

In Search of Quantum Reality

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Chapter 1

Beginning Ideas and Thoughts

I wish to guide you on an excursion which is long and rather difficult but worth the trouble, so I am going to climb ahead of you, slowly.

Golem's Inaugural Lecture
in **Imaginary Magnitude**
by Stanislaw Lem

1.1 How does the universe work?

What are the principles that underlie natural phenomena?

Philosophers and physicists have pondered such questions for millennia. Their answers generally reflect the *world view* of modern civilization, i.e., how we perceive ourselves in relation to the universe.

Prior to the 20th century, the dominant world view was *determinism*, a tenet that had its origins in the philosophical thinking of Descartes. Descartes metaphor for the universe was a gigantic clockwork machine, a Rube Goldberg device that grinds relentlessly onward, towards eternity. According to its interpretation, the future is preordained and fully predictable. All of existence is described precisely by physical laws, and, *in principle*, can be known by us.

Nature, however, had a surprise in store for philosophers and physicists. In the first decades of the 20th century, they were to see this world view subverted, uprooted, and toppled by a physical theory called *quantum mechanics*. Theoretical physics has come a long way since those amazing days in the 1920's and 1930's when physicists were taking the first tentative steps towards a radical new definition of reality.

Now, the foundation of all advanced physical theory is quantum mechanics,

which is the subject matter of this book.

1.2 What is quantum mechanics?

It turns out that if you want to understand how a transistor works or the principles behind the laser in your compact disc player you cannot use classical physics. Newton's mechanics and Maxwell's electromagnetic theory can explain a wide range of *macroscopic* phenomena, such as the motion of billiard balls and rockets or the operation of an electric circuit, but they fail spectacularly when applied to *microscopic* phenomena, such as proton-atom scattering or the flow of electrons in a semiconductor.

The world is not what it seems. Behind the apparent solidity of everyday objects lies an exotic shadow world of *potentiality* and *uncertainty*. This world, as we will see, defies simple description since its foundations are so different from our everyday experience. Yet our world of solid tables, bowling balls, stars, and galaxies somehow arises from whatever is going on at some micro-level underneath. Even today, we do not know, as we will see, how the transition between the microworld and the macroworld occurs, i.e., how the macro world emerges from the microcworld.

There exists a theory that explains how the microworld works: it is called quantum mechanics. It is the most successful scientific theory that has ever been created and it has completely changed our view of the world. Yet, for all of its success, there are aspects of quantum theory that remain utterly baffling, even to physicists.

We think that we can understand the macroworld and we think it seems to make sense. The ideas used to understand the macroworld, do not work in the microworld. Thus, an understanding of such micro-processes requires, as we will see, a completely new way of thinking, namely, quantum mechanics.

As we will see, quantum mechanics is a collection of postulates based on a huge number of experimental observations and the set of tools and ideas derived from those postulates.

We will use these tools to analyze, predict, and understand microscopic phenomena. Quantum theory forms the bedrock of the modern physics of matter - atoms, molecule and solids - and is at the core of such diverse sciences as astrophysics and biochemistry. In its more pragmatic guises, quantum mechanics plays a vital role in a vast array of technological applications, some of which we use everyday - e.g., the microchips in the computer that I used to write this book.

Thus, in one form or another, quantum physics pervades the life of everyone

in our high-tech world. Discussing the importance of quantum mechanics to non-physicists, Heinz R. Pagels has written in the **Cosmic Code**

When the history of this century is written, we see that political events - in spite of their immense cost in human lives and money - will not be the most influential events. Instead, the main event will be the first human contact with the invisible quantum world and the subsequent biological and computer revolutions.

In this book you will learn how this quantum world works, why it must work in this particular way, and how we might understand it.

In this introductory chapter we will ease into this bizarre world. We will begin with a short discussion of classical mechanics. We will see the way in which this classical structure supported the deterministic ideas of philosophers of the early 1900's and we will learn about the classical systems that gave early indications of the impending troubles. Then we will take a whirlwind tour of the world according to quantum physics, focussing on some of the new ideas that so devastated the Newtonian view.

This introductory chapter and the next chapter of this book will provide a bird's eye view of quantum theory. In them, we will examine qualitatively the central ideas of the theory. Then, in the following chapters of this book, we will set off on a voyage of discovery, formulating these quantum mechanical ideas mathematically (I will teach you the necessary mathematics) and applying them to the microscopic universe of photons, electrons, atoms, K-mesons, neutrinos and so on.

In the 90 years since quantum theory was first proposed, many physicists have attempted to explain quantum physics to non-physicists. This is an important undertaking. The microworld, which exists at a length scale smaller than that of the world we experience with our senses (i.e., the macroworld), is profoundly mysterious, and there are some very important philosophical messages about the nature of reality and the limits of science that everyone needs to understand. I hope that this book can contribute to that effort.

Quantum theory has implications about the nature of reality; this has led to so-called quantum hype - the use of quantum theory to justify ideas about extrasensory perception (ESP), consciousness, the nature of God and the creation of the universe. As we will see, quantum theory cannot (and should not) be used to support any of these ideas.

The goal of this book is to give you sufficient understanding of what quantum theory is about and where the philosophical lines are drawn so you can judge for yourself on the various issues that arise.

We will assume that everyone has taken standard high school mathematics

courses and can remember at least some of it. Any more mathematics than this, I will introduce and explain (based on high school mathematics only) as we go along.

I need to say something about philosophy. If we are going to have a sensible discussion about the philosophy of quantum physics we need to agree on some ideas from the beginning.

This is mainly a matter of terminology, i.e., a few technical terms that act as reasonable shorthand for complicated ideas. For example, philosophers have many theories concerning the nature of knowledge: how we know something, how reliable our knowledge is, whether all our knowledge comes from the world via our senses, or are there some things that we just *know*. Discussions such as this are covered by a branch of philosophy called **epistemology**. A closely connected, but distinct, area is **ontology**. This is the inquiry into what is *actually out there* for us to know. For example, the existence of electrons is dealt with by ontology; how we know about them and their properties is dealt with by epistemology.

Epistemologists have come up with two ideas about how science works, or what science actually attempts to do.

If you are a **realist**, then you believe that science is a true representation of what is *really* out there. The concepts and pictures that we develop (such as electrons, black holes, the big bang, and DNA) are elements of reality and we are discovering true facts about the world. In this point of view, the purpose of science is clear: to determine as much as possible about what is going on in the world. To a realist, a good theory shows us that the objects it discusses are not just figments of our scientific imaginations.

However, you could be an **instrumentalist**, i.e., you do not worry too much about the accuracy or reality of your ideas as long as they fit the data and allow accurate predictions to be made about what will happen next. An instrumentalist may not believe that electrons are real, existing objects. They will agree, however, that experiments generate *clumps* of data that can be gathered together under the heading *that's an electron* and use this data to predict another set of experimental readings under slightly different circumstances. To an instrumentalist, a good theory allows us to play the *game* well.

Various scientists belong to one these two groups. A few quotations make the differences clear.

REALISTS

Physicists believe that there exist real material things independent of our minds and our theories. We construct theories and invent words (such

as electron and positron, etc) in an attempt to explain to ourselves what we know about our external world ... we expect a satisfactory theory, as a good image of objective reality, to contain a counterpoint for every element of the physical world. — B. Podolsky

A complete, consistent, unified theory is only the first step: our goal is a complete understanding of the events around us, and of our own existence. — S. Hawking

The great wonder in the progress of science is that it has revealed to us a certain agreement between our thoughts and things. — L. deBroglie

INSTRUMENTALISTS

I take the positivist viewpoint that a physical theory is just a mathematical model and that it is meaningless to ask whether it corresponds to reality. All that one can ask is that its predictions should be in agreement with observations. — S. Hawking

In science we study the linkage of pointer readings with pointer readings. — A. Eddington

There are good arguments on both sides. A realist says that the only reasonable way of explaining whether science succeeds is that the objects we are discussing in the theory are really there. An instrumentalist would point out that when Newton was alive we believed that time was absolute, i.e., the same for everyone no matter what; Einstein later proved that time is different for different observers depending on their relative state of motion or if they happen to be at different places in a gravity field. So maybe “being really there” is not so important! What next?

Often our ideas of what is *out there* change radically over time, so why believe any of it? As long as the ideas allow us to develop new technologies, who cares?

I think that the most satisfactory viewpoint at the moment might correspond to **critical realism**. Critical realists acknowledge that it is difficult to be sure which parts of the theories actually correspond to the world. They think that the theory must have some elements of *objective reality* if it explains things well, explains seemingly unconnected things and correctly predicts new science.

The important thing is not whether we can make a *picture* about what the theory is telling us. Instead, the most important aspect is the *range* of data(experimental) that it links together and correctly explains.

Critical realists believe, first, it is difficult to do science and maintain motivation while attempting very difficult work, unless you(deep down) think that we are actually finding out about the world, not playing an interpretive game and second, experiments must be the sources that give us the needed clues. Quantum

physics has very weird ideas that come out of experimental data and, as we will see, we could not have proposed any other theory to explain the data as well as quantum mechanics.

In general, scientists work without being worrying about the philosophical niceties

”Shut up and calculate”

is their motto (actually said by Feynman, who had little tolerance for philosophy).

The problem is that it is very difficult to adhere to Feynman’s motto and that quantum physics forces us to think about some very weird ideas, if we look into it too deeply.

As we will find out in this book, much of our discussion will center around a concept called the *state of the quantum system*.

A realist will have trouble believing that a quantum state is an ontologically real thing, since it will seem to depend on *what we know* about the system.

An instrumentalist will have no problem believing that the state is just information that we are linking together and thus the objects under study behave in radically different ways if their state(or information) changes, which suggests that some aspects are ontologically true about the state.

Throughout this book I am going to try and remain as neutral as possible and point out where realism and instrumentalism have their strengths when applied to quantum theory. Hopefully, you will be able to come to your own conclusions.

1.3 The Classical Point of View

Consider Newtonian classical mechanics. In their simplest form, the laws of classical mechanics are written in terms of particle trajectories(paths of motion). So the concept of a *trajectory* underlies the structure of classical physics and the concept of a *particle* underlies its associated model of physical reality.

1.3.1 Some Opening Thoughts

Macroworld objects such as trees, bushes, and bowling balls are made up of small-scale (microscopic) things such as protons, neutrons and electrons. The laws of physics that describe the large-scale macroworld have been known and understood since the 1700’s and the physics of the small-scale microworld has been known since the 1900’s. The problem we face is that the small-scale microworld laws describe a behavior that, judged by the standards of everyday experience(the macroworld and its classical laws), is very strange. It will be

very difficult to see how all the strange behavior going on at the atomic scale can lead to the regular, reliable world we spend our lives in.

The contrast between the microworld(*seen* via experiment) and the macroworld(*experienced* via our senses) is a theme we will return to often throughout the book.

1.3.1.1 Particles and their Trajectories

Physicists, classical or otherwise, study the universe by investigating isolated fragments, which are called *systems*. Classical physics applies to macroscopic systems, quantum physics to microscopic systems. A *system* is just a collection of particles that interact among themselves via internal forces and that may interact with the world outside the system.

To a classical physicist, a *particle* is an indivisible point mass(occupies zero volume) possessing a variety of physical properties that can be measured. In a physical theory, measurable quantities are called *observables*. By listing the values of all of the observables of a particle at any time we can specify its *state*. The *trajectory* is an equivalent and more convenient way to specify a particle's state. The *state of the system* is just the collection of all of the individual particle states making up the system.

1.3.1.2 Extrinsic versus Intrinsic Properties

Classical physicists often characterize properties of a particle as **intrinsic** or **extrinsic**. *Intrinsic* properties do not depend on the particle's location, do not evolve with time, and are not influenced by its physical environment - rest mass and charge are intrinsic properties. *Extrinsic* properties, on the other hand, evolve with time in response to the forces acting on the particle - position and momentum are extrinsic properties.

According to classical physics, all properties, intrinsic and extrinsic, of a particle *could be known* with *infinite* precision. For example, in classical physics, we could certainly(we believe) measure precise values of the position and the momentum of a particle at the same time.

Of course, precise knowledge of everything is an illusion in the real world where neither the measuring apparatus nor the experimental technique is perfect and experimental errors trouble physicists as they do all scientists. But, *in principle*, both can be made perfect, that is, classical physicists think that our knowledge of the physical universe is limited only by ourselves and our instrumental limitations, not by nature.

Let us be more explicit about these ideas via some detailed **definitions**:

1. A **system** is that part of the universe under investigation. Systems can be

very large (stars and galaxies) or very small (electrons and photons). They can have lots of pieces(parts) within them (a living body) or only a few (a hydrogen atom). We try to isolate any system that we are investigating from the rest of the universe, so we can study and interpret its behavior more easily. This is not always completely possible. Attempting to isolate systems is what makes experimental physics so expensive.

2. **Physical properties** are the aspects of a system that we can measure or detect. Examples include mass, color, density, speed, and position. Using measurement we assign to these properties quantitative values (a number and a unit). A system might, for example, have a speed of 20 m/s .
3. **Physical variables** are the symbols that stand for physical properties in a mathematical theory. Speed (velocity), for example, is generally given by the symbol v when we want to refer to it without assigning a particular quantitative value. If a theory is *complete*, then all the important physical properties of a system are represented by variables in the theory.
4. **System properties** are the physical properties that describe a system and help us distinguish one system from another. An electron has system properties such as electric charge ($-1.6 \times 10^{-19}\text{ C}$) and mass ($9.1 \times 10^{-31}\text{ kg}$).
5. **State properties** are the physical properties of a system that can change without changing the intrinsic nature of the system. An electron can have a whole variety of different speeds and still be an electron. Thus, speed is part of the electron's state.
6. A **classical state** specifies the quantitative values of all the state properties relevant to a given system. In some situations we can know the state of the system without being sure about the states of all the parts in the system. A gas, for example, is a collection of molecules. The state of the gas, in terms of its pressure, volume, and temperature, can be specified perfectly without knowing the exact state - in terms of velocity and position, of each molecule, because the state properties are averages in this case, i.e., temperature is proportional to the average value of the speed squared.

We now need start the process of learning needed mathematics. As we will see, mathematics is the language of quantum mechanics. We start with some mathematics you learned in high school.

1.3.1.3 Mathematical Interlude #1: Vectors

A **vector** has many levels of complexity and is a very abstract mathematical (geometrical) object. A vector is representable by two numbers in two dimensions, three numbers in three dimensions, and so on. One characterization is to specify its magnitude or length and its orientation or direction - think of a directed line segment. As we shall see, quantum mechanics will be formulated

in terms of vectors, but they will *not* be related to these simple directed line segments. We will present a better definition later.

1.3.1.4 The Standard Language of Vectors

As we said, in ordinary space, i.e., on a piece of paper, we can represent a vector by a directed line segment(an arrow). The standard(old) symbol for a vector is \vec{A} .

A straightforward property of a vector is multiplication of the vector by a scalar (a real number) α . A scalar is just a number (like 7, 35, temperature, minutes after noon,). In this case the magnitude(length) of the vector changes and the direction stays the same (it might reverse if $\alpha < 0$). This is illustrated in Figure 1.1 below:

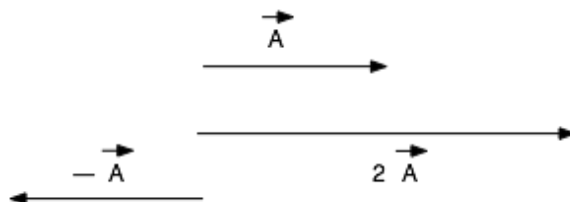


Figure 1.1: Multiplication by a scalar.

Now given two vectors as shown in Figure 1.2 below

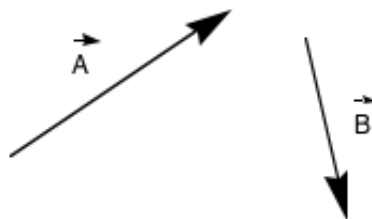


Figure 1.2: Two distinct vectors.

we *define* the sum and difference of the two vectors or the general property of *vector addition* by the *tip-to-tail* diagrams shown in Figure 1.3 below. Clearly, for vector addition as defined below in the two diagrams, we have

$$\vec{C} = \vec{A} + \vec{B} \quad \text{or} \quad \vec{C} = \vec{A} - \vec{B} = \vec{A} + (-\vec{B}) \quad (1.1)$$

which yields a new vector in each case. This new vector can have both a different direction and a different magnitude than either of the two vectors that are used to create it.

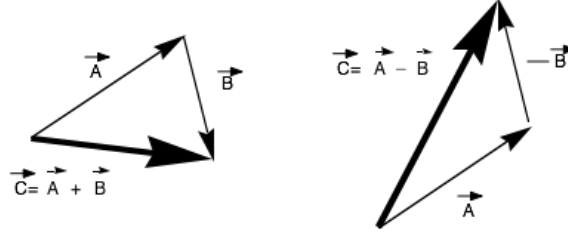


Figure 1.3: Definition of sum and difference of two vectors.

These properties allow us to define a general **linear combination(sum)** of vectors as

$$\vec{C} = \alpha \vec{A} + \beta \vec{B} \quad (1.2)$$

which is also a well-defined vector. An example ($\alpha = 2$ and $\beta = 5$) is shown Figure 1.4 below:

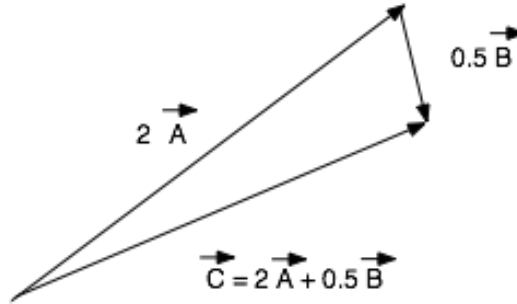


Figure 1.4: Linear combination of two vectors.

We note that the coefficients α, β must be real numbers in this definition. This will not be true in later discussions about quantum theory when we generalize the idea of a vector.

With these new ideas now available to us (this is how we will proceed with learning mathematics, i.e., we will introduce new ideas as we need them), we now return to our earlier discussion:

How does a classical physicist predict the outcome of a measurement? She uses *trajectories*. The trajectory of a single particle consists of the values of a pair of vectors, namely, its *position* vector, $\vec{r}(t)$, which is the vector from some reference point (the origin) to the location of the particle as it moves and its *momentum* vector (defined as its mass times its velocity vector) $\vec{p}(t)$. Formally, we write

$$\{\vec{r}(t), \vec{p}(t); t \geq t_0\} = \text{trajectory} \quad (1.3)$$

where the (linear) momentum is, by definition (as mentioned above),

$$\vec{p}(t) = m\vec{v}(t) = m \frac{d\vec{r}(t)}{dt} \quad (1.4)$$

with

$$\begin{aligned} \vec{r}(t) &= \text{position vector} \\ \vec{v}(t) &= \text{velocity vector} \\ m &= \text{mass of the particle} \end{aligned} \quad (1.5)$$

Formally, the quantity

$$\frac{d\vec{r}(t)}{dt} \quad (1.6)$$

is the first derivative (or rate of change) of the position vector with respect to time. We will discuss simple ideas of calculus later in Chapter 6. For now we only need to know that these quantities exist and can be calculated.

Although this is a perfectly good way to proceed for ordinary vectors in the macroworld, it will not allow us to generalize the notion of vectors beyond ordinary physical space, which is an arena (adequate for classical mechanics) that will turn out to be *much too confining* in our effort to understand quantum mechanics.

We need to formulate these same concepts in another way. But, first let us learn some new mathematical language that will help us understand some of the quantities we have been using up to now without any detailed explanations.

1.3.1.5 Mathematical Interlude #2: The Space of Physics and Simple Calculus

As we said: a vector = a set of 3 numbers (in 3-dimensional space). This implies that a vector can be used to characterize a point in the 3-dimensional world we live in since each point in that world is also characterized by three numbers.

As we stated above, the vector representing the location of a point in 3-dimensional space relative to a given *origin* (a reference point) is called the *position* vector.

To proceed further in a way that will allow generalization, we must define three (for 3 dimensions) special vectors. We use the symbols

$$\hat{e}_1, \hat{e}_2, \hat{e}_3 \quad \text{or} \quad \hat{i}, \hat{j}, \hat{k} \quad \text{or} \quad \hat{x}, \hat{y}, \hat{z} \quad (1.7)$$

to represent these special vectors.

These are unit vectors (length = 1) that *define a right-handed coordinate system*

as shown in Figure 1.5 below. Then the position vector, also shown in Figure 1.5 below, is represented by the 3-tuple (3 numbers)

$$\vec{r} = (x, y, z) = (x_1, x_2, x_3) \quad (1.8)$$

which is a shorthand notation for the linear combination of the unit vectors given by

$$\vec{r} = x\hat{i} + y\hat{j} + z\hat{k} = x_1\hat{e}_1 + x_2\hat{e}_2 + x_3\hat{e}_3 = x\hat{x} + y\hat{y} + z\hat{z} \quad (1.9)$$

These are all equivalent representations of the position vector. We have written the position vector as the sum (linear combination or superposition) of three distinct vectors. The numbers (x, y, z) or (x_1, x_2, x_3) are called the *components* of the vectors with respect to the chosen set of unit vectors. The unit vectors are chosen to be orthogonal (perpendicular) for convenience as we shall see.

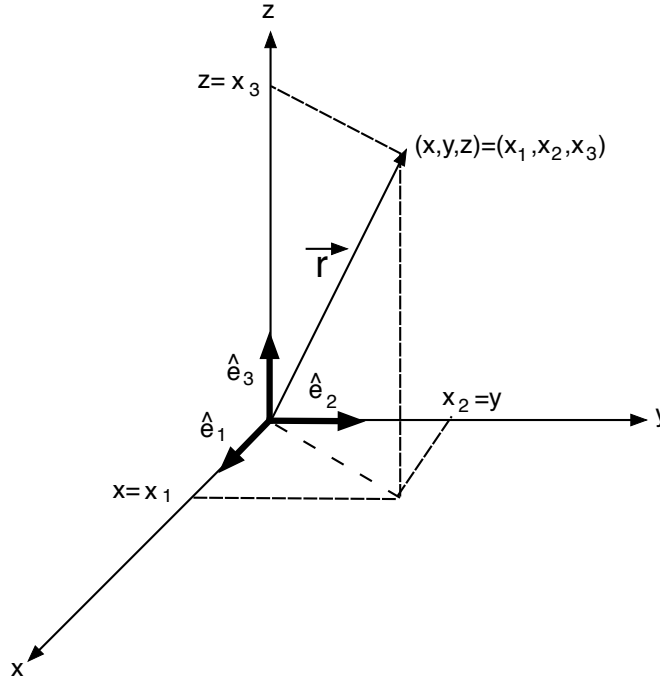


Figure 1.5: Standard right-handed coordinate system.

The length of the position vector is defined (using the Pythagorean theorem) by

$$r = |\vec{r}| = \sqrt{x^2 + y^2 + z^2} \quad (1.10)$$

i.e., the square-root of the sum of the squares of the components.

Let us elaborate on these important ideas. Consider the vectors (in 2 dimensions) shown in Figure 1.6 below:

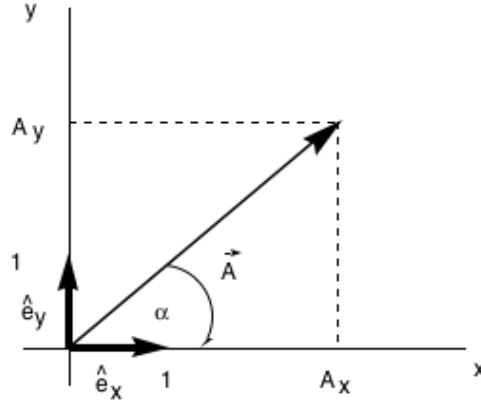


Figure 1.6: A typical 2-dimensional vector.

In this figure, we have specified two unit vectors, namely,

$$\begin{aligned}\hat{e}_x &= \text{unit(length} = 1) \text{ vector in } x - \text{direction} \\ \hat{e}_y &= \text{unit(length} = 1) \text{ vector in } y - \text{direction}\end{aligned}\quad (1.11)$$

In terms of these unit vectors we can write(as we did for the position vector in Figure 1.5) the vector \vec{A} as

$$\vec{A} = A_x \hat{e}_x + A_y \hat{e}_y \quad (1.12)$$

where

$$\begin{aligned}A_x \hat{e}_x &= \text{vector of length } A_x \text{ in the } x - \text{direction} \\ A_y \hat{e}_y &= \text{vector of length } A_y \text{ in the } y - \text{direction}\end{aligned}\quad (1.13)$$

and the sum of these two vectors equals \vec{A} because of the tip-to-tail rule for adding vectors that we defined earlier.

We then have, from an earlier definition, that

$$\begin{aligned}A_x &= \text{component of vector } \vec{A} \text{ in the } x - \text{direction} \\ A_y &= \text{component of vector } \vec{A} \text{ in the } y - \text{direction}\end{aligned}\quad (1.14)$$

From the diagram and trigonometric definitions of the sine and cosine functions we then have

$$A_x = A \cos \alpha \quad , \quad A_y = A \sin \alpha \quad (1.15)$$

where A = length of the vector \vec{A} (by Pythagorean theorem) and α is the angle between the vector \vec{A} and the x -axis (\hat{e}_x) as shown.

The purpose of introducing these new ideas is that we can then redefine(develop

a better method) vector addition in terms of components and unit vectors as follows:

$$\begin{aligned}\vec{A} &= A_x \hat{e}_x + A_y \hat{e}_y \quad , \quad \vec{B} = B_x \hat{e}_x + B_y \hat{e}_y \\ \vec{A} + \vec{B} &= (A_x + B_x) \hat{e}_x + (A_y + B_y) \hat{e}_y \\ \vec{A} - \vec{B} &= (A_x - B_x) \hat{e}_x + (A_y - B_y) \hat{e}_y\end{aligned}\tag{1.16}$$

i.e., we can just add and subtract components. This way of thinking about vector addition will generalize for the strange representation of vectors we will develop in quantum theory later.

Back to our discussion:

Trajectories are the *state descriptors* of Newtonian physics. Conventionally, we think of a trajectory as a path in geometrical space. In classical physics, however, a trajectory, as we said earlier, means a path in a space defined as *momentum versus position* (called **phase space**) for all times $t \geq t_0$.

To study the evolution of the state represented by the trajectory one uses Newton's Second Law of motion

$$m \frac{d\vec{v}(t)}{dt} = \vec{F} = \text{external force} = m\vec{a}(t)\tag{1.17}$$

where $\vec{a}(t)$ is the acceleration vector. The process works like this: the acceleration vector $\vec{a}(t)$ tells us how the velocity vector changes with time, which allows us to determine $\vec{v}(t)$. The velocity vector tells us how the position vector changes with time, which allows us to determine $\vec{r}(t)$. These two calculations then give the trajectory.

In addition, in classical physics the energy of a particle is given by

$$E = \frac{1}{2}mv^2 + V(\vec{r})\tag{1.18}$$

where

$$\begin{aligned}\frac{1}{2}mv^2 &= \frac{\vec{p}^2}{2m} = \text{kinetic energy} \\ V(\vec{r}) &= \text{potential energy function}\end{aligned}\tag{1.19}$$

The force function and hence the acceleration vector and hence the trajectory are all determined by the potential energy function.

Thus, to obtain the trajectory for $t \geq t_0$, we need only know the potential energy function and the initial conditions (the values of the position and momentum at the initial time t_0). With the trajectory in hand, we can study the various properties of the particle in the state that is described by the trajectory, for

example, its energy.

Notice that classical physics implicitly assumes that we can measure the initial conditions without disturbing the motion of the particle, that is, that in measuring the momentum of the particle, we transfer to it only a negligible amount of momentum. To determine the initial momentum we must measure the initial velocity. The velocity is the rate of change of position, so to measure the velocity we must observe the position at two nearby times making the time interval between them as small as our instrument will allow. Such position measurements necessarily involve a change in the particle's momentum, but, as we will see, this effect is negligible for the macroscopic particles considered in classical physics.

Thus, the job of classical (or Newtonian) physics is to enable us to calculate a projected final state at some future time, given an initial state and a complete specification of all forces acting (to calculate the trajectory). In practice, however, there are several potential problems with this process.

1. In principle the collection of properties associated with any interesting physical system is very large. Something as mundane as a rock has mass, velocity (in three different directions), position (with three different coordinates), volume, size (very hard to be very precise about, given that a rock is usually not a simple shape), temperature, surface reflectivity, surface smoothness, and other properties. However, we don't always have to worry about most of these properties. It depends on what we are trying to achieve. Some properties don't affect the motion of the rock; they can be left out of the calculation (e.g., its temperature). The quantitative values of others can be approximated; although the exact shape of the rock will modify the details of its path, we can usually be sufficiently accurate by treating it as a sphere or even a point.
2. The full details of all the forces acting can be rather complicated. In the case of a rock, gravity and air resistance are the most important forces once it is in flight. Fortunately, the gravitational force will be much larger than the air resistance at typical rock speeds, so we can approximate the situation by ignoring air resistance. This process of simplifying things by ignoring the details of physical properties and forces is called *making a model* of the situation, and it is one of the most important techniques in macroworld science.
3. We might not be able to specify the initial state precisely. There is always some uncertainty connected with measurement. No matter how accurate, complicated, or expensive our apparatus may be, there will always be some amount of error. This in turn will affect any calculations that are made using the measurements as part of the system's initial state. In detailed work, this error is taken into account. For example, when one throws a rock we may not know precisely the value of velocity at which it left our

hand. This means that the best we can do is to produce a range of possible landing points, together with some estimation of how likely each one is. We accept this limitation on our predictive power as being the price we pay for the ability to do a sensible calculation. Our knowledge is uncertain and we have to rely on predicting probabilities of the range of outcomes because we cannot include all the details with perfect accuracy. This does not represent any fundamental problem.

Although we can't always know the exact values of all the physical quantities in a classical state, or the fine details of all the forces acting, the process of model making and approximating has generally proven to be a highly successful strategy for dealing with the large-scale world. For example, it enabled us to put astronauts on the moon. However, the predictability of Newtonian physics has been challenged not only by quantum physics. In recent decades, we have become aware of *delicately balanced systems* that are more intimately linked with the surrounding universe than most.

1.3.1.6 Chaos

These *finely tuned systems* are exquisitely sensitive to their precise initial state; so in practice it is impossible to make any sensible predictions about them at all. The rings surrounding the planet Saturn are an excellent example of such a system.

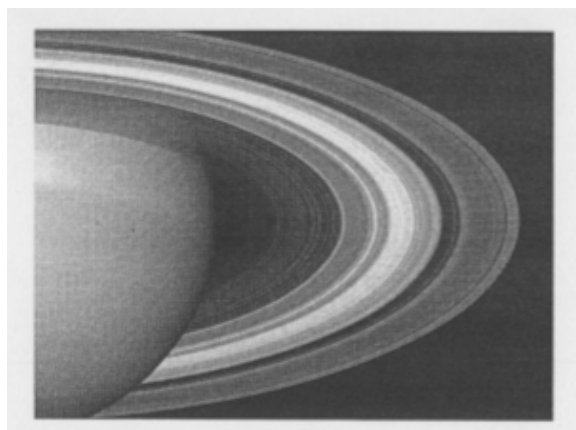


Figure 1.7: The rings of Saturn.

Saturn's rings(as photographed by the Cassini probe above) are composed of different sized chunks of rock and ice. At first glance you would think that calculating the orbit of any rock in a ring would be nearly as straightforward as calculating the parabolic path of a rock(projectile) thrown on the earth. However, this is not the case. Although Saturn's gravity accounts for the dominant force acting on such a rock, there are also other significant forces. The rocks

will exert tiny gravitational forces on one another, and the orbiting moons of Saturn will also pull them in different directions. Unlike the rock on the earth situation where we could ignore many of the smaller forces, the motion here is very *critically balanced*. It turns out that there are certain regions in the rings where the precise orbit followed by a chunk of rock depends very sensitively on its *exact* velocity. Two rocks placed in the same place would soon end up moving in a totally different manner if they had slightly different velocities - in fact, there would be *no correlation* between the two motions eventually). One might fall toward the planet and the other fly off into space. This is why there are empty regions in the rings. Finely balanced systems, such as this one, are called **chaotic systems**.

Actually, the name gives the wrong impression of what is going on. Chaotic systems are unpredictable, as we can never specify the initial state precisely enough to single out one final state, but they are not lawless. In principle, everything about a chaotic system is exactly determined, but in practice all we can do is estimate the probability of various outcomes. The same was true when we threw a rock, but in that case the uncertainty was quite small. If it was a chaotic system, it might be the case that we could not be sure of the field the rock would land in! It would be as if infinitesimal changes in the way in which the rock was thrown could change the landing point by several kilometers instead of a few centimeters!

Another commonly quoted example of a chaotic system is the weather. The global atmospheric system is finely balanced and small disturbances can produce vast changes in the outcome. We can never measure what is going on in the atmosphere to the level of precision that would be needed for a reliable weather prediction extending more than a few days into the future.

Chaotic systems derive their unpredictability from the practical limitations on how well we can pick out the initial state. There is no genuine randomness at the heart of chaotic systems. This is in contrast with quantum physics where, at least in some interpretations, the unpredictability is thought to come from genuine randomness at the heart of nature as it exists in the microworld, as we will see later.

Thus, the *scheme of classical physics*, which we may describe as **The Newtonian Universe Clock**, which when fed the proper information (particle masses, forces on and between the particles, initial conditions), predicts the future of the universe, is based on precise specification of the position and momentum of a particle. This machine is now known to be incorrect and obsolete as we will see!

I do not mean to imply by this short description that classical physics is easy. Solving the equations of motion for a system with lots of particles interacting among themselves or exposed to complicated external fields is a formidable task.

Contemporary applications of Newtonian mechanics to problems like the motion of planets in the solar system or galaxy-galaxy collisions, require massive parallel computing systems. In many cases, one may be unable, using present technology, to solve these equations.

The important point, however, is that, *in principle*, given sufficient time and computing resources, we could predict from the initial conditions of all the particles the precise future behavior of any system or even the entire universe. *That is the classical view.*

1.3.1.7 The Determinate Universe

The underlying assumptions and philosophical implications of classical physics are so familiar that you may have never given them a second thought. For example, classical physics ascribes to the universe an *objective reality*, an existence of properties external to and independent of any measurements that might be made. This assumption reassures us that when we do research in physics we are studying what is actually *out there* and that we can design experiments that do not affect in any significant way the systems they measure. That is, in an objective universe we can control the interaction between the *measuring apparatus* and the *system being measured* and, if clever enough, can make this interaction negligibly weak.

Our central assumption about the nature of the classical universe is that it is predictable. Knowing the initial conditions of the constituents of any system, however complicated, we can use Newton's Laws to predict the future precisely, without ambiguity or uncertainty. This notion is the essence of *determinism*, which supported by Newtonian mechanics, dominated western philosophical thinking until the advent of quantum theory.

If the universe is determinate, then for every effect there must be a cause. After all, if *all* events, *all* phenomena can be predicted and explained precisely by physics, then it must be possible to backtrack from any event to find, somewhere in the dim recesses of history, its cause. We may have to look long and hard - the bird that just fell off the tree limb outside my window may have been influenced by an event during the Peloponnesian wars - but somewhere there *is* a cause.

That is what the principle of **causality** says.

Causality was an important element of 19th century western philosophy. It had important implications for physicists of that era for it guaranteed the reproducibility of experiments, that is, that two *identical* systems with the *same* initial conditions (*same* state) subject to the *same* measurement will yield identical results. *Same* causes - *same* effects. Very neat and tidy!

I suppose the deterministic world view implied by Newtonian mechanics could, even today, seem comforting, for it implies that the universe can be fully understood and dealt with rationally. But it has a dark side. For example, if the universe is ruled by causality, then free will is a meaningless concept, for the universe is a vast, mindless machine that controls our every action, our every decision. Everything that happens, happens because of something that happened in the past, not because we chose to make it happen. According to this view, if you *decide* to get married or to take a job or collect water buffalo, you do so not by choice but because of past events. In such a universe, our loves, hopes, and dreams are but delusions, hiding the grim reality that we are but cogs in Descartes' clockwork machine. Goals are irrelevant. Human aspirations are pointless.

Thus, determinism is a dehumanizing philosophy. It describes a universe that is infinitely predictable, holding few surprises. All can be known. Nothing is unexpected. Determinism is boring.

It is also wrong!

1.4 Through the Looking Glass: The Quantum Point of View

We have seen that Newtonian mechanics is constructed from particle trajectories. One reason classical physics fails when applied to microscopic systems is that the constituents of such systems are not particles in the classical sense of the word. Moreover, they do not have trajectories. Thus, to understand the physics of the microworld, that is, to understand the results of experiments on microscopic *particles*, we must radically revise our conceptual description of a *particle*.

1.4.1 When is a Particle Not a Particle?

In describing the quantum world, we must abandon the classical notion of a *particle* as an indivisible mass point with an independent existence and well-defined measurable extrinsic properties. Whatever microscopic entities are, they are certainly not indivisible mass points.

We can verify this statement in the laboratory. In suitably designed experiments quantum *particles* seem to act like classical particles - appearing, for example, as *spots* on a screen or *clicks* in a detector. But in other experiments, their transit through space is such that they seem to act like a *wave*, manifesting behavior such as diffraction and interference, as though they were diffuse wave fronts, as we will show later.

This apparently contradictory behavior is a manifestation of the so-called **wave-**

particle duality that many physicists think characterizes the domain where quanta dwell.

In our study of this duality later, we will see why it poses such a challenge to the student of quantum physics. It renders useless the conventional mental images with which we visualize physical phenomena. Thus, an electron is not a tiny planet orbiting a nuclear sun, as in the Rutherford and Bohr models of the atom from the early 20th century. But neither is it a fuzzy thing smeared out over a region of space as it is portrayed in many introductory physics or chemistry books.

The electron is *something else*, neither particle nor wave, but eerily reminiscent of both. However, we must also keep a completely open mind - it is possible that an electron has nothing to do with particles or waves at all! In any case, the seemingly dual nature of subatomic particles subverts the classical concept of a particle.

The true nature of microscopic entities, however, is even more nebulous than is implied by a wave-particle duality, for *the properties of quantum particles are not, in general, well-defined until they are measured*. In a sense, as we shall see later, the physical properties of electrons, protons, etc., seem to be *potential* or *latent properties (propensities)* until a macroscopic experiment does a measurement.

In this chapter, we will be noting many new ideas like those mentioned above, but we will not fully discuss them until later in the book. This first pass is simply to try to get an initial grasp on the problem.

You will encounter the following disquieting aspect of quantum mechanics if you ask a quantum physicist to predict the value you would obtain were you to measure, say, the position of an electron in a metal. She cannot give you a definite answer, even if she *completely* knows the state of the electron just prior to the proposed measurement. The inability of quantum theory to provide precise answers to such simple questions will not turn out to be a deficiency of the theory. *Rather, as we will see, it is a reflection of its essential nature!*

We can see this if we look at how quantum mechanics specifies the state of a particle.

Unlike a classical state, a quantum state will turn out to be a *mixture* of all of the *possible* outcomes of measurement of physical properties.

At most, quantum physicists will be able to tell you only the *possible* outcomes and the *probability* that you will obtain one or another of them. Quantum mechanics is expressed in the language of *probabilities*, not certainties. A grammar for this new language will be formulated later. It seems, according to many

physicists, to be inherently *statistical* in nature, describing not definite results of a measurement on an individual system, but instead possible results of measurements on a large number (an ensemble) of identical systems, but, as we will see later, maybe this idea is not correct either.

What then will control what actually happens in a particular measurement, that is, which of the possible values of position a particle possesses will actually appear when we measure this quantity?

Random chance will seem to be the correct answer.

Of course, were we to carry out a position measurement on a single particle, we would get a single value. So immediately after the measurement, if we can repeat the measurement on the same system (if the measurement has not destroyed the system), we can meaningfully talk about the position of the particle - its position is the number we got in the measurement. But what about immediately before the measurement? According to quantum mechanics, as we shall see later, *the particle does not have a position*. Rather, its position prior to measurement is *latent* - a mere possibility, waiting to be made actual! In this standard way of thinking, by the act of measurement, we *change* the state of the particle from one which is characterized by a range of possible positions to one in which it has a single, well-defined position.

Clearly, measurement will play a more important role in quantum physics than in classical physics. When we study the microworld, experimentation will not be just a way of discovering the nature of external reality, but rather it will seem to be a way of *creating* certain aspects of reality or maybe we do not understand what *reality* is and that last statement will be seen to make no sense!

In contrast to the assumptions of classical physics, *it will seem that an experiment cannot observe a microscopic system without altering some of its properties*.

Intrinsically, indeterminate interactions between the measurement system and the physical system under observation are an inevitable feature of the quantum universe; a feature that applies not just to position, but to all properties of microscopic particles.

Some physicists even believe that we macroscopic observers *create* the microscopic building blocks of the universe by actualizing them via measurement of their various physical properties. What you will end up believing after reading this book remains to be seen!

The interaction is *unavoidable* - the effect of the measurement on the observed system *cannot be reduced to zero*, in principle or in practice. This fact, which is reflected in the mathematical structure of quantum theory and has been veri-

fied by countless experiments, seems to demolish the philosophical notion of an objective universe or the idea that what we study in physics is necessarily a *real world* external to and independent of our perceptions, but maybe not - we shall see in our studies.

These ideas also give rise to a host of fascinating metaphysical questions:

1. Do particles exist if their properties are not being measured?
2. Is what we study in physics, reality or merely our perceptions of reality?

The measurement/observed-system or observer/observed interaction is also *uncontrollable*. Although we can be sure that when we measure the properties of a microscopic particle we will change its state, we can neither predict nor influence precisely how the state will be changed.

Once again, it is determined by **random chance**.

In fact, randomness governs microscopic phenomena even if the system is not being studied. A famous example of this seeming perversity of nature is radioactive decay of an atom. Quantum mechanics prohibits us from predicting precisely when a particular atom will decay, emitting radiation. At most, we can determine the probability that it will decay in a given time interval. The role of randomness in microscopic physical processes shatters the illusion that the universe is deterministic!

1.4.1.1 The Decline and Fall of the Trajectory

Thus, the idea of using the classical model of a particle to describe a microscopic entity seems not to be possible. But can we salvage the basic state descriptor of classical physics, the trajectory?

The first step in determining the trajectory of a particle is measuring its initial conditions $x(t_0)$ and $p_x(t_0)$ (actually we need to also measure the other components in the y and z directions, but we can make all of our arguments only using one dimension with no loss of generality). To determine the accuracy of our results, we would perform such a measurement not just on one particle, but on a large number of *identical* particles, all (in this case) in the same state. Such an aggregate of identical systems in the same state is called an **ensemble**. We will discuss this concept in greater detail later.

Each individual measurement yields a value for x and a value for p_x (subject to experimental uncertainties). But the results of different measurements are not the same, even though the systems are identical. If graphed, these results are seen to fluctuate about a central peak as shown in Figures 1.8 and 1.9 below.

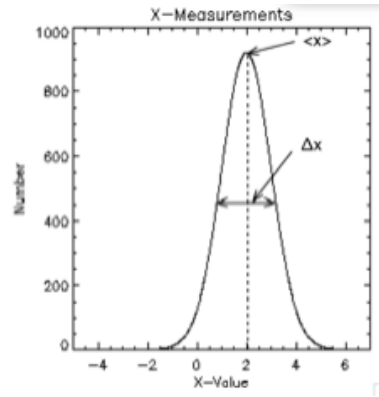


Figure 1.8: Experimental result: x -measurements.

The first figure shows the results of measurements of the x components of the position of a large number of identical quantum particles. The results are seen to fluctuate about a central peak, the *mean value*.

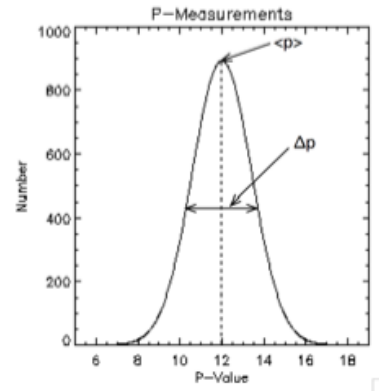


Figure 1.9: Experimental result: p_x -measurements.

The second figure shows the results of measurements of the x components of the momentum of a large number of identical quantum particles. The results are also seen to fluctuate about a central peak, the *mean value*.

A similar spread of results characterizes the measurement of all other variables. At first sight, the fact that the results of many identical experiments are not the same does not worry us. We think it is just a manifestation of the experimental error that troubles all measurements.

According to classical physics, we can reduce the errors in x and p_x to zero and thereby determine the initial conditions precisely.

But, it will turn out that *we cannot unambiguously specify the values of both of these observables for a microscopic particle*. This peculiarity of nature in the microscopic regime follows from the **Heisenberg Uncertainty Principle (HUP)**. In its simplest form, the HUP shows that any attempt to *simultaneously* (say at time t_0) measure $x(t_0)$ and $p_x(t_0)$ for any system in the ensemble necessarily introduces an imprecision in the value of each observable. No matter how the experiment is designed, the results are *inevitably* uncertain, and the *uncertainties* (to be defined carefully later) $\Delta x(t_0)$ and $\Delta p_x(t_0)$, which are measures of fluctuations like those in the figures above, cannot be reduced to zero. Instead, as we shall derive later, their product must satisfy the condition

$$\Delta x(t_0)\Delta p_x(t_0) \geq \frac{\hbar}{2} \quad (1.20)$$

where $\hbar = 6.626 \times 10^{-34} \text{ J} \cdot \text{sec}$ = Planck's constant. Not a very big number, but not zero either! Similar constraints hold in the other directions.

Position and momentum are thus *fundamentally incompatible observables*, in the sense that knowing the precise value of one precludes knowing anything about the other.

But there is a deeper dimension to the Heisenberg Uncertainty principle. Quantum mechanics reveals that the limitation reflected by the uncertainty relation on our ability to simultaneously measure x and p_x is *implicit in nature*. It is a fundamental property of the microworld. It has nothing to do with a particular apparatus or with experimental technique. Quantum mechanics proves, as we shall see, that a particle cannot *simultaneously* have a precise value of x and a precise value of p_x .

Uncertainty relations are not veiled criticisms of experimental physicists. They are *fundamental limitations on knowledge*. *The universe is inherently uncertain*. We cannot know all of existence. We might think of uncertainty relations as nature's way of restraining our ambitions!

The Heisenberg Uncertainty Principle strikes at the very heart of classical physics, namely, the trajectory.

Obviously, if we cannot know the position and the momentum of a particle at t_0 , we cannot specify the initial conditions of the particle and hence cannot calculate its trajectory. Indeed, since the HUP applies at any time, it makes no sense to ascribe a trajectory to a microscopic particle. We are forced, however, reluctantly, to conclude that microscopic particles do not have trajectories. But, once we throw out trajectories, we must also discard Newton's Laws and nothing is left in classical theory.

Stripped of its basic elements and fundamental laws, the whole structure of classical physics collapses.

The demise of classical physics occurred around 1920. Sitting amidst the rubble, physicists of that era realized that their only alternative (other than to change careers) was to rebuild - to construct a new theory from scratch, one based on elements other than trajectories and on laws other than those of Newton and Maxwell.

Thus began the quantum revolution and we are still part of an ongoing revolution as you will see in this book.

1.4.1.2 Classical and Quantum Physics Get Together

To say that classical physics died around 1920 is a bit too dramatic. The physics of Newton and Maxwell still accurately and beautifully describes the macroscopic world. Knowing this, physicists developing quantum mechanics demanded (possibly incorrectly as we will see) that when applied to macroscopic systems, the new physics must reduce to old physics. They felt that as the size of the system being studied increases, the quantum laws of motion (which we will write down shortly) must go over smoothly into those of Newtonian mechanics, and non-classical phenomena such as uncertainty and duality must become undetectable. Remember, however, this was just a guess!

Neils Bohr specified this requirement into his **Correspondence principle**, the essential elements of which are sketched in Figure 1.10 below.

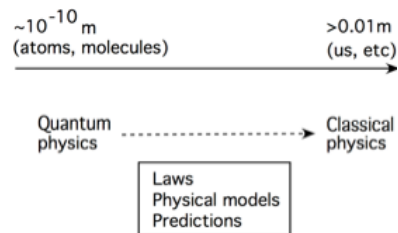


Figure 1.10: The Correspondence Principle

The ability of quantum mechanics to satisfy this principle was taken as an important theoretical justification of the new physical theory. This is another point where we should keep an open mind as we discuss quantum mechanics. Is this principle truly universal, valid for all systems? If so, where do we draw the line between microscopic systems obeying quantum mechanics and macroscopic system obeying classical physics. Modern experiments, as we shall see keep pushing this line towards larger and larger systems. It might be the case that no such line exists and quantum mechanics applies to all systems of any size!

The *experimental* justification of quantum theory is that it works. The predictions, qualitative and quantitative, of quantum mechanics have been verified

in 10000's of experiments on a wide ranging collection of systems. These verifications are of paramount importance to physics, for in some ways quantum theory is a fragile creation. It is an *inferential* theory, in which we will devise a small set of postulates and from them derive equations, which can be put to the test of experimental verification. If the equations pass the test, then we will have some confidence that the postulates, which cannot be directly tested, are consistent and correct. But it would take *only one repeatable experiment* whose results disagreed with the equations of quantum mechanics to bring the whole structure tumbling down. To date, the edifice stands (although some think it is very shaky). Quantum mechanics remains the only theory we have that explains how matter is constructed and how physical processes at the atomic level work.

1.4.1.3 The Indeterminate Universe

As this worldwind overview may suggest, the new physics, quantum physics, differs from classical physics in nearly every way imaginable - from its elements and laws to the kind of knowledge it provides. It is in this last respect that the implications of the quantum revolution are most profound.

Classical physics yields *precise* information about the properties and behavior of individual, independent systems. It holds out to the scientist the promise that, in principle at least, she can know everything. Quantum physics says that this is just not so, that nature imposes fundamental limitations on knowledge via constraints such as the Heisenberg Uncertainty Principle.

These limitations derive from the *probabilistic nature of quantum mechanics*. The new physics, in the *standard view* (as we shall see), yields only *statistical* information about ensembles or aggregates of identical systems. Moreover, the statistical information provided by quantum theory is limited to the results of measurements. Some physicists put it in strong statements such as

Do not make any statements that can not be verified.

We can only know properties that can be measured.

That is, quantum physicists are not allowed to infer facts about a system unless these facts can be verified by experiment. This is a severe limitation - for example, it prohibits us from ascribing an orbit (a path) to a particle, because (as we shall see later) measurements of position are necessarily performed at discrete times. Even if we measure the position of a particle at two times t_1 and t_2 , we cannot even make the simple inference that it traveled from $\vec{r}(t_1)$ to $\vec{r}(t_2)$ via a path in ordinary (geometric) space. We can only say that we found it at $\vec{r}(t_1)$ at t_1 and then at $\vec{r}(t_2)$ at t_2 . We cannot talk, as we will see, about it being *in between* at any time unless we can measure it to be there at those times!

This limitation, that physics describes only observed phenomena forces us to

think about reality in a strange new way. At its most fundamental level, reality seems to be discontinuous. Here is Erwin Schrödinger on this most non-classical feature of the theory:

... it is better to regard a particle not as a permanent entity but as an instantaneous event. Sometimes these events form chains that give the illusion of permanent beings - but only in particular circumstance and only for any extremely short period of time in every single case.

Quantum physics is a harsh taskmaster!

In closing this section of the book, I should say that all this has not set well with many physicists. Even today, some find the world view implied by quantum mechanics, namely, a subjective universe, intolerably offensive. The battle over the interpretation of quantum mechanics goes on (this is my research area). All, however, agree on the usefulness of the theory for predicting and understanding the physics of matter. It is, after all, the only game in town!

1.4.1.4 Final Thoughts: What is It All About?

From this overview, you may have concluded that quantum mechanics is not a particularly easy subject to study. That is true. To pretend otherwise would be untruthful. But why is learning quantum mechanics hard?

There are, I think, three reasons. First, we grew up in and now inhabit a macroscopic world. Our intuition - our sense of how things ought to behave - has been reinforced every waking minute by experiences in a world that follows classical physics. Quantum physics is an affront to that intuition. To understand it, to use it effectively, we must develop a new way of thinking about the ways things work, because as Richard Feynman has written:

Things on a very small scale behave like nothing you have any direct experience about. They do not behave like waves, they do not behave like particles, they do not behave like clouds, or billiard balls, or weights on springs, or like anything that you have ever seen.

Second, quantum physics operates at a level that is one step removed from everyday reality. It is more abstract than classical physics. While classical physicists can deal with well-defined trajectories that describe particles they can visualize, quantum physicists must forever wander through a haze of uncertainty, probabilities, and indeterminacy, trying to understand a universe they cannot directly observe. The microworld can be understood, but it cannot be seen.

Third, quantum mechanics is inherently mathematical. There is an important distinction here between classical and quantum physics. In classical physics physicists use mathematical methods to implement the ideas of the theory, but we can discuss, using words, those ideas without recourse to mathematics. This is not possible in quantum mechanics. Notwithstanding the achievements of

writers who have recently tried to popularize quantum theory, I believe it is impossible to fully grasp the principles of quantum theory without seeing them expressed mathematically. Mathematics is more than a tool for solving quantum mechanics problems - **mathematics is the language of quantum physics**. As we move deeper into quantum theory, we will see physics and mathematics become inextricably intertwined. Thus, quantum physics demands that we think in a new, abstract, inherently mathematical way - no easy task. We will learn this new language in this book; it was invented by Dirac. Finally, we must re-think and redefine many familiar words and concepts, and when we use words to discuss quantum concepts, we must do so with great care and precision. Familiar terms such as *particle* and *motion* assume, in the quantum domain, subtle overtones and shades of meaning that we ignore at our peril. We have already seen an example of this in our discussion of the *position* of a microscopic particle. The *position* of a quantum particle prior to its measurement is not a single, well-defined number, such as $10.7m$. Rather, it must be specified as a collection of several - maybe an infinity of - values, *none of which represent the position of the particle*. Instead, each value represents a *possibility*, a location at which the particle *might* be found.

In spite of these roadblocks - our classical intuition, the inherently mathematical nature of quantum mechanics, and the need to use old words in new ways - I know that you can understand quantum mechanics. Even if you cannot visualize what goes on in the microworld of atoms and molecules, you can grasp the beautiful and powerful physical laws that govern that world.

This is our world and welcome to it.

1.5 Into the Microworld

I have no data yet.
 It is a capital mistake to theorize
 before one has data.
 Insensibly one begins to twist facts
 to suit theories, instead of theories
 to suit facts.

Sherlock Holmes to Doctor Watson
 in **A Scandal in Bohemia**
 by Sir Arthur Conan Doyle

We now embark on our first pass through some of the details concerning these new ideas. As you will see, we will make several passes over similar material in this book in the hope that multiple exposures improves your understanding.

1.5.1 Duality and The Double Slit

Quantum physics is chock full of bizarre, non-classical ideas; weird concepts haunt nearly every aspect of the subject. Three of these ideas - quantization, uncertainty and duality - deserve special treatment, for they are among the fundamental ideas in quantum theory.

Quantization is probably familiar term to you, but you would not have encountered it in a classical physics book or in your everyday experience. The observables of macroscopic systems are not quantized or so it seems. The energy of a ball on a string, the linear momentum of a hockey puck, and the angular momentum of an astronaut in a centrifuge - all can take on any of a *continuum* of values, subject only to whatever constraints are imposed by the forces acting on the system. In the macroscopic world *nature is continuous (or seems to be)*.

Not so in the microworld, where there is abundant evidence that nature is inherently discrete. Physicists have been aware of this fact since pre-quantum days. By 1900, for example, spectroscopists knew that radiation was emitted by atoms and molecules at discrete frequencies(wavelengths). But the first direct evidence of *quantization of energy* appeared in collision experiments performed in the early 1900's by Franck and Hertz.

For several years, Franck and Hertz had been measuring the ionization potential of atoms (the amount of energy needed to remove an electron from the atom) and this experience influenced their interpretation of the results of their collision experiments. In these experiments, they scattered electrons from various atoms; for example, in their most famous experiment, Franck and Hertz accelerated electrons being emitted from a heated platinum wire and sent the resulting beam through a gas of mercury vapor. By measuring the electric current(number of electrons per second) in the scattered electron beam as a function of the energy of the incident electrons, Franck and Hertz could study the energy loss suffered by the electrons in their collisions with atoms of the gas. They found that the scattered current exhibited a series of sharp drops, each occurring at an incident energy equal to an integral multiple of 4.9 eV .

Being initially led astray by their prior experience studying ionization, they concluded that 4.9 eV is the ionization energy of mercury. But Neils Bohr, on learning of the Franck and Hertz results, realized that the electrons in the beam were not ionizing the mercury atoms but were rather exciting them - losing energy to the atoms through collisions. Drawing on his model of the atom, Bohr further deduced that the energy spacing at which the current drops occur, 4.9 eV , is the separation of two *discrete* energy levels of the mercury atom.

In 1914, when Franck and Hertz reported their work, physicists thought that it supported the Bohr theory of the atom - which has since been superseded by

quantum theory. Although the Bohr model of the atom, the heart of what is called *the old quantum theory*, is of enormous historical importance, we will not talk about it in this book because this model turns out to be both unphysical and very misleading!

Nevertheless, the Franck-Hertz experiment stands as one of the first demonstrations of energy quantization in atoms, a striking example of non-classical shenanigans in the microworld.

Another underlying concept of this world is *uncertainty*. Earlier, we showed an example of this principle. Nature imposes a peculiar indeterminacy on any attempt to simultaneously measure the position and momentum of a quantum particle. The mathematical manifestation of this indeterminacy is the **Heisenberg Uncertainty Principle**.

Duality, the third major quantum idea, is the focus of this part of this book. The so-called **wave-particle duality** is one of the more confounding ideas of quantum physics, for it most directly challenges our classical intuition about how the world behaves. So we must face the challenge of duality. Before we can understand the ways of the microworld, we must get rid of the idea that quantum particles can be understood as either classical particles or classical waves. The essence of wave-particle duality is beautifully encapsulated in a single experiment, the famous double-slit experiment. After first getting some needed background ideas, we will then investigate this provocative experiment. Again we will make multiple passes through this and equivalent experiments until we think that we understand what is happening.

1.5.1.1 A Short Digression: How Science Works

Most people have a rather unrealistic view of how science works. It's not their fault. In the media, on the TV, and in the movies, scientists are often portrayed as being dispassionate searchers of the truth, applying a rigorous scientific method that, in the end, will explain everything. Some scientists do what they can to promote this view, when they write books or present public lectures. However, not all scientists agree with this picture. They recognize that things are usually far more complicated than that.

Science, as we generally have it explained to us at school, starts with some experimental data. The scientists then have to come up with some hypothesis to explain these results. Using that hypothesis, a prediction is made about what might happen in a slightly different experiment. An experimental check is made, and if the prediction turns out to be correct, the hypothesis is upgraded into a theory. You then return to **GO**, collect \$200(get new funding) and start again with a new set of experiments and so on.

Actually, you don't have to work in science for very long to realize that this pic-

ture of how things work is pretty unsophisticated and definitely oversimplified. Sometimes it can be extraordinarily difficult to find a hypothesis that explains the data; sometimes there are many hypotheses and the data are insufficient to decide between them. Often we have to start with a rough idea of what is going on, under very simplified circumstances, and try to slowly add in more detail. Occasionally the theories that we use get too mathematically difficult to apply and get exact answers. Then the theoretician has to struggle to get some sort of partial answer with ingenious approximations, limited attention to detail, and, normally, a great deal of coffee.

One technique that sometimes helps is to imagine a simplified experiment, that, if it could be made to work, would illuminate certain aspects of the theory. Einstein was an absolute master of producing such experimental ideas. He called them **gedanken** experiments, which translates as **thought** experiments. During the development of quantum mechanics in the 1920s, Einstein would often argue with Bohr and Heisenberg about the nature of quantum theory and would produce brilliant gedanken experiments designed to point out errors in the theory and that the theory produces inconsistent results. In the end, as we will see, this turned out to be a losing battle and Einstein had to admit that quantum theory was at least consistent, although he never accepted that it was the correct theory of the microworld.

Occasionally, simplified experiments of this sort become part of the scientific culture and are used as teaching aids when the ideas are being passed on to the next generation. The danger is that mistakes and misinterpretations can be inherited as part of the folklore. This is why it is very timely when technology catches up with the creativity of the scientist and a gedanken experiment experiment is turned into a real experiment.

Quantum theory has such an experiment. It is integrated into the folk memory, used as a teaching aid, and widely reproduced in books. Richard Feynman believed that all the mysteries of quantum theory could be seen in this one experiment. It is known as the **double-slit experiment**.

1.5.1.2 Waves versus Particles

The behavior of a microscopic *particle* differs in subtle ways from that of a classical particle; in some situations, it seems to exhibit the behavior of a classical wave. So before we plunge into the microworld, we need to discuss and understand the classical picture of particles and waves.

Earlier, we reviewed the characteristics of a classical particle and the analysis of its motion using Newtonian mechanics. For example, a macroscopic particle has a well-defined position and linear momentum at any time and from these observables we can calculate its energy. Essential to this description is the notion of spatial localization. The idea that a particle is a localized thing is implicit, for

example, in the description of transport of energy through space by a particle as a localized lump. This quality of the classical description of a particle is, in turn, reflected in the *state descriptor* of Newtonian theory: **the trajectory**.

The characteristics of a *wave* are quite different from those of a particle (we will discuss waves and their properties in detail later). A wave is not spatially localized - this quality is reflected in the properties by which we characterize a wave, such as the *wavelength*. Like a particle, a wave carries energy and momentum, but it does so in a *non-localized* manner, distributed over a region of space called a *wave front*. A wave exhibits distinctive, non-particle-like behavior such as diffraction, interference and polarization. Not surprisingly, then, the theory classical physicists use to describe the propagation of an electromagnetic wave and its interaction with matter - Maxwell's theory of electromagnetism - is quite different from that of Newtonian particle dynamics. So at the macroscopic level, classical physics elegantly and cleanly separates into wave propagation and particle dynamics.

Alas, this division does not apply to microscopic particles, which adamantly refuse to adhere to either the classical wave model or the classical particle model. In some circumstances microscopic particles behave according to the laws of classical mechanics. For example, some collisions of highly energetic atoms with molecules can be explained using classical collision theory. Yet in other circumstances quantum particles behave like waves: e.g., electrons that have been scattered by a crystal exhibit a diffraction pattern when they are detected. Analysis of this pattern reveals that in this experiment the electrons propagate precisely, as we will see later, as though they had a well-defined wavelength and frequency - as though they are waves.

This situation, we might think, is a mess. We are told that light is not a wave. And electrons are not particles. Well then, what are they? And how can we understand the behavior of electrons if not with Newtonian mechanics, and waves if not with Maxwell's theory? What is going on here?

1.5.1.3 First Thoughts about Light

When you set out to understand something new in physics, it is a good idea to start by comparing it with something that you have already figured out. In the case of light, there are two possible comparisons. As we said, some physicists think light is either a wave (a spread out, flappy sort of thing that varies in both space and time like a ripple on a pond) or a stream of particles (localized hard lumps, like marbles, that simply change their position with time). Each view has its supporters, and with no clear experimental way of settling the issue (until the 1800s), most physicists took sides based on philosophical or theoretical grounds.

Historically, the big hitters squaring up in opposite corners were Thomas Young

and Isaac Newton. In 1665, Newton made some fundamental discoveries about light while taking leave from his studies at Cambridge, which was under threat from the plague that was spreading throughout the country. In one of his classic experiments, Newton allowed a thin shaft of sunlight to fall on a glass prism, producing a spectrum of colors as shown in Figure 1.11 below.

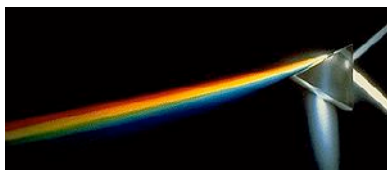


Figure 1.11: White light incident on a prism.

He proposed that white light was a mixture of particles that gave rise to the various colors. As these particles passed through the prism, they interacted with the glass in different ways and as a result were separated out.

With Newton as a public supporter, the particle view was bound to hold a certain influence; but what also helped was the observed existence of sharp shadows. A casual glance at the shadows cast by objects shows that they have well-defined edges. This was difficult (at the time) to explain if light was a wave effect. Waves, such as water waves, clearly bend around objects that get in their way (see Figure 1.12 below).

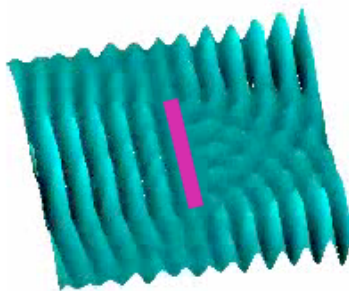


Figure 1.12: Water waves bending around an object.

If light was a wave, then it was thought that shadows should have rather fuzzy outlines.

However, not all were convinced, and in 1801 Young carried out an experiment that was sensitive enough to reveal the wave aspects of light. The key to Young's experiment was to use two linked sources of light to produce an *interference pattern*. We will discuss the details of how interference works later on, but for a simple illustration imagine dropping two pebbles into an otherwise smooth

surface of water. Ripples would spread out from each impact point. Inevitably, they would overlap somewhere, and the result would be a complex pattern of motion on the surface of water: *an interference pattern* as shown in Figure 1.13 below.

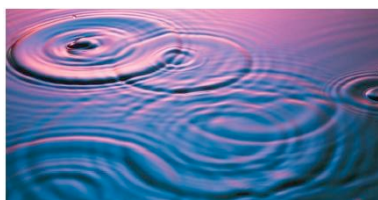


Figure 1.13: Interference pattern in water.

In Young's version, specially prepared light from two sources lit up a screen. In the region where the light from both sources overlapped, instead of a patch of illumination, a series of bands were seen. The natural explanation was that the waves from the two sources were overlapping in a complex manner, like the ripples on water, causing bright patches where they somehow reinforced each other and dark regions where they somehow canceled each other. On the left of Figure 1.14 below we see the interference pattern from water waves and on the right a schematic of a two-slit experiment.

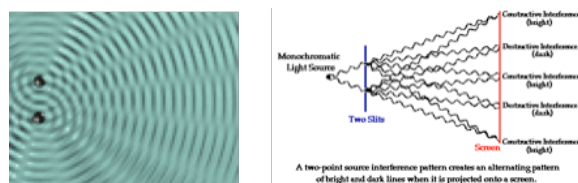


Figure 1.14: Two source experiment with water waves.

Figure 1.15 figure below shows Young's original sketch of the experiment.

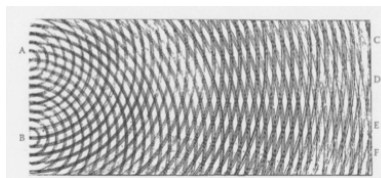


Figure 1.15: Young's original idea.

As a final point, it is noteworthy that a wave view of light explains the existence of different colors by suggesting that color is related to the wavelength of the light(not different particles).

1.5.2 Some Second Thoughts

1.5.2.1 On the Nature of Light

To probe deeper into the wave-particle duality, we are going to make a quick pass through the history of our evolving ideas about the nature of electromagnetic radiation.

Corpuscular theories of light, which treated light as though it were composed of particles, have been around since the days of Newton and Laplace. But light has an irritating tendency to exhibit distinctively non-particle-like behavior, such as diffraction and interference, which corpuscular theories cannot explain. Once Maxwell introduced the wave theory of electromagnetic radiation (1870) and it became clear that this theory could beautifully explain such phenomena, most physicists abandoned corpuscular theories of light.

According to Maxwell, all electromagnetic radiation - light included - consists of real waves propagating through space, waves that carry energy distributed over continuous, non-localized spherical wave fronts. In the late 19th century, it seemed that Maxwell's theory could explain even the most complicated electromagnetic phenomena.

1.5.2.2 Walking the Planck

It was Albert Einstein who, in 1905, resurrected the notion that electromagnetic radiation is particle-like rather than wave-like in nature. But where did this idea originate? Einstein has written that the seeds of his 1905 theory were planted by research carried out at the turn of the century by Max Planck.

Although encouraged by his physics teacher to pursue a career as a musician, Planck persevered in physics. Planck's studies of radiation inside a heated cavity led, via a line of reasoning he himself described as an act of desperation, to the concept of quantization of energy and then to the birth of quantum physics.

Planck did not set out to revolutionize physics. Instead, following in the footsteps of his teacher Kirchhoff, he sought to understand why hot bodies glow. This phenomenon, which is called black-body radiation, may be familiar to you if you ever did any pottery. Suppose you making a clay pot. To harden the clay, you fire the pot, that is, put it in a kiln (an oven) and heat it to roughly 2000° F for about 10 to 12 hours. Suppose that there is a tiny hole in the oven. As the pot heats up, at first you see darkness and then as the pot gets hotter and hotter, it begins to glow red. As the temperature of the pot increases further, this glow becomes orange, then yellow, then white, and fills the oven, obliterating all detail of the pot. Why?

Planck formulated this question in slightly more abstract terms, asking: what is the spectrum (distribution of wavelengths or frequencies) of electromagnetic

radiation inside a heated cavity? More specifically: how does the spectrum depend on the temperature T of the cavity, on its shape, size and chemical makeup, and on the frequency f of the electromagnetic radiation in it? By the time Planck began his studies, part of the answer was known. Kirchhoff and others had shown that once the radiation in the cavity attains equilibrium (reaches a steady (unchanging) state) with the walls, the energy in the field depends on f and T but, surprisingly, is independent of the physical characteristics of the cavity such as its size, shape or chemical composition.

The cavity, of course, encloses a finite volume. Planck was interested in the radiative energy inside the cavity, not on the effects that depend on its volume, so he worked in terms of an energy density (energy/volume). In particular, he sought an expression for the radiative energy density per unit volume $\rho(f, T)$. If we multiply this quantity by an small range of frequency df , we obtain $\rho(f, T)df$, the energy per unit volume in the radiation field with frequencies between f and $f + df$ at cavity temperature T .

Rather than confront the distracting complexities of a real heated cavity, Planck based his work on a model originally introduced by Kirchhoff. Kirchhoff called his model of a heated cavity in thermal equilibrium a *black-body radiator*. A black body is simply any object that absorbs all radiation incident on it. Thus, a black-body radiator neither reflects nor transmits; it just absorbs or emits radiation.

From the work of Wien, Planck knew that the radiative energy density $\rho(f, T)$ for a black body is proportional to f^2 and, from the work of Stefan, that the integrated (sum over all the frequency intervals) or total energy density is

$$\int_0^{\infty} \rho(f, T) df \propto T^4 \quad (1.21)$$

This quantity is an integral, which, at this point, is simply a symbol representing the sum over all the intervals. We will study the integral in more detail in Chapter 6 and understand how it works.

But this information did not fully describe the dependence of $\rho(f, T)$ on f and T ; experimental evidence implied a further, unknown dependence on the ratio f/T . Typically, the data sets are as shown in Fig 1.16 below. In the plot the horizontal axis is wavelength $\lambda = c/f$, where c = speed of light.

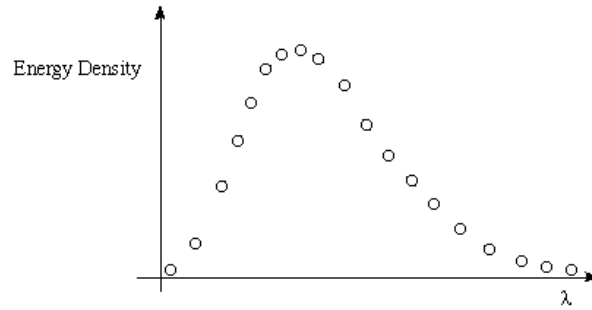


Figure 1.16: Typical black-body radiation spectrum.

Wien had actually proposed an equation for the energy density of a black-body radiator, but the theoretical foundation of his theory was shaky. Moreover, his equation worked only in certain circumstances; it correctly explained the f and T dependence of $\rho(f, T)$ for low temperatures and low frequencies (high wavelengths). But it predicted that heated black bodies should emit a blue (high frequency/low wavelength) glow at all temperatures (that is the dotted curve getting very large at low wavelengths in Fig 1.17 below) - a prediction not supported by experiment. Planck knew of this defect in Wien's theory. The actual theoretical result due to Wien is

$$\rho(f, T) = \frac{8\pi k_B T}{c^3} f^2 = \frac{8\pi k_B T}{c} \lambda^{-2} \quad (1.22)$$

For low frequencies (or high wavelengths) this agrees spectacularly with experiment as shown in Figure 1.17 below:

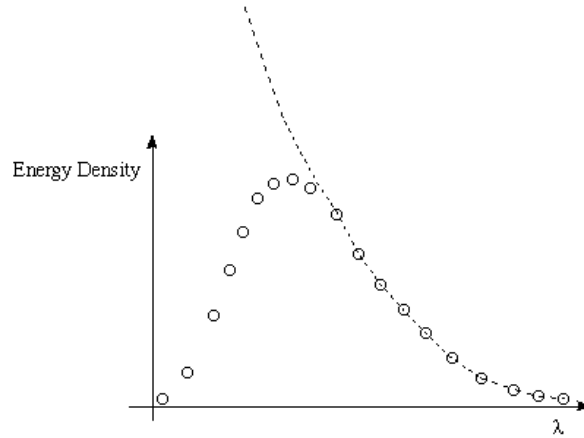


Figure 1.17: Wien theory (dotted line) compared to experiment

Clearly, however, we see that the model totally fails for high frequencies or

small wavelengths. The blue glow mentioned above would appear because of the dramatic increase in the energy density ρ for high frequencies or low wavelengths (blue end of spectrum).

Furthermore, on purely theoretical grounds alone, this result must be wrong since it predicts that for a cavity of volume V at temperature T the total radiant energy in this volume (sum over all frequencies - we will learn how to do the calculation shown below in Chapter 6) is

$$E = V \int_0^{\infty} \rho(f, T) df = V \frac{8\pi k_B T}{c^3} \int_0^{\infty} f^2 df = \infty \quad (1.23)$$

which is clearly a nonsensical result. Our eyes are not seared by the erroneously predicted x-rays and gamma rays when we look into a cold stove or even a hot stove.

In his research, Planck focussed on the exchange of energy between the radiation field (in the cavity) and the walls. He developed a simple model of this process by imagining that the molecules of the cavity walls are electrical charges undergoing oscillations called simple harmonic motion. As a consequence of their oscillations, these charges emit electromagnetic radiation at their oscillation frequency, which, at thermal equilibrium, equals the frequency of the radiation field. According to classical electromagnetic theory, energy exchange between the oscillators and the walls is a continuous process, that is, the oscillators can exchange any amount of energy with the field, provided, of course, that energy is conserved in the process.

By judiciously applying classical thermodynamics and a healthy dose of physical intuition, Planck deduced the form of an empirical formula for the radiative energy density:

$$\rho(f, T) = \frac{A f^3}{e^{Bf/T} - 1} \quad (1.24)$$

In this equation, A and B are constants to be determined by fitting the experimental data; that is why it is called an *empirical* formula.

This result agreed beautifully with experimental data for a wide range of frequencies and temperatures. And, in the limit $f \rightarrow 0$ or $T \rightarrow \infty$, it reduced properly to Wien's law.

But Planck was concerned that he could not rigorously justify this formula.

For his second attempt to derive the energy density of a black body, Planck adopted well-known statistical physics methods due to Boltzmann. At one point in the new derivation, Planck introduced a simplifying assumption, that is, a trick to allow him to carry out the necessary mathematics (to do the calculations). His ploy was a conventional trick in mathematical analysis and Planck

expected to take appropriate limits and remove his simplifying assumption at the end. Planck was in for a rude shock.

His assumption was both simple and radical. He knew that a classical black body could exchange any amount of energy with the walls of the cavity. Nevertheless, for the purposes of his derivation, Planck assumed that only *discrete* amounts of energy can be absorbed or emitted by the oscillating atoms that comprise the walls of the black body (changing a continuous variable into a discrete variable, doing the calculation, and then going back to continuous variables was well-established mathematical technique). He called these discrete amounts of energy **quanta**. To each quantum, Planck assigned an energy equal to an integral multiple of hf , where h is a constant with an empirical value of $h = 6.63 \times 10^{-34} \text{ J} \cdot \text{sec}$.

Having made this assumption, Planck could easily carry out the needed mathematics and derived the radiation law

$$\rho(f, T) = \frac{8\pi f^2}{c^3} \frac{hf}{e^{hf/k_B T} - 1} \quad (1.25)$$

where $c = 3.00 \times 10^8 \text{ m/sec}$ is the speed of light and $k_B = 1.38 \times 10^{-23} \text{ J/K}$ is Boltzmann's constant. Comparing this result with the earlier guess (Eq. 1.24), we see that in his new equation, Planck had now derived expressions for the constants A and B that appeared in his earlier empirical guess. The theory now agreed with the data perfectly!

This derivation was the theoretical justification that Planck sought for the distribution of radiation in a black body. But in setting up the foundation for the theory, Planck paid an enormous price, for try as he might, he could not get rid of his artificial constant h - he could not get rid of quantization. Setting $h = 0$ (taking the expected limits, i.e., using the standard procedures in mathematics for removing the tricks needed to do the calculation) inevitably led to a result that disagreed with much of the experimental data. Yet if h is non-zero, then Planck's theory seemed to be seriously at odds with a physicist's understanding of energy exchange as a continuous process.

Planck's rash assumption heralded the strange new physics of the quantum, which dominated the physics community for the next three decades. But physicists, who were then and are today a rather conservative lot, did not appreciate being told that their understanding of so basic a process as energy exchange was fundamentally incorrect. Attempts to derive Planck's result without making his drastic assumption always failed and for several years Planck's quanta languished in obscurity, largely ignored. Yet Planck's assumption was nothing compared to the surprise that Einstein had in store.

1.5.2.3 Particles of Light

Einstein thought he saw an inconsistency in the way Planck used Maxwell's wave theory of electromagnetic radiation in his derivation. With characteristic intellectual courage Einstein decided that this inconsistency implied a flaw not in Planck's theory but in Maxwell's theory. This radical contention shifted the emphasis in research on black bodies from the oscillators that make up the walls to the electromagnetic radiation field inside the cavity itself. Ultimately, Einstein's insight completely altered the way we think about light.

In 1905 Einstein proposed that the energy in an electromagnetic field is not spread out over a spherical wave front, as Maxwell would have it, but instead is localized in indivisible clumps - in *quanta*. Each quantum of frequency f , travels through space with the speed of light, $c = 3.00 \times 10^8 \text{ m/sec}$, carrying a discrete amount of energy hf and momentum hf/c . Thus, in Einstein's model, light transports energy in the same way particles do. G.N. Lewis subsequently dubbed Einstein's quantum of radiation energy a **photon**, the name we use today.

Einstein thought that light only appeared as a wave if one observed it over fairly long time intervals ($\Delta t \gg 1/f$) or if it was very intense light. If one could *freeze* the light wave in time (this has now been done photographically in experiments), he felt that one would observe the quanta or *photons* or alternatively, one should be able to reduce the light intensity until there was only one photon around at a time and see the discreteness directly (experimentalists could not do this when Einstein was alive, but can now do it as we will see later).

The photon model cast Planck's theory of black-body radiation in, so to speak, a new light. Planck thought that energy exchange between the oscillators of the cavity and the field occurs in units of hf because of some strange property of the oscillators. To this Einstein said: **No, the explanation is that the radiation field itself is quantized.** Planck's result is consistent with this extraordinary notion; if the energy in the field is contained in photons - quanta of magnitude hf - then of course only integral multiples of the photon energy can be exchanged with the walls.

The photon model explained more than just black-body radiation (as all good theories should do).

One of Einstein's greatest achievements was using it to understand the **photo-electric effect** - the ejection of electrons from a metal, such as sodium, when light impinges (shines) on it as shown in Figure 1.18 below.

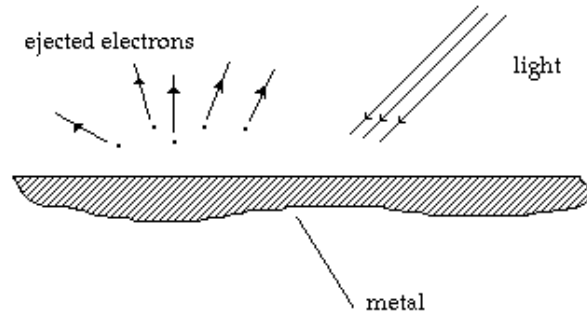


Figure 1.18: The photoelectric effect

What happens is this. The material (actually the electrons in the material) absorbs the light and hence its energy and when they have acquired an energy above a certain minimum value (dependent on the material) called the *work function* they are able to escape from the material and be detected in the laboratory.

1.5.2.4 Experimental results:

1. there exists a threshold frequency f_0
2. no matter how large the value of the light intensity (energy/time if light is a wave) no electrons are ejected if $f < f_0$
3. if $f > f_0$, then the electrons are detected almost instantaneously (as soon as the light is turned on). The delay is less than 10^{-12} sec
4. electrons are detected and the detected electron energy is given by the relationship

$$h(f - f_0) \quad (1.26)$$

independent of the light intensity, where h is a constant.

If light were a wave, then its energy (according to classical theory) is proportional to its intensity (brightness). Thus, if we raise the intensity (without changing the frequency with $f < f_0$), then when we have enough energy available (when the intensity is large enough) to eject the electrons, they should appear.

BUT THEY DO NOT!

Also if the electrons were absorbing energy from waves, then they could not acquire enough energy instantaneously (10^{-12} sec) to be ejected. Energy transfer in wave interactions is a relatively slow process.

The wave analogy here is that the bigger the wave (the larger its intensity) the

harder a swimmer is thrown out of the water. Whereas, a lot of waves (high frequency) are bothersome but will not toss you out of the water. Frequency is of no importance in determining the energy content of classical waves. Try it out experimentally. Consider a cork bobbing in bathtub. We must create huge sloshing waves in order to eject the cork. But if you hit it with another particle(your toe for example), it can instantaneously jump out.

The photon model, however, seems to explain every feature of the experiment!

First, the threshold value is explained because, in the case $f < f_0$ a single photon does not contain enough energy to eject the electron (the probability of a single electron absorbing 2 photons simultaneously is essentially zero) or

$$\text{threshold energy} = \text{minimum energy for ejecting an electron}$$

The threshold frequency value f_0 is where the photons just have enough energy. Electrons immediately appear (even if we reduce the intensity to zero) because we only need a single photon of the correct energy to eject an electron.

In the wave analogy, i.e., if light were a wave, then this result would say that a ripple and a tidal wave(of same frequency) would both throw you onto the beach with the same energy - clearly not true!

Second, if photons have energy hf and it takes energy hf_0 to get out, then the electrons have $h(f - f_0)$ left after being ejected, which is what is observed for the ejected electrons.

Third, photon absorption is an instantaneous(essentially) process. This means that as soon as the beam is turned on and $f > f_0$ any electron that absorbs a photon has enough energy to get out and they do so instantaneously as observed.

So once again light behaves like a packet or bundle of energy and momentum or like a particle and waves do not work.

Light seems to be able to be a wave when it needs to be a wave (interference and diffraction experiments) and a particle when it needs to be a particle(photoelectric effect) or *so it seems to our classical minds*.

Yet, the photon was too radical for physicists of the early 1900's, and Einstein's model of the electromagnetic field encountered strong opposition. Even as late as 1913 - years after the publication of Einstein's work on the photoelectric effect - four German physicists (including Planck) wrote in a petition recommending

Einstein's appointment to the Prussian Academy of Science:

.... That he may sometimes have missed the target in his speculations, as, for example, in his hypothesis of light quanta, cannot be held too much against him, for it is not possible to introduce fundamentally new ideas, even in the most exact sciences, without occasionally taking a risk.

One year later Millikan reported a precise verification of Einstein's equation for the energy of a photon $E = hf$, and the first measurement of Planck's constant. Yet physicists still resisted abandoning their long-cherished idea that light was a wave.

Then in 1923, Compton published the results of his x-ray scattering experiments, and drove the last nail into the coffin of the wave theory of light. Compton scattered x-rays (electromagnetic radiation with a wavelength around $10^{-10} m$ and a frequency around $10^{18} sec^{-1}$) from a thin layer of a light element such as carbon and measured *the shift in the wavelength of the x-rays due to the scattering*. His results were seriously at odds with the predictions of Maxwell's beleaguered theory.

Compton's data clearly showed that the wavelength of the scattered radiation is larger than that of the incident radiation. After several foredoomed attempts to explain the result with classical theory, Compton tried the photon idea. If x-rays carry energy in localized clumps, he reasoned, then we can apply classical collision theory to their interaction with electrons in the target. Compton used the classical laws of conservation of energy and linear momentum - as though he were analyzing a game of billiards - and was able to derive the correct expression for the wavelength shift. This analysis vindicated Einstein's idea. It was too much even for the diehard opponents: the photon was accepted!

1.5.2.5 What is light?

Einstein's brilliant notion still does not fully illuminate the nature of light. The photon is a particle-like model, but clearly light does not actually consist of classical particles. Particles do not diffract. They do not interfere. But light does. Yet, this model demolishes the idea that light is a classical wave. Indeed, the nature of electromagnetic radiation after Einstein seemed more ephemeral than ever; depending on the physical conditions, light seemed to behave either like a classical wave or like a classical particle.

The more one thinks about this so-called wave-particle duality, the more confusing it seems.

1.5.2.6 Understanding Diffraction the Classical Way - First Pass

Diffraction, which was first observed by Leonardo daVinci, is often considered to be the signature of a wave. Diffraction occurs when ripples in a pond encounter a pair of logs that are close together, when light passes through a narrow slit in a window shade, or when x-rays scatter from a crystal. In each case, we can explain the distinctive pattern that forms using classical wave theory. Let us quickly review the most important characteristics of wave phenomena.

A schematic of a single-slit diffraction experiment with light is shown in Figure 1.19 below.

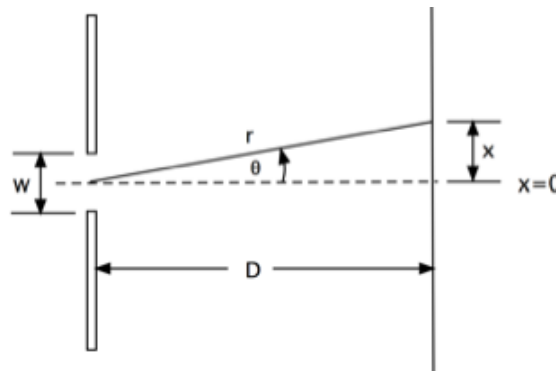


Figure 1.19: Single slit experimental setup

The above diagram represents a highly simplified single-slit diffraction apparatus. At the detector, the distance x is measured from a point on a perpendicular from the midpoint of the slit. The analysis of the experiment is performed in terms of the radial distance r from the midpoint of the slit to the point at x and the corresponding angle θ . In the actual experiment $D \gg w$, i.e., the width of the slit is very much smaller than the distance to the screen(detector).

Monochromatic (single frequency or wavelength) light of frequency f is incident on a barrier in which there is a single slit of width w . We will assume that the light source is far to the left of the barrier, so that the incident radiation can be represented by a *plane wave* (a normal spherical wave of very large radius looks like a plane wave). The width of the slit must be comparable to wavelength $\lambda = c/f$ of the radiation (typically $5 \times 10^{-5} \text{ cm}$) if the slit is to appreciably diffract the light; for example, to diffract visible light enough to observe this phenomenon, we require a slit of width $w \approx 10^{-4} \text{ cm}$.

Light diffracted by the slit falls on a detector such as a photographic plate or a photocell or a screen, located at a distance D far to the right of the slit. The detector measures the energy delivered by the diffracted wave as a function of the distance x as shown in Figure 1.20 below.

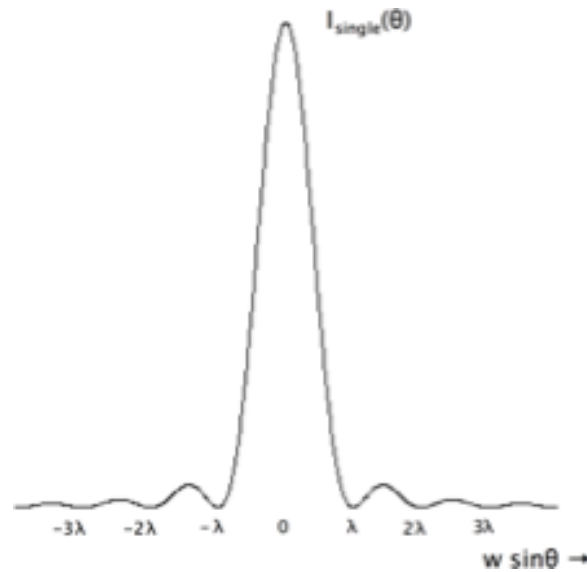


Figure 1.20: Single slit diffraction pattern.

Light diffracted by the single-slit apparatus forms a beautiful pattern at the detector as shown above. This pattern is characterized by a very bright central band located directly opposite the center of the slit, surrounded by a series of alternating bright and dark regions. The bright regions on either side of the central band are called *secondary bands*, because they are much less intense than the central band. Indeed, the secondary bands drop off so dramatically on either side of the central band that often only one pair of secondary bands is visible to the unaided eye.

Additional weak secondary bands exist, though, as can be seen by sensitive detectors. If we experiment with the frequency control of the light source and studies the resulting diffraction patterns, then we find that the separation between adjacent bright bands is proportional to the wavelength λ of the incident radiation. The phenomenon is called Fraunhofer diffraction.

To understand the origin of this pattern, we must digress and spend some time studying wave motion. First, we ask what is a wave?

The essential feature of wave motion is that a *disturbance* of some kind is transmitted from one place to another. A local effect can be linked to a distant cause and there is a time lag between cause and effect that depends on the properties of the medium and finds its expression in the velocity of the wave.

The most important wave for our purposes is the so-called *traveling wave* (as-

sume propagation in the x -direction) described mathematically by the expression

$$y(x, t) = A \sin\left(\frac{2\pi}{\lambda}(x - vt)\right) \quad (1.27)$$

where $y(x, t)$ describes the **shape** of the wave in space and time, A is the wave **amplitude**, λ is the **wavelength**, v is **velocity of propagation** of the wave, and $f = v/\lambda$ is the **frequency** of the wave.

If we imagine that time is frozen at some particular instant (i.e., we take a photograph of the wave), say at $t = 0$, the shape of the wave in space (as shown by the solid or dashed line in Figure 1.21 below) is a sine wave

$$y(x, 0) = A \sin\left(\frac{2\pi}{\lambda}x\right) = A \sin(kx) \quad (1.28)$$

with a distance λ between any pair of identical (having the same value and slope) points on the wave (the wavelength).

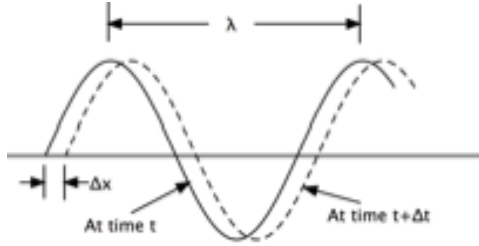


Figure 1.21: Traveling wave at a fixed instant of time.

Now let us fix attention on any one value of y , corresponding to certain values of x and t , and ask where we find that *same* value of y at a slightly later time $t + \Delta t$. If the appropriate location is designated as $x + \Delta x$, then we must have

$$y(x, t) = y(x + \Delta x, t + \Delta t) \quad (1.29)$$

or

$$\begin{aligned} \sin\left(\frac{2\pi}{\lambda}(x - vt)\right) &= \sin\left(\frac{2\pi}{\lambda}(x + \Delta x - v(t + \Delta t))\right) \\ &= \sin\left(\frac{2\pi}{\lambda}(x - vt) + \frac{2\pi}{\lambda}(\Delta x - v\Delta t)\right) \end{aligned} \quad (1.30)$$

This says that the values of Δx and Δt are related by the equation

$$\Delta x - v\Delta t = 0 \Rightarrow v = \frac{\Delta x}{\Delta t} \quad (1.31)$$

This implies that the wave (the propagating disturbance) as a whole is moving in the positive x -direction with speed v as shown in Figure 1.21 above, where we

see the incremental displacement of wave traveling in the positive x -direction. If we look at the wave at only one location (say $x = 0$) we have the expression

$$y(0, t) = -A \sin\left(\frac{2\pi}{\lambda} vt\right) = -A \sin(2\pi ft) = -A \sin(\omega t) \quad (1.32)$$

or the shape (any point on the wave) of the wave oscillates with frequency f . Note that $\omega = 2\pi f$ is called the angular frequency.

The wave is usually written in the useful form

$$y(x, t) = A \sin(kx - \omega t) \quad k = \frac{2\pi}{\lambda}, \quad \omega = 2\pi f \quad (1.33)$$

It turns out that waves can be combined or added together. The process is called **superposition**.

Suppose that we have two waves traveling over the same path (x -direction). Then the resultant shape of the propagating disturbance at any instant of time is given by the *simple sum* of the two shapes, that is, if

$$\begin{aligned} y_1(x, t) &= A \sin\left(\frac{2\pi}{\lambda_1}(x - vt)\right) \\ y_2(x, t) &= A \sin\left(\frac{2\pi}{\lambda_2}(x - vt)\right) \end{aligned} \quad (1.34)$$

then the total disturbance at any point in space and time is given by

$$y(x, t) = y_1(x, t) + y_2(x, t) = A \sin\left(\frac{2\pi}{\lambda_1}(x - vt)\right) + A \sin\left(\frac{2\pi}{\lambda_2}(x - vt)\right) \quad (1.35)$$

Since we have assumed that the two waves are propagating with the same speed, it turns out that the combined disturbance will move with unchanging shape. The shape of the combination or superposition is most easily determined if we put $t = 0$ (since we get the same shape for any t value). We then have

$$y(x, 0) = A \sin\left(\frac{2\pi}{\lambda_1}x\right) + A \sin\left(\frac{2\pi}{\lambda_2}x\right) \quad (1.36)$$

If the two wavelengths are not very different from one another, then we get the superposition of two traveling waves of slightly different wavelength as shown Figure 1.22 below, that is, we get a high frequency sinusoidal wave modulated by a low frequency sinusoidal wave.



Figure 1.22: Superposition of two traveling waves of slightly different wavelengths.

Clearly the superposed wave shape is a combination of a very high frequency (small wavelength) wiggle modulated by a low frequency (large wavelength) outer envelope.

In discussing superposed waves (and interference and diffraction later) it is convenient to introduce the reciprocal of the wavelength. The quantity $\bar{k} = 1/\lambda$ is called the wave number; it is the number of complete wavelengths per unit distance (not necessarily an integer). In terms of wave numbers, the equation for the superposed wave form can be written as follows:

$$y(x, 0) = A [\sin(2\pi\bar{k}_1x) + \sin(2\pi\bar{k}_2x)] \quad (1.37)$$

where $\bar{k}_1 = 1/\lambda_1$ and $\bar{k}_2 = 1/\lambda_2$.

Using the trigonometric identity

$$\sin A + \sin B = 2 \cos \frac{1}{2}(A - B) \sin \frac{1}{2}(A + B) \quad (1.38)$$

that you learned in high school, we can now write this as

$$y(x, 0) = 2A \underbrace{\cos[\pi(\bar{k}_1 - \bar{k}_2)x]}_{\text{low frequency}} \underbrace{\sin[\pi(\bar{k}_1 + \bar{k}_2)x]}_{\text{high frequency}} \quad (1.39)$$

The distance from zero to zero of the modulating factor (low frequency wave)

$$\cos[\pi(\bar{k}_1 - \bar{k}_2)x] \quad (1.40)$$

is defined by the change of x corresponding to an increase of π in the quantity $\pi(\bar{k}_1 - \bar{k}_2)x$, which corresponds to locating two successive zeros of the modulating

factor. Denoting this distance by D , we have

$$\pi(\bar{k}_1 - \bar{k}_2)D = \pi \rightarrow D = \frac{1}{\bar{k}_1 - \bar{k}_2} = \frac{\lambda_1 \lambda_2}{\lambda_2 - \lambda_1} \quad (1.41)$$

If the wavelengths are almost equal and we write them as λ and $\lambda + \Delta\lambda$ with $\Delta\lambda$ small, we then have (approximately)

$$D = \frac{\lambda_1 \lambda_2}{\lambda_2 - \lambda_1} \approx \frac{\lambda^2}{\Delta\lambda} \quad (1.42)$$

which means that a number of wavelengths given by $\lambda/\Delta\lambda$ is contained between successive zeros of the modulation envelope.

With this basic knowledge of waves we can now return to the discussion of the single slit diffraction pattern.

1.5.2.7 The Huygens-Fresnel Principle

Suppose that a disturbance occurs at some point in a tank of water - a small object is dropped into the water, for example, or the surface is touched with a pencil point. Then an expanding circular wave pulse is created. Clearly, the pulse expands at some well-defined speed v . If the pulse is created at the origin at $t = 0$, then particles of the medium (water) at a distance r from the origin are set in motion at $t = r/v$. It was Huygens' view that the effects occurring at $r + \Delta r$ at time $t + \Delta r/v$ were directly caused by the agitation of the medium at r at time t (cause and effect), thus treating the disturbance very explicitly as something handed on from point to adjacent point through the medium. This picture of things was probably suggested by the observed behavior of ripples on water. In particular, if wave traveling outward from a source encounter a barrier with only a tiny aperture in it (tiny meaning a width small compared to the wavelength), then this aperture appears to act just like a *new point source*, from which circular wave spread out as shown in Figures 1.23 and 1.24 below.

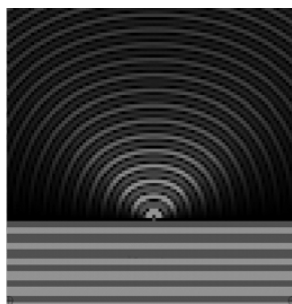


Figure 1.23: Theoretical simulation



Figure 1.24: Experimental water wave

1.5.2.8 Double-Slit Interference using Huygens Principle

We now consider what happens when an advancing wavefront is obstructed by barriers. From the standpoint of Huygens' principle, each unobstructed point on the original wavefront acts as a new source and the disturbance beyond the barrier is the superposition(sum) of all the waves spreading out from these secondary sources.

For a traveling circular(spherical) wave (not one-dimensional as we have been discussing) starting out from $r = 0$ at $t = 0$, we have the form

$$y(r, t) = A \cos \left(\frac{2\pi}{\lambda} (r - vt) + \beta \right) = A \cos (\omega(t - r/v) - \beta) \quad (1.43)$$

The quantity $\frac{2\pi}{\lambda} (r - vt) + \beta$ is called the **phase** of the wave and β is the initial phase or the value of the phase at $r = 0$ and $t = 0$. Because all of the secondary sources are derived from the same original wave, there is a well-defined relation between their initial phases. This says that all the sources, primary and secondary, are **in phase** or are **coherent**. If this were not true, they would be **incoherent**.

This condition of **coherence** implies, in turn, a definite phase relation among the secondary disturbances as they arrive at some distance point beyond the barrier. As a result there exists a characteristic interference pattern in the region on the far side of the barrier that does not fluctuate in appearance.

The simplest situation, and one that is basic to the analysis of all others, is to have the original wave completely obstructed except at two arbitrarily narrow apertures.

In this two-dimensional system, the two slits act as new point sources as shown in Figure 1.25 below.

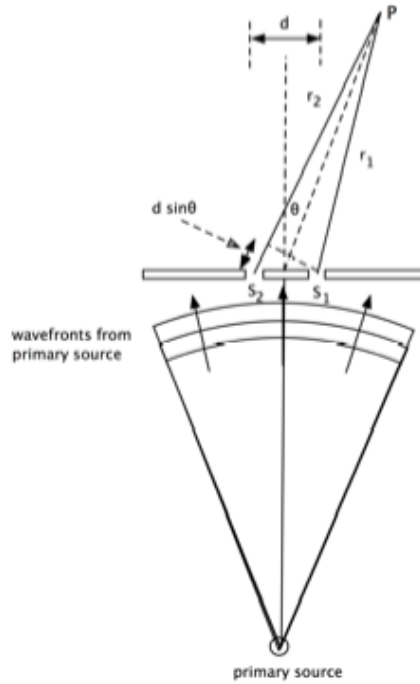


Figure 1.25: Spherical wave interacting with two slits and generating a pattern

In the figure above we indicate a wavefront approaching two slits S_1 and S_2 , which are assumed to be very narrow (but identical).

For simplicity we assume that the slits are the same distance from some point source which acts as the primary source of the wave. Thus, the secondary sources are completely in phase with each other, that is, the phase $\omega(t - r/v)$ is the same for the primary wavefront when it arrives at both slits and thus for for each new source (we choose $\beta = 0$ for simplicity).

If the original source generates sinusoidal waves, then the secondary sources also generate sinusoidal waves.

At an arbitrary point P , the disturbance is obtained by adding together the contributions arriving at a given instant from S_1 and S_2 . In general we need to consider two characteristic effects:

1. The disturbances arriving at P from S_1 and S_2 , are different in amplitude (value of A) for two reasons. First, the distances r_1 and r_2 are different, and the amplitude generated by an expanding disturbance falls off with increasing distance from the source (like $1/r$). Second, the angles θ_1 and θ_2 are different and this also affects the amplitudes.

We will concentrate on situations for which the distances r_1 and r_2 are very large compared to the separation between the slits d . In these situations, the differences between the amplitudes from the two slits at P is negligible and we ignore the difference.

2. There is a phase difference between the disturbances at P corresponding to the different amounts of time it takes each wave to arrive at P . The time difference is $(r_2 - r_1)/v$ where v is the wave speed.

It is this phase difference which dominates the general appearance of the resultant interference pattern. Ripple tank examples for two and three slits are shown in Figure 1.26 and Figure 1.27 below.

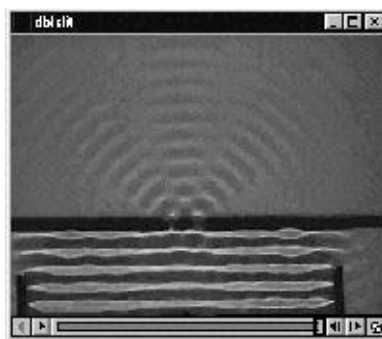


Figure 1.26: Two slit pattern - water waves

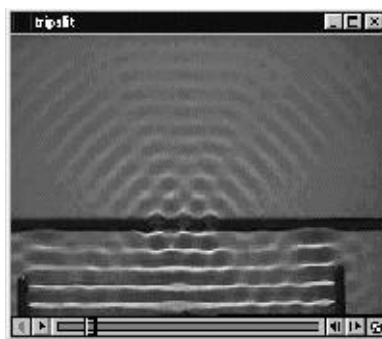


Figure 1.27: Three slit pattern - water waves

Clearly there exist *nodal* lines along which the resultant disturbance is almost zero (called **destructive interference**) at all times. It is easy to calculate their positions. At any point P , the disturbance (displacement) as a function of time is of the form

$$y_P(t) = A_1 \cos(\omega(t - r_1/v)) + A_2 \cos(\omega(t - r_2/v)) \quad (1.44)$$

This equation embodies the fact that a given sequence of displacements at each source gives rise, at a time r/v later, to a similar sequence at a point a distance r away. Thus, if we put $A_1 \approx A_2 = A_0$, we then have

$$\begin{aligned} y_P(t) &= A_0 [\cos(\omega(t - r_1/v)) + \cos(\omega(t - r_2/v))] \\ &= 2A_0 \cos \omega t \cos \left[\frac{\omega}{2v}(r_2 - r_1) \right] \end{aligned} \quad (1.45)$$

Introducing the wavelength $\lambda = v/f = 2\pi f/\omega$ we have

$$y_P(t) = 2A_0 \cos \omega t \cos \left[\frac{\pi(r_2 - r_1)}{\lambda} \right] \quad (1.46)$$

A given nodal line is defined by the condition $y_P(t) = 0$ or that the quantity

$$\frac{\pi(r_2 - r_1)}{\lambda} = (2n + 1)\frac{\pi}{2} \rightarrow r_2 - r_1 = (n + 1/2)\lambda \quad (\text{nodal lines}) \quad (1.47)$$

where n is any integer. Between the nodal lines there is another set of lines of *maximum* displacement, where the resultant disturbance reaches its greatest value (called **constructive interference**). In the same way as for minima, it is easy to see that the condition for this to occur is

$$r_2 - r_1 = n\lambda \quad (\text{interference maxima}) \quad (1.48)$$

The important parameter that governs the general appearance of the interference pattern is the dimensionless ratio of the slit separation d to the wavelength λ . This fact is manifested in its simplest form if we consider the conditions at a large distance from the slits, that is, $r \gg d$. Then, the value of $r_2 - r_1$ can be set equal to $d \sin \theta$ (see Figure 1.25 above) with negligible error. Therefore, the condition for interference maxima becomes

$$d \sin \theta_n = n\lambda \rightarrow \sin \theta_n = \frac{n\lambda}{d} \quad (1.49)$$

and the amplitude at some arbitrary direction is given by

$$A(\theta) = 2A_0 \cos \left(\frac{\pi d \sin \theta}{\lambda} \right) \quad (1.50)$$

We then see that the interference at a large distance from the slits is essentially a directional effect, that is, if the positions of the nodes and the interference maxima are observed along a line parallel to the line joining the two slits (we put a screen out there), the *linear separation* of adjacent maxima (or zeroes) increase in proportion to the distance D from the slits ($\sin \theta \approx x/D$).

If we now turn to the schematic for the double slit setup shown in Figure 1.28 below

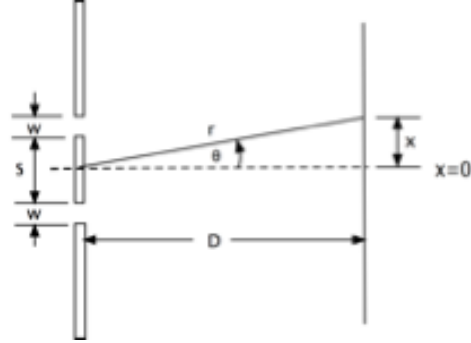


Figure 1.28: Two slit schematic

then, in this case, the detector or screen shows an interference pattern like the one in Figure 1.29 below ($s \gg \lambda$)

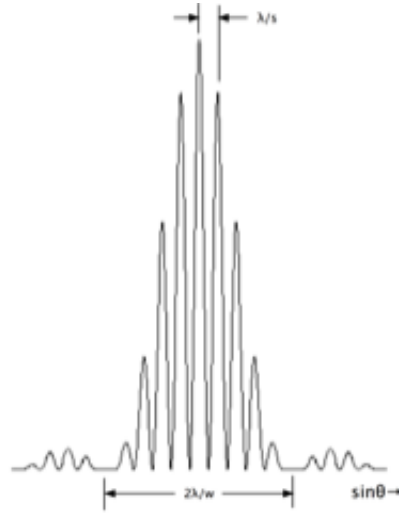


Figure 1.29: Screen interference pattern

The separation between maxima is

$$\sin \theta = \frac{\lambda}{s} \rightarrow x = D \sin \theta = \frac{D\lambda}{s} \left(\text{or } \frac{D\lambda}{d} \right) \quad (1.51)$$

The pattern above does not assume the slit width w is zero. The equation for this pattern (without any derivation) is

$$I_{double}(\theta) = 4I_0 \left[\frac{\sin \left(\pi \frac{w \sin \theta}{\lambda} \right)}{\pi \frac{w \sin \theta}{\lambda}} \right]^2 \cos^2 \left(\pi \frac{s \sin \theta}{\lambda} \right) \quad (1.52)$$

where $I_0 = A_0^2$. The intensity wiggles are shown in Figure 1.30 below where they are modulated by the single-slit pattern

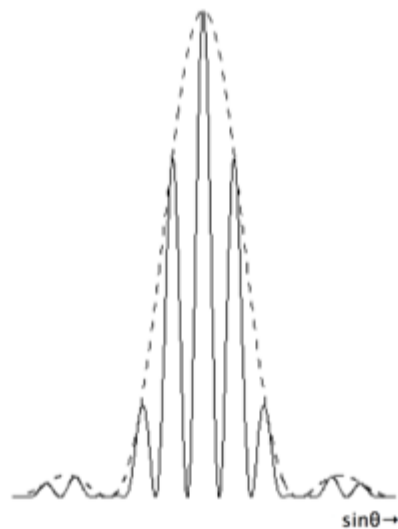


Figure 1.30: Theoretical prediction

A real picture of this result is shown in Figure 1.31 below

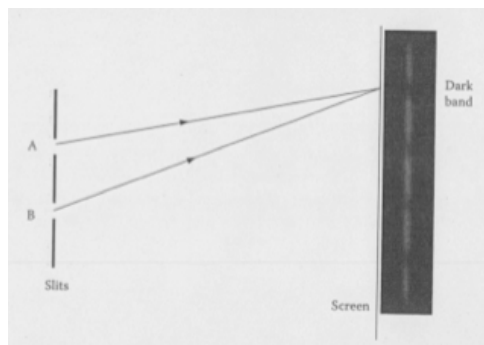


Figure 1.31: Actual experimental data

You might think that the same effect could be achieved by firing two lasers (why bother with the slits?). Unfortunately, this doesn't work. As the lasers are independent light sources, there is no guarantee that the phases of the waves from each laser start out in a fixed pattern. The path difference still produces a phase difference at the screen, but whether this is constructive or destructive depends on how the waves started out, which could vary from one moment to the next. All you would get is a rapidly and randomly shifting pattern, which just looks like featureless illumination on the screen. A single laser beam covering both

slits will split into two parts with the same phase as the light passes through the slits.

It is worth emphasizing this aspect of the experiment: the effect can only be made to work when waves from a single source pass through both slits at the same time.

Thus, we have shown that the double-slit interference pattern can be completely explained using Maxwell's electromagnetic wave theory.

But wait! According to Einstein, a light beam consists of *photons* and therefore transports energy in *spatially-localized clumps* with particle-like properties. But no model based on particle dynamics can explain interference or diffraction. The implications of the double-slit experiments appear to contradict Einstein's theory of light.

Yet a model based purely on classical wave theory is also inadequate for it cannot explain phenomena such as the photoelectric effect and x-ray (Compton) scattering. These experiments support a model in which light interacts with other subatomic particles (for example electrons) according to the laws of classical particle dynamics.

Is there direct evidence of particle-like photons? Some modern developments say yes!

1.5.2.9 Lasers and Video Cameras

In the 20th century, the study of light has been revolutionized by the development of the **laser**. Lasers produce a precisely controlled beam that is very narrow, straight, and made of light that is all the same color and is coherent.

Another remarkable technological development has been the **CCD camera**. CCD stands for charge-coupled device. They are very sensitive detectors of light, which convert the light falling on them into electrical signals that can be stored in the memory of a computer.

From our point of view, it is the combination of the laser's ability to produce controlled beams of light and the CCD's ability to detect very faint amounts of light that is crucial. This enables us to carry out experiments similar to Young's basic design, but in ways that he could not have imagined. The results of these new experiments are so radical that they will call into question everything in classical physics.

1.5.2.10 Particle-like Photons

A very simple experiment would be to point a laser beam directly at a CCD detector (just *detectors* from now on) as shown in Figure 1.32 below and see what happens. We assume that the output of the detector is transferred to a computer and displayed graphically on its screen.

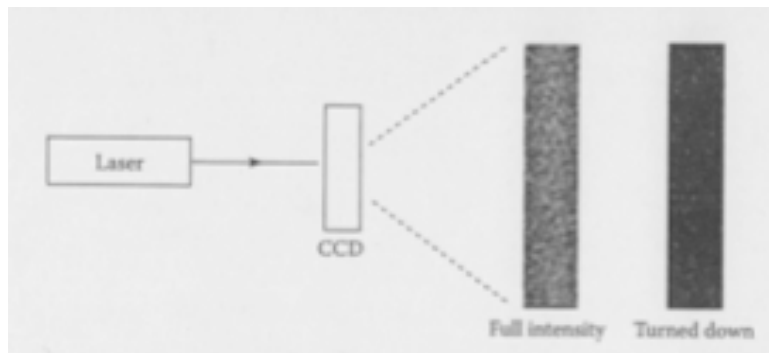


Figure 1.32: Laser directed at a CCD detector

The detector registers the arrival of energy. At moderate intensities, the light energy seems to spread equally over the sensitive surface of the detector. However, as we reduce the intensity of the beam, the image on the screen starts to break up into a sequence of tiny speckles as shown above.

Rather than the light energy being uniformly spread over the detector, it seems to be arriving in localized lumps. Reducing the intensity further makes the speckles appear less frequently, and consequently they seem to be scattered randomly across the screen. With a suitable laser source, the intensity of the beam can be reduced to the point at which only a single speckle occurs at any one time with a notable interval between it and the next one.

A natural way of interpreting these results, aside from thinking that the detector is broken, would be to suggest that the light is a stream of particles. When a particle strikes the detector, it deposits its energy and produces a single speckle on the screen. At high intensities there are millions of particles, all of them arriving within small intervals of time, and the detector records a uniform illumination. These particles have been given the name **photons**.

1.5.2.11 Now electrons as waves.....

Maybe we can resolve this puzzle by performing the double-slit experiment using a beam of *particles* - say, electrons. The behavior of these particles in the experiment should differ strikingly from that of light. This was a good idea, but as we will now see, the experiment deepens rather than solves the mystery (as often happens in physics).

1.5.2.12 Double Trouble

Our strategy in this new double-slit experiment is to send electrons through a *double-slit* and see how the intensity measured by the detector differs from the interference pattern formed by light. To implement this strategy, we must make a few modifications in the apparatus used to perform the experiment with light.

First, we replace the light source with an electron gun - a device that produces a (nearly monoenergetic) beam of electrons of energy E . A heated tungsten wire, for example, produces a stream of electrons which we can form into a beam (collimate) and accelerate to any desired speed. Second, we replace the photographic plate with an electron detector - a device that counts the number of electrons that arrive in each square meter per unit area per sec. Like the photographic plate, this detector measures the rate at which energy arrives at each point on the detector. A screen covered with a phosphor will do - when an electron arrives on the screen, it produces a bright spot (we can take pictures of the screen as time progresses).

What would we expect to see at the detector if the electrons were particles, subject to the same physical laws as, say, marbles or bowling balls? Imagine for a moment, that we block one slit so that all the electrons must come through the other, open slit. Most electrons that make it through will go straight through this slit, *piling up* at the detector directly opposite it. We therefore expect to see a maximum in the measured intensity opposite the open slit. But some particles will scatter from the edges of the slit, so we expect some amount of spread in the pattern. A reasonable guess for the intensity of a beam of particles passing through the apparatus with only one (or the other) slit open is one of the two curves $I_u(\theta)$ or $I_l(\theta)$ as shown in Figure 1.33 below each of which has a maximum directly behind one slit. Note that there is no position on the screen where no particles appear in either case.

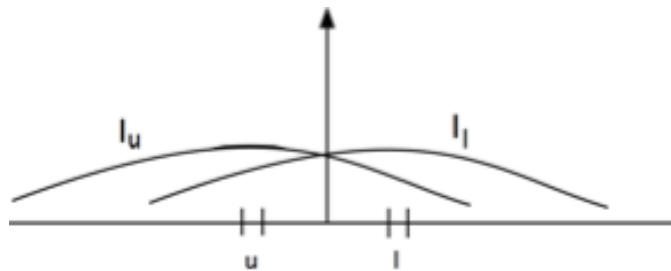


Figure 1.33: Guess for single slit patterns for particles

What *should* happen when both slits are open? Well, if the electrons are indeed particles, then the measured intensity should simply be $I_u(\theta) + I_l(\theta)$. This rather featureless curve is shown in Figure 1.34 below.

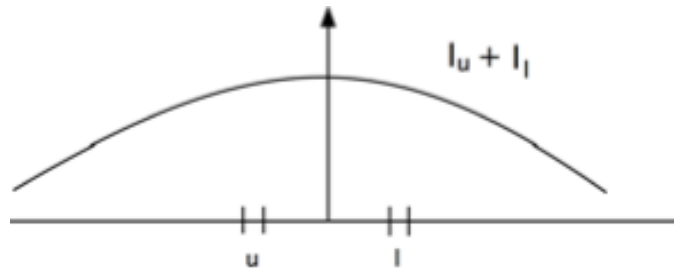


Figure 1.34: Expected particle intensity with both slits open

If you were to scale the apparatus to macroscopic size and send through a uniform beam of marbles - with, of course, a suitable detector - this is exactly what you see in an experiment.

But what we *actually* see when the experiment is run with electrons is altogether different.

The actual modern experimental electron diffraction apparatus setup is shown below (Hitachi Labs). This is a modern-day version of the original Davisson and Germer experiments in 1920 where electrons were sent through a crystal lattice (set of parallel planes of atoms acting like slits).

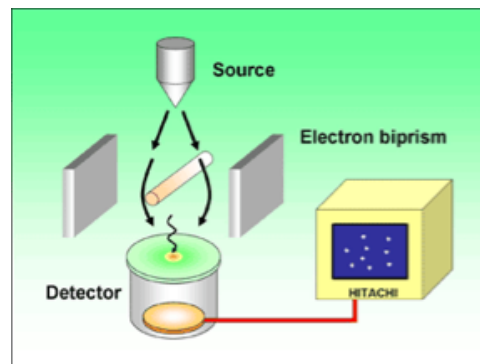


Figure 1.35: Hitachi experiment

The experiment was carried out in 1989 in Tokyo by Tonomura et al at the Hitachi Advanced Research Lab. In the experimental set-up, electrons are generated on a hot wire with a well determined energy (velocity) and then a beam is created using electrostatic lenses. The monoenergetic (single wavelength) electron beam is then sent through an electron biprism to simulate a double slit geometry. A schematic of the biprism based electron diffraction apparatus is shown in Figure 1.36 below:

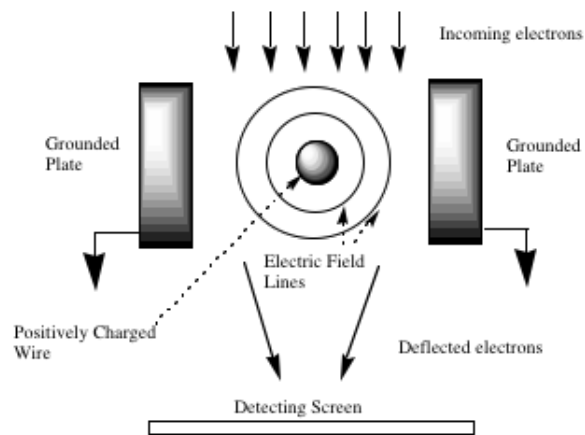


Figure 1.36: Schematic diagram of double-slit part of the apparatus

The experimental results are shown below in Figure 1.37 (sequence of images made at different times during the experiment).

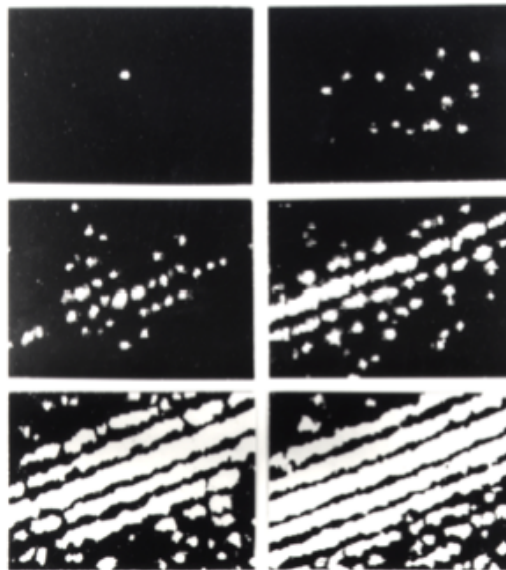


Figure 1.37: Experimental data

The measured intensities clearly exhibit bands of alternating high and low intensity - an interference pattern, like the one formed by light. This experiment seems to imply that the electrons are *diffracted* by the slits and then interfere in the region between the slits and the detector. If one fits the measured intensity of the scattered electrons to the double-slit intensity formula we get a perfect fit if we assign to each electron (of mass m and energy E) a wavelength given by

$$\lambda = \frac{h}{\sqrt{2mE}} = \frac{h}{p} \quad (1.53)$$

To a classical physicist, steeped in the idea that electrons are particles, this equation is nonsense!

Another set (over time) of experimental results is shown in Figure 1.38 below.

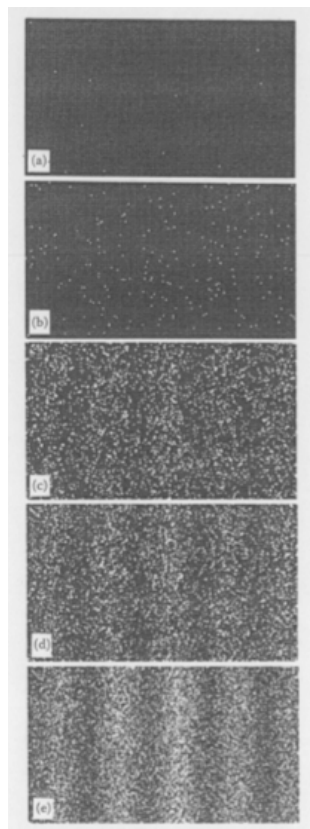


Figure 1.38: More dramatic experimental data

These images from the electron double-slit experiment performed by the Hitachi team show successive instants in time. Numbers of electrons are (a) 10, (b) 200, (c) 600, (d) 40,000, (e) 140,000.

From (a) and (b), you can clearly see the individual dots produced by the arrival of a single electron at the detector. Such dots reinforce our impression that electrons are simply lumps of matter travelling through space like marbles thrown across a room. If all we had to look at were (a) and (b), we would have no problem interpreting these results. A single electron produced by the source travels to the screen. If it happens to hit the screen, it will be absorbed and that is it. If the electron is lucky enough to arrive at one of the slits, it can pass through and enjoy life a little longer until it smacks into the detector, producing a spot of light.

However, we can't just ignore (c), (d), and (e) from the pattern sequence. As more and more electrons arrive, it becomes clear that there are some parts of the detector that just don't see any electrons and parts where lots of them arrive. The resulting pattern looks just like the interference bands produced from the laser light. Yet, and this is important, each electron arrives and makes a single dot somewhere in the pattern.

These are truly amazing pictures when one remembers these are electrons that are producing the patterns! Note that there are regions in the data sets where no electrons arrive on the screen!

1.5.2.13 Maybe they are waves?

At first, the results of the electron double-slit experiment seem consistent with the (deviant) notion that electrons are waves, not particles. This is a quite radical idea - a wealth of experimental evidence to the contrary exists. Early experiments on electrons such as Thomson's measurements of the charge to mass ratio e/m , Millikan's 1917 measurement of the electron charge e , and Rutherford's 1911 scattering experiments, strongly support the **model** of the electron as a discrete, indivisible unit of electric charge - not a wave.

If we investigate these new experiments further, however, we discover a problem with a wave hypothesis.

Suppose we turn down the intensity of the *incident* electron beam so that *very few electrons per second pass through the slit*. Were electrons waves, the interference pattern that forms at the detector after a few seconds would be weak (but it would still be the full interference pattern). As time passes and more and more electrons are scattered by the double-slit, this pattern would intensify, ultimately looking like the last frame in the two above pictures.

But this is not what happens.

As can be seen in the frame sequences above, shortly after we switch on the electron gun, we see at the detector not a (weak) diffraction pattern, but *spots* - just what we would expect to see if the electrons were particles! This result is incompatible with the notion that electrons are waves since waves transport energy via non-localized wave fronts, not concentrated lumps. Only concentrated lumps of energy can produce spots! You can see similar behavior - spots at the detector - if we perform the experiment with light at low enough intensity that only a few photons per second arrive at the photographic plate.

Curiously, the spots initially show no particular pattern, neither *interference* or *plain bumps*. It looks like electrons are particles that arrive **randomly**.

But they are not! With the passage of time, the electrons begin to form the interference pattern. The frame sequences show this pattern forming as if by magic. These pictures are eerie - it is as though each electron knows precisely where it should contribute to the interference pattern. This gives rise to the question: **If the electrons are particles, what guides them to just the right place on the detector?** Remember, if they are all classical particles with the same initial conditions, then they should all be doing the same thing - following the same path of motion. They do not!

We can summarize our observations in this way:

When an electron arrives at the detector, its interaction with the material of the detector produces a spot, a spatially-localized point - behavior we associate with a classical particle.

Yet, when a number of electrons propagate from the slit to the detector, they somehow form a distinctive interference pattern - behavior we associate with classical waves. Perhaps strangest of all, **this pattern appears only after sufficient time has elapsed that a statistically significant number of electrons has arrived at the detector.**

Saying this again

If we interpret the individual dots on the screen as evidence that electrons are little lumps of matter (we call them particles), then we also have to face the paradox that the interference pattern produced by the dots seems to show that they're waves.

The notion that the pattern of dots is a genuine interference effect can be confirmed by blocking off one of the slits. In this case, the bands disappear: you simply get a distribution of dots opposite the open slit, just what one might expect from particles flying through the gap.

What makes things so mysterious is that the experiment was very carefully set

up to allow only one electron through at a time. Yet each electron, from the very first onward, seems to have *knowledge* of the final interference pattern. They never arrive at the center of one of the dark bands. This eliminates any notion that the bands are due to pairs of electrons influencing each other as each of them pass through one of the slits. It's hard to avoid an interpretation that has the electrons moving through the equipment as a wave (hence passing through both slits at the same time, resulting in an interference pattern), but arriving at the detector as a particle.

We note the experimental indication that individual electrons *understand* the whole interference pattern will be the most direct challenge to any interpretation that regards quantum states as referring to collections of objects and not individuals as we will discuss later.

This is a situation worthy of Gilbert and Sullivan. In the same apparatus, we can see electrons behaving like waves or like particles, depending on how long we let the experiment run. The short-term behavior of the electrons is incompatible with the *wave model*, but their long-term behavior is incompatible with the *particle model*.

So what are they? (Is this even the correct question to be asking?)

In these experiments, we might say that we are seeing light or electrons appearing to behave as **both** a wave and particle in the same experiment or maybe we are just **misinterpreting** the whole thing!

Maybe it has nothing to do with particles and waves which are classical ideas and is the result of something totally new happening.

We must keep our *minds open* when we are investigating new physics.

Remember, that when we say that a physical object can be both a particle and a wave we are *mixing* two very, very different classical attributes.

1. A wave can spread out over an enormous area
2. Particles are confined to small regions (they are localized)
3. A wave is easily split into parts going in all directions (beam splitters)
4. Particles cannot be split up.
5. Two waves can overlap in space and time and emerge unchanged
6. Particles collide if they attempt to occupy the same point in space and time

But experiment seems to say that objects can be *both* at the same time!

If this is bothersome, remember that this statement may make no sense...it may simply be our last **desperate attempt** to maintain classical descriptions as we proceed to find classical physics does not work.

We will soon have to discard this way of doing things. We will have to find totally new ways of describing the world if we are going to have any chance of understanding it.

1.5.2.14 The Mystery Deepens

Whatever theory we dream up to make sense of these observations must preserve the spatially-localized property of electrons and yet explain the pattern formed when many electrons arrive at the detector. Let us try the hypothesis that an electron is a new kind of particle, one that somehow propagates according to wave dynamics. This hypothesis, at least, would let us explain the observed pattern as due to the interference of two electrons, one from the upper slit and one from the lower slit. To test this idea, we devise another variation on the double-slit experiment.

If this *model* of the electron is correct, we should be able to get rid of the interference pattern by turning the incident beam density *so low that only one electron goes through the slits at a time*. A single electron, after all, has nothing to interfere with. But the results of the experiment are not what we expect. *Even at the lowest possible incident density, an interference pattern forms (eventually)*. Any such *model* implicitly assumes that the electron has a trajectory, that is, that each electron goes through one slit or the other. Yet, in this experiment each electron acts as though it were interfering with itself (whatever that statement might mean). Such results force us to accept that in no sense can an electron be thought of as a classical particle or a classical wave.

The double-slit experiment beautifully illustrates one of the central mysteries of quantum physics: the **dual nature** of microscopic entities.

I believe that the difficulties many people have understanding the results of this experiment arise because we are hidebound by our classical training and intuition. We persist in trying to force electrons and photons to fit *either* the classical particle model *or* the classical wave model. It is perhaps unfortunate that electrons behave *like* classical particles in some experiments and *like* waves in others, for this behavior can seduce us into thinking that there must be some way to retain one of these classical models. But there is not; *neither* model by itself is correct, for *neither* model conforms to the observed behavior of electrons. **To explain the double-slit results we will need a completely new theory. We will need to rethink all of our ideas about the physical world. We will need to learn a new language to understand this new world!**

1.5.2.15 More Trouble with Trajectories

We argued earlier that the very idea of ascribing a trajectory to a microscopic particle is rendered nonsensical by the Heisenberg Uncertainty Principle - on the grounds that if we cannot know precisely a particle's position and momentum at any time, then we cannot even define its trajectory. The implications of this argument are far-reaching: it requires us to jettison the entire machinery of Newtonian physics! The double-slit experiment provides further insight into this problem by showing us how misleading is the idea that microscopic particles follow paths in geometrical space.

If the incident electrons did follow paths through the slits to the detector, then each would have to pass through *either* the upper slit *or* the lower slit. Yet, the results of the double-slit experiment imply that the electrons *seem to go through both slits*, for an interference pattern forms at the detector even if the incident intensity is so low that electrons traverse the region from source to detector one at a time. But interference is understood (in classical physics) as arising from the superposition of two (or more) waves, and such an explanation is inconsistent with the notion that electrons follow classical paths.

1.5.2.16 Aside: Failed Attempts to Trick the Electrons

You may be wondering if the issue of whether trajectories can be ascribed to electrons could be settled by a variation on this experiment - one would *trick* the electrons into revealing which slit they went through. Suppose, for example, that we put an electron detector immediately behind each slit. By seeing which detector registers, we could determine once and for all which slit each electron went through.

This gambit works! If we carry out such an experiment, we find that one or the other device (not both!) registers for each electron that arrives at the detector. But after many electrons have undergone the journey through the slits, if we look for an interference pattern at the detector we do not find one. Instead, we find that the measured intensity forms the *hump* pattern characteristic of particles. So this experiment in no way explains the wave-like behavior of the propagation of electrons in the original apparatus, for in this experiment the behavior of the electrons is consistently particle-like.

What went wrong was that we interfered with the electrons. By measuring the position immediately behind the slits, we altered the state of the incident electrons, changing their subsequent behavior and therefore the pattern they form in the detector. In particular, our observation of which slit the electrons went through imparted momentum to them. This transfer of momentum destroyed the interference pattern (we will work out the details of this later). This experiment illustrates the interaction between observer and the observed that we discussed earlier: a measurement on a microscopic system inevitably alters the

state in an uncontrollable way.

The Heisenberg Uncertainty Principle affords some insight into this interaction. To be sure which slit the electrons pass through, we must measure position (just behind the slits) accurately to within an uncertainty Δx that is less than the spacing between the slits. But since the uncertainty product $\Delta x \Delta p_x$ must be positive, a non-zero position uncertainty implies a non-zero momentum uncertainty. A detailed quantitative analysis (as we will see) along these lines reveals that the resulting Δp_x is just large enough to wash out the interference pattern at the detector (just large enough to make the phase of the waves involved uncertain enough to wash out the interference).

Duality characterizes the whole range of quantum particles: protons, neutrons, atoms, molecules, etc. Invariably, microscopic entities seem to propagate according to wave dynamics but to interact with each other according to particle dynamics. **Or maybe we are thinking about the whole thing in the wrong way!**

A significant step on the road to understanding this duality was taken in 1923 by Prince Louis Victor Pierre Raymond de Broglie.

1.5.2.17 Wave Nature of Electrons

The idea that particles might display some wavelike properties dates back to the mid-1920s. About then, Louis de Broglie was thinking about the apparent dual wave and particle nature of light. Working on the lines of *what's sauce for the goose is sauce for the gander*, de Broglie felt that, in the right conditions, electrons might show some wavelike properties. In his Ph.D thesis, he proposed a couple of formulas to link the wavelength and frequency of **electrons waves** to the more familiar energy and momentum of a particle:

$$\lambda = \frac{h}{p} \quad , \quad f = \frac{E}{h} \quad (1.54)$$

where λ is the wavelength of the *electron wave*; p is the magnitude of the electron's momentum; f the frequency of the *electron wave*; E the energy of the electron; and h a quantitative constant, which had already been introduced into physics by Max Planck in 1900.

The de Broglie formulas catch the weirdness of wave/particle duality in a very striking manner. Momentum and energy are *particle-like* ideas; frequency and wavelength belong to conversations about *waves*.

de Broglie's formulas link these ideas together; they show us how the particle is related to the wave. At least they do this in a mathematical way; nothing that de Broglie has done gives us an idea of how to *picture* this if any such picture is possible!. We are still left struggling to see how the same object can appear like

a wave at one moment and a particle the next. We note that de Broglie's notion of an *electron wave* would soon be abandoned in favor of something called *amplitudes*.

Returning to the double-slit experiment, it's easy to show that the gap between bright and dark bands in an interference pattern is directly related to the wavelength of the wave. An approximate formula (derived earlier) that produces very good results near the center of the pattern is

$$\text{wavelength} = \frac{(\text{distance between bands}) \times (\text{distance between slits})}{\text{distance from screen to detector}}$$

In their experiment, the Hitachi team produced electrons from an electron gun, similar to that used in a Stern-Gerlach experiment. They used 50,000 *Volts* to accelerate the electrons to a speed of 120,000 *km/s* ($0.4c$) giving them a wavelength of about $6.1 \times 10^{-12} m$.

1.5.2.18 More details concerning the ideas of de Broglie

The experiments we have been discussing raise a host of questions. If electromagnetic radiation consists of photons - localized lumps of energy - how can we explain phenomenon such as diffraction and interference? If not, why did Compton have to use classical collision theory to explain the scattering of x-rays by metals? On the other hand, if electrons are particles, why do they produce an interference pattern at the detector in the double-slit experiment? The behavior of electrons and photons in these experiments seems provocatively similar - crazy, to be sure, but crazy in the same way. Are electrons and photons in some sense the same?

Einstein was deeply puzzled by this question until he noticed a possible answer in the doctoral thesis of a young French physicist. In 1924, Einstein wrote in a letter to his Dutch colleague Hendrik Lorentz that the research of Prince Louis de Broglie "*... is the first feeble ray of light to illuminate this, the worst of our physical riddles*". de Broglie's achievement was to synthesize the wave-like and particle-like aspects of microscopic matter. Although de Broglie seems to have only dimly understood the nature of quantum particles and his rather nebulous physical models of quanta have since been superseded, the importance of his contribution has not diminished. It initiated the development of modern quantum mechanics.

1.5.2.19 Sometimes a Great Notion

In 1910, de Broglie began studying history at the University of Paris; soon, however, he switched to physics. His studies were interrupted in 1913 by a six-year stint in the French army, during which he and his brother Maurice worked on wireless telegraphy. Then in 1919 he returned to Paris for his doctoral research.

From his work on the x-ray spectra of heavy elements, de Broglie knew of photons and the Bohr model of atomic structure. And he was particularly intrigued by *Planck's mysterious quanta*. So he set himself the task of *uniting the corpuscular and undulatory points of view and thus penetrating a bit into the real nature of quanta*.

In 1923, lightning struck. As de Broglie tells it:
As in my conversations with my brother we always arrived at the conclusion that in the case of x-rays one had both waves and corpuscles, thus suddenly - I cannot give the exact date when it happened, but it was certainly in the course of summer 1923 - I got the idea that one had to extend this duality to material particles, especially to electrons.

Thus, did de Broglie come up with the idea of **matter waves**. This idea led him to the important notion that **all microscopic material particles are characterized by a wavelength and a frequency, just like photons**.

Aesthetic considerations seem to have influenced de Broglie's thinking towards the idea of matter waves. He evidently felt that nature should be symmetrical (now everyone knows that this is a valid way to think - he was so far ahead of his time!), so if *particles of light* (photons) were to be associated with electromagnetic radiation, then so should *waves of matter* be associated with electrons. Simply stated, his hypothesis is this: **There is associated with the motion of every material particle a "fictitious wave" that somehow guides the motion of its quantum of energy**.

In spite of its rather vague character, this idea was remarkably successful. For example, using the methods of classical optics (such as Fermat's principle of least time) to describe the propagation of quanta, de Broglie was able to explain how photons (and, for that matter, electrons) diffract and interfere: It is not the particles themselves but rather their *guide waves* that diffract and interfere. In de Broglie's words, "*the fundamental bond which unites the two great principles of geometrical optics and of dynamics is thus fully brought to light*".

de Broglie put forth these ideas in his Ph.D dissertation, which he wrote at age 31. His thesis did not fully convince his examiners, who were impressed but skeptical of the physical reality of de Broglie's matter waves. One examiner later wrote, "at the time of the defense of the thesis, I did not believe in the physical reality of the waves associated with the particles of matter. Rather, I regarded them as very interesting objects of imagination". Nevertheless, de Broglie passed.

It is not clear that de Broglie himself knew what he meant by matter waves. In his thesis he notes that "the definitions of the phase wave and of periodic

phenomenon were purposely left somewhat vague". In subsequent papers, de Broglie tried several different interpretations of his elusive waves.

1.5.2.20 Beautiful Equations

de Broglie's equations for the wavelength and frequency of his matter waves are elegant and simple. Even their derivations are not complicated. In his seminal paper of 1923, de Broglie began with light quanta - photons - so let us discuss the equations governing the wavelength and momentum of a photon and then extend that to material particles.

The photon is a relativistic particle of zero rest mass, $m_0 = 0$. Hence the momentum p of a photon is related to its total energy E through the speed of light by

$$p = \frac{E}{c} \quad (1.55)$$

To introduce the frequency f of a photon, we use Einstein's equation for the photon energy

$$E = hf \quad (1.56)$$

so that

$$p = \frac{hf}{c} \quad (1.57)$$

For a wave in free space, the wavelength is $\lambda = c/f$ so that we have

$$p = \frac{h}{\lambda} \quad (1.58)$$

Now, in contrast to a photon, a material particle such as an electron has a non-zero rest mass $m_0 \neq 0$. Therefore the relationship between the energy and momentum of such a particle moving at relativistic velocities (in a region of zero potential energy) is given (from relativity) by

$$E^2 = p^2c^2 + m_0^2c^4 \quad (1.59)$$

and its kinetic energy is simply

$$K = E - m_0c^2 = \sqrt{p^2c^2 + m_0^2c^4} - m_0c^2 \quad (1.60)$$

If the velocity of the particle is non-relativistic ($v \ll c$), then its kinetic energy is simply

$$K = \frac{p^2}{2m_0} = \frac{1}{2}m_0v^2 \quad (1.61)$$

as we mentioned earlier. In either form, the simple photon derivation cannot be applied to a material particle.

Nonetheless, de Broglie proposed that we use the photon results for material

particles also. Thus, for electrons, atoms, photons and all other quantum particles, the energy and momentum are related to the frequency and wavelength by

$$p = \frac{h}{\lambda} \quad , \quad E = hf \quad (1.62)$$

which are the de Broglie-Einstein equations we introduced earlier. Notice that the de Broglie equation $\lambda = h/p$ implies an inverse relationship between the total energy E of a particle and its wavelength

$$\lambda = \frac{hc/E}{\sqrt{1 - \left(\frac{m_0 c^2}{E}\right)^2}} \quad (1.63)$$

If applied to a photon (by setting the rest mass to zero) this equation reduces to the earlier result. Hence, the larger the energy of a particle, the smaller the wavelength and vice versa.

The Unanswered Question

de Broglie's notion that some sort of wave guides the motion of every quantum enabled him to explain a variety of hitherto inexplicable phenomena, such as quantization of the orbital angular momentum of an electron in a Bohr orbit of the hydrogen atom. It also led him to suggest that the existence of matter waves could be verified by looking for electron diffraction patterns. The experiments of Davisson and Germer mentioned earlier vindicated de Broglie's ideas. Matter waves were real or so it seemed at the time.

But de Broglie's research left unanswered deep and important questions: **what is a matter wave?** Of what is λ the wavelength? How do these mysterious waves control the propagation of a microscopic particle? The answers are not to be found in de Broglie's writings.

Nonetheless, by raising such questions and focusing the attention of the physics community on the need to associate some sort of wave with microscopic material particles, de Broglie initiated the quest for a new physical theory. The quest led physicists on a tortuous path during the early 1920's that was often called the Stone Age of Quantum Mechanics.

But rather than follow this tortuous path that is full of useless dead-ends, we will jump to the successful theories of Schrödinger, Heisenberg and Dirac.

In fact, we will approach the subject from a very abstract viewpoint due to Dirac, that is, we will learn a new language - the language of quantum mechanics - and then derive the ideas and equations of the theory. At that point we will try to decide whether the idea of matter waves makes any sense.

1.5.3 The Controversial Concept of Complementarity

As for knowledge, it's the scandal of our age
that philosophy has been whittled away to a
barebones epistemology, and thence to an even
barer agnoiology.

Have I found a word you don't know?

Agnoiology is the philosophy of ignorance, a
philosophy for philosophers.

from **Camp Concentration**
by Thomas M. Disch

Seemingly, to explain the behavior of quantum particles, we must evidently use both the classical wave and particle models - in spite of the apparent contradictions between them. To say that this situation poses logical problems is to understate wildly. In the early 1920s, this predicament lay heavy on the minds of physicists, until the Danish physicist Neils Bohr proposed a way out.

1.5.3.1 Bohr to the Rescue

Bohr was one of the intellectual giants of early quantum theory. His ideas and his personality were enormously influential. During the 1920s and 1930's, the Bohr Institute in Copenhagen became a haven for scientists who were developing the new physics.

Bohr was not always receptive to quantum ideas; like many of his colleagues, he initially rejected Einstein's photons. But by 1925 the overwhelming experimental evidence that light actually has a dual nature had convinced him. So for the next several years, Bohr concentrated on the logical problem implied by the duality, which he considered the central mystery of the interpretation of quantum theory.

Unlike many of his colleagues, Bohr did not emphasize the mathematical formalism of quantum mechanics. Like de Broglie, he considered it vital to reconcile the apparently contradictory aspects of quanta. Bohr's uneasy marriage of the wave and particle models was the **Principle of Complementarity**. The principle entails two related ideas:

1. A complete description of the observed behavior of microscopic particles requires concepts and properties that are mutually exclusive.
2. The mutually exclusive aspects of quanta do not reveal themselves in the same observations.

The second point was Bohrs' answer to the apparent paradox of wave-particle duality: There is no paradox. In a given observation, *either* quanta behave like

waves or like particles - never both!

How, you may wonder, could Bohr get away with this - eliminating a paradox by claiming that it does not exist because it cannot be observed? Well, he has slipped through a logical loophole provided by the limitation of quantum physics that we mentioned earlier: **quantum mechanics describes only observed phenomena**. From this vantage point, the central question of wave-particle duality is not “*can a thing be both a wave and a particle?*” Rather, the question is “*can a thing be both a particle and a wave in the same measurement?*” Bohr’s answer is no: in a given observation quantum particles exhibit *either* wave-like behavior (if we observe their propagation) *or* particle-like behavior (if we observe their interaction with matter).

And, sure enough, no one has yet found an exception to this principle. We will have much more to say about complementarity later in this book.

Notice, that by restricting ourselves to observed phenomena, we are dodging the question, “**what is the nature of the reality behind the phenomena?**”

Many quantum physicists answer, “**there is no reality behind phenomena**”. We will try to decide this question for ourselves in this book.

1.5.3.2 Complementary Observables

Before leaving complementarity, I want to mention another aspect of this topic, one that relates it to the Heisenberg Uncertainty Principle. This principle implies a special relationship between position and momentum. The uncertainties in these observables are related by $\Delta x \Delta p \geq \hbar/2$ so if we obtain (via measurement) *precise knowledge* of either observable, we do so at the expense of *any* knowledge of the other. Bohr considered this mutual uncertainty as a *manifestation* of complementarity in the mathematical formalism of quantum mechanics.

We will have to decide in this book whether this interpretation of the uncertainty principle is correct - whether it has anything to do with individual measurements.

The relationship between position and momentum, as expressed in the Heisenberg Uncertainty Principle, differs from the complementarity relationship of the wave and particle nature of quanta: position and momentum are both *particle-like* attributes of quanta. Rather than describe position and momentum as complementary, perhaps it would be better to describe them as **incompatible**.

1.5.3.3 A Philosophical Cop-Out?

The Principle of Complementarity may seem a little vague. Indeed, that is how it struck the audience of distinguished physicists at the international confer-

ence in 1927 where Bohr first presented his ideas. These ideas are undeniably subtle, and Bohr did not always express himself clearly. Nevertheless, in spite of some initial confusion, the physicists developing and using quantum theory adopted complementarity, and today it is one of the central tenets of the so-called **Copenhagen Interpretation of Quantum Mechanics**.

The Copenhagen interpretation, which we will discuss later, has its detractors, but it is a way of making sense (more or less) of the physics of the microworld, and it remains the dominant interpretation of quantum mechanics (of course, that does not make it correct - physics is not democracy).

In spite of the wide adoption of the Principle of Complementarity, many thinkers have found it philosophically offensive, perhaps because rather than confront the problem of duality head on, Bohr's principle seems to sneak around it, taking recourse in the limitation of quantum mechanics to observed phenomena. James R. Newman has expressed the uneasiness some feel with complementarity:

In this century the professional philosophers have let the physicists get away with murder. It is a safe bet that no other group of scientists could have passed off and gained acceptance for such an extraordinary principle as complementarity.

1.6 Final Thoughts: A Few Words about Words.

I suspect that some of the difficulties people have with complementarity stem from classical thinking - from their understandable determination to cling to *classical models*. After all, the wave and particle descriptions of nature *are merely models*. There is no reason to expect them to apply to the whole physical world (a limitation of all models is their applicability to restricted sets of phenomena). The results we have been discussing tell us that in the microworld, each of these models is *part of the truth*, but each by itself is incomplete. In some cases, the *wave model* must be invoked to understand observations; in others, the *particle model*.

Electrons are not particles. They are not waves, either. They are something else, for which we neither have a name nor a classical model. Properly, we should follow de Broglie's lead and refer to them as **fragments of energy**, but that would be awkward. Or we could follow Eddington and call them **wavicles**, but that sounds silly. So we stick with **particles** and do the best we can.

But we must not overlook the influence of the language we use on how we think. In the microworld, nature transcends our familiar language and the technical

language of the classical physicist. On this point Werner Heisenberg wrote:

The problems of language are really serious.
We wish to speak in some way about the structure
of atoms... But we cannot speak about atoms in
ordinary language.

1.6.1 Quantum Mechanics, Ordinary Language and Mathematical Language

It is not possible to reduce the quantum universe to everyday ways of thinking (usually called **common sense**). In fact, in order to understand the ideas and implications of the theory we will have to adjust all of our ways of thinking at the most fundamental level.

Imagine, for a moment, that you are attempting to understand a new culture. If you are serious about it, the first thing you would do is to learn the language appropriate to that culture so that you can put your experiences in the proper context.

Understanding the universe of quantum phenomena is much like understanding a new culture where the appropriate language is mathematics and the experiences we are attempting to put into context are microscopic experiments.

We have to use a mathematical language to describe the quantum world since ordinary language, which was developed to explain everyday occurrences (experiments on macroscopic objects), will turn out to be totally inadequate. There are no *models* or *classical analogues* that will ever give us any insight into the workings of the quantum world.

Since it makes no sense to attempt any understanding of the nature of quantum phenomena without first learning to speak and use the language of the quantum world, one should spend some time very early on in learning the appropriate mathematics, in particular, the subject of linear vector spaces (we will in this book).

The adjustment of our ways of thinking at the fundamental level that will be needed is not simply a mathematical matter, however. The development of the necessary mathematical language will not come into conflict with our everyday modes of thinking in any major way. Although, the mathematics of linear vector spaces is very elegant, you will be able to understand it without much difficulty and without having your basic view of the world changed at any fundamental level.

You will be troubled, however, when you apply the mathematics to physical systems that develop according to quantum rules. You will need to attach

physical meaning to the mathematical formalism in ways that will conflict with your well-developed views (I will call these *classical views*) about how the world works.

Dirac was able to join the conceptual structure with the mathematical structure. He invented a mathematical language (I purposely do not use the word *notation*) that directly embeds the philosophy of quantum mechanics into the mathematical structure used to do calculations. The new language directly exhibits what is being said about nature in quantum mechanics. Dirac language exposes the internal logic of quantum mechanics in a way that mere words cannot possibly accomplish. It displays the sense, the physical meaning of the theory in every equation one writes without the need for further explanation or any need for inadequate models.

It is very important to understand that the Dirac language is not simply a new notation for quantum mechanics (as many physicists seem to think). It is not merely a way of writing. A way of writing expresses a way of thinking. Dirac language is a way of thinking.

It will allow us to use the physical ideas of quantum mechanics to develop the appropriate mathematical language rather than the other way around. This allows the very mathematical quantum theory to be more closely connected to experiment than any other physical theory.

Dirac language expresses the quantum mechanical way of thinking. With it one can proceed from the philosophy of the subject to its mathematical expression rather than the other way around. That is the way one should study quantum mechanics. One should proceed from meaning and Dirac language is perfectly suited to this task.

Meaning does not reside in mathematical symbols, however. It resides somehow in the thoughts surrounding these symbols. It is conveyed in words, which assign meaning to the symbols.

Dirac language is able to take notions expressed in words and replace them with simple mathematical statements that we are eventually able to place within a complete and logical structure that allows for a fundamental understanding of what quantum mechanics means and is saying about nature.

This task is impossible without mathematics. Mathematics is the true language of all of physics. Words alone only suffice for thinking about the physics of everyday objects.

These statements about the importance of understanding the mathematical language appropriate to the physics under consideration do not only apply to the quantum world. It is true, I believe, for all areas of physics and other sciences.

One should always learn the appropriate language before studying any field that relies on that language for its understanding.

So be careful. Beginning now we shall buckle down and take a serious look at the mathematical and physical structure of quantum mechanics. But tread warily, lest you slip back into the black abyss of classical thinking and consequent confusion. With this warning out of the way, we can proceed.

Chapter 2

Quantum Thoughts

How do we start our discussion of quantum physics?

Our goal is to delineate in a clear manner a theory of quantum phenomena and then determine if this theory is supported by real world experiments(which is the only test for validity that we will accept).

We will approach the problem without prejudice towards any ideas.

The goal of this discussion is for all of us to reach the point where we can understand what quantum physics is all about and how it proposes to explain the experiments that will clearly defy classical physics.

We will first present a quick overview of the ideas that will occupy our attention for most of this book. Don't worry if there are things in the overview that do not make sense, we will come back to all of them in detail later and you *will* understand them eventually.

2.1 Quick Overview:

I will note (usually with some form of emphasis) the appearance of many words when we use them during this overview so that we realize that we do not really understand their meaning at that point in our discussions even though we may think we do!

Two major facts dominate the entire quantum physics story.....

First, quantum theory works !!!!!

It is an extraordinarily accurate theory. It accurately describes (as we shall see) the microworld of atoms and beyond(smaller). It works better than any previous

physical theory. Quantum theory works from aggregates of atoms like crystals (sizes of order 10^{-1} cm) to fundamental particles (sizes of order 10^{-21} cm). This is a truly amazing range of validity - a factor of 10^{20} - that is the same as the ratio between diameter of our galaxy (10^{22} cm) and a meter stick (10^2 cm)! Its predictive capabilities are shown clearly in an experiment that measures a property of the electron called a magnetic moment

$$\begin{aligned}\text{experiment} &\rightarrow 1.0011596521 \pm 0.0000000093 \\ \text{theory} &\rightarrow 1.001159652 \pm 0.000000046\end{aligned}$$

Quantum theory is able to clearly explain the stability of atoms, quantized energy levels in atom, emission of light at definite wavelengths, chemical forces determining all molecular properties, reliability of inheritance in DNA, lasers, superconductors and superfluids, semiconductor electronics, computers and so on

Quantum mechanics(QM) is at the heart of all areas of modern advanced technology.

Second, no one fully understands quantum theory !!!!!

When we apply the theory to calculate various quantities associated with a physical system we will always get the correct (agreement with all experiments) answer. Although this is true even after 88 years of successful predictions, there is still significant argument about

- (a) the meaning of its assumptions
- (b) what happens during a measurement
- (c) how the assumptions relate to **reality** (as we shall see after we are able define it)

We will find out that all these arguments are about **interpretation**.

By this I mean that everyone, no matter how they might choose to interpret quantum theory (and they will do it in very different and sometime exceedingly strange ways), calculates the **SAME** answers for **ALL** phenomena under consideration. They **ALL** get the same answers when they make predictions!

We will spend most of our time in four areas:

1. the basic postulates
2. time evolution of quantum systems
3. measurement
4. interpretations and reality

because these represent the heart of quantum physics.

When people are doing physics or when non-physicists think about what physicists are doing, they sometimes think that physicists are

finding out the way things are

As we shall see, this is a sensible thing to say in *classical* or *pre-quantum* physics, where we are able to

relate the REAL world to our EVERYDAY experiences

which is **one way to define reality**.

Classical physics relies on the (usually unstated) assumption that an **observer**

**can know BOTH *where* an electron
(or a cow or a 747) is and *what* it is doing**

Making this statement more rigorously, we would state that a classical observer **can know the POSITION and VELOCITY of an object simultaneously**.

This statement turns out to be very nearly true. In fact, we can do it with seemingly arbitrary accuracy for cows and 747s. But it will turn out **NOT** to be true for electrons or any other objects in the microworld! As we shall see in our upcoming discussions, quantum theory will completely destroy any analogy we might try to make between electrons and cows!

Among other things, the theory will imply that **BOTH** position and velocity cannot be simultaneously known with arbitrary accuracy no matter what we do or how clever we are! Think about the implications of that statement for a second. Think about what that statement means for subsequent predictions of ordinary motion!

Now, based on the special theory of relativity, all physicists believe that no information can be propagated at speeds faster than that of light. Yet we will be faced with quantum experiments that seemingly have no other explanation (or so it seems) than the requirement that one quantum system has instantaneously influenced all other quantum systems anywhere in the universe....in what Einstein called **spooky action at a distance**.

What then is the **reality** that we will eventually associate with an electron? What will quantum theory have to say? The act of measurement (*we will have to be very, very careful about how we define measurement later on*) in quantum theory introduces inescapable **random** (need to be careful about meaning) elements into the measured system.

Consider the following situation where we have a large number of **identical** particles (systems).

Classical measurements give **EXACTLY**(within experimental uncertainty) the **SAME** value of all dynamical variables, the position, for example, for each identical particle - **that is what the classical physicist means by the word identical**. On the other hand, quantum measurements give **DIFFERENT** and **UNPREDICTABLE** values for each particle **even though we said they were identical, so I guess we are going to have to carefully define the word *identical***.

It will turn out, however, that in the quantum world I can, after making a very large number of measurements on these **identical** systems, only state a **probability** that the position will have a particular value.....that is, for the next measurement to be made of the position x , we have

$$probability(x) = \frac{\text{number of times value } x \text{ was measured}}{\text{total number of measurements}} \quad (2.1)$$

This type of statement is one that is based on the results of *all previous measurements*. The goal of quantum mechanics is to predict these probabilities before the measurements are done.

This is different than classical mechanics. In classical mechanics, we know where a particle is, but experimental uncertainty can *fuzz out* the results. In quantum mechanics, however, the only possible results are a *fuzz* of some sort!

Let us take a first look at how this probability stuff works. Consider this example. Suppose we measure the heights of Swarthmore students and we find: $N = 1300 = \text{total number of measured heights(in cm)}$ and obtain the data set

n_h	h
50	150
100	160
200	170
300	180
300	190
200	200
100	210
60	220

where n_h = number of times height h was measured. Then the probability that we will measure $h = 190 \text{ cm}$ if another student (if we missed one) walks in is

$$probability(x) = \frac{\text{number of times value 190 was measured}}{\text{total number of measurements}} = \frac{3}{13}(23\%) \quad (2.2)$$

This is a very simple and intuitive definition and it seems to work very well (it is exact in the limit of $N = \text{total number} \rightarrow \infty$, **which we cannot really do**). Being comfortable with it, however, does not mean that it is correct!

Now, we consider an example of an experiment that exhibits quantum mechanical effects. We return to our earlier discussion of slits and interference patterns. We have a source of photons(single slit O = laser) + double slits (B and A) and a screen(C), which detects photons individually as discrete events(flashes).

Some very curious quantum behavior occurs as follows.

Suppose only slit B is open. Many places on the screen are reached by photons(photons are detected at these places). The region is centered directly behind B.

If only slit A is open, we get similar results in different places with some overlap of the two photon detection regions of A and B. The region is centered directly behind A.

If we open both slits, then a strange thing occurs. Some spots where photons had been detected with only one slit open(A or B) now have NO photons being detected, that is, opening more slits causes less photons to reach some spots on the screen!

This same experiment can be done with electrons with the same results!

We get this interference pattern buildup even when the intensity gets very small or we reduce the number of photons per second to a very small number.

In particular, let us reduce the intensity so that the number of photons in the apparatus at any given time is just 1! These experiments have only become possible in the last decade and we will discuss them in detail shortly.

How do we know only 1 photon or electron is in the vicinity of the apparatus?

Say the apparatus has a length $L = 3m$. Since the speed of light is $c = 3 \times 10^8 m/sec$, the time it takes a photon to pass through the apparatus is about $T = L/c = 10^{-8} sec$.

Therefore, if we want only 1 photon in apparatus at any time, then the time between photons coming out of the source and entering the apparatus must be greater than $10^{-8} sec$ or equivalently, the number of photons per second (from the source) is less than 10^8 per sec (that is the intensity of the incoming beam). Now for a typical photon, using $E = hf$, we have an energy $= 10^{-19} Joule/photon$. Thus, 10^8 photons per sec corresponds to $10^{-11} Joules/sec = 10^{-11} watts$ (note that a typical light bulb is 60-100 watts).

If we surround the source with a spherical shell that has a small pinhole in it, then the ratio of the area of the pinhole (diameter = $10^{-6} m$) to the area of the sphere (radius = $10 m$) is approximately $10^{-6}/10 = 10^{-13}$.

Therefore, a source delivering a total of 100 watts (in all directions) will deliver $100 \times 10^{-13} = 10^{-11}$ *watts* to the apparatus through the pinhole.

So it is easily possible create an experiment where only one photon is in the apparatus at a given time, although it is generally done with much cleverer techniques.

In this case, one can actually observe the screen flashes from individual particle impacts as the pattern builds up!!!

So let us say again what happens.

In this experiment a stream of particles is directed toward a screen. A second screen containing parallel slits is put in between the source and the detector screen. In this way, each particle must pass through one slit or the other in order to reach the final screen (**or so we think**). Each time a particle reaches the screen it causes a flash to appear or a detector to click.

Yet the most amazing thing (amazing according to classical physicists) is that if you close down one of the slits more particles make their way to certain places on the final screen than if we leave both slits open.

There is no way to understand this paradox if you insist on regarding the beam as simply made up of little particles (bullets), especially as we reduce the intensity towards zero.

Let me ask what will turn out to be poorly worded questions (questions of this type are often asked at this point).

How does a single particle **KNOW** if you have one or two slits open?

If this is an interference effect (wave theory of light) ... what is the single photon interfering with?

Photons cannot split, so it cannot be one piece interfering with another.

The photon goes through one slit or the other (**maybe?**) and if we wait long enough (even days) the proper interference pattern appears anyway.

If we try to detect (no matter how clever we are) which slit it went through, we destroy the interference pattern and end up with the sum of two single slit patterns.

Some **totally new way of thinking** will be necessary in order to understand this!!!

Let us step back a second and consider a comparable completely classical experiment.

Imagine pouring a container of sand onto a flat plate with a small centrally located hole. A few centimeters below the plate is a tiny movable detector that counts the number of sand grains hitting it per unit of time. It would show, as we expect, that the greatest number of sand grains is registered directly under the hole and the number decreases as the detector is moved transversely (parallel to the plate) away from the hole.

If we make another hole in the plate near the first one, cover the first hole and repeat the experiment we get the same results just shifted so that the maximum number is now under the second hole.

If we open both holes then the total number of grains reaching the detector at any location is the sum of the number of grains reaching the detector at the location from each hole independently.

In other words, opening up more holes can only increase, and never decrease, the total amount of sand reaching the detector per unit time at any location.

In the experiment with photons or electrons, no photons or electrons can be created or destroyed by the apparatus (same as for sand grains).

Yet somehow less photons can reach a spot on the screen when both slits are open than the sum of the numbers from when each slit was open separately.

Somehow, scaling the properties of the particles down from macroscopic to microscopic radically alters the way in which the particles get distributed (they must still be somewhere).

We never see two things that can happen independently somehow conspiring to cancel each other out in the macroscopic world! But such occurrences seem to happen constantly in the microworld.

How will quantum theory want us to think about all of this so that we have some hope of understanding what is happening?

As we shall see, quantum theory will give the following explanation (if I have to use inadequate **words**): when the photon is **going between the source and**

screen (whatever that means) the state of the photon *cannot* be described as

having gone through slit B
having gone through slit A
having gone through both slits simultaneously
having gone through neither slit

which exhausts all the **logical possibilities** we can imagine in the macroscopic world (using ordinary language).

As we shall see, the photon is a mysterious combination (**superposition**) of **all** these possibilities or maybe **none of the above** in any fashion.

A **superposition** will **only be understandable** via the mathematical language we will develop. We will not be able to make a model of what is happening because, as we shall see, there are no models (in the classical sense) available to us in the quantum world. We will not be able to find words from everyday language that will allow us to give an accurate description of what is happening. It will not be possible!!! Words are an incorrect language for describing the microworld.

Since that has never happened to you before, it has to seem mighty strange.

Not really, however, since you have never tried to describe what electrons and such are doing.

The fact that this result holds even if we reduce the intensity of the photon beam so that only one photon is entering the apparatus per year will force us to think in terms of **probabilities** instead of **classical paths**, which might allow us to say which slit the photon passed through. Each photon, which does something different than the other **identical** photons, will be seen to behave probabilistically.

We will consider many different experiments in our discussions. They will exhibit the very strange quantum behavior of systems in the microworld.

Our attitude will have to be.....

Well, if the microscopic world works in these strange ways no matter what quantities we are measuring, then so be it.

We must let our theories accommodate themselves to this new kind of **reality**.

So, later in our discussions of the quantum world, we will accept the experimentally observed properties that we find and try to work out a theory that incorporates them fully. We feel that if we can it will be a theory that can be used to make predictions about other phenomena in the microworld.

Alas, if it only was going to be so easy. It turns out that the microworld is much worse than we can imagine even if you were having a nightmare from too much beer and pizza.

To see this.....consider the following:

Let us try to measure the position of an electron. Suppose we know that an electron is in some box. Then, schematically our measuring process must look something like Figure 2.1 below:

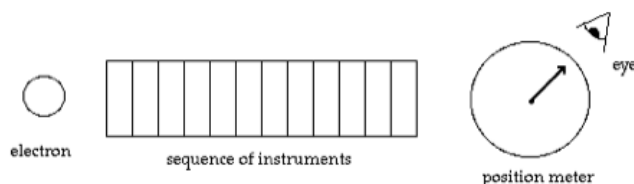


Figure 2.1: The measurement process.

The point here is that you will **NOT** have observed the electron **DIRECTLY!!!!**

Some as yet undefined sequence of *expensive instruments* is between the observed electron and your eye looking at some pointer.

This means that we do not **see** things in the quantum world the way we think we **see** them in the classical world (**where we seem to see objects directly or so we think**).

Actually, as we shall see in our discussions, the two worlds are really exactly the same, but it will turn out that they will behave very differently in the way the act of **seeing** interacts with the system being **seen**.

One of our crucial questions will be the following.

Where in the sequence of instruments (measurements) is the information or action or cause which makes the position meter dial point to a definite value replacing the quantum uncertainties of the electron with the definiteness of the pointer?

It will turn out that what we really should say is happening is shown in Figure 2.2 below:

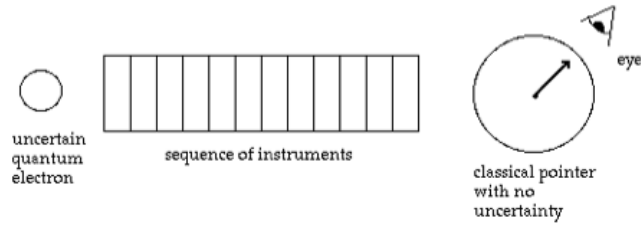


Figure 2.2: The measurement process adjusted.

The crucial question will be what happens in between?

Some kind of **discontinuity** will have to occur to abruptly remove the uncertainties of the quantum measurements.

But where does it occur?

This will be among the most puzzling parts of our discussions. Many great minds have fallen by the road side in trying to tackle this question.

So, these ideas are where the much of the discussion in this book will have to dwell.

This question is what all the interpretation debate in quantum theory is really all about !!!

Among other things that we will find out, perhaps the strangest will be that an electron can pass through a solid wall (so could you by the way...just more difficult (less probable) and certainly more painful) in a very strange way.

It simply **vanishes** on one side and **reappears** on the other side and I mean that statement very **literally, if I must use words again**).

Why should that be disturbing?

It is that we will not be able to say (measure) that it was ever at any place (position) in between.

Here and there and NEVER in between.

In fact, if we try to **see** if it is in between, then it will not be able to get through!!!! It will behave classically and no matter how much I try to throw any object that we are **watching** through the wall it will never make it.

Nothing in our everyday experience prepares us for this kind of phenomena.

By the way, suppose we put an object on the table and do not observe in any manner. Can it suddenly appear on the other side of the wall? The answer will be YES!!! The probability will be very small however...so small that we probably would not see it occur in the lifetime of the universe.

Now, the classical explanation of interference works for intense beams (intense \rightarrow wave behavior).

When we do not have an intense beam (lots of photons), then the wave model fails. However, for a very weak beam of photons, i.e., one photon per century, as we said earlier, we eventually get the same pattern.

What then is interfering with what? Or is interference *not* the right idea?

Remember a single photon can only produce one bright dot on screen and not a pattern. Any one photon simply ends up at a particular spot on the screen.

Each photon is identically prepared.

We cannot predict where a particular photon will end up.

The end result after centuries is the same pattern as if interference had taken place.

How do they each know what to do? (this will turn out to be a poor question).

The only satisfying explanation will use probability.

Each photon has a probability $P(x)$ (where $P(x)$ implies the arrival pattern at the detector discussed earlier) of ending up at position x on the screen.

We might say that each photon independently uses $P(x)$ to choose an impact point. We might say that each photon independently generates a part of interference pattern.

Another useful way to think about single-photon interference is as follows:

Suppose that a photon is a superposition of all things it can possibly do. Then it passes through the slits in a state that is a superposition of passing through slit b and passing through slit a .

Photons will not produce the interference pattern if we know (must measure) they are going through a particular slit.

Somehow they will **know** if the other slit is open/closed and change the probabilities of doing things.

If we try to check which it goes through then quantum behavior disappears and they are like sand grains.

In quantum physics you cannot know which slit it passes through - this question will make no sense - it will, in fact, be meaningless.

If you check to see if it goes through a particular slit, then it either hits your detector(went through that slit) and no photon gets to the screen which implies no pattern or it does not hit your detector and hence it went through the other slit.

But a single photon going through a single slit produces a different pattern, which, of course, it then does. We would obtain the pattern corresponding to the slit without the detector being open!

Your extra experiment forces the photon to behave as if it goes through one slit or the other and the interference pattern changes.

What was initially a photon with many possibilities (many probabilities to do different things) is now a photon doing a definite(single thing) because **you measured it doing that particular thing**(or not doing that thing!).

We have **collapsed** possibilities into definiteness by trying to know what it is doing and in the process the experimental result is always destroyed.

If we wish to retain quantum effects, then we cannot know what is happening in between measurements – we can only have probabilities of final outcomes.

So if we do not look at photons they interfere, but if we look, then they behave like sand grains and do not interfere.

That is the way we will find that the quantum world works.

Clearly, this behavior will have devastating effects on our notions of reality.

Before we jump into developing the theory, let me present some more food for thought so that our minds are in the right frame to proceed.

What will we find in the quantum theory?

Things will seem to move without following any mechanical law.

Things will seem to move in a disjointed or discontinuous manner. They will

jump from one place to another, seemingly without effort and without bothering to go between the two places.

Quantum theory will suggest that what one uses to observe nature on an atomic scale **created** and determined what one saw. That nothing has properties independent of the observer (measurement). The values one observes will appear to depend upon what one chooses to observe.

Despite the natural disorder apparent in these experiments, quantum theory will indicate that there is an order to the universe.

It simply is not the order we might expect.

In the microworld, we will find that any path from causes to effects is constantly blurred by uncertainty and jogged from side to side by randomness and chance.

How can this be the ultimate theory that underlies the ordered and inevitable universe revealed by classical physics? We will answer that question in this book.

Now let us say a little more about the early quantum theory according to Schrödinger, Heisenberg and Bohr.

2.1.1 The Wave Equation.....

The first development of a formal quantum theory was due to Schrödinger. He used analogies with standard classical wave theory to come up with a new **wave** equation analogous to the existing classical wave equations for sound, light, vibrating strings, etc.

Schrödinger's **wave** equation provided a continuous mathematical description (via the mathematics of differential equations) of how quantum probabilities develop in time.

The problem was that no one could imagine what these new **waves** looked like. They had no recognizable form in ordinary physical space. They did not behave like water or sound waves. They seemed to be only mathematical thingsonly mathematical functions of space and time.

This is why Schrödinger disliked the theory he devised! He was looking for a real physical wave..... a de Broglie **matter** wave of some kind in physical 3-dimensional space.

By adding these waves together (like mathematical vector addition as we shall see) physicists found out that they could represent particles (objects of limited extent) that behaved correctly (as observed in the actual world).

Heisenberg and Dirac (almost simultaneously) came up with alternative formulations of quantum theory using matrices and vectors, which are other mathematical objects that we will learn about later. Dirac developed most of the general principles we shall use in this book.

Born and Bohr developed the so called **standard** or **Copenhagen** interpretation of these theories in terms of probabilities and measurements. The principles espoused in this standard interpretation are the cause of most of the vigorous debates about interpretation.

Central to the problems of interpretation will be the idea of a measurement.

We now look at some examples in order to clarify some of these thoughts:

When you look at something, you are detecting reflected light that has come from some source, **bounced** or **scattered** off the object and then entered your eye.

We do not normally think about seeing in this way since in our everyday world we can safely assume that light bouncing off something macroscopic does not change that object in any measurable way since the photon energy is insignificant compared the macroscopic object energy.

When we get to the quantum world, however, this comfortable assumption no longer works. If we want to **see** the bundle of matter (bunch of energy and momentum) that we **call** an electron, then we have to **bounce** another bundle off it. In the process the electron is significantly changed, since the bundle energy is comparable to the electron energy.

To understand this better, consider the following:

Suppose that you wanted to find out if there was a car in a long tunnel. Also suppose that the **ONLY** (this is the equivalent situation for electrons) way that you could do this was to send another car into the tunnel and listen for the crash.

crash \rightarrow a car was in the tunnel
no crash \rightarrow no car was in the tunnel

Obviously our detection scheme will work and just as obviously, our detection scheme has a rather **drastic** effect on the object being detected (in this case it changes the object velocity to zero).

In the QUANTUM WORLD, this is the **ONLY** measurement we can do!

They are called **destructive** measurements(the classical world is full of seemingly **non-destructive** measurements).

This will be our first rule of QM:

You cannot observe something without changing it in some way during the measurement process (this is related to the famous Uncertainty Principle of Heisenberg in action as we shall see later)

Think again about the car in the tunnel. When we chose to observe one thing.....the location of a car in the tunnel.....our measurement procedure was such that we had to forever be uncertain about something else (some other property of the car). In this case, we lose all information about how fast the car was moving before the collision.

When we walk into the tunnel, we can accurately locate the crash and thus we know what the position of the car at the instant of the crash and we have time to measure it exactly or $\Delta(position) = 0$.

However, we know nothing about the velocity before the measurement (collision in this case).

The inability to observe things in the microscopic world without at the same time disturbing them has some surprising consequences when you start to think about the way particles move from one point to another.

Again let us use cars as an **example**.

Suppose I ask where a particular car will be **TOMORROW**.

In the ordinary everyday world, we would just look to see where it is now and **THEN** look to see how fast it is moving and in what direction. Then we use our calculator and figure out the answer - we get a **DEFINITE ANSWER**.

If the car is replaced by an electron, **you cannot look at it more than once** - the first look changes everything.

You cannot know with precision both where it is **AND** how fast it is going at any instant of time. The best you can do is to play one uncertainty against the other so you know both quantities **reasonably well** in some sense.

You might say(after a measurement) that the car is in the Chicago area and heading in a generally easterly direction at about 40 – 60 *mph*. More measurements imply more disturbances thereby increasing uncertainties and not helping us at all.

In order to talk about where the car will be tomorrow, we are forced to speak in terms of **PROBABILITIES**.

The car might be in Detroit or Cleveland or even NYC, but it is not likely to

be in Miami or London. We can make similar statements about when it might be at these places.

The collection of all probability information will be everything we can know about the electron(car).

We will call this maximal set of information the **STATE** of the electron.

IT WILL BE ALL THAT WE CAN KNOW!

Up to this point, you have probably been following along pretty easily, perhaps thinking that you might as well humor the writer of this book since he is a professor of physics.

Well hold on, things are about to become really strange.

The reason you are **not bothered** by having to describe the car(electron) in terms of probabilities is that **DEEP DOWN** you **KNOW** that the car is **really** somewhere **ALL** the time and if you could just peek, you would see it moving along any time that you wanted to.

Of course, if you did, then you would change it and mess up the experiment, but you still have that confident feeling that in some manner the car is **REALLY** there, even if you don't **SEE** it (this is called **objective reality**).

You might even imagine the entire country as an underground parking garage in which you can see the car **ONLY** at the exits. You may not be able to see it **BETWEEN** the exits, but, if you saw it enter the garage, then you **KNOW** it is always somewhere inside the garage.

This is not the way, however, that a physicist envisions electrons.

Their view, as we will see, is that **UNTIL** you look (perform a measurement) on a particle you have to treat it as **ONLY** a set of probabilities (that is the **maximal possible information**).

The car **IS NOT** really at **ANY** particular place **UNLESS** it is being measured and found to be at that place.

In between, it is just a set of probabilities that describe what could happen if a new measurement were to take place – in between, it is **ONLY** a **STATE**.

This assumption will, as we will see, have directly measurable consequences. It is not just idle talk! If we assume anything different, then our predictions will not agree with experiment, as we shall see.

The idea that there **HAD** to be some sort of underlying reality beneath these *states* and their associated *probabilities* was what led Einstein to make his famous comment that:

"God does not play dice with the universe"

Less famous is Bohr's reply:

"Albert, stop telling God what to do"

Finally, let us consider the saga of two gloves.....this tale illustrates one central feature(very important) of quantum theory.

2.1.2 The Tale of 2 Gloves (read carefully)

You and a friend are at the airport in Atlanta. You each have a locked box containing a glove. One box contains a right-handed glove of the pair, the other the left-handed glove, but you do not know which. Both of you also have keys, but they are not the keys to the boxes you are carrying.

Carrying your box, you each board a Delta airlines plane. You fly to Chicago and your friend flies, at the same time, to Philadelphia.

When you get to Chicago you use your key to open a locker at the airport, and inside you find another key. This is the key to your box, which you now open to discover that the glove you have brought to Chicago is the right-handed one.

As soon as you know this, of course, you know also that your friend's box, by now in Philadelphia, contains the left-handed glove. With that instantaneous realization, you have acquired a piece of knowledge about a state of affairs on the other side on the east coast.

Perfectly straightforward, you may say, and so it is. You may have heard of Einstein's rule that nothing, not even information, can travel faster than the speed of light, but no part of this story contradicts this rule in any way.

You have made a deduction, using information available to you at the Chicago airport, about a fact that pertains to your friend in Philadelphia. We make this kind of **long-distance inference**, in big ways and small ways, all the time.

An astronomer observing the weak light that reaches a telescope here on earth uses it to deduce the surface temperature of stars many light years away. You get out of the shower one morning, look at your watch, and realize that a class meeting that you had to attend has already started.

Figuring out what is happening in some distant place is a **different** thing from **transferring** that knowledge from one place to another.

If, having discovered that your glove is right-handed, you wanted to tell your friend that she has a left-handed one, you would have to use a cellphone, or send a telegram, or send her email or mail her a postcard. Some of these might even travel at close to the speed of light (under ideal conditions).

You have no way, however, of knowing whether she has already opened her box or not - unless you get a message from her telling you that you must have a right-handed glove.

The fact that you have found out which glove she has does not allow you to beat the laws of physics and get that information to her faster than Einstein allows.

But still, you think that there might be some way of exploiting your knowledge to influence your friend's behavior. Suppose, before you both set off on your plane trips, you had agreed with your friend that if she found the left-handed glove in her box she would proceed onto London, but if she found the right-handed one she would fly to Paris.

Does your opening the box in Chicago determine where she ends up?

Not a chance!

Whichever glove was in her box was there from the outset (objective reality), so whether she has to fly to London or Paris is **predetermined**.

When you open your box in Chicago you instantly know where she must be going next, but her destination is as much a surprise to her as it is to you.

As before, you have found out what happens next, but you have no influence over it.

Now let us change this story.

The gloves in the two boxes are, you are informed, of a strange and quantum-mechanical kind, **unlike** any gloves you have ever come across before.

They still make up a pair, but for as long as they are sealed up in the boxes, they are neither right-handed nor left-handed, but in an unfixed, indeterminate state.

Only when a box is **opened**, letting in the light, does the glove inside **instantaneously become** either right-handed or left-handed and there is a 50-50 chance of either eventuality.

During the few hours you are in the plane flying to Chicago, you may well be puzzling over what the glove in your box - this strange glove, neither right-

handed nor left handed but potentially either - actually looks like. But you do not have the key that would let you open the box and peek inside, and, in any case, as soon as you **peeked** the glove **would have** to take on a definite shape, right-handed or left handed.

The quantum-mechanical nature of the glove is such that you **can never see** it in its unformed state, because as soon as you look, it turns(**collapses**) into something familiar and recognizable.

A frustrating catch-22.

On the other hand, as soon as you arrive in Chicago and open your box to find, let us suppose, a right-handed glove, you begin to think that things are not as straightforward as before. You immediately know that when your friend opens her box, she must discover a left-handed glove.

But now, apparently, some sort of signal or information must have traveled from your glove to hers, must it not?

If both gloves were truly indeterminate before you opened your box and looked inside, then presumably as soon as your glove decided to be(remember it is a 50-50 chance) a right-handed one, hers must have become left-handed, so that the two would be guaranteed to remain a pair. **That is the rule for these quantum-mechanical gloves.**

Does this mean that your act of observing the glove in Chicago **instantaneously** reduced the indefiniteness of its partner in Philadelphia to a definite state of left-handedness?

It now occurs to you that there is another possibility.

How do you know that your friend did not get to Philadelphia first and open her box before you had a chance to open yours?

In that case, she evidently found a left-handed glove, which caused yours to be right-handed even before you looked inside your box. So, if there was an instantaneous transmission of information, it might have gone the other way. Your friend's act of opening her box determined what sort of glove you would find and not the other way around.

Now you realize that the only way to find out which way the instantaneous transmission of information went, from your glove to hers or from hers to yours, is to use your cellphone and call Philadelphia and find out at what time she opened her box. That cellphone call, however, travels slower than light. Now you are really getting confused.

There seems to have been some kind of instantaneous communication between the two gloves, but you cannot tell which way it went, and to find out you have to resort to old-fashioned, slower-than-light means of communication, which seems to spoil any interesting tricks you might be able to figure out if there **really** had been an instantaneous glove to-glove signal.

If you think again of the strategy whereby your friend had to get on a plane to either London or Paris, depending on which glove she found in her box, then you realize you are no more able than before to influence her choice by your action in Chicago.

The rules of the game are such that you have a 50-50 chance of finding either a right-handed or a left-handed glove in your box, so even if you are sure that you have opened your box before she opened hers, and even if you think that opening your box sends an instantaneous signal to hers, causing her glove to be the partner of yours, you will still have no control over which glove you find.

It remains a 50-50 chance whether she will end up in London or Paris.

You have no say in the matter!

So now you are even more confused.

You think there has been some sort of instantaneous transmission of information, but you cannot tell which way it went, and you cannot seem to find a way to communicate anything to your friend by means of this secret link between the gloves.

Perhaps you might even conclude at this point that it is a good thing that real gloves are not like this.

In that case you would be in agreement with Einstein.

It is true that gloves do not behave this way, but according to quantum theory, as we shall see, electrons, photons and other elementary particles do!

These particles have properties which, apparently, lie in some unresolved indeterminate (**entangled**) state until an observer comes along and does an experiment that causes them to be one thing or the other(**collapses their state in some way**). The observer cannot know in advance what the result of any particular measurement is going to yield; quantum theory predicts only the probabilities of possible results.

This greatly offended Einstein's view of what physics should be like.

Before quantum theory, it was taken for granted that when we measure some-

thing, we were **gaining knowledge of a pre-existing state**. That is, gloves are always either right handed or left-handed, whether we are observing them or not, and when you discover what sort of glove you have, you are simply taking note of an independent fact about the world (objective reality).

Quantum theory says otherwise. Some things are not determined except when they are measured, and it is **only by being measured** that they take on their specific values. The gloves are neither right-handed nor left-handed until we check.

Einstein and his colleagues actually devised an experiment of this sort(not with gloves) as a way to show how absurd and unreasonable quantum theory really is. They hoped to convince their physicist colleagues that something must be wrong with a theory that seemed to demand signals traveling faster than light.

Notwithstanding the genius of Einstein, in this case he was sadly wrong. Nothing genuinely unacceptable is actually happening with the gloves. The whole thing may seem very odd, and it may seem quite inescapable that some sort of instantaneous communication between gloves is essential for everything to work, but in the end it seems impossible to do anything with this communication. We will discuss a real version of this experiment in detail later.

Quantum theory arrives at what it deemed an acceptable interpretation of this sort of puzzle by insisting that we stick to practicalities.

It is no good, and indeed very dangerous, to speculate about what **seems** to happen in such a case. Stick to what actually occurs, and can be recorded and verified, and you will be all right. If you cannot actually send an instantaneous message of your own devising, then it is meaningless to guess at what might or might not have been secretly going on between the two gloves.

You might think that if we do not **understand** all aspects of what is going on then we will not be able to do anything useful with this quantum theory stuff. It turns out just the **opposite!**

Well, so much for our overview.

Now for the details of how quantum theory works..... Quantum Mechanics is a branch of physics that has a **well-defined set of rules** which tell physicists how to set up a certain class of problems and how to do the calculations needed to solve the problems. In **all cases**, if the rules are followed, then the calculated results always agree with experiment.

Physicists generally do not need to engage in a debate about the meaning of the assumptions of QM and most do not since it makes them very uncomfortable to realize that they really do not understand what it is they are using everyday.

As we shall see, the interpretations of the principles of Quantum Mechanics easily inspire a very vigorous debate about their meaning. The outcome of the debate, as we shall see, will have no effect on the values obtained from our calculations, i.e., the calculation rules are independent of their interpretations!

This is very convenient for the practicing physicist. They can discover fundamental effects, use them to create neat new devices, make lots of money and gain lots of fame while never understanding the meaning of their assumptions at all.

In this book, however, we are interested in the meanings and interpretation of the principles. In order to do this we must understand how to do Quantum Mechanics first.

We will now develop an understanding of the tools used by the physicist to do Quantum Mechanics. Only after we understand how to do Quantum Mechanics and see some of its dazzling and astounding effects will we discuss the interpretations.

We approach this discussion from a real **theorist's** viewpoint.

Not many of you have ever seen a theoretical physicist in action, so some of this will seem very much off the wall. It is important to remember that the theorist has only one goal.....to understand the universe in some manner.

No assumption is considered too crazy to be included.

Invention of new ways of thinking will be commonplace.

Strange interpretations will be given all over the place.

What is correct? Only that which agrees with measurements!

We proceed along the lines set out by Paul Dirac in the 1920s modified by much hindsight from the intervening 85 years of discovery.

Chapter 3

Introducing Linear Algebra

Philosophy is written in this all-encompassing book that is constantly open before our eyes, that is the universe; but it cannot be understood unless one first learns to understand the language and knows the characters in which it is written. It is written in mathematical language, and its characters are triangles, circles, and other geometrical figures; without these it is humanly impossible to understand a word of it, and one wanders around pointlessly in a dark labyrinth.

- Galileo

3.1 Thinking about vectors

We define a vector (with symbol $|\dots\rangle$) in 2 dimensions as a set of 2 numbers as shown below:

$$|V\rangle = (v_1, v_2) \tag{3.1}$$

The real numbers v_1 and v_2 are called the *components* of the vector $|V\rangle$. v_1 is the 1-component and v_2 is the 2-component. The number of components equals the *dimension* of the space.

As we will see in our later discussions of Quantum Mechanics, such vectors will represent the quantum states of physical systems.

The vectors have the following properties (these properties completely define the vector mathematically).

3.1.1 Addition of vectors

$$\begin{aligned} \text{If } |V_1\rangle &= (7, -2) \text{ and } |V_2\rangle = (-5, 3) \\ \text{then the sum } |V\rangle &= |V_1\rangle + |V_2\rangle = (7 + (-5), (-2) + 3) = (2, 1) \end{aligned} \quad (3.2)$$

Thus, vector addition is accomplished by the addition of components.

3.1.2 Difference of vectors

$$\begin{aligned} \text{If } |V_1\rangle &= (7, -2) \text{ and } |V_2\rangle = (-5, 3) \\ \text{then the difference } |V\rangle &= |V_1\rangle - |V_2\rangle = (7 - (-5), (-2) - 3) = (12, -5) \end{aligned} \quad (3.3)$$

Thus, vector difference is accomplished by the subtraction of components.

3.1.3 Length

The *length* of a vector is defined by

$$\text{If } |V\rangle = (v_1, v_2) \text{ then length} = \sqrt{v_1^2 + v_2^2} \quad (3.4)$$

3.1.4 A new operation and the generalized length

We can generalize this definition of “length” in the following way. Let us label a new mathematical property or operation on vectors by the symbol $\langle \dots | \dots \rangle$ called a “bra-c-ket or bracket” and define the new operation as follows:

$$\begin{aligned} \text{If } |V\rangle &= (v_1, v_2) \quad , \quad |U\rangle = (u_1, u_2) , \\ \text{then } \langle V | U \rangle &= v_1 u_1 + v_2 u_2 \end{aligned} \quad (3.5)$$

Therefore, using the new operation, the length of a vector is given by

$$\langle V | V \rangle = v_1 v_1 + v_2 v_2 = v_1^2 + v_2^2 = (\text{length})^2 \quad (3.6)$$

or

$$\text{length} = \sqrt{\langle V | V \rangle} = \sqrt{v_1^2 + v_2^2} \quad (3.7)$$

Note that, by definition, $\langle V | V \rangle \geq 0$, i.e., it is the sum of squares of real numbers. The particular type of vector we have defined up to this point is called a *Euclidean* vector with *real* components in 2 dimensions.

3.1.5 More than 2 dimensions

These definitions are easily extended to more than two dimensions as follows:

$$\begin{aligned} |V\rangle &= (v_1, v_2, \dots, v_n) \quad , \quad |U\rangle = (u_1, u_2, \dots, u_n) \\ \langle V | U \rangle &= v_1 u_1 + v_2 u_2 + \dots + v_n u_n = \sum_{k=1}^n v_k u_k \end{aligned} \quad (3.8)$$

$$\text{length} = \sqrt{\langle V | V \rangle} = \sqrt{v_1 v_1 + v_2 v_2 + \cdots + v_n v_n} = \sqrt{\sum_{k=1}^n v_k^2} \quad (3.9)$$

Note that, by definition, we still have $\langle V | V \rangle \geq 0$. The particular type of vector we have defined in this case is called a *Euclidean* vector with *real* components in n dimensions.

The mathematical name for this new operation $\langle \cdots | \cdots \rangle$ is the *scalar* or *inner* or *dot* product.

We can generalize these definitions even further by allowing the components of the vectors to be complex numbers (this will be the case in Quantum Mechanics).

3.1.6 Digression on complex numbers

We first specify some simple properties about complex numbers which are determined by the *defined* properties of a new mathematical object i . We have (by definition)

$$i^2 = -1, \quad i^3 = -i, \quad i^4 = +1, \quad i^5 = i, \quad i^6 = -1, \quad \text{and so on} \quad (3.10)$$

A complex number z is then defined in terms of i by the expression $z = a + bi$ where a, b are real numbers. a is called the *real part* of z and b is called the *imaginary part* of z . Using (1.10) we can do arithmetic with complex numbers, i.e., we can add two complex numbers

$$(7 + 4i) + (-2 + 9i) = 5 + 13i$$

i.e., we just add/subtract the real and imaginary parts separately.

We can also multiply two complex numbers

$$\begin{aligned} (7 + 4i)(-2 + 9i) &= (7)(-2) + (7)(9i) + (4i)(-2) + (4i)(9i) \\ &= 14 + 54i - 36 = -22 + 54i \end{aligned}$$

Next, we define the *conjugate* z^* of z by $z^* = a - bi$.

Finally, we define the *absolute value* $|z|$ of a complex number by

$$|z|^2 = z^* z = (a - bi)(a + bi) = a^2 + b^2 \quad (3.11)$$

or

$$|z| = \sqrt{a^2 + b^2} \quad (3.12)$$

We can then define Euclidean vectors in n dimensions with complex numbers as coefficients if we generalize the definition scalar product of two vectors as shown below:

$$\langle V | U \rangle = v_1^* u_1 + v_2^* u_2 + \cdots + v_n^* u_n = \sum_{k=1}^n v_k^* u_k \quad (3.13)$$

and thus the new definition of length becomes

$$\text{length} = \sqrt{\langle V | V \rangle} = \sqrt{\sum_{k=1}^n v_k^* v_k} = \sqrt{\sum_{k=1}^n |v_k|^2} \quad (3.14)$$

These new definitions are still valid if the components are real numbers since $v_k^* = v_k$ and $|v_k|^2 = v_k^2$ for real components and thus the equations are identical to the earlier versions.

Vectors in Quantum Mechanics are Euclidean vectors with complex components.

3.1.7 Non-Euclidean vectors

As an aside, however, we note that special relativity deals with *non-Euclidean* vectors with real components. A non-Euclidean vector arises when we redefine the scalar product as follows. Suppose we have 4 dimensions and we define

$$\begin{aligned} |V\rangle &= (v_1, v_2, v_3, v_4) \quad , \quad |U\rangle = (u_1, u_2, u_3, u_4) \\ \langle V | U \rangle &= v_1 u_1 - v_2 u_2 - v_3 u_3 - v_4 u_4 = \sum_{k=1}^n c_k v_k u_k \end{aligned} \quad (3.15)$$

where, in this case, $c_1 = 1$ and $c_2 = c_3 = c_4 = -1$.

Note, however, that the “square of the length” now is no longer a positive quantity, i.e.,

$$\langle V | V \rangle = v_1^2 - v_2^2 - v_3^2 - v_4^2 = \sum_{k=1}^n c_k v_k^2 \quad (3.16)$$

can now take on positive, negative and zero values. Clearly, the standard Euclidean vectors defined earlier simply have all $c_k = 1$.

3.1.8 Unit vectors

We can always create a Euclidean vector that has length = 1 in the following way:

If $|V\rangle = (v_1, v_2)$

then old length = $V = \sqrt{v_1^2 + v_2^2}$

Now define $|\hat{V}\rangle = \frac{|V\rangle}{V} = \left(\frac{v_1}{V}, \frac{v_2}{V}\right)$. We then have

new length = $\hat{V} = \sqrt{\left(\frac{v_1}{V}\right)^2 + \left(\frac{v_2}{V}\right)^2} = \sqrt{\frac{v_1^2 + v_2^2}{V^2}} = \sqrt{\frac{V^2}{V^2}} = 1$ as desired.

3.1.9 Basis vectors

There always exists a special set of unit vectors called *fundamental basis vectors* which have only a single component, i.e., in 2 dimensions we have the fundamental basis vectors

$$|1\rangle = (1, 0) \quad , \quad |2\rangle = (0, 1) \quad (3.17)$$

This easily generalizes to n dimensions, i.e., for 3 dimensions we have

$$|1\rangle = (1, 0, 0) \quad , \quad |2\rangle = (0, 1, 0) \quad , \quad |3\rangle = (0, 0, 1) \quad (3.18)$$

and so on.

A *vector space* is a mathematical structure formed by a collection of elements (called vectors), which may be added together and multiplied by numbers such that the new vectors thus created are in the collection. A vector space may be endowed with additional structure, such as an inner or scalar product. Quantum mechanics operates in this type of vector space.

Any vector in the vector space can be written in terms of the basis vectors (the reason for the name “basis”). For example.

$$|V\rangle = (v_1, v_2) = v_1(1, 0) + v_2(0, 1) = v_1|1\rangle + v_2|2\rangle \quad (3.19)$$

We use the terminology: v_1 is the component of $|V\rangle$ in the 1-direction and v_2 is the component of $|V\rangle$ in the 2-direction.

We also note an interesting relationship between components and the scalar product as shown below:

$$\langle 1|V\rangle = v_1\langle 1|1\rangle + v_2\langle 1|2\rangle \quad (3.20)$$

Now, according to our rules for evaluating the scalar product, we have

$$\langle 1|1\rangle = (1, 0) \cdot (1, 0) = (1)(1) + (0)(0) = 1 \quad (3.21)$$

$$\langle 1|2\rangle = (1, 0) \cdot (0, 1) = (1)(0) + (0)(1) = 0 \quad (3.22)$$

Thus, we see that

$$\langle 1|V\rangle = v_1 \quad (3.23)$$

In a similar way we also have

$$\langle 2|V\rangle = v_1\langle 2|1\rangle + v_2\langle 2|2\rangle \quad (3.24)$$

with

$$\langle 2|1\rangle = (0, 1) \cdot (1, 0) = (0)(1) + (1)(0) = 0 \quad (3.25)$$

$$\langle 2|2\rangle = (0, 1) \cdot (0, 1) = (0)(0) + (1)(1) = 1 \quad (3.26)$$

and thus,

$$\langle 2 | V \rangle = v_2 \quad (3.27)$$

Thus, the components of a vector in a particular direction are simply given by the scalar product of the vector with the corresponding basis vector. Thus, we can always write

$$|V\rangle = \langle 1 | V \rangle |1\rangle + \langle 2 | V \rangle |2\rangle \quad (3.28)$$

I have illustrated all these relations with real components but all the derivations still hold for complex components using the appropriate scalar product rules.

3.1.10 Orthogonality

Before defining “orthogonality” in general, let us specialize to a case where you are familiar with its meaning. Consider the ordinary 2-dimensional space of vectors that you can draw on a sheet of paper.

The usual procedure that we use goes as follows:

1. Two coordinates are needed to describe what happens on a piece of paper(a plane). The usual convention is to call them x and y .
2. Define an origin of coordinates: $(x,y)=(0,0)$, Define x - and y -axes.
3. Every point on the paper (in the plane) relative to the chosen origin is specified by the x - and y -coordinates of the point.
4. Vectors relative to the origin are specified by the components in the x - and y -directions. Thus, (using standard notation now) the vector $\vec{V} = (7, 4)$ corresponds to vector you would draw on the paper with x -component = 7 and y -component = 4 as shown in Figure 3.1 below. Note that we have chosen the x - and y -axes to be orthogonal(perpendicular).

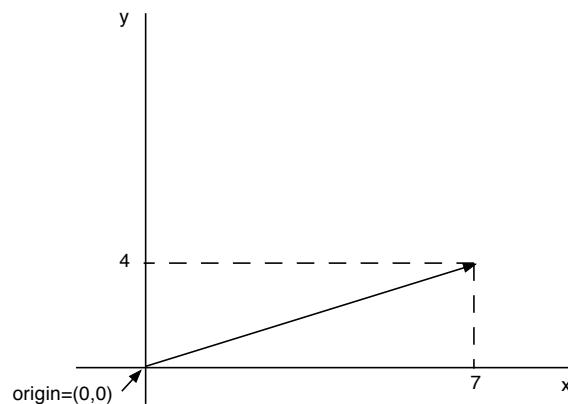


Figure 3.1: Vector properties

5. We now define the basis vectors for this space. They correspond to unit vectors in the coordinate directions (along the axes), i.e.,

$$\hat{x} = (1, 0) \quad , \quad \hat{y} = (0, 1) \quad (3.29)$$

6. We can then write

$$\vec{V} = 7\hat{x} + 4\hat{y} \quad (3.30)$$

i.e., the sum of a vector of length 7 in the +x-direction plus a vector of length 4 in the +y-direction. and where

$$7 = v_x = \hat{x} \cdot \vec{V} \quad , \quad 4 = v_y = \hat{y} \cdot \vec{V} \quad (3.31)$$

as before. The length of the vector is $\sqrt{v_x^2 + v_y^2} = \sqrt{65}$. This just corresponds to the Pythagorean theorem!

7. We now note that

$$7 = v_x = \hat{x} \cdot \vec{V} = \text{length}(\hat{x}) \times \text{length}(\vec{V}) \times \frac{v_x}{\text{length}(\vec{V})}$$

But

$$\frac{v_x}{\text{length}(\vec{V})} = \text{cosine of angle between } \vec{V} \text{ and } \hat{x}$$

Thus, for any two vectors

$$\vec{A} \cdot \vec{B} = AB \cos \theta \quad (3.32)$$

where $A = \text{length}(\vec{A})$, $B = \text{length}(\vec{B})$ and θ is the angle between \vec{A} and \vec{B} .

This works as shown below:

$$\hat{x} \cdot \hat{x} = \text{length}(\hat{x}) \times \text{length}(\hat{x}) \cos(0^\circ) = 1$$

as expected since the vectors are in the same direction.

Similarly, we have

$$\hat{x} \cdot \hat{y} = \text{length}(\hat{x}) \times \text{length}(\hat{y}) \cos(90^\circ) = 0$$

as expected since the vectors are orthogonal.

We now generalize and define the cosine of the angle between two vectors (even if we cannot draw them in real space(on a sheet of paper)) by the relationship

$$\langle A | B \rangle = AB \cos(\theta_{AB}) \quad (3.33)$$

The basis vectors $\{|1\rangle, |2\rangle\}$ we defined earlier for the general vector space were chosen to be orthogonal for convenience in calculations. In general, we will always choose a basis to be a set of *orthonormal* vectors, i.e., they are all of length = 1 and orthogonal to each other. This orthogonality for basis vectors is expressed mathematically using a new symbol called the “Kronecker-delta” as shown below

$$\langle n | m \rangle = \delta_{nm} = \begin{cases} 1 & n = m \\ 0 & n \neq m \end{cases} \quad (3.34)$$

so that

$$\begin{aligned} \langle 1 | 1 \rangle &= \delta_{11} = 1 \\ \langle 1 | 2 \rangle &= \delta_{12} = 0 \\ \langle 2 | 1 \rangle &= \delta_{21} = 0 \\ \langle 2 | 2 \rangle &= \delta_{22} = 1 \end{aligned}$$

3.1.11 Spacelike, timelike, null properties

Returning to non-Euclidean vectors, which as we said earlier can have a negative $(length)^2$, we make the following definitions whose meaning becomes clear when one studies special relativity. We define

1. $(length)^2 > 0$ timelike
2. $(length)^2 = 0$ null
3. $(length)^2 < 0$ spacelike

We now need to rewrite our notation so that it conforms to the standard notation used by practicing physicists. In order to do this we must introduce a completely new mathematical idea, namely, *matrices*.

3.2 Matrices

An $m \times n$ *matrix* is an $m \times n$ array (m rows and n columns) of numbers (matrix elements) with a well-defined set of associated mathematical rules. For example, we have the matrices shown below

1. 2×1 matrix (2 rows and 1 column) or column vector

$$\begin{pmatrix} 2 \\ 5 \end{pmatrix}$$

2. 1×2 matrix or row vector

$$(2 \quad 5)$$

3. 2×2 matrix

$$\begin{pmatrix} 2 & 5 \\ -3 & 10 \end{pmatrix}$$

4. 2×3 matrix

$$\begin{pmatrix} 2 & 5 & -1 \\ -3 & 10 & 5 \end{pmatrix}$$

and so on. If we have two matrices (will use 2×2 as an example)

$$\mathbf{A} = \begin{pmatrix} 2 & 5 \\ -3 & 10 \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} -8 & 15 \\ 7 & 4 \end{pmatrix}$$

then we define these operations

$$\mathbf{A} + \mathbf{B} = \begin{pmatrix} (2) + (-8) & (5) + (15) \\ (-3) + (7) & (10) + (4) \end{pmatrix} = \begin{pmatrix} -6 & 20 \\ 4 & 14 \end{pmatrix}$$

i.e., we just add corresponding matrix elements.

$$\mathbf{AB} = \begin{pmatrix} 2 & 5 \\ -3 & 10 \end{pmatrix} \begin{pmatrix} -8 & 15 \\ 7 & 4 \end{pmatrix} = \begin{pmatrix} (2)(-8) + (5)(7) & (2)(15) + (5)(4) \\ (-3)(-8) + (10)(7) & (-3)(15) + (10)(4) \end{pmatrix} = \begin{pmatrix} 19 & 50 \\ 94 & -5 \end{pmatrix}$$

This last operation is called *matrix multiplication* and is defined for general elements by

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

$$\mathbf{AB} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} = \begin{pmatrix} a_{11}b_{11} + a_{12}b_{21} & a_{11}b_{12} + a_{12}b_{22} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} \end{pmatrix}$$

We now define some special matrices and matrix properties.

$$\mathbf{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \text{identity matrix}$$

$$\det \mathbf{A} = a_{11}a_{22} - a_{12}a_{21} = \text{determinant of } \mathbf{A}$$

$$\mathbf{A}^{-1} = \frac{1}{\det \mathbf{A}} \begin{pmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{pmatrix} = \text{inverse matrix}$$

where we have the property $\mathbf{AA}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$. This particular equation is only valid for 2×2 matrices.

$$\mathbf{A}^T = \begin{pmatrix} a_{11} & a_{21} \\ a_{12} & a_{22} \end{pmatrix} = \text{transpose matrix}$$

$$\mathbf{A}^\dagger = \begin{pmatrix} a_{11}^* & a_{21}^* \\ a_{12}^* & a_{22}^* \end{pmatrix} = \text{Hermitian conjugate matrix}$$

If $\mathbf{A}^\dagger = \mathbf{A}$, then the matrix is said to be *Hermitian*. If $\mathbf{A}^\dagger = \mathbf{A}^{-1}$, then the matrix is said to be *unitary*. These terms will arise later in Quantum Mechanics.

We are now in a position to fix our notation so that it conforms to standards.

3.3 Putting it all together

We have these definitions (from Dirac):

$$|V\rangle = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \text{"ket" vector} \quad (3.35)$$

$$\langle V| = (v_1^* \quad v_2^*) = \text{"bra" vector} \quad (3.36)$$

$$\langle V|U\rangle = (v_1^* \quad v_2^*) \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = v_1^* u_1 + v_2^* u_2 = \text{"braket"} \quad (3.37)$$

where we used matrix multiplication in the last equation.

We now assume that all vectors are unit vectors since this will be the case in Quantum Mechanics.

3.4 Thinking about operators

3.4.1 Definition

There exists another very important mathematical object in the study of linear algebra that we will need in Quantum Mechanics. This object is an *operator*, which we define in this way:

An *operator* is a mathematical object which acts on a vector in the vector space and results in another vector in the *same* vector space.

For example, consider the operation shown below:

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \quad , \quad |V\rangle = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$$

$$\mathbf{A}|V\rangle = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} a_{11}v_1 + a_{12}v_2 \\ a_{21}v_1 + a_{22}v_2 \end{pmatrix} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = |U\rangle$$

Thus, \mathbf{A} acting on vector $|V\rangle$ results in another vector $|U\rangle$ and this implies that \mathbf{A} is an operator in the vector space that contains the vectors $|V\rangle$ and $|U\rangle$. All 2×2 matrices are operators in the vector space of 2×1 column vectors.

Operators are very important because *observables* or quantities that can be measured will be represented in Quantum Mechanics by Hermitian operators (matrices) and *transformations* or physical changes of the vectors will be represented in Quantum Mechanics by Unitary operators (matrices).

3.4.2 Properties of operators

If we have an operator $\hat{\mathbf{O}}$ (note boldface + “hat” notation), then we can define the following properties:

1. The matrix that corresponds to an operator in the $\{|1\rangle, |2\rangle\}$ basis (the matrix representation in this basis) is given by

$$\mathbf{O} = \begin{pmatrix} \langle 1 | \hat{\mathbf{O}} | 1 \rangle & \langle 1 | \hat{\mathbf{O}} | 2 \rangle \\ \langle 2 | \hat{\mathbf{O}} | 1 \rangle & \langle 2 | \hat{\mathbf{O}} | 2 \rangle \end{pmatrix} = \begin{pmatrix} o_{11} & o_{12} \\ o_{21} & o_{22} \end{pmatrix}$$

where $o_{nm} = \langle n | \hat{\mathbf{O}} | m \rangle$ is the nm matrix element (n^{th} row - m^{th} column) of $\hat{\mathbf{O}}$. If we assume, for illustration, that

$$\hat{\mathbf{O}} |1\rangle = |q\rangle \quad , \quad \hat{\mathbf{O}} |2\rangle = |r\rangle$$

where $|u\rangle$ and $|r\rangle$ are two new vectors in the vector space, then we evaluate the matrix elements as shown below:

$$o_{11} = \langle 1 | \hat{\mathbf{O}} | 1 \rangle = \langle 1 | r \rangle$$

$$o_{12} = \langle 1 | \hat{\mathbf{O}} | 2 \rangle = \langle 1 | q \rangle$$

$$o_{21} = \langle 2 | \hat{\mathbf{O}} | 1 \rangle = \langle 2 | q \rangle$$

$$o_{22} = \langle 2 | \hat{\mathbf{O}} | 2 \rangle = \langle 2 | r \rangle$$

2. If an operator acts on a vector and the result is the *same* vector, possibly multiplied by a constant number, i.e., if

$$\hat{\mathbf{A}} |V\rangle = a |V\rangle$$

then $|V\rangle$ is called an *eigenvector* of the operator $\hat{\mathbf{A}}$ with *eigenvalue* a . For Hermitian operators, used for observables in Quantum Mechanics, the set of eigenvectors of an operator always forms an orthonormal basis - they are called a *complete* set. If the basis used to calculate the matrix representing an operator is the set of eigenvectors of that operator, i.e., if

$$\hat{\mathbf{O}} |1\rangle = o_1 |1\rangle \quad , \quad \hat{\mathbf{O}} |2\rangle = o_2 |2\rangle$$

i.e., the eigenvalues are the set $\{o_1, o_2\}$, then we have

$$o_{11} = \langle 1 | \hat{\mathbf{O}} | 1 \rangle = o_1 \langle 1 | 1 \rangle = o_1$$

$$o_{12} = \langle 1 | \hat{\mathbf{O}} | 2 \rangle = o_2 \langle 1 | 2 \rangle = 0$$

$$o_{21} = \langle 2 | \hat{\mathbf{O}} | 1 \rangle = o_1 \langle 2 | 1 \rangle = 0$$

$$o_{22} = \langle 2 | \hat{\mathbf{O}} | 2 \rangle = o_2 \langle 2 | 2 \rangle = o_2$$

or the matrix looks like

$$\mathbf{O} = \begin{pmatrix} \langle 1 | \hat{\mathbf{O}} | 1 \rangle & \langle 1 | \hat{\mathbf{O}} | 2 \rangle \\ \langle 2 | \hat{\mathbf{O}} | 1 \rangle & \langle 2 | \hat{\mathbf{O}} | 2 \rangle \end{pmatrix} = \begin{pmatrix} o_1 & 0 \\ 0 & o_2 \end{pmatrix}$$

in the representation given by the operator's own eigenvectors. In this case, it is a *diagonal* matrix (only nonzero elements are on the diagonal) and the diagonal elements are the eigenvalues. For general basis vectors, i.e., not eigenvectors, the matrix representing an operator is generally not diagonal.

3. An alternate method for representing operators uses the “ket” and “bra” vectors as shown below. Consider the quantity $\mathcal{P}_{fg} = |f\rangle\langle g|$. We have

$$\mathcal{P}_{fg}|V\rangle = (|f\rangle\langle g|)|V\rangle = \langle g|V\rangle|f\rangle = \text{number} \times |f\rangle$$

This object satisfies the definition for an operator which means it is an operator! They are called “ket-bra”s. If the labels f and g are the same, then we have $\mathcal{P}_f = |f\rangle\langle f|$. This object is called a *projection operator*. It also acts on any vector and always turns it into the vector $|f\rangle$ multiplied by a number equal to the component of the vector in the direction of $|f\rangle$, i.e.,

$$\mathcal{P}_f|V\rangle = (|f\rangle\langle f|)|V\rangle = \langle f|V\rangle|f\rangle$$

Projection operators also have the following property.

$$\mathcal{P}_f^2 = (|f\rangle\langle f|)(|f\rangle\langle f|) = \langle f|f\rangle|f\rangle\langle f| = |f\rangle\langle f| = \mathcal{P}_f$$

Notice the algebraic rule (2 consecutive vertical bars become 1 vertical bar) that was used in the last equation is

$$(\langle f|)(|f\rangle) = \langle f|f\rangle$$

This will happen many times in our derivations.

Let us now consider the projection operators for our basis vectors $\{|n\rangle\}$, $n = 1, 2, 3, \dots, N$. We must have (for $\mathcal{P}_k = |k\rangle\langle k|$)

$$\begin{aligned}\mathcal{P}_k^2|n\rangle &= \mathcal{P}_k|n\rangle \\ (\mathcal{P}_k - \mathcal{P}_k^2)|n\rangle &= 0 \\ \mathcal{P}_k(1 - \mathcal{P}_k)|n\rangle &= 0\end{aligned}$$

which says that

$$\mathcal{P}_k|n\rangle = (|k\rangle\langle k|)|n\rangle = \langle k|n\rangle|k\rangle = \delta_{nk}|k\rangle = \begin{cases} |k\rangle & n = k \\ 0 & n \neq k \end{cases}$$

This also says that the only eigenvalues of \mathcal{P}_k are 0, 1 for any value of k , i.e.,

$$\begin{aligned}\mathcal{P}_k|k\rangle &= \langle k|k\rangle|k\rangle = |k\rangle \\ \mathcal{P}_k|n \neq k\rangle &= \langle k|n\rangle|k\rangle = 0|k\rangle = 0\end{aligned}$$

Another very useful property of projection operators is the following. Consider, for the basis $\{|k\rangle\}$, $k = 1, 2, 3, \dots, n$, the quantity (called the “ket-bra sum”)

$$\sum_{k=1}^n |k\rangle \langle k|$$

We have, for any vector $|V\rangle$,

$$\left(\sum_{k=1}^n |k\rangle \langle k| \right) |V\rangle = \sum_{k=1}^n \langle k|V\rangle |k\rangle = |V\rangle$$

Thus, we find that this operator does not change anything, i.e., it is the *Identity* operator.

$$\sum_{k=1}^n |k\rangle \langle k| = \hat{\mathbf{I}}$$

This will be a very useful property later on when we study Quantum Mechanics and do any algebra involving vectors and operators.

4. Another very useful quantity will be the *expectation value* of an operator. The expectation value is a property of the operator and a vector. It is defined and calculated as follows.

The expectation value $\langle \hat{\mathbf{O}} \rangle$ of operator $\hat{\mathbf{O}}$ in the state $|V\rangle$ is given by

$$\langle \hat{\mathbf{O}} \rangle = \langle V | \hat{\mathbf{O}} | V \rangle \quad (3.38)$$

As we will see later in our discussion of Quantum Mechanics, the expectation value as defined above will correspond to the *average value* of a set of measurements of the observable O represented by the operator $\hat{\mathbf{O}}$ when the system being measured is in a system state represented by the vector $|V\rangle$.

5. We can use projection operators to obtain a very powerful and useful representation of an operator. Assume that we have some Hermitian operator $\hat{\mathbf{B}}$ and that $\hat{\mathbf{B}}$ has a set of eigenvectors and eigenvalues labeled as shown

$$\hat{\mathbf{B}} |b_k\rangle = b_k |b_k\rangle \quad k = 1, 2, 3, \dots, n$$

i.e., the eigenvectors are the set of states $\{|b_k\rangle\}$, $k = 1, 2, 3, \dots, n$ and the corresponding eigenvalues are the set of numbers $\{b_k\}$, $k = 1, 2, 3, \dots, n$. As we stated earlier, the set of eigenvectors of a Hermitian operator forms a complete, orthonormal set, which means that

$$\langle b_i | b_j \rangle = \delta_{ij}$$

Thus, the set of eigenvectors can be used as a set of basis vectors. In addition, for such a set of vectors we have the relationship

$$\sum_{k=1}^n |b_k\rangle \langle b_k| = \hat{\mathbf{I}}$$

Using this result we can write

$$\begin{aligned}\hat{\mathbf{B}} &= \hat{\mathbf{B}}\hat{\mathbf{I}} = \hat{\mathbf{B}} \sum_{k=1}^n |b_k\rangle \langle b_k| \\ &= \sum_{k=1}^n \hat{\mathbf{B}} |b_k\rangle \langle b_k| = \sum_{k=1}^n b_k |b_k\rangle \langle b_k|\end{aligned}$$

This gives a representation of an operator in terms of its eigenvalues and eigenvectors (or corresponding projection operators)

$$\hat{\mathbf{B}} = \sum_{k=1}^n b_k |b_k\rangle \langle b_k| = \sum_{k=1}^n b_k \mathcal{P}_{b_k} \quad (3.39)$$

6. This result allows us to discuss the properties of a function of an operator. Let us first consider the simple operators $\hat{\mathbf{B}}^2$, $\hat{\mathbf{B}}^3$, and $\hat{\mathbf{B}}^m$. We have

$$\begin{aligned}\hat{\mathbf{B}}^2 &= \left(\sum_{k=1}^n b_k |b_k\rangle \langle b_k| \right) \left(\sum_{m=1}^n b_m |b_m\rangle \langle b_m| \right) \\ &= \sum_{k=1}^n \sum_{m=1}^n b_k b_m |b_k\rangle \langle b_k | b_m\rangle \langle b_m| = \sum_{k=1}^n \sum_{m=1}^n b_k b_m |b_k\rangle \langle b_m| \delta_{km} \\ &= \sum_{k=1}^n b_k^2 |b_k\rangle \langle b_k|\end{aligned}$$

In a similar manner we find

$$\hat{\mathbf{B}}^3 = \sum_{k=1}^n b_k^3 |b_k\rangle \langle b_k|$$

and

$$\hat{\mathbf{B}}^n = \sum_{k=1}^n b_k^n |b_k\rangle \langle b_k|$$

Now, many functions can be represented as *power series*, i.e.,

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots = \sum_{k=0}^{\infty} a_k x^k$$

In particular, we have the results

$$\begin{aligned}
e^x &= \sum_{k=0}^{\infty} \frac{1}{k!} x^k \\
e^{\alpha x} &= \sum_{k=0}^{\infty} \frac{1}{k!} \alpha^k x^k \\
\sin x &= \sum_{k=0}^{\infty} \frac{1}{(2k+1)!} (-1)^k x^{2k+1} \\
\sin \alpha x &= \sum_{k=0}^{\infty} \frac{1}{(2k+1)!} (-1)^k \alpha^{2k+1} x^{2k+1} \\
\cos x &= \sum_{k=0}^{\infty} \frac{1}{(2k)!} (-1)^k x^{2k} \\
\cos \alpha x &= \sum_{k=0}^{\infty} \frac{1}{(2k)!} (-1)^k \alpha^{2k} x^{2k}
\end{aligned}$$

These power series are the actual definitions of the functions. The tables of these functions in books are calculated using these power series and your computer calculates them using the power series. These power series expansions allow us to find representation of some functions of operators.

7. In Quantum Mechanics we will be particularly interested in the exponential function of an operator. From the above results we can write

$$e^{\alpha \hat{\mathbf{O}}} = \sum_{k=0}^{\infty} \frac{1}{k!} \alpha^k \hat{\mathbf{O}}^k$$

In a special case, which arises often in Quantum Mechanics, we find that if $\hat{\mathbf{O}}^2 = \hat{\mathbf{I}}$, then

$$\begin{aligned}
e^{i\theta \hat{\mathbf{O}}} &= \sum_{k=0}^{\infty} \frac{1}{k!} (i\theta)^k \hat{\mathbf{O}}^k = \sum_{k=0}^{\infty} \frac{1}{k!} (i)^k \theta^k \hat{\mathbf{O}}^k \\
&= \hat{\mathbf{I}} + i\theta \hat{\mathbf{O}} + \frac{1}{2!} i^2 \theta^2 \hat{\mathbf{O}}^2 + \frac{1}{3!} i^3 \theta^3 \hat{\mathbf{O}}^3 + \frac{1}{4!} i^4 \theta^4 \hat{\mathbf{O}}^4 + \dots \\
&= \hat{\mathbf{I}} + i\theta \hat{\mathbf{O}} - \frac{1}{2!} \theta^2 \hat{\mathbf{O}}^2 - i \frac{1}{3!} \theta^3 \hat{\mathbf{O}}^3 + \frac{1}{4!} \theta^4 \hat{\mathbf{O}}^4 + \dots \\
&= \left(\hat{\mathbf{I}} - \frac{1}{2!} \theta^2 \hat{\mathbf{O}}^2 + \frac{1}{4!} \theta^4 \hat{\mathbf{O}}^4 + \dots \right) + i \left(\theta \hat{\mathbf{O}} - \frac{1}{3!} \theta^3 \hat{\mathbf{O}}^3 + \dots \right) \\
&= \left(\hat{\mathbf{I}} - \frac{1}{2!} \theta^2 \hat{\mathbf{I}} + \frac{1}{4!} \theta^4 \hat{\mathbf{I}} + \dots \right) + i \left(\theta \hat{\mathbf{O}} - \frac{1}{3!} \theta^3 \hat{\mathbf{O}} + \dots \right) \\
&= \cos \theta \hat{\mathbf{I}} + i \hat{\mathbf{O}} \sin \theta
\end{aligned} \tag{3.40}$$

where we have used

$$\hat{\mathbf{O}}^2 = \hat{\mathbf{O}}^4 = \hat{\mathbf{O}}^6 = \dots = \hat{\mathbf{I}}$$

and

$$\hat{\mathbf{O}} = \hat{\mathbf{O}}^3 = \hat{\mathbf{O}}^5 = \dots = \hat{\mathbf{O}}$$

The relationship Eq. (3.40) (it is a generalized Euler relation (from calculus) for an operator) will be very useful later on in our study of Quantum Mechanics.

It is only possible to prove this procedure works for a function of an operator if the function has a power series expansion. In Quantum Mechanics, however, one usually make the assumption that the process holds for any function, i.e., that we can always write

$$f(\hat{\mathbf{B}}) = \sum_{k=1}^n f(b_k) |b_k\rangle \langle b_k| \quad (3.41)$$

8. When working with ordinary numbers (a, b) , it is always true that $ab = ba$. However, this is not the case for operators and since Quantum Mechanics involves operators, this leads to some amazing consequences.

We now define a property called the *commutator* for two operators $\hat{\mathbf{A}}$ and $\hat{\mathbf{B}}$ as

$$\text{commutator} = [\hat{\mathbf{A}}, \hat{\mathbf{B}}] = \hat{\mathbf{A}}\hat{\mathbf{B}} - \hat{\mathbf{B}}\hat{\mathbf{A}} \quad (3.42)$$

The value of this commutator can be 0 in which case the two operators commute or it can be a number or another operator in which case the two operators do not commute.

9. We now show two other properties that will be useful.

$$\begin{aligned} |V\rangle &= v_1 |1\rangle + v_2 |2\rangle \quad , \quad |U\rangle = u_1 |1\rangle + u_2 |2\rangle \\ \langle V | U \rangle &= v_1^* u_1 + v_2^* u_2 \\ \langle U | V \rangle &= u_1^* v_1 + u_2^* v_2 = \langle V | U \rangle^* \end{aligned} \quad (3.43)$$

$$\begin{aligned} |V\rangle &= \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \\ \langle V| &= (v_1^* \quad v_2^*) = |V\rangle^\dagger \end{aligned} \quad (3.44)$$

3.4.3 Finding eigenvalues and eigenvectors

Since eigenvalues and eigenvectors are so important in Quantum Mechanics let us develop the procedure for determining them. We will only consider 2×2 matrices in our discussion. This means that the vector space we are working with is 2-dimensional and has basis sets with 2 vectors. We will only need properties of a 2-dimensional vector space in our later discussions.

The first operator we consider is $\hat{\sigma}_3$ which has these properties

$$\hat{\sigma}_3 |1\rangle = |1\rangle \quad , \quad \hat{\sigma}_3 |-1\rangle = -|-1\rangle \quad (3.45)$$

i.e., the vectors $|\pm 1\rangle$ are eigenvectors of $\hat{\sigma}_3$ with eigenvalues ± 1 , respectively. Remember they are orthonormal, i.e.,

$$\langle 1 | -1 \rangle = 0 = \langle -1 | 1 \rangle \quad \text{and} \quad \langle 1 | 1 \rangle = 1 = \langle -1 | -1 \rangle \quad (3.46)$$

The matrix representing $\hat{\sigma}_3$ in the basis $\{|1\rangle, |-1\rangle\}$ is given by

$$\sigma_3 = \begin{pmatrix} \langle 1 | \hat{\sigma}_3 | 1 \rangle & \langle 1 | \hat{\sigma}_3 | -1 \rangle \\ \langle -1 | \hat{\sigma}_3 | 1 \rangle & \langle -1 | \hat{\sigma}_3 | -1 \rangle \end{pmatrix} = \begin{pmatrix} \langle 1 | 1 \rangle & -\langle 1 | -1 \rangle \\ -\langle -1 | 1 \rangle & -\langle -1 | -1 \rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (3.47)$$

i.e., the matrix representation will be diagonal with the eigenvalues as matrix elements, as we indicated earlier, when we are using the basis of eigenvectors. In this case, the corresponding eigenvectors are

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad |-1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (3.48)$$

i.e., we have

$$\hat{\sigma}_3 |1\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |1\rangle \quad (3.49)$$

as expected.

We now consider the operator $\hat{\sigma}_1$ which has these properties

$$\hat{\sigma}_1 |1\rangle = |-1\rangle \quad , \quad \hat{\sigma}_1 |-1\rangle = -|1\rangle \quad (3.50)$$

The matrix representing $\hat{\sigma}_1$ in the basis $\{|1\rangle, |-1\rangle\}$ is given by

$$\sigma_1 = \begin{pmatrix} \langle 1 | \hat{\sigma}_1 | 1 \rangle & \langle 1 | \hat{\sigma}_1 | -1 \rangle \\ \langle -1 | \hat{\sigma}_1 | 1 \rangle & \langle -1 | \hat{\sigma}_1 | -1 \rangle \end{pmatrix} = \begin{pmatrix} \langle 1 | -1 \rangle & \langle 1 | 1 \rangle \\ \langle -1 | -1 \rangle & \langle -1 | 1 \rangle \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (3.51)$$

Let us define the two eigenvectors of $\hat{\sigma}_1$ by

$$|\pm\rangle = \begin{pmatrix} a_{\pm} \\ b_{\pm} \end{pmatrix} \quad (3.52)$$

We then have for either eigenvector

$$\hat{\sigma}_1 |\pm\rangle = \lambda_{\pm} |\pm\rangle \quad (3.53)$$

where the λ_{\pm} are the corresponding eigenvalues. Using the matrix representations we have

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a_{\pm} \\ b_{\pm} \end{pmatrix} = \lambda_{\pm} \begin{pmatrix} a_{\pm} \\ b_{\pm} \end{pmatrix} = \lambda_{\pm} \hat{I} \begin{pmatrix} a_{\pm} \\ b_{\pm} \end{pmatrix} = \lambda_{\pm} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} a_{\pm} \\ b_{\pm} \end{pmatrix} = \begin{pmatrix} \lambda_{\pm} & 0 \\ 0 & \lambda_{\pm} \end{pmatrix} \begin{pmatrix} a_{\pm} \\ b_{\pm} \end{pmatrix}$$

or

$$\left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \begin{pmatrix} \lambda_{\pm} & 0 \\ 0 & \lambda_{\pm} \end{pmatrix} \right] \begin{pmatrix} a_{\pm} \\ b_{\pm} \end{pmatrix} = \begin{pmatrix} -\lambda_{\pm} & 1 \\ 1 & -\lambda_{\pm} \end{pmatrix} \begin{pmatrix} a_{\pm} \\ b_{\pm} \end{pmatrix} = 0 \quad (3.54)$$

This represents two homogeneous simultaneous equations for the numbers (a_{\pm}, b_{\pm}) , i.e.,

$$\begin{aligned} -\lambda_{\pm}a_{\pm} + b_{\pm} &= 0 \\ a_{\pm} - \lambda_{\pm}b_{\pm} &= 0 \end{aligned} \quad (3.55)$$

There is a non-trivial solution only if the determinant of the matrix is $= 0$, i.e., if

$$\det \begin{pmatrix} -\lambda_{\pm} & 1 \\ 1 & -\lambda_{\pm} \end{pmatrix} = \lambda_{\pm}^2 - 1 = 0 \quad (3.56)$$

The last equation is called the *characteristic equation* and it says that $\lambda_{\pm} = \pm 1$ are the eigenvalues. We determine the eigenvectors as follows. We must have

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a_{\pm} \\ b_{\pm} \end{pmatrix} = \lambda_{\pm} \begin{pmatrix} a_{\pm} \\ b_{\pm} \end{pmatrix} = \pm \begin{pmatrix} a_{\pm} \\ b_{\pm} \end{pmatrix}$$

or

$$\begin{pmatrix} b_{\pm} \\ a_{\pm} \end{pmatrix} = \pm \begin{pmatrix} a_{\pm} \\ b_{\pm} \end{pmatrix} \quad (3.57)$$

This gives $a_{\pm} = b_{\pm}$ or $a_{\pm} = -b_{\pm}$. Since we want the eigenvectors to have unit length we choose $a_{\pm} = b_{\pm} = 1/\sqrt{2}$ in the first case and $a_{\pm} = -b_{\pm} = 1/\sqrt{2}$ in the second case. The eigenvectors are then give by

$$|\pm\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} \quad (3.58)$$

The procedure is tedious but straightforward.

3.4.4 An interesting thought

Earlier we defined the expectation value or average value for some observable $\hat{\mathbf{B}}$ in the state $|V\rangle$ as

$$\langle \hat{\mathbf{B}} \rangle = \langle V | \hat{\mathbf{B}} | V \rangle \quad (3.59)$$

Since the eigenvectors of the operator $\hat{\mathbf{B}}$ form a basis we can always write any vector in the space in terms of the eigenvectors of $\hat{\mathbf{B}}$, i.e., we can write

$$\begin{aligned} |V\rangle &= \sum_{k=1}^n d_k |b_k\rangle \quad , \quad d_k = \langle b_k | V \rangle \\ \langle V| &= \sum_{k=1}^n d_k^* \langle b_k| \end{aligned} \quad (3.60)$$

Therefore, we get

$$\begin{aligned}
\langle \hat{\mathbf{B}} \rangle &= \left(\sum_{k=1}^n d_k^* \langle b_k | \right) \hat{\mathbf{B}} \left(\sum_{m=1}^n d_m | b_m \rangle \right) = \sum_{k=1}^n \sum_{m=1}^n d_k^* d_m \langle b_k | \hat{\mathbf{B}} | b_m \rangle \\
&= \sum_{k=1}^n \sum_{m=1}^n d_k^* d_m \langle b_k | b_m \rangle = \sum_{k=1}^n \sum_{m=1}^n d_k^* d_m b_m \langle b_k | b_m \rangle \\
&= \sum_{k=1}^n \sum_{m=1}^n d_k^* d_m b_m \delta_{km} = \sum_{k=1}^n b_k d_k^* d_k \\
&= \sum_{k=1}^n b_k |d_k|^2
\end{aligned} \tag{3.61}$$

Now in general, however, the average value of any set of measurements is given by the expression

$$\langle \hat{\mathbf{B}} \rangle = \sum_{\text{allowed values}} (\text{allowed value of } \mathbf{B}) \times (\text{Probability of that value}) \tag{3.62}$$

Comparing (1.45) and (1.46) we might make the guess that the allowed values of $\hat{\mathbf{B}}$ are its eigenvalues, i.e., you can only measure eigenvalues, and the probability of measuring a particular eigenvalue is given by $|d_k|^2$. These results will, in fact, be two of our postulate when we formulate Quantum Mechanics later.

We also note that

$$|d_k|^2 = d_k^* d_k = (\langle b_k | V \rangle)^* \langle b_k | V \rangle = |\langle b_k | V \rangle|^2 = \langle V | b_k \rangle \langle b_k | V \rangle \tag{3.63}$$

This says that $|\langle b_k | V \rangle|^2$ is the probability of observing value b_k when in the state $|V\rangle$. It also says that $\langle V | b_k \rangle \langle b_k | V \rangle = \langle V | \mathcal{P}_{b_k} | V \rangle$ is the probability of observing value b_k when in the state $|V\rangle$. This last expression is the expectation value of the corresponding projection operator.

That is almost all of the mathematics we will need to begin our study of Quantum Mechanics. Try the problems at the end of this chapter.

3.5 Problems

3.5.1 Complex Numbers

Prove the following properties of complex numbers:

- (a) $\text{Real}(z) = \frac{z+z^*}{2}$, $\text{Imag}(z) = \frac{z-z^*}{2}$
- (b) z is a pure real number if and only if $z^* = z$ and z is a pure imaginary number if and only if $z^* = -z$
- (c) $z^{**} = z$, $(z_1 + z_2)^* = z_1^* + z_2^*$, $(z_1 z_2)^* = z_1^* z_2^*$

- (d) $|z|^2 = (\text{Real}(z))^2 + (\text{Imag}(z))^2$
- (e) $|z| \geq |\text{Real}(z)|$ and $|z| \geq |\text{Imag}(z)|$
- (f) $|z_1 + z_2| \leq |z_1| + |z_2|$

3.5.2 Complex Expressions

- (a) $z = (2 + 3i)^3$
- (b) $z = \frac{1}{i-1}$

3.5.3 More Vectors

Given two vectors

$$\vec{A} = 7\hat{e}_1 + 6\hat{e}_2 - 13\hat{e}_3 \quad , \quad \vec{B} = -2\hat{e}_1 + 16\hat{e}_2 + 4\hat{e}_3$$

- (a) Determine $\vec{A} \pm \vec{B}$
- (b) Determine $\vec{A} \cdot \vec{B}$
- (c) Determine a unit vector in the same direction as \vec{A}

3.5.4 Simple Basis Vectors

Given two vectors

$$\vec{A} = 7\hat{e}_1 + 6\hat{e}_2 \quad , \quad \vec{B} = -2\hat{e}_1 + 16\hat{e}_2$$

written in the $\{\hat{e}_1, \hat{e}_2\}$ basis set and given another basis set

$$\hat{e}_q = \frac{1}{2}\hat{e}_1 + \frac{\sqrt{3}}{2}\hat{e}_2 \quad , \quad \hat{e}_p = -\frac{\sqrt{3}}{2}\hat{e}_1 + \frac{1}{2}\hat{e}_2$$

- (a) Show that \hat{e}_q and \hat{e}_p are orthonormal.
- (b) Determine the new components of \vec{A} , \vec{B} in the $\{\hat{e}_q, \hat{e}_p\}$ basis set.

3.5.5 Operators Acting

Given two operators

$$\hat{O}_1 = \begin{pmatrix} 1 & 2 \\ 3 & 6 \end{pmatrix} \text{ and } \hat{O}_2 = \begin{pmatrix} 10 & 4 \\ -5 & -2 \end{pmatrix}$$

and two vectors

$$|X\rangle = \begin{pmatrix} 3 \\ -1 \end{pmatrix} \text{ and } |Y\rangle = \begin{pmatrix} 2 \\ 4 \end{pmatrix}$$

Determine $\hat{O}_1 |X\rangle$, $\hat{O}_2 |X\rangle$, $\hat{O}_1 |Y\rangle$, and $\hat{O}_2 |Y\rangle$

3.5.6 Eigenvectors

Here is an operator and four vectors

$$\hat{O} = \begin{pmatrix} 3 & 2 \\ 1 & 2 \end{pmatrix}, |A\rangle = \begin{pmatrix} 1 \\ -1 \end{pmatrix}, |B\rangle = \begin{pmatrix} 1 \\ 2 \end{pmatrix}, |C\rangle = \begin{pmatrix} 2 \\ 1 \end{pmatrix}, |D\rangle = \begin{pmatrix} 1 \\ -2 \end{pmatrix}$$

Which of the four vectors are eigenvectors of the operator \hat{O} and what are their eigenvalues?

3.5.7 Linear Functional

We call $|\psi\rangle$ a ket-vector and $\langle\psi|$ its dual vector or bra-vector. Technically the dual vector is a linear functional, that is, a new mathematical object which has the property of turning ket-vectors into numbers (complex). An “operational” way to define (as in the text) the linear functional or bra-vector is as follows.

In a 2-dimensional vector space, if $|\psi\rangle = a_1|1\rangle + a_2|2\rangle$, the set $\{|1\rangle, |2\rangle\}$ form an orthonormal basis, then $\langle\psi| = a_1^*\langle 1| + a_2^*\langle 2|$. It then acts on a ket-vector to produce a scalar. Show that $\langle\psi|\psi\rangle = |a_1|^2 + |a_2|^2$.

3.5.8 Eigenvectors

Find the eigenvalues and eigenvectors of the operator

$$\hat{O} = \begin{pmatrix} 0 & 2 \\ 2 & 3 \end{pmatrix}$$

3.5.9 Matrix Properties

Given two operators

$$\hat{B} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{C} = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix}$$

Show that

- (a) $\hat{C} = \hat{I} + 2\hat{B}$
- (b) Show that $[\hat{B}, \hat{C}] = 0$
- (c) Find the eigenvectors and eigenvalues of \hat{B} and \hat{C}

3.5.10 Multiplying Matrices

- (a) Multiply the two matrices

$$\hat{A} = \begin{pmatrix} 1 & 5 & 4 \\ 7 & 2 & 1 \\ 9 & 2 & 3 \end{pmatrix}, \quad \hat{B} = \begin{pmatrix} 6 & 9 & -2 \\ 5 & 5 & -3 \\ -3 & -5 & 1 \end{pmatrix}$$

- (b) Determine the commutator $[\hat{A}, \hat{B}]$

3.5.11 Operator Algebra

An operator for a two-state system is given by

$$\hat{H} = a (|1\rangle \langle 1| - |2\rangle \langle 2| + |1\rangle \langle 2| + |2\rangle \langle 1|)$$

where a is a number. Find the eigenvalues and the corresponding eigenkets.

3.5.12 Eigenvalues and Eigenvectors

Find the eigenvalues and normalized eigenvectors of the matrix

$$A = \begin{pmatrix} 1 & 2 & 4 \\ 2 & 3 & 0 \\ 5 & 0 & 3 \end{pmatrix}$$

Are the eigenvectors orthogonal? Comment on this.

3.5.13 Operator Matrix Representation

If the states $\{|1\rangle, |2\rangle, |3\rangle\}$ form an orthonormal basis and if the operator \hat{G} has the properties

$$\begin{aligned}\hat{G}|1\rangle &= 2|1\rangle - 4|2\rangle + 7|3\rangle \\ \hat{G}|2\rangle &= -2|1\rangle + 3|3\rangle \\ \hat{G}|3\rangle &= 11|1\rangle + 2|2\rangle - 6|3\rangle\end{aligned}$$

What is the matrix representation of \hat{G} in the $|1\rangle, |2\rangle, |3\rangle$ basis?

3.5.14 Matrix Representation and Expectation Value

If the states $\{|1\rangle, |2\rangle, |3\rangle\}$ form an orthonormal basis and if the operator \hat{K} has the properties

$$\begin{aligned}\hat{K}|1\rangle &= 2|1\rangle \\ \hat{K}|2\rangle &= 3|2\rangle \\ \hat{K}|3\rangle &= -6|3\rangle\end{aligned}$$

- (a) Write an expression for \hat{K} in terms of its eigenvalues and eigenvectors (projection operators). Use this expression to derive the matrix representing \hat{K} in the $|1\rangle, |2\rangle, |3\rangle$ basis.
- (b) What is the *expectation or average value* of \hat{K} , defined as $\langle \alpha | \hat{K} | \alpha \rangle$, in the state

$$|\alpha\rangle = \frac{1}{\sqrt{83}} (-3|1\rangle + 5|2\rangle + 7|3\rangle)$$

3.5.15 Projection Operator Representation

Let the states $\{|1\rangle, |2\rangle, |3\rangle\}$ form an orthonormal basis. We consider the operator given by $\hat{P}_2 = |2\rangle\langle 2|$. What is the matrix representation of this operator? What are its eigenvalues and eigenvectors. For the arbitrary state

$$|A\rangle = \frac{1}{\sqrt{83}} (-3|1\rangle + 5|2\rangle + 7|3\rangle)$$

What is the result of $\hat{P}_2|A\rangle$?

3.5.16 Spectral Decomposition

Find the eigenvalues and eigenvectors of the matrix

$$M = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

Construct the corresponding projection operators, and verify that the matrix can be written in terms of its eigenvalues and eigenvectors. This is the spectral decomposition for this matrix.

3.5.17 Measurement Results

Given particles in state

$$|\alpha\rangle = \frac{1}{\sqrt{83}} (-3|1\rangle + 5|2\rangle + 7|3\rangle)$$

where $\{|1\rangle, |2\rangle, |3\rangle\}$ form an orthonormal basis, what are the possible experimental results for a measurement of

$$\hat{Y} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & -6 \end{pmatrix}$$

(written in this basis) and with what probabilities do they occur?

3.5.18 Expectation Values

Let

$$R = \begin{bmatrix} 6 & -2 \\ -2 & 9 \end{bmatrix}$$

represent an observable, and

$$|\Psi\rangle = \begin{bmatrix} a \\ b \end{bmatrix}$$

be an arbitrary state vector (with $|a|^2 + |b|^2 = 1$). Calculate $\langle R^2 \rangle$ in two ways:

- (a) Evaluate $\langle R^2 \rangle = \langle \Psi | R^2 | \Psi \rangle$ directly.
- (b) Find the eigenvalues(r_1 and r_2) and eigenvectors($|r_1\rangle$ and $|r_2\rangle$) of R^2 or R . Expand the state vector as a linear combination of the eigenvectors and evaluate

$$\langle R^2 \rangle = r_1^2 |c_1|^2 + r_2^2 |c_2|^2$$

Chapter 4

A Simple Introduction to Quantum Ideas via Experiments

4.1 Superposition - World of Color and Hardness

We start our discussion of quantum mechanics with a story about something that can happen to various particles in the microworld, which we will call *electrons*. All the experiments that will be described in this story have actually been performed. We will discuss real experiments corresponding to some of them later. The story is about two *physical properties* of electrons that we can measure with great accuracy. The precise physical definitions of these properties will not matter. They do however, correspond to real properties of electrons or photons as we shall see later. We will call them *hardness* and *color*.

4.1.1 The Strange World of Color and Hardness

It is *experimental fact* that color property of electrons can assume only two values, namely, *green* or *magenta*. This simply means that *nothing else has ever been observed (measured)* for the color property of an electron. A similar situation exists for the hardness property. Electrons are either *hard* or *soft* (the only possibilities). *Nothing else has ever been observed*.

It is possible to build a device we will call a *color box*, which measures the color of an electron. It is a box (expensive, complicated stuff inside) with three apertures as shown below.

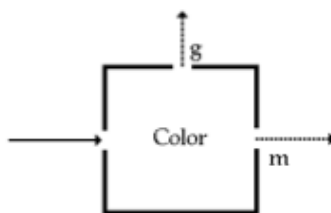


Figure 4.1: Color Box

We can also build a hardness measuring box that works in a similar way. It is shown below.

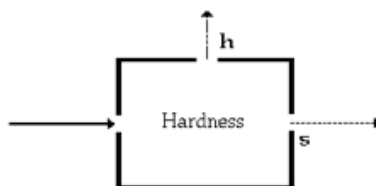


Figure 4.2: Hardness Box

For real electrons, these hardness and color boxes are called *Stern-Gerlach devices* and for real photons these hardness and color boxes are called *Polaroids*, as we will see later.

The world of color and hardness exhibits all the same physics as the real world devices without introducing any of the real world complications, i.e., we do not need to discuss in detail how these boxes work.

In both cases, electrons enter the boxes through the left aperture and the boxes separate the electrons *in physical space* (put them onto different paths) according to the value of the color or hardness as shown. Thus, in either case, we can distinguish the electrons after they pass through one of the boxes by their final position(path) in real physical space, i.e., *we have separate beams at the end*.

EXPERIMENTAL PROPERTY: *Measurements with hardness or color boxes are repeatable.*

That is, if one color box determines that an electron is magenta and if that electron (without having been tampered (we will see later exactly what that statement means) with in between measurements) is subsequently (immediately) sent into the left aperture of another color box, then that electron will (*with probability* = 1) emerge from the second box through the magenta aperture. This is

illustrated below.

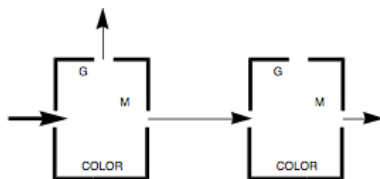


Figure 4.3: Repeatability Experiment

The *same property* of repeatability *holds* for green electrons and color boxes and for hard or soft electrons with hardness boxes.

This is simply a statement of the way the real microworld and its measuring devices work in the laboratory. We want our representation of the real world to behave that way also.

Now, suppose that we *suspect* there is a possibility that the color and hardness properties of electrons are *related* in some way. One way to look for such a relation is to check for *correlations* (or relationships) between the measured values of the hardness and color properties of electrons. Our boxes (*real world experiments*) make it very easy to check whether such correlations exist.

After much experimentation, it turns out that no such correlations exist, i.e.,
of any large collection of, say, magenta electrons, all of which are fed into the left aperture of a hardness box, precisely half emerge through the hard aperture, and precisely half emerge through the soft aperture.

The same result occurs for green electrons and similar results hold if we send hard or soft electrons into a color box. This is shown below.

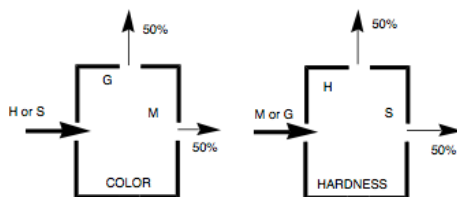


Figure 4.4: Correlation Experiment

The color (hardness) of an electron *apparently gives no information* about its hardness (color). There does not seem to be any correlations.

Now, suppose we set up a *sequence of three boxes*. First a color box, then a hardness box and finally another color box as shown below:

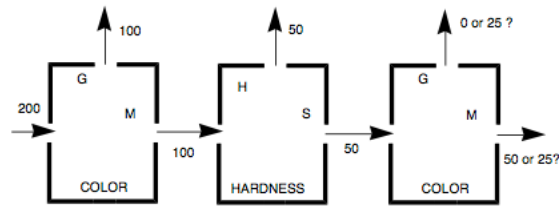


Figure 4.5: Measurements Disturb

In this experiment, suppose an electron that emerges from the magenta aperture of the first color box then goes into the left aperture of the hardness box (remember it must not be tampered with in between or there must be no other measurements of any kind or essentially no time interval).

Suppose it then emerges from the hardness box through the soft aperture (as half of the magenta electrons will do) and it is sent into the left aperture of the last color box (again no measurements or time intervals allowed).

Presumably, the electron that enters that last box is known to be both magenta and soft, which were the results of the two previous measurements just made on it.

If this were so, then we would expect the electron to emerge from the magenta aperture (with *probability* = 1), *confirming* the result of the first measurement.

Any reputable *classical* physicist would say at this point that electrons entering the last color box are known to be

magenta AND soft

In the classical world, particles have objective reality - they have *real* properties and we *measure to find out* the values of the properties.

THE PROBLEM: *this is not what happens in the real world in this experiment!*

Precisely *half* of the electrons entering the last box emerge from the magenta aperture and precisely *half* emerge from the green aperture!!

Therein lies the fundamental puzzle of the quantum world.

In fact, if the first two measurements give

magenta AND soft
or magenta AND hard
or green AND soft
or green AND hard

which represents *all* the possible cases, then, when any of these beams is sent into the last box, precisely half emerge from each aperture!!

The *same* kind of results hold if we switch the hardness and color boxes.

It seems as if the presence of the hardness box between the two color boxes constitutes some sort of color measurement or color tampering and vice versa.

The hardness box *seems* to be *changing half* of the magenta electrons into green electrons. As we will see, this will turn out to be an incorrect way of thinking about the results of the experiment!

The hardness box *must be the blame* since if it not there, then the last box would only see magenta electrons(a *different* experiment that corresponds to repeatability) as shown below.

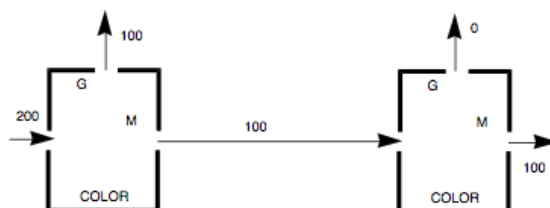


Figure 4.6: No Hardness Box = Repeatability

Now all this seems so *weird (non-classical)* that we must *question (challenge)* all features of the experiment *before* we accept the story as truth.

Perhaps the hardness box is *poorly built* (we did not get enough \$\$\$\$ from Congress in our research grant).

Maybe it is measuring hardness correctly, but while doing that job it apparently *does disrupt color* because of bad design.

This raises *two fundamental questions*:

- (1) Can hardness boxes be built that will measure hardness without disrupting color?

- (2) In the case of a poorly built apparatus it seems as if half of the electrons change color....what is it that determines which electrons have their color changed and which do not change?

We address the second question first.

The way to discover the determining factor(s) (*if there are any to be discovered!*) is to carefully monitor the *correlations* between all the measurable properties of the electrons that are sent into the first color box and found to be magenta and which aperture of the final color box they come out of.

Any *correlation* will tell us which property is the determining one. *All known experiments say no such correlations exist.*

Those electrons that have their color changed by passage through the hardness box and those electrons whose color is not changed by passage through the hardness box *do not differ* from one another in *any measurable way*.

So the second question has no answer that we can figure out from measurements.

If we believe, as I do, that we can only know properties that we can measure, then this would mean that there is NO answer to this question, i.e., there is no property of the electrons that determines which electrons get their color changed, which is completely counter to our classical notion of cause and effect and objective reality!!!

What about the first question?

It turns out that no matter how we build hardness boxes..... *remember that a device qualifies as a hardness box if it can separate electrons by their hardness value* they *all* disrupt color measurements in the same way.... they all change *precisely* half ... *exactly*, as far as any experiment can determine. Any hardness (color) measurement seems to *randomize* the next color (hardness) measurement, i.e., make it *50% green/ 50% magenta*.

Suppose we want to build a *color-AND-hardness box*.... a box that could determine both color and hardness for a single electron simultaneously (and we could convince some funding source to support us). This box would need *five* apertures as shown below.

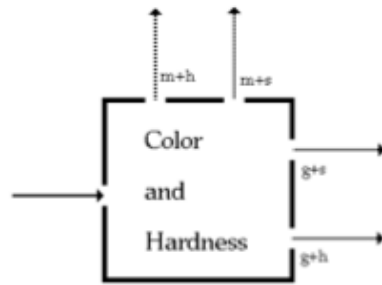


Figure 4.7: Color AND Hardness Box

Let us try to build this device.

In *some manner* it has to consist of a hardness box *and* a color box (or their equivalents) because we must be measuring hardness and color in some way. But as we have already seen, whichever box the electrons pass through last provides reliable information *ONLY* about that measured quantity and the other quantity is *randomized* (i.e., half/half). *No one has succeeded* in building a device which can simultaneously measure both color and hardness. It seems to *fundamentally* be beyond our means *no matter how clever we are*. The universe just seems to work in this peculiar manner!! As we will see later, this is just a reflection of the **Uncertainty Principle of Heisenberg**. *Measurable quantities* like hardness and color are said to be *incompatible* with one another since a measurement of one *ALWAYS NECESSARILY disrupts(randomizes)* the other.

4.1.2 Probing Deeper

Let us probe into this situation more deeply. Consider the more complicated experimental device shown below.

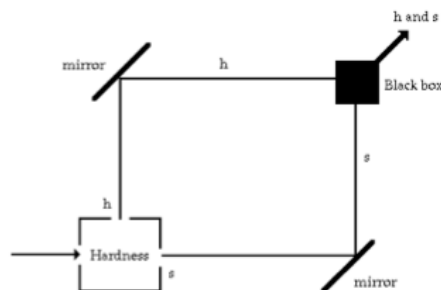


Figure 4.8: Two Path Experiment

The *mirrors* in this device are just reflecting devices of some kind which only change the electron direction and do nothing else (in particular they *do not* change hardness or color during the direction changing process). We have drawn the device in this way so that you could easily see what it is doing. No real mirrors are necessarily involved. This experiment is the equivalent, in the color/hardness world, of the two slit interference experiment with light(photons) that we will discuss later.

In this device, hard and soft electrons *follow different paths in physical space* and eventually the electrons are recombined into a single beam again in the *black box* at the end, i.e., all the *black box* does is to recombine the two beams back into one beam by direction changes (again without changing hardness or color values). So if we start with a mixed (hard + soft) beam of electrons, then we end up with a mixed (hard + soft) beam at the end.

The effectiveness of the device can be checked separately for both hard and soft electrons and it works.

That is, if hard or soft electrons are sent in separately, they simply travel along different paths and end up in the same place with their hardness property *unchanged*.

Here are some experiments we might *imagine* could be done with this apparatus. All of these experiments have actually been done in real laboratories with equivalent setups. **Listen carefully to see where your classical mind is misleading you.**

- (1) Send *magenta electrons* into the first hardness box. At the end (after beams are recombined) we *add* a final hardness box and thus we are *measuring their hardness* at that point. See figure below.

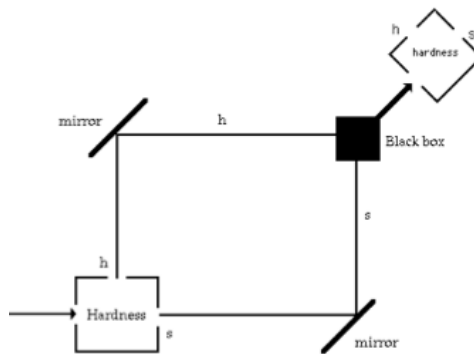


Figure 4.9: Magenta in - Measure Hardness at End

Analysis: For magenta electrons, 50% will take the h route and 50% will

take the s route so that at the end(recombined beam) 50% are hard electrons (remember nothing bothers hardness along the routes) and 50% are soft electrons.

- (2) Send *hard electrons* into the hardness box. At the end we *add* a color box (replace the final hardness box) and we measure their *color*. See figure below.

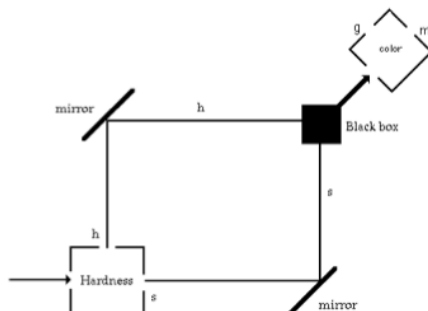


Figure 4.10: Hard in - Measure Color at End

Analysis: All hard electrons follow the h route. When you measure the color of a hard electron it is 50-50 green-magenta. Similarly for a soft electrons. Therefore we end up with 50-50 green/magenta coming out of the color box.

These experimental outcomes are what we would expect from our earlier results and they *do happen exactly as described* above in real world experiments. *So no problems yet!!!*

- (3) Now send *magenta electrons* into the hardness box. At the end we *add* a color box and we measure their *COLOR*. See figure below.

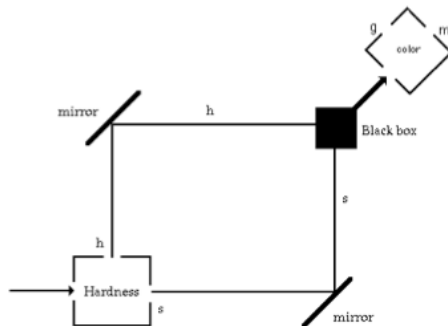


Figure 4.11: Magenta in - Measure Color at End

What do you expect? The *true classical physicist* would give this argument.

Since, for magenta electrons, 50% are hard and 50% are soft (*that is what happens to magenta electrons when they are sent into a hardness box* - they are *randomized*) and each kind of electron take the appropriate h and s routes, at the end, 50% of h (those on h route) electrons or 25% of the total are magenta and 50% of s (those on s route) electrons or 25% of total are magenta.

Thus, for 100% magenta sent in, our *classical reasoning* says that only 50% are magenta at the end.

This seems to be an valid conclusion since hardness boxes(*first box*) supposedly randomize color.

The problem is that this last part of the story, which your classical mind so desperately wants to accept as correct, *is false*. When you actually do this experiment, *all(100%) of the electrons at the end are magenta!!!*

This is very odd. It is hard to imagine (classically) what can possibly be going on in this system.

Of course, maybe our classically oriented minds *cannot imagine* what is happening and need to be *retrained!!!*

- (4) Let us try another experiment in the hopes of understanding what is going on.

We rig up a small, movable, electron-stopping wall that can be inserted in and out of route s.

When the wall is *out*, we have precisely our earlier apparatus. When the wall is *in*, only those electrons moving along the h route get through to the beam recombination device.

What should we expect to happen when we slide the wall in?

Analysis: First, there are 50% less electrons reaching the beam recombination device.

When wall is out all(100%) of the electrons that get to the beam recombination device are magenta at the end (the *earlier experimental result*).

That means (or *seems to mean*) that all the electrons that take the s route (or *we think they are taking the s route*) end up magenta and all that take

the h route (or *we think they are taking the h route*) end up magenta at the beam recombination device when no wall is inserted.

This means that with the wall inserted, we should end up with 50% (*1/2 lost impacting the inserted wall*) magenta at the beam recombination device. Based on the earlier experiment, they should all be magenta since the inserted wall *cannot affect* the electrons on the h path! This is an assumption called *locality*, which means the following:

we can separate the hard and soft paths by a large distance and therefore make sure that nothing we do on the soft path (like inserting a wall) can affect electrons on the hard path during the time they are on the hard path - this is possible because the maximum speed of information transfer is the speed of light - as one learns from the study of relativity.

What is the actual result? Again we are wrong in the classical way we are analyzing things. *The result is only 25%.*

The h route beam (*if there really is one*) seems to end up *randomized* (50-50 green-magenta) and 50% of 50% is 25%.

If we insert the wall in the h route, the same thing happens. We still end up only with 25% magenta!

Clearly, we have real trouble with the classical way of reasoning!

If we do not insert the wall, then 100% magenta sent into the device, ends up as 100% magenta out of the device.

If we put a wall on one path, then 100% magenta into the device, ends up as 25% magenta out of the device. Same result if we put the wall in the other path.

So it *seems* that if we check (*do a measurement*) to see on which path the electrons are passing through the device (i.e., *if we check to see whether a magenta electron is passing through the apparatus as a hard or soft electron*) we get 25% magenta (50% change to green) at the end and if we *DO NOT* check we get 100% magenta (0% change to green).

Our classical minds are spinning at this point!!

To begin to try to resolve this dilemma, we turn to a quantum system containing only *one particle* at any instant of time instead of using beams with many particles at any instant of time.

So now consider a *single* magenta electron which passes through our apparatus when the wall is out.

Can it have taken the h route? *No*, since all such electrons are hard and hard electrons are 50-50 green-magenta (and we need 100% magenta). If on hard path, then they are hard - *it is a measurement*.

Can it have taken the s route? *No*, since all such electrons are soft and soft electrons are 50-50 green-magenta (and we need 100% magenta). If on soft path, then they are soft - *it is a measurement*.

Can it somehow have taken *BOTH* routes at the *same time*?

If we look (*measure*), then half the time we find an electron on the h route and half the time we find an electron on the s route, but we *never find* two electrons in the apparatus, or *two halves* of a single, split electron, one-half on each route, or anything like that.

There just is *not any experimental way* in which the electron seems to be taking both routes simultaneously. Therefore, as physicists, we must rule out this possibility.

Can it have taken *neither route* (*got there some other way*)?

Certainly not.

If we put *walls in both routes*, then *NOTHING* gets through at all. Thus, the results had to have *something* to do with the box and paths.

Let us *summarize* these results to see the dilemma we (as classical physicists) are faced with in this experiment.

Electrons passing through this apparatus, in so far as we are able to figure out (*measure*) so far, *do not take route h and do not take route s and do not take both routes at the same time and do not take neither of the routes*, i.e., they have *zero probability* for doing all of these things (*from experiment*).

Our problem is that those *four possibilities* are simply *all of the logical possibilities* we have any notion of how to entertain using the *everyday language of classical physics*!

What can these electrons be doing?

They must be doing something which has simply never been thought of before by classical physics (assuming the experiments are correct and they

are!).

Electrons seem to have *modes of being*, or *modes of moving*, available to them which are *quite unlike* anything we know how to think about using *words derived from everyday ideas and classical physics*. The name of the new mode (*a name for something we do not understand at the moment*) is **SUPERPOSITION**.

What we now say about our initially magenta electron, which is passing through our apparatus with the wall out, is that it is *NOT* on the *h* path and *NOT* on the *s* path and *NOT* on both paths and *NOT* on neither, but rather it is in a *SUPERPOSITION of being on h and being on s*. What this last statement *means*, other than *none of the above*, we do not know at this time.

That is what we shall be trying to find out as we develop quantum theory in these notes.

It will force us, as we will see, to think in terms of *probabilities*, i.e., the magenta electron will have a probability of being hard or soft but is only observed to be magenta at the end if we do not check to see whether it is hard or soft during any intermediate stage of the experiment.

If we check to see if it is hard, then the probability that it is hard is *irreversibly realized* and we have hard electrons in the apparatus (*because we looked or measured?*).

Because this is a very important point in our discussions, we will now look at it in another way. The hope is that we will learn more about it and be able to decide how to build a theory that describes what is happening.

- (5) Let us construct a new experimental box which we will call a *do-nothing* box. It has only two apertures. An electron goes into one aperture and emerges from the other aperture with *ALL* of its measurable properties (color, hardness, energy, momentum, whatever) *UNCHANGED*.

This box does not measure anything itself. If we measure the properties of electrons before entering this box and then after passing through the box, no measured properties are changed. Also the time it takes for the electron to get through the box is *identical* to the time it would have taken if the box were not there. So *nothing mysterious* seems to be delaying it and messing around with it while it is in the box.

Such a *do-nothing* box can actually be constructed in the laboratory.

Now recall our two-path apparatus from our earlier discussions and hold

on to your seats. It is possible to build such a *do-nothing* box, which, when inserted into either one of the two paths of our apparatus, will *change* all of the electrons that were magenta at the end into green electrons at the end.

When the box is removed they go back to all being magenta. So inserting such a box into *one of those paths* will change the resultant color of an electron passing through the apparatus.

What is going on here?

Do-nothing boxes *do not change* any measurable property of electrons that pass through them (*by definition*) *AND of course*, do-nothing boxes *do not change* any measurable property of electrons that *DO NOT* pass through them. That would not make any sense at all.

So once again the only explanation will go like.....

It is not possible for the electron to have passed through the do-nothing box since we already said that cannot change anything. It is not possible for the electron to have passed outside the box since the box certainly does not have a chance to bother anything that does not even pass through it (*even though it would not do anything anyway*). It is not possible that the electron passes both inside and outside of the box or neither as before.

The only answer is that the electron passes through our apparatus in a superposition of passing through the do-nothing box and not passing through the do-nothing box and this must cause the color change somehow.

This theory has got to be really neat when we finally figure out what it is we are saying about the world.

4.2 Applying linear algebra ideas to Quantum Mechanics

Let us now develop a simple mathematical formalism that allows us to give a possible explanation of the non-classical results of the color/hardness experiments.

We define a *quantum state* as the set of information (obtained from measurements) that we know about a system. We represent such quantum states by a mathematical object called a *ket* (symbol = $|\dots\rangle$) with the properties that we have already discussed. This mathematical formalism is due to Dirac.

If an electron is in some arbitrary (we have not performed any measurements

on the electron yet) quantum state, we describe or represent it by a mathematical object given by the ket $|undetermined\rangle$. If we send this electron through a color box and it emerges from the magenta aperture (we know it is magenta because we did a measurement), then it is represented by the ket $|magenta\rangle = |m\rangle$. If it had emerged from the green aperture, then it is represented by the ket $|green\rangle = |g\rangle$. If, instead, we sent this electron through a hardness box and it emerges from the hard aperture, then it is represented by the ket $|hard\rangle = |h\rangle$. Finally, if it had emerged from the soft aperture, then it is represented by the ket $|soft\rangle = |s\rangle$.

This will be **Postulate #1** of quantum theory.

We describe a measuring device by the mathematical object called an *operator* that we have been discussing. As we saw earlier, operators have properties with respect to kets (or vectors) similar to the properties of *functions* in algebra. Remember that functions take numbers and change them into a new (or the same) number, i.e., the function f takes x into y , or $y = f(x)$, where x and y are numbers. Operators behave the same way for kets, i.e., for an operator \hat{O} we have the defining equation $|y\rangle = \hat{O}|x\rangle$. Let us now define four operators relevant to the experiments we have been discussing.

Let us try to imagine a simple model (probably incorrect but still instructive) of a measuring device, in particular, a *color box*. We first note the following properties of the vectors and operators we have been discussing.

$$\begin{aligned}\mathcal{P}_g|hard\rangle &= (|g\rangle\langle g|)|h\rangle \\ &= \langle g|h\rangle|g\rangle \rightarrow |g\rangle\end{aligned}\tag{4.1}$$

where the last step just removes the number $\langle g|h\rangle$ multiplying the final state vector since all state vectors in Quantum Mechanics must be unit vectors and $|g\rangle$ is already a unit vector. Thus the projection operator \mathcal{P}_g seems to represent a measurement of the green property of the electron in some manner. We can observe “how” it does this, but we cannot answer the question “why” it does it. This just reflects the dilemma of physics - that physics can explain “how” but not “why” - “why” questions are left to philosophers because they are impossibly hard questions to answer - maybe unanswerable!

In a similar manner we have

$$\begin{aligned}\mathcal{P}_m|h\rangle &= (|m\rangle\langle m|)|h\rangle \\ &= \langle m|h\rangle|m\rangle \rightarrow |m\rangle\end{aligned}\tag{4.2}$$

With these results let me propose the following model of a color box. I am going to represent a color box by the operator

$$\hat{C} = \delta\mathcal{P}_g + (1 - \delta)\mathcal{P}_m\tag{4.3}$$

where δ randomly takes only the values 0 or 1 unless the entering electron has a definite color value - it then just lets the electron leave by the appropriate aperture unchanged in any way.

How might this device work in the “real” world? Here is a possible scenario.

As a hard electron $|h\rangle$ enters the left aperture of a color box, some interaction(unknown) between the electron(a microscopic quantum system) and the color box (a macroscopic system) generates a value for δ . This value is random and unpredictable in the range $[0,1]$ with average value $1/2$. Thus, the color box randomly sends the electrons out the “green” aperture as $|g\rangle$ or out the “magenta” aperture as $|m\rangle$, unless, as mentioned above the electron has a definite color value already. Similar results hold for “soft” electrons entering the color box. Similar results also hold for “magenta/green” electrons entering a hardness box.

Now when we send a magenta electron into a hardness box it comes out either hard or soft (50%-50%) and so on. A magenta electron was described earlier as a *SUPERPOSITION* of hard and soft, although we did not specify what was meant by the term “superposition”.

We now represent a superposition mathematically by *addition* of kets (vector addition)as follows:

$$\begin{aligned} |m\rangle &= \frac{1}{\sqrt{2}} |h\rangle - \frac{1}{\sqrt{2}} |s\rangle \\ |g\rangle &= \frac{1}{\sqrt{2}} |h\rangle + \frac{1}{\sqrt{2}} |s\rangle \\ |h\rangle &= \frac{1}{\sqrt{2}} |g\rangle + \frac{1}{\sqrt{2}} |m\rangle \\ |s\rangle &= \frac{1}{\sqrt{2}} |g\rangle - \frac{1}{\sqrt{2}} |m\rangle \end{aligned} \tag{4.4}$$

The reasons for the particular numerical coefficients will become clear shortly.

This will be **Postulate #2** of quantum theory.

I note that this is way theory works - we make assumptions, i.e., the meaning of the term “superposition” in this case, develop measurable consequences from the assumptions and then test them experimentally, which determines their validity.

Before proceeding we need to digress to discuss simple ideas of probability.

4.2.1 Digression on Simple Classical Probability Ideas

Let us imagine that we have a box which contains N balls, each marked with some number, which we denote generically by ν . In general, the same ν -value may appear on more than one ball. The set of values for ν is assumed to be (ν_1, ν_2, \dots) , i.e., a set like $(\nu_1 = 1, \nu_2 = 5, \nu_3 = 7, \nu_4 = 13, \nu_5 = 21)$. We let n_k be the number of balls on which there appears the particular ν -value ν_k . The box of balls is therefore described by two sets of numbers

$$\{\nu_i\} = \nu_1, \nu_2, \nu_3, \nu_4, \dots, \quad \{n_i\} = n_1, n_2, n_3, n_4, \dots \quad (4.5)$$

Since the total number of balls is N , we must have

$$\sum_k n_k = n_1 + n_2 + n_3 + n_4 + \dots = N \quad (4.6)$$

Suppose that we select a ball at random from the box. What is the probability p_k that the selected ball will show the value ν_k ? Since out of N possible selections, n_k of these would yield the ν -value ν_k , we conclude that

$$p_k = \frac{n_k}{N} \quad (4.7)$$

Thus, if $n_k = 0$, then it would be *impossible* to select a ball showing ν_k , and we would have $p_k = 0$. On the other hand, if $n_k = N$, then it would be an *absolute certainty* that the selected ball would show ν_k , and we would have $p_k = 1$. These results all agree with our *common sense* notions of probability, which as we have seen is not always correct!. In general, the numbers $\{p_k\}$ satisfy the conditions

$$0 \leq p_k \leq 1 \text{ for all } k, \quad \sum_k p_k = 1 \quad (4.8)$$

Connection to quantum theory: It will turn out that in the quantum world we will be able to, after making a very large number of measurements of observable Q on an ensemble of *identical* systems, calculate a *probability* that the observable will have a particular value....., that is, for the next measurement to be made of the observable to be q , we have

$$\text{probability}(q) = \frac{\text{number of times value } q \text{ was already measured}}{\text{total number of measurements so far}} \quad (4.9)$$

The goal of quantum mechanics is to predict these probabilities before the measurements are carried out.

This type of probability statement is one that is based on the results of *all previous measurements* and is fundamental to all of science. It is called the *frequency model* and is strictly valid only if the number of identical measurements tends to infinity, which, of course, is impossible!.

The mean or average value of M measured ν -values, which we label by $\nu^{(i)}$ $i =$

1, 2, ..., M) is defined as

$$\langle \nu \rangle = \frac{\sum_{i=1}^M \nu^{(i)}}{M} \quad (4.10)$$

which is the standard definition of the *average or best value* of a series of measurements. However, one must be very careful not to imply that $\langle \nu \rangle$ has any truth or legitimacy beyond that of any of the individual measured $\nu^{(i)}$ values.

The *root-mean-square (or rms) deviation* of these values is defined as

$$\Delta \nu = \sqrt{\frac{\sum_{i=1}^M (\nu^{(i)} - \langle \nu \rangle)^2}{M}} = \sqrt{\langle \nu^2 \rangle - \langle \nu \rangle^2} \quad (4.11)$$

where

$$\langle \nu^2 \rangle = \frac{\sum_{i=1}^M (\nu^{(i)})^2}{M} \quad (4.12)$$

If we have knowledge of the two sets of numbers $\{\nu_k\}$ and $\{p_k\}$, it would seem that we ought to be able to predict approximately what values would be obtained for $\langle \nu \rangle$ and $\Delta \nu$. The key to making such a prediction is the following assumption: since n_k of the N balls have the number ν_k , then in M random samplings of these balls we ought to obtain the value ν_k approximately m_k times where

$$\frac{m_k}{M} \approx \frac{n_k}{N} \quad (4.13)$$

We then find the approximate number of times the value ν_k should appear in the set of values $\nu^{(1)}, \nu^{(2)}, \dots, \nu^{(M)}$ is

$$m_k = \frac{n_k}{N} M = p_k M \quad (4.14)$$

and therefore we can write

$$\langle \nu \rangle = \frac{1}{M} \sum_{i=1}^M \nu^{(i)} = \frac{1}{M} \sum_k m_k \nu_k = \frac{1}{M} \sum_k (p_k M) \nu_k = \sum_k p_k \nu_k \quad (4.15)$$

This result expresses $\langle \nu \rangle$ as a *weighted sum* of the possible ν_k values; the weight assigned to any particular value ν_k is just the probability of its occurrence p_k , as we indicated in earlier discussion. This value is the *theoretically expected* value; the *experimental* value determined from the measurements will generally differ somewhat from this theoretical value owing to the randomness involved. However, in the limit of very many experimental samplings ($M \rightarrow \infty$), the two values may be expected to get arbitrarily close in value, that is, the rms deviation $\Delta \nu$ should approach zero.

This result may be generalized to another important result. Let f be a given

function of ν , and let this function be evaluated for each of the $\nu^{(i)}$ -values. The average or mean of the resulting set of $f(\nu^{(i)})$ -values is given by

$$\langle f(\nu) \rangle = \sum_k p_k f(\nu_k) \quad (4.16)$$

Returning to the Quantum Theory Discussion

In quantum theory, it will turn out that the fundamental quantity associated with probability is not the probability itself, but a new quantity called the *probability amplitude*, which we introduce now.

If the electron to be measured was in an arbitrary state represented by $|\psi\rangle$, then the probability amplitude that we will measure magenta if we send this electron into a color box is given by a new mathematical object represented by the symbol

$$\langle \text{property to be measured} | \text{state being measured} \rangle = \langle m | \psi \rangle \quad (4.17)$$

It is a *complex number*, which is called a *braket* (symbol= $\langle \dots | \dots \rangle$ that we defined and discussed earlier).

We thus have the complex number $A = \langle m | \psi \rangle = \text{probability amplitude}$ and the corresponding probability is defined by $P = |A|^2 = |\langle m | \psi \rangle|^2$ as we mentioned earlier.

This will be **Postulate #3** of quantum theory.

We now send electrons into a color box and select the electrons (a beam) coming out of the magenta aperture. They are all in the state $|m\rangle$. We then put the magenta electrons into another color box and find, using the last postulate idea, that

Probability that a magenta electron emerges from the magenta aperture of a color box

$$P = |\langle m | m \rangle|^2 = 1 \quad (4.18)$$

and thus $\langle m | m \rangle = 1$.

Similarly, the probability that a magenta electron emerges from the green aperture of a color box

$$P = |\langle m | g \rangle|^2 = 0 \quad (4.19)$$

and thus $\langle m | g \rangle = 0$.

Similarly, the probability that a hard electron emerges from the hard aperture of a hardness box

$$P = |\langle h | h \rangle|^2 = 1 \quad (4.20)$$

and thus $\langle h | h \rangle = 1$.

In the same way, the probability that a hard electron emerges from the soft aperture of a color box

$$P = |\langle h | s \rangle|^2 = 0 \quad (4.21)$$

and thus $\langle h | s \rangle = 0$.

Similarly, we have

Probability that a green electron emerges from the green aperture of a color box

$$P = |\langle g | g \rangle|^2 = 1 \quad (4.22)$$

and thus $\langle g | g \rangle = 1$.

Probability that a green electron emerges from the magenta aperture of a color box is

$$P = |\langle g | m \rangle|^2 = 0 \quad (4.23)$$

and thus $\langle g | m \rangle = 0$.

Probability that a soft electron emerges from the soft aperture of a hardness box is

$$P = |\langle s | s \rangle|^2 = 1 \quad (4.24)$$

and thus $\langle s | s \rangle = 1$.

Probability that a soft electron emerges from the hard aperture of a hardness box is

$$P = |\langle s | h \rangle|^2 = 0 \quad (4.25)$$

and thus $\langle s | h \rangle = 0$.

We can now understand the meaning of these results obtained from a very special set of restricted experiment from our earlier discussions.

We see that the kets $\{|m\rangle, |g\rangle\}$ or the kets $\{|h\rangle, |s\rangle\}$ are just two different orthonormal bases for all quantum states in the world of color/hardness. That is why we can write any arbitrary quantum state as $|\psi\rangle = a|m\rangle + b|g\rangle$ or $|\psi\rangle = c|h\rangle + d|s\rangle$. In particular, we earlier wrote

$$\begin{aligned} |m\rangle &= \frac{1}{\sqrt{2}} |h\rangle - \frac{1}{\sqrt{2}} |s\rangle \\ |g\rangle &= \frac{1}{\sqrt{2}} |h\rangle + \frac{1}{\sqrt{2}} |s\rangle \\ |h\rangle &= \frac{1}{\sqrt{2}} |g\rangle + \frac{1}{\sqrt{2}} |m\rangle \\ |s\rangle &= \frac{1}{\sqrt{2}} |g\rangle - \frac{1}{\sqrt{2}} |m\rangle \end{aligned} \quad (4.26)$$

The mysterious property we called SUPERPOSITION is, as we stated earlier, just vector addition!

Does this formalism work? Does it allow us to say correct things about quantum experiments?

Consider a hard electron sent into color box, then, using the rules we have developed, the probability that it will be (emerge as or be measured as) a magenta electron is given by (this is how the algebra works)

$$\begin{aligned}
 |\langle \text{magenta} | \text{hard} \rangle|^2 &= \left| \langle \text{magenta} | \left[\frac{1}{\sqrt{2}} |\text{green}\rangle + \frac{1}{\sqrt{2}} |\text{magenta}\rangle \right] \right|^2 \\
 &= \left| \frac{1}{\sqrt{2}} \langle \text{magenta} | \text{green} \rangle + \frac{1}{\sqrt{2}} \langle \text{magenta} | \text{magenta} \rangle \right|^2 \\
 &= \left| \frac{1}{\sqrt{2}}(0) + \frac{1}{\sqrt{2}}(1) \right|^2 = \frac{1}{2}
 \end{aligned} \tag{4.27}$$

and the probability that it will emerge as a green electron is given by

$$\begin{aligned}
 |\langle \text{green} | \text{hard} \rangle|^2 &= \left| \langle \text{green} | \left[\frac{1}{\sqrt{2}} |\text{green}\rangle + \frac{1}{\sqrt{2}} |\text{magenta}\rangle \right] \right|^2 \\
 &= \left| \frac{1}{\sqrt{2}} \langle \text{green} | \text{green} \rangle + \frac{1}{\sqrt{2}} \langle \text{green} | \text{magenta} \rangle \right|^2 \\
 &= \left| \frac{1}{\sqrt{2}}(1) + \frac{1}{\sqrt{2}}(0) \right|^2 = \frac{1}{2}
 \end{aligned} \tag{4.28}$$

Thus, a hard electron has a 50-50 chance of coming out of the magenta and green apertures which agrees with the results of earlier experiments. That is why we chose the particular numerical coefficients (components values) $\pm 1/\sqrt{2}$. In fact, this formalism agrees with all of the earlier experiments. For example, let us look at the repeatability experiment.

First, a hard electron $|h\rangle$ is sent into a color box. The probability that it will emerge from the magenta aperture is

$$|\langle m | h \rangle|^2 = \frac{1}{2} \tag{4.29}$$

Then, the electron emerging from the magenta aperture is sent into another color box. It is now a magenta electron and represented by the ket $|m\rangle$. The probability that it will emerge from the magenta aperture of the second color box is

$$|\langle m | m \rangle|^2 = 1 \tag{4.30}$$

which corresponds to the repeatability property.

During this experiment, the hard electron which is initially in a superposition of magenta and green properties, i.e.,

$$|h\rangle = \frac{1}{\sqrt{2}} |g\rangle + \frac{1}{\sqrt{2}} |m\rangle \quad (4.31)$$

appears as an electron in the state $|m\rangle$ when it emerges from the magenta aperture of the first color box.

The *standard or Copenhagen interpretation* of quantum theory will say that during the first measurement (the first color box), the state of the electron(hard) is *collapsed* or *reduced* from a superposition of possibilities to a definite value(magenta) corresponding to the value just measured, i.e., to the aperture we *looked at!* This interpretation seems to say that the measurement *caused* the collapse to occur. This also fits with the ideas behind my simple model of the color box described earlier.

This will correspond to **Postulate #4** of quantum theory.

4.2.2 Two-Path Experiment using New Formalism

We now redo the two-path color-hardness experiment in more detail. See the figure below:

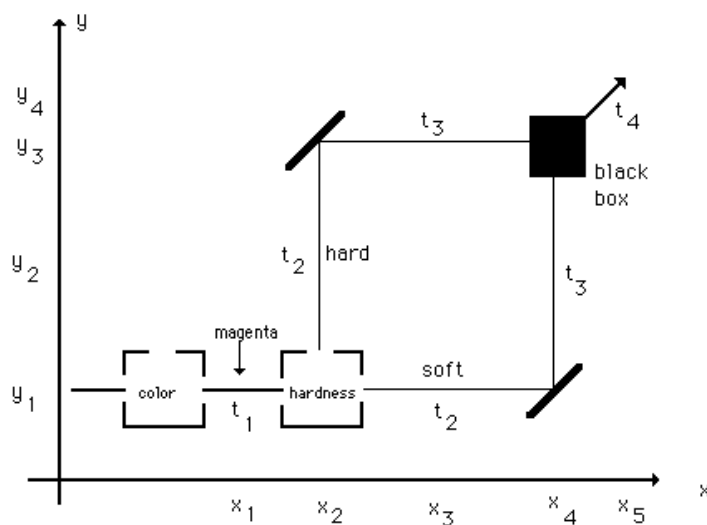


Figure 4.12: Two Path Setup

We have added time and position values to the diagram.

We will need to use states or kets which correspond to the electrons having color

or hardness AND positions. This is allowed because they are *compatible* properties, i.e., it is valid in quantum systems to say a magenta electron is located at a particular position. Thus, the electron can have a color (or hardness) and simultaneously be at a definite position. However, as we saw earlier, an electron CANNOT be hard AND magenta, which are *incompatible* properties. These states take the form:

$$\begin{aligned} |color, x, y\rangle &= |color\rangle |x, y\rangle \\ |hardness, x, y\rangle &= |hardness\rangle |x, y\rangle \end{aligned} \quad (4.32)$$

At time t_1 , when the particle is about to enter the apparatus, its state is (having just left a color box via the magenta aperture):

$$\begin{aligned} |color = magenta, x = x_1, y = y_1\rangle &= |m\rangle |x_1, y_1\rangle \\ &= \left(\frac{1}{\sqrt{2}} |h\rangle - \frac{1}{\sqrt{2}} |s\rangle \right) |x_1, y_1\rangle = \frac{1}{\sqrt{2}} |h\rangle |x_1, y_1\rangle - \frac{1}{\sqrt{2}} |s\rangle |x_1, y_1\rangle \end{aligned} \quad (4.33)$$

Here is how quantum theory *says* to calculate what happens next.

Consider the following: If the state at time t_1 were just the *hard* part

$$\frac{1}{\sqrt{2}} |h\rangle |x_1, y_1\rangle \quad (4.34)$$

and if the hardness box behaves properly, then the state at time t_2 would be

$$\frac{1}{\sqrt{2}} |h\rangle |x_2, y_2\rangle \quad (4.35)$$

i.e., the electron would have just emerged through the hard aperture and be on what we will call the *hard path*.

Similarly, if the state at time t_1 were just the *soft* part

$$\frac{1}{\sqrt{2}} |s\rangle |x_1, y_1\rangle \quad (4.36)$$

and if the hardness box behaves properly, then the state at time t_2 would be

$$\frac{1}{\sqrt{2}} |s\rangle |x_3, y_1\rangle \quad (4.37)$$

i.e., the electron would have just emerged through the soft aperture and be on what we will call the *soft path*. This is what we said the apparatus does to hard/soft electrons!

However, as the state at t_1 is in fact neither just the *soft* part nor just the *hard* part, but the superposition

$$|m\rangle |x_1, y_1\rangle = \frac{1}{\sqrt{2}} |h\rangle |x_1, y_1\rangle - \frac{1}{\sqrt{2}} |s\rangle |x_1, y_1\rangle \quad (4.38)$$

it follows from the above discussion (formally called the *linearity* property of Quantum Mechanics, i.e., we are operating in a mathematical vector space which satisfies the axioms of linear algebra) that the state at time t_2 must be (if the hardness box behaves properly)

$$\frac{1}{\sqrt{2}} |h\rangle |x_2, y_2\rangle - \frac{1}{\sqrt{2}} |s\rangle |x_3, y_1\rangle \quad (4.39)$$

This state is an *entanglement* between hardness/color and position (coordinate space) properties of the electron (note that the color and position properties were separated to start with - they had definite values, namely, magenta and (x_1, y_1)).

This state involves *nonseparable* correlations between hardness/color and coordinate-space properties of the electron.

No hardness or color properties of the electron in this state nor any of its coordinate-space properties (position, momentum, etc) has any definite value in this case!

This is a superposition of states, where one part of the electron state indicates a probability amplitude for being on the hard path and the other of the electron state indicates a probability amplitude for being on the soft path. Note that we are not saying that the electron itself is actually on either path.

This is the reason that earlier we had to make the statements about not hard, not soft, not both and not neither. Those ideas are *not only false, they are meaningless!*

We have entangled two classical states that cannot exist at the same time for a single electron! This state is called an *entangled state*. It will get our thoughts and ideas very entangled later on when we discuss the Einstein paradox and the Bell inequality!!

Continuing on..... the last state of the electron above (at t_2) leads to the state of the electron at t_3

$$\frac{1}{\sqrt{2}} |h\rangle |x_3, y_3\rangle - \frac{1}{\sqrt{2}} |s\rangle |x_4, y_2\rangle \quad (4.40)$$

and then the state at time t_4 is

$$\begin{aligned} & \frac{1}{\sqrt{2}} |h\rangle |x_5, y_4\rangle - \frac{1}{\sqrt{2}} |s\rangle |x_5, y_4\rangle \\ &= \left(\frac{1}{\sqrt{2}} |h\rangle - \frac{1}{\sqrt{2}} |s\rangle \right) |x_5, y_4\rangle \\ &= |m\rangle |x_5, y_4\rangle \end{aligned} \quad (4.41)$$

We see that the color state and the coordinate-space state have *become separate* again. The position of the electron once again has a definite value and the color

once again has a definite value.

So the fact that a hard electron fed into the total device will come out hard, and that a soft electron will come out soft (at the same point), together with our quantum assumptions, means that a magenta electron fed into the total device will come out (just as we found it did) magenta! That is the way quantum mechanics works!

What if we were to stop the experiment in the middle by measuring the position of the electron at, say, t_3 ?

We could insert a wall on the soft path. This implies, for example, that if any electron gets through the device, it must have traveled on the hard path. This is a measurement of position. The same goes for inserting a wall on the hard path.

Then the superposition would go away.

According to our postulates, a *collapse* would occur and the state just after the measurement would be either

$$|h\rangle|x_3, y_3\rangle \quad \text{or} \quad |s\rangle|x_4, y_2\rangle \quad (4.42)$$

each with probability 1/2 (in accordance with our probability assumption).

Then the state at t_4 would be either

$$|h\rangle|x_5, y_4\rangle \quad \text{or} \quad |s\rangle|x_5, y_4\rangle \quad (4.43)$$

respectively. After this point in time, only one part of the state continues to evolve in time, while the other remains unchanged (due to the wall that was inserted).

We emphasize that we collapsed the particle to *hard or soft* by measuring its position in an entangled state. That is the way entangled or nonseparable states work - **collapsing one property (position in this case) collapses all the other properties (hardness in this case).**

The state vector

$$\frac{1}{\sqrt{2}}|h\rangle|x_5, y_4\rangle - \frac{1}{\sqrt{2}}|s\rangle|x_3, y_1\rangle \quad (4.44)$$

is nonseparable between hardness/color properties and coordinate-space properties. This means it is not associated with any definite values for hardness or color or position or momentum or anything like that.

Note that if we have inserted a wall on one path, then we have electrons of

definite hardness, which are 50/50 magenta/green. This agrees with the experiments we described earlier.

Let me finally say something about how to build a *do-nothing* box.

If we are in a state $|A\rangle$ and measure color, then the probability of measuring magenta is determined as shown below.

Write $|A\rangle$ as a superposition of color states (since color is the thing we want to measure). This can always be done since color kets are a basis (anything measurable provides a basis).

$$|A\rangle = \alpha |magenta\rangle + \beta |green\rangle \quad (4.45)$$

where

$$\begin{aligned} \langle magenta | A \rangle &= \alpha \langle magenta | magenta \rangle + \beta \langle magenta | green \rangle = \alpha \\ \langle green | A \rangle &= \alpha \langle green | magenta \rangle + \beta \langle green | green \rangle = \beta \end{aligned} \quad (4.46)$$

and the probability that the measurement will indicate that the electron is magenta is given by

$$|\langle magenta | A \rangle|^2 = |\alpha|^2 \quad (4.47)$$

Now consider the state

$$-|A\rangle = -\alpha |magenta\rangle - \beta |green\rangle \quad (4.48)$$

If we measure color on this state, we will get all the same probabilities for every possible outcome as we did with the state $|A\rangle$, i.e.,

$$|\langle magenta | A \rangle|^2 = |\alpha|^2 = |-\langle magenta | A \rangle|^2 \quad (4.49)$$

So if a vector $|A\rangle$ changes to the vector $-|A\rangle$ there are **NO OBSERVABLE EFFECTS - NO PROBABILITIES CHANGE - NOTHING HAPPENS** as far as quantum theory is concerned!!!.

So any box which changes the state of any incoming electron into -1 times that incoming state will be a *do-nothing* box, since it will not change any of the measurable values, i.e., any probabilities of the values of any of the observables of any electron which passes through it. Obviously, it will also not effect any electron which passes outside of it. As we will see later in our discussion, we are changing a quantity called the “phase” of the complex number corresponding to the amplitude.

But the effects of such a box on an electron which is in a superposition of passing through it and outside of it may be quite a different matter.

Suppose the box is inserted in the soft path of the two-path device at (x_3, y_1) .

Then, if the initial input electron were magenta, the state at t_2 will be (earlier discussion)

$$\frac{1}{\sqrt{2}} |h\rangle |x_2, y_2\rangle - \frac{1}{\sqrt{2}} |s\rangle |x_3, y_1\rangle \quad (4.50)$$

and the state at t_3 (after the *passage* through the box) *will be not be*

$$\frac{1}{\sqrt{2}} |h\rangle |x_3, y_3\rangle - \frac{1}{\sqrt{2}} |s\rangle |x_4, y_2\rangle \quad (4.51)$$

as in earlier discussion, but *will be*

$$\frac{1}{\sqrt{2}} |h\rangle |x_3, y_3\rangle + \frac{1}{\sqrt{2}} |s\rangle |x_4, y_2\rangle \quad (4.52)$$

where the sign of the second term has been changed by the *do-nothing* box in the soft path.

If we now follow this new state to t_4 as before we will find

$$\begin{aligned} & \frac{1}{\sqrt{2}} |h\rangle |x_5, y_4\rangle + \frac{1}{\sqrt{2}} |s\rangle |x_5, y_4\rangle \\ &= \left(\frac{1}{\sqrt{2}} |h\rangle + \frac{1}{\sqrt{2}} |s\rangle \right) |x_5, y_4\rangle \\ &= |g\rangle |x_5, y_4\rangle \end{aligned} \quad (4.53)$$

instead of

$$\begin{aligned} & \frac{1}{\sqrt{2}} |h\rangle |x_5, y_4\rangle - \frac{1}{\sqrt{2}} |s\rangle |x_5, y_4\rangle \\ &= \left(\frac{1}{\sqrt{2}} |h\rangle - \frac{1}{\sqrt{2}} |s\rangle \right) |x_5, y_4\rangle \\ &= |m\rangle |x_5, y_4\rangle \end{aligned} \quad (4.54)$$

So the *do-nothing* box has changed the color of all the electrons from magenta to green (as we had reported earlier) even though it has no measurable effect on the electrons that *passed though it* !!!!.

That is the way quantum mechanics works!!

Our new mathematical formalism seems to work very well since the theory it provides agrees with experiment, which is the only valid test!

4.2.3 Some further mathematical thoughts

Some loose ends from our prior discussion will now be fixed up. Suppose we define an operator

$$\hat{G} = |g\rangle \langle g| \quad (4.55)$$

We then have these properties

$$\hat{G}|g\rangle = |g\rangle \langle g|g\rangle = |g\rangle \quad , \quad \hat{G}|m\rangle = |g\rangle \langle g|m\rangle = 0 \quad (4.56)$$

or the states representing the green and magenta electrons are the eigenvectors of \hat{G} with eigenvalues 1 and 0 respectively.

We also find that the expectation value of \hat{G} in the green state is

$$\langle g|\hat{G}|g\rangle = |\langle g|g\rangle|^2 = 1 \quad (4.57)$$

and the expectation value of \hat{G} in the magenta state is

$$\langle m|\hat{G}|m\rangle = |\langle g|m\rangle|^2 = 0 \quad (4.58)$$

These results make sense if we **interpret**

$$\hat{G} = |g\rangle \langle g| \quad (4.59)$$

as the operator corresponding to a measurement of the green property of electrons, i.e., an observer looking at the output of a green aperture of a color box.

The first result then says, using the earlier result

$$prob(b_k) = |\langle b_k|\psi\rangle|^2 \quad (4.60)$$

that if we measure the probability that the color of a green electron is green we get the value 1 as expected and the second result then says if we measure the probability that the color of a green electron is magenta we get the value 0 as expected. Things make sense! Pushing these strange ideas even further, if we assume, as earlier, that a hard electron is a superposition of green and magenta electrons,

$$|hard\rangle = |h\rangle = \frac{1}{\sqrt{2}}|g\rangle + \frac{1}{\sqrt{2}}|m\rangle \quad (4.61)$$

then the expectation value of \hat{G} in the hard state is

$$\begin{aligned} \langle h|\hat{G}|h\rangle &= \left(\frac{1}{\sqrt{2}}\langle g| + \frac{1}{\sqrt{2}}\langle h| \right) \hat{G} \left(\frac{1}{\sqrt{2}}|g\rangle + \frac{1}{\sqrt{2}}|m\rangle \right) \\ &= \frac{1}{2}\langle g|\hat{G}|g\rangle + \frac{1}{2}\langle g|\hat{G}|m\rangle + \frac{1}{2}\langle m|\hat{G}|g\rangle + \frac{1}{2}\langle m|\hat{G}|m\rangle \\ &= \frac{1}{2}\langle g|\hat{G}|g\rangle = \frac{1}{2} \end{aligned} \quad (4.62)$$

i.e., equal parts 0 and 1.

Another way of saying this is, using the earlier result

$$\langle \hat{B} \rangle = \sum_k b_k prob(b_k) = \sum_k b_k |\langle b_k|\psi\rangle|^2 \quad (4.63)$$

is

$$\begin{aligned}
\langle h | \hat{G} | h \rangle &= \sum (\text{eigenvalue } g) (\text{probability of } g \text{ in } |h\rangle) \\
&= (1) |\langle \text{eigenvalue} = 1 | h \rangle|^2 + (0) |\langle \text{eigenvalue} = 0 | h \rangle|^2 \\
&= (1) |\langle g | h \rangle|^2 + (0) |\langle m | h \rangle|^2 = (1) \frac{1}{2} + (0) \frac{1}{2} = \frac{1}{2} \quad (4.64)
\end{aligned}$$

which again makes sense, i.e., if we have a beam of hard electrons, then we will measure an electron to be green 1/2 of the time as we observed earlier!

Clearly, this formalism is both neat and very powerful and certainly seems to have the potential to describe our earlier observations. We will see shortly that the formalism, based on a set of postulates, can completely represent quantum systems and quantum measurements. Let us summarize some of the ideas we have been discussing. The more times we think about it, the better we will understand it.

Sometimes a theory is just guessed (educated guesses based on experiments) as a set of postulates. Let us take this approach now.

4.2.4 Quantum Mechanics Postulates (in color/hardness world)

Let us make a first pass at sewing up the postulates of quantum mechanics based on the results we have obtained from the color/hardness world.

There are **five parts (ASSUMPTIONS OR AXIOMS)** to the **Quantum Mechanics algorithm**.

(A) Physical States

All physical systems are represented by ket vectors normalized to 1.

They are called “**state vectors**” $\rightarrow |\psi\rangle$ where $\langle\psi|\psi\rangle = 1$.

This literally means ALL. A green or hard electron is represented by a vector. An atom is represented by a vector. A banana is represented by a vector. A car is represented by a vector. YOU are represented by a vector (albeit a very complex one).

(B) Measurable Properties

Measurable properties (dynamical variables) of physical systems are called “**observables**”.

Observables are represented by linear operators.

If the vector associated with a particular physical state $|\psi\rangle$ happens to be an eigenvector, with eigenvalue α , of an operator \hat{A} associated with some particular measurable property of the system, i.e., if

$$\hat{A}|\psi\rangle = \alpha|\psi\rangle \quad (4.65)$$

then the system in that state has the value α of that particular measurable property.

That is, if you were to perform a measurement corresponding to \hat{A} on a system in a state represented by $|\psi\rangle$, then with **certainty** (probability = 1) you would measure the value α .

Since the eigenvalues of operators representing observables are supposed to be measurable numbers, they must also always be **real**.

This means that we can only choose a certain kind of operator to represent observables, namely, HERMITIAN, which is guaranteed to always have real eigenvalues.

This requirement produces an added bonus for quantum theory.

It turns out that the eigenvectors of any HERMITIAN operator always comprise a **complete, orthonormal set**.

This means that they always comprise a set of **mutually orthonormal vectors** that can be used as a **basis** (number is dimension of space).

It also turns out that **any** HERMITIAN operator will represent a possible observable of the physical system.

Turning this statement around, we can say that the **eigenvectors of any observable can be used as the basis vectors** for our space.

This feature will have an important connection to measurement.

4.2.4.1 Example: back to color and hardness.....

Since the operators \hat{H} and \hat{C} that represent the observables **hardness** and **color** must be Hermitian, we can use either set of corresponding eigenvectors as a basis set for the quantum theory of color and hardness.

One such basis is then

$$|hard\rangle = |h\rangle \quad , \quad |soft\rangle = |s\rangle \quad (4.66)$$

where (by definition)

$$\begin{aligned}\hat{H}|h\rangle &= |h\rangle \rightarrow \text{eigenvalue} = 1 \quad (\text{by convention}) \\ \hat{H}|s\rangle &= -|s\rangle \rightarrow \text{eigenvalue} = -1 \quad (\text{by convention})\end{aligned}\tag{4.67}$$

or, in words, $|h\rangle$ is a state with a measured value of hardness = 1 and $|s\rangle$ is a state with a measured value of hardness = -1.

Since these states form a basis (orthonormal set) they satisfy

$$\begin{aligned}\langle h|h\rangle &= 1 = \langle s|s\rangle \\ \langle h|s\rangle &= 0 = \langle s|h\rangle\end{aligned}\tag{4.68}$$

The operator \hat{H} clearly represents a way to obtain all the information we can have about a state.

Since, as we showed earlier, any operator can be written in terms of its eigenvalues and projection operators we have

$$\hat{H} = (+1)|h\rangle\langle h| + (-1)|s\rangle\langle s| = |h\rangle\langle h| - |s\rangle\langle s|\tag{4.69}$$

so that

$$\begin{aligned}\hat{H}|h\rangle &= (|h\rangle\langle h| - |s\rangle\langle s|)|h\rangle = |h\rangle\langle h|h\rangle - |s\rangle\langle s|h\rangle = |h\rangle(1) - |s\rangle(0) = |h\rangle \\ \hat{H}|s\rangle &= (|h\rangle\langle h| - |s\rangle\langle s|)|s\rangle = |h\rangle\langle h|s\rangle - |s\rangle\langle s|s\rangle = |h\rangle(0) - |s\rangle(1) = -|s\rangle\end{aligned}\tag{4.70}$$

as expected.

The eigenvector/eigenvalue equations above just say that the hardness operator and hence the hardness box acting on a state vector does not change the states of definite hardness, namely, $|h\rangle$ and $|s\rangle$ (as we saw earlier an overall minus sign does not change any measurable properties of the $|s\rangle$ state) as required.

We can write the matrices representing these objects in the hardness basis (called a **matrix representation**)

$$\begin{aligned}|h\rangle &= \begin{pmatrix} \langle h|h\rangle \\ \langle s|h\rangle \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |s\rangle = \begin{pmatrix} \langle h|s\rangle \\ \langle s|s\rangle \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ [H] &= \begin{pmatrix} \langle h|\hat{H}|h\rangle & \langle h|\hat{H}|s\rangle \\ \langle s|\hat{H}|h\rangle & \langle s|\hat{H}|s\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\end{aligned}\tag{4.71}$$

where we have used $\langle h|\hat{H}|s\rangle = \langle h|(-1)|s\rangle = -\langle h|s\rangle = 0$, etc.

Remember that in terms of matrices, Hermitian means the following: If

$$[A] = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}\tag{4.72}$$

then

$$[A^+] = \begin{pmatrix} a_{11}^* & a_{21}^* \\ a_{12}^* & a_{22}^* \end{pmatrix} \quad (4.73)$$

is the Hermitian conjugate matrix and it is the same matrix, i.e., $[A] = [A^+]$.

Similarly, another such basis(equivalent) is then

$$|magenta\rangle = |m\rangle \quad , \quad |green\rangle = |g\rangle \quad (4.74)$$

where (by definition)

$$\begin{aligned} \hat{C}|g\rangle &= |g\rangle \rightarrow \text{eigenvalue} = 1 \quad (\text{by convention}) \\ \hat{C}|m\rangle &= -|m\rangle \rightarrow \text{eigenvalue} = -1 \quad (\text{by convention}) \end{aligned} \quad (4.75)$$

or, in words, $|g\rangle$ is a state with a measured value of color = 1 and $|m\rangle$ is a state with a measured value of color = -1. The operator \hat{C} represents the entire color box. Since any operator can be written in terms of its eigenvalues and projection operators we have

$$\hat{C} = |g\rangle\langle g| - |m\rangle\langle m| \quad (4.76)$$

Since these states form a basis (orthonormal set) they satisfy

$$\begin{aligned} \langle g | g \rangle &= 1 = \langle m | m \rangle \\ \langle g | m \rangle &= 0 = \langle m | g \rangle \end{aligned} \quad (4.77)$$

The eigenvector/eigenvalue equations above just say that a color box does not change $|g\rangle$ and $|m\rangle$ states (again, we will see shortly that an overall minus sign does not change any measurable properties of the $|m\rangle$ state).

We can write the matrices representing these objects in the color basis (called a matrix representation)

$$\begin{aligned} |g\rangle &= \begin{pmatrix} \langle g | g \rangle \\ \langle g | m \rangle \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad |m\rangle = \begin{pmatrix} \langle m | g \rangle \\ \langle m | m \rangle \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ [C] &= \begin{pmatrix} \langle g | \hat{C} | g \rangle & \langle g | \hat{C} | m \rangle \\ \langle m | \hat{C} | g \rangle & \langle m | \hat{C} | m \rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{aligned} \quad (4.78)$$

where we have used $\langle g | \hat{C} | m \rangle = -\langle g | m \rangle = 0$, etc.

Let us now write the $|g\rangle$ and $|m\rangle$ vectors in terms of the $|h\rangle$ and $|s\rangle$ vectors. This is always possible since $|h\rangle, |s\rangle$ is a basis and $|g\rangle, |m\rangle$ are just some other vectors in the same space(in the world).

This is just the principle of SUPERPOSITION, that we mentioned earlier, in action. We write

$$\begin{aligned} |g\rangle &= a|h\rangle + b|s\rangle \\ |m\rangle &= c|h\rangle + d|s\rangle \end{aligned} \quad (4.79)$$

Normalization: the states must be normalized to 1 (we assume a, b, c, d are real numbers) so that

$$\begin{aligned}\langle g | g \rangle &= 1 = (a \langle h | + b \langle s |) (a | h \rangle + b | s \rangle) = a^2 + b^2 \\ \langle m | m \rangle &= 1 = (c \langle h | + d \langle s |) (c | h \rangle + d | s \rangle) = c^2 + d^2\end{aligned}\quad (4.80)$$

Orthogonality: the states must be orthogonal (eigenvectors of a Hermitian operator) so that

$$\langle g | m \rangle = 0 = (a \langle h | + b \langle s |) (c | h \rangle + d | s \rangle) = ac + bd \quad (4.81)$$

One possible solution to these equations (which as we will see later represents the color states) is

$$a = b = c = -d = \frac{1}{\sqrt{2}} \quad (4.82)$$

so that we obtain

$$|g\rangle = \frac{1}{\sqrt{2}} |h\rangle + \frac{1}{\sqrt{2}} |s\rangle \quad , \quad |m\rangle = \frac{1}{\sqrt{2}} |h\rangle - \frac{1}{\sqrt{2}} |s\rangle \quad (4.83)$$

Similarly, we can express the $|h\rangle$ and $|s\rangle$ vectors in terms of the $|g\rangle$ and $|m\rangle$ vectors as a basis. We obtain

$$|h\rangle = \frac{1}{\sqrt{2}} |g\rangle + \frac{1}{\sqrt{2}} |m\rangle \quad , \quad |s\rangle = \frac{1}{\sqrt{2}} |g\rangle - \frac{1}{\sqrt{2}} |m\rangle \quad (4.84)$$

So, sums and differences of vectors represent superpositions of physical states.

States of definite color are superpositions of different hardness states.

States of definite hardness are superpositions of different color states.

The hardness and color operators are incompatible observables in the sense that states of definite hardness (eigenvectors of the hardness operator) apparently have no definite color value (since they are not eigenvectors of the color operator) and vice versa. This means that color and hardness are incompatible and that their representative operators do not commute. We can see that by determining the matrix for \hat{H} in the color basis and then computing the commutator. We have

$$[H] = \begin{pmatrix} \langle g | \hat{H} | g \rangle & \langle g | \hat{H} | m \rangle \\ \langle m | \hat{H} | g \rangle & \langle m | \hat{H} | m \rangle \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (4.85)$$

where we have used

$$\begin{aligned}
\langle g | \hat{H} | m \rangle &= \left(\frac{1}{\sqrt{2}} \langle h | + \frac{1}{\sqrt{2}} \langle s | \right) \hat{H} \left(\frac{1}{\sqrt{2}} | h \rangle - \frac{1}{\sqrt{2}} | s \rangle \right) \\
&= \frac{1}{2} (\langle h | \hat{H} | h \rangle - \langle h | \hat{H} | s \rangle + \langle s | \hat{H} | h \rangle - \langle s | \hat{H} | s \rangle) \\
&= \frac{1}{2} (\langle h | h \rangle + \langle h | s \rangle + \langle s | h \rangle + \langle s | s \rangle) = \frac{1}{2} (1 + 0 + 0 + 1) = 1
\end{aligned} \tag{4.86}$$

and so on. We then have

$$\begin{aligned}
[\hat{C}, \hat{H}] &= \hat{C}\hat{H} - \hat{H}\hat{C} \\
&= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\
&= 2 \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \neq 0
\end{aligned} \tag{4.87}$$

So it looks like it will be possible to work out the descriptions of color and hardness and of all the relations between them within the framework of a these 2-dimensional vector space ideas.

The final part of this postulate is

**if the system is in any arbitrary state $|\psi\rangle$
and we measure the observable \hat{B} (where $|\psi\rangle$
is NOT an eigenstate of \hat{B} , then the ONLY
possible results are the eigenvalues of \hat{B}
that is, the set $\{b_k\}$**

Read that statement again!. It is a truly amazing statement.

(C) Dynamics

There is a dynamics of state vectors.

There are “**deterministic**” laws (you know the kind of laws where if you know everything at the start, then you can predict everything that will happen in the future exactly) about how a state vector of any given system changes with time.

Since every state vector representing a real physical system must have length = 1, the changes of the state vectors dictated by the dynamical laws (called the **Schrödinger equation or time-development equation**) are exclusively changes of direction (and never of length).

We define the “**time evolution or development**” operator that governs

how a state vector changes in time by the relationship

$$|A, t + \Delta t\rangle = \hat{U}(\Delta t) |A, t\rangle \quad (4.88)$$

or, in words,

**the state vector at time $t + \Delta t$ is given by
the time evolution operator \hat{U} operating on
the state vector at time t**

Note how the things inside the vector symbol change when I have to indicate that there is new information known about the state (the “**when**” in this case).

In general, the only thing that changes - is the labels - which contain whatever we know(have measured) about the state.

The time evolution operator is also a **linear** operator. It is a unitary operator \hat{U} , which means that

**if $\hat{U}\hat{U}^{-1} = \hat{I}$ or \hat{U}^{-1} is the inverse of \hat{U}
then the Hermitian conjugate $\hat{U}^\dagger = \hat{U}^{-1}$**

As we said earlier, the time evolution operator is related to the energy operator. More about this later.

(D) **The Connection with Experiment** So far, none of our assumptions have touched upon the results of measurements.

All we have said so far, in this arena, is that the particular physical state whose state vector is an eigenvector, with eigenvalue α , of the operator associated with some particular measurable property will “**have**” the value α for that property and that a measurement of that property, carried out on a system which happens to be in that state, will produce the result α with certainty(probability = 1) and that if we are not in an eigenvector of the observable being measured, then we can only measure one of its eigenvalues.

But we will need much more than that to deal with experiments.

What if we measure a certain property of a physical system at the moment when the state vector of the system does not happen to be an eigenvector of that property operator? (this will, in fact, be the case most of the time).

What if we measure the color of a hard electron(which is an electron in a superposition of being green and being magenta)?

What happens then?

All of our earlier assumptions are no help here.

We need a **new assumption**.

Suppose we have a system in some state $|\psi\rangle$, and we carry out a measurement of the value of a property (observable) associated with the operator \hat{B} .

We assume that the eigenvectors of \hat{B} are the states $|b_i\rangle$ which means that

$$\hat{B} |b_i\rangle = b_i |b_i\rangle \quad , \quad i = 1, 2, 3, 4, \dots \quad (4.89)$$

where the b_i are the corresponding eigenvalues.

Quantum theory then says, as we have seen, that the outcome of any such a measurement is strictly a matter of “**probability**”.

In particular, quantum theory stipulates that the **probability that the outcome** of the measurement of \hat{B} on state $|\psi\rangle$ (not an eigenvector) will yield the result b_i (remember the only possible results are the eigenvalues of \hat{B} , no matter what state we are in), is **equal** to

$$|\langle b_i | \psi \rangle|^2 \quad (4.90)$$

or the absolute-square of the corresponding component!

This postulate means the following:

- (a) The probability as so defined is always ≤ 1 as it must be, which results from the requirement that all allowable states be of length = 1 (normalized to 1). This is the reason for the normalization requirement.
- (b) If $|\psi\rangle = |b_i\rangle$ (the state we are in corresponds to an eigenvector), then the probability that we will measure b_i is

$$\text{probability} = |\langle b_i | b_i \rangle|^2 = 1 \quad (4.91)$$

and the probability that we will measure any other eigenvalue b_k , $k \neq i$ is

$$\text{probability} = |\langle b_k | b_i \rangle|^2 = 0 \quad , \quad k \neq i \quad (4.92)$$

due to orthonormality.

This is just the special case when the state we are measuring is an eigenvector of the observable being measured and corresponds to Postulate #2. Postulate #4 agrees with Postulate #2 as it must.

- (c) The probability that a green electron will be found during a hardness measurement to soft is $1/2$ (this must be true to explain earlier experimental results). This follows as shown below. the state being measured is

$$|g\rangle = \frac{1}{\sqrt{2}} |h\rangle + \frac{1}{\sqrt{2}} |s\rangle \quad (4.93)$$

and the probability to be soft, i.e., the $prob(soft|green)$ is given by

$$\begin{aligned} prob(soft|green) &= |\langle s|g\rangle|^2 = \left| \langle s| \left(\frac{1}{\sqrt{2}} |h\rangle + \frac{1}{\sqrt{2}} |s\rangle \right) \right|^2 \\ &= \left| \frac{1}{\sqrt{2}} (\langle s|h\rangle + \langle s|s\rangle) \right|^2 = \left| \frac{1}{\sqrt{2}} (0 + 1) \right|^2 = \frac{1}{2} \quad (4.94) \end{aligned}$$

That is why we chose the particular superposition earlier.

- (d) Similarly, the probability that a green electron will be found during a hardness measurement to be hard is $1/2$.

The probability that a hard electron will be found during a color measurement to be green is $1/2$.

The probability that a hard electron will be found during a color measurement to be magenta is $1/2$.

and so on.

The new formalism correctly predicts the required (experimental) results for hardness and color measurements.

Does that make sense?

It is important to realize that we cannot say anything definite about the color if we are in a hardness state and vice versa. We can only make probability statements. Before we measure the color of the electron, the electron does not have a color, according to quantum theory! Our information about the electron color is only a set of probabilities. But all of your experience says that objects have values for measured quantities before they are measured, i.e., your experience tells you that the electron has a color even if we do not measure it.

That is your view (the standard classical view) about what is real and what is not real.

Quantum theory says that you are wrong in both cases!! If

you believe otherwise, then all quantum effects would not work...but they do!!!

We will eventually devise experiments to show that quantum theory is correct and your classical views about reality are incorrect!!

We must also devise a theory to show why it seems this way for electrons but does not **seem** to be true for macroscopic objects.

These first 4 postulates are not even the controversial ones!!!

Finally, we state the last, and as we shall see the most controversial postulate.

(E) Collapse

Measurements are always repeatable. This seems like a very innocuous statement!

Once a measurement is carried out and a result obtained for some observable, the state of the system must be such as to guarantee (with probability = 1) that if the same measurement is repeated, the exact same result will be obtained. Since systems evolve in time, this is literally only true if the second measurement follows the first instantaneously or, at least, within such a small time that the system in question does not have a chance to evolve.

What does this mean about the state vector of the measured (after measurement) system?

One view is that something must happen to the state vector when the measurement occurs.

If a measurement of an observable \hat{O} is carried out on a system S , and if the outcome of the measurement is the value o_q (one of the many possible measured values of the operator \hat{O} one of its eigenvalues) then, whatever the state vector of S was before the measurement of \hat{O} , the only way to guarantee (with probability = 1) that another measurement of \hat{O} will give the same result is that the state vector of S after the measurement must necessarily be the eigenvector of \hat{O} with eigenvalue o_q . **This must be so according to Postulate #2.**

Thus, in this view, the effect of measuring an observable must necessarily be to “**change**” the state vector of the measured system, to **COLLAPSE** it, to make it “**jump**” from whatever it may have been prior to the measurement into some eigenvector of the measured observable operator.

This is called

collapse of state vector or reduction of state vector

It says that the state vector changes(discontinuously) during a measurement from representing a range of possibilities (a superposition of all possible states) to a definite state or only one possible outcome.

Which particular eigenvector it gets changed into is determined by the outcome of the measurement and it cannot be known until then!!!!!! It cannot be predicted!!!!

Since that outcome, according to our earlier assumption, is a matter of probability, it is at this point and at no other point in the discussion, that an element of “**pure chance**” enters into the time evolution of the state vector and **determinism goes out the window**.

Our postulates thus assume that the time evolution of a system is continuous and deterministic between measurements, and discontinuous and probabilistic(random) during measurements.

It is clear why this postulate is controversial. It will dominate some of our later discussions.

Those are the principles(postulates) of quantum theory. They are the most precise mechanism for predicting the outcomes of experiments on physical systems ever devised.

No exceptions to them have ever been discovered. NOBODY expects any.

We will now spend some time making these principles into operational tools that we can use to carry out quantum theory and make predictions.

We will see, in detail, how quantum theory makes predictions and how the strange results of various experiments are easily accounted for by the theory.

We are about to enter a very strange world where quantum systems behave in rather mysterious and non-intuitive ways.

Remember, however, that any behavior we predict and observe will just be a consequence of the 5 postulates we have just stated.

That is how theoretical physics works!

Now let us look at some real world experiments that exhibit the same

phenomena as we have seen in the color-hardness experiments.

4.3 An Interference Experiment with Photons

In this experiment a laser beam is directed at a half-silvered mirror. For intense light beams, these mirrors reflect half of the light striking them and allow half to pass straight through. When the intensity of the laser beam is high, two beams can be seen emerging from the mirror, each one having half the intensity of the incoming beam. This arrangement is called a *beam-splitter*.

If we turn the intensity of the laser down, so that we have photons emerging with a notable time gap between them (only one photon around at any given time), and use a pair of C(harged)C(oupled)D(device) detectors (similar to those in modern digital cameras) to catch the reflected and transmitted beams, we see something very interesting.

For each photon that leaves the laser, one is detected either at the transmission CCD (on the transmitted path) or at the reflection CCD (on the reflected path). The photons are not *split* in some odd manner so that half a photon goes one way at the mirror and half the other way. Instead, there seems to be a 50:50 chance(probability) that an individual photon will be transmitted or reflected by the half-silvered mirror. Moreover, there is no measurable difference between the photons as they approach the mirror, i.e., no property that seems to determine which way they will go (hopefully, *by now*, that sounds familiar!).

This is a *fundamental point* that will come up repeatedly in the context of quantum theory.

The next step is to remove the detectors and replace them with two mirrors (fully silvered) that divert the two beams(change their directions by 90°) to a second half-silvered mirror as shown in the figure below.

At this point the same thing happens, with half of the light arriving at the half-silvered mirror passing straight through and the other half being reflected. The upshot of this is that two new beams emerge and travel to a pair of detectors placed at X and Y.

The beam heading to detector X is a combination of the light that was *reflected* by the first half-silvered mirror (and so travelled the *top* path), then *transmitted* by the second half-silvered mirror with the light that was *transmitted* by the first half-silvered mirror(along the *bottom* path) and *reflected* by the second one. Detector Y collects light that is a similar mixed combination.

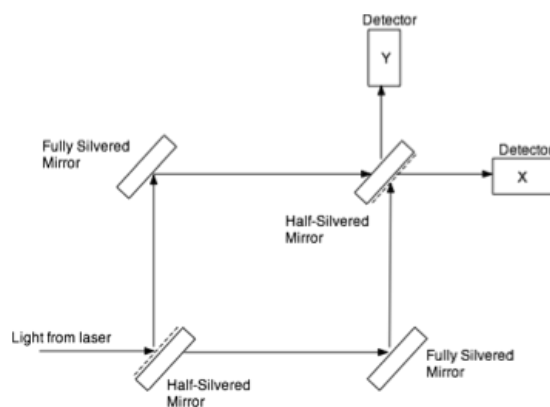


Figure 4.13: Splitting a Laser beam

This arrangement of mirrors and detectors is called a **Mach-Zehnder interferometer**. Once the interferometer is set up, it is easy to confirm that the intensity of the light reaching each detector depends very critically on the *distances* travelled by the light along the top and bottom paths. If the equipment can be finely adjusted so that these paths are *exactly* the same length, detector Y records no light at all while detector X records all of the intensity (all of the photons) entering the experiment. Without this very critical adjustment, X and Y collect light in varying relative amounts: the more light that arrives at X, the less that reaches Y (and vice versa). Using classical physics methods these effects can be *completely* explained by saying that light is a *wave*.

Interference as a Wave Effect (a reminder)

Consider some ripples crossing the surface of a lake. These ripples consist of places where the water level is higher than normal (peaks) and places where it has dropped below normal (troughs). The *wavelength* of the ripple is the distance between successive peaks(P), which is the same as the distance between successive troughs(T). The *frequency* of the wave is the rate at which complete cycles (from peak to trough to peak again) pass a fixed point, and the *period* is the time taken for one cycle. See figure below.

Light is a much more complicated thing than a water wave as it is composed of electric and magnetic fields. The peaks and troughs of a light wave are not physical distances as in the height of a water wave; instead they are variations in the *strength* of the fields. Mathematically, however, they are the same phenomena and that, as we will see, is all that matters.

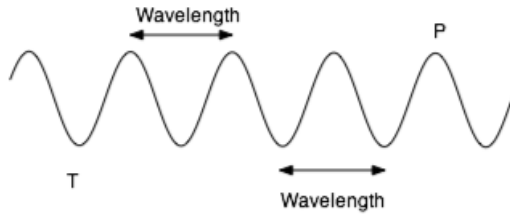


Figure 4.14: A Wave

Because of this, light waves are very sensitive measures of distance. Thinking back to the interference experiment with the interferometer, imagine dividing the distance travelled by a light wave on route to a detector into sections, each one of which had a length equal to the wavelength of the wave. The chances are that the distance will not be a whole number of wavelengths. Furthermore, the two different possible routes through the experiment would have to be precisely the same length for them to be precisely the same number of wavelengths long.

If the distances are not precisely the same, the light traveling along each route will consequently have gone through a different number of complete waves by the time it gets to the detector.

As the light has a common source at the first half-silvered mirror, the two beams will set off on their different routes in *phase* (i.e., in step - simplest definition of phase - both at the same point on the wave) with each other as shown in the figure below.

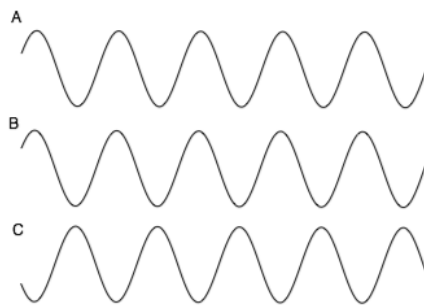


Figure 4.15: In Phase and Out of Phase

The waves labelled A and B are in phase with each other (peak to peak and trough to trough), waves B and C are exactly out of phase with each other (peak

to trough). If we could see their peaks and troughs directly, they would have set off marching along peak for peak and trough for trough - they were in phase. However, by the time they get to the detector the two beams may no longer be in phase (due to the different distances travelled). One could be arriving at a peak, and the other at a trough (like B and C in the figure). If this happens, then the waves will cancel each other out and there will be little energy entering the detector - called *destructive interference* (if they were still in phase they would add up - called *constructive interference*). Exact cancellation would only happen if the waves met precisely peak to trough, which is not possible for any extended length of time due to small variations in the distance (the mirrors will be shaking slightly) and fluctuations in the laser output.

In a detailed analysis of the interference experiment we also need to take into account what happens to the light at the various mirrors as they *also* influence the phase of the waves. Generally, when light reflects off a mirror, the reflected wave is out of phase with the incoming wave by half a wavelength. Using λ to stand for wavelength, we would say that the wave has undergone a $\lambda/2$ phase shift (shift by $1/2$ wavelength) on reflection. Things are slightly different with the half-silvered mirror, which is a surface that can reflect from either side mounted on a thin block of glass. The dashed line in Figure 4.13 indicates the reflecting surface. If the reflection takes place off the surface before the light enters the glass block, then the ordinary $\lambda/2$ phase shift takes place. However, any light that has to pass through the block before reaching the reflecting surface is not phase shifted on reflection.

Have a look at the two figures below.

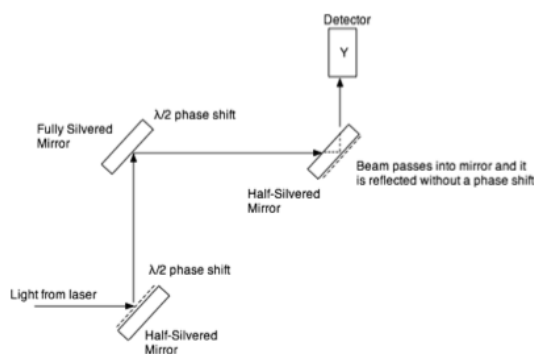


Figure 4.16: Top Path

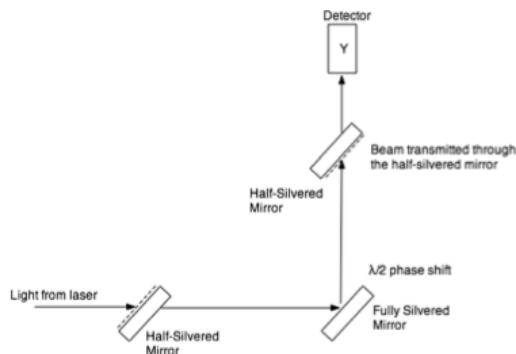


Figure 4.17: Bottom Path

As you can see from the figures, the two light beams reaching detector Y will be (overall) $\lambda/2$ out of phase with one another. Consequently, they will look like waves B and C in Figure 4.15 and will completely cancel each other out (if they travelled equal distances).

If you carry out the same analysis for detector X, i.e., chart the progress of the waves through the interferometer to detector X (try it), you should find that they arrive in phase with each other, provided they have travelled equal distances.

In most experimental setups, the paths through the interferometer are not exactly equal and so the waves arrive not quite exactly in/out of phase. Consequently, you get some light reaching both X and Y. If the equipment allowed you to move one of the fully silvered mirrors, so that the relative path lengths were changed, then the variation in brightness of the light in X and Y could be studied as the mirror moved - as the relative paths changed.

Although Young (remember earlier discussion) did not have access to a Mach-Zehnder interferometer (they had not been invented yet), his experiments could only be explained by using a wave theory of light. Young may not have had the sophistication of lasers and half-silvered mirrors to work with, but he did manage to combine light from two sources to produce an interference pattern on a screen.

Mach-Zehnder with Photons

Now we turn to a very modern version of the Mach-Zehnder interferometer in which it is possible to turn down the laser intensity so that the light beam is made up of single photons in the apparatus at any given time.

Suppose we reduce the laser's intensity so that the time interval between photons coming out is so large that there is enough time for one photon to get to a detector before the next one is emitted from the source. Then we can say that there is only one photon in the experiment at any one time. However, we cannot *determine* exactly when a photon will be emitted by a laser; it is a random event. Sometimes a few come close together in time; sometimes there is quite a long time interval between them. We only have control over the *average rate*.

One might expect that the photons arriving at the half-silvered mirror have a 50:50 chance of going through or reflecting off. Another perfectly logical possibility would be that two reduced energy photons emerge from the mirror, one heading in each direction. It is easy enough to determine experimentally exactly what happens: all we have to do is place some photon detectors just after the mirror in the path of each possible beam.

This simple experiment produces an interesting result. Half the time the photon is reflected, and half the time it is transmitted; you never get two photons coming out at the same time. However, there seems to be no inherent difference between those photons that get through and those that reflect. There seems to be no pattern at all to the sequence, except that after a long time half reflect and half get through. Sounds familiar!

We will find that this sort of effect is reasonably common in quantum physics. There seems to be some aspects of nature's behavior that lie beyond our ability to predict (e.g., which way the photon will go). The question is - does this reflect a fundamentally random aspect to nature, or is there something more subtle going on that we have not discovered yet?

Having established that a photon reaching the first half-silvered mirror in a Mach-Zehnder interferometer will either *reflect* and travel the *top path* through the device, or *transmit* and follow the *bottom path*, we now turn our attention to what happens at the detector end of the device.

The first thing we find is that between them, the detectors pick up every photon that enters the experiment. However, the number of photons arriving at either detector in a given time depends on the two path lengths, i.e., if they are exactly equal then *no photons ever* arrive at Y.

If the paths are not exactly equal, then we find that the detection rate at each detector reflects the intensity of the interference pattern that would be observed when the intensity is turned up. What do we mean by that? Let's imagine that we had arranged for the path lengths to be such that 70% of the total light intensity entering the experiment arrives at X and 30% at Y. There is never a double photon firing (as long as we have the laser turned down so there is only one photon in the system at a time). This experiment has been done under extremely well-controlled conditions and there is no doubt that the photon arrival

rate directly reflects an interference pattern as described above.

It doesn't sound like there is much of a problem with this, but there is.

If a photon is genuinely a *small particle* of light, then how can the different path lengths have any effect on *one single photon*?

We confirmed that photons randomly choose reflection or transmission at the half-silvered mirror. After that, they surely proceed along one path or the other to the detector. It is hard to imagine a single photon going along both paths at the same time - remember this seems to be rejected by the experimental results (when we put detectors in the paths after the half-silvered mirror, they only registered one photon at a time down one or the other path).

Now a wave can do this. It can spread out throughout the experiment (think of ripples formed when you toss a pebble into a lake) so that parts of the wave travel along each path at the same time (i.e., the wave energy divides between the paths). When the two parts of the wave combine at the far side of the experiment, the information about both paths is being compared, which leads to the interference pattern.

A single photon must surely have information about only one path, so how can single photon experiments produce interference patterns?

There is a flaw in our arguments. It is extremely subtle and leads us to another of the primary issues that physicists face when dealing with the quantum world. We confirmed that the photons divert at the half-silvered mirror by placing detectors in the two paths. However, doing this eliminated any chance of picking up the interference pattern. If the detectors have stopped the photons, then they have not travelled the paths. In principle, this does not tell us anything about what might happen when no detectors are present.

It would be common sense to assume that the photons do the same thing with or without the detectors, but as we have already seen, the interference pattern for photons does not seem to be a matter of common sense. In addition, the color/hardness experiments lead us to believe that it matters whether or not the detectors are present!

There is a way to investigate this further.

All one has to do is place one photon detector after the half-silvered mirror - say in the path of the reflected beam. If we detect a photon there, then we certainly would not get one at the far side of the experiment. On the other hand, if we do not pick one up at the detector then we can assume that it has passed through the mirror rather than reflecting and so we can expect to see it at the far end. The experiment is easily done and confirms that for every photon leaving the

laser we pick one up either at the far end or in the reflected beam as shown in the figure below.

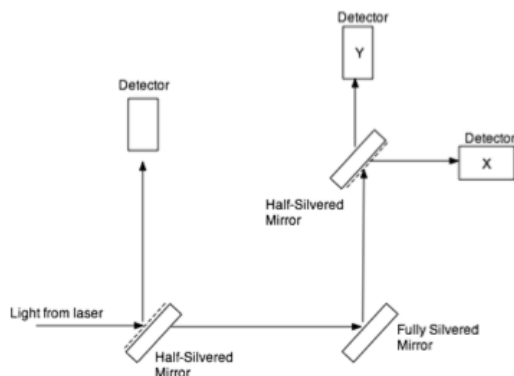


Figure 4.18: Bottom Path

What we find for the transmitted photons is that half of them arrive at Y and the other half at X, no matter what the length of the path is. In other words, there is no interference that takes place. Removing the detector on the reflected path (and replacing the corresponding half-silvered mirror) opens up that route to the far side of the experiment again. At the same time it removes any direct knowledge that we might have about the behavior of the photons at the half-silvered mirror. We observe however, that doing this restores the interference pattern!

It is worth summarizing the *logic* of this so we can expose what is happening.

- (1) The rate of photons arriving at the far side of the experiment is related to the intensity of a bright beam.
- (2) Moving a mirror with a bright beam maps out an interference pattern in the detectors.
- (3) Reducing the intensity of the beam does not affect the interference pattern - instead the arrival rate of the photons now depends on the position of the mirror
- (4) If we set up the experiment so that we can tell which path was taken by the photon (directly or indirectly), then the interference pattern is destroyed.
- (5) If we are unable to tell the paths of photons, then there is an interference pattern, which seems to imply that the photons arriving have information about both routes through the experiment.

- (6) Opening up the top path (by removing the detector) can actually reduce the number of photons arriving at Y. In fact, if the paths' lengths are the same, opening up the top path means that you never get any photons at Y.

All of these experimental results are equivalent to those of a Young-type two-slit interference experiment and the two-path color-hardness experiment discussed earlier.

Delayed Choice

It is possible to make the results of an interference experiment even stranger. To do this we introduce a device called a Pockels cell(PC) into one of the routes. See figure below where the PC is in reflected(top) route.

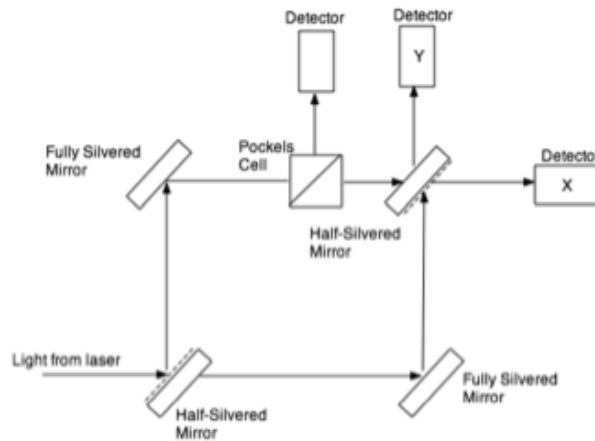


Figure 4.19: Delayed Choice Experiment

PCs are crystals that change their optical properties when an electrical current is applied to them. Without the current, the cell allows photons to pass. Applying a current changes the cell so that it diverts photons, which can then be picked up by another detector. The advantage of this is that the electrical currents can be turned on and off very quickly, which means that should be able to investigate time scales that allow us to find out what the photons are doing while they are in the interferometer.

Consider the following scenario where the PC is set to divert photons(to the added Pockels detector). A photon leaves the laser and arrives at the first half-silvered mirror. If it is reflected, then the setting of the PC will divert it so we don't see it at X or Y. However, if the photon is transmitted by the first half-silvered mirror, it misses the PC, and then eventually it turns up at either

X or Y.

In either case there is no interference pattern (since we have which-path information). If instead we set the PC to pass photons, then in some mysterious manner this changes what happens and we get an interference pattern. In the extreme case of equal path lengths, no photons ever arrive at Y.

Let us assume in the rest of the discussion that the two path lengths are exactly the same.

So what we are saying is:

- (1) If the PC is set to transmit, then we get no photons at Y and all of them at X.
- (2) If the PC is set to divert, then only half of the photons get detected at the far end but they have an equal chance of being picked up at either X or Y.

This result alone is enough to make us stop and think. If the photon takes the lower route with the PC set to divert, then it can get to X or Y. If it takes the lower route with the PC set to pass, then the photon can never arrive at Y. But if it takes the lower route it doesn't go anywhere near the PC, so how can the setting of that device affect things? Is this a further hint that somehow or other the photon travels both routes at the same time? Again this should sound familiar!

Now we start to get devious. Let us set the PC to divert photons, but while the photon is in flight, switch the cell over to the transmit setting. Our ability to do this very rapidly means that we can make the change *after* the photon has interacted with the first half-silvered mirror. There is no magic in doing this. If we know when the photon has left the laser, we can estimate how long it takes to get to the half-silvered mirror. Provided we switch the PC *after* this time, but *before* the photon has had time to reach the detectors X and Y, then we can perform the experiment as described.

If the setting of the PC has in some manner influenced the photon, then the original setting should have determined that the photon take one path or the other and certainly not both at once. Now we have changed the setting after the decision has been made [NOTE: Of course, the word *decision* is not really very appropriate here. Photons do not make decisions (at least we do not think they do). Clearly, it is very hard not to be a somewhat *anthropomorphic* when describing these experiments]. In fact, what we can do is trigger the PC in a random manner. All we need to do is record the setting of the PC and match the arrival of photons at one detector or another. We can then run the experiment for many photons and record their arrival at different detector positions.

After the experiment has run for a while, we can use a computer to sort through the data. What we have is some photons arriving at the Pockels detector (this always happens when the PC is set to divert) and some at the far end of the experiment. This latter group can be sorted out into those that arrived when the PC was set to divert, and those that made it when the PC was set to transmit. Remarkably, when the data are separated out in this manner, the photons that arrived at the far side with the PC set to transmit show an interference pattern. The other photons that arrived with the PC set to divert (but obviously were committed to the other path and so missed it) show no interference pattern.

In every case the PC was set to divert photons and was switched only *after* they left the first mirror. With the PC set to divert, we have seen that the photons follow one route or the another. But we then switched the PC, *destroying* our ability to know which path the photons travelled, and producing an interference pattern. It is hard to believe that changing the setting of the PC can have an influence that *seems to travel backward in time* to when the photon reaches the first mirror. This last statement may be total nonsense of course!

Although this section of the notes has only been a starting point in our exploration of quantum physics, we have already tackled many fundamental issues. We have faced the fact that a description of light must recognize both its wavelike- and particle-like nature, depending on circumstances. The underlying randomness that can appear in the quantum world has also made itself known via our inability to tell which way a photon will travel at a half-silvered mirror (in an experiment set up to detect its path).

But, most importantly, from both the photon experiments and the color/hardness experiments we have seen that quantum physics is going to be a *contextual theory* by which we mean that an adequate description of the behavior of a quantum object (light or electrons in this case) will require an understanding of the *whole* (the context) experimental setup.

The quantum behavior seems to depend on context! The experimental results (answers to questions) seem to depend on what questions we are asking!

Another Interference Experiment

In this discussion we will present another interference experiment that allows us to control the pattern's appearance by making adjustments to a beam that doesn't even take part in the interference itself. Hopefully, the discussion of this somewhat more complicated modern experiment enhances our understanding of the weird nature of the quantum world.

As we saw in the last discussions, one gets into difficulty with experiments when one tries to piece together an understanding of the whole by looking at the com-

ponent parts on their own. When we put everything together, things can behave differently. Equally, the results of one experiment are certainly not an accurate guide to what will happen in another. If that were the case, then we would conclude that photons *always* take only one route, as indicated in experiments that look for the route followed. However, we know full well that as soon as we do not have the ability to tell the path of the photons (directly or indirectly) they *seem* to take both routes at once or something that is equivalent to that.

Another recent experiment has pushed this notion somewhat further by showing that an interference pattern can be destroyed without any direct influence on the photons creating it. This experiment relies on a type of crystal lens known as a *down-shifter*. These devices absorb any photons that enter them and use the energy obtained to produce two new photons, each with half the energy. The experimental arrangement is shown in the figure below.

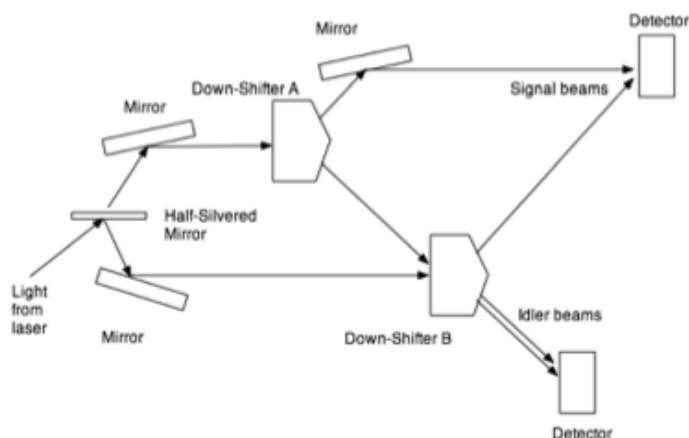


Figure 4.20: Introducing Idler beams

Laser light is sent onto a half-silvered mirror and the two beams are separately directed into down-shifters. Each down-shifter produces a signal beam and an idler beam, the difference between the two beams being nothing more than the subsequent way they are used.

The two signal beams are directed to a detector where they produce an interference pattern due to their different path lengths (same as earlier Mach-Zehnder interferometer, but even more obvious here). The idler beam from down-shifter A is then mixed with that from down-shifter B and both beams arrive at the second detector. The upshot is that every time a photon leaves the laser, a photon of half energy arrives at each detector.

The very fact that an interference pattern emerges at all tells us that, in some manner, each photon appears to have travelled along both signal beam paths. The same was true of the Mach-Zehnder experiments earlier, but now it is clearer.

Let's say that a photon arrives at the half-silvered mirror and from there goes along the top path - and only that path. This photon would eventually arrive at down-shifter A and produce two further photons, one of which ends up at the signal detector and the other at the idler. There would be no interference pattern as no information has been carried to the signal detector about the other route. The same would be true if the photon took the lower route through the experiment. The only way to get an interference pattern at the signal detector is for information to arrive from both routes, in other words, there have to be two signal beams, one from each down-shifter. If this is the case, then the down-shifters have to be *activated* by *something* arriving at each one, which makes it appear that the photon from the laser went both ways at the half-silvered mirror.

However, the presence of the two signal beams, as specified earlier, doesn't imply that the two photons are arriving at the signal detector, as we pick up only one at a time arriving.

Perhaps the most bizarre feature of this experiment is the way in which an interference pattern can be destroyed if we have the ability to tell the path of the photons, even if we don't choose to use this information. The mere threat of doing this, or rather that fact that the experiment is set up in such a way to allow the possibility, is enough to destroy the interference.

This can be dramatically confirmed by blocking one of the idler signals, say from down-shifter A as shown below.

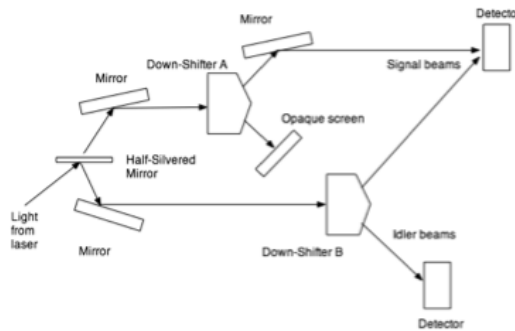


Figure 4.21: Blocking an Idler Beam

The logic here is remarkable.

Whenever a photon is picked up at the idler detector we know it must have come from down-shifter B. This means that a photon from the half-silvered mirror must have hit the down-shifter to be converted into the photon that arrives at the idler detector. From this, we can further deduce that the other photon from down-shifter B must have travelled to the signal detector and therefore that is the photon detected there. Tracing the argument further back, the photon that definitely hits down-shifter B must have come from the half-silvered mirror. Consequently there is no ambiguity about the route that this photon takes from the mirror. Nothing goes along the top route; nothing is produced from down-shifter A, so the interference pattern disappears.

As long as the idler route from down-shifter A is open, we have no way of telling which shifter a photon came from. This ambiguity is sufficient to guarantee an interference pattern at the signal detector. If we don't know that the photon at the idler detector came from B (or A for that matter), then we don't know about the signal photon either. Under those circumstances, we can't say which route the photon took at the half-silvered mirror, so it *takes both routes* or "something" like that.

It seems that the behavior of the photon is being determined by the context of the experiment as a whole. After all, if we know that there are no photons coming from down-shifter A, why does it matter that the idler route from A is blocked? How is this information conveyed back to the half-silvered mirror so as to determine what happens there?

In the experiment with the Pockels cell discussed earlier, we destroyed the interference by changing something directly in the path, leading to the pattern. Here we are placing a block in a path that does not lead to the pattern and furthermore can only directly affect the photons that are not involved with the formation of the pattern anyway!

All of the experiments we have discussed here, whether taking place in the invented world of color/hardness (this will become the world of Stern-Gerlach experiments with electrons shortly) or the real world of photons clearly illustrate the strange requirements that any theory we devise must satisfy.

4.4 Stern-Gerlach Experiments

We now repeat everything again using electrons and Stern-Gerlach devices (you will be able to see the similarities to our color/hardness and photon interference discussions) so that we can reinforce the knowledge we have learned so far and also expand our understanding of quantum theory along the way.

We are now going to discuss the results of a classic experiment performed in 1922. The Stern-Gerlach (S-G) experiment, was designed to study how electrons behave in magnetic fields. We want to illustrate how quantum objects, in this case electrons, behave in another context and in the process do some ground work for further developing the idea of quantum states and the assumptions of quantum theory so that we can proceed later to discuss the modern quantum experiments and ideas which seem so paradoxical to classical physicists.

A quote from Feynman sets the stage for our new discussions.

Newton thought that light was made up of particles, but then it was discovered, as we have seen, that it behaves like a wave. Later(20th century) it was found that light did indeed sometimes behave like a particle. The electron, on the other hand, was thought to behave like a particle and then it was found that in many respects it behaved like a wave. So it really behaves like neither. Now we have given up. We say: "it is like neither". There is one lucky break, however - electrons behave like light. The quantum behavior of atomic objects (electrons, protons, neutrons, photons, and so on) is the same for all, they are all "particle waves" or whatever you want to call them.

This seemingly paradoxical nature of light/electrons is usually called the *wave-particle duality*. They could *appear* to be a wave in one situation and a stream of particles in another. To get to the bottom of this, we have to *give up* in the sense that Feynman suggests. We need to discard the classical descriptions of waves or particles (maybe there are no such things quantum mechanically) and develop a new set of rules and concepts to cover this strange microworld. As we have seen, this is not something we can easily discuss, write down and understand. We need to build our understanding slowly.

As we will see, there is no *wave-particle duality*. Electrons can exhibit wave-like properties during measurements if that is what we are looking for (if that is how we set up the experiment or that is the question we are asking). On the other hand, electrons can exhibit particle-like properties during measurements if that is what we are looking for (if that is how we set up the experiment or that is the question we are asking). The context of the experiment will determine the experimental results - the quantum theory of the microworld is *contextual* in nature.

4.4.1 Stern-Gerlach Experiment

As far as quantum physics is concerned, electrons are fundamental particles, i.e., they are not composites of other particles. Electrons have a negative charge and a very tiny mass ($\sim 1/2000$ of a proton's mass). They are found isolated or inside atoms where they are held to the positively charged nucleus by electric forces. If the atoms are subjected to a large electric field, then we can strip (ionize) the electron from the atoms. Old style CRT tubes are large glass containers with the air taken out (vacuum inside) as shown in the figure below.

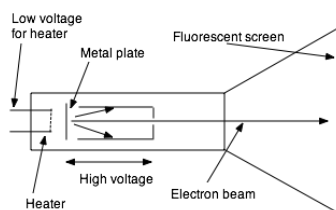


Figure 4.22: An Electron Gun

The tube is generally cylindrical at one end and broadens out to a large flat panel (the screen) at the other. The narrow end contains an *electron gun*, made up of a piece of metal, a heater, and a high-voltage supply. The purpose of the electron gun is to produce a beam of electrons, that is, a continual supply of electrons that are traveling in the same direction with similar speeds. The number of electrons per second moving along the beam as well as their energy can be controlled. Such an electron beam is used to perform the S-G experiment.

Atoms and electrons behave like bar magnets when sent into a magnetic field, i.e., if we send some bar magnets into a non-uniform magnetic field (stronger at the top than the bottom of the field region) then the field both deflects the path of the magnets and aligns (N-S axis) the magnets with the fields. See figure below.

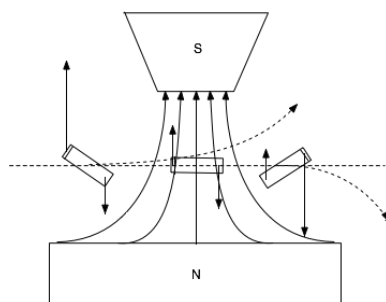


Figure 4.23: Bar Magnets in Non-Uniform Field

The leftmost magnet experiences a combination of forces that tend to turn it in a clockwise direction, so that it aligns with the field. However, due to the nonuniformity of the field, the force on the north pole of the small magnet is stronger than the force on the south pole, so the small magnet will move upward as well as rotate (align with field motion). The right-hand magnet (moving left to right) will experience the same rotation (alignment motion) but the opposite deflection. The small magnet in the center will simply rotate until it is aligned. This deflection provides an ideal way of investigating the magnetic properties of atoms.

Now, we can assume that the S-G magnet exerts a similar magnetic force on electrons (they have a property called a magnetic moment which makes them act like microscopic bar magnets) passing between its poles and that this force will deflect the electron's path as shown in the figure below.

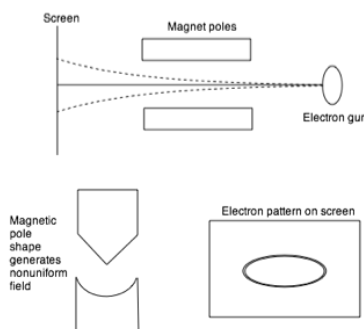


Figure 4.24: Deflecting Electron Paths

The purpose of our hypothetical experiment is to see how much deflection takes place when we pass an electron beam between the poles of one of these magnets. We also assume that we can detect the deflected electrons after they pass through the field region. The electron detectors are assumed to be capable of detecting a single electron at a time.

If we were to run an experiment along these lines, we would observe two things:

- (1) There seems to be no pattern determining which way the electrons are deflected; they go either up or down - apparently at random.
- (2) Each electron is deflected, upward or downward, by a fixed amount (final deflection angle).

The second point is very surprising to a classical physicist: the amount of deflection is same for each electron. If an electron were acting like some sort of tiny magnet (classical picture), we would expect this magnet to be pointing in a more or less random direction when it enters the S-G field. Consequently, the amount of deflection, which depends on the initial orientation of the electron's

magnet, would be slightly different for each one. The end result would be a range(in space) of detected deflection angles by the electron detector, not just two fixed deflections.

One way of interpreting these results is to assume that the electrons have some *internal property* that determines which way they are deflected by the magnet. As they emerge from the electron gun, *up* and *down* types are produced at random, with approximately equal numbers of each. At the end of the experiment, we have two roughly equal-sized sets of sorted electrons. The sets will probably not be exactly the same size due to random experimental variations, but this does not alter the basic principle.

To save making the discussion more complicated than it needs to be (and also to use the quantum terminology we have already developed), we refer to electrons that are deflected upward as *UP state* electrons and give them the state (Dirac ket vector) $|U\rangle$ and those that are deflected downward as *DOWN state* electrons and refer to them by the state $|D\rangle$. For the moment we assume that the state of the electron is determined by some internal property as mentioned above, although we will see shortly that there are some problems with this idea.

We have already stated many properties of states like these and we will have a great deal more to say as we proceed, but a few quick comments are worthwhile at the moment.

One of the great strides forward in the description of nature came when we realized that some physical properties could be specified in a quantitative manner, that is, a numerical value coupled with an appropriate unit. Classical physics (physics from Newton to the discovery of quantum physics) uses a whole set of properties that can be quantitatively specified: mass, velocity, momentum, position, temperature, volume, density, etc.

Some of these properties directly describe the system that we are interested in. These are properties that you can't change without altering the nature of the system. A curling stone would not be a curling stone unless it had particular values of mass, size, shape, etc.

However, some properties describe the particular state that the system happens to be in; position, velocity, and temperature are good examples of such state properties.

One of the key assumptions behind classical physics is that measuring the state of a system does little to alter the values of the state properties; it simply *reveals* the quantitative values of these properties (in suitable units) to some degree of accuracy. In particular, it is always assumed that the system had quantitative values of the state properties, whether they were measured or not. One of the key themes that we will find (and have already seen some examples with

color/hardness) is that such assumptions are called into question when we try to use classical type states to describe quantum systems, such as electrons.

For the moment we assume that the $|U\rangle/|D\rangle$ state describes an electron moving along the top/bottom path through an S-G magnet and that there is some state property belonging to the electron that determines the path that it takes. Observing the path of the electron is the only way we can measure this state property.

Presumably the electron gun feeding the experiment is producing electrons that randomly emerge in either the $|U\rangle$ or $|D\rangle$ state. These electrons pass through the poles of the S-G magnet and are sorted by being deflected according to their labels. This is shown in the figure below.

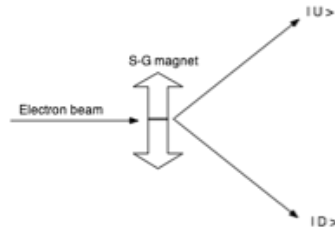


Figure 4.25: A Stern-Gerlach Magnet

At this point we can ask if the results of this experiment are genuinely *measuring* some state property of the electrons, or if the magnet is simply randomly deflecting them one way or the other. One way of answering this question is to consider a modification to the experiment in which the electron detector is removed and replaced by a further pair of S-G magnets arranged in such a way that the electrons passing out of the first magnet pass through one of the two further magnets as shown below.

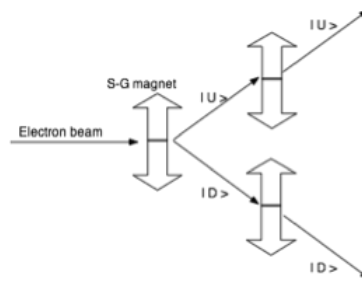


Figure 4.26: Adding Stern-Gerlach Magnets

The results of this modified experiment (corresponds to the repeatability measurements we discussed earlier) are quite conclusive. Electrons that emerge along the UP channel of the first magnet then pass through the topmost second magnet and all of them emerge from that magnet's UP channel. None of these electrons are deflected downward. *Some should be down if the magnet is randomly deflecting electrons.*

In similar fashion, the DOWN electrons emerging from the first magnet are all subsequently deflected down by their second magnet.

The second magnets, and any others that we wish to add to the chain, seem to confirm the sorting carried out by the first magnet. These results definitely give the *impression* that the S-G magnets are *measuring* some state property belonging to the electrons.

4.4.1.1 Turning Things Around

So far we have been using S-G magnets vertically so that they are deflecting electrons upward or downward. The magnets can also be turned through 90° so they deflect electrons right or left. In fact, the S-G magnets can be oriented at any angle, but we will only need (UP,DOWN) and (LEFT, RIGHT).

The results of running an experiment with the S-G magnet turned horizontally are exactly the same as the previous experiments but now in reference to the new orientation of the magnets. Half the electrons passing through the poles of the magnet are deflected to the right, and half to the left. Once again there is no obvious pattern that predicts which electron will go which way.

The same line of argument as earlier then suggests that there are two possible states for an electron to be in, $|R\rangle$ and $|L\rangle$, and the magnet is sorting them out. Thus, the electrons seem to have a second state property that helps to determine which way they get deflected. Adding two further magnets, also arranged horizontally, to check out the electrons in either deflected beam can confirm this. The results are not surprising. The $|R\rangle$ electrons from the first magnet are deflected only to the right by the second magnet and the $|L\rangle$ electrons are deflected to the left again by the second magnet. The similarities to Hardness and Color is striking!

For any physicist, the next step would be to see if the $|U\rangle$ and $|D\rangle$ states are linked (correlated) in some way to the $|R\rangle$ and $|L\rangle$ states. In other words, are the “determining” state properties connected in some manner? This would be easy to check by constructing a further experiment that uses an (UP,DOWN) S-G magnet with two (LEFT,RIGHT) magnets so that the electrons in the UP and DOWN channels of the first magnet are tested to see if they are either $|L\rangle$ or $|R\rangle$. See figure below.

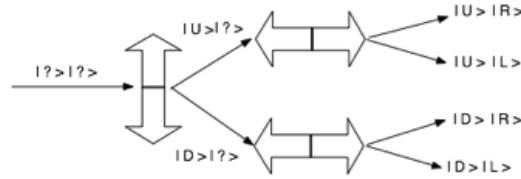


Figure 4.27: Sorting out different electrons

The results of such an experiment are very interesting. It turns out that a $|D\rangle$ passing into a (LEFT,RIGHT) magnet can come out either channel, and similarly for an $|U\rangle$ electron. Think back to the color/hardness boxes and this result should be familiar.

Now if this is true, it would appear that we are actually dealing with *four* different combinations of electron states determined by the two state properties. For example, an electron in state $|U\rangle$ could also be in either state $|L\rangle$ or state $|R\rangle$. The possible combinations are

$$|U\rangle|R\rangle \quad |U\rangle|L\rangle \quad |D\rangle|R\rangle \quad |D\rangle|L\rangle$$

and the electron gun is evidently producing them in equal numbers. The combination of two differently oriented (perpendicular) magnets sorts out these electrons as shown in Figure 4.27.

In Figure 4.27, we have used the symbol $|?\rangle$ to show when we're not sure what state the electron is in. When the electrons in the beam arrive at the first magnet, we have no way of knowing either their (UP,DOWN) or (LEFT,RIGHT) state, hence they are $|?\rangle|?\rangle$. The first magnet sorts them into $|U\rangle$ or $|D\rangle$, but tells us nothing about their $|R\rangle$ or $|L\rangle$ state. The final pair of magnets completes the sorting so that we now have four piles of distinct state combinations, with roughly equal numbers of electrons in each.

4.4.1.2 Things Get More Puzzling

The experiment illustrated in the last figure shows how a combination of three magnets could be used to sort electrons into groups of each of the four possible states. As an extension to this experiment, we might consider adding another two magnets to further check the results as shown in the figure below.

In this experiment we have used some more (UP,DOWN) S-G magnets to check the two beams. The extra magnets have been placed in the path of the $|U\rangle|R\rangle$ and $|D\rangle|L\rangle$ beams. Any of the four beams could have been chosen or even all four of them using two more magnets, but that would just clutter up the diagram and, as it turns out, not add anything to the discussion.

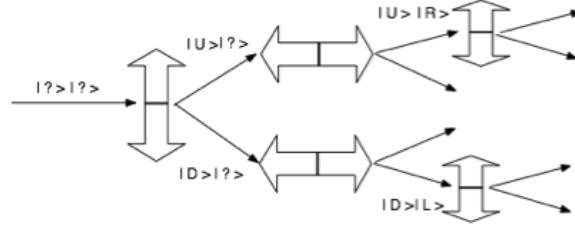


Figure 4.28: Another Experiment - Are we right?

The results of this experiment are truly *remarkable*.

Electrons from the beam that we have labelled as $|U\rangle|R\rangle$ (i.e., we thought that it contained electrons only in the $|U\rangle$ state) now pass through this last magnet and emerge from either the UP- or DOWN-channel. It is as if some $|D\rangle$ state electrons somehow got mixed with the beam that we thought was pure $|U\rangle$. This cannot be a valid explanation since there are no extra electrons in the beam. The results show that each of the emerging beams contains roughly half of the electrons. A more plausible explanation would be that the (LEFT,RIGHT) magnet has somehow changed the state of some of the electrons passing through it. All the electrons arriving at this magnet are in the $|U\rangle$ state, but perhaps after passing through the (LEFT,RIGHT) magnet, a few of them have been flipped into the $|D\rangle$ state.

This immediately suggests a whole new set of experiments. What is it about the angle that changes the state? Does the magnet have to be at 90° to do this? Will any other angle do? What if the magnet is only slightly turned away from being vertical? All of these suggestions could be tested by appropriate experiments. None of these, though, would be as illuminating (and as puzzling) as the experiment we are actually going to look at now.

4.4.1.3 So, Where Did It Go?

The next experiment (in the figure below)

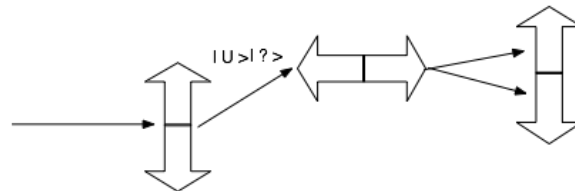


Figure 4.29: Both Beams into Same Magnet

starts with a pure beam of the $|U\rangle$ state electrons (we can do this by selecting the UP channel of an (UP,DOWN) S-G magnet) passing through a (LEFT,RIGHT) magnet, producing two beams, with roughly half the number of electrons in each.

Now by moving another (UP,DOWN) magnet very close in, we can arrange for both beams to pass through the next magnet. This is not as difficult as it sounds; the deflections produced by an S-G magnet are actually quite small - it is only by allowing the electrons to travel some distance after the magnet that the beams separate by measurable amounts.

Before we discuss what actually happens, let us summarize our thinking up to this point.

- (1) Passing through an (UP,DOWN) magnet splits a beam into two samples.
- (2) This implies that an electron can be in any one of two states and the magnet is sorting them out.
- (3) We called these states $|U\rangle$ and $|D\rangle$.
- (4) A horizontally arranged magnet also sorts electrons into $|R\rangle$ and $|L\rangle$ states.
- (5) This suggests that there are four different combinations of electron states: those that are $|U\rangle$ and $|R\rangle$, those that are $|U\rangle$ and $|L\rangle$, and so on.
- (6) However, passing a beam of electrons that should be only $|U\rangle|R\rangle$ (having come from an UP channel and a RIGHT channel in that order) into another (UP,DOWN) magnet divides the beam into two again.
- (7) The *conclusion* from this experiment is that passing a $|U\rangle$ beam through a (LEFT,RIGHT) magnet can somehow flip the (UP,DOWN) state of some of the electrons(if so which electrons get switched?).

Based on this line of thought, you can predict that allowing both beams from the (LEFT,RIGHT) magnet to pass through a single (UP,DOWN) magnet produces the same result as having an (UP,DOWN) magnet on each beam. We should get two beams emerging from the single (UP,DOWN) magnet as the magnet has flipped the state of some of the electrons.

Now, you probably realized that we wouldn't go through all the trouble of explaining this if we were not setting things up for an unexpected result! In fact, using one magnet to catch both emerging beams produces just a single beam of pure $|U\rangle$ electrons as shown below.

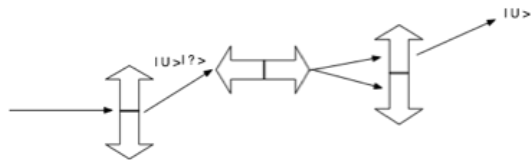


Figure 4.30: Beam is Unchanged! - UP is Preserved

Similar results hold for $|D\rangle$ states. See figure below.

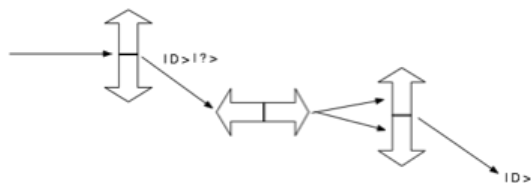


Figure 4.31: Beam is Unchanged! - DOWN is Preserved!

The conclusion is clear. If the beams from the (LEFT,RIGHT) magnet are passed into separate (UP,DOWN) magnets, then the $|U\rangle/|D\rangle$ state of the electrons is modified. However, if both beams from the (LEFT,RIGHT) magnet pass through the same (UP,DOWN), then there is no state flip. The original state of the electrons that entered the (LEFT,RIGHT) magnet is preserved. Remember the hard/soft electrons in the 2-path experiment.

This is very puzzling. Up to now, everything that we have said about electron states and the way electrons are deflected (sorted) by S-G magnets could be a simple extension to classical ideas about electrons. Now with this experiment we're starting to see that these states have a quantum nature, which makes them behave in a rather different (non-classical) way.

One way of trying to retain some *common sense* would be to speculate that the *flipping* of the electron's state is a process that needs a certain distance over which to happen. Hence by moving the (UP,DOWN) S-G magnet nearer we have not given enough opportunity for the flip to happen.

This might be a reasonable speculation, but we can kill it off, and any similar lines of thought with it, by making a simple modification to the experiment.

A small metal plate is sufficient to block either of the channels in the (LEFT,RIGHT) magnet and prevent any electrons from getting through (similar to what we did in the color/hardness experiments). You would just have to make sure that it was not wide enough to stop both channels at the same time. It should be possible to set things up so that we can choose to block either channel, but let's

say we pick the LEFT channel for the moment as shown below.

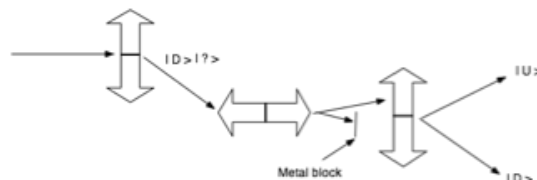


Figure 4.32: BLOCK \rightarrow Scramble (UP,DOWN) Property

We have not moved the magnet any further away, so all the $|D\rangle|L\rangle$ electrons will presumably, if our guess about distance being needed is correct, stay in the $|D\rangle$ state and come out of the second magnet along the bottom channel.

Wrong again!

Making this modification just throws another puzzle in our face. Blocking the LEFT channel restores *flipping* the (UP,DOWN) state. As the experiment doesn't alter the distance travelled by the electrons in the RIGHT channel, we have eliminated any argument based on *flipping* needing a certain distance to work.

We can turn the *flipping* on or off by simply blocking one of the paths and doing nothing to the distance.

As a matter of routine you could check that similar results are obtained if the RIGHT channel is blocked instead, as indeed they are.

We summarize the results of all of these experiments below.

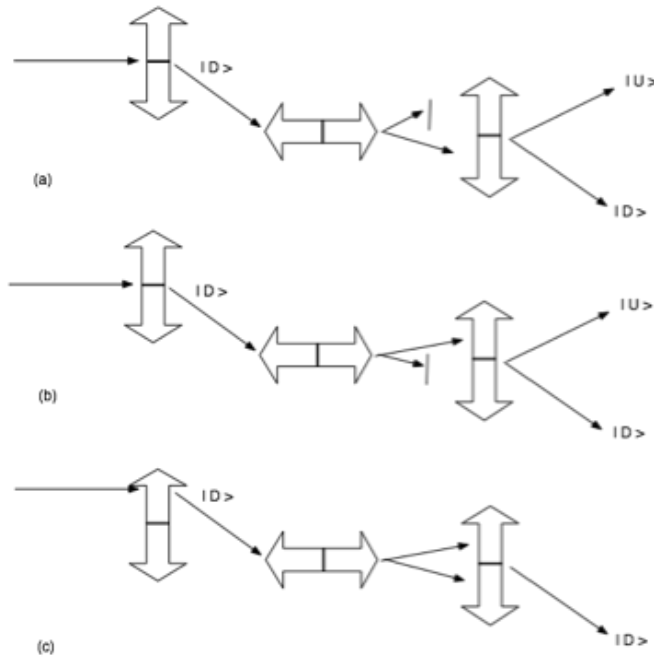


Figure 4.33: Our Results

- (a) Blocking the RIGHT channel produces a mixture of $|U\rangle$ and $|D\rangle$ states in the electrons that pass through the LEFT channel.
- (b) Blocking the LEFT channel produces a mixture of $|U\rangle$ and $|D\rangle$ states in the electrons that pass through the RIGHT channel.
- (c) Having both LEFT and RIGHT channels open produces only $|D\rangle$ state electrons.

4.4.1.4 What Does It All Mean?

We started with the idea that electrons possess a certain state property that determines their path through an S-G magnet. Presumably some electrons start in the $|U\rangle$ state and some in the $|D\rangle$ state, and when the electrons are formed into a beam, the $|U\rangle$ and $|D\rangle$ electrons will be randomly distributed in the beam, so that we can't tell which type is coming next. Roughly half of them are $|U\rangle$ and half are $|D\rangle$, so on the average the beam divides equally when passing through the magnet. This idea was extended to include the results of a (LEFT,RIGHT) magnet, suggesting that every electron has two states and that a beam contains equal numbers of all four different combinations of states.

Crucially, we are assuming that the state of the electron is fully determined

before it enters any magnet that we might put in its path. This is the assumption behind the classical idea of a state (that a measurement reveals what is already there).

The results of the experiments shown in the last figure completely undermine this idea.

- (1) Passing a collection (beam) of $|D\rangle$ state electrons through a (LEFT,RIGHT) magnet separates them into $|D\rangle|L\rangle$ and $|D\rangle|R\rangle$ states, each with equal numbers of each.
- (2) Passing the $|D\rangle|L\rangle$ and $|D\rangle|R\rangle$ electrons into separate (UP,DOWN) magnets produces both $|U\rangle$ and $|D\rangle$ electrons at each magnet, suggesting that the $|D\rangle$ state does not always survive passing through a (LEFT,RIGHT) magnet.
- (3) Passing the $|D\rangle|L\rangle$ and $|D\rangle|R\rangle$ electrons into the *same* (UP,DOWN) magnet produces a pure $|D\rangle$ beam, suggesting that the $|D\rangle$ state is now preserved.
- (4) This undermines the thought expressed in point (1) that we can specify the (UP,DOWN) and (LEFT,RIGHT) states at the same time. Perhaps there are no such things as $|D\rangle|L\rangle$ and $|D\rangle|R\rangle$ states after all, just $|U\rangle/|D\rangle$ or $|R\rangle/|L\rangle$ states.
- (5) Any suggestion that it is the distance travelled by the electrons or the passage through the magnet that causes these effects is contradicted by the experimental results produced by blocking one of the beams.
- (6) Blocking the left- or right-hand beam through the (LEFT,RIGHT) magnet separately before they reach the same single (UP,DOWN) magnet as used in point (3) results in some of the electrons going up and some going down.
- (7) The nature of the electron's state seems to depend on the *context* of the experiment.

There is one point that we have not mentioned yet, and it makes things even stranger. If, for example, we block the LEFT channel, then the electrons passing along the RIGHT channel into the (UP,DOWN) magnet emerge in either $|U\rangle$ or $|D\rangle$ states. However, if they passed along the RIGHT channel, how can they have known that the LEFT channel was closed? Put it another way, if we suddenly open up the LEFT channel, we *add* more electrons passing into the (UP,DOWN) magnet - those that would have gone through the RIGHT channel anyway and those that were probably blocked in the LEFT channel. Suddenly all electrons are now in the $|D\rangle$ state. Remember the magenta electrons coming out all magenta!

None of the results we have been discussing depend in the slightest way on the intensity of the beam. If we choose, the beam can be turned down so low

that only one electron is present in the apparatus at any one time. All our experiments work perfectly well under these conditions and produce the same results. This disposes of any notion that the electrons are *interacting* or *getting in each others way* or any other theory of this sort, which produces particular difficulty with experiments of the sort in the last figure. As I pointed out before, there is no obvious way that an electron passing through one channel could be influenced by the other channel being blocked, unless there was another electron in that channel at the same time to mediate the influence. Clearly, as the experiment gives the same result with a low-intensity beam, that idea can't work either.

One way in which all of these results can be put into a coherent whole is to consider what *information* we can obtain from each experiment in turn.

When one of the channels through the (LEFT,RIGHT) magnet is blocked, it is clear that any electron emerging from the experiment must have passed through the open channel.

However, with both channels open, we cannot tell which path the electrons followed through the (LEFT,RIGHT) magnet.

Remember that electrons are subatomic particles, so it is not simply a case of leaning close over the experiment and watching them go past. Any equipment that we might add into the experiment to figure out which path the electrons take has the same result as blocking the path.

Here, there are clear similarities with the photon experiments discussed earlier. *Once again the context of the whole experiment is proving crucial.*

Evidently, knowing that an electron is in either a $|L\rangle$ or $|R\rangle$ state prevents us from saying for certain that it is in a $|U\rangle$ or $|D\rangle$ state.

Look at Figure 4.33: having one path blocked after the second magnet tells us that an electron entering into the (UP,DOWN) magnet is clearly in either the $|L\rangle$ or $|R\rangle$ states, in which case we have lost any notion of it being $|U\rangle$ or $|D\rangle$. With both paths open there is no information from the experiment that tells us the $|L\rangle/|R\rangle$ state of the electrons. In this case, it seems that we can retain some information about the $|U\rangle/|D\rangle$ state.

This interpretation is not forced on us simply by the results of the experiments discussed so far, but as we look further into quantum physics and discuss other experiments, we will see the consistency of this approach. It ties in with what we were discussing earlier with color/hardness. Those experiments showed us that getting different results depended on not being able to tell which path the electrons were using. Here we can tell if it is $|U\rangle/|D\rangle$ as long as we cannot tell if it is $|L\rangle/|R\rangle$. We will see this again later when we talk about photons and

two-slit(corresponding to two-path) interference phenomena.

All these results are showing us something important about the nature of the quantum state.

Chapter 5

Further Discussion - Mathematical Language of Quantum Mechanics

5.1 Dirac Language

We now need to develop the *full* quantum formalism that explains these experiments. As we said earlier, this requires that we develop the mathematical language necessary to understand the formalism. We now make another pass over the details of the mathematical formalism we have introduced and add a few more needed ideas. We will introduce any other mathematical ideas as needed in later parts of the text.

This is a repeat(sometimes with less details) of some of the ideas we have already presented and we will be repeating much of this discussion throughout the rest of the book, so consider this section one more pass over these very new concepts. I hope that by covering this material many times, we can come to a firmer understanding of these important ideas.

Let us introduce the standard way of writing(from Dirac) vectors in Quantum Physics. The **ket** $|A\rangle$ will be the symbol representing the vector \vec{A} (the old notation) where the **ket-label** A contains **all the information we know about the ket vector**.

For example, we might have labels like (if we were talking about ordinary 2-dimensional vectors)

$$|Q\rangle = |r, \theta\rangle = |x, y\rangle \quad (5.1)$$

for kets representing *position* information.

Vector addition is written as

$$|A\rangle + |B\rangle = |C\rangle \quad (5.2)$$

This addition property is very important.

These ket vectors will represent **real physical systems** in the universe, that is, their mathematical properties will be so extensive that real physical systems can be completely represented by them!

The addition of ket vectors will be connected with the idea of **superposition** of physical systems that will be central to our understanding of quantum physics.

This property of two vectors that they can be added together to form a third vector in the same space will allow us, later on, to construct physical systems that are **sums** of other physical systems such that new, very strange properties, which will be needed to explain experiment, appear.

In particular, it allows us to construct **magenta electrons as superpositions of hard and soft electrons** as we have seen earlier!

So this very simple and basic property of vectors will be connected to powerful properties of real physical systems.

For the moment, however, the Dirac language **simply** looks like a change of notation. ($\vec{A} \rightarrow |A\rangle$)

Let us continue.

Some of the equations that we have developed so far are rewritten in the following way in Dirac language:

$$\begin{aligned}
 \hat{e}_i &\rightarrow |i\rangle \\
 \hat{e}_i \cdot \hat{e}_j &\rightarrow (|i\rangle, |j\rangle) = \langle i | j \rangle = \text{"bra - ket"} = \delta_{ij} \\
 \vec{A} &= \sum_{j=1}^3 A_j \hat{e}_j \rightarrow |A\rangle = \sum_{j=1}^3 A_j |j\rangle \\
 \hat{e}_k \cdot \vec{A} &= A_k \rightarrow \langle k | A \rangle = A_k \\
 \vec{A} &= \sum_{j=1}^3 (\hat{e}_j \cdot \vec{A}) \hat{e}_j \rightarrow |A\rangle = \sum_{j=1}^3 \langle j | A \rangle |j\rangle = \sum_{j=1}^3 |j\rangle \langle j | A \rangle
 \end{aligned} \tag{5.3}$$

The actual choice of any basis set is arbitrary as shown in Figure 5.1 below, where we have (for the 2-dimensional case)

$$|A\rangle = A_1 |1\rangle + A_2 |2\rangle = A'_1 |1'\rangle + A'_2 |2'\rangle \tag{5.4}$$

Clearly, the vector is the same for different bases - only the components change; any **orthonormal** basis set is equivalent in quantum mechanics, i.e., any basis set can be used to represent any vector (or physical system).

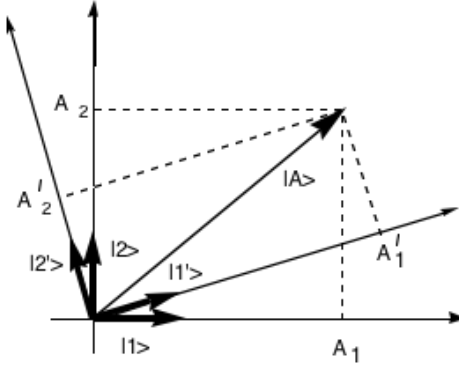


Figure 5.1: Different Bases

As we have seen, in quantum physics, the A_i numbers (the vector components) will represent **real physically measurable** quantities, namely probability amplitudes.

To generalize to an N -dimensional space (this is no longer any real space that you can move around in), we must use N mutually orthonormal vectors to describe it, say the set

$$|1\rangle, |2\rangle, |3\rangle, \dots, |N-1\rangle, |N\rangle \quad (5.5)$$

where the orthonormality is expressed by the scalar product relations

$$\langle i | j \rangle = \delta_{ij} \quad (5.6)$$

where δ_{ij} is the Kronecker-delta function introduced earlier.

Property: for scalar products we have

$$\langle A | (|B\rangle - |C\rangle) = \langle A | B \rangle - \langle A | C \rangle \quad (5.7)$$

We now use this property in an ordinary 2-dimensional space example, i.e., suppose we have the pair of vectors $|x\rangle, |y\rangle$ where

$$\langle x | x \rangle = 1 = \langle y | y \rangle \quad , \quad \langle x | y \rangle = 0 = \langle y | x \rangle \quad (\text{orthonormal}) \quad (5.8)$$

and where the (x, y) labels indicate the direction of the vector in real 2-dimensional space - a real physically measurable thing. Since the vectors $|x\rangle, |y\rangle$ form a orthonormal pair of vectors, we can use the pair of vectors $|x\rangle, |y\rangle$ as **basis** vectors for the 2-dimensional plane (all vectors in the plane can be written in terms of them). They are just the old unit basis vectors (\hat{e}_x, \hat{e}_y) introduced earlier.

Now, suppose we have two vectors $|M\rangle$ and $|Q\rangle$ where

$$\begin{aligned}
 |M\rangle &= m_x |x\rangle + m_y |y\rangle \\
 m_x &= \sqrt{\langle M | M \rangle} \cos \theta_M = L_M \cos \theta_M = \langle x | M \rangle \\
 m_y &= \sqrt{\langle M | M \rangle} \sin \theta_M = L_M \sin \theta_M = \langle y | M \rangle \\
 |Q\rangle &= q_x |x\rangle + q_y |y\rangle \\
 q_x &= \sqrt{\langle Q | Q \rangle} \cos \theta_Q = L_Q \cos \theta_Q = \langle x | Q \rangle \\
 q_y &= \sqrt{\langle Q | Q \rangle} \sin \theta_Q = L_Q \sin \theta_Q = \langle y | Q \rangle
 \end{aligned} \tag{5.9}$$

as shown below:

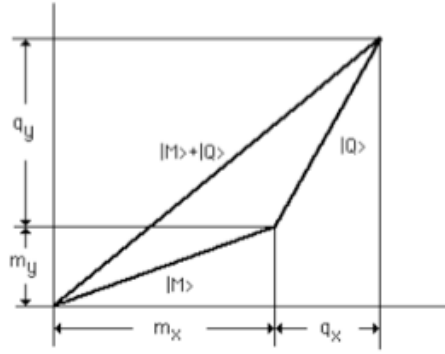


Figure 5.2: 2-Dimensional Example

Now as can be seen from the figure

$$|M\rangle + |Q\rangle = (m_x + q_x) |x\rangle + (m_y + q_y) |y\rangle \tag{5.10}$$

where we have just added components.

The scalar product of these two vectors is given by

$$\langle M | Q \rangle = m_x q_x + m_y q_y \tag{5.11}$$

The value of the scalar product is an **invariant** independent of the choice of basis vectors.

Proof: If we choose a rotated axis pair (rotate by angle ϵ as shown below), then we get (assuming L_M and L_Q are the vector lengths) the component expressions

$$m_x = L_M \cos \theta_M, \quad m_y = L_M \sin \theta_M, \quad q_x = L_Q \cos \theta_Q, \quad q_y = L_Q \sin \theta_Q \tag{5.12}$$

so that

$$\langle M | Q \rangle = m_x q_x + m_y q_y = L_M L_Q (\cos \theta_M \cos \theta_Q + \sin \theta_M \sin \theta_Q) \tag{5.13}$$

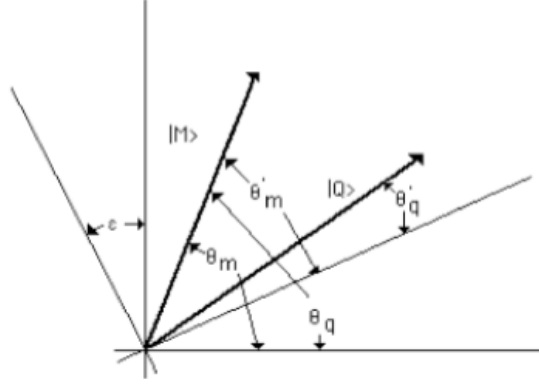


Figure 5.3: 2-Dimensional Example

and similarly for $\langle M' | Q' \rangle$. Then using $\theta_M - \theta_Q = \varepsilon$ as shown in Figure 5.3, we get

$$\begin{aligned} \langle M' | Q' \rangle &= L_M L_Q \cos(\theta'_M - \theta'_Q) = L_M L_Q \cos((\theta_M - \varepsilon) - (\theta_Q - \varepsilon)) \\ &= L_M L_Q \cos(\theta_M - \theta_Q) = \langle M | Q \rangle \end{aligned} \quad (5.14)$$

so that the scalar product is **independent of choice of basis vectors. The scalar product is an invariant.**

Now suppose we want $\langle M | M \rangle = 1$, i.e., suppose that we want a vector that is not necessarily a unit vector (normalized to 1) to become a vector normalized to 1. What does that mean (think length!)? From the previous result

$$\langle M | Q \rangle = m_x q_x + m_y q_y \quad (5.15)$$

we have

$$\langle M | M \rangle = m_x^2 + m_y^2 \quad (5.16)$$

or the sum of the squares of the components the $(\text{length})^2$. This is just the Pythagorean theorem (see diagram in Figure 5.4 below).

If $\langle M | M \rangle \neq 1$, then we can **normalize** the vector by dividing as shown below

$$|M\rangle = \frac{1}{\sqrt{m_x^2 + m_y^2}} (m_x |x\rangle + m_y |y\rangle) \quad (5.17)$$

So we only need to know the two numbers (the two orthogonal components) for each vector and everything else can be determined.

The components seem to contain all the possible information about a vector.

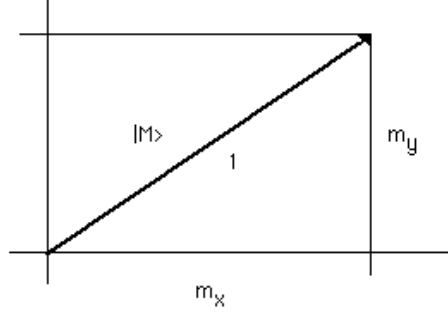


Figure 5.4: Pythagorous

Now, generalizing to N dimensions (where we would need N mutually orthonormal basis vectors). Let us again designate the basis vectors by

$$|1\rangle, |2\rangle, |3\rangle, \dots, |N-1\rangle, |N\rangle \quad (5.18)$$

Suppose we have the two vectors

$$\begin{aligned} |M\rangle &= m_1 |1\rangle + m_2 |2\rangle + m_3 |3\rangle + \dots + m_N |N\rangle \\ |Q\rangle &= q_1 |1\rangle + q_2 |2\rangle + q_3 |3\rangle + \dots + q_N |N\rangle \end{aligned} \quad (5.19)$$

then(as before),

$$|M\rangle + |Q\rangle = (m_1 + q_1) |1\rangle + (m_2 + q_2) |2\rangle + \dots + (m_N + q_N) |N\rangle \quad (5.20)$$

i.e., just add **components** and

$$\langle M | Q \rangle = m_1 q_1 + m_2 q_2 + \dots + m_N q_N \quad (5.21)$$

which = an invariant (independent of the choice of basis).

Our discussion in this chapter up to this point has involved what is called a **real vector space**, i.e., the vector components are real numbers. Quantum mechanics, as we saw earlier, involves components which can be complex numbers or a complex vector space, so we will need a generalization to create the correct vectors and vector properties appropriate for quantum theory.

In particular, the coefficients (components) of the basis vectors will need to be complex numbers, i.e., in the expression

$$|M\rangle = m_x |x\rangle + m_y |y\rangle \quad (5.22)$$

m_x and m_y will need to be complex numbers(discussed earlier).

To allow for the possibility that quantum vectors might have complex components, we **generalize** the definition of the scalar product to

$$\langle M | Q \rangle = m_x^* q_x + m_y^* q_y \quad (5.23)$$

and

$$\langle M | M \rangle = m_x^* m_x + m_y^* m_y = |m_x|^2 + |m_y|^2 \quad (5.24)$$

which means that the length is still a real number!

An **alternative** and very powerful way of looking at the inner products goes as follows: given two ket vectors $|A\rangle, |B\rangle$ we define new mathematical objects given by the symbols $\langle A|, \langle B|$ called **bra** vectors(from "bra-ket" as defined earlier). If the ket vectors $|A\rangle, |B\rangle$ belong to a vector space, the bra vectors $\langle A|, \langle B|$ also belong to a vector space called the **dual** space and

$$\langle A| \text{ is the dual vector for } |A\rangle \quad (5.25)$$

If we have the ket vector

$$|A\rangle = A_1 |1\rangle + A_2 |2\rangle \quad (5.26)$$

then its corresponding dual or bra vector is defined as

$$\langle A| = A_1^* \langle 1| + A_2^* \langle 2| \quad (5.27)$$

and the bra(-c-)ket or inner product is defined as

$$\langle A | B \rangle = (\langle A|) |B\rangle = (\langle A| , |B\rangle) \quad (5.28)$$

The bra vector is also called a **linear functional**. When acting on a ket vector it produces a number (the inner product). Using this idea, we can write the equations above explicitly, i.e.,

$$\begin{aligned} \langle M | M \rangle &= (m_x^* \langle x| + m_y^* \langle y|) (m_x |x\rangle + m_y |y\rangle) \\ &= m_x^* m_x \langle x | x \rangle + m_x^* m_y \langle x | y \rangle + m_y^* m_x \langle y | x \rangle + m_y^* m_y \langle y | y \rangle \\ &= m_x^* m_x + m_y^* m_y = |m_x|^2 + |m_y|^2 \end{aligned} \quad (5.29)$$

We also have the important property

$$\langle V | W \rangle = \langle W | V \rangle^* \quad (5.30)$$

5.1.1 Illustration using Color and Hardness Properties

The above formalism is easily able to describe the world of color and hardness that we discussed earlier.

Suppose that we choose the ket vector $|g\rangle$ to represent the state of an electron with color = green, the ket vector $|m\rangle$ to represent the state of an electron with color = magenta, the ket vector $|h\rangle$ to represent the state of an electron with

hardness = hard, and the ket vector $|s\rangle$ to represent the state of an electron with hardness=soft.

We will assume that

$$\begin{aligned}\langle g | g \rangle &= 1 = \langle m | m \rangle \\ \langle g | m \rangle &= 0 = \langle m | g \rangle\end{aligned}\tag{5.31}$$

i.e., they are an orthonormal basis set and

$$\begin{aligned}\langle h | h \rangle &= 1 = \langle s | s \rangle \\ \langle h | s \rangle &= 0 = \langle s | h \rangle\end{aligned}\tag{5.32}$$

so that they are an orthonormal basis set also.

Physically these statements mean that magenta and green represent the only possible color values (there are only two colors because there are only two vectors in the basis set) that can be measured and hard and soft represent the only possible hardness values that can be measured.

Since we observed that hard electrons can appear to be both green and magenta electrons we might make a first guess (this is what theoretical physicists do - we try things and see if they work!) that

$$|hard\rangle = |h\rangle = a|g\rangle + b|m\rangle\tag{5.33}$$

i.e., a hard electron is a **SUPERPOSITION** of both color states or a hard electron is a **LINEAR COMBINATION** of both color states where the components are

$$\langle g | h \rangle = a \langle g | g \rangle + b \langle g | m \rangle = a \text{ and } \langle m | h \rangle = a \langle m | g \rangle + b \langle m | m \rangle = b\tag{5.34}$$

Can this simple correspondence really work? Is it possible that SUPERPOSITION is just a linear combination or just vector addition!

We shall see later in our discussion of real experiments that it does work!!

We will find many different mathematical ways to represent these fundamental vector objects.

If we know the basis we are using (we shall see later that it will be chosen according to what we are trying to measure) then we only need the two numbers a and b , i.e., the components.

Two different and equivalent ways to represent the superposition are

$$|hard\rangle = a|g\rangle + b|m\rangle = \begin{pmatrix} a \\ b \end{pmatrix}\tag{5.35}$$

where

$$\begin{pmatrix} a \\ b \end{pmatrix} \quad (5.36)$$

is a column vector or 1 x 2 matrix that we discussed earlier (more about matrices later).

That is almost all we will need to know about vectors in order to do quantum theory.

So lots of new words, but really just high school ideas of vectors, components, length(Pythagorus), perpendicular, etc along with an open mind willing to accept new uses for these old ideas and new ways of expressing them.

As we shall see, **ket vectors will represent physical systems in quantum mechanics.**

5.1.2 Operators in a Vector Space

There is one other kind of mathematical object we will need to know about to do quantum theory. They are called **operators**. This one may not be familiar to you from H.S. but the concept should be, as we will now see.

In a vector space, **an operator is a definite rule for taking every vector in the space into some other vector in the space.**

An operator will be represented by the \hat{Q} symbol, i.e., \hat{Q} , so that the action of an operator \hat{Q} is given by the relation

$$|B'\rangle = \hat{Q} |B\rangle \quad (5.37)$$

Think about reading this expression from right to left —

$$\text{vector } |B\rangle \text{ acted upon by operator } \hat{Q} \text{ is changed into vector } |B'\rangle \quad (5.38)$$

Think of an operator as some kind of box, where you put a vector in and get another(**either different or the same**) vector out. This is similar to the definition of an ordinary function for the space of numbers.

5.1.2.1 Some properties of operators in QM:

$$\begin{aligned} \hat{Q}(|A\rangle + |B\rangle) &= \hat{Q}|A\rangle + \hat{Q}|B\rangle \quad (\text{linearity}) \\ \hat{Q}(c|A\rangle) &= c\hat{Q}|A\rangle \quad , \quad c = \text{complex number} \\ \langle C|(\hat{Q}|B\rangle) &= \langle C|B'\rangle = \text{number} = \langle C|\hat{Q}|B\rangle \quad (\text{matrix element}) \\ (\hat{Q}_1 + \hat{Q}_2)|A\rangle &= \hat{Q}_1|A\rangle + \hat{Q}_2|A\rangle \quad (\text{linearity}) \\ (\hat{Q}_1\hat{Q}_2)|A\rangle &= \hat{Q}_1(\hat{Q}_2|A\rangle) \quad (\text{order matters}) \end{aligned} \quad (5.39)$$

These properties imply that all of our operators are what the mathematicians call **LINEAR** operators. The fact that quantum mechanics can be understood using only linear operators is truly amazing because they are the simplest kind of operator that mathematicians can think of.

All observables or “quantities that we can measure” will be represented by operators in quantum mechanics.

Now we introduce a **completely new property** using vectors and operators.

This new property of operators involves mathematical objects called **eigenvalues and eigenvectors**.

In some special cases it turns out that we find the following result:

$$\hat{B}|B\rangle = b|B\rangle \quad (5.40)$$

where b = a number, that is, we get the **exact same vector** back when using the operator (possibly multiplied by a number $\neq 1$).

In this case, $|B\rangle$ is an **eigenvector** of the operator \hat{B} with **eigenvalue** b .

These ideas will be very important in quantum mechanics because the **only possible results that can be obtained from the measurement of a physical quantity or observable** that can be represented by the operator \hat{W} will be the **eigenvalues** of \hat{W} (a postulate we will make later).

The set of eigenvalues is called the **spectrum** of the operator.

It will also turn out that the **eigenvectors** of the operator representing an observable can **always** be used as the **basis** for the vector space.

5.1.2.2 Average Values in Quantum Mechanics Another Way to Represent Operators

Suppose that we have N **identically prepared** physical systems, each represented by the **same** state vector $|\psi\rangle$ – that we can do this will be one of our postulates later.

Suppose that we make measurements of an observable represented by the operator \hat{B} with eigenvalues/eigenvectors given by

$$\hat{B}|b_j\rangle = b_j|b_j\rangle \quad j = 1, 2, 3, 4, \dots \quad (5.41)$$

Suppose the measurement results(remember they must be the eigenvalues as we shall see later) are the b_k , occurring n_k times with $k = 1, 2, 3, 4, \dots$ where

$$\sum_k n_k = N = \text{total number of measurements} \quad (5.42)$$

Now from the definition we derived earlier, the average value of \hat{B} is

$$\begin{aligned}\langle \hat{B} \rangle &= \text{average or expectation value of } \hat{B} \\ &= \frac{1}{N} \sum_k n_k b_k = \sum_k \frac{n_k}{N} b_k = \sum_k b_k \text{prob}(b_k)\end{aligned}$$

In quantum theory, this will given by (another postulate) the expression

$$\langle \hat{B} \rangle = \sum_k b_k \text{prob}(b_k) = \sum_k b_k |\langle b_k | \psi \rangle|^2 \quad (5.43)$$

Since the set $\{|b_k\rangle\}$ is a basis we can write

$$|\psi\rangle = \sum_k \langle b_k | \psi \rangle |b_k\rangle \quad (5.44)$$

This says that $\langle b_k | \psi \rangle$ is the component of the vector $|\psi\rangle$ along the "**direction**" specified by the basis vector $|b_k\rangle$.

Thus, we will have the important result

$$\begin{aligned}\text{prob}(b_k) &= |\langle b_k | \psi \rangle|^2 \\ &= \text{absolute value squared of the component of } |\psi\rangle \text{ along } |b_k\rangle\end{aligned} \quad (5.45)$$

Now by definition

$$|\langle b_k | \psi \rangle|^2 = \langle b_k | \psi \rangle^* \langle b_k | \psi \rangle \quad (5.46)$$

and

$$\langle b_k | \psi \rangle^* = \langle \psi | b_k \rangle \quad (5.47)$$

so we get

$$|\langle b_k | \psi \rangle|^2 = \langle \psi | b_k \rangle \langle b_k | \psi \rangle \quad (5.48)$$

and therefore

$$\langle \hat{B} \rangle = \sum_k b_k |\langle b_k | \psi \rangle|^2 = \sum_k b_k \langle \psi | b_k \rangle \langle b_k | \psi \rangle = \langle \psi | \left[\sum_k b_k |b_k\rangle \langle b_k| \right] | \psi \rangle \quad (5.49)$$

Now the quantity

$$\sum_k b_k |b_k\rangle \langle b_k| = \hat{Q} \quad (5.50)$$

must be some operator in the vector space since when it acts on any vector the result is another vector.

Proof:

Now we can always write

$$|a\rangle = \sum_s d_s |b_s\rangle = \text{arbitrary vector}$$

since the set $\{|b_k\rangle\}$ is a basis. This gives

$$\begin{aligned}\hat{Q}|a\rangle &= \left(\sum_k b_k |b_k\rangle \langle b_k|\right)|a\rangle = \left(\sum_k b_k |b_k\rangle \langle b_k|\right)\left(\sum_s d_s |b_s\rangle\right) \\ &= \sum_{k,s} d_s b_k |b_k\rangle \langle b_k | b_s\rangle = \sum_{k,s} d_s b_k |b_k\rangle \delta_{ks} = \sum_k b_k d_k |b_k\rangle\end{aligned}$$

so that the operation by \hat{Q} on an arbitrary vector returns a vector indicating that \hat{Q} is an operator.

But we also have

$$\hat{B}|a\rangle = \sum_k d_k \hat{B}|b_k\rangle = \sum_k b_k d_k |b_k\rangle$$

This is the same result as for the operator \hat{Q} , which says (since the vector $|a\rangle$ is arbitrary) that we can always write

$$\hat{B} = \sum_k b_k |b_k\rangle \langle b_k| \quad (5.51)$$

This is another(very important) way of representing the operator , i.e., **any operator can be written in terms of its eigenvalues and eigenvectors**. It is called the **spectral decomposition** of the operator.

Therefore, the average value expression becomes

$$\langle \hat{B} \rangle = \langle \psi | \left[\sum_k b_k |b_k\rangle \langle b_k| \right] | \psi \rangle = \langle \psi | \hat{B} | \psi \rangle \quad (5.52)$$

Thus, when we do an experiment of this type, i.e., identical measurements on many identical systems, the (expected) average of those measurements is just this **average or expectation value** given by $\langle \psi | \hat{B} | \psi \rangle$.

5.1.2.3 Projection Operators

Operators of the form

$$\hat{P} = |b_k\rangle \langle b_k| \quad (5.53)$$

where the $|b_k\rangle$ are eigenvectors of the operator \hat{B} , i.e.,

$$\hat{B}|b_j\rangle = b_j |b_j\rangle \quad j = 1, 2, 3, 4, \dots \quad (5.54)$$

are called **projection operators**. They have some very interesting and useful properties.

First, let us determine the eigenvalues of a projection operator? We have

$$\hat{P}^2 = (|b_k\rangle \langle b_k|)(|b_k\rangle \langle b_k|) = |b_k\rangle \langle b_k | b_k\rangle \langle b_k| = |b_k\rangle \langle b_k| = \hat{P} \quad (5.55)$$

or if

$$\hat{P}|\alpha\rangle = \lambda|\alpha\rangle \quad (5.56)$$

so that $|\alpha\rangle$ = eigenvector and λ = the corresponding eigenvalue, then we have

$$\begin{aligned} \hat{P}^2|\alpha\rangle &= \lambda\hat{P}|\alpha\rangle = \lambda^2|\alpha\rangle = \hat{P}|\alpha\rangle = \lambda|\alpha\rangle \\ (\lambda^2 - \lambda)|\alpha\rangle &= 0 \\ \lambda^2 - \lambda = 0 &\rightarrow \lambda = 0 \text{ or } 1 \rightarrow \text{eigenvalues} \end{aligned} \quad (5.57)$$

Second, consider the following operator

$$\hat{I} = \sum_k |b_k\rangle \langle b_k| \quad (5.58)$$

We have

$$\hat{I}|\beta\rangle = \sum_k |b_k\rangle \langle b_k | \beta\rangle = \sum_k \langle b_k | \beta\rangle |b_k\rangle = |\beta\rangle$$

or

$$\hat{I} = \sum_k |b_k\rangle \langle b_k| \quad (5.59)$$

is the so-called **identity operator**. The identity operator being defined as that operator which does not change anything!

Our earlier results now make sense since

$$|\psi\rangle = \sum_k \langle b_k | \psi\rangle |b_k\rangle = \sum_k |b_k\rangle \langle b_k | \psi\rangle = \left(\sum_k |b_k\rangle \langle b_k| \right) |\psi\rangle = \hat{I}|\psi\rangle \quad (5.60)$$

5.1.2.4 Operator Examples

Suppose we define an operator

$$\hat{G} = |g\rangle \langle g| = |green\rangle \langle green| \quad (5.61)$$

We then have these properties

$$\hat{G}|g\rangle = |g\rangle \langle g | g\rangle = |g\rangle \quad , \quad \hat{G}|m\rangle = |g\rangle \langle g | m\rangle = 0 \quad (5.62)$$

or the states representing the green and magenta electrons are the eigenvectors of \hat{G} with eigenvalues 1 and 0 respectively.

We also find that the expectation value of \hat{G} in the green state is

$$\langle g | \hat{G} | g\rangle = |\langle g | g\rangle|^2 = 1 \quad (5.63)$$

and the expectation value of \hat{G} in the magenta state is

$$\langle m | \hat{G} | m\rangle = |\langle g | m\rangle|^2 = 0 \quad (5.64)$$

These results make sense if we **interpret**

$$\hat{G} = |g\rangle \langle g| \quad (5.65)$$

as the operator corresponding to a measurement of the green property of electrons, i.e., an observer looking at the output of a green aperture of a color box.

The first result then says, using the earlier result

$$prob(b_k) = |\langle b_k | \psi \rangle|^2 \quad (5.66)$$

that if we measure the probability that the color of a green electron is green we get the value 1 as expected and the second result then says if we measure the probability that the color of a green electron is magenta we get the value 0 as expected. Things make sense! Pushing these strange ideas even further, if we assume, as earlier, that a hard electron is a superposition of green and magenta electrons,

$$|hard\rangle = |h\rangle = \frac{1}{\sqrt{2}} |g\rangle + \frac{1}{\sqrt{2}} |m\rangle \quad (5.67)$$

then the expectation value of \hat{G} in the hard state is

$$\begin{aligned} \langle h | \hat{G} | h \rangle &= \left(\frac{1}{\sqrt{2}} \langle g | + \frac{1}{\sqrt{2}} \langle h | \right) \hat{G} \left(\frac{1}{\sqrt{2}} |g\rangle + \frac{1}{\sqrt{2}} |m\rangle \right) \\ &= \frac{1}{2} \langle g | \hat{G} | g \rangle + \frac{1}{2} \langle g | \hat{G} | m \rangle + \frac{1}{2} \langle m | \hat{G} | g \rangle + \frac{1}{2} \langle m | \hat{G} | m \rangle \\ &= \frac{1}{2} \langle g | \hat{G} | g \rangle = \frac{1}{2} \end{aligned}$$

Another way of saying this is, using the earlier result

$$\langle \hat{B} \rangle = \sum_k b_k prob(b_k) = \sum_k b_k |\langle b_k | \psi \rangle|^2 \quad (5.68)$$

is

$$\begin{aligned} \langle h | \hat{G} | h \rangle &= \sum (\text{eigenvalue } g) (\text{probability of } g \text{ in } |h\rangle) \\ &= (1) |\langle \text{eigenvalue} = 1 | h \rangle|^2 + (0) |\langle \text{eigenvalue} = 0 | h \rangle|^2 \\ &= (1) |\langle g | h \rangle|^2 + (0) |\langle m | h \rangle|^2 = (1) \frac{1}{2} + (0) \frac{1}{2} = \frac{1}{2} \end{aligned} \quad (5.69)$$

which again makes sense, i.e., if we have a beam of hard electrons, then we will measure an electron to be green 1/2 of the time as we observed earlier!

Clearly, this formalism is both neat and very powerful and certainly seems to have the potential to describe our earlier observations. We will see shortly that the formalism can completely represent quantum systems and quantum measurements.

5.1.3 More Useful Mathematical Ideas

5.1.3.1 Matrices

We have been representing an operator by the way it acts on vectors.

An operator can also be represented by an array of numbers. In mathematics such an array is called a **matrix**, i.e., a matrix is a mathematical object which takes the form

$$[O] = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \quad (5.70)$$

which is a 2×2 matrix representing the operator \hat{O} and the numbers $\alpha, \beta, \gamma, \delta$ are called the matrix elements of \hat{O} . Their numerical values depend on which set of basis vectors we are using and the corresponding operator \hat{O} .

Let us assume the two basis vectors are labelled by $|1\rangle, |2\rangle$. We then define

$$\begin{aligned} \alpha &= O_{11} = \langle 1 | \hat{O} | 1 \rangle = O_{\text{row label, column label}} \\ \beta &= O_{12} = \langle 1 | \hat{O} | 2 \rangle \\ \gamma &= O_{21} = \langle 2 | \hat{O} | 1 \rangle \\ \delta &= O_{22} = \langle 2 | \hat{O} | 2 \rangle \end{aligned} \quad (5.71)$$

or

$$[O] = \begin{pmatrix} O_{11} & O_{12} \\ O_{21} & O_{22} \end{pmatrix} = \begin{pmatrix} \langle 1 | \hat{O} | 1 \rangle & \langle 1 | \hat{O} | 2 \rangle \\ \langle 2 | \hat{O} | 1 \rangle & \langle 2 | \hat{O} | 2 \rangle \end{pmatrix} \quad (5.72)$$

This is called the **matrix representation** of the operator \hat{O} in the $|1\rangle, |2\rangle$ basis.

A vector in the space is then represented by a 2-element column matrix (vector) of the form

$$|a\rangle = a_1 |1\rangle + a_2 |2\rangle = \langle 1 | a \rangle |1\rangle + \langle 2 | a \rangle |2\rangle \equiv \begin{pmatrix} \langle 1 | a \rangle \\ \langle 2 | a \rangle \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \quad (5.73)$$

This implies that the basis vectors themselves are represented (in the $|1\rangle, |2\rangle$ basis) by the particular column matrices

$$|1\rangle = \begin{pmatrix} \langle 1 | 1 \rangle \\ \langle 2 | 1 \rangle \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |2\rangle = \begin{pmatrix} \langle 1 | 2 \rangle \\ \langle 2 | 2 \rangle \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (5.74)$$

i.e.,

$$|a\rangle = a_1 |1\rangle + a_2 |2\rangle = a_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + a_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \quad (5.75)$$

Now consider the color basis. In this case, we have

$$|1\rangle = |g\rangle = \begin{pmatrix} \langle g | g \rangle \\ \langle m | g \rangle \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |2\rangle = |m\rangle = \begin{pmatrix} \langle g | m \rangle \\ \langle m | m \rangle \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (5.76)$$

and

$$|hard\rangle = |h\rangle = \frac{1}{\sqrt{2}}|g\rangle + \frac{1}{\sqrt{2}}|m\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (5.77)$$

We also have

$$|soft\rangle = |s\rangle = \frac{1}{\sqrt{2}}|g\rangle - \frac{1}{\sqrt{2}}|m\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (5.78)$$

Note that the hard and soft states are also orthonormal. Both sets are bases as can be seen explicitly by the example below (written in the color basis):

$$\begin{aligned} |\psi\rangle &= \begin{pmatrix} a \\ b \end{pmatrix} = a\begin{pmatrix} 1 \\ 0 \end{pmatrix} + b\begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ &= \frac{1}{\sqrt{2}}(a+b)\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{1}{\sqrt{2}}(a-b)\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \\ &= a|g\rangle + b|m\rangle = \frac{1}{2}(a+b)|h\rangle + \frac{1}{2}(a-b)|s\rangle \end{aligned} \quad (5.79)$$

The operator \hat{G} was defined to be

$$\hat{G} = |g\rangle\langle g| \quad (5.80)$$

and it represented measuring the **"green"** property of electrons.

The matrix representing \hat{G} (in the color basis) can now be written down:

$$\begin{aligned} (\hat{G})_{11} &= \langle g|\hat{G}|g\rangle = \langle g|(|g\rangle\langle g|)|g\rangle = 1 \\ (\hat{G})_{12} &= \langle g|\hat{G}|m\rangle = \langle g|(|g\rangle\langle g|)|m\rangle = 0 \\ (\hat{G})_{21} &= \langle m|\hat{G}|g\rangle = \langle m|(|g\rangle\langle g|)|g\rangle = 0 \\ (\hat{G})_{22} &= \langle m|\hat{G}|m\rangle = \langle m|(|g\rangle\langle g|)|m\rangle = 0 \end{aligned} \quad (5.81)$$

or

$$[\hat{G}] = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad (5.82)$$

We then have

$$\begin{aligned} \hat{G}|g\rangle &= (|g\rangle\langle g|)|g\rangle = |g\rangle \\ \text{or} \\ \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \rightarrow \text{matrix multiplication} \end{aligned} \quad (5.83)$$

where **matrix multiplication** is defined by these relations: if

$$[A] = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \quad [B] = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \quad (5.84)$$

then

$$[A][B] = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} = \begin{pmatrix} a_{11}b_{11} + a_{12}b_{21} & a_{11}b_{12} + a_{12}b_{22} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} \end{pmatrix} \quad (5.85)$$

or

$$[AB]_{ij} = \sum_k a_{ik} b_{kj} \quad (5.86)$$

Thus, we have **two equivalent ways** of doing calculations, i.e., using **operator algebra** or **matrix algebra**.

5.1.3.2 Another Example in a Finite Dimensional Vector Space

Let us consider the 2-dimensional vector space spanned by the orthonormal basis set

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (5.87)$$

We can define two projection operators as

$$\hat{P}_1 = |1\rangle \langle 1| \quad , \quad \hat{P}_2 = |2\rangle \langle 2| \quad (5.88)$$

The matrix representation of these two projection operators is easily found. We have

$$\begin{aligned} (\hat{P}_1)_{11} &= \langle 1 | \hat{P}_1 | 1 \rangle = \langle 1 | (|1\rangle \langle 1|) | 1 \rangle = 1 \\ (\hat{P}_1)_{12} &= \langle 1 | \hat{P}_1 | 2 \rangle = \langle 1 | (|1\rangle \langle 1|) | 2 \rangle = 0 \\ (\hat{P}_1)_{21} &= \langle 2 | \hat{P}_1 | 1 \rangle = \langle 2 | (|1\rangle \langle 1|) | 1 \rangle = 0 \\ (\hat{P}_1)_{22} &= \langle 2 | \hat{P}_1 | 2 \rangle = \langle 2 | (|1\rangle \langle 1|) | 2 \rangle = 0 \end{aligned} \quad (5.89)$$

or

$$[\hat{P}_1] = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad (5.90)$$

and in a similar manner

$$[\hat{P}_2] = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad (5.91)$$

Now consider an arbitrary vector in this space

$$|\psi\rangle = a|1\rangle + b|2\rangle = \begin{pmatrix} a \\ b \end{pmatrix} \quad (5.92)$$

We then have (using both Dirac and matrix language)

$$\begin{aligned} \hat{P}_1 |\psi\rangle &= a\hat{P}_1 |1\rangle + b\hat{P}_1 |2\rangle = a|1\rangle \langle 1 | 1 \rangle + b|1\rangle \langle 1 | 2 \rangle = a|1\rangle \\ \hat{P}_1 |\psi\rangle &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = a \begin{pmatrix} 1 \\ 0 \end{pmatrix} = a|1\rangle \end{aligned} \quad (5.93)$$

and the projection operator performs as advertised. We note that (at least in this **special case**)

$$(\hat{P}_1) + (\hat{P}_2) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \hat{I} = \text{identity operator}$$

or

$$(\hat{P}_1 + \hat{P}_2) |a\rangle = (|1\rangle \langle 1| + |2\rangle \langle 2|) |a\rangle = \sum_{j=1}^2 |j\rangle \langle j | a \rangle = |a\rangle = \hat{I} |a\rangle \quad (5.94)$$

where we have made use of the expansion formula for an arbitrary state in an orthonormal basis.

We now introduce another useful mathematical object.

5.1.3.3 The Commutator

We define the **commutator** between two operators as

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \quad (5.95)$$

For ordinary numbers the commutator is zero, but for operators it is not always zero.

If two operators have a **zero** commutator, then we say that they **commute**.

If we have

$$\hat{A} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \hat{B} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (5.96)$$

then

$$\begin{aligned} [\hat{A}, \hat{B}] &= \hat{A}\hat{B} - \hat{B}\hat{A} \\ &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = 2 \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \neq 0 \end{aligned} \quad (5.97)$$

so that they do not commute!

5.2 A More Mathematical Digression

Learning the explicit process for finding eigenvectors/eigenvalues is useful easy to show. We presented this process earlier and repeat it now to make sure that everyone understands it.

Let us now devise a **general procedure** for finding the eigenvalues and eigenvectors of an operator. We will use the matrices that represent operators. In particular, we consider the matrices (operators)

$$\hat{A} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \hat{B} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \hat{C} = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix} \quad (5.98)$$

We consider the operator \hat{A} first. The eigenvalue/eigenvector problem can be written in the following way:

$$\hat{A}|\alpha\rangle = \alpha|\alpha\rangle \quad (5.99)$$

or in terms of matrices

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a \\ -b \end{pmatrix} = \alpha \begin{pmatrix} a \\ b \end{pmatrix} \quad (5.100)$$

The last matrix equation corresponds to two simple algebraic equations (equating matrix elements)

$$a = \alpha a \quad , \quad b = -\alpha b \quad (5.101)$$

The solutions to these equations are:

$$\begin{aligned} a \neq 0 &\rightarrow \alpha = 1 \\ &\rightarrow b = -b \rightarrow b = 0 \end{aligned} \quad (5.102)$$

and

$$\begin{aligned} b \neq 0 &\rightarrow \alpha = -1 \\ &\rightarrow a = -a \rightarrow a = 0 \end{aligned} \quad (5.103)$$

This says that the eigenvalues of \hat{A} are $\alpha = \pm 1$ and the corresponding eigenvectors (normalized to 1) are

$$|+1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad |-1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (5.104)$$

So, for diagonal matrices (where the only non-zero matrix elements lie along the diagonal) the eigenvalue/eigenvector problem is trivial. The eigenvalues are just the diagonal matrix elements and the eigenvectors are just column vectors with a single entry = 1 and all other entries = 0. This generalizes to any number of dimensions.

Let us use this simple case to illustrate the general procedure for non-diagonal matrices. We had

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \alpha \begin{pmatrix} a \\ b \end{pmatrix} \quad (5.105)$$

This can be written as

$$\begin{pmatrix} 1-\alpha & 0 \\ 0 & -1-\alpha \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = 0 \quad (5.106)$$

This set of equations is called homogeneous (zeroes on the right-hand side). A trivial solution always exists - it is $a = b = 0$. This solution is of no interest to physicists. We will have a non-trivial solution if and only if

$$\text{determinant} \begin{pmatrix} 1-\alpha & 0 \\ 0 & -1-\alpha \end{pmatrix} = \det \begin{pmatrix} 1-\alpha & 0 \\ 0 & -1-\alpha \end{pmatrix} = \begin{vmatrix} 1-\alpha & 0 \\ 0 & -1-\alpha \end{vmatrix} = 0 \quad (5.107)$$

where

$$\det \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc \quad (5.108)$$

In the above case we get

$$\begin{vmatrix} 1-\alpha & 0 \\ 0 & -1-\alpha \end{vmatrix} = 0 = (1-\alpha)(-1-\alpha) \rightarrow \alpha = \pm 1 \rightarrow \text{eigenvalues} \quad (5.109)$$

Proof: Suppose that we have a pair of linear equations in two unknowns

$$\begin{aligned} a\alpha_1 + b\alpha_2 &= q_1 \\ c\alpha_1 + d\alpha_2 &= q_2 \end{aligned} \quad (5.110)$$

We can write these equations in matrix notation as

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} \quad (5.111)$$

or

$$A\alpha = Q \quad (5.112)$$

where

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad \alpha = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}, \quad Q = \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} \quad (5.113)$$

The inverse of a matrix(or operator) A^{-1} is defined by

$$A^{-1}A = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \text{identity} \quad (5.114)$$

If the inverse exists, then we can write

$$A^{-1}A\alpha = I\alpha = \alpha = A^{-1}Q \quad (5.115)$$

which represents a solution for the unknowns α_1 and α_2 .

For a 2×2 matrix

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad (5.116)$$

the inverse is given by

$$A^{-1} = \frac{1}{\det A} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} \quad (5.117)$$

where

$$\det A = ad - bc \quad (5.118)$$

since

$$A^{-1}A = \frac{1}{\det A} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (5.119)$$

The solution of the original equation is then given by

$$\begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \frac{1}{\det A} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} \quad (5.120)$$

Example: Suppose we have

$$\begin{aligned} x + 2y &= 5 \\ 2x - 3y &= 4 \end{aligned} \quad (5.121)$$

or

$$\begin{pmatrix} 1 & 2 \\ 2 & -3 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 5 \\ 4 \end{pmatrix} \quad (5.122)$$

We then have

$$A = \begin{pmatrix} 1 & 2 \\ 2 & -3 \end{pmatrix}, \quad \det A = -7, \quad A^{-1} = -\frac{1}{7} \begin{pmatrix} -3 & -2 \\ -2 & 1 \end{pmatrix} \quad (5.123)$$

Check:

$$A^{-1}A = -\frac{1}{7} \begin{pmatrix} -3 & -2 \\ -2 & 1 \end{pmatrix} \begin{pmatrix} 1 & 2 \\ 2 & -3 \end{pmatrix} = -\frac{1}{7} \begin{pmatrix} -7 & 0 \\ 0 & -7 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (5.124)$$

as it should.

We therefore have the solution

$$\begin{pmatrix} x \\ y \end{pmatrix} = A^{-1} \begin{pmatrix} 5 \\ 4 \end{pmatrix} = -\frac{1}{7} \begin{pmatrix} -3 & -2 \\ -2 & 1 \end{pmatrix} \begin{pmatrix} 5 \\ 4 \end{pmatrix} = -\frac{1}{7} \begin{pmatrix} -23 \\ -6 \end{pmatrix} \quad (5.125)$$

or

$$x = \frac{23}{7}, \quad y = \frac{6}{7} \quad (5.126)$$

Now let us return to the case of the eigenvalue/eigenvector equation where we have

$$\hat{A}|\alpha\rangle = \alpha|\alpha\rangle = \alpha\hat{I}|\alpha\rangle \quad (5.127)$$

or

$$(\hat{A} - \alpha\hat{I})|\alpha\rangle = 0 \quad (5.128)$$

If we define

$$\hat{R} = \hat{A} - \alpha\hat{I} \quad (5.129)$$

then we have the equation

$$\hat{R}|\alpha\rangle = 0 \quad (5.130)$$

or

$$\begin{aligned} & \left[\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} - \begin{pmatrix} \alpha & 0 \\ 0 & \alpha \end{pmatrix} \right] \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\ & \begin{pmatrix} A_{11} - \alpha & A_{12} \\ A_{21} & A_{22} - \alpha \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \end{aligned} \quad (5.131)$$

Thus, we have a formal solution

$$\begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \frac{1}{\det \begin{pmatrix} A_{11} - \alpha & A_{12} \\ A_{21} & A_{22} - \alpha \end{pmatrix}} \begin{pmatrix} A_{11} - \alpha & A_{12} \\ A_{21} & A_{22} - \alpha \end{pmatrix} \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad (5.132)$$

The only possibility that this gives a nonzero(or nontrivial) result is when

$$\det \begin{pmatrix} A_{11} - \alpha & A_{12} \\ A_{21} & A_{22} - \alpha \end{pmatrix} = 0 \quad (5.133)$$

which completes the proof.

A more general procedure(matrix not diagonal) for finding eigenvalues goes like the following:

$$\begin{aligned} \hat{G} &= \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix} \\ \hat{G}|\lambda\rangle &= \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} = \lambda \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} = \lambda|\lambda\rangle \end{aligned} \quad (5.134)$$

$$\begin{aligned} &\begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} - \lambda \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} \\ &= \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} - \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} \\ &= \begin{pmatrix} g_{11} - \lambda & g_{12} \\ g_{21} & g_{22} - \lambda \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} = 0 \end{aligned} \quad (5.135)$$

Once again, this last set of equations is pair of homogeneous linear equations. Again, there is a always the trivial solution ($\lambda_1 = \lambda_2 = 0$). A non-trivial solution exists only if

$$\det \begin{pmatrix} g_{11} - \lambda & g_{12} \\ g_{21} & g_{22} - \lambda \end{pmatrix} = 0 \quad (5.136)$$

which is a **quadratic equation** for the eigenvalues.

Let us apply this procedure to the other two operators. First we work with \hat{B} .

$$\hat{B} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \rightarrow \det(\hat{B} - \alpha \hat{I}) = 0 = \begin{vmatrix} -\alpha & 1 \\ 1 & -\alpha \end{vmatrix} = \alpha^2 - 1 \rightarrow \alpha = \pm 1 \quad (5.137)$$

To find the eigenvectors(subscripts indicate basis) we then proceed as follows:

$$\begin{aligned} \alpha &= +1 \\ \rightarrow \hat{B}|+1\rangle_B &= |+1\rangle_B \rightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix} \\ \rightarrow b &= a \end{aligned} \quad (5.138)$$

To normalize this eigenvector we must have

$${}_B \langle +1 | +1 \rangle_B = 1 = a^2 + b^2 = 2a^2 \rightarrow a = \frac{1}{\sqrt{2}} = b \quad (5.139)$$

so that

$$|+1\rangle_B = \begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (5.140)$$

and similarly,

$$|-1\rangle_B = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (5.141)$$

Second, we work with \hat{C} .

$$\hat{C} = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix} \rightarrow \begin{vmatrix} 1-\alpha & 2 \\ 2 & 1-\alpha \end{vmatrix} = 0 = (1-\alpha)(1-\alpha) - 4 \rightarrow \alpha^2 - 2\alpha - 3 = 0 \rightarrow \alpha = 3, -1 \quad (5.142)$$

To find the eigenvectors we then proceed as follows:

$$\begin{aligned} \alpha &= +3 \\ \rightarrow \hat{C}|+3\rangle_C &= 3|+3\rangle_C \rightarrow \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = 3 \begin{pmatrix} a \\ b \end{pmatrix} \\ \rightarrow a + 2b &= 3a \\ \rightarrow 2a + b &= 3b \\ \rightarrow b = a, \quad a^2 + b^2 &= 1 \rightarrow a = \frac{1}{\sqrt{2}} = b \end{aligned} \quad (5.143)$$

so that

$$|+3\rangle_C = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |-1\rangle_C = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (5.144)$$

A strange thing has happened. Both operators \hat{B} and \hat{C} have the same eigenvectors (different eigenvalues).

It turns out that the following important property is true:

if two operators commute, then they share a common set of eigenvectors

This the case for \hat{B} and \hat{C} .

5.2.1 Special Matrices (operators)

Two special types of operators will dominate our discussion of quantum mechanics. For later use we define:

$$\begin{aligned} \text{Transpose} : \hat{A}^{Tr} &\rightarrow (A^{Tr})_{ji} = A_{ij} \\ \text{Hermitian} : \hat{A} &= \hat{A}^\dagger = \hat{A}^{*Tr} \rightarrow A_{ij} = A_{ji}^* \\ \text{Unitary} : \hat{A}^{-1} &= \hat{A}^\dagger = \hat{A}^{*Tr} \rightarrow (A^{-1})_{ij} = A_{ji}^* \end{aligned} \quad (5.145)$$

5.2.2 More Mathematical Details

Definition: A set of vectors is said to be **linearly independent** if a linear relation of the form

$$\sum_{k=1}^n c_k |k\rangle = 0 \quad (5.146)$$

implies that $c_k = 0$ for all k ; otherwise the set of vectors is **linearly dependent**.

If a set of vectors is linearly dependent, then we can express a member of the set as a linear combination of the other members of the set.

Examples:

1. Consider the set of vectors(3-tuples in this case)

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad (5.147)$$

This set is linearly independent since

$$a_1 |1\rangle + a_2 |2\rangle + a_3 |3\rangle = \begin{pmatrix} a_1 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ a_2 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ a_3 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \quad (5.148)$$

implies that the only solution is

$$a_1 = a_2 = a_3 = 0 \quad (5.149)$$

2. Consider the set of vectors(3-tuples in this case)

$$|1\rangle = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, |2\rangle = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad (5.150)$$

This set is linearly independent since

$$a_1 |1\rangle + a_2 |2\rangle + a_3 |3\rangle = \begin{pmatrix} a_1 \\ a_1 \\ 0 \end{pmatrix} + \begin{pmatrix} a_2 \\ -a_2 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ a_3 \end{pmatrix} = \begin{pmatrix} a_1 + a_2 \\ a_1 - a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \quad (5.151)$$

implies that the solution is

$$a_1 + a_2 = a_1 - a_2 = a_3 = 0 \rightarrow a_1 = a_2 = a_3 = 0 \quad (5.152)$$

3. Consider the set of vectors(3-tuples in this case)

$$|1\rangle = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, |2\rangle = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, |3\rangle = \begin{pmatrix} 2 \\ 0 \\ 1 \end{pmatrix} \quad (5.153)$$

This set is linearly dependent since

$$a_1 |1\rangle + a_2 |2\rangle + a_3 |3\rangle = \begin{pmatrix} a_1 \\ a_1 \\ a_1 \end{pmatrix} + \begin{pmatrix} a_2 \\ -a_2 \\ 0 \end{pmatrix} + \begin{pmatrix} 2a_3 \\ 0 \\ a_3 \end{pmatrix} = \begin{pmatrix} a_1 + a_2 + 2a_3 \\ a_1 - a_2 \\ a_1 + a_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \quad (5.154)$$

implies that the solution is

$$a_1 + a_2 + 2a_3 = a_1 - a_2 = a_1 + a_3 = 0 \rightarrow a_3 = -a_1, a_2 = a_1 \quad (5.155)$$

and we have (for example)

$$|1\rangle = -|2\rangle + |3\rangle \quad (5.156)$$

We say that an infinite set of vectors is linearly independent if **every finite subset** is linearly independent.

Definition: The maximum number of linearly independent vectors in a space V is called the **dimension** of the space $\dim(V)$.

Definition: A set of vectors $\{|k\rangle, k = 1, 2, 3, \dots, n\}$ **spans** the space if **every** vector $|Q\rangle$ in the space can be written as a linear combination of vectors in the set

$$\sum_{k=1}^n q_k |k\rangle = |Q\rangle \quad (5.157)$$

This linear combination, which is given by the coefficients $q_k, k = 1, 2, \dots, n$ is **unique**.

Definition: A set of vectors is a **basis** for the space if it is a linearly independent set **and** spans the space, that is, if $\dim(V) = m$, a set of m linearly independent vectors is called a basis on V .

The set of vectors

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad (5.158)$$

is the maximal set of linearly independent vectors since any other vector $|g\rangle$ in the space can always be written as a linear combination of them as

$$|g\rangle = a_1 |1\rangle + a_2 |2\rangle + a_3 |3\rangle = \begin{pmatrix} a_1 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ a_2 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ a_3 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \quad (5.159)$$

Therefore the dimension of this vector space is 3. This set of vectors is also a basis. The basis is **not unique** since the set of linearly independent vectors

$$|1\rangle = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, |2\rangle = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad (5.160)$$

also spans the space, i.e.,

$$|g\rangle = c_1 |1\rangle + c_2 |2\rangle + c_3 |3\rangle = \begin{pmatrix} c_1 + c_2 + 2c_3 \\ c_1 - c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \quad (5.161)$$

implies that

$$c_1 = a_1 + a_2 - 2a_3, \quad c_2 = a_1 - 2a_3, \quad c_3 = a_3 \quad (5.162)$$

and, thus, this set is also a basis. Clearly, a basis spans the whole of V

Example: In the space of 3-tuples, a basis is represented by the three vectors

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad (5.163)$$

so that an arbitrary vector in the space

$$|g\rangle = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \quad (5.164)$$

can be written

$$|g\rangle = a_1 |1\rangle + a_2 |2\rangle + a_3 |3\rangle = \begin{pmatrix} a_1 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ a_2 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ a_3 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \quad (5.165)$$

so that a_1 , a_2 , and a_3 are the components.

5.2.3 Gram-Schmidt Orthogonalization Process

An orthonormal basis set for an n -dimensional vector space can always be constructed from any set of n linearly independent vectors using the Gram-Schmidt orthogonalization method. We will not be using this procedure in this book but it is important to know it exists and we could use it if needed.

Suppose that we have a set of n linearly independent vectors $|\alpha_i\rangle$, $i = 1, 2, \dots, n$ that are not a mutually orthonormal set. We can construct a mutually orthonormal set $|\beta_i\rangle$, $i = 1, 2, \dots, n$ using the following steps:

1. let $|\beta_1\rangle = |\alpha_1\rangle$
2. let $|\beta_2\rangle = |\alpha_2\rangle + a_1 |\beta_1\rangle$ where we choose a_1 such that $\langle \beta_1 | \beta_2 \rangle = 0$
3. since we want the vectors $|\beta_1\rangle$ and $|\beta_2\rangle$ to be orthogonal, we require that

$$\begin{aligned} \langle \beta_1 | \beta_2 \rangle &= 0 = \langle \beta_1 | \alpha_2 \rangle + a_1 \langle \beta_1 | \beta_1 \rangle \\ \text{or } a_1 &= -\frac{\langle \beta_1 | \alpha_2 \rangle}{\langle \beta_1 | \beta_1 \rangle} \end{aligned} \quad (5.166)$$

Now proceed by **induction**. Suppose we have constructed k mutually orthogonal vectors $|\beta_i\rangle$, $i = 1, 2, \dots, k$. If we let

$$|\beta_{k+1}\rangle = |\alpha_k\rangle + \sum_{j=1}^k a_j |\beta_j\rangle \quad (5.167)$$

with

$$a_j = -\frac{\langle \beta_j | \alpha_{k+1} \rangle}{\langle \beta_j | \beta_j \rangle} \quad (5.168)$$

then we have $\langle \beta_j | \beta_{k+1} \rangle = 0$ for $j = 1, 2, \dots, k$. These steps are repeated until we have n mutually orthogonal vectors. We then normalize them to 1 and create an orthonormal set.

For example, suppose we have the set

$$|\alpha_1\rangle = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, |\alpha_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, |\alpha_3\rangle = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \quad (5.169)$$

These vectors are not orthonormal.

1. let

$$|\beta_1\rangle = |\alpha_1\rangle = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \quad \langle \beta_1 | \beta_1 \rangle = 2 \quad (5.170)$$

2. let $|\beta_2\rangle = |\alpha_2\rangle + a_1 |\beta_1\rangle$ with

$$a_1 = -\frac{\langle \beta_1 | \alpha_2 \rangle}{\langle \beta_1 | \beta_1 \rangle} = -\frac{1}{2} \quad (5.171)$$

and thus

$$|\beta_2\rangle = |\alpha_2\rangle - \frac{1}{2} |\alpha_1\rangle = \frac{1}{2} \begin{pmatrix} -1 \\ 1 \\ 2 \end{pmatrix}, \quad \langle \beta_2 | \beta_2 \rangle = \frac{3}{2}, \quad \langle \beta_1 | \beta_2 \rangle = 0 \quad (5.172)$$

3. let $|\beta_3\rangle = |\alpha_3\rangle + a_1 |\beta_1\rangle + a_2 |\beta_2\rangle$ with

$$a_1 = -\frac{\langle \beta_1 | \alpha_3 \rangle}{\langle \beta_1 | \beta_1 \rangle} = -\frac{1}{2}, \quad a_2 = -\frac{\langle \beta_2 | \alpha_3 \rangle}{\langle \beta_2 | \beta_2 \rangle} = -\frac{1}{3} \quad (5.173)$$

and thus

$$|\beta_3\rangle = \frac{2}{3} \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}, \quad \langle \beta_3 | \beta_3 \rangle = \frac{4}{3}, \quad \langle \beta_1 | \beta_3 \rangle = 0, \quad \langle \beta_2 | \beta_3 \rangle = 0 \quad (5.174)$$

The orthonormal set is then

$$|\gamma_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, |\gamma_2\rangle = \frac{1}{\sqrt{6}} \begin{pmatrix} -1 \\ 1 \\ 2 \end{pmatrix}, |\gamma_3\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} \quad (5.175)$$

5.2.4 Functions of Operators

Functions of operators are used all the time in quantum mechanics. We will always assume that it is possible to find a given function of an operator in this book. It is important, however, to see the process carried out in detail at least once.

Suppose that we have the eigenvector/eigenvalue equations for a self-adjoint operator

$$\hat{A} |k\rangle = a_k |k\rangle \quad , \quad k = 1, 2, \dots, N \quad (5.176)$$

We then assume that

$$f(\hat{A}) |k\rangle = f(a_k) |k\rangle \quad , \quad k = 1, 2, \dots, N \quad (5.177)$$

for the eigenvectors.

We can show that this works for polynomials and power series as follows:

$$\begin{aligned} |\psi\rangle &= \sum_{k=1}^N |k\rangle \langle k | \psi \rangle \\ \hat{A} |\psi\rangle &= \hat{A} \sum_{k=1}^N |k\rangle \langle k | \psi \rangle = \sum_{k=1}^N \hat{A} |k\rangle \langle k | \psi \rangle = \sum_{k=1}^N a_k |k\rangle \langle k | \psi \rangle = \left(\sum_{k=1}^N a_k |k\rangle \langle k| \right) |\psi\rangle \\ &\rightarrow \hat{A} = \sum_{k=1}^N a_k |k\rangle \langle k| \rightarrow \text{spectral resolution of the operator} \end{aligned} \quad (5.178)$$

Now define the projection operator

$$\hat{P}_k = |k\rangle \langle k| \rightarrow \hat{P}_k \hat{P}_j = \hat{P}_k \delta_{kj} \quad (5.179)$$

We then have

$$\hat{A} = \sum_{k=1}^N a_k |k\rangle \langle k| = \sum_{k=1}^N a_k \hat{P}_k \quad (5.180)$$

or any operator is represented by a sum over its eigenvalues and corresponding projection operators.

We then have

$$\begin{aligned} \hat{A}^2 &= \left(\sum_{k=1}^N a_k \hat{P}_k \right) \left(\sum_{j=1}^N a_j \hat{P}_j \right) = \sum_{k,j=1}^N a_k a_j \hat{P}_k \hat{P}_j \\ &= \sum_{k,j=1}^N a_k a_j \hat{P}_k \delta_{kj} = \sum_{k=1}^N a_k^2 \hat{P}_k \rightarrow \hat{A}^n = \sum_{k=1}^N a_k^n \hat{P}_k \end{aligned} \quad (5.181)$$

Therefore, for

$$f(x) = \sum_{n=1}^N q_n x^n \quad (5.182)$$

we have

$$f(\hat{A}) = \sum_{n=1}^N q_n \hat{A}^n = \sum_{n=1}^N q_n \sum_{k=1}^N a_k^n \hat{P}_k = \sum_{k=1}^N \left(\sum_{n=1}^N q_n a_k^n \right) \hat{P}_k = \sum_{k=1}^N f(a_k) \hat{P}_k \quad (5.183)$$

This says that, in general, that we have

$$\begin{aligned} f(\hat{A})|\psi\rangle &= f(\hat{A}) \sum_{k=1}^N |k\rangle \langle k | \psi \rangle = \sum_{k=1}^N f(\hat{A}) |k\rangle \langle k | \psi \rangle \\ &= \sum_{k=1}^N f(a_k) |k\rangle \langle k | \psi \rangle = \left(\sum_{k=1}^N f(a_k) |k\rangle \langle k| \right) |\psi\rangle \end{aligned} \quad (5.184)$$

which implies that

$$f(\hat{A}) = \sum_{k=1}^N f(a_k) |k\rangle \langle k| \quad (5.185)$$

which is the *spectral resolution of a function of an operator*.

Numerical example:

$$\hat{A} = \begin{pmatrix} 4 & 3 \\ 3 & 4 \end{pmatrix} \quad (5.186)$$

has eigenvalues 7,1 with eigenvectors

$$|7\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad , \quad |1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (5.187)$$

This gives

$$\hat{P}_7 = |7\rangle \langle 7| = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \quad , \quad \hat{P}_1 = |1\rangle \langle 1| = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \quad (5.188)$$

and therefore

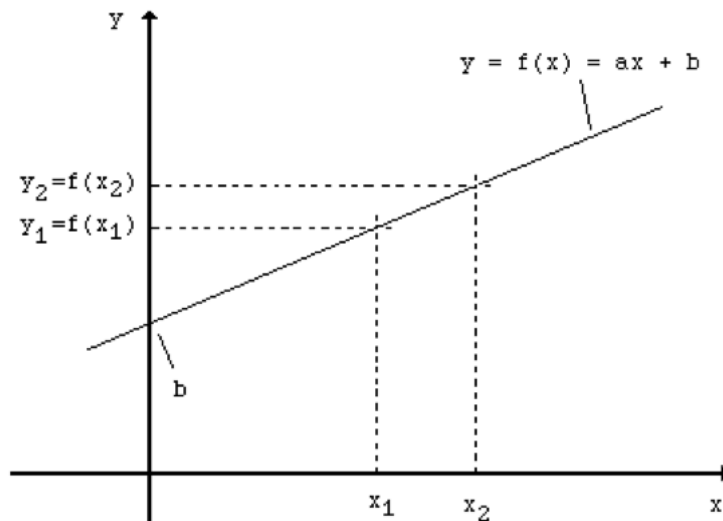
$$\begin{aligned} \hat{A} &= 7\hat{P}_7 + \hat{P}_1 = \frac{7}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 4 & 3 \\ 3 & 4 \end{pmatrix} \text{ as expected!} \\ \hat{A}^2 &= 7^2 \hat{P}_7 + \hat{P}_1 = \frac{7^2}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 25 & 24 \\ 24 & 25 \end{pmatrix} = \begin{pmatrix} 4 & 3 \\ 3 & 4 \end{pmatrix} \begin{pmatrix} 4 & 3 \\ 3 & 4 \end{pmatrix} \\ \log \hat{A} &= \log(7) \hat{P}_7 + \log(1) \hat{P}_1 = \frac{\log(7)}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \\ \sqrt{\hat{A}} &= \sqrt{7} \hat{P}_7 + \sqrt{1} \hat{P}_1 = \frac{\sqrt{7}}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \sqrt{7}+1 & \sqrt{7}-1 \\ \sqrt{7}-1 & \sqrt{7}+1 \end{pmatrix} \end{aligned}$$

Before proceeding to the formal statement of the postulates of quantum theory and another pass through some material, let us digress to learn some calculus, which will be of use as we continue our studies.

5.3 A One Hour Tour of Calculus

5.3.1 Preliminaries

The rule $y = f(x) = ax + b$ has a graph called a **straight line** as shown in the figure below:



captionStraight line graph.

where

$$a = \text{slope of the line} = \frac{y_2 - y_1}{x_2 - x_1} = \frac{f(x_2) - f(x_1)}{x_2 - x_1} \quad (5.189)$$

and

$$b = \text{intercept on the } y\text{-axis} = f(0) \quad (5.190)$$

Now, the problem of finding the equation of that line which is tangent to a function $y = f(x)$ at the point (c, d) , where $d = f(c)$ is central to CALCULUS. The most general straight line passing through the point (c, d) is given by $y - d = m(x - c)$.

Proof: This certainly represents a straight line since we can rewrite it as $y = mx + (d - mc)$, which is the standard form of the equation of a straight line with slope $= m$ and intercept $(d - mc)$. The line passes through the point (c, d) since when we choose $x = c$, we have $y = mc + (d - mc) = d$. This completes the proof. It represents the most general straight line through (c, d) since its slope m is arbitrary.

Suppose we plot two graphs as shown in the figure below:

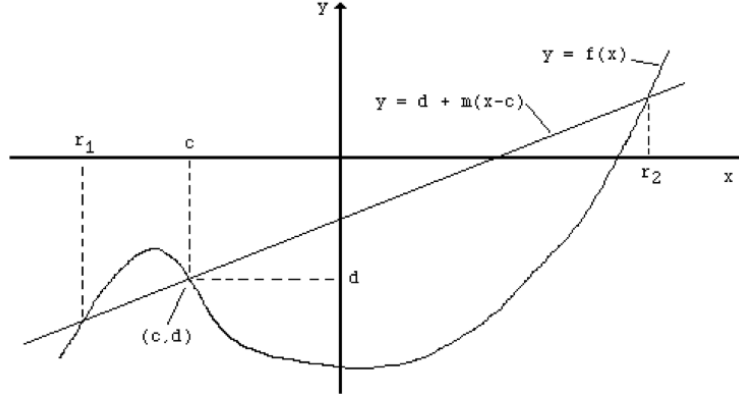


Figure 5.5: Finding intersections

where we have indicated three intersections labelled by their x -values, namely, r_1 , c and r_2 . More than three intersections are possible, but that case only represent an unnecessary complication for the present discussion.

The intersections r_1 , c and r_2 represent the zeroes of the function $p(x) = f(x) - d - m(x - c)$. Now, very close to the point $x = c$, $p(x)$ must have the form $p(x) = (x - c)g(x)$ since it equals 0 at $x = c$. Similarly, near $x = r_1$, $p(x)$ must have the form $p(x) = (x - r_1)g(x)$.

If we rotate (change the slope) of the line about the point (c, d) until the straight line becomes tangent to the curve at (c, d) , then, since this means that r_1 approaches c , we must have

$$\begin{aligned} p(x) &= (x - c)(x - r_1)g(x) \quad \text{near } x = c = r_1 \\ &= (x - c)(x - c)g(x) = (x - c)g(x) \end{aligned} \quad (5.191)$$

In other words, when the line is tangent to the curve at (c, d) we must have $g(c) = 0$. From the definition of $g(x)$, we then have

$$g(x) = \frac{p(x)}{x - c} = \frac{f(x) - d}{x - c} - m = q(x) - m \quad (5.192)$$

When $x = c$, this implies that $g(c) = 0 = q(c) - m$ or $m = q(c)$ = the slope of the tangent line to $f(x)$ at (c, d) , where

$$q(x) = \frac{f(x) - d}{x - c} = \frac{f(x) - f(c)}{x - c} \quad (5.193)$$

For simple functions this rule is easily applied. Consider the case $y = f(x) = x^3$. We have

$$q(x) = \frac{f(x) - f(c)}{x - c} = \frac{x^3 - c^3}{x - c} = \frac{(x - c)(x^2 + cx + c^2)}{x - c} = x^2 + cx + c^2 \quad (5.194)$$

This implies that m = slope of the line tangent to $f(x) = x^3$ at the point $(c, c^3) = q(c) = 3c^2$. Then, the equation

$$y - c^3 = 3c^2(x - c) \rightarrow y = 3c^2x - 2c^3 \quad (5.195)$$

represents the tangent line! The case $c = 1$ is plotted below:

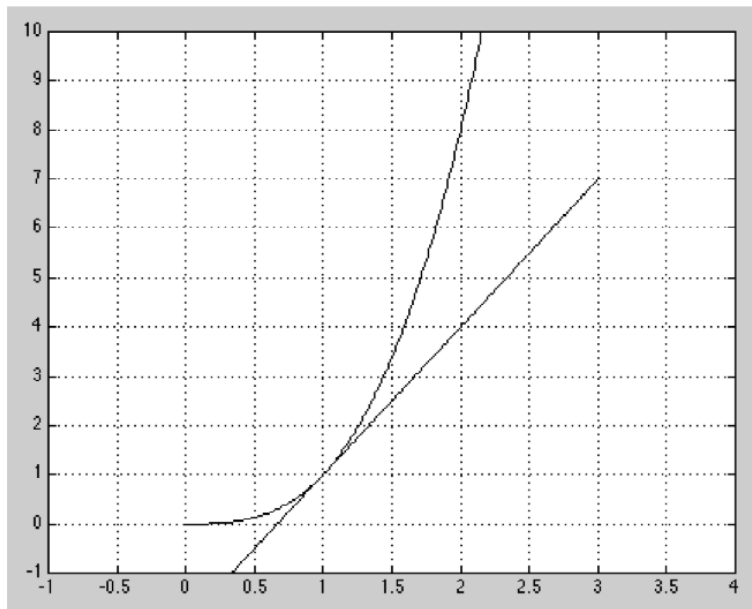


Figure 5.6: Case $c = 1$

In this case, the tangent line at the point $(1, 1)$ is given by the line $y = 3x - 2$.

5.3.2 The Derivative

The above procedure, while transparent, is hard to apply for more complicated functions. We now develop an alternative approach (called the **derivative**) which enables us to find the slope of the tangent line for arbitrary functions. Consider the figure below:

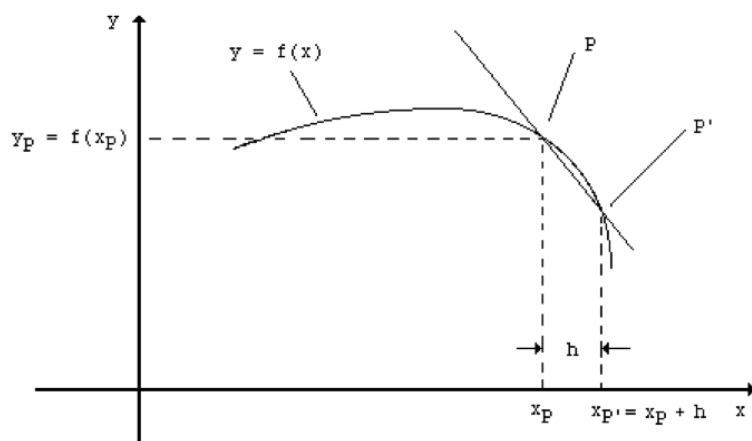


Figure 5.7: Approximating the tangent line

Now follow this procedure:

1. Choose a point P corresponding to $(x_P, f(x_P))$
2. Choose a second point P' such that $x_{P'} = x_P + h$
3. Find the equation of the straight line through P and P'
4. As P' approaches P , the slope of the line PP' approaches a limiting value equal to the slope of the tangent line at point P . This is shown schematically in the diagram below:

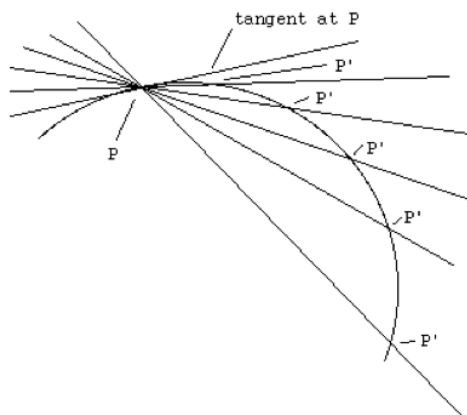


Figure 5.8: Limit approaches the tangent line

Now the slope of PP' is

$$m_h = \frac{f(x_{P'}) - f(x_P)}{x_{P'} - x_P} = \frac{f(x_P + h) - f(x_P)}{h} \quad (5.196)$$

and the slope of the tangent line at P is

$$m_P = \lim_{h \rightarrow 0} m_h = \lim_{h \rightarrow 0} \frac{f(x_P + h) - f(x_P)}{h} \quad (5.197)$$

To illustrate these ideas, let us return to our previous example $f(x) = x^3$. We then have

$$\begin{aligned} m_P &= \lim_{h \rightarrow 0} \frac{(x_P + h)^3 - x_P^3}{h} = \lim_{h \rightarrow 0} \frac{x_P^3 + 3hx_P^2 + 3h^2x_P + h^3 - x_P^3}{h} \\ &= \lim_{h \rightarrow 0} \frac{3hx_P^2 + 3h^2x_P + h^3}{h} = \lim_{h \rightarrow 0} (3x_P^2 + 3hx_P + h^2) = 3x_P^2 \end{aligned} \quad (5.198)$$

For the point $x_P = c$, we have $m = 3c^2$ as before.

Before proceeding, we state (without proof) some useful rules involving limits.

1. $\lim_{h \rightarrow a} cF(h) = c \lim_{h \rightarrow a} F(h) = cF(a)$ for $c = \text{constant}$
2. $\lim_{h \rightarrow a} (F(h) \pm G(h)) = \lim_{h \rightarrow a} (F(h) \pm \lim_{h \rightarrow a} G(h)) = F(a) \pm G(a)$
3. $\lim_{h \rightarrow a} (F(h)G(h)) = (\lim_{h \rightarrow a} (F(h)))(\lim_{h \rightarrow a} G(h)) = F(a)G(a)$
4. $\lim_{h \rightarrow a} \left(\frac{F(h)}{G(h)} \right) = \frac{\lim_{h \rightarrow a} F(h)}{\lim_{h \rightarrow a} G(h)} = \frac{F(a)}{G(a)}$ if $G(a) \neq 0$

In general, the derivative of the function $f(x)$ at the arbitrary point x is defined by

$$f'(x) = \frac{df}{dx} = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h} \quad (5.199)$$

The derivative is also called the **rate of change**, i.e., $df/dx = \text{rate of change of } f(x) \text{ with respect to } x$. From our previous discussion we have $f'(q) = \text{slope of the tangent line to the graph } y = f(x) \text{ at the point } (q, f(q))$.

Simple Example: Let $f(x) = cx^2$. Then

$$\begin{aligned} f'(x) &= \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h} = \lim_{h \rightarrow 0} \frac{c(x+h)^2 - cx^2}{h} \\ &= \lim_{h \rightarrow 0} \frac{2cxh + ch^2}{h} = \lim_{h \rightarrow 0} (2cx + h) = 2cx \end{aligned} \quad (5.200)$$

This is the slope of the line tangent to $f(x) = cx^2$ at $(x, f(x))$.

Although this procedure is straightforward, we do not wish to do all of this work for every $f(x)$ that arises in this course. We need to develop some general rules

that we can use.

Consider the function $f(x) = x^n$, which includes the previous example. We have

$$f'(x) = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - f(x)}{\Delta x} = \lim_{\Delta x \rightarrow 0} \frac{(x + \Delta x)^n - x^n}{\Delta x} \quad (5.201)$$

where we have made a change to standard notation, i.e., h to Δx . In order to evaluate this we need the following algebraic result:

$$(x + \Delta x)^n = x^n + nx^{n-1}\Delta x + \frac{n(n-1)}{2}x^{n-2}(\Delta x)^2 + \frac{n(n-1)(n-2)}{6}x^{n-3}(\Delta x)^3 + \dots \quad (5.202)$$

This is the so-called **Binomial expansion**. It can be proved by simple multiplication. Using it we then have

$$\begin{aligned} f'(x) &= \lim_{\Delta x \rightarrow 0} \frac{(x + \Delta x)^n - x^n}{\Delta x} \\ &= \lim_{\Delta x \rightarrow 0} \frac{\left(x^n + nx^{n-1}\Delta x + \frac{n(n-1)}{2}x^{n-2}(\Delta x)^2 + \frac{n(n-1)(n-2)}{6}x^{n-3}(\Delta x)^3 + \dots \right) - x^n}{\Delta x} \\ &= \lim_{\Delta x \rightarrow 0} \left(nx^{n-1} + \frac{n(n-1)}{2}x^{n-2}\Delta x + \dots \right) = nx^{n-1} \end{aligned} \quad (5.203)$$

or

$$\frac{d(x^n)}{dx} = nx^{n-1} \quad (5.204)$$

This result agrees with the special case that we did explicitly earlier.

Given the functions $u(x)$ and $v(x)$ we can now state several important derivative rules (we will prove a couple of them to illustrate the methods involved).

1. $\frac{d}{dx}(cu(x)) = c \frac{du}{dx}$
2. $\frac{d}{dx}(u(x) \pm v(x)) = \frac{du}{dx} \pm \frac{dv}{dx}$
3. $\frac{d}{dx}(u(x)v(x)) = v(x) \frac{du}{dx} + u(x) \frac{dv}{dx}$
4. $\frac{d}{dx} \left(\frac{u(x)}{v(x)} \right) = \frac{v(x) \frac{du}{dx} - u(x) \frac{dv}{dx}}{(v(x))^2}$
5. $\frac{d}{dx}(u^p) = pu^{p-1} \frac{du}{dx}$

Another very important rule that is used all the time is called the **chain rule**. If $y = f(u)$ and $u = g(x)$, then we can define the **composite function** $y =$

$f(g(x)) = H(x)$. We can then write

$$\begin{aligned}\frac{dH(x)}{dx} &= \frac{df(g(x))}{dx} = \lim_{\Delta x \rightarrow 0} \frac{f(g(x + \Delta x)) - f(g(x))}{\Delta x} \\ &= \lim_{\Delta x \rightarrow 0} \frac{f(g(x + \Delta x)) - f(g(x))}{g(x + \Delta x) - g(x)} \frac{g(x + \Delta x) - g(x)}{\Delta x} \\ &= \lim_{\Delta x \rightarrow 0} \frac{f(g(x + \Delta x)) - f(g(x))}{g(x + \Delta x) - g(x)} \lim_{\Delta x \rightarrow 0} \frac{g(x + \Delta x) - g(x)}{\Delta x} \\ &= \lim_{\Delta x \rightarrow 0} \frac{f(g(x + \Delta x)) - f(g(x))}{g(x + \Delta x) - g(x)} \frac{dg}{dx}\end{aligned}$$

Now as $\Delta x \rightarrow 0$, $g(x + \Delta x) \rightarrow g(x)$. therefore we have $\Delta g = g(x + \Delta x) - g(x) \rightarrow 0$ as $\Delta x \rightarrow 0$. We can then write

$$\begin{aligned}\frac{dH(x)}{dx} &= \frac{df(g(x))}{dx} = \lim_{\Delta x \rightarrow 0} \frac{f(g(x + \Delta x)) - f(g(x))}{g(x + \Delta x) - g(x)} \frac{dg}{dx} \\ &= \lim_{\Delta g \rightarrow 0} \frac{f(g(x + \Delta x)) - f(g(x))}{\Delta g} \frac{dg}{dx} = \frac{df}{dg} \frac{dg}{dx}\end{aligned}$$

which is a very powerful and useful rule.

Example: Find the derivative of $y = g^3 + g - 5$ where $g = x^2 + 6x$. We have

$$\frac{dy}{dx} = \frac{dy}{dg} \frac{dg}{dx} = (3u^2 + 1)(2x + 6) = (3(x^2 + 6x)^2 + 1)(2x + 6)$$

5.3.2.1 Properties Derivable from Derivatives

First, we must define higher derivatives. $f'(x) = df/dx$ is called the first derivative of $f(x)$ with respect to x . We define the second derivative by

$$f''(x) = \frac{df'(x)}{dx} = \frac{d}{dx} \left(\frac{df(x)}{dx} \right) = \frac{d^2 f(x)}{dx^2} \quad (5.205)$$

and so on for third, fourth, derivatives, etc.

Now, if the graph of a function $f(x)$ has a minimum (maximum) at some point $x = a$, then $f'(a) = 0$ as can be seen in the figures below.

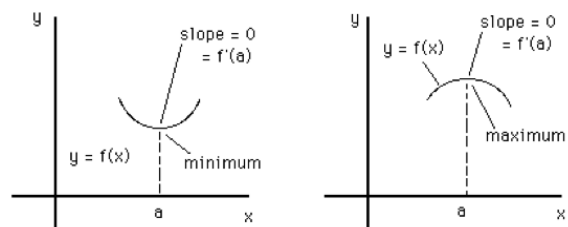


Figure 5.9: Maxima and minima

The slope of these graphs are clearly zero at the minimum and the maximum. If, in each case, we plot $f'(x)$ versus x , then the graphs would look like the figures below:

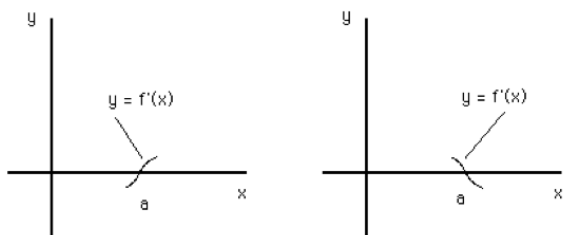


Figure 5.10: First derivative at maximum/minimum

The graphs pass through zero at the minimum and the maximum. If, in each case we plot $f''(x)$ (which is just the slope of the $f'(x)$ graph) versus x , then the graphs would look like the figures below:

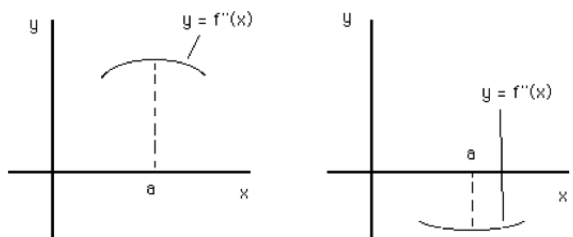


Figure 5.11: Second derivative at maximum/minimum

The second derivative is positive for a minimum and negative for a maximum. Summarizing, in words, near a minimum

$$f'(x) = 0 \quad \text{and} \quad f''(x) > 0 \quad (5.206)$$

and near a maximum

$$f'(x) = 0 \quad \text{and} \quad f''(x) < 0 \quad (5.207)$$

Some useful derivatives are given below:

$$\begin{aligned}\frac{d}{dx}(e^{ax}) &= ae^{ax} \quad , \quad \frac{d}{dx}(\log x) = \frac{1}{x} \\ \frac{d}{dx}(\sin ax) &= a \cos ax \quad , \quad \frac{d}{dx}(\cos ax) = -a \sin ax\end{aligned}\tag{5.208}$$

5.3.3 Integration

Now, if we can write

$$h(x) = \frac{d}{dx}(g(x))\tag{5.209}$$

then the quantity $g(x) + c$, where c = an arbitrary constant is called the antiderivative of $h(x)$, i.e., $g(x) + c$ is the function whose derivative is $h(x)$.

Suppose we now ask the following question: what is the area (shaded region in the figure below) under the curve $y = f(x)$ between $x = a$ and $x = b$?

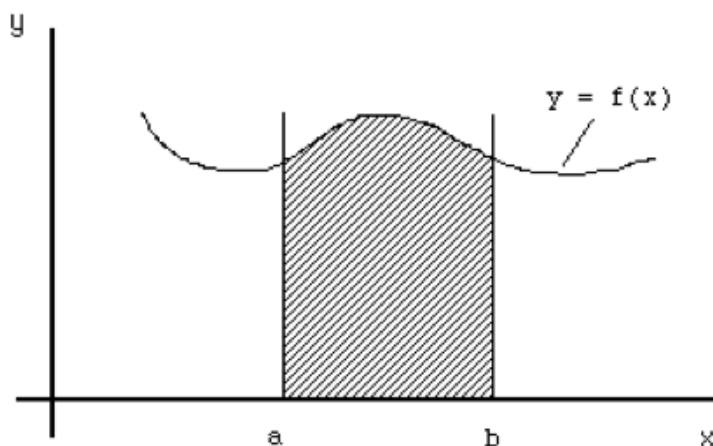


Figure 5.12: Area under a curve

A good approximation to this area is given by the following procedure:

1. divide the interval $a \leq x \leq b$ into N equal segments each of length

$$\Delta = \frac{b - a}{N}\tag{5.210}$$

2. define $x_k = a + k\Delta$ for $k = 1, 2, 3, 4, \dots, N$

3. calculate the corresponding values of $f(x)$, namely,

$$f(x_k) = f(a + k\Delta) \quad k = 1, 2, 3, 4, \dots, N\tag{5.211}$$

4. then an approximation to the area is given by

$$AREA = \sum_{k=1}^N f(x_k) \Delta \quad (5.212)$$

as shown in the figure below:

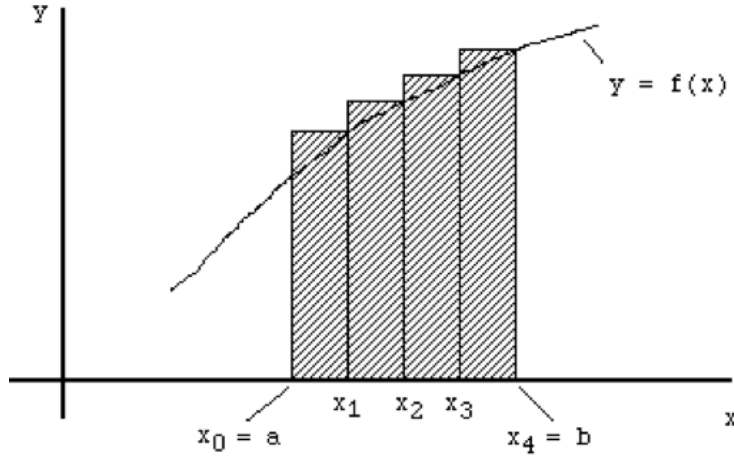


Figure 5.13: Approximate area

where for the case $N = 4$ we have

$$\Delta = \frac{b-a}{4} \quad (5.213)$$

and

$$x_0 = a, x_1 = a + \Delta, x_2 = a + 2\Delta, x_3 = a + 3\Delta, x_4 = a + 4\Delta = a + (b-a) = b \quad (5.214)$$

As can be seen from the figure, our approximation for the area equals the sum of the shaded rectangles. In the case shown, the calculated area is greater than the actual area.

Alternatively, we could have used

$$AREA = \sum_{k=1}^N f(x_{k-1}) \Delta \quad (5.215)$$

which underestimates the area as shown in the figure below:

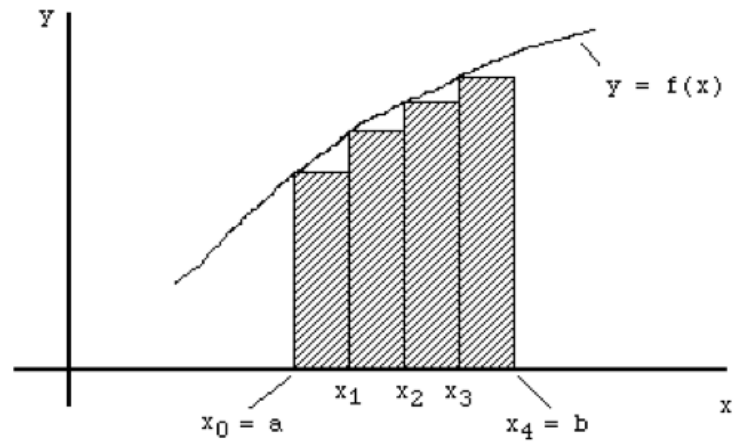


Figure 5.14: An alternate approximation

For an even better result, we could have used

$$AREA = \frac{1}{2} \sum_{k=1}^N (f(x_{k+1}) + f(x_{k-1})) \Delta \quad (5.216)$$

which is called the trapezoid rule. The is rule calculates the area shown in the figure below:

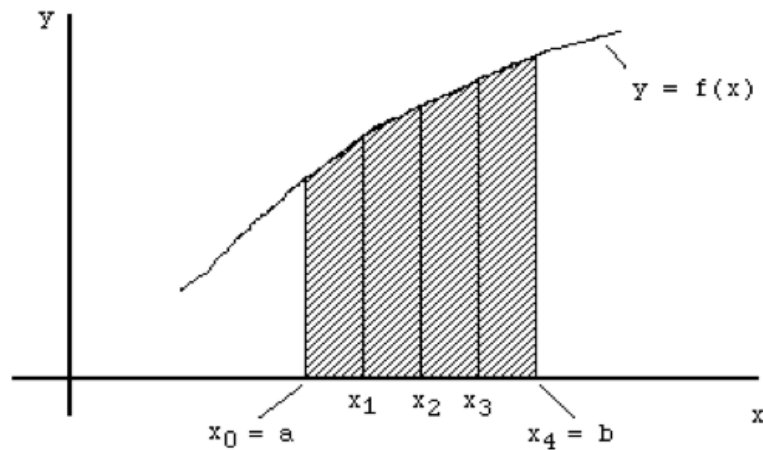


Figure 5.15: Trapezoid approximation

It uses straight lines between points on the actual curve rather than horizontal lines. It is clearly the best approximation of these three.

In the limit $N \rightarrow \infty$, all of these approximations give identical results (= to the actual area under the curve). The limit $N \rightarrow \infty$ is usually written as

$$AREA = \int_a^b f(x) dx = \text{integral of } f(x) \text{ from } a \text{ to } b = \lim_{N \rightarrow \infty} \Delta f(x_k) \quad (5.217)$$

and a and b are called the limits of integration.

Simple Integral: Let $f(x) = cx$ (a straight line) as shown in the figure below:

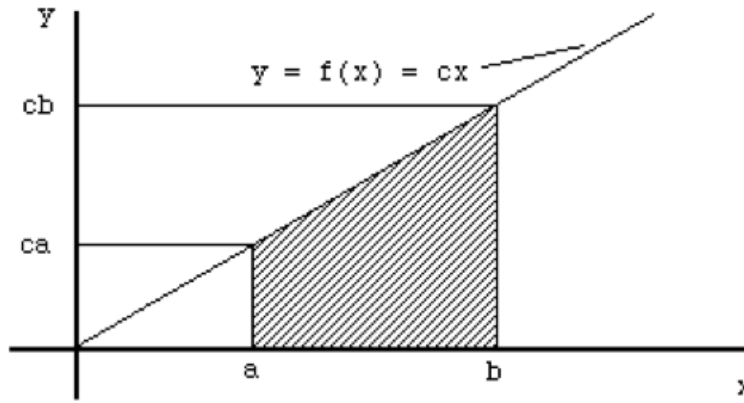


Figure 5.16: Integral of a straight line function

In this case we have

$$\begin{aligned} \int_a^b f(x) dx &= \int_a^b cx dx = \lim_{N \rightarrow \infty} \Delta f(x_k) = \lim_{N \rightarrow \infty} cx_k \Delta \\ &= c \lim_{N \rightarrow \infty} \frac{b-a}{N} \sum_{k=1}^N (a + k\Delta) = c \lim_{N \rightarrow \infty} \frac{b-a}{N} \sum_{k=1}^N a + c \lim_{N \rightarrow \infty} \frac{b-a}{N} \frac{b-a}{N} \sum_{k=1}^N k \\ &= c \lim_{N \rightarrow \infty} \frac{b-a}{N} aN + c \lim_{N \rightarrow \infty} \frac{b-a}{N} \frac{b-a}{N} \frac{N(N+1)}{2} \\ &= \lim_{N \rightarrow \infty} c(b-a) + \lim_{N \rightarrow \infty} \frac{1}{2} c(b-a)^2 \left(1 + \frac{1}{N}\right) \\ &= c(b-a) + \frac{1}{2} c(b-a)^2 = \frac{1}{2} c(b^2 - a^2) \end{aligned} \quad (5.218)$$

The shaded area is easy to calculate directly in this case and is given by

$$(b-a)ca + \frac{1}{2}(b-a)(cb-ca) = \frac{1}{2}c(b^2 - a^2) \quad (5.219)$$

So it works!

In this manner, we could evaluate any integral (find the area under the corresponding curve). The procedure quickly becomes very cumbersome and tedious, however. A better method is to realize that there is a connection between integrals and derivatives.

5.3.4 The Fundamental Theorem of Calculus

If

$$\frac{dF}{dx} = f(x) \quad (5.220)$$

i.e., if $F(x) + c$ is the antiderivative of $f(x)$, then

$$\int_a^b f(x) dx = F(b) - F(a) = F(x)|_{x=a}^{x=b} = \text{definite integral(a number)} \quad (5.221)$$

Alternatively, another way of saying the same thing is to use the definition

$$\int f(x) dx = F(x) + c = \text{indefinite integral(a function of } x) \quad (5.222)$$

The indefinite integral represents the most general antiderivative of $f(x)$.

Examples:

1. Since

$$\cos x = \frac{d}{dx}(\sin x) \quad (5.223)$$

we have

$$\int_a^b \cos x dx = \sin b - \sin a \quad (5.224)$$

or

$$\int \cos x dx = \sin x + c \quad (5.225)$$

2. Since

$$x^n = \frac{d}{dx} \left(\frac{x^{n+1}}{n+1} \right) \quad n \neq -1 \quad (5.226)$$

we have

$$\int_a^b x^n dx = F(b) - F(a) = \frac{x^{n+1}}{n+1} \Big|_{x=a}^{x=b} = \frac{b^{n+1}}{n+1} - \frac{a^{n+1}}{n+1} \quad (5.227)$$

or

$$\int x^n dx = \frac{x^{n+1}}{n+1} + c \quad (5.228)$$

5.3.4.1 More Mathematical Stuff

We now introduce a convenient notation and define the **differential**. Define

$$du = u'(x)dx = \left(\frac{du}{dx}\right)dx \quad \text{this is NOT cancellation} \quad (5.229)$$

where the quantity dx is called the differential of x . Using this notation our last example can be written as follows: let $y = qx$, which implies that

$$dy = \left(\frac{dy}{dx}\right)dx = qdx \quad (5.230)$$

or

$$\int_a^b \cos(qx) dx = \frac{1}{q} \int_{qa}^{qb} \cos y dy = \frac{1}{q} \int_{qa}^{qb} \frac{d}{dy}(\sin y) dy = \frac{1}{q}(\sin(qb) - \sin(qa)) \quad (5.231)$$

Note the change in the integration limits at one point.

5.3.4.2 Some Useful Properties of the Differential

$$\begin{aligned} d(u+v) &= du + dv \\ d(cu) &= cdu \\ d(f(u)) &= \left(\frac{df}{du}\right)du \\ d(uv) &= u dv + v du \end{aligned} \quad (5.232)$$

The trick to doing most integrals is to evaluate the antiderivative, i.e., Let us call $x = \sin \theta$. We can then write

$$dx = \cos \theta d\theta = d\theta \sqrt{1 - \sin^2 \theta} = d\theta \sqrt{1 - x^2} \rightarrow \frac{dx}{\sqrt{1 - x^2}} = d\theta \quad (5.233)$$

Therefore, we are able to do a complicated integral rather straightforwardly, as shown below

$$\int \frac{dx}{\sqrt{1 - x^2}} = \int d\theta = \theta + c = \sin^{-1} x + c \quad (5.234)$$

Similarly, if we choose $x = \tan \theta$, we can write $dx = (1 + \tan^2 \theta)d\theta = d\theta(1 + x^2)$ so that

$$\int \frac{dx}{1 + x^2} = \theta + c = \tan^{-1} x + c \quad (5.235)$$

Algebraic manipulation also works in many integrals. Consider

$$\int \frac{dx}{1 - x^2} = \int \frac{dx}{(1+x)(1-x)} = \int \frac{dx}{2} \left(\frac{1}{1+x} + \frac{1}{1-x} \right) = \frac{1}{2} \ln \left(\frac{1+x}{1-x} \right) \quad (5.236)$$

A very useful result is a procedure called **integration by parts**. It goes as follows. Since

$$\frac{d}{dx}(u(x)v(x)) = v(x)\frac{du}{dx} + u(x)\frac{dv}{dx} \quad (5.237)$$

we have

$$\begin{aligned}\int_a^b u(x) \frac{dv}{dx} &= \int_a^b \frac{d}{dx} (u(x)v(x)) \\ &\quad - \int_a^b v(x) \frac{du}{dx} = u(b)v(b) - u(a)v(a) - \int_a^b v(x) \frac{du}{dx}\end{aligned}\quad (5.238)$$

An example is shown below:

$$\begin{aligned}\int_a^b x \cos x \, dx &= \int_a^b \frac{d}{dx} (x \sin x) \\ &\quad - \int_a^b \sin x \, dx = b \sin b - a \sin a + \cos b - \cos a\end{aligned}\quad (5.239)$$

Another useful result follows when

$$\frac{d}{dx} (F(g(x))) = \frac{dF}{dg} \frac{dg}{dx} \quad (5.240)$$

We then have

$$\int_a^b \frac{dF}{dg} \frac{dg}{dx} dx = \int_a^b \frac{d}{dx} (F(g(x))) dx = F(g(b)) - F(g(a)) \quad (5.241)$$

Chapter 6

Quantum States and Postulates

Real Meaning of the Formalism

We will now set up the formal axiomatic structure of quantum theory and along the way review most of the stuff we have already talked about. Hopefully, we understand it all after this final pass and can then begin to use it!

6.1 Quantum States and the Real Meaning of the Formalism

Now we will start to develop(redevelop) the theoretical machinery of quantum physics. We will do this by building on the experimental insight from the present discussions, accepting them as valid statements about the nature of quantum objects (no matter how confusing that nature seems to be) and see if we can develop some simple scheme for calculating the likely outcomes of new experiments. After that we will try to understand the reality we have devised.

6.1.1 Where Are We Now?

Over the last several sections of the book, we have considered various experimental results that force us to rethink how matter behaves, at least at atomic scales. For example, an individual photon can apparently follow both paths from a half-silvered mirror as long as the experiment is not set up to detect the photon's direction of flight(which path it is on). It is as if reality is slightly *out of focus*, until a specific experiment forces the picture to sharpen into one possibility or another.

Perhaps being *out of focus* is an issue with the theory and not a reflection of what is actually happening *out there*. It is the theory that is out of focus. Maybe in the future, new experiments will expose some physical variables that we have not spotted up to now, and these will allow us to make a more advanced theory

that resolves what appears to be paradoxical.

Physicists call such hypothetical ideas *hidden variable theories*.

Of course it's possible that our current experiments are saying something genuine about the nature of reality. The problem then would lie with our *expectations* about reality.

Up to now, our experience has been centered on the large-scale world (macroworld) that we have been living in. We are used to throwing rocks and observing that they follow a single path. This *common sense* understanding colors our view of all reality, irrespective of scale, but there is *no guarantee* that it will apply outside our everyday world. Indeed, as we have seen when we experiment with photons and electrons, we find that they do not act like tiny rocks. Consequently, the challenge is to explain how a rock (which is after all made of particles such as electrons) can manage to behave in the *common sense* way, given the underlying strangeness of the quantum world.

Before we can discuss such puzzles in any greater detail, we need to completely specify the scheme for describing our experimental results in a consistent way, which allows some measure of predictability. In other words, we need to develop a *quantum theory* from first principles that we can apply. We have covered most of the ideas earlier and now we will expand on those discussions so that all aspects of the full theory are clearly delineated.

6.1.1.1 Describing Quantum Systems

Earlier, we saw how using a classical type of state could get us into trouble when trying to describe experiments in the quantum world. A classical state is effectively a list of quantitative values of various physical properties, so it is hard to see how this can be applied to a photon in an interference experiment *apparently* traveling on two paths at the same time. Similarly, any physical property determining the direction of an electron through a Stern-Gerlach (S-G) experiment seems to be influenced by the exact details of how the experiment was set up(the context), which runs contrary to the classical idea that experiments reveal what is already there.

Let us explore how we can construct a quantum state to replace the normal classical description of a system. If this is going to work, it's important that certain basic characteristics are designed in from the beginning.

1. The inherent *randomness* found in some situations must be represented. For example, the description of a photon arriving at a half-silvered mirror has to allow the photon to have an equal chance of being transmitted or reflected, without stating that it will definitely do one or the other.
2. The *contextuality* of quantum behavior must be incorporated. We have

seen how experimental results are influenced by the overall setup of the equipment. If a photon detector is placed beyond the half-silvered mirror, then the photon will either reflect or transmit. If there is no detector present, then the results seem to imply that the photon explores both possibilities.

3. Quantum systems *seem to be able to exist in a mixed state that combines classical states* in a way that we would have regarded as being impossible (e.g., reflecting and transmitting at the half-silvered mirror), i.e., they combine classical states that are incompatible with each other!

In the figure below we have tried to summarize what needs to be achieved in a quantum description.

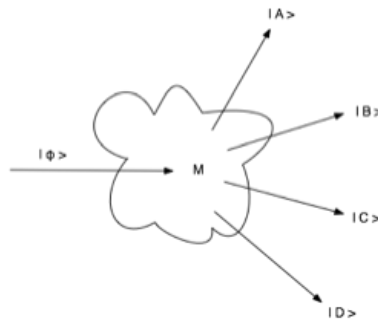


Figure 6.1: Measurement Idea

On the left-hand side of the figure we have a system, such as an electron, in some quantum state symbolized by the ket $|\phi\rangle$. The electron then interacts with some measuring apparatus, M , and as a result one of several possibilities can occur, each with a different probability. A specific example might be a $|U\rangle$ state electron interacting with a (LEFT,RIGHT) S-G magnet and as a result emerging in an $|L\rangle$ or $|R\rangle$ state.

Taking a direct approach to the problem, we could try writing the initial state in the following form:

$$|\phi\rangle = p_1 |A\rangle + p_2 |B\rangle + p_3 |C\rangle + p_4 |D\rangle + \dots \quad (6.1)$$

where the numbers p_1, \dots, p_4, \dots represent in some way (we do not know how at this point) the probability that the electron would end up in each state $|A\rangle$, $|B\rangle$, etc. We are not saying that the numbers are probabilities; just that they are *related* to the probabilities in some way, which is yet to be determined. This is an attractive formulation as it already catches some of the flavor of quantum behavior. It seems to be saying that the state $|\phi\rangle$ is made up of all the possibilities $|A\rangle$, $|B\rangle$, etc, which may subsequently come about. For example, with our S-G experiment, we would write

$$|U\rangle = p_1 |L\rangle + p_2 |R\rangle \quad (6.2)$$

to represent the initial state of the electron shown in the figure below.

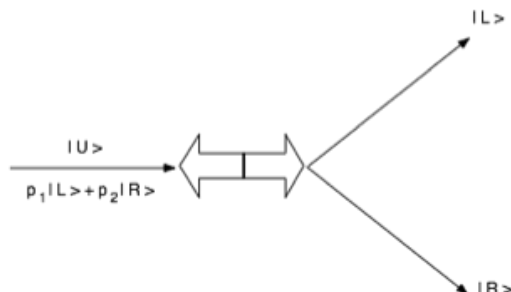


Figure 6.2: Initial State in terms of Final States

After the electron has passed through the magnet, it's no longer appropriate to describe it by the state $|U\rangle$: now it's either state $|L\rangle$ or $|R\rangle$, so our initial description *seems to have collapsed* (after measurement) into one of the two alternatives that it is composed of.

This way of expressing quantum states looks rather similar to the manner in which probabilities can be combined. Imagine that we are trying to calculate the average number of words per page in this book. One way of doing this would be to count up the number of words and divide by the number of pages.

However, an equivalent way would be to group the pages into sets where each page in the set had the same number of words on it. The average then becomes

average number of words =

$$\frac{(\text{number pages}(700 \text{ words})) \times 700 + (\text{number pages}(600 \text{ words})) \times 600 + \dots}{\text{total number of pages}}$$

average number of words =

$$\frac{(\text{number pages}(700 \text{ words})) \times 700}{\text{total number of pages}} + \frac{(\text{number pages}(600 \text{ words})) \times 600}{\text{total number of pages}} + \dots$$

average number of words = (Probability of 700 words) \times 700

+ (Probability of 600 words) \times 600 + ..

which looks just like the formula that one uses when different possibilities are being considered. It is the same formula as the one we used earlier in our mathematical discussions. Given an event E_1 with probability P_1 , event E_2 with probability P_2 and event E_3 with probability P_3 , the rules of probability state

$$\text{Probability}(E_1 \text{ or } E_2 \text{ or } E_3) = P_1 + P_2 + P_3$$

If these events correspond to measuring different values of a physical property (e.g., V_1 , V_2 , and V_3), then the average value of that property after many trials

is

$$\text{average value of } V = (V_1 \times P_1) + (V_2 \times P_2) + (V_3 \times P_3)$$

which certainly looks like the quantum mechanical state. If the two formulations were exactly the same, then the terms p_1, p_2, p_3 , etc in

$$|\phi\rangle = p_1 |A\rangle + p_2 |B\rangle + p_3 |C\rangle + p_4 |D\rangle + \dots\dots\dots$$

would have to be probabilities, but there is a **problem** with this interpretation.

6.1.1.2 Specific Example: Mach-Zehnder Again

Having figured out some idea of how to represent a quantum state, we need to see if it works in an experimental situation. A useful example to choose is the Mach-Zehnder interferometer from our earlier discussions. You will remember, this experiment seems to need both wave and particle descriptions of light, so it will be a good test of our quantum state formulation.

We will assume that the intensity of the laser beam has been turned down so that only one photon at a time is crossing the setup.

At the first half-silvered mirror, photons can be reflected or transmitted (pass straight through). So, it would be appropriate to write the quantum state of an arriving photon as

$$|\phi\rangle = a |T\rangle + b |R\rangle \quad (6.3)$$

where $|T\rangle$ represents the transmitted state and $|R\rangle$ the reflected one. The numbers a and b will be related to the probability that the photon is transmitted or reflected, respectively. These numbers will be determined by the construction of the mirror.

The part of the state $|\phi\rangle$ we designated as $|R\rangle$ contains all the information about photons that are reflected at the half-silvered mirror - that is the best we can say in this type of description. Unless there is a measurement device on either arm of the experiment, we cannot say that the photon has either been transmitted or reflected. Consequently, we should not imply that the photon is going in any particular direction. The alternative would be to say something like *the reflected photon state moves along the upper arm*, but states *do not move*. We settle on saying things like *the reflected photon property or information* meets the fully silvered mirror at A (see figure below). Consequently, its quantum state must change at this mirror to $|G\rangle$. At the next half-silvered mirror, the state can be either one of *transmission through* or *reflection up*:

$$|G\rangle = b |L\rangle + a |K\rangle \quad (6.4)$$

Here, we have used the same factors, a (for transmission) and b (for reflection), as in the first half-silvered mirror. See figure below.

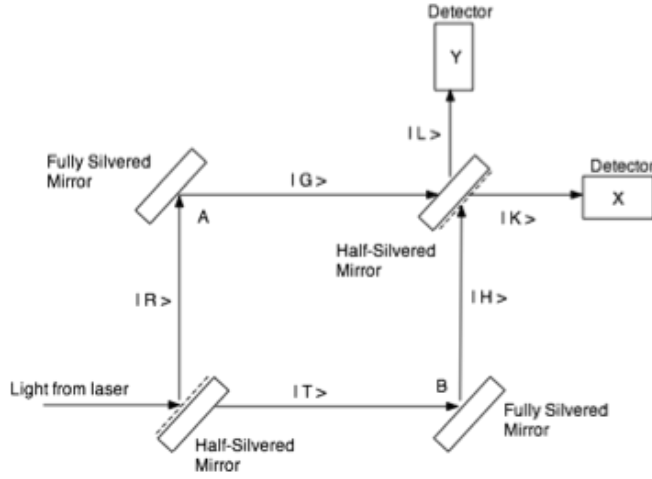


Figure 6.3: Mach-Zehnder Again

Meanwhile the other property of the photon is in state $|T\rangle$. This property will *reach* the mirror at position B, where it will be reflected and so change into state $|H\rangle$. However, according to our system, it must be possible to write $|H\rangle$ in terms of $|K\rangle$ and $|L\rangle$ as these are the possible outcomes when $|H\rangle$ interacts with the half-silvered mirror. The above figure shows that we have to be slightly careful when constructing this representation. From the point of view of $|H\rangle$, $|L\rangle$ is the transmitted state and $|K\rangle$ is the reflected one. So, we have to write

$$|H\rangle = b|K\rangle + a|L\rangle \quad (6.5)$$

Now we have $|H\rangle$ and $|G\rangle$ written in terms of $|K\rangle$ and $|L\rangle$, which means that we can go back to the original state $|\phi\rangle$ and figure out how to write it in terms of $|K\rangle$ and $|L\rangle$.

$$\begin{aligned} |\phi\rangle &= a|T\rangle + b|R\rangle = a|H\rangle + b|G\rangle \\ &= a(b|K\rangle + a|L\rangle) + b(b|L\rangle + a|K\rangle) \\ &= ab|K\rangle + ab|K\rangle + a^2|L\rangle + b^2|L\rangle \\ &= 2ab|K\rangle + (a^2 + b^2)|L\rangle \end{aligned} \quad (6.6)$$

This is an example of the kind of algebra we will be doing all the time.

We have now produced a representation of the initial photon state $|\phi\rangle$ in terms of the two possible final outcomes $|K\rangle$ and $|L\rangle$. The numbers $2ab$ and $(a^2 + b^2)$ represent (in some way) the probabilities that the photon will be detected at X and Y, respectively, i.e., that we end up with the state $|K\rangle$ or the state $|L\rangle$ for the single photon.

At this point we need to think back to the actual experimental results. If the distances in the detector are balanced out, then all photon passing through the device are picked up at detector X; none of them reach Y. Consequently, the final state of the photon cannot include $|L\rangle$.

If the formalism is to work, then $(a^2 + b^2) = 0$, which poses an immediate problem. If a and b are probabilities, then they must be positive numbers. As the square of any positive number is bound to be positive (as indeed is the square of a negative number), there is no way in which we can obtain $(a^2 + b^2) = 0$. Consequently, the terms a and b themselves cannot be probabilities. Of course, we could have $a = b = 0$, which makes no physical sense, i.e., it says that the half-silvered mirror does not work as observed in real experiments.

At this point it might seem better to abandon this approach for representing quantum systems. That, however, would be premature.

It turns out that mathematicians looking at the equation $(a^2 + b^2) = 0$ would not be so fainthearted. They would realize immediately that a and b are examples of *complex numbers* as we have discussed earlier.

When we attempted to write down a consistent representation of a photon's state on the far side of the Mach-Zehnder experiment, we reached the point at which we had

$$|\phi\rangle = (a^2 + b^2)|L\rangle + 2ab|K\rangle$$

with the proviso that the $|L\rangle$ state was never observed in practice if the lengths of the two arms of the experiment were equal. Consequently, we needed to have $(a^2 + b^2) = 0$, which was a puzzle. Now we can see that this can work, however, using imaginary numbers. If $a = bi$ so that $a^2 = -b^2$, then $(a^2 + b^2) = 0$. There is a price to pay, however. If these numbers multiplying the states are imaginary (or even possibly complex numbers), what can they *mean*? They certainly cannot directly represent a probability, which is a real, non-negative number.

We started out with the notion that the numbers we used to multiply states were *related* to the probability that the state would come about as a result of a measurement. Any hope that the numbers might actually *be* the probability has just been dashed by applying the idea to the Mach-Zehnder experiment. We must use complex numbers if we are going to represent all possible experimental situations. This move is required by the experimental results. That is the way the theoretical physicist makes progress.

As we have now seen that they cannot be probabilities, we can give these numbers their proper names. In quantum theory, they are called *probability amplitudes* (as we saw earlier).

$$|\phi\rangle = a_1|A\rangle + a_2|B\rangle + a_3|C\rangle + a_4|D\rangle + \dots\dots\dots$$

where a_1, a_2, a_3 , etc are the probability amplitudes for states $|A\rangle, |B\rangle, |C\rangle$, etc.

Now we must see how these probability amplitudes are related to probabilities. The probability that we obtain from an amplitude must have all the factors i removed from it. It is impossible to have i connected directly with probability. Now of course we already know of a procedure that will remove all factors of i from a complex number: multiplying the number by its conjugate. We therefore have a possible interpretation (we do not know if our guess is correct as yet): to convert *probability amplitudes* into *probabilities*, we multiply the amplitude by its complex conjugate.

RULE 1:

If

$$|\phi\rangle = a_1 |A\rangle + a_2 |B\rangle + a_3 |C\rangle + a_4 |D\rangle + \dots \quad (6.7)$$

then

$$Prob(|\phi\rangle \rightarrow |A\rangle) = a_1^* a_1 = |a_1|^2, \quad Prob(|\phi\rangle \rightarrow |B\rangle) = b_1^* b_1 = |b_1|^2, \quad etc \quad (6.8)$$

This is one of the fundamental rules (postulates) of quantum theory as we saw in our earlier discussions.

Rules like these can't be proven in any mathematical sense. Mathematics can't tell us what probability amplitudes *mean*. That is the job of physics and the only way of doing it is to relate the mathematics to experimental results. We have to *assume* the rule, use it to do some calculations and then check and see if all predictions are correct. If all works out, then the rule gets accepted. In this case, the relationship between amplitudes and probabilities is the cornerstone of quantum theory; the success of the whole theory relies on its being correct. Quantum theory has been around for nearly 100 years now and it works, so we can regard this rule as being confirmed by experiments.

6.1.1.3 States in Stern-Gerlach Experiment

Now let us see if we can apply our ideas to S-G experiments.

If we send a $|U\rangle$ state electron through a (LEFT,RIGHT) magnet, it can emerge from either channel with equal probability. Similarly, if we send a $|D\rangle$ state electron into a (LEFT,RIGHT) magnet, it will also emerge from either channel with equal probability. So using the ideas from the previous section, we must be able to write the two quantum states $|U\rangle$ and $|D\rangle$ in the form (remember color/hardness discussion)

$$\begin{aligned} |U\rangle &= a |R\rangle + b |L\rangle \\ |D\rangle &= c |R\rangle + d |L\rangle \end{aligned} \quad (6.9)$$

where a , b , c , and d are the probability amplitudes. Now we need to figure out what the values of these numbers might be. We have some clues to help us out.

First, a must be different from c , and b must be different from d . This has to be the case as $|U\rangle$ and $|D\rangle$ must be different from one another although both of them are combinations of $|L\rangle$ and $|R\rangle$.

Second, if the probability of emerging from either channel is the same, then Rule 1 (amplitude absolute squared = probability) tells us

$$aa^* = bb^* = cc^* = dd^* = \frac{1}{2} \quad (6.10)$$

A simple way of solving these equations would be to have

$$a = b = c = d = \frac{1}{\sqrt{2}} \quad (6.11)$$

The problem with making a , b , c , and d all $1/\sqrt{2}$ is that we just indicated they must all be different. We have to be more careful and use the fact that $\sqrt{1/2}$ can be $+1/\sqrt{2}$ or $-1/\sqrt{2}$ to construct

$$\begin{aligned} |U\rangle &= \frac{1}{\sqrt{2}} |R\rangle + \frac{1}{\sqrt{2}} |L\rangle \\ |D\rangle &= \frac{1}{\sqrt{2}} |R\rangle - \frac{1}{\sqrt{2}} |L\rangle \end{aligned} \quad (6.12)$$

Remember the color/hardness states. We could switch the $+$ and $-$ signs if we wished with no change in the physical content. These are correct combinations, but unfortunately we can't prove that formally at this stage. To figure out the values of a , b , c , and d we have actually used the following:

RULE 2: NORMALIZATION

If

$$|\phi\rangle = a_1 |A\rangle + a_2 |B\rangle + a_3 |C\rangle + a_4 |D\rangle + \dots \quad (6.13)$$

then

$$|a_1|^2 + |a_2|^2 + |a_3|^2 + |a_4|^2 + \dots = 1 \quad (6.14)$$

You can see how this works out easily in the case of the $|U\rangle$ state where

$$|a_1|^2 + |a_2|^2 = \frac{1}{2} + \frac{1}{2} = 1 \quad (6.15)$$

In general, Rule 2 is telling us that the total probability obtained by adding the probability for each possibility in the state must add to 1. In other words, something has to happen! If the probabilities added up to a number < 1 , this would mean there was a probability that something would happen that was not

included in the list of possibilities (states in linear combination making up the state under consideration), which violates Rule 1.

Rule 2 puts a constraint on the amplitudes, which can help work out their values. If we have got things right and all probabilities associated with the amplitudes in the state add up to 1, we say the state has been *normalized*.

General Stern-Gerlach States

When we talked about the S-G experiment earlier, we discussed only the positions of the magnets that were at 90° with respect to one another, when it is clearly possible to have any orientation.

Consider a beam of $|U\rangle$ state electrons arriving at an S-G magnet with its axis tilted at some angle θ to the vertical. Electrons will emerge from this magnet along one of the two paths as before. Let us call the states $|1\rangle$ and $|2\rangle$. In this case, a different number of electrons pass down each channel, indicating that the amplitudes are *not the same*:

$$|U\rangle = a|1\rangle + b|2\rangle \quad (6.16)$$

with the constraint that $aa^* + bb^* = |a|^2 + |b|^2 = 1$, which follows from Rule 2.

A detailed mathematical analysis(beyond scope of this book) of the angled S-G magnet shows that the correct states and amplitudes are

$$\begin{aligned} |U\rangle &= \cos\left(\frac{\theta}{2}\right)|1\rangle + \sin\left(\frac{\theta}{2}\right)|2\rangle \\ |D\rangle &= \sin\left(\frac{\theta}{2}\right)|1\rangle - \cos\left(\frac{\theta}{2}\right)|2\rangle \end{aligned} \quad (6.17)$$

where, in general, θ measures the angle between the axis of the magnet and a vertical reference line.

These states have to be consistent with our earlier results. So if we send the $|U\rangle$ and $|D\rangle$ states into a (LEFT,RIGHT) magnet, then $\theta = 90^\circ$ and $\theta/2 = 45^\circ$. Now,

$$\sin(45^\circ) = \cos(45^\circ) = \frac{1}{\sqrt{2}} \quad (6.18)$$

Thus, we get the states we had earlier. Also

$$\sin^2\left(\frac{\theta}{2}\right) + \cos^2\left(\frac{\theta}{2}\right) = 1 \quad (6.19)$$

for any θ , which is consistent with Rule 2.

Some Further Thoughts

Summarizing what we have come up with so far about *quantum states*:

The mathematical representation of an initial quantum state uses a ket symbol such as $|\phi\rangle$, and an expansion (summed list) over a series of possible final quantum states as follows $|\phi\rangle = a_1 |1\rangle + a_2 |2\rangle + a_3 |3\rangle + a_4 |4\rangle + \dots$. The amplitudes are a collection of complex numbers related to the probability that the initial state $|\phi\rangle$ will change into one of the final states $|n\rangle$ as a result of a measurement. Rule 1 gives us the relationship between amplitudes and probabilities. The list of possible final states is called the *basis* (the **HOME** space) of the expansion.

So we know how to represent the amplitudes and what they mean; but what about basis states? How can we write down what the $|n\rangle$ are in mathematical terms? Is there some equation or formula for the $|n\rangle$?

Up to now we have simply written states such as $|\phi\rangle$ in terms of basis states, and these in turn have been written as a combination of a further basis, for example we wrote $|U\rangle$ as a combination of $|L\rangle$ and $|R\rangle$. In turn $|L\rangle$ can be written as a combination of $|U\rangle$ and $|D\rangle$ as can $|R\rangle$. The system that we have seems to lead to a regression of writing one thing in terms of another without actually getting anywhere. However, this is not entirely true.

For one thing the structure of our quantum state is a reflection of the *contextuality* of quantum physics, something that we referred to earlier. A state such as $|U\rangle$ can be written as

$$|U\rangle = \frac{1}{\sqrt{2}} |R\rangle + \frac{1}{\sqrt{2}} |L\rangle \quad (6.20)$$

in the *context* of a (LEFT,RIGHT) magnet, or as

$$|U\rangle = \cos\left(\frac{\theta}{2}\right) |1\rangle + \sin\left(\frac{\theta}{2}\right) |2\rangle \quad (6.21)$$

in the *context* of a magnet is at some other angle θ .

Furthermore, each of the $|n\rangle$ states in our basis represents a possible result of measurement in that context!. Although we have been talking about S-G magnets and interference experiments, these states have not been linked to a specific quantitative value of a physical property, but as we go further into quantum theory this link will come up(as it did in our earlier discussion).

What we are missing at the moment is some way of extracting quantitative information about a physics property (an observable) from a state such as $|n\rangle$. We will discuss this later.

6.1.1.4 What Are Quantum States?

The average quantum mechanic is about a philosophically sophisticated as the average automobile mechanic.

John Polkinghorne

According to the picture we have built up so far in this book, the quantum state of a system contains a series of complex numbers related to the probability that the system will *collapse* into a new state when a measurement takes place. Each of these new states represents a possible result of the measurement, which might be a path or a specific quantitative value of some physical variable. However, this simple description of a quantum state hides a **number of difficulties**.

If we make a measurement on a specific system, for example, an electron, then the result will be a distinct value of the physical property being measured. However, such a measurement cannot confirm the probability of finding an electron with that value. We have to make the same measurement many times and see how often each specific value comes up. This gives us some practical difficulties to deal with. For example, how do we ensure that the electron is in *exactly* the same state every time we make a measurement? We might be better off using a collection of electrons, if we can put all of them in the same initial state, and perform one measurement on each. But, if this is the best way of carrying out the measurement we must ask what the quantum state actually represents.

Given a collection of electrons in the same state prior to measurement, does the quantum state describe *each* electron in the collection or can the state only meaningfully refer to the collection *as a whole*?

This is more than just a debate over terminology: it raises important questions about the nature of probability itself. Let us expand on our earlier discussion of probability.

Probabilities occur in science in many different ways. Sometimes when we have to deal with probabilities, there is some physical aspect of the system that reflects this. A good example would be throwing a fair dice, which will result in each face coming up $1/6$ of the time, precisely because there are 6 faces to choose from. However, if we have a collection of balls in a bag and half of them are red and the other half are white, then the probability of drawing a red ball out of the bag (without looking) is $1/2$. In this case the probability is not a direct reflection of some property of each ball. The probability only exists when the balls are placed in the collection. Perhaps we might prefer to say that the probability state describes only the collection and not the individual balls within it.

So, if the quantum state refers only to a collection of systems, the probability involved might come from having systems within the collection that are not

quite identical. Then the amplitudes would not be representing a genuine unpredictability that is inherent to a system. They would be expressing our ignorance of what is going on at a *deeper level*. Perhaps there are some *hidden variables* at work and if we only knew what they were and what values they take, exact predictions would be possible. The collection of systems would actually have various possible values of these hidden variables, we just couldn't tell which one was which. The probability would simply be telling us how many of each type was in the collection.

However, if the quantum state refers to a single system, the probabilities involved might reflect the physical nature of the system. This is a more intriguing possibility as it may open up a new way of looking at reality. If the quantum state of a system is represented by a set of probability amplitudes, then, in a manner of speaking, we are describing the state in terms of what it can *become* as a result of measurement or interaction. After the measurement, one of the possibilities has taken place (manifested itself); so the system is in a new state. This state in turn is best described in terms of what it can become after the next measurement. We are therefore continually describing systems in terms of what they become or change into, arguably never what they are. Perhaps there is nothing more to describing what something is than saying what it can become or what it can do. The quantum description is then one of these *processes*. Somehow the current state of a quantum system has its future implicit within it. Once a measurement has taken place, one of the implicit possibilities becomes explicit.

This is a very abstract picture, but do not worry about that. The classical state of a system is also abstract, in the strict sense of the word, as the state is represented by a series of quantities abstracted from the physical properties of the system. Nevertheless, it seems more real since the speed, position, mass, etc., of an object are familiar terms, and we are quite used to the idea that they can be determined in quantitative terms.

The meaning we give to a quantum state is a philosophical question. Provided that the quantum description allows us to make calculations that correctly predict the outcome of an experiment (given the random nature of some quantum outcomes), there is no experimental way in which different ways of thinking about the quantum state can be distinguished.

The majority of physicists take a very pragmatic view of this. As far as they are concerned, quantum theory works: it allows them to make calculations, do experiments, and build a career in science. The deeper questions about what it all means are rather fruitless (as they are not accessible to experimental resolution). This, however, is not the approach that all take, including me.

There is no denying that there is a distinct element of weirdness about this. The probability amplitudes still seems to be detached from any tangible reality.

At one level, this is simply the normal puzzlement that we feel when learning about an unfamiliar subject. On another level our unease reflects a genuine problem in quantum theory: how can it be that the familiar everyday world that we experience results from the underlying quantum reality described by probability amplitudes?

When quantum mechanics was first developed, physicists struggled to understand how the bizarre outcomes of their experiments could be described in terms of the familiar classical world. As their understanding and experience deepened they learned to replace some classical concepts, but the direction of their thinking always tended to be from the familiar classical toward the bizarre quantum. Now, physicists have become more used to dealing with the quantum world and the thinking is more from the other direction: accepting quantum reality and wondering how the everyday world can be understood from it.

Amplitudes

Let us now look at amplitudes in more detail and particularly the ways in which amplitudes have to be combined in certain circumstances. This will allow us to make a significant step forward in understanding the way quantum theory works.

Amplitudes play a key role in quantum mechanics. They are the link between theory and experiment. The theorist use quantum mechanics to calculate amplitudes for various situations, and then the experimenters have to set up those situations and make measurements.

Experiments in fundamental physics tend to be very costly and complicated. Normally the same particle, or the same atom, or whatever it is that is being studied, is passed through a sequence of measuring systems, each one of which will try and extract some information about what is going on. The chances are that each measuring device will have an effect on the state of the system. The set of amplitudes describing what might happen at one measuring device will depend on the outcome of the previous measurement. If we are going to be able to deal with this, we need some way of tracing amplitudes through a sequence of situations. We need to know how to combine and convert amplitudes.

Physicists have had to abstract the basic rules for combining amplitudes from experimental results. As with Rules 1 and 2 from earlier, these principles can not be proven in a strict mathematical sense (they are like postulates). We have to follow nature's lead and guess the correct way to proceed.

RULE 3:

Changes in states(transitions) are governed by amplitudes.

When one transition follows another, the amplitudes are multiplied to-

gether.

When two alternatives are possible, the *probabilities add* if the alternatives can be *distinguished* in the experiment.

When two alternatives *cannot* be distinguished, the *amplitudes add* and then the probability is calculated by *taking the absolute square of the total amplitude*.

The best way to understand this rule is to see how it works in practice.

Let's go back to the S-G experiments again, but this time we are going to start with a state $|\phi\rangle$ where

$$|\phi\rangle = a|U\rangle + b|D\rangle \quad (6.22)$$

We have chosen $|U\rangle$ and $|D\rangle$ as the basis for the state expansion as the first part of the experiment is going to be an (UP,DOWN) magnet - (UP,DOWN) states are called the HOME space for this part of the experiment (they are the possible results of measurement). After that, we will allow each beam from the first magnet to pass into other magnets arranged at some angle θ , so the emerging states are $|L'\rangle$ and $|R'\rangle$. It then makes sense to expand the $|U\rangle$ and $|D\rangle$ states over a new basis $|L'\rangle$ and $|R'\rangle$ as follows:

$$|U\rangle = m|L'\rangle + n|R'\rangle \quad , \quad |D\rangle = p|L'\rangle + r|R'\rangle \quad (6.23)$$

At the first magnet, the beam of electrons in state $|\phi\rangle$ divides into an UP beam containing a fraction $|a|^2$ of the original beam, and a DOWN beam containing a fraction $|b|^2$ of the original beam. At the second magnet, the $|U\rangle$ states collapse into either $|L'\rangle$ with probability $|m|^2$ or $|R'\rangle$ with probability $|n|^2$. A similar sort of thing happens to the $|D\rangle$ electrons, as you can see in the figure below.

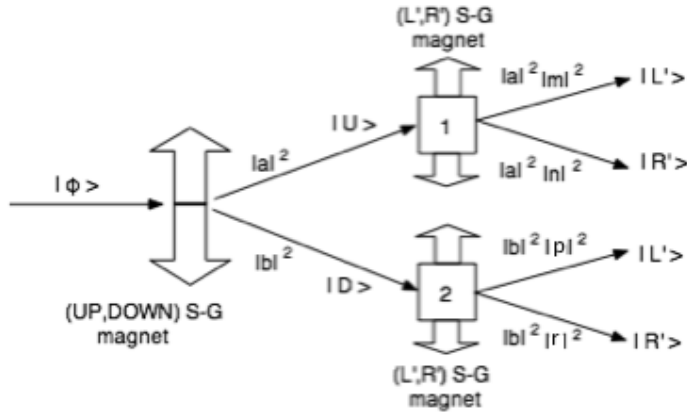


Figure 6.4: Rules for Combining Amplitudes

So, the probability that an electron starting in state $|\phi\rangle$ will end up in state $|L'\rangle$ having gone through magnet 1 is

$$Prob\left(|\phi\rangle \xrightarrow{\text{via magnet 1}} |L'\rangle\right) = |a|^2 \times |m|^2 \quad (6.24)$$

A result that is simply obtained by considering the fraction of the original beam that makes it through each stage. Note, though, that we would get exactly the same result if we constructed the amplitude governing the state change from $|\phi\rangle$ to $|L'\rangle$ as

$$\begin{aligned} & \text{amplitude}\left(|\phi\rangle \xrightarrow{\text{via magnet 1}} |L'\rangle\right) \\ &= \text{amplitude}(|\phi\rangle \rightarrow |U\rangle) \times \text{amplitude}(|U\rangle \rightarrow |L'\rangle) = a \times m \end{aligned} \quad (6.25)$$

and then calculated the probability by complex squaring the amplitude, i.e., $|a \times m|^2 = (a m) \times (a^* m^*) = aa^* \times mm^* = |a|^2 \times |m|^2$. The end result is just what Rule 3 said it has to be: when one transition (change of state) follows another, the amplitudes multiply. So, the first part of the rule works as advertised.

Now let's ask a slightly different question: what would be the probability of an electron ending up in state $|L'\rangle$ if we were not worried about which (L', R') magnet it went through? It's simple enough to see what this should be if we look back at the last figure.

$$\begin{aligned} Prob\left(|\phi\rangle \xrightarrow{\text{via magnet 1}} |L'\rangle\right) &= |a|^2 \times |m|^2 \\ Prob\left(|\phi\rangle \xrightarrow{\text{via magnet 2}} |L'\rangle\right) &= |b|^2 \times |p|^2 \end{aligned} \quad (6.26)$$

So that the overall probability is

$$Prob(|\phi\rangle \rightarrow |L'\rangle) = |a|^2 \times |m|^2 + |b|^2 \times |p|^2 \quad (6.27)$$

This is actually an application of a standard rule in probability calculations, which we mentioned earlier: when you have one event **or** another, the probabilities add. Rule 3 states, *When two alternatives are possible, the probabilities add if the alternatives can be distinguished in the experiment.* The crucial part here is the phrase *can be distinguished in the experiment.*

Information about which alternative a particular system follows has to be available, *even if we don't choose to use that information in the experiment.*

That just leaves us with the final part of Rule 3, which applies in situations where we cannot tell which alternative is happening. We need an example to see how it works. The most convenient situation to use is the previous experiment with a slight alteration. What we need to do is get rid of one of the (L', R') S-G magnets and pull the other one forward, so it gets both beams from the (UP,DOWN) magnet, as in the figure below.

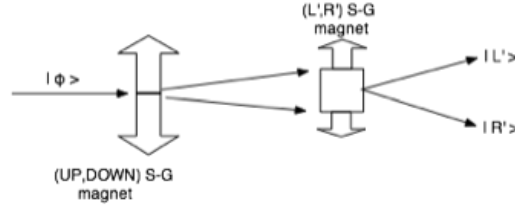


Figure 6.5: Cannot distinguish paths

Now we ask once again: what is the probability of an electron starting in the state $|\phi\rangle$ and ending up in state $|L'\rangle$? In this situation, we have no way to tell which channel is used by the electron on its way from the (UP,DOWN) magnet to the (L',R') magnet. The possibilities are indistinguishable. As we have seen in earlier discussions, when possibilities cannot be distinguished, the quantum systems seem to take all the options at once. The final part of Rule 3 is there to reflect this.

Rule 3 tells us that we need to trace the amplitude through each possible path individually

$$\begin{aligned} \text{amplitude} \left(|\phi\rangle \xrightarrow{\text{top path}} |L'\rangle \right) &= a \times m \\ \text{amplitude} \left(|\phi\rangle \xrightarrow{\text{bottom path}} |L'\rangle \right) &= b \times p \end{aligned} \quad (6.28)$$

and then add the amplitudes together

$$\text{amplitude} \left(|\phi\rangle \xrightarrow{\text{cannot tell which path}} |L'\rangle \right) = a \times m + b \times p \quad (6.29)$$

From this it is a straightforward job to calculate the probability by complex squaring the total amplitude

$$\text{Prob} \left(|\phi\rangle \xrightarrow{\text{cannot tell which path}} |L'\rangle \right) = |a \times m + b \times p|^2 \quad (6.30)$$

This final part of Rule 3 is a very important aspect of quantum theory. The rule that we add the amplitudes before complex squaring if the paths are indistinguishable has *no equivalent in normal probability calculations or classical physics*.

Basically this is the theoretical representation of what happens in an interference experiment. We will talk about this a lot more when we discuss interference later, but let us make this one comment now.

As we are adding the amplitudes before they are squared (when we cannot tell which path is being followed), the two amplitudes can *interfere* with each other. If both $a \times m$ and $b \times p$ are positive, then the combined amplitude is bigger. However, if any one of them is negative, then the amplitude decreases. In a standard interference experiment, the amplitudes will change depending on the length of the path through the experiment. This change affects the sign of the amplitude, so we have an overall probability that gets bigger and smaller depending on path length. This will be exactly the property we are looking for later when we try to explain the experiments we discussed earlier.

6.1.1.5 Change of Basis

There is another way of looking at the indistinguishable path probability calculation. It involves a little mathematical manipulation. Let us do it in detail. It is a good way to learn/practice the mathematics and the kind of algebraic procedures we need to use later on.

The idea that states can be expanded over a any basis is a very important aspect of quantum theory. It is part of the way that the *contextuality* of quantum physics gets reflected in the theory. When you expand a state, it is always a good idea to choose a basis that is useful in describing the measurement that is going to take place - we have called this process *going to the HOME space*. Every quantum state can be expanded in many ways, depending on what sort of experiment is involved. To illustrate this idea, let's have another look at the indistinguishable path experiments as shown in the Figure 6.5.

The first thing that the electrons in the state $|\phi\rangle$ come across is an (UP,DOWN) S-G magnet. So, it's sensible to expand this state in terms of $|U\rangle$ and $|D\rangle$ states(use them as the basis for expansion).

$$|\phi\rangle = a|U\rangle + b|D\rangle \quad \text{Expansion 1} \quad (6.31)$$

The electrons then hit the (L', R') magnet, which makes it sensible to consider an expansion of the $|U\rangle$ and $|D\rangle$ states in terms of $|L'\rangle$ and $|R'\rangle$.

$$\begin{aligned} |U\rangle &= m|L'\rangle + n|R'\rangle \\ |D\rangle &= p|L'\rangle + q|R'\rangle \end{aligned} \quad \text{Expansion 2} \quad (6.32)$$

As far as the overall situation is concerned, our initial state is $|\phi\rangle$ and the final state we are interested in is $|L'\rangle$. Then, what we really need is is an expansion of $|\phi\rangle$ in terms of $|L'\rangle$ and $|R'\rangle$. We can get this expansion by pulling together the information that we already have. After all, we can plug Expansion 2 into Expansion 1. It is a bit of slightly messy algebra, so let us step through it in detail.

$$\begin{aligned} |\phi\rangle &= a|U\rangle + b|D\rangle = a[m|L'\rangle + n|R'\rangle] + b[p|L'\rangle + q|R'\rangle] \\ &= (am + bp)|L'\rangle + (an + bq)|R'\rangle \end{aligned} \quad (6.33)$$

The result is very interesting, so let us look at it carefully.

$$|\phi\rangle = (am + bp) |L'\rangle + (an + bq) |R'\rangle \quad (6.34)$$

This expansion is telling us the amplitude for $|\phi\rangle$ to collapse to $|L'\rangle$ by the end of the experiment (and in same expansion, the amplitude for $|\phi\rangle$ to collapse to $|R'\rangle$). If you look closely, you can see that the amplitude $(am + bp)$ is exactly what we calculated using Rule 3 earlier.

Can you think why this calculation produces the same answer? The primary reason is as follows.

If the paths are distinguishable, Expansion 1 is no longer valid. What happens instead is that $|\phi\rangle$ turns into one of $|U\rangle$ or $|D\rangle$, whereas Expansion 1 is assuming that both are valid at the same time; in other words, the state has not collapsed so we cannot tell which path is happening.

So we can see from this that the same quantum state can be expanded in many ways, depending on the circumstances or experiment being performed. It is also possible to switch from one basis to another with a little bit of algebra.

6.1.1.6 Expanding the Dirac Language

As we mentioned earlier, the first person to work with the symbol $|\phi\rangle$ was the English physicist Paul Henri Dirac. As we said, he named the mathematical objects $|\rangle$ *kets*.

Dirac's creativity did not stop with the introduction of kets into the physicist's vocabulary; he also brought *bras* into our thinking (you can make your own jokes at this point....although it is not what you are thinking!) as we discussed earlier. To Dirac a bra, $\langle|$, is just an alternative way of representing and expanding a state by using the complex conjugates of the amplitudes rather than the amplitudes themselves

$$\langle\phi| = a_1^* \langle 1| + a_2^* \langle 2| + a_3^* \langle 3| + \dots + a_n^* \langle n| \quad (6.35)$$

Dirac language has become the standard language for working in quantum theory. Aside from its elegance, which will become more apparent as we move on, it has the virtue of directly illuminating important quantum physics.

The first thing that we can do is to use it to express another important rule for dealing with amplitudes. We will eventually be able to think "quantum mechanically" when writing equations using the Dirac language.

RULE 4:

If a system starts off in state $|\phi\rangle$ and ends up in state $|\psi\rangle$, then the amplitude that determines the transition from one to the other can be calculated

by taking the bra of the final state and acting on the ket of the initial state (mathematically we are actually evaluating the inner product - we use the \times sign to indicate the action).

$$\text{amplitude}(|\phi\rangle \rightarrow |\psi\rangle) = \langle\psi| \times |\phi\rangle \quad (6.36)$$

Let's see how this works in a specific case. The simplest situation is the one we started off with.

$$|\phi\rangle = a|U\rangle + b|D\rangle \quad (6.37)$$

According to Rule 4, the amplitude governing the collapse of $|\phi\rangle$ into $|U\rangle$ should be

$$\text{amplitude}(|\phi\rangle \rightarrow |U\rangle) = \langle U| \times |\phi\rangle = \langle U| \times (a|U\rangle + b|D\rangle) \quad (6.38)$$

We have to expand out the last bracket to see what we get

$$\begin{aligned} \text{amplitude}(|\phi\rangle \rightarrow |U\rangle) &= \langle U| \times (a|U\rangle + b|D\rangle) \\ &= a\langle U| \times |U\rangle + b\langle U| \times |D\rangle \end{aligned} \quad (6.39)$$

In this case we actually know what the answer should be. The definition of state expansion tells us that the amplitude for $|\phi\rangle$ changing into $|U\rangle$ is a . If our rule is going to be consistent with what we already know, then we must have

$$\langle U| \times |U\rangle = 1 \quad , \quad \langle U| \times |D\rangle = 0 \quad (6.40)$$

Actually this is totally consistent. According to Rule 4, $\langle U| \times |U\rangle$ should be telling us the amplitude for $|U\rangle$ to change into $|U\rangle$, which if we have normalized the states properly should give us 1. However, $|U\rangle$ cannot change into $|D\rangle$ (at least not directly), so $\langle U| \times |D\rangle = 0$. These last two statements are just an expression of the orthonormality of the (UP,DOWN) basis states as we discussed earlier. Hence

$$\text{amplitude}(|\phi\rangle \rightarrow |U\rangle) = a\langle U| \times |U\rangle + b\langle U| \times |D\rangle = a \times 1 + b \times 0 = a \quad (6.41)$$

There is one further refinement to this. When we take a bra and act on a ket, we tend to leave the multiplication sign out of the middle (since it really is an inner product) and write $\langle\psi|\phi\rangle$ not $\langle\psi| \times |\phi\rangle$. Note this is where the names *bra-ket* comes from, i.e., *bra-c-ket*. This is a physicist kind of whimsical humor.

6.1.1.7 Orthogonal Bases

Let's see what happens when we take a bra and act on the ket for the same state

$$\begin{aligned} \langle\phi|\phi\rangle &= \{a_1^* \langle 1| + a_2^* \langle 2| + \dots + a_n^* \langle n|\} \{a_1 | 1\rangle + a_2 | 2\rangle + \dots + a_m | m\rangle\} \\ &= a_1^* a_1 \langle 1| 1\rangle + a_1^* a_2 \langle 1| 2\rangle + \dots + a_n^* a_m \langle n| m\rangle \end{aligned} \quad (6.42)$$

Here we have used a collection of states $|1\rangle, |2\rangle, |3\rangle$, etc as the basis. From now on, when we want to refer to such a collection of states, we will use the abbreviation $\{|n\rangle\}$. The curly brackets tell us that we are dealing with a collection of

states, not just one single state. The labeling $|n\rangle$ shows us that the states are going to be numbered 1, 2, 3, etc.

The final term in the second line of this expansion looks a bit odd: $a_n^* a_m \langle n | m \rangle$. Mathematicians use this sort of thing to show how all the terms are put together with $n = 1, 2, 3, \dots$ and $m = 1, 2, 3, \dots$. This saves having to write out all the terms, with the telling us that we have not reached the end yet.

If we have made a sensible choice (an orthonormal basis as we discussed earlier) about the set of basis states to expand over, two things follow.

1. Terms such as $\langle n | m \rangle$, where n and m are different, vanish since $\langle n | m \rangle = 0$.
2. Terms of the form $\langle 1 | 1 \rangle$ or $\langle n | m \rangle$, where n and m are the same, should be $\langle 1 | 1 \rangle = \langle n | n \rangle = \langle m | m \rangle = 1$, etc.

These rules are not pulled out of thin air; they directly reflect experimental facts. If the states $|1\rangle, |2\rangle, |3\rangle$, etc represent different measurement results and the experiment has separated out distinct paths or quantitative values of a physical variable, one state cannot *overlap* with another (they have nothing in common - they are orthogonal). Hence the amplitude for a transition from $|m\rangle$ to $|n\rangle$ ($m \neq n$) is zero.

Thus, there is a physical basis for the orthonormality of basis states corresponding to the measurements.

As we saw earlier, physicists describe any two states for which $\langle n | m \rangle = 0$ as *orthogonal* states. In a good basis set, all the states are orthogonal to one another and the collection is called an orthogonal basis.

Assuming that the basis $\{|n\rangle\}$ is orthogonal, the calculation of $\langle \phi | \phi \rangle$ reduces nicely to

$$\begin{aligned} \langle \phi | \phi \rangle &= a_1^* a_1 \langle 1 | 1 \rangle + a_1^* a_2 \langle 1 | 2 \rangle + \dots + a_n^* a_m \langle n | m \rangle \\ &= a_1^* a_1 + a_2^* a_2 + a_3^* a_3 + \dots + a_n^* a_n + \dots \\ &= 1 \end{aligned} \tag{6.43}$$

where the last line follows from Rule 2.

Let me now illustrate an algebraically better way to do the calculation. We will be using this new way most of the time later on. Let

$$|\phi\rangle = a_1 |1\rangle + a_2 |2\rangle + \dots + a_n |n\rangle = \sum_{i=1}^K a_i |i\rangle$$

and

$$\langle \phi | = a_1^* \langle 1 | + a_2^* \langle 2 | + \dots + a_n^* \langle n | = \sum_{j=1}^K a_j^* \langle j |$$

where K is the size (dimension) of the basis. Then

$$\langle \phi | \phi \rangle = \left(\sum_{j=1}^K a_j^* \langle j | \right) \left(\sum_{i=1}^K a_i | i \rangle \right) = \sum_{j=1}^K \sum_{i=1}^K a_i a_j^* \langle j | i \rangle$$

But the basis is *orthonormal* which means that $\langle j | i \rangle = \delta_{ij}$ and therefore

$$\langle \phi | \phi \rangle = \sum_{j=1}^K \sum_{i=1}^K a_i a_j^* \delta_{ij} = \sum_{i=1}^K a_i a_i^* = \sum_{i=1}^K |a_i|^2$$

or

$$\langle \phi | \phi \rangle = a_1^* a_1 + a_2^* a_2 + a_3^* a_3 + \dots + a_n^* a_n + \dots = 1$$

as in Eq. (6.43).

6.1.1.8 It Really is the Language

The elegance of Dirac's language starts to reveal itself if we return to an earlier argument and recast it (briefly) using the bra and ket language.

The starting point was to write $|\phi\rangle = a|U\rangle + b|D\rangle$, which would now become

$$|\phi\rangle = \langle U | \phi \rangle |U\rangle + \langle D | \phi \rangle |D\rangle \quad (6.44)$$

since

$$\begin{aligned} \langle U | \phi \rangle &= a \langle U | U \rangle + b \langle U | D \rangle = a \times 1 + b \times 0 = a \\ \langle D | \phi \rangle &= a \langle D | U \rangle + b \langle D | D \rangle = a \times 0 + b \times 1 = b \end{aligned} \quad (6.45)$$

The next thing we did was to write $|U\rangle$ and $|D\rangle$ in terms of $|L'\rangle$ and $|R'\rangle$

$$\begin{aligned} |U\rangle &= m|L'\rangle + n|R'\rangle = \langle L' | U \rangle |L'\rangle + \langle R' | U \rangle |R'\rangle \\ |D\rangle &= p|L'\rangle + q|R'\rangle = \langle L' | D \rangle |L'\rangle + \langle R' | D \rangle |R'\rangle \end{aligned} \quad (6.46)$$

and substitute them into the $|\phi\rangle$ expansion. As a result of this work we produced an expression for the amplitude governing the transition $|\phi\rangle \rightarrow |L'\rangle$, which was, as we found earlier, $(am + bp) = (ma + pb)$. In Dirac language this would be written as

$$\begin{aligned} |\phi\rangle &= \langle U | \phi \rangle |U\rangle + \langle D | \phi \rangle |D\rangle \\ |\phi\rangle &= \langle U | \phi \rangle (\langle L' | U \rangle |L'\rangle + \langle R' | U \rangle |R'\rangle) \\ &\quad + \langle D | \phi \rangle (\langle L' | D \rangle |L'\rangle + \langle R' | D \rangle |R'\rangle) \\ |\phi\rangle &= [\langle L' | U \rangle \langle U | \phi \rangle + \langle L' | D \rangle \langle D | \phi \rangle] |L'\rangle \\ &\quad + [\langle R' | U \rangle \langle U | \phi \rangle + \langle R' | D \rangle \langle D | \phi \rangle] |R'\rangle \\ |\phi\rangle &= [ma + pb] |L'\rangle + [na + qb] |R'\rangle \end{aligned} \quad (6.47)$$

so that

$$\begin{aligned} \text{amplitude} \left(|\phi\rangle \xrightarrow{\text{cannot tell which path}} |L'\rangle \right) &= \langle L' | U \rangle \langle U | \phi \rangle + \langle L' | D \rangle \langle D | \phi \rangle \\ &= ma + pb \end{aligned} \quad (6.48)$$

This expression beautifully illustrates how the amplitudes combine together.

Look at it closely.

The first term is the amplitude that takes $|\phi\rangle \rightarrow |L'\rangle$ via intermediate state $|U\rangle$. The second term is the amplitude that takes $|\phi\rangle \rightarrow |L'\rangle$ via intermediate state $|D\rangle$.

This expression is actually an example of the another important rule.

RULE 5:

Any amplitude governing a transition from an initial state to a final state via an intermediate state can be written in the form

$$\begin{aligned} \langle \text{final state} | \text{initial state} \rangle &= \\ \langle \text{final state} | \text{intermediate state} \rangle \langle \text{intermediate state} | \text{initial state} \rangle \end{aligned} \quad (6.49)$$

If the various intermediate states (labelled by i) are indistinguishable, we have to add up all of them to get the overall amplitude

$$\langle \text{final state} | \text{initial state} \rangle = \sum_i [\langle \text{final state} | i \rangle \langle i | \text{initial state} \rangle] \quad (6.50)$$

Rule 5 is really an extension of Rule 3 written in a more formal way.

6.1.1.9 Going the Other Way

In Dirac language, the amplitude for a transition between some initial state and a final state is

$$\langle \text{final state} | \text{initial state} \rangle \quad (6.51)$$

Of course, it is always possible that the process is running in the opposite direction from the *final* to the *initial* state. Before we get too confused about what's initial and what's final, let's agree to call them i and j .

In general,

RULE 6(very important):

The amplitude to go from $|i\rangle$ to $|j\rangle$ is the complex conjugate of the amplitude to go from $|j\rangle$ to $|i\rangle$.

$$\langle i | j \rangle = \langle j | i \rangle^* \quad (6.52)$$

This can be seen below.

$$\begin{aligned} \langle i | j \rangle &= (a^* \langle U | + b^* \langle D |) (c | U \rangle + d | D \rangle) = a^* c + b^* d \\ \langle j | i \rangle^* &= [(c^* \langle U | + d^* \langle D |) (a | U \rangle + b | D \rangle)]^* \\ &= [c^* a + d^* b]^* = a^* c + b^* d = \langle i | j \rangle \end{aligned}$$

6.1.2 Measurement

We now tackle one of the most profound puzzles in quantum physics. The process of measurement takes a quantum state, expressed as a collection of possibilities, and makes one of the possibilities actual. Without measurement, we could not relate theory to reality. Yet, despite the crucial nature of measurement, there is still no widely agreed theory of how it takes place in the microworld.

6.1.2.1 Embracing Change

Change is built into the structure of a quantum state. We have seen how a state can be expanded over a set of basis states, which represent the different possible outcomes of an experiment. Once the experiment has been performed, the original state has collapsed into one of the basis states.

State collapse is a very peculiar process, and we will have a lot more to say about it in this book. However, it is not the only way that quantum states can change. For most of the time, the various quantum systems in nature exist in the universe not being involved in experiments, yet clearly things can and do change. Any valid theory must be capable of describing the normal processes of the world in which things interact with one another, change, and develop. Part of our dealings in this section will be to develop and expand our knowledge and understanding of the machinery that quantum theory uses to portray the changes corresponding to ordinary time development and the, rather more mysterious, changes due to the measurement process.

6.1.2.2 Types of States

When thinking about quantum states it is useful to divide them into two broad groups. A state such as $|U\rangle$ represents a particle with a definite fixed value

of a certain property (although we have not yet been clear about what these particular properties are). In the terminology of quantum physics, such states are called *eigenstates*. A state such as $|\phi\rangle$ tends to be a combination of many basis states and so does not have a definite fixed value when a measurement is carried out. Such states are called *mixed states or superpositions*. Sometimes the terms *pure* and *non-pure* are used instead.

Eigenstates

Eigenstates describe systems as having a definite fixed value of a given physical property. Such states are very important. If we know that an object is in an eigenstate, we can predict with absolute certainty what a measurement is going to produce. We saw this in earlier discussions of the postulates and when we sent electrons in the state $|U\rangle$ into an (UP,DOWN) S-G magnet. All such electrons emerged from the magnet along the top path. If we followed this up with a second (UP,DOWN) measurement, once again all the electrons emerged on the top path. This is another important property of an eigenstate: if we make a measurement of the physical property associated with some particular eigenstate, then that measurement does not change the state of the object, no matter how many times we repeat the measurement. This is just the repeated measurement postulate we discussed earlier.

If we choose to measure a property different from the one fixed by the eigenstate, we cannot predict with certainty what will happen. For example, if we send a $|U\rangle$ state electron into a (LEFT,RIGHT) magnet, we do not know on which of the two paths it will eventually emerge.

Sometimes the system can be in an eigenstate of more than one physical property at the same time. An example of this will arise later in which we will find that the free-particle state(not interacting with anything) is an eigenstate of both energy and momentum. Another example was a magenta electron having a definite position. With such a state you can measure either property, predict with certainty what will happen, and not change the state during the measurement. Such a state has definite values of both physical quantities.

Mixed States

The state

$$|R\rangle = \frac{1}{\sqrt{2}} (|U\rangle + |D\rangle) \quad (6.53)$$

is an example of a mixed state. If we choose to measure an electron in this state using an (UP,DOWN) S-G magnet, we will get either $|U\rangle$ or $|D\rangle$ with a 50:50 probability. After a long run of such experiments, we would expect to observe $|U\rangle$ and $|D\rangle$ with about equal frequency, but as the process is random, we would not be surprised or bothered if the fractions were not exactly 50:50.

Mixed states give us a lot of trouble when we want to understand what quantum mechanics is trying to say about the world. Crucially, the mixture is often a sort that would not be allowed in a classical situation. For example, when we considered the Mach-Zehnder device earlier, we ended up with a mixed state that combined two different paths through the device. Any self-respecting classical particle would only follow one path and not seem to be in two places at the same time. Yet the mixed state was unavoidable. Without it we couldn't explain the experimental fact that none of the photons ended up in one of the detectors (with two equal path lengths through the device).

Paul Dirac identified the existence of quantum mixed states as the central puzzle of quantum theory. He points out that a quantum mixed state is not some sort of average. It doesn't describe an existence that is a blend of the separate states, which a classical *mixed state* would. When you try to observe a quantum mixed state, what actually happens is that the mixture collapses into one of the component states. The mixture simply tells us the relative probability of finding the separate component states via the amplitudes that go into the mixture.

A convenient way of thinking about mixed states is to recognize that they show us a set of *tendencies(or potentialities)* for something to happen. A way of expressing this would be to say that the state was *loaded with possibilities* and that when a measurement is made, one of the possibilities is *turned into an actuality*. Most physicists probably think of mixed states on similar lines. Where they tend to *disagree* is on the extent to which they believe this propensity or latency in the state is related to the physical nature of the object.

The distinction between a mixed state and an eigenstate is not an absolute divide. States $|U\rangle$ and $|D\rangle$ are eigenstates as far as (UP,DOWN) measurements are concerned, but are mixed states for (LEFT,RIGHT) measurements. Similarly, states $|L\rangle$ and $|R\rangle$ are eigenstates for (LEFT,RIGHT) measurements, but mixed states for (UP,DOWN) measurements.

Expectation Values

Let us imagine that we have a large number of electrons available to us, all of which are in the same state $|U\rangle$, and then we send a some of them at an (UP,DOWN) S-G device. We know with absolute certainty that the results will always be UP. The state $|U\rangle$ is an eigenstate of (UP,DOWN). However, if we choose to send the remainder of the electrons at a (LEFT,RIGHT) device, our ability to predict what happens becomes more limited. Given a specific electron all we can say is that half the time it will emerge from the LEFT channel and half the time it will emerge from the RIGHT channel. We have no way of telling what is going to happen to each electron in turn. This is how *randomness* finds its expression in the quantum world.

This doesn't stop us from saying what will happen on *average*. If we give RIGHT

the value (+1) and LEFT(-1), then after a run of such measurements the average value across all the electrons taking part will be close to zero (exactly zero except for randomness and/or experimental precision).

Now imagine that our set of electrons is in some other state $|\phi\rangle$ where

$$|\phi\rangle = a|L\rangle + b|R\rangle \quad \text{with} \quad |a|^2 + |b|^2 = 1 \quad \text{but} \quad a \neq b \quad (6.54)$$

On subjecting this collection of electrons to a (LEFT,RIGHT) measurement, we will find that a fraction of them equal to $|a|^2$ will come out LEFT and another fraction equal to $|b|^2$ will come out RIGHT. Again we have no way of knowing what will happen to each individual electron, but in this instance the average value has a more interesting result. If $|a|^2$ of them have (+1) and $|b|^2$ of them have (-1), then we can compute the average value as

$$\text{average value} = |a|^2 \times (1) + |b|^2 \times (-1) = |a|^2 - |b|^2 \quad (6.55)$$

In quantum theory, the average value of a series of measurements made on a collection of identically prepared systems (in the same state) is called the *expectation value*, as we defined earlier. Note that the expectation value applies only to a series of measurements. In the case of a set of electrons, each individual electron in the set will give either (+1) or (-1) and so cannot be compared with the expectation value, *which belongs to the set as a whole*.

This connection between the expectation values and the results of a set of measurements leads some people to the view that states represent only collections of systems. According to them, when we say that the electrons are in the state $|\phi\rangle$ we are not saying each individual electron is in the state $|\phi\rangle$; it is the set as a whole that has that state. Indeed, such thinking would put to rest the view that *any* state applies to an individual system!

There is clearly some sense to this view. After all, and to some people this is the crucial point, we can never tell from a single measurement what state a system is in. Sending an electron at an (UP,DOWN) magnet and seeing it come out UP does not allow us to distinguish between $|U\rangle$ as the initial state, which is bound to give us UP, and an initial state of $|R\rangle$, where it was made actual as $|U\rangle$ by the measurement. It would not help to repeat the experiment on the same electron; once it emerged from the UP channel we know that it now has to be in the state $|U\rangle$, no matter what state it started off in. The only way of telling what was going on would be to have a set of these electrons and measure each one in turn. Finding one came out in the DOWN channel would enable us to tell the difference between $|U\rangle$ and $|R\rangle$. It would not allow us to tell the difference between $|R\rangle$ and $|L\rangle$, however. We would have to look at the (LEFT,RIGHT) property for that.

So, there is clearly something to be said for the idea that states refer only to

collections of systems. Such a view tends toward an instrumentalist interpretation of quantum theory. A realist would certainly want to know what was happening to the *real* individual electrons out there.

Operators

It's very important to be able to tell if a state is a mixed state or an eigenstate with respect to a given measurement. The mathematical machinery of quantum theory must allow for a way of doing that, otherwise all we can do is construct a state after the fact. This is where the mathematical objects called *operators* we discussed earlier play a crucial role.

As we said earlier, an operator takes some sort of mathematical expression and transforms it into something else. In quantum theory operators take us from one state to another, a process governed by strict rules for each operator. There are many different types of operators in quantum theory, which have different jobs to do. Perhaps the most important ones are the operators that represent the process of measuring a physical property.

An immediate example of such an operator would be the (UP,DOWN) S-G operator, called \hat{S}_z , where we are assuming, without loss of generality, that the UP-DOWN direction is the z -axis. The $\hat{}$ over the symbol (used earlier) indicates an operator. The role of this operator is to *pull out* of a state information about how the state will react to an (UP,DOWN) measurement. The rules that govern how it works are very simple. $|U\rangle$ and $|D\rangle$ are the eigenstates of (UP,DOWN) measurements. This means that the (UP,DOWN) measurement or its corresponding operator does not change these states. Thus, we have

$$\hat{S}_z |U\rangle = +1 |U\rangle \quad \text{and} \quad \hat{S}_z |D\rangle = -1 |D\rangle \quad (6.56)$$

The operator takes an eigenstate and multiplies it by a number equal to the value of the quantity that would be found by a measurement of the particle in that state. The action of the operator is to pull the *value* from the state. Remember that we assigned values (+1) to UP and (-1) to DOWN.

This is really a definition of what we mean by an operator in this context. By the way, the value that ends up multiplying the state, which is the value that an experiment would reveal with certainty, is called the *eigenvalue* of the eigenstate, as we discussed earlier. We note that the complete set of eigenstates for an operator connected with a physical variable always can be used as a good basis set. This is because all operators for physical variables are Hermitian operators as we discussed earlier.

If the state concerned is not an eigenstate of vertical(z -axis) S-G measurements,

then \hat{S}_z will make a mess of it. For example,

$$\begin{aligned}\hat{S}_z |R\rangle &= \hat{S}_z \left(\frac{1}{\sqrt{2}} |U\rangle + \frac{1}{\sqrt{2}} |D\rangle \right) = \left(\frac{1}{\sqrt{2}} \hat{S}_z |U\rangle + \frac{1}{\sqrt{2}} \hat{S}_z |D\rangle \right) \\ &= \left(\frac{1}{\sqrt{2}} |U\rangle - \frac{1}{\sqrt{2}} |D\rangle \right) = |L\rangle\end{aligned}\quad (6.57)$$

Although this does not look like it is much use to anyone, the action of an operator on states that are *not* one of its eigenstates has an important role to play. Look at what happens when we expand out the mathematical construction

$$\begin{aligned}\langle R | \hat{S}_z | R \rangle &= \left(\frac{1}{\sqrt{2}} \langle U | + \frac{1}{\sqrt{2}} \langle D | \right) \hat{S}_z \left(\frac{1}{\sqrt{2}} |U\rangle + \frac{1}{\sqrt{2}} |D\rangle \right) \\ &= \left(\frac{1}{\sqrt{2}} \langle U | + \frac{1}{\sqrt{2}} \langle D | \right) \left(\frac{1}{\sqrt{2}} \hat{S}_z |U\rangle + \frac{1}{\sqrt{2}} \hat{S}_z |D\rangle \right) \\ &= \left(\frac{1}{\sqrt{2}} \langle U | + \frac{1}{\sqrt{2}} \langle D | \right) \left(\frac{1}{\sqrt{2}} |U\rangle - \frac{1}{\sqrt{2}} |D\rangle \right) \\ &= \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \langle U | U \rangle - \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \langle D | D \rangle \\ &= \frac{1}{2} - \frac{1}{2} = 0\end{aligned}\quad (6.58)$$

Note that we have used the fact that $\langle U | D \rangle = \langle D | U \rangle = 0$ (a property of any set of basis states).

As it stands, this still does not look like an especially useful calculation. However, before we jump to conclusions, let's do it again using $|\phi\rangle$ instead of $|R\rangle$. Then we have

$$\begin{aligned}\langle \phi | \hat{S}_z | \phi \rangle &= (a^* \langle U | + b^* \langle D |) \hat{S}_z (a |U\rangle + b |D\rangle) \\ &= (a^* \langle U | + b^* \langle D |) (a \hat{S}_z |U\rangle + b \hat{S}_z |D\rangle) \\ &= (a^* \langle U | + b^* \langle D |) (a |U\rangle - b |D\rangle) \\ &= a^* a \langle U | U \rangle - b^* b \langle D | D \rangle \\ &= |a|^2 - |b|^2\end{aligned}\quad (6.59)$$

In other words, mathematical constructions such as $\langle \phi | \hat{S}_z | \phi \rangle$ or $\langle R | \hat{S}_z | R \rangle$ give us the expectation (or average) values that apply to a series of measurements made on a state such as $|\phi\rangle$ or $|R\rangle$.

\hat{S}_z is not the only example of an operator representing a measurement of a physical quantity. There are operators for the other S-G magnet directions, and also for position, momentum, energy, and all the normal things that one would want to measure in physics. Although these other operators exist and function in a very similar way to \hat{S}_z , we will not look at them in detail until much later.

Up to that point, if we need to refer to the energy operator, for example, we will just use the symbol \hat{E} .

The connection between a physical quantity and an operator in quantum theory is very different from the way in which classical physics deals with such things.

In classical physics, as we have said, a state is a collection of quantities that describe an object at a given moment. Those quantities can be speed (momentum), mass, energy, etc., and each is given a numerical value that represents the amount of this quantity on some scale. The classical laws of nature provide rules that connect the various quantities together so that when we put the actual values in place, we can predict future values.

In quantum mechanics, a state is a collection of amplitudes for the object to have values of physical quantities. Any physical quantity is represented by an operator \hat{O} , which can be used to find out the expectation value of that physical variable. There is a strong temptation to call this the average value of the *quantity*, but it's not really. It is the average value obtained from a repeated run of measurements on identical systems, but none of the systems will necessarily have a value equal to the expectation value.

Operators tell us nothing by themselves; they need to act on states for any information to be forthcoming.

RULE 7:

Every physical variable has an operator \hat{O} associated with it. Such operators have eigenstates $|\psi\rangle$ defined by

$$\hat{O}|\psi\rangle = a|\psi\rangle \quad (6.60)$$

where a is the value of the physical variable you would get if you measured state $|\psi\rangle$. The complete set of eigenstates $\{|\psi\rangle\}$ for a given operator always forms a basis.

The operator associated with a physical variable can be used to calculate the expectation value of a series of measurements made on a collection of systems in the same state $|\phi\rangle$. It is given by

$$\langle\hat{O}\rangle = \langle\phi|\hat{O}|\phi\rangle \quad (6.61)$$

How can we represent operators?

As we said earlier, think of an operator as some kind of box, where you put a vector in and get another (either different or the same) vector out. This is similar to the definition of a function for the space of numbers.

Some properties of operators in Quantum Mechanics(from earlier discussions):

$$\begin{aligned}
\hat{Q}(|A\rangle + |B\rangle) &= \hat{Q}|A\rangle + \hat{Q}|B\rangle \quad (\text{linearity}) \\
\hat{Q}(c|A\rangle) &= c\hat{Q}|A\rangle \quad , \quad c = \text{complex number} \\
\langle C|(\hat{Q}|B\rangle) &= \langle C|B'\rangle = \text{number} \equiv \langle C|\hat{Q}|B\rangle \quad (\text{matrix element}) \\
(\hat{Q}_1 + \hat{Q}_2)|A\rangle &= \hat{Q}_1|A\rangle + \hat{Q}_2|A\rangle \quad (\text{linearity}) \\
(\hat{Q}_1\hat{Q}_2)|A\rangle &= \hat{Q}_1(\hat{Q}_2|A\rangle) \quad (\text{order matters})
\end{aligned} \tag{6.62}$$

These properties imply that all of our operators are what the mathematicians call *LINEAR* operators. The fact that quantum mechanics can be understood using only linear operators is truly amazing because they are the simplest kind of operator that mathematicians can think of.

All observables or *quantities that we can measure* will be represented by operators in quantum mechanics.

Let us repeat the discussion we presented earlier. This additional pass, now that we have had many discussions in between, should greatly enhance our understanding.

In order to find a way to represent operators, we need to restate and expand our knowledge of some of the properties that we have already specified.

Suppose that we make measurements on a state $|\psi\rangle$ of an observable represented by the operator \hat{B} with eigenvalues/eigenvectors given by

$$\hat{B}|b_j\rangle = b_j|b_j\rangle \quad j = 1, 2, 3, 4, \dots \tag{6.63}$$

and

$$|\psi\rangle = \sum_k a_k |b_k\rangle \tag{6.64}$$

where

$$a_k = \langle b_k | \psi \rangle \tag{6.65}$$

Suppose the measurement results(they must be the eigenvalues) are the values b_k , each occurring n_k times where $k = 1, 2, 3, 4, \dots$ and where

$$\sum_k n_k = N = \text{total number of measurements} \tag{6.66}$$

Now from the definition of the average value, we have

$$\begin{aligned}
\langle \hat{B} \rangle &= \text{average or expectation value of } \hat{B} \\
&= \frac{1}{N} \sum_k n_k b_k = \sum_k \frac{n_k}{N} b_k = \sum_k b_k \text{prob}(b_k)
\end{aligned} \tag{6.67}$$

From our postulates (or rules) we then have that $prob(b_k) = |\langle b_k | \psi \rangle|^2$ so that

$$\langle \hat{B} \rangle = \sum_k b_k prob(b_k) = \sum_k b_k |\langle b_k | \psi \rangle|^2 \quad (6.68)$$

Now $\langle b_k | \psi \rangle^* = \langle \psi | b_k \rangle$. Therefore, $|\langle b_k | \psi \rangle|^2 = \langle \psi | b_k \rangle \langle b_k | \psi \rangle$ and

$$\langle \hat{B} \rangle = \sum_k b_k |\langle b_k | \psi \rangle|^2 = \sum_k b_k \langle \psi | b_k \rangle \langle b_k | \psi \rangle = \langle \psi | \left[\sum_k b_k |b_k\rangle \langle b_k| \right] | \psi \rangle \quad (6.69)$$

Our definition of the expectation value, however, was

$$\langle \hat{B} \rangle = \langle \psi | \hat{B} | \psi \rangle \quad (6.70)$$

which then says that we can represent the operator \hat{B} by the expression

$$\hat{B} = \sum_k b_k |b_k\rangle \langle b_k| \quad (6.71)$$

This is very important way of representing the operator, i.e., any operator can be written in terms of its eigenvalues and eigenvectors. It is called the *spectral decomposition* of the operator.

Projection Operators

Operators of the form

$$\hat{P}_\beta = |\beta\rangle \langle \beta| \quad (6.72)$$

are called *projection operators*. Thus, we can write any operator \hat{B} as

$$\hat{B} = \sum_k b_k P_{b_k} \quad (6.73)$$

where

$$P_{b_k} = |b_k\rangle \langle b_k| \quad (6.74)$$

We also have the very important property of projection operators given by the following operator

$$\hat{I} = \sum_k |b_k\rangle \langle b_k| \quad (6.75)$$

Using this operator we have

$$\hat{I} |\beta\rangle = \sum_k |b_k\rangle \langle b_k | \beta \rangle = \sum_k \langle b_k | \beta \rangle |b_k\rangle = |\beta\rangle \quad (6.76)$$

Thus, the operator \hat{I} is the *IDENTITY* operator or the operator that leaves all kets *unchanged*.

Some Operators

If we define the color operator as \hat{O}_{color} with the properties in the color space

$$\hat{O}_{color} |m\rangle = (+1) |m\rangle \quad , \quad \hat{O}_{color} |g\rangle = (-1) |g\rangle \quad (6.77)$$

Then we have

$$\hat{O}_{color} = |m\rangle \langle m| - |g\rangle \langle g| \quad (6.78)$$

Does it work? We have

$$\begin{aligned} \hat{O}_{color} |m\rangle &= (|m\rangle \langle m| - |g\rangle \langle g|) |m\rangle = |m\rangle \\ \hat{O}_{color} |g\rangle &= (|m\rangle \langle m| - |g\rangle \langle g|) |g\rangle = -|g\rangle \end{aligned} \quad (6.79)$$

as expected! We note that the $|h\rangle$ state has equal amounts of magenta/green. Therefore the expectation value of the color operator in a hard state should equal zero. This is confirmed below.

$$\begin{aligned} \langle h | \hat{O}_{color} | h \rangle &= \frac{1}{\sqrt{2}} (\langle m | + \langle g |) \hat{O}_{color} \frac{1}{\sqrt{2}} (|m\rangle + |g\rangle) \\ &= \frac{1}{2} [\langle m | \hat{O}_{color} | m \rangle + \langle m | \hat{O}_{color} | g \rangle + \langle g | \hat{O}_{color} | m \rangle + \langle g | \hat{O}_{color} | g \rangle] \\ &= \frac{1}{2} [\langle m | m \rangle - \langle m | g \rangle + \langle g | m \rangle - \langle g | g \rangle] \\ &= \frac{1}{2} [1 - 0 + 0 - 1] = 0 \end{aligned} \quad (6.80)$$

This Dirac language is very powerful!

In a similar manner, we can represent an (UP,DOWN) S-G magnet or the operator \hat{S}_z by

$$\hat{S}_z = |U\rangle \langle U| - |D\rangle \langle D| \quad (6.81)$$

6.1.2.3 How States Evolve

There is a range of different types of operators in quantum theory, each with its own role to play. We have already seen how some operators are tied to physical variables. Their job is to act on a state to see if it is an eigenstate of the physical variable. If it is, the operator pulls out the eigenvalue and puts it in front of the state. If not, the operator will change the state to another one.

There is another very important operator that is not directly tied to a physical variable: the *time evolution operator*. This operator, $\hat{U}(t)$, takes a state and moves it forward in time:

$$\hat{U}(t) |\Psi(T)\rangle = |\Psi(T+t)\rangle \quad (6.82)$$

where $|\Psi(T)\rangle$ represents the state of a system at time T .

Here the time evolution operator $\hat{U}(t)$ has taken the state $|\Psi(T)\rangle$ and pushed it forward an interval of time t to become $|\Psi(T+t)\rangle$

Clearly if $\hat{U}(t)$ is to do this accurately, it must have all of the details of the behavior of the system is doing and how it is interacting with the environment.

To take a simple example, imagine our typical electron in state $|U\rangle$ moving through space toward an S-G magnet. Now, it's very unlikely that this electron will move through a complete vacuum with no gravitational, electrical, or magnetic fields lying around. Such fields will exert a force on the electron and quite possibly disturb its S-G orientation. As a result, the state will evolve from $|U\rangle$ to different state, say $|\phi\rangle$, in a smooth and deterministic manner. As it turns out, the energy of the electron as it interacts with these fields (or any other particle for that matter) will determine the manner in which the state evolves, i.e., the time evolution operator will be constructed from the energy operator for the electron.

To be clearer about what the time evolution operator does, remember that we can always describe any S-G state using the $\{|U\rangle, |D\rangle\}$ basis.

$$|\Psi\rangle = a|U\rangle + b|D\rangle \quad (6.83)$$

So, what really happens when the $\hat{U}(t)$ operator acts is

$$\begin{aligned} \hat{U}(t)|\Psi(T)\rangle &= \hat{U}(t)[a(T)|U\rangle + b(T)|D\rangle] \\ &= [a(T+t)|U\rangle + b(T+t)|D\rangle] \end{aligned} \quad (6.84)$$

In other words, $\hat{U}(t)$ changes the amplitudes from their values at time T to new ones at time $T+t$. Now imagine we take this extra time interval t and divide it into many smaller intervals, which are of size δt . If there are 100 such small pieces, then $t = 100 \times \delta t$. Nothing that we have said about the time evolution operator has suggested that it works in any way differently for very small time intervals compared with longer ones. So, rather than applying $\hat{U}(t)$ once to take the state from $|\Psi(T)\rangle$ to $|\Psi(T+t)\rangle$, we ought to be able to get the same answer by applying $\hat{U}(\delta t)$ 100 times, one after the other. When we apply $\hat{U}(\delta t)$ for the first time we get

$$\begin{aligned} \hat{U}(\delta t)|\Psi(T)\rangle &= \hat{U}(\delta t)[a(T)|U\rangle + b(T)|D\rangle] \\ &= [a(T+\delta t)|U\rangle + b(T+\delta t)|D\rangle] \end{aligned} \quad (6.85)$$

and it is not very likely that $a(T+\delta t)$ will be very different from $a(T)$ (same is true for the amplitude b). Applying $\hat{U}(\delta t)$ again gives us

$$\begin{aligned} \hat{U}(\delta t)|\Psi(T+\delta t)\rangle &= \hat{U}(\delta t)[a(T+\delta t)|U\rangle + b(T+\delta t)|D\rangle] \\ &= [a(T+2\delta t)|U\rangle + b(T+2\delta t)|D\rangle] \end{aligned} \quad (6.86)$$

and so forth. So, the state's evolution from $|\Psi(T)\rangle$ to $|\Psi(T+t)\rangle$ takes place via a *continuously smooth* (limit as $\delta t \rightarrow 0$) *change from one moment to the next*.

Furthermore, and this is very important, this evolution is perfectly determined by the physics of the system, as expressed in the structure of $\hat{U}(t)$. There is *no randomness* involved here.

Of course, this smooth evolution is not the only way that a state can evolve. States also evolve in a sharp(discontinuous) and unpredictable manner when a measurement takes place. Indeed, a possible definition of a measurement is that it produces a *sharp and unpredictable change in the state of the system*.

When an electron in a state such as $|\Psi\rangle$ reaches an (UP,DOWN) S-G magnet, the state will change into $|U\rangle$ with probability $|a|^2$ or into $|D\rangle$ with probability $|b|^2$. After the measurement we can say that the state has *evolved* into $|U\rangle$ (i.e., $a \rightarrow 1$, $b \rightarrow 0$) or $|D\rangle$ (i.e., $a \rightarrow 0$, $b \rightarrow 1$). In this instance, the amplitudes a and b have not changed in a continuously smooth manner (or so it seems) as produced by the $\hat{U}(t)$ operator. The dramatic and unpredictable change in quantum state as a result of a measurement is often referred to as the *collapse or reduction of the state*.

State collapse is a radically different sort of process from $\hat{U}(t)$ evolution, as it can't be broken down into a smooth progression of small steps. This makes it mathematically impossible for the equations of quantum theory as we currently understand them, to describe state collapse (a non-linear process cannot be described by a linear operator). It remains an *add on* assumption, rather than something that can be predicted from within the theory.

This is a significant point.

Quantum theory can correctly describe the evolution of states from one moment to the next; it just doesn't describe the world we live in, unless we add in something that allows for measurement processes and state collapse. The world is not a set of evolving possibilities. The possibilities encoded in a quantum state have to be linked to actual events in the world.

Some physicists (Roger Penrose among them) have suggested that what we need to do is modify quantum theory and introduce some new equations that can describe measurement in a satisfactory manner. States would not then collapse (discontinuous change), but would evolve in a different manner over very short time scales.

If this is true, then there must be some physics that we have missed up to now. It would have to remain as a very small-scale effect until the particle (or whatever) is interacting with a measuring device, as the current equations work very well, except under those circumstances. Clearly the physicists who are working to modify the theory along these lines are looking for a realistic view of state collapse.

The collapse of a state as a result of a measurement is an encouragement to some physicists to seek an instrumentalist view of quantum states. They would argue that a discontinuous change in the state of a system shows that the state simply represents our information about the system. After all, before a dice is thrown, our information about it is that there is a 1/6 probability of each face coming up. After the throw, our information state collapses, as we now know which face has actually landed uppermost. The dice has not changed in any physical manner. Correspondingly when a quantum state collapses this does not necessarily signal any physical difference in the system being described, just a change in our knowledge about it.

To counter this, a realist would say that the quantum state cannot just be our knowledge of the system, since how can our knowledge have a direct effect on the system's behavior? We have previously considered various *delayed choice* experiments in which our ability/lack of ability to infer information about the state of a photon had a direct result on the outcome of the experiment. Therefore our knowledge must be a reflection of something real to do with the system.

Quantum states may well be rather weird and spooky compared to the cozy classical reality that we have all been brought up in, but there is no reason to give up believing that science is revealing truths about the world just because we find the truths surprising.

SUMMARY

The $\hat{U}(t)$ operator evolves a state forward in time in a *smooth and predictable manner*

$$\hat{U}(t) |\Psi(T)\rangle = |\Psi(T+t)\rangle \quad (6.87)$$

The exact form of the $\hat{U}(t)$ operator depends on the physics of the system. State collapse is the *sharp and unpredictable* change in a state as a result of a measurement (if a state is not an eigenstate of the physical quantity being measured).

6.1.2.4 Why is State Reduction Necessary?

It is reasonable to ask ourselves how we ever managed to get into this mess in the first place. Why are we driven to construct a theory that requires such an odd concept as state collapse? The argument reduced to its essentials, would run as follows:

- (1) Certain events in the microworld, such as reflection or transmission of photons from a half-silvered mirror, seem to be random (at least to our level of current understanding). We are forced to represent the state of microscopic objects in terms of probabilities. We assign a number to each possibility, and this number tells us the probability that things will turn out this way.

- (2) A detailed analysis of the Mach-Zehnder experiment shows us that these numbers (we call them amplitudes) have to be complex numbers, so they can't in themselves be probabilities. The link between amplitudes and probabilities is guessed (that $probability = |amplitude|^2$) and subsequently checked by experiment.
- (3) We are therefore led to represent the quantum state of a system using a collection of amplitudes.
- (4) In certain situations we see that the appropriate quantum state is a mixture of states that would have to be separate classically. For example, there are many experiments that can only be understood if the intermediate state of a photon appears to follow two different classical paths at the same time. Without this, interference effects would not take place and the actual experimental results could not be explained.
- (5) Although quantum theory allows these mixed states to occur, we seem to be protected from them, as they are never directly observed as outcomes of experiments. The photon is never observed on both paths at the same time.
- (6) It is clear that the quantum state of a system is prone to change. If we prepare an appropriate beam of electrons for a Stern-Gerlach (S-G) experiment, we find that 50% of them exit the device along each channel, indicating that the electrons were in one of these mixed states to start with. However, if we pass all the electrons from one channel into another identical S-G device, then all of them emerge from the same channel. The first experiment has changed their quantum state from one of these, apparently, unobservable mixed states into a classical-like eigenstate that is definitely $|U\rangle$ or $|D\rangle$.
- (7) This is the crux of the problem. Certain experiments can only be explained if classically forbidden mixtures are allowed. However, we live in a classical world so that quantum mixed states must collapse into more classical-like states that we can directly observe.

The realists among us would say that state collapse is what is really going on out there, so we had better just get used to it. Instrumentalists would probably confess that they don't like the idea, but after all a theory is only a way of getting experimental predictions out and they have to do what works. Very troubling from both points of view!

Now let us use all of this formalism to explain a real experiment.

6.1.3 Explaining the Double-Slit Experiment with Amplitudes

A quantum mechanical description of the double-slit experiment must involve a set of amplitudes governing the passage of an electron through the slits to the

far detector. We have already seen how to deal with amplitudes of this sort: they are covered by Rule 5.

We start by writing down

$$\langle x | I \rangle = \langle x | A \rangle \langle A | I \rangle + \langle x | B \rangle \langle B | I \rangle \quad (6.88)$$

where $|x\rangle$ is the state corresponding to an electron arriving at a position x of a detector, $|A\rangle$ corresponds to passing through slit A, $|B\rangle$ corresponds to passing through slit B, and $|I\rangle$ corresponds to the initial state of an electron emerging from the electron gun as shown below.

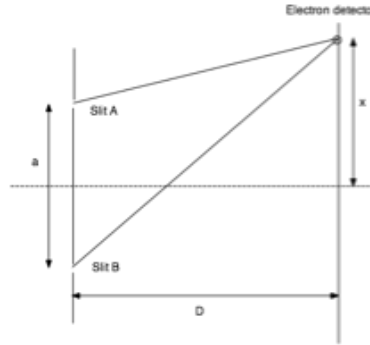


Figure 6.6: Two Slit Experiment

Experimentally, there are bright and dark interference bands. The dark band separation is given by $D\lambda/a$ where λ is the wavelength.

We have to add together two terms in the overall amplitude, as the two possibilities (traveling through one slit or the other) cannot be distinguished in the context of the experiment as it is set up. Normally, when we combine amplitudes in this fashion some sort of interference results. If we block a slit, then one of the terms will *disappear* and hence there can be no interference.

The probability that an electron arrives at x is the complex square of the total amplitude.

$$|\langle x | I \rangle|^2 = [\langle x | A \rangle \langle A | I \rangle + \langle x | B \rangle \langle B | I \rangle]^* [\langle x | A \rangle \langle A | I \rangle + \langle x | B \rangle \langle B | I \rangle] \quad (6.89)$$

Expanding this out is a tedious job as shown below:

$$\begin{aligned} |\langle x | I \rangle|^2 &= \langle x | A \rangle^* \langle A | I \rangle^* \langle x | A \rangle \langle A | I \rangle + \langle x | B \rangle^* \langle B | I \rangle^* \langle x | B \rangle \langle B | I \rangle \\ &\quad + \langle x | A \rangle^* \langle A | I \rangle^* \langle x | B \rangle \langle B | I \rangle + \langle x | B \rangle^* \langle B | I \rangle^* \langle x | A \rangle \langle A | I \rangle \end{aligned} \quad (6.90)$$

The first two terms give the conventional (classical) sum of probabilities that we might expect for an electron that goes through one slit or the other. The final

term in square brackets is where the interesting stuff resides: *it is an interference term*.

6.1.3.1 Phase and Physics

Let us digress for a moment to review and reconsider complex numbers in a different form so that they will be more useful for our discussion of phase.

The Complex Plane - As we have seen, complex numbers are needed if certain mathematical objects in quantum mechanics are going to represent reality. We now want to think about the ideas already introduced and explore the exponential way of writing complex numbers further and introduce a geometrical picture to help us understand what is going on. This will make our later study of quantum interference clearer and easier.

It is sometimes more convenient to think of a complex number as denoting a point on a special type of graph.

Mathematicians sometimes picture the real numbers as lying on a line stretching out to infinity. As we work our way along this line (from either direction) we must, at some point, come across the number zero. Then, if we sit and contemplate life on the zero point, any points on the line to the right of us are positive real numbers and those to the left are negative real numbers.

Now, when complex numbers appeared, mathematicians started to think in terms of two lines at right angles to one another.

A purely real number would lie on the horizontal line, and a purely imaginary numbers (e.g., $3i$ or $5i$ or $-2.1678i$) would lie somewhere on a vertical line running through the zero point.

Clearly, any two lines at right angles to one another *map out* or *define* a two-dimensional (2-D) region, and in this case we call it the *complex plane*.

Any complex number, such as $a + ib$, can then be identified with a point on the complex plane. To get to this point you walk along the real line a distance a , turn at right angles, and walk parallel to the imaginary line a distance b .

The figure below shows a graphical representation of the complex plane.

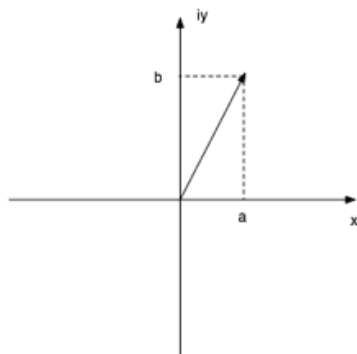


Figure 6.7: Point in Complex Plane

In this figure, we have taken a small liberty that we will talk about in a moment. In some ways this figure looks just like an ordinary graph. The horizontal arrow with an x next to it shows that we are plotting the x coordinate along this direction. On a normal graph, there is also a vertical arrow with a y next to it showing that we are plotting the y coordinate along the vertical direction. In this case, though, we have labelled the vertical line as iy , which we are not really allowed to do. You see, you cannot plot a coordinate iy as there is no such distance. The point of the graph is to represent quantities (numbers with units) as lengths according to some scale. Really we should have just put y on the vertical axis and then say that any complex number is going to be of the form

$$z = (x \text{ coordinate}) + i(y \text{ coordinate}) \quad (6.91)$$

The reason we have not done this is quite simple. We want to emphasize that in the above figure and the figure below (and so on) *neither* the x direction nor the y direction is an actual physical direction in space. The figures just represent the way of picturing the complex numbers.

On any flat surface (plane) there is always more than one way of getting to a particular point. Rather than walking specific distances along multiple lines, we can approach the same point by a more direct route.

Imagine standing on the zero point looking along the real line. If you turn in a counterclockwise (or anticlockwise) direction through an angle θ and proceed to walk in that direction a distance R , you will end up at exactly the same point $a + ib$ as shown in the figure below.

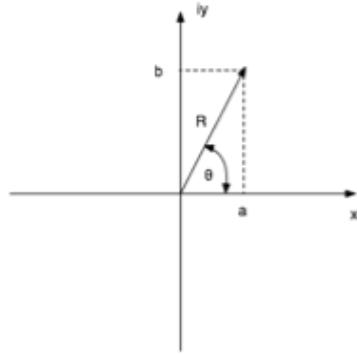


Figure 6.8: An Alternate Path

If you like, you can think of the line of length R as the hand of a clock and θ the angle that the hand sweeps out (note that it starts sweeping out at 3 o'clock (positive x -axis) and goes backward(anticlockwise)!).

Clearly, if R and θ are to get you to the same place as a and b , there must be some formulas that connects the two sets of numbers together. A moment's thought using some high school geometry(Pythagoras) and trigonometry(sines and cosines) shows that

$$a = R \cos \theta, \quad b = R \sin \theta \rightarrow \frac{b}{a} = \tan \theta, \quad R^2 = a^2 + b^2 \quad (6.92)$$

It is worth noting that R must always be positive. You cannot move a negative distance away from the zero point. Sometimes people do not get this the first time and assume that negative R means walking in the opposite direction. Think instead of "positive" as meaning the arrow points outward.

What this all means in the end is that we now have two ways of writing the same complex number, either as $z = a + ib = (a, b)$ or $z = (R, \theta)$. We will come up with a mathematical form for the second way soon.

Magnitude and Phase

For the moment, let's think about this *distance to walk*, R .

The complex conjugate of the number $z = a + ib$ is $z^* = a - ib$. As you know, if you multiply a complex number by its conjugate, you always get a real number. Now we can see specifically what this number is

$$zz^* = (a + ib)(a - ib) = a^2 + b^2 = R^2 \quad (6.93)$$

Clearly, this is a mathematical way to *convert* a complex number into a real number. As we have already seen this is an important operation that gives us

probabilities from probability amplitudes.

But now we ought to think about what happens if we switch things around. It's clear from considering the complex plane that there will be many complex numbers that have the same R . All we need to do is draw a circle around the zero point of radius R ; all the points on the circumference of that circle will be complex numbers with the same R .

The figure below illustrates this idea. The complex numbers $z = a + ib$ and $Z = A + iB$ have the same value of R , which is called their *magnitude*. Consequently, they would both lead to the same absolute value. Indeed there are an infinite number of complex amplitudes that would lead to the same absolute value.

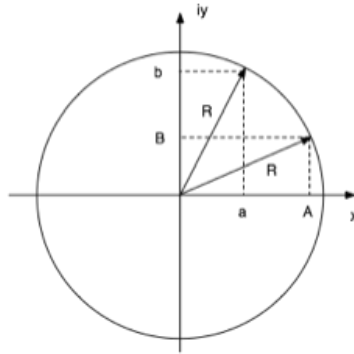


Figure 6.9: Same magnitude

All the complex numbers with the same R differ only in the value of θ , which is called the *argument* of the complex number by mathematicians, but to build a link with physics we will call θ the *phase* (it will correspond to the phase we defined earlier in the interference experiments). It will turn out that the magnitude of the complex numbers will be related to the observable probability and the phase will tell us about quantum interference as we will see later.

Multiplying Complex Numbers

If we can write a complex number $z = a + ib$ in the form (R, θ) , how would we write iz ?

Well, iz would be $i(a + ib) = ia - b$ or $-b + ia$, which is very interesting, as the complex numbers z and iz would then clearly have the same magnitude, R . However, their phases would be different. The two numbers are illustrated in the figure below.

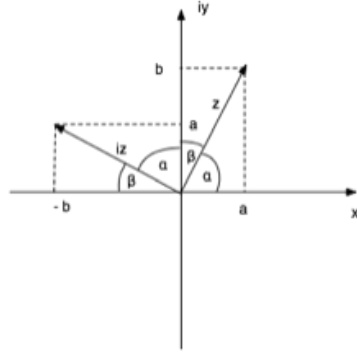


Figure 6.10: Multiply by i

As you can see the phases of z and iz differ by 90° , i.e.,

$$2\alpha + 2\beta = \pi \rightarrow \alpha + \beta = \pi/2 \rightarrow \text{orthogonal} \quad (6.94)$$

Thus, whenever you multiply by i you rotate the phase anticlockwise by 90° , but leave the magnitude alone.

We can push this a little bit further. After all, i is simply the number that lies one unit along the imaginary axis. There are lots of complex numbers that have the same magnitude as i (i.e., $R = 1$) but different phases. The number 1 ($= 1 + 0i$) is an example. What happens if we multiply by one of these other numbers instead?

Take our number $z = a + ib$ and multiply by another number $w = p + iq$ given that $p^2 + q^2 = 1$.

$$zw = (a + ib)(p + iq) = ap + iaq + ibp - bq = (ap - bq) + i(aq + bp) \quad (6.95)$$

Next, we ask ourselves what is the magnitude of this new number? To get the square of the magnitude we add the square of the real part to the square of the imaginary part.

$$\begin{aligned} R^2 &= (ap - bq)^2 + (aq + bp)^2 = a^2p^2 + b^2q^2 - 2apbq - a^2q^2 - b^2p^2 - 2aqbp \\ &= a^2p^2 + b^2q^2 + a^2q^2 + b^2p^2 = a^2(p^2 + q^2) + b^2(p^2 + q^2) \\ &= a^2 + b^2 \end{aligned} \quad (6.96)$$

using $p^2 + q^2 = 1$.

In other words, multiplying any complex number z by another number w , when w has magnitude 1, doesn't change the magnitude of z .

What about the phase though? Well, although it is tougher to prove, one can

show that the phases add (the proof is will be easy later using the exponential form of the complex numbers and slightly harder using trigonometry (see below). In fact, the general rule is as follows:

MULTIPLYING COMPLEX NUMBERS

When two complex numbers z and w are multiplied together, their magnitudes *multiply* and their phases *add*.

$$\text{If } z = (R_1, \theta_1) \text{ and } w = (R_2, \theta_2), \text{ then } zw = (R_1 R_2, \theta_1 + \theta_2) \quad (6.97)$$

Proof: (uses trigonometry)

$$\begin{aligned} z &= a + ib, & w &= p + iq \\ \tan \theta_z &= \frac{b}{a}, & \tan \theta_w &= \frac{q}{p} \\ zw &= (ap - bq) + i(aq + bp) \\ \tan \theta_{zw} &= \frac{aq + bp}{ap - bq} = \frac{\frac{q}{p} + \frac{b}{a}}{1 - \frac{q}{p} \frac{b}{a}} = \frac{\tan \theta_z + \tan \theta_w}{1 - \tan \theta_z \tan \theta_w} = \tan(\theta_z + \theta_w) \\ \Rightarrow \theta_{zw} &= \theta_z + \theta_w \end{aligned} \quad (6.98)$$

More Phase Stuff

The figure below shows how the two complex numbers $z = a + ib$ and $-z = -a - ib$ are related to one another on the complex plane.

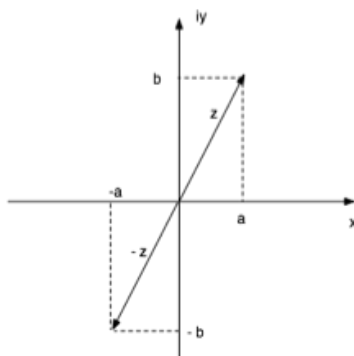


Figure 6.11: z and $-z$

You probably already realized that z and $-z$ have the same value of R . That the phases would be different by 180° may also have occurred to you. If you don't see this straight away, think about multiplying z by i and then again by i , as $i^2 = -1$. Each multiplication by i shifts the phases by 90° , hence 180° overall.

And Pulling It All Together

All the work up to now has been to develop the idea that complex numbers can be represented in two different, but equivalent ways. We choose to use either the two numbers a and b (and write $z = a + ib$) or the two numbers R and θ (and write (R, θ)).

However, there is another way of writing complex numbers, which combines elements of both forms.

Before proceeding we need to review some other mathematics. Various functions in mathematics are represented by something called *power series* - actually these series are the real definitions of the functions, i.e., how we actually calculate them. We have

$$e^{\alpha x} = 1 + \alpha + \frac{1}{2}\alpha^2 + \frac{1}{6}\alpha^3 + \dots = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} x^n \quad (6.99)$$

$$\sin \alpha x = \alpha x - \frac{1}{6}(\alpha x)^3 + \frac{1}{24}(\alpha x)^5 + \dots = \sum_{n=0}^{\infty} (-1)^n \frac{\alpha^{2n+1}}{(2n+1)!} x^{2n+1} \quad (6.100)$$

$$\cos \alpha x = 1 - \frac{1}{2}(\alpha x)^2 + \frac{1}{16}(\alpha x)^4 + \dots = \sum_{n=0}^{\infty} (-1)^n \frac{\alpha^{2n}}{(2n)!} x^{2n} \quad (6.101)$$

These expansions are valid even if the parameter α is a complex number. This leads us to a most important mathematical result for quantum mechanics.

Complex Exponentials

We then have the very important relation

$$\begin{aligned} e^{i\alpha x} &= \sum_{n=0}^{\infty} \frac{i^n \alpha^n}{n!} x^n = 1 + i\alpha x - \frac{\alpha^2}{2!} x^2 - i\frac{\alpha^3}{3!} x^3 + \frac{\alpha^4}{4!} x^4 + i\frac{\alpha^5}{5!} x^5 - \dots \\ &= \left(1 - \frac{\alpha^2}{2!} x^2 + \frac{\alpha^4}{4!} x^4 - \dots\right) + \left(i\alpha x - i\frac{\alpha^3}{3!} x^3 + i\frac{\alpha^5}{5!} x^5 - \dots\right) \\ &= \cos \alpha x + i \sin \alpha x \end{aligned} \quad (6.102)$$

which is called the *Euler relation*.

Using the Euler relation we have the important results

$$\sin \alpha x = \frac{e^{i\alpha x} - e^{-i\alpha x}}{2i}, \quad \cos \alpha x = \frac{e^{i\alpha x} + e^{-i\alpha x}}{2}$$

The Euler relation allows us to define i in a better manner instead of via the square root. We have

$$e^{i\pi} = \cos \pi + i \sin \pi = -1 \quad (6.103)$$

and

$$e^{i\pi/2} = \cos \pi/2 + i \sin \pi/2 = i \quad (6.104)$$

We also have the properties

$$\begin{aligned} e^{a+b} &= e^a e^b \\ e^a &= e^{a/2} e^{a/2} \rightarrow e^{a/2} = \sqrt{e^a} \\ (e^a)^n &= e^{na} \end{aligned} \quad (6.105)$$

so that

$$\sqrt{e^{i\pi}} = e^{i\pi/2} = \cos \pi/2 + i \sin \pi/2 = i \quad (6.106)$$

Now from earlier we had

$$a = R \cos \theta, \quad b = R \sin \theta \rightarrow \frac{b}{a} = \tan \theta, \quad R^2 = a^2 + b^2 \quad (6.107)$$

so that

$$z = a + ib = R \cos \theta + i R \sin \theta = R(\cos \theta + i \sin \theta) = R e^{i\theta} \quad (6.108)$$

One further useful wrinkle will be to see how to write the complex conjugate z^* using the exponential form. We have

$$z^* = a - ib = R \cos \theta - i R \sin \theta = R[\cos(-\theta) + i \sin(-\theta)] = R e^{-i\theta} \quad (6.109)$$

where the last step relied on the properties of $\cos \theta$ and $\sin \theta$ when the angles are negative (i.e., measured in a clockwise direction from the real line), which you may not have come across before, i.e.,

$$\cos(-\theta) = \cos \theta, \quad \sin(-\theta) = -\sin \theta \quad (6.110)$$

Since we will find the exponential form to be extremely useful, let us say a couple more things about it.

When you use $\cos \theta$ and $\sin \theta$ in this sort of context, which is not directly related to geometrical shapes, it is more convenient to use a different measure for θ instead of angle in degrees. Mathematicians and physicists call this measure the *radian*.

The normal way to measure an angle is to take a circle and divide its circumference up in to 360 pieces (see figure below). Then you draw a set of lines from the ends of these pieces to the center of the circle, and there you have a protractor as shown below. The angle between any pair of lines is then 1° .

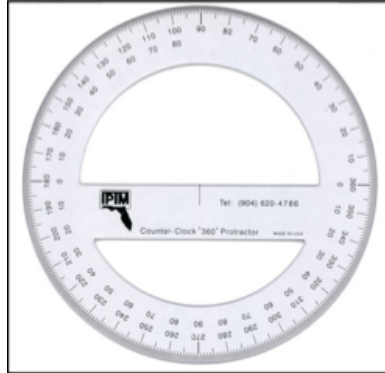


Figure 6.12: Protractor

If you stop to think about it, there is no real reason to pick 360 pieces, as distinct from any other number. We have just gotten so used to 360, it seems like the only choice. There is, however, a more interesting possibility. After all, the circumference of a circle is $2\pi \times \text{radius}$, so why not divide the circumference into 2π pieces rather than 360. Now we cannot actually do this in practice, at least not exactly, since the number π requires an infinite decimal expansion to completely specify it. But actually, we are not interested in making a real protractor here as much as providing a mathematically convenient measure of angle.

If we imagine that we had divided the circle into 2π pieces, then the angle between any two of our imaginary lines would be 1 radian. A complete trip around the whole circle, which would be 360° , is the same as 2π radians. More specifically, 90° cuts out $1/4$ of the circle and this would be $2\pi/4 = \pi/2$ radians. In the same way, 180° is π radians, etc. There are some specific advantages to using the radian, especially when it comes to the properties of sine and cosine as we will see later.

Finally, let us show(again) a very useful property of the exponential form of complex numbers. If you look back at the multiplication rule you will see that when we multiply z_1 by z_2 , the magnitudes multiply and the *phases add*(as we proved earlier using trigonometry). In other words,

$$z_1 z_2 = R_1 \exp(i\theta_1) R_2 \exp(i\theta_2) = (R_1 R_2) \exp(i(\theta_1 + \theta_2)) \quad (6.111)$$

which we had proved earlier.

Returning to Phase and Physics

We are trying to explain the electron interference pattern revealed by the detector, given the amplitudes that govern the two possible routes from slits to

detector. The existence of dark bands, parts of the detector where no electrons arrive, is a key point that we need to factor into our thinking. Clearly, when we add up the amplitudes for getting to such a dark point on the detector, the total must be zero. How can we be sure that this happens? If we were thinking of water waves interfering, or something like that, we would be saying that the path difference between the two routes was equivalent to some multiple of half of a wavelength, so that the waves arrived out of phase with each other. Perhaps something similar is happening with the amplitudes.

To explain a dark band at position x on the detector, we must have

$$\langle x | I \rangle = \langle x | A \rangle \langle A | I \rangle + \langle x | B \rangle \langle B | I \rangle = 0 \quad (6.112)$$

We can simplify this relationship slightly by setting $\langle A | I \rangle$ and $\langle B | I \rangle$ equal to each other and writing them as $\langle slits | I \rangle$. This is not very contentious; if the source is placed midway between the slits, these amplitudes should be pretty much the same. So our relationship factors down to

$$\langle x | I \rangle = [\langle x | A \rangle + \langle x | B \rangle] \langle slits | I \rangle = 0 \quad (6.113)$$

Now there are two ways in which this can be true. Either $\langle slits | I \rangle = 0$, which isn't very interesting since then the electrons aren't even getting to the slits in the first place, or $\langle x | A \rangle + \langle x | B \rangle = 0$, which must be related to the interference.

Of course, both might be true, but that would mean that we've really set up a poor experiment.

If $\langle x | A \rangle + \langle x | B \rangle = 0$, then $\langle x | A \rangle = -\langle x | B \rangle$, which is rather reminiscent of our earlier discussion of two complex numbers with the same magnitude, but opposite phases (z and $-z$).

Now imagine that we had some way of changing the position of one slit in the screen without moving the second one. We could do this by having a very wide slit covered by some shutters. The shutters could then slide back and forth over the slit, opening up different parts of it. This would have the same effect as moving the slit.

This enables us to alter the length of one path compared to the other, so we could convert a point of destructive interference into one with constructive interference. To do this we would have moved the slit to alter the path by a distance equal to half of a wavelength. The question is, does this alter the phase of the amplitude, or the magnitude, or both?

Well, we can imagine moving the slit even further so that the path difference is $3\lambda/2$. This would be destructive interference, so the two amplitudes must have, once again, the same magnitude but opposite phases. It seems unlikely that simply increasing the path difference can make the *magnitude* go up and

down. However, we can imagine alterations to the path changing the *phase* of the amplitude - remember how the phase was defined.

If the structure of the amplitude is of the form $R \exp(i\theta)$ and θ is determined by the path length, then a steadily increasing path would increase the angle, taking us round and round a circle in the complex plane. Mathematicians don't limit angles to $\leq 360^\circ$ (or 2π radians). For example, an angle of 370° would be once round the circle and 10° more. Comparing two amplitudes of this type could quite easily move us from a situation where their phases are identical to out of phase and back again as the path length changed. If this is right, then the wavelength associated with the electron must, in some manner, be *coded into the phase*.

An Experiment with Phase

Let's give this idea a try. If we write the two amplitudes in the form

$$\langle x | A \rangle = R_1 \exp(i\theta_1(x, t)) \quad , \quad \langle x | B \rangle = R_2 \exp(i\theta_2(x, t)) \quad (6.114)$$

suggesting that the phase θ depends on position and time, we can then put them into the probability calculation and see what we get. We write (this is a piece of wild algebra - you can ignore it and jump to the result or if you are more mathematically inclined work through the algebra).

$$\begin{aligned} |\langle x | I \rangle|^2 &= |\langle x | A \rangle + \langle x | B \rangle|^2 |\langle slits | I \rangle|^2 \\ &= |R_1 \exp(i\theta_1(x, t)) + R_2 \exp(i\theta_2(x, t))|^2 |\langle slits | I \rangle|^2 \\ &= [R_1 \exp(i\theta_1(x, t)) + R_2 \exp(i\theta_2(x, t))]^* [R_1 \exp(i\theta_1(x, t)) + R_2 \exp(i\theta_2(x, t))] |\langle slits | I \rangle|^2 \\ &= [R_1 \exp(-i\theta_1(x, t)) + R_2 \exp(-i\theta_2(x, t))] [R_1 \exp(i\theta_1(x, t)) + R_2 \exp(i\theta_2(x, t))] |\langle slits | I \rangle|^2 \\ &= [R_1 (\cos(-\theta_1(x, t)) + i \sin(-\theta_1(x, t))) + R_2 (\cos(-\theta_2(x, t)) + i \sin(-\theta_2(x, t)))] \\ &\quad \times [R_1 (\cos(\theta_1(x, t)) + i \sin(\theta_1(x, t))) + R_2 (\cos(\theta_2(x, t)) + i \sin(\theta_2(x, t)))] |\langle slits | I \rangle|^2 \\ &= [R_1 (\cos(\theta_1(x, t)) - i \sin(\theta_1(x, t))) + R_2 (\cos(\theta_2(x, t)) - i \sin(\theta_2(x, t)))] \\ &\quad \times [R_1 (\cos(\theta_1(x, t)) + i \sin(\theta_1(x, t))) + R_2 (\cos(\theta_2(x, t)) + i \sin(\theta_2(x, t)))] |\langle slits | I \rangle|^2 \\ &= \left[\begin{aligned} &R_1^2 (\cos^2(\theta_1(x, t)) + \sin^2(\theta_1(x, t))) + R_2^2 (\cos^2(\theta_2(x, t)) + \sin^2(\theta_2(x, t))) \\ &+ 2R_1 R_2 (\cos(\theta_1(x, t)) \cos(\theta_2(x, t)) + \sin(\theta_1(x, t)) \sin(\theta_2(x, t))) \\ &+ iR_1 R_2 (\cos(\theta_1(x, t)) \sin(\theta_2(x, t)) + \sin(\theta_1(x, t)) \cos(\theta_2(x, t))) \\ &- iR_1 R_2 (\cos(\theta_1(x, t)) \sin(\theta_2(x, t)) + \sin(\theta_1(x, t)) \cos(\theta_2(x, t))) \end{aligned} \right] |\langle slits | I \rangle|^2 \\ &= [R_1^2 + R_2^2 + 2R_1 R_2 (\cos(\theta_1(x, t)) \cos(\theta_2(x, t)) + \sin(\theta_1(x, t)) \sin(\theta_2(x, t)))] |\langle slits | I \rangle|^2 \\ &= [R_1^2 + R_2^2 + 2R_1 R_2 (\cos(\theta_1(x, t) - \theta_2(x, t)))] |\langle slits | I \rangle|^2 \quad (6.115) \end{aligned}$$

The first two terms just give a uniform probability for an electron to arrive at the detector (this corresponds to the classical probability). If slit 2 (or B) was blocked off we would just have R_1^2 and if slit 1 (or A) was blocked off, the probability would be R_2^2 . It's the last term (with the cosine) that provides the

interference pattern of light and dark bands across the detector.

The Interference Term

Although the whole interference effect relies on the path difference between the two routes from slit to screen, the size of this path difference is not large enough to affect the intensity of electrons arriving at the screen from each slit. In a fully detailed mathematical analysis of the double-slit experiment, we would have to account for different path lengths having an impact on the magnitude of the amplitude as well as the phase. However, provided the two slits are close together, we don't need to worry about this and can say with confidence that $R_1 = R_2 = R$. Using this in our probability calculation, we get

$$|\langle x | I \rangle|^2 = 2R^2 [1 + (\cos(\theta_1(x, t) - \theta_2(x, t)))] |\langle slits | I \rangle|^2 \quad (6.116)$$

This will be zero (a dark band) when $(\cos(\theta_1(x, t) - \theta_2(x, t))) = -1$, i.e., when $\theta_1(x, t) - \theta_2(x, t) = \pi$.

The next dark band pops up when $\theta_1(x, t) - \theta_2(x, t) = 3\pi$ and another at 5π , etc.

So the interference term guarantees a series of dark bands at regular intervals across the electron detector. Thus, our theoretical formalism seems to work out as far as explaining this particular experiment.

We still need to figure out how the phase relates to physical quantities. That will come later.

6.2 Quantum Theory redux

Let us repeat our earlier discussion and summarize the ideas we have been discussing. This final pass is make sure that there are no points left that are not fully understood by all.

Although theories are most often developed as we saw in the last section, sometimes a theory is just guessed as a set of postulates. Let us take this latter approach now.

6.2.1 Quantum Mechanics Postulates (using color/hardness world)

There are **five parts**(**ASSUMPTIONS OR AXIOMS**) to the **Quantum Mechanics algorithm**.

(A) **Physical States**

All physical systems are represented by ket vectors normalized to 1.

They are called “**state vectors**” $\rightarrow |\psi\rangle$ where $\langle\psi|\psi\rangle = 1$.

This literally means ALL. A green or hard electron is represented by a vector. An atom is represented by a vector. A banana is represented by a vector. A car is represented by a vector. YOU are represented by a vector (albeit a very complex one).

(B) Measurable Properties

Measurable properties(dynamical variables) of physical systems are called “**observables**”.

Observables are represented by linear operators.

If the vector associated with a particular physical state $|\psi\rangle$ happens to be an eigenvector, with eigenvalue α , of an operator \hat{A} associated with some particular measurable property of the system, i.e., if

$$\hat{A}|\psi\rangle = \alpha|\psi\rangle \quad (6.117)$$

then the system in that state has the value α of that particular measurable property.

That is, if you were to perform a measurement corresponding to \hat{A} on a system in a state represented by $|\psi\rangle$, then with **certainty** (probability = 1) you would measure the value α .

Since the eigenvalues of operators representing observables are supposed to be measurable numbers, they must also always be **real**.

This means that we can only choose a certain kind of operator to represent observables, namely, HERMITIAN, which is guaranteed to always have real eigenvalues.

This requirement produces an added bonus for quantum theory.

It turns out that the eigenvectors of any HERMITIAN operator always comprise a **complete, orthonormal set**.

This means that they always comprise a set of **mutually orthonormal vectors** that can be used as a **basis** (number is dimension of space).

It also turns out that **any** HERMITIAN operator will represent a possible observable of the physical system.

Turning this statement around, we can say that the **eigenvectors of any observable can be used as the basis vectors** for our space.

This feature will have an important connection to measurement.

6.2.1.1 Example: back to color and hardness.....

Since the operators \hat{H} and \hat{C} that represent the observables **hardness** and **color** must be Hermitian, we can use either set of corresponding eigenvectors as a basis set for the quantum theory of color and hardness.

One such basis is then

$$|hard\rangle = |h\rangle \quad , \quad |soft\rangle = |s\rangle \quad (6.118)$$

where (by definition)

$$\begin{aligned} \hat{H}|h\rangle &= |h\rangle \rightarrow \text{eigenvalue} = 1 \quad (\text{by convention}) \\ \hat{H}|s\rangle &= -|s\rangle \rightarrow \text{eigenvalue} = -1 \quad (\text{by convention}) \end{aligned} \quad (6.119)$$

or, in words, $|h\rangle$ is a state with a measured value of hardness = 1 and $|s\rangle$ is a state with a measured value of hardness = -1.

Since these states form a basis (orthonormal set) they satisfy

$$\begin{aligned} \langle h | h \rangle &= 1 = \langle s | s \rangle \\ \langle h | s \rangle &= 0 = \langle s | h \rangle \end{aligned} \quad (6.120)$$

The operator \hat{H} clearly represents the entire hardness box.

Since, as we showed earlier, any operator can be written in terms of its eigenvalues and projection operators we have

$$\hat{H} = (+1)|h\rangle\langle h| + (-1)|s\rangle\langle s| = |h\rangle\langle h| - |s\rangle\langle s| \quad (6.121)$$

so that

$$\begin{aligned} \hat{H}|h\rangle &= (|h\rangle\langle h| - |s\rangle\langle s|)|h\rangle = |h\rangle\langle h|h\rangle - |s\rangle\langle s|h\rangle = |h\rangle(1) - |s\rangle(0) = |h\rangle \\ \hat{H}|s\rangle &= (|h\rangle\langle h| - |s\rangle\langle s|)|s\rangle = |h\rangle\langle h|s\rangle - |s\rangle\langle s|s\rangle = |h\rangle(0) - |s\rangle(1) = -|s\rangle \end{aligned} \quad (6.122)$$

as expected.

The eigenvector/eigenvalue equations above just say that a hardness box (hardness operator acting on a state vector) does not change $|h\rangle$ and $|s\rangle$ states (we will see shortly that an overall minus sign does not change any measurable properties of the $|s\rangle$ state) as required.

We can write the matrices representing these objects in the hardness basis (called a **matrix representation**)

$$\begin{aligned} |h\rangle &= \begin{pmatrix} \langle h|h\rangle \\ \langle s|h\rangle \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |s\rangle = \begin{pmatrix} \langle h|s\rangle \\ \langle s|s\rangle \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ [H] &= \begin{pmatrix} \langle h|\hat{H}|h\rangle & \langle h|\hat{H}|s\rangle \\ \langle s|\hat{H}|h\rangle & \langle s|\hat{H}|s\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{aligned} \quad (6.123)$$

where we have used $\langle h|\hat{H}|s\rangle = \langle h|(-1)|s\rangle = -\langle h|s\rangle = 0$, etc.

Remember that in terms of matrices, Hermitian means the following: If

$$[A] = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \quad (6.124)$$

then

$$[A^+] = \begin{pmatrix} a_{11}^* & a_{21}^* \\ a_{12}^* & a_{22}^* \end{pmatrix} \quad (6.125)$$

is the Hermitian conjugate matrix and it is the same matrix, i.e., $[A] = [A^+]$.

Similarly, another such basis(equivalent) is then

$$|magenta\rangle = |m\rangle, \quad |green\rangle = |g\rangle \quad (6.126)$$

where (by definition)

$$\begin{aligned} \hat{C}|g\rangle &= |g\rangle \rightarrow \text{eigenvalue} = 1 \quad (\text{by convention}) \\ \hat{C}|m\rangle &= -|m\rangle \rightarrow \text{eigenvalue} = -1 \quad (\text{by convention}) \end{aligned} \quad (6.127)$$

or, in words, $|g\rangle$ is a state with a measured value of color = 1 and $|m\rangle$ is a state with a measured value of color = -1. The operator \hat{C} represents the entire color box. Since any operator can be written in terms of its eigenvalues and projection operators we have

$$\hat{C} = |g\rangle\langle g| - |m\rangle\langle m| \quad (6.128)$$

Since these states form a basis (orthonormal set) they satisfy

$$\begin{aligned} \langle g|g\rangle &= 1 = \langle m|m\rangle \\ \langle g|m\rangle &= 0 = \langle m|g\rangle \end{aligned} \quad (6.129)$$

The eigenvector/eigenvalue equations above just say that a color box does not change $|g\rangle$ and $|m\rangle$ states (again, we will see shortly that an overall minus sign does not change any measurable properties of the $|m\rangle$ state.

We can write the matrices representing these objects in the color basis (called a matrix representation)

$$\begin{aligned} |g\rangle &= \begin{pmatrix} \langle g|g\rangle \\ \langle g|m\rangle \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad |m\rangle = \begin{pmatrix} \langle m|g\rangle \\ \langle m|m\rangle \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ [C] &= \begin{pmatrix} \langle g|\hat{C}|g\rangle & \langle g|\hat{C}|m\rangle \\ \langle m|\hat{C}|g\rangle & \langle m|\hat{C}|m\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{aligned} \quad (6.130)$$

where we have used $\langle g|\hat{C}|m\rangle = -\langle g|m\rangle = 0$, etc.

Let us now write the $|g\rangle$ and $|m\rangle$ vectors in terms of the $|h\rangle$ and $|s\rangle$ vectors. This is always possible since $|h\rangle, |s\rangle$ is a basis and $|g\rangle, |m\rangle$ are just some other vectors in the same space(in the world).

This is just the principle of SUPERPOSITION, that we mentioned earlier, in action. We write

$$\begin{aligned} |g\rangle &= a|h\rangle + b|s\rangle \\ |m\rangle &= c|h\rangle + d|s\rangle \end{aligned} \quad (6.131)$$

Normalization: the states must be normalized to 1 (we assume a, b, c, d are real numbers) so that

$$\begin{aligned} \langle g|g\rangle &= 1 = (a\langle h| + b\langle s|)(a|h\rangle + b|s\rangle) = a^2 + b^2 \\ \langle m|m\rangle &= 1 = (c\langle h| + d\langle s|)(c|h\rangle + d|s\rangle) = c^2 + d^2 \end{aligned} \quad (6.132)$$

Orthogonality: the states must be orthogonal (eigenvectors of a Hermitian operator) so that

$$\langle g|m\rangle = 0 = (a\langle h| + b\langle s|)(c|h\rangle + d|s\rangle) = ac + bd \quad (6.133)$$

One possible solution to these equations (which as we will see later represents the color states) is

$$a = b = c = -d = \frac{1}{\sqrt{2}} \quad (6.134)$$

so that we obtain

$$|g\rangle = \frac{1}{\sqrt{2}}|h\rangle + \frac{1}{\sqrt{2}}|s\rangle \quad , \quad |m\rangle = \frac{1}{\sqrt{2}}|h\rangle - \frac{1}{\sqrt{2}}|s\rangle \quad (6.135)$$

Similarly, we can express the $|h\rangle$ and $|s\rangle$ vectors in terms of the $|g\rangle$ and $|m\rangle$ vectors as a basis. We obtain

$$|h\rangle = \frac{1}{\sqrt{2}}|g\rangle + \frac{1}{\sqrt{2}}|m\rangle \quad , \quad |s\rangle = \frac{1}{\sqrt{2}}|g\rangle - \frac{1}{\sqrt{2}}|m\rangle \quad (6.136)$$

So, sums and differences of vectors represent superpositions of physical states.

**States of definite color are superpositions
of different hardness states.**

**States of definite hardness are superpositions
of different color states.**

The hardness and color operators are incompatible observables in the sense that states of definite hardness (eigenvectors of the hardness operator) apparently have no definite color value (since they are not eigenvectors of the color operator) and vice versa. This means that color and hardness are incompatible and that their representative operators do not commute. We can see that by determining the matrix for \hat{H} in the color basis and then computing the commutator. We have

$$[H] = \begin{pmatrix} \langle g | \hat{H} | g \rangle & \langle g | \hat{H} | m \rangle \\ \langle m | \hat{H} | g \rangle & \langle m | \hat{H} | m \rangle \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (6.137)$$

where we have used

$$\begin{aligned} \langle g | \hat{H} | m \rangle &= \left(\frac{1}{\sqrt{2}} \langle h | + \frac{1}{\sqrt{2}} \langle s | \right) \hat{H} \left(\frac{1}{\sqrt{2}} | h \rangle - \frac{1}{\sqrt{2}} | s \rangle \right) \\ &= \frac{1}{2} (\langle h | \hat{H} | h \rangle - \langle h | \hat{H} | s \rangle + \langle s | \hat{H} | h \rangle - \langle s | \hat{H} | s \rangle) \\ &= \frac{1}{2} (\langle h | h \rangle + \langle h | s \rangle + \langle s | h \rangle + \langle s | s \rangle) = \frac{1}{2} (1 + 0 + 0 + 1) = 1 \end{aligned} \quad (6.138)$$

and so on. We then have

$$\begin{aligned} [\hat{C}, \hat{H}] &= \hat{C}\hat{H} - \hat{H}\hat{C} \\ &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ &= 2 \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \neq 0 \end{aligned} \quad (6.139)$$

So it looks like it will be possible to work out the descriptions of color and hardness and of all the relations between them within the framework of a these 2-dimensional vector space ideas.

The final part of this postulate is

**if the system is in any arbitrary state $|\psi\rangle$
and we measure the observable \hat{B} (where $|\psi\rangle$
is NOT an eigenstate of \hat{B} , then the ONLY
possible results are the eigenvalues of \hat{B}
that is, the set $\{b_k\}$**

Read that statement again!. It is a truly amazing statement.

(C) Dynamics

There is a dynamics of state vectors.

There are “**deterministic**” laws (you know the kind of laws where if you know everything at the start, then you can predict everything that will happen in the future exactly) about how a state vector of any given system changes with time.

Since every state vector representing a real physical system must have length = 1, the changes of the state vectors dictated by the dynamical laws (called the **Schrodinger equation or time-development equation**) are exclusively changes of direction (and never of length).

We define the “**time evolution or development**” operator that governs how a state vector changes in time by the relationship

$$|A, t + \Delta t\rangle = \hat{U}(\Delta t) |A, t\rangle \quad (6.140)$$

or, in words,

**the state vector at time = $t + \Delta t$ is given by
the time evolution operator \hat{U} operating on
the state vector at time = t**

Note how the things inside the vector symbol change when I have to indicate that there is new information known about the state (the “**when**” in this case).

**In general, that is the only thing that changes.... the labels
.... which contain whatever we know (have measured) about the
state.**

The time evolution operator is also a **linear** operator. It is a unitary operator \hat{U} , which means that

**if $\hat{U}\hat{U}^{-1} = \hat{I}$ or \hat{U}^{-1} is the inverse of \hat{U}
then the Hermitian conjugate $\hat{U}^+ = \hat{U}^{-1}$**

As we said earlier, the time evolution operator is related to the energy operator. More later.

(D) **The Connection with Experiment** So far, none of our assumptions have touched upon the results of measurements.

All we have said so far, in this arena, is that the particular physical state whose state vector is an eigenvector, with eigenvalue α , of the operator associated with some particular measurable property will “**have**” the value

α for that property and that a measurement of that property, carried out on a system which happens to be in that state, will produce the result α with certainty(probability = 1) and that if we are not in an eigenvector of the observable being measured, then we can only measure one of its eigenvalues.

But we will need much more than that to deal with experiments.

What if we measure a certain property of a physical system at the moment when the state vector of the system does not happen to be an eigenvector of that property operator? (this will, in fact, be the case most of the time).

What if we measure the color of a hard electron(which is an electron in a superposition of being green and being magenta)?

What happens then?

All of our earlier assumptions are no help here.

We need a **new assumption**.

Suppose we have a system in some state $|\psi\rangle$, and we carry out a measurement of the value of a property (observable) associated with the operator \hat{B} .

We assume that the eigenvectors of \hat{B} are the states $|b_i\rangle$ which means that

$$\hat{B} |b_i\rangle = b_i |b_i\rangle \quad , \quad i = 1, 2, 3, 4, \dots \quad (6.141)$$

where the b_i are the corresponding eigenvalues.

Quantum theory then says, as we have seen, that the outcome of any such a measurement is strictly a matter of “**probability**”.

In particular, quantum theory stipulates that the **probability that the outcome** of the measurement of \hat{B} on state $|\psi\rangle$ (not an eigenvector) will yield the result b_i (remember the only possible results are the eigenvalues of \hat{B} , no matter what state we are in), is **equal** to

$$|\langle b_i | \psi \rangle|^2 \quad (6.142)$$

or the absolute-square of the corresponding component!

This postulate means the following:

- (a) The probability as so defined is always ≤ 1 as it must be, which results from the requirement that all allowable states be of length = 1

(normalized to 1). This is the reason for the normalization requirement.

- (b) If $|\psi\rangle = |b_i\rangle$ (the state we are in corresponds to an eigenvector), then the probability that we will measure b_i is

$$\text{probability} = |\langle b_i | b_i \rangle|^2 = 1 \quad (6.143)$$

and the probability that we will measure any other eigenvalue b_k , $k \neq i$ is

$$\text{probability} = |\langle b_k | b_i \rangle|^2 = 0 \quad , \quad k \neq i \quad (6.144)$$

due to orthonormality.

This is just the special case when the state we are measuring is an eigenvector of the observable being measured and corresponds to Postulate #2. Postulate #4 agrees with Postulate #2 as it must.

- (c) The probability that a green electron will be found during a hardness measurement to soft is 1/2 (this must be true to explain earlier experimental results). This follows as shown below. the state being measured is

$$|g\rangle = \frac{1}{\sqrt{2}} |h\rangle + \frac{1}{\sqrt{2}} |s\rangle \quad (6.145)$$

and the probability to be soft, i.e., the $\text{prob}(\text{soft}|\text{green})$ is given by

$$\begin{aligned} \text{prob}(\text{soft}|\text{green}) &= |\langle s | g \rangle|^2 = \left| \langle s | \left(\frac{1}{\sqrt{2}} |h\rangle + \frac{1}{\sqrt{2}} |s\rangle \right) \right|^2 \\ &= \left| \frac{1}{\sqrt{2}} (\langle s | h \rangle + \langle s | s \rangle) \right|^2 = \left| \frac{1}{\sqrt{2}} (0 + 1) \right|^2 = \frac{1}{2} \end{aligned} \quad (6.146)$$

That is why we chose the particular superposition earlier.

- (d) Similarly, the probability that a green electron will be found during a hardness measurement to be hard is 1/2.

The probability that a hard electron will be found during a color measurement to be green is 1/2.

The probability that a hard electron will be found during a color measurement to be magenta is 1/2.

and so on.

The new formalism correctly predicts the required (experimental) results for hardness and color measurements.

Does that make sense?

It is important to realize that we cannot say anything definite about the color if we are in a hardness state and vice versa. We can only make probability statements. Before we measure the color of the electron, the electron does not have a color, according to quantum theory! Our information about the electron color is only a set of probabilities. But all of your experience says that objects have values for measured quantities before they are measured, i.e., your experience tells you that the electron has a color even if we do not measure it.

That is your view (the standard classical view) about what is real and what is not real.

Quantum theory says that you are wrong in both cases!! If you believe otherwise, then all quantum effects would not work...but they do!!!

We will eventually devise experiments to show that quantum theory is correct and your classical views about reality are incorrect!!

We must also devise a theory to show why it seems this way for electrons but does not **seem** to be true for macroscopic objects.

These first 4 postulates are not even the controversial ones!!!

Finally, we state the last, and as we shall see the most controversial postulate.

(E) Collapse

Measurements are always repeatable. This seems like a very innocuous statement!

Once a measurement is carried out and a result obtained for some observable, the state of the system must be such as to guarantee (with probability = 1) that if the same measurement is repeated, the exact same result will be obtained. Since systems evolve in time, this is literally only true if the second measurement follows the first instantaneously or, at least, within such a small time that the system in question does not have a chance to evolve.

What does this mean about the state vector of the measured (after measurement) system?

One view is that something must happen to the state vector when the

measurement occurs.

If a measurement of an observable \hat{O} is carried out on a system S , and if the outcome of the measurement is the value o_q (one of the many possible measured values of the operator \hat{O} one of its eigenvalues) then, whatever the state vector of S was before the measurement of \hat{O} , the only way to guarantee (with probability = 1) that another measurement of \hat{O} will give the same result is that the state vector of S after the measurement must necessarily be the eigenvector of \hat{O} with eigenvalue o_q . **This must be so according to Postulate #2.**

Thus, in this view, the effect of measuring an observable must necessarily be to **“change”** the state vector of the measured system, to **COLLAPSE** it, to make it **“jump”** from whatever it may have been prior to the measurement into some eigenvector of the measured observable operator.

This is called

collapse of state vector or reduction of state vector

It says that the state vector changes(discontinuously) during a measurement from representing a range of possibilities (a superposition of all possible states) to a definite state or only one possible outcome.

Which particular eigenvector it gets changed into is determined by the outcome of the measurement and it cannot be known until then!!!!!!. It cannot be predicted!!!!

Since that outcome, according to our earlier assumption, is a matter of probability, it is at this point and at no other point in the discussion, that an element of **“pure chance”** enters into the time evolution of the state vector and **determinism goes out the window**.

Our postulates thus assume that the time evolution of a system is continuous and deterministic between measurements, and discontinuous and probabilistic(random) during measurements.

It is clear why this postulate is controversial. It will dominate some of our later discussions.

Those are the principles(postulates) of quantum theory. They are the most precise mechanism for predicting the outcomes of experiments on physical systems ever devised.

No exceptions to them have ever been discovered. **NOBODY** expects any.

We will now spend some time making these principles into operational tools that we can use to carry out quantum theory and make predictions.

We will see, in detail, how quantum theory makes predictions and how the strange results of various experiments are easily accounted for by the theory.

We are about to enter a very strange world where quantum systems behave in rather mysterious and non-intuitive ways.

Remember, however, that any behavior we predict and observe will just be a consequence of the 5 postulates we have just stated.

That is how theoretical physics works!

6.3 Quantum Theory - How it works.....Some Details

Suppose that we want to predict the behavior of a physical system using the QM algorithm. How, exactly, do we go about it?

6.3.1 General Approach

1. Identify the vector space associated with that system—this is the space where all possible physical states of the system can be represented – this simply means that we must find a **suitable basis** set of vectors.
2. Identify the operators associated with various measurable properties of the system — this means calculate **eigenvectors and eigenvalues** of appropriate observables.
3. Map out the specific correspondences between individual physical states and individual vectors – this means to decide how to label the state vectors (or **what goes inside the ket**).
4. Ascertain the present state vector of the system by means of measurements — this means to determine what are its **initial labels**. This is called **state preparation**.
5. The **time evolution** of the systems is then determined by the time evolution operator \hat{U} — this is a **deterministic** equation until the next measurement. \hat{U} must be specified for each system.
6. The **probabilities of particular outcomes** of a measurement carried out at a future time can then be calculated by using Postulate #4 which says that the probability of measuring the eigenvalue b of the observable \hat{B} at time t when we are in the state $|\psi\rangle$ at time t is given by $|\langle b|\psi\rangle|^2$.

7. The **effects of measurement** are taken into account using Postulate #5
– this implies that the state **collapses** to an appropriate (determined by value measured) eigenvector of measured observable.
8. Then [5]-[7] are just **repeated** over and over again.....

Remember:

Postulate #5 says that the state vector is “**collapsed**” into an eigenvector of the measured observable operator.

Postulate #3 tells us how a state evolves in time.

This is the standard or **Copenhagen interpretation** of quantum theory due to Bohr, Dirac, Born and von Neumann.

I can now state the standard way of talking, which students of physics are traditionally required to master, about what superpositions are.

The way to deal with the apparent contradictions we saw in our earlier discussion of color and hardness measurements boils down to this explanation

The right way to think about superpositions of, say, being green and being magenta is to think of them as situations where **color predictions** cannot be made, situations where **color talk** is unintelligible.

Talking and inquiring about the color of an electron in such circumstances (in the standard view) makes no sense whatsoever.

As long as you follow this rule all of our earlier contradictions go away.

In this view, it just is not so that hard electrons are not green and not magenta and not both and not neither, since color talk of any kind, about hard electrons, simply has no meaning at all and the same is true for all other incompatible observables.

That is the way it is that is the way the world works according to the quantum physicist!

Of course, once an electron has been “**measured**” to be green or magenta, then it “**is**” green or magenta (**color talk now applies**) according to this standard interpretation.

Measuring the color of a hard electron, then, is **not a matter of determining** what the color of that hard electron is ... **it has none - it only has probabilities to have color values if we measure color.**

Rather, it is a matter of “**collapsing**” the state of the measured electron into one where color talk applies, and “**then**” determining the color of the newly created, color-applicable state.

Measurements in QM (and particularly within the standard view) are very **active processes**.

They are not processes of **merely learning** something about the system they are invariably processes which **drastically change** the measured system.

The most important rule that we can state is as follows:

If you are going to measure some observable \hat{C} , then choose as your basis vectors the eigenvectors of the \hat{C} operator since it is only with these states that \hat{C} -talk makes any sense, i.e., if you are discussing color measurements than use the color basis where color-talk makes sense! The same holds true if you are going to measure anything else!

6.3.1.1 Some Consequences

We are allowed to use **any orthonormal set** (provided their number = dimension of the space) as a basis. If such other sets exist, then they must be eigenvectors of some other observables (not color). For examples here are two other orthonormal sets.....

$$\begin{aligned} \text{Set \#1} \\ |1\rangle = \frac{1}{2}|g\rangle + \frac{\sqrt{3}}{2}|m\rangle \text{ and } |2\rangle = \frac{\sqrt{3}}{2}|g\rangle - \frac{1}{2}|m\rangle \end{aligned} \quad (6.147)$$

$$\begin{aligned} \text{Set \#2} \\ |1\rangle = \frac{1}{2}|g\rangle - \frac{\sqrt{3}}{2}|m\rangle \text{ and } |2\rangle = \frac{\sqrt{3}}{2}|g\rangle + \frac{1}{2}|m\rangle \end{aligned}$$

Either set can be used as a basis(they both are orthonormal pairs). Prove that for yourself.

Since all basis sets correspond to some operator, let us choose to call their associated observables **direction** \hat{d} and **truth** \hat{t} , where set #1 are eigenstates of direction operator \hat{d} with associated eigenvalues +1(up) and -1(down) and set #2 are eigenstates of truth operator \hat{t} with associated eigenvalues +1(true) and -1(false). Thus, we can write

$$\begin{aligned} \text{Set \#1} \\ |1\rangle = |\text{direction} = +1\rangle = |\text{up}\rangle = \frac{1}{2}|g\rangle + \frac{\sqrt{3}}{2}|m\rangle \\ |2\rangle = |\text{direction} = -1\rangle = |\text{down}\rangle = \frac{\sqrt{3}}{2}|g\rangle - \frac{1}{2}|m\rangle \\ \text{Set \#2} \\ |1\rangle = |\text{truth} = +1\rangle = |\text{true}\rangle = \frac{1}{2}|g\rangle - \frac{\sqrt{3}}{2}|m\rangle \\ |2\rangle = |\text{truth} = -1\rangle = |\text{false}\rangle = \frac{\sqrt{3}}{2}|g\rangle + \frac{1}{2}|m\rangle \end{aligned} \quad (6.148)$$

Remember we already had the other basis sets:

$$\begin{aligned} |color = +1\rangle &= |g\rangle = \frac{1}{\sqrt{2}} |h\rangle + \frac{1}{\sqrt{2}} |s\rangle \\ |color = -1\rangle &= |m\rangle = \frac{1}{\sqrt{2}} |h\rangle - \frac{1}{\sqrt{2}} |s\rangle \end{aligned} \quad (6.149)$$

$$\begin{aligned} |hardness = +1\rangle &= |h\rangle = \frac{1}{\sqrt{2}} |g\rangle + \frac{1}{\sqrt{2}} |m\rangle \\ |hardness = -1\rangle &= |s\rangle = \frac{1}{\sqrt{2}} |g\rangle - \frac{1}{\sqrt{2}} |m\rangle \end{aligned} \quad (6.150)$$

Now think of these states as representing a real physical system and think about probabilities. We can make these statements (based on our rules):

1. probability that an electron that is “up” will be measured to be “magenta” = 3/4
2. probability that an electron that is “false” will be measured to be “magenta” = 1/4
3. probability that an electron that is “soft” will be measured to be “magenta” = 1/2
4. probability that an electron that is “green” will be measured to be “hard” = 1/2

and so on.

Let us now look at some details and some examples, that is, let us apply all of this stuff and expand our knowledge and capabilities as we proceed.

We begin with an example that includes only familiar classical properties like position, velocity, momentum, energy, etc, then return to explain the color-hardness experiments and finally in the later sections of the book we investigate photon polarization experiments, electron interference experiments and Stern-Gerlach electron spin experiments.

We know from hundreds of years of experience, that the behavior of relatively big particles, with large masses (like rocks and shampoo bottles) is very well described by the classical mechanics of Newton. This says something about the quantum theory of particles, i.e., whatever the theory ends up saying about microworld particles it ought to predict that everyday particles, subject to everyday circumstances, will behave in the everyday, Newtonian way we all know and love.

Now the **position** operator \hat{x} and the **momentum** operator \hat{p} are incompatible (i.e., they are not simultaneously measurable - this is the famous Heisenberg uncertainty principle as we will show later). This means that

$$[\hat{x}, \hat{p}] \neq 0 \quad (6.151)$$

In fact, the value is known to be

$$[\hat{x}, \hat{p}] = i\hbar \quad (6.152)$$

where

$$\hbar = \frac{h}{2\pi} = 1.05 \times 10^{-34} \text{ Joule} - \text{sec} , \quad h = \text{Planck's constant} \quad (6.153)$$

Note the appearance of the factor i where $i^2 = -1$.

Since \hat{x} is an operator representing a physical observable, a possible basis of the space is the set of eigenvectors of the \hat{x} operator.

Similarly, for the eigenvectors of the \hat{p} operator.

They each form a possible basis because they are observables represented by Hermitian operators.

Because their corresponding operators do not commute, a state of definite momentum (an eigenvector of \hat{p}) will be a superposition of states of definite position (eigenvectors of \hat{x}) or, in other words, a state of definite momentum can only have probabilities of having definite x -values. Similarly, a state of definite position (an eigenvector of \hat{x}) will be a superposition of states of definite momentum (eigenvectors of \hat{p}).

The vector space when the \hat{x} eigenvectors are the basis is called the *coordinate representation*.

The vector space when the \hat{p} eigenvectors are the basis is called the *momentum representation*.

Now, the most important operator in quantum mechanics is the energy operator or **Hamiltonian** \hat{H} . It will determine the time evolution operator as we will see later.

The vector space when the \hat{H} eigenvectors are the basis is called the *energy representation*.

All are **equivalent** basis sets.

Our choice will depend on the questions we are asking or the measurements we are carrying out.

That choice is called **going to the HOME SPACE**.

Now the possible eigenvalues (allowed measured values) of \hat{x} and \hat{p} form a continuum extending from $-\infty \rightarrow \infty$ (called a continuous spectrum). The basis is

infinite(non-denumerable) dimensional. In general, this presents many difficult mathematical problems. For the systems we will be discussing, the infinite dimension causes no difficulties and so we can treat all properties as if the space had a finite dimension. The one exception will be normalization as we will discuss later.

The state $|x\rangle$ corresponds to a system with a definite value of the position, namely, x . It is an eigenvector of the \hat{x} operator. The state $|p\rangle$ corresponds to a system with a definite value of the momentum, namely, p . It is an eigenvector of the \hat{p} operator. The state $|E\rangle$ corresponds to a system with a definite value of the energy, namely, E . It is an eigenvector of the \hat{H} operator.

In general, the set of energy eigenvalues are both a **discrete** set over some range and a **continuous** set over a disjoint range. The operators position \hat{x} and \hat{C} are compatible and, therefore, we can simultaneously measure these observables.

This means that we can say that a magenta electron is located at $x = 7$ and it makes sense to do so.

We write the state representing this case in the form

$$|color - value\rangle |x - value\rangle \quad (6.154)$$

i.e., $|m\rangle|7\rangle$ for a magenta electron located at $x = 7$. (the formal name for this product is a **tensor-product**). When operators act on such states their operation takes the form

$$\begin{aligned} \hat{C}|m\rangle|7\rangle &= -|m\rangle|7\rangle \text{ i.e., } \hat{C} \text{ only acts on the color space part} \\ \hat{x}|m\rangle|7\rangle &= 7|m\rangle|7\rangle \text{ i.e., } \hat{x} \text{ only acts on the position space part} \end{aligned} \quad (6.155)$$

Similarly statements can be made for position and hardness, momentum and color, momentum and hardness, energy and color, and energy and hardness. They all represent simultaneously measurable pairs.

As we said, the operator corresponding to the observable energy is called the Hamiltonian \hat{H} where

$$\hat{H}|E\rangle = E|E\rangle \quad (6.156)$$

As I mentioned, the energy basis is the most fundamental one in quantum theory. We will see why shortly.

The quantity

$$\psi_E(x) = \langle x | E \rangle \quad (6.157)$$

for some state vector $|E\rangle$, is called the energy **wave function**, that is, since it takes on different values for each value of x , it is a function of x .

It satisfies a famous equation that governs its time and space dependence - the

Schrodinger equation. The Schrodinger equation in 1-dimension is an “ordinary differential equation” given by

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_E(x,t)}{dx^2} + V(x)\psi_E(x,t) = E\psi_E(x,t) = i\hbar \frac{d\psi_E(x,t)}{dt} \quad (6.158)$$

where $V(x)$ is the potential energy of the system. We will not need to solve this equation in this book, but we show how it arises later in the book.

The time evolution operator for simple systems is expressed in terms of the Hamiltonian operator \hat{H} by the relation $\hat{U} = e^{-i\hat{H}t/\hbar}$, which is an operator function of \hat{H} . We will derive this result later.

As shown in earlier in these notes, in simple cases, functions of operators are easy to deal with. If

$$\hat{B}|b\rangle = b|b\rangle \quad (6.159)$$

i.e., $|b\rangle$ is an eigenstate of \hat{B} , then we have

$$f(\hat{B})|b\rangle = f(b)|b\rangle \quad (6.160)$$

for a function of the operator.

This implies that the energy eigenvectors have a very simple time dependence or time evolution, i.e.,

$$|E, t\rangle = \hat{T}|E, 0\rangle = e^{-i\hat{H}t/\hbar}|E, 0\rangle = e^{-iEt/\hbar}|E, 0\rangle \quad (6.161)$$

where the complex exponential form means

$$e^{-iEt/\hbar} = \cos \frac{E}{\hbar}t - i \sin \frac{E}{\hbar}t \quad (6.162)$$

as we showed earlier.

Using the eigenvectors and eigenvalues of the Hamiltonian, namely,

$$\hat{H}|E_n\rangle = E_n|E_n\rangle \quad (6.163)$$

as a basis we can work out the time dependence of an arbitrary state vector. It goes as follow. We have

$$\begin{aligned} |\psi(0)\rangle &= \sum_n c_n |E_n\rangle \quad \text{expand in energy basis} \\ |\psi(t)\rangle &= e^{-i\hat{H}t/\hbar} |\psi(0)\rangle = e^{-i\hat{H}t/\hbar} \sum_n c_n |E_n\rangle \quad \text{operate with evolution operator} \\ |\psi(t)\rangle &= \sum_n c_n e^{-i\hat{H}t/\hbar} |E_n\rangle = \sum_n c_n e^{-iE_n t/\hbar} |E_n\rangle \quad \text{eigenvectors/eigenvalues} \\ |\psi(t)\rangle &= \hat{U}(t) |\psi(0)\rangle = \hat{U}(t) \sum_n c_n |E_n\rangle = \sum_n c_n \hat{U}(t) |E_n\rangle = \sum_n c_n e^{-iE_n t/\hbar} |E_n\rangle \end{aligned} \quad (6.164)$$

Let us now explore the coordinate-space. Since we have continuous eigenvalues we must replace sums by integrals (simply continuous sums for our purposes here).

In the discrete spectrum case, we have, using a basis set $\{|n\rangle\}$, that

$$\begin{aligned} |\psi\rangle &= \sum_n c_n |n\rangle \quad , \quad c_m = \langle m | \psi \rangle \\ |\psi\rangle &= \sum_n \langle n | \psi \rangle |n\rangle = \sum_n |n\rangle \langle n | \psi \rangle = \left(\sum_n |n\rangle \langle n| \right) |\psi\rangle \\ &\rightarrow \sum_n |n\rangle \langle n| = \hat{I} = \text{identity operator} \end{aligned} \quad (6.165)$$

and if

$$\hat{A} |a_n\rangle = a_n |a_n\rangle \quad , \quad |\psi\rangle = \sum_n c_n |a_n\rangle \quad (6.166)$$

then

$$\begin{aligned} \hat{A} |\psi\rangle &= \sum_n c_n \hat{A} |a_n\rangle = \sum_n c_n a_n |a_n\rangle = \sum_{n,m} c_n a_m |a_m\rangle \delta_{nm} \\ &= \sum_{n,m} c_n a_m |a_m\rangle \langle a_m | a_n \rangle = \sum_n c_n \left(\sum_m a_m |a_m\rangle \langle a_m| \right) |a_n\rangle \end{aligned}$$

so that

$$\hat{A} = \sum_m a_m |a_m\rangle \langle a_m| \quad (6.167)$$

which is the *spectral representation* of the operator \hat{A} in terms of its eigenvalues and eigenvectors.

Some of the changed relations (we will derive these later) look like

$$\hat{I} = \int_{-\infty}^{\infty} |x\rangle \langle x| dx \quad \text{instead of} \quad \hat{I} = \sum_n |n\rangle \langle n| \quad (6.168)$$

where, for our purposes, the \int symbol just means a sum over a continuous variable (more later) and

$$\int_{-\infty}^{\infty} g(x') \langle x | x' \rangle dx' = g(x) \quad \text{instead of} \quad \sum_n a_m \langle m | n \rangle = a_n \quad (6.169)$$

These relations imply a trick normalization for these states

$$\langle x | x' \rangle = \delta(x - x') \quad (6.170)$$

(called the Dirac delta function) where we have the defining property

$$\int f(x') \delta(x - x') dx' \equiv f(x) \quad (6.171)$$

Any arbitrary state can be written in terms of the basis states,

$$|\psi\rangle = \hat{I}|\psi\rangle = \left(\int_{-\infty}^{\infty} |x\rangle \langle x| dx \right) |\psi\rangle = \int_{-\infty}^{\infty} \langle x | \psi \rangle |x\rangle dx = \int_{-\infty}^{\infty} \psi(x) |x\rangle dx \quad (6.172)$$

The probability (from Postulate #4) that we will find the system (particle) at $x = q$ is given by

$$\begin{aligned} \text{prob}(x = q|\psi) &= P(q) = |\langle q | \psi \rangle|^2 = \left| \langle q | \left(\int_{-\infty}^{\infty} \psi(x) |x\rangle dx \right) \right|^2 \\ &= \left| \left(\int_{-\infty}^{\infty} \psi(x) \langle q | x \rangle dx \right) \right|^2 = |\psi(q)|^2 = |\langle q | \psi \rangle|^2 \end{aligned}$$

or in general we say that

$$P(x) = |\langle x | \psi \rangle|^2 = |\psi(x)|^2 \quad (6.173)$$

or the probabilities are given by the wave functions which will be solutions of the Schrodinger equation (these are actually probability densities).

Now we are beginning to get somewhere!

The next derivation is more mathematical, but it is very important. You now have the needed tools so work your way through it.

The general procedure for figuring out the time dependence of a states and then answering the questions posed in experiments goes as follows (**this is tricky algebra but well worth spending time on**):

1. Ask the question — it usually takes the form — if we are in the state $|\phi\rangle$ at the time $t = 0$, then what is the probability of being in the state $|b_7\rangle$ at time $= t$?
2. Assume that $|b_7\rangle$ is one of the eigenvectors of the operator \hat{B} .
3. We solve for the energy eigenvectors of the system, i.e. we find the Hamiltonian (energy operator) and do the mathematics.
4. We write $|\phi\rangle$ in terms of the energy eigenvector basis

$$|\phi\rangle = \sum_E c_E |E\rangle \quad \text{where } c_{E'} = \langle E' | \phi \rangle \quad (6.174)$$

5. Since the time dependence of the energy eigenstates is easy we can write down the time dependence of the state $|\phi\rangle$ as

$$|\phi, t\rangle = \sum_E c_E |E, t\rangle = \sum_E c_E e^{-iEt/\hbar} |E\rangle \quad (6.175)$$

6. We write $|E\rangle$ in terms of the \hat{B} eigenvector basis

$$|E\rangle = \sum_j d_j |b_j\rangle \quad \text{where } d_k = \langle b_k | E \rangle \quad (6.176)$$

7. We write $|\phi, t\rangle$ in terms of the \hat{B} eigenvector basis

$$|\phi, t\rangle = \sum_E c_E e^{-iEt/\hbar} |E\rangle = \sum_E \langle E | \phi \rangle e^{-iEt/\hbar} \sum_j \langle b_j | E \rangle |b_j\rangle \quad (6.177)$$

8. Then the probability of finding b_7 is given by

$$\begin{aligned} P = |\langle b_7 | \phi, t \rangle|^2 &= \left| \sum_E \langle E | \phi \rangle e^{-iEt/\hbar} \sum_j \langle b_j | E \rangle \langle b_7 | b_j \rangle \right|^2 \\ &= \left| \sum_j \langle b_7 | b_j \rangle \left(\sum_E \langle b_j | E \rangle \langle E | \phi \rangle e^{-iEt/\hbar} \right) \right|^2 \\ &= \left| \sum_E \langle b_7 | E \rangle \langle E | \phi \rangle e^{-iEt/\hbar} \right|^2 \end{aligned} \quad (6.178)$$

This final result expresses the answer in terms of the initial and final states and the properties of the energy eigenvectors and energy eigenvalues, all of which are known.

Thus after several passes (to better understand things) through the various topics involved, we see our formulation of quantum theory is capable of making the necessary predictions. We won't be doing this in general, but it is important to know that we can!

6.4 Relating to Physical Quantities and Time Evolution

Let us now bring all of the ideas we have been talking about together and answer some fundamental questions (some review and some new).

Earlier we saw how the rules for combining amplitudes could be used to explain the electron interference patterns. However, we couldn't follow this line of argument through completely as we didn't have an amplitude that told us the probability of finding an electron at a particular point at a given time. We now try to correct this by looking at a somewhat simpler situation - that of a particle which is not being acted on by any forces - a free particle.

6.4.1 Using the Position Basis

If we want to work out the probability of finding a particle at any location x , then we have to expand the particle's state over a set of appropriate basis

states, each one of which corresponds to the particle being found at a given point (choose the appropriate HOME space). This corresponds to the position basis made up of the eigenvectors of the position operator.

$$|\phi\rangle = a_1 |x_1\rangle + a_2 |x_2\rangle + a_3 |x_3\rangle + \dots + a_n |x_n\rangle + \dots \quad (6.179)$$

In this expression, we have listed the various possible locations as x_1, \dots, x_n, \dots . In practice, this list will be infinitely long. After all, there are an infinite number of points along even the shortest line.

Obviously we can't write down an expansion (summation) that is infinitely long, which is why mathematicians have developed a couple of helpful pieces of shorthand. We have already used one of these in the preceding expansion. The term $a_n |x_n\rangle$ shows us how each piece of the expansion has the same form, just with different numbers in place (in sequence) instead of the n . The \dots at the end of the expansion is the hint that it should be going on forever.

Actually though, all we need to know is the form that each term takes, $a_n |x_n\rangle$. If we have that form, there is no need to put down any examples (like $a_1 |x_1\rangle$ or $a_2 |x_2\rangle$). Instead, we can simply write

$$|\phi\rangle = \sum_{n=1}^{\infty} a_n |x_n\rangle \quad \left(\text{formally} \equiv \int dx a_n |x_n\rangle \right) \quad (6.180)$$

Continuous Bases

Up to now, most of our expansions over basis sets $\{|i\rangle\}$ have had a finite set of values to deal with (most often two, such as $|U\rangle$ and $|D\rangle$). We need to use a continuous basis to illustrate some properties and so we want to expand on the properties of continuous bases.

With something like position, there are an infinite number of possibilities since even the shortest range of positions can be split up into an infinite number of mathematical points. In this case, the position should not really be specified by an infinite set of numbers x_n , but rather as a variable x , which can take up a continuous range of values.

Equally it is more convenient to write the amplitudes as $a(x)$ (which translates to *a is a function of x* or *a of x*) than as a set of numbers a_1, a_2, \dots , etc. This is not a complicated idea: $a(x)$ is a number and the value of that number changes for different choices of another number x . In this case, x is a physical quantity - distance.

We also must allow for the possibility that the amplitude will change over time as well, in which case we should be writing our expansion of the state as follows:

$$|\Psi(x, t)\rangle = \sum_x a(x, t) |x\rangle \quad (6.181)$$

Even with this expansion, we still have not got things quite right. When you have an infinite number of points to deal with, the chances of finding a particle at any one point exactly are effectively zero. If it was not = zero, then since there is an infinite number, the total probability would also be infinite!

What we have to do instead, for things to make sense, is calculate the probability of finding a particle in a small region surrounding the specified point. We will work out how to do this later.

The Amplitude for a Free Particle

The expansion

$$|\Psi(x, t)\rangle = \sum_x a(x, t) |x\rangle \quad (6.182)$$

is very general. If we're going to get any specific information out of it, we need to know what $a(x, t)$ actually is: we need a mathematical expression for $a(x, t)$ in a specified physical situation.

In cases like the double-slit experiment from the last section, it can be quite difficult to find the mathematical form of $a(x, t)$. We have to solve the equations of quantum mechanics and put in some initial conditions to get the right answer.

Since we are not yet ready to talk about such things in detail, we use a simple example - that of a particle moving in one dimension with no forces acting on it: the so-called free particle.

Unfortunately, even in this simple situation, we cannot derive the form of the free-particle amplitude $a(x, t)$.

In traditional quantum mechanics textbooks, one of the following two approaches is generally taken:

1. To write down the equations of quantum theory, which help to derive amplitudes in certain situations, and then produce the free-particle amplitudes from them.
2. To write down the free-particle amplitude and use it to obtain a sensible form for the equations.

In either case, something has to be taken as *given* or, equivalently, an *assumption* has to be made. This is the nature of science. The originators of the theory inched their way to a satisfactory version of quantum theory by a series of inspired guesses, half thought-out models and mathematical insight. The equations of quantum theory can't be proven; they are the starting point of the theory. Their only justification can be the correct predictions they make about nature. We will use approach #2 here.

So we guess the free-particle amplitude.

FREE-PARTICLE AMPLITUDE

$$a(x, t) = A \exp\left(\frac{2\pi i x}{\lambda} - 2\pi i f t\right) \quad (6.183)$$

A is the magnitude of the complex number and since it does not depend on x or t it remains constant. As we suspected, the phase (argument of the exponential function) changes with both x and t and is connected to the *wavelength* λ and *frequency* f .

Wavelength

It is hard to visualize what this amplitude *looks like*, without a drawing such as the figure below.

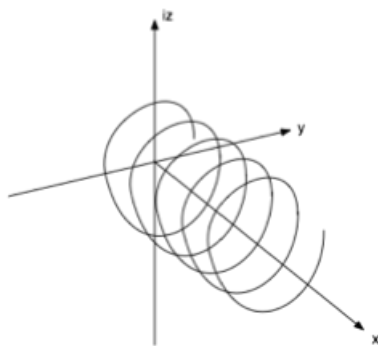


Figure 6.13: Representation of a Free-Particle Amplitude

In the figure three arrows have been labelled (x, y, iz) . The arrow labelled x represents the line along which, in classical terms, the particle is moving.

The other arrows are the real(y) and imaginary(iz) axes of a complex plane representing the amplitude(a complex number for each x and t value). One particular complex plane has been drawn slicing through the x line at the position $x = 0$. The amplitude itself is the spiral winding round the x -direction. However, to fully understand what this amplitude looks like, you must realize that the figure should be a collection of complex planes stacked up parallel to one another slicing through every point on the x -axis.

Clearly as we move along the x -direction, the amplitude keeps a constant magnitude (the spiral is always the same distance from the x -axis), but its phase is continually changing.

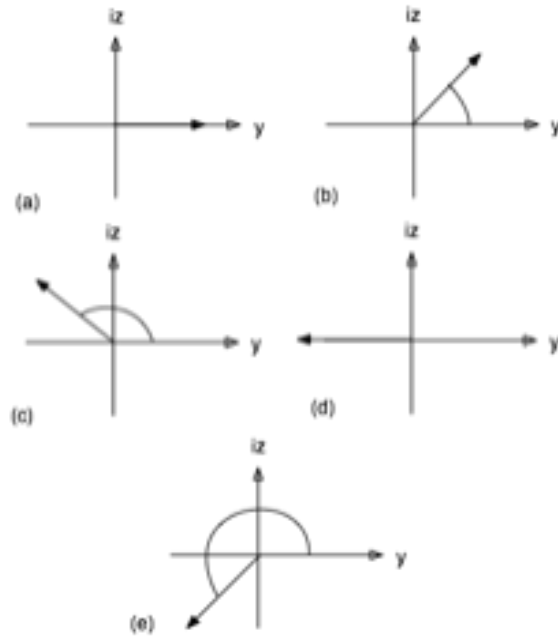


Figure 6.14: Slices of Free-Particle Amplitude

To see how this works, consider what would happen if we took various vertical slices through the figure at different distances along the x -axis as in figure above. In each figure, the amplitude at the given x value is represented by an arrow (which points from a place on the x -axis to the spiral line in the first figure). Figure (a) above is for $x = 0$. The phase of the amplitude at $x = 0$ is fixed by the $2\pi ft$ part of the formula as the $2\pi x/\lambda$ part clearly vanishes if $x = 0$. If we arrange to start a clock timing the particle as it crosses the $x = 0$ point, then this contribution to the phase will be zero ($t = 0$), which is why the arrow representing the amplitude points along the y -axis. Provided each other slice is taken at the same moment, the $2\pi ft$ part will be the same in each part of the figure, and so we can forget about its contribution.

This is a crucial point. The various complex planes in the above figure show what the amplitude looks like at *different points at the same moment*. There is no implied actual motion of the particle here. In fact, what the amplitude tells us about how the particle is moving is rather surprising as we will see shortly.

In part (b) of the figure we are looking at a point further along the x -axis, so the phase of the amplitude is different by an amount $2\pi x/\lambda$. The arrow in the figure has rotated around by a fraction x/λ , of a complete circle. As we move still further down the x -axis, the phase continues to change, until as in part (d) of the figure the phase has advanced by 180° (π radians) compared to part (a).

The phase in (d) is given by $2\pi x/\lambda$, and as this is evidently π radians, which is greater than the phase at (a), we can see that $2\pi x/\lambda = \pi$, so $x/\lambda = 1/2$ and $x = \lambda/2$.

We have advanced down the x -axis a distance equal to half of a wavelength. Eventually the amplitude's phase will reach 360° when $x = \lambda$, as shown below.

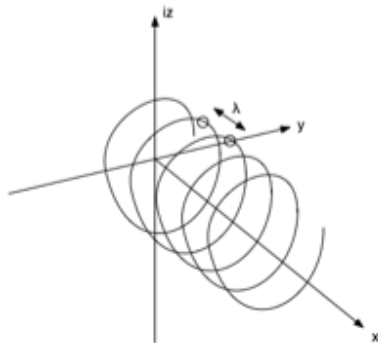


Figure 6.15: Wavelength of a Free-Particle

The two *small circles* drawn on the spiral in the above figure indicate the places where the phase differs by 360° ; the distance between these places is what we call a *wavelength*.

Here is one hint on how to read these figures. Go back to the electron interference experiment we discussed earlier. If one of the paths (say the top one) from slit to screen was distance x_1 , which corresponded to the first small circle in the figure, then we know what the phase would be for that path. A second drawing like the above figure might represent the amplitude from the other slit (the bottom one). If its path to the screen was a distance x_2 , corresponding to the second small circle, then the two amplitudes would have the same phase and constructive interference would occur.

This is what is meant by the *wavelength* of the particle.

Frequency

In the previous discussion, we set our clock so that $t = 0$ corresponded to the particle crossing the $x = 0$ point. What would happen if we didn't set things up so conveniently?

Actually not much: if in part (a) of the figure we didn't have $t = 0$, then the phase would be set to an amount equal to $2\pi ft$ rather than zero. We could just rotate(clockwise) the arrow to give that phase. Then we would have to shift all the arrows on (b) through (e) by the same amount. The discussion wouldn't

change, provided all the figures were drawn at the same moment so that $2\pi ft$ is the same for all of them.

Alternatively, we could sit on one x value and watch what happens to the phase as time goes on. This behavior is governed by the $2\pi ft$ part of the formula. Basically it works just like the x variation.

The frequency f of a wave (the number of cycles the wave goes through in 1 second) is related to the period of the wave (the time taken for one cycle) by

$$f = \frac{1}{T} \quad (6.184)$$

Now we can write the time factor in the phase as $2\pi t/T$. The ratio t/T tells us what fraction of a period we have been sitting on the x value for and by what fraction of a circle we need to rotate the phase by.

When we compared slices along the x -axis at one time, the phase changed in an anticlockwise direction. Sitting on an x point and watching the time go by sees the phase rotating backwards (clockwise) due to the negative sign.

$$Amplitude = A \exp\left(\underbrace{\frac{2\pi ix}{\lambda}}_{\substack{\nearrow \\ \text{Drives phase} \\ \text{anticlockwise}}} - \underbrace{\frac{2\pi it}{T}}_{\substack{\nwarrow \\ \text{Drives phase} \\ \text{clockwise}}}\right) \quad (6.185)$$

Imagine a long spring (a slinky) stretched out so that there are gaps between the coils as in figure below.

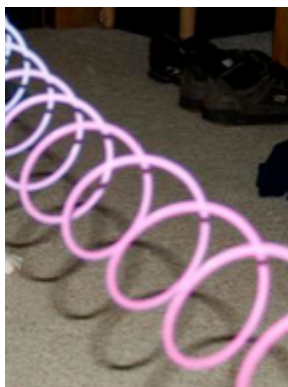


Figure 6.16: Slinky Model

The long axis of the slinky is the x -direction in the figure so that the coils represent the amplitude (remember, in reality, that amplitude is not in a *physical* direction in space). If you can picture this, then you can *see* that the wavelength is the distance between the coils. Now picture the slinky slowly rotating about its long axis. If a dot is painted onto the top of one of the coils, then this will rotate downward (say clockwise as we are looking at it) until the dot is at the bottom of the slinky and then round back to the top again. The time it takes to do this is the period of the rotation. The frequency is the rate at which the dot comes back to the top and is measured in *returns per second*.

What Does the Amplitude Tell Us about the Motion of a Free Particle?

The *free-particle amplitude* does not represent a particle showing *visible* motion. Consider the following. Earlier we wrote down the following general expansion over position eigenstates:

$$|\Psi(x, t)\rangle = \sum_x [a(x, t) |x\rangle] \quad (6.186)$$

Now we can use the specific $a(x, t)$ we assumed for a free particle.

$$|\Psi(x, t)\rangle = \sum_x \left[A \exp\left(i \frac{2\pi x}{\lambda} - 2\pi i f t\right) |x\rangle \right] \quad (6.187)$$

To calculate the probability of finding our particle at a given point X , our rules say that we need to find the amplitude $\langle X | \Psi \rangle$ and complex square (absolute square) it. The first step is to get $\langle X | \Psi \rangle$

$$\begin{aligned} \langle X | \Psi \rangle &= \langle X | \sum_x \left[A \exp\left(\frac{2\pi i x}{\lambda} - 2\pi i f t\right) |x\rangle \right] \\ &= \sum_x \left[A \exp\left(\frac{2\pi i x}{\lambda} - 2\pi i f t\right) \langle X | x \rangle \right] \\ &= A \exp\left(\frac{2\pi i X}{\lambda} - 2\pi i f t\right) \end{aligned} \quad (6.188)$$

where we have used the relationships $\langle X | x \rangle = 0$ unless $x = X$ and $\sum_x [g(x) \langle X | x \rangle] = g(X)$. Since the summation here adds up terms that have every x value, one by one, this operation effectively removes each term in the summation except the one where $x = X$.

Now the probability we need is $|\langle X | \Psi \rangle|^2 = \langle X | \Psi \rangle^* \langle X | \Psi \rangle$, which is

$$\begin{aligned}
|\langle X | \Psi \rangle|^2 &= A \exp\left(\frac{2\pi i X}{\lambda} - 2\pi i f t\right)^* A \exp\left(\frac{2\pi i X}{\lambda} - 2\pi i f t\right) \\
&= A^2 \exp\left(-\frac{2\pi i X}{\lambda} + 2\pi i f t\right) \exp\left(\frac{2\pi i X}{\lambda} - 2\pi i f t\right) \\
&= A^2 \exp\left(-\frac{2\pi i X}{\lambda} + 2\pi i f t + \frac{2\pi i X}{\lambda} - 2\pi i f t\right) \\
&= A^2 \exp(0) = A^2
\end{aligned} \tag{6.189}$$

where we have used the rule for multiplying complex numbers, i.e., multiply the magnitudes and add the phases.

This is a *striking result*. The probability of finding the particle at a given point X is $|A|^2$, *no matter* what X we pick. The particle is equally likely to be found anywhere along the *direction of flight* at any time. *This does not sound much like a particle moving along at constant speed.*

As always with quantum mechanics, we have to stop and think carefully about what we are actually doing. If we were to carry out an experiment to measure the position of a particle in the state $|\phi\rangle$, then we would collapse into one of the position eigenstates, $|x\rangle$. If we then want to follow this up with a future position measurement on the same particle, we would have to let the $\hat{U}(t)$ operator act on it. The state produced would not be the same as the previous $|\phi\rangle$. Hence $|\phi\rangle$ cannot represent a particle smoothly moving through space in a classical sense.

Amplitudes, Energy and Momentum

Earlier, we wrote the amplitude of a free particle in the following form:

$$a(x, t) = A \exp\left(\frac{2\pi i x}{\lambda} - 2\pi i f t\right) \tag{6.190}$$

However, this is not the only way of writing the amplitude down. We have, from earlier discussions, the de Broglie relationships:

$$\lambda = \frac{h}{p} \quad , \quad f = \frac{E}{h} \tag{6.191}$$

which we can use to replace frequency and wavelength in the amplitude.

$$\begin{aligned}
a(x, t) &= A \exp\left(\frac{2\pi i x}{\lambda} - 2\pi i f t\right) \\
&= A \exp\left(\frac{2\pi i}{h} p x - \frac{2\pi i}{h} E t\right) = A \exp\left(\frac{i}{\hbar} (p x - E t)\right)
\end{aligned} \tag{6.192}$$

where $\hbar = h/2\pi$.

In this final form we can see how the amplitude is determined by the various physical quantities that we would directly measure. It is a *particle(property) version* rather than a *wave(property) version* of the amplitude.

Energy and Momentum Eigenstates

Returning to the state expansion, we can now write

$$|\Psi(x, t)\rangle = \sum_x \left[A \exp\left(\frac{i}{\hbar}(px - Et)\right) |x\rangle \right] \quad (6.193)$$

What sort of state is this? Well, it clearly can't be a position eigenstate. Two things count against that. First, the expansion is over a range of position states, so the overall state can't have a distinct position value. Second, the amplitude produces the same probability for all positions at all times, which is not what one would expect for a position eigenstate.

Of course, it doesn't have to be an eigenstate of anything, but it is amusing to consider the possibilities. The other physical variables present are time(t), momentum(p) and energy(E). Now, it's entirely unclear what a time eigenstate might be (an object frozen in time?), so we will discount that possibility. The other two are much better candidates. In fact, this state turns out to be an eigenstate of *both* momentum and energy as we will see later.

Returning to the Phase and its relation to Physical Variables

We have found that the amplitude to be at a particular position for a free particle is $\langle X | \Psi \rangle$ and we found

$$\langle X | \Psi \rangle = A \exp\left(\frac{2\pi i X}{\lambda} - 2\pi i f t\right) \quad (6.194)$$

This of the form $R \exp(i\theta)$ that we assumed for this amplitude in the two-slit interference experiment. Therefore, the spatial dependence of the phase is given by

$$\theta = px/\hbar = 2\pi x/\lambda \quad (6.195)$$

If the distance x is different for two amplitudes, then we could get an interference pattern given by

$$A' = A e^{2\pi i x_1/\lambda} + A e^{2\pi i x_2/\lambda} \quad (6.196)$$

This gives an intensity or brightness on the screen of

$$\begin{aligned} I &= |A'|^2 = |A|^2 \left| \left(e^{2\pi i x_1/\lambda} + e^{2\pi i x_2/\lambda} \right) \right|^2 \\ &= 4 |A|^2 \left(1 + \cos(2\pi(x_2 - x_1)/\lambda) \right) \end{aligned} \quad (6.197)$$

which agrees with the classical result for the interference pattern!

Time Evolution

We can also see that the energy eigenvectors evolve in time with an exponential factor

$$e^{-iEt/\hbar} \quad (6.198)$$

This says that for an energy eigenvector $|E\rangle$ we have (as we already mentioned earlier)

$$\hat{U}(t)|E\rangle = e^{-iEt/\hbar}|E\rangle \quad (6.199)$$

Thus, if we want to find the time evolution of any arbitrary state, then we follow this procedure we stated earlier:

1. Write the arbitrary initial ($t = 0$) state $|\psi\rangle$ in terms of the energy eigenvectors, i.e., use the energy basis.

$$|\psi(0)\rangle = \sum_n a_n |E_n\rangle \quad (6.200)$$

where $a_n = \langle E_n | \psi \rangle$.

2. Operate with the time development operator

$$\begin{aligned} |\psi(t)\rangle &= \hat{U}(t)|\psi\rangle = \hat{U}(t) \sum_n a_n |E_n\rangle \\ &= \sum_n a_n \hat{U}(t) |E_n\rangle \\ &= \sum_n a_n e^{-iE_n t/\hbar} |E_n\rangle \end{aligned} \quad (6.201)$$

3. Do a measurement of some observable, say \hat{B} . This means that we must now change the basis to the eigenvectors of \hat{B} . We have

$$|E_n\rangle = \sum_k c_{kn} |b_k\rangle \quad (6.202)$$

where $\hat{B}|b_k\rangle = b_k|b_k\rangle$ and $c_{kn} = \langle b_k | E_n \rangle$.

4. Finally, we have the probability amplitude for measuring b_k if we are in the state $|\psi\rangle(t)$ is given by

$$\begin{aligned} \langle b_k | \psi(t) \rangle &= \sum_n a_n e^{-iE_n t/\hbar} \langle b_k | E_n \rangle \\ &= \sum_n a_n e^{-iE_n t/\hbar} c_{kn} \end{aligned} \quad (6.203)$$

In a formal sense we have answered the question, although the actual computation might be very difficult.

Another way of thinking about time evolution is to work directly with the time-evolution operator $\hat{U}(t)$. This makes the above discussion more formal.

Most of the operators we have been discussing correspond to observables. In mathematics all of these operators are of a certain type called *Hermitian operators*. This is so because their eigenvalues are the possible results of measurements of those observables and their eigenvalues must be real numbers, which is always true for Hermitian operators.

The time-evolution operator is representative of a second class of operators in quantum theory. These operators do not represent observables, but instead transform kets (states) into different kets (states).

Because the coefficients of basis states in the representation of an arbitrary state are related to probability amplitudes and therefore the sum of their absolute squares must equal 1, these *transformation*-type operators, in mathematics, must of a kind called *unitary operators*.

Unitary operators in mathematics have eigenvalues whose absolute value always equals 1.

From our study of complex numbers, we know that if $z = e^{i\alpha} = \cos \alpha + i \sin \alpha$, then $|z|^2 = \cos^2 \alpha + \sin^2 \alpha = 1$ or $|z| = 1$. Thus, the eigenvalues of any unitary operator can always be represented by a complex exponential.

If the eigenvectors/eigenvalues of $\hat{U}(t)$ are represented by the equation below

$$\hat{U}(t) |\beta_n\rangle = e^{i\beta_n} |\beta_n\rangle \quad (6.204)$$

then we can write

$$\hat{U}(t) = \sum_n e^{i\beta_n} |\beta_n\rangle \langle \beta_n| \quad (6.205)$$

Now in many physical systems, the energy operator does not change with time. In quantum theory, that means that both the energy operator and the time-evolution operator have the same eigenvectors.

If, in this case, we have $\hat{E} |E_k\rangle = E_k |E_k\rangle$, then it turns out that we can write

$$\hat{U}(t) = \sum_n e^{-iE_n t/\hbar} |E_n\rangle \langle E_n| \quad (6.206)$$

This implies that for an energy eigenvector we have

$$\hat{U}(t) |E_k\rangle = \left[\sum_n e^{-iE_n t/\hbar} |E_n\rangle \langle E_n| \right] |E_k\rangle = e^{-iE_k t/\hbar} |E_k\rangle \quad (6.207)$$

i.e., the only change by a phase factor. It turns out that no probabilities changes during the time evolution of these states and hence they are called *stationary states*.

More importantly, this property gives us the method for finding the time evolution for an arbitrary state. it goes as follows:

1. Write the initial arbitrary state in the energy basis

$$|\psi(0)\rangle = \sum_n a_n |E_n\rangle \quad (6.208)$$

where $a_n = \langle E_n | \psi \rangle$

2. Operate with the time development operator

$$\begin{aligned} |\psi(t)\rangle &= \hat{U}(t) |\psi\rangle = \hat{U}(t) \sum_n a_n |E_n\rangle \\ &= \sum_n a_n \hat{U}(t) |E_n\rangle \\ &= \sum_n a_n e^{-iE_n t/\hbar} |E_n\rangle \end{aligned} \quad (6.209)$$

3. and so on as before.....

6.5 Problems

6.5.1 Color Operator

If we know what an operator does, then we can construct it. Let us do this for the color operator. We work in the hardness basis:

$$|hard\rangle = |h\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } |soft\rangle = |s\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

with hardness operator

$$\hat{O}_h = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Using this basis, the color states are given by

$$|green\rangle = |g\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \text{ and } |magenta\rangle = |m\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

All we need to remember in order to construct the color operator is how it acts on the color states

$$\hat{O}_c |g\rangle = |g\rangle \text{ and } \hat{O}_c |m\rangle = -|m\rangle$$

Write out these last two equations treating the four elements of the color operator as unknowns. You should get four equations that allow you to calculate the four elements of the color operator. Do you get the same operator as in the textbook?

6.5.2 Probabilities

We stated that if a particle is in the state $|\psi\rangle$ and you measure its color, for example, the outcome of the measurement is either $|green\rangle$ with probability $|\langle g|\psi\rangle|^2$ or $|magenta\rangle$ with probability $|\langle m|\psi\rangle|^2$. Let us try this out on a few states.

What are the possible outcomes and with what probability do they occur if the color is measured of a particle in

- (a) the state $|hard\rangle$
- (b) the state $|soft\rangle$
- (c) the state

$$|\psi\rangle = \sqrt{\frac{3}{4}}|hard\rangle + \frac{1}{2}|soft\rangle$$

Use the $(hard, soft)$ basis for the calculation.

6.5.3 Orthogonal Basis Vectors

Compute the eigenvectors of the matrix operator

$$A = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 5 & 0 & 3 \end{pmatrix}$$

Using Gram-Schmidt, construct an orthonormal basis set from the eigenvectors of this operator.

6.5.4 Hardness World

Let us define a state using the hardness basis $(|h\rangle, |s\rangle)$

$$|A\rangle = \cos\theta|h\rangle + e^{i\phi}\sin\theta|s\rangle$$

where θ and ϕ are constants.

- (a) Is this state normalized? Show your work.
- (b) Find the state $|B\rangle$ that is orthogonal to $|A\rangle$. Make sure that $|B\rangle$ is normalized.
- (c) Express $|h\rangle$ and $|s\rangle$ in the $(|A\rangle, |B\rangle)$ basis.
- (d) What are the possible outcomes of a hardness measurement on state $|A\rangle$ and with what probability will each occur?
- (e) Express the hardness operator in the $(|A\rangle, |B\rangle)$ basis.

6.5.5 Two-Path Experiment

Consider the following situations based on the two path color-hardness experiment in the notes:

- (a) just as in the figure
- (b) a wall in one path at (x_3, y_1)
- (c) a wall in one path at (x_2, y_2)

Make a chart with each row representing one of these situations. In the columns of the chart, give

- (1) the state of the particles that emerge at (x_5, y_4)
- (2) the probability that a hardness box at (x_5, y_4) measures the hardness to be hard
- (3) the probability that a hardness box at (x_5, y_4) measures the hardness to be soft
- (4) the probability that a color box at (x_5, y_4) measures the color to be green
- (5) the probability that a color box at (x_5, y_4) measures the color to be magenta

6.5.6 Time Evolution

A state $|X\rangle$ is given in the hardness basis as

$$|X\rangle = \frac{1}{3}|h\rangle + \frac{2i\sqrt{2}}{3}|s\rangle$$

- (a) What are the possible outcomes and probabilities for measurement of hardness and color on this state at $t = 0$?
- (b) Imagine that due to an external field, the two color states $|g\rangle$ and $|m\rangle$ are eigenstates of the energy operator with the energy of the green state being zero and the energy of the magenta state being $1.0 \times 10^{-34} J$. What are the possible outcomes and probabilities for measurement of hardness and color on this state after 1 second?

Chapter 7

Polarization

Now let us use all the formalism that we have developed to completely deal with a real-world property associated with photons, namely, *polarization*.

Before starting out, we need to digress and learn a few more mathematical things about matrices.

7.1 More about Matrix Operators

As we have seen, operators are very important objects in quantum theory; some operators directly represent physical properties, others transform states. Whatever type of operator we are dealing with, they can all be written down in various ways or representations. We now expand on our earlier discussion of ways of writing operators with some additional facts about matrices.

A *matrix* is an array of numbers such as

$$\begin{pmatrix} 1 & 4 \\ 7 & 9 \end{pmatrix} \quad (7.1)$$

which is a *two by two* or 2×2 matrix or

$$\begin{pmatrix} 1 & 34 \\ 9 & 18 \\ 5 & 12 \end{pmatrix} \quad (7.2)$$

which is a *three by two* or 3×2 matrix.

A matrix can have any number of rows and columns, including one by something or something by one.

Each number in the matrix is called an element. Of course, we can always use

letters to represent elements when we are not sure what the number is, or when we deliberately do not want to refer to a specific number.

To make such arrays useful, mathematicians invented a series of rules that allow us to add, subtract, and multiply matrices together.

You can add and subtract matrices if they have the same number of rows and columns. All you have to do is add the elements.

$$\begin{pmatrix} 1 & 4 \\ 7 & 9 \end{pmatrix} + \begin{pmatrix} 4 & 2 \\ 5 & 1 \end{pmatrix} = \begin{pmatrix} 5 & 6 \\ 12 & 10 \end{pmatrix} \quad (7.3)$$

We will not have to add or subtract matrices; we will only need to multiply them together.

You can multiply two matrices if the number of columns in one is the same as the number of rows in another. For example

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} aA + bC & aB + bD \\ cA + dC & cB + dD \end{pmatrix} \quad (7.4)$$

which looks fiendishly complicated, but its actually not so bad. What you are doing is multiplying the row in the first matrix by the column in the second. Look at the top left element of the resulting matrix, $aA + bC$. You can see that we combined elements from the top row of the first matrix and those from the left column of the second. Similarly, the top right element, $aB + bD$, is built from the top row of the first matrix and the right column of the second. Work your way through the elements and you will see how they are put together.

Quantum states can be written in matrix form (remember color/hardness discussion). For example, the eigenstates of the vertical Stern-Gerlach (S-G) operator \hat{S}_z can be written

$$|U\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |D\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (7.5)$$

Think of the top row as containing the amplitude for the particle to be in the state $|U\rangle$ and the bottom row as the amplitude for it to be in the state $|D\rangle$. In a formal sense, this says that a state can be thought of as an array of amplitudes for transitions to other states (normally eigenstates).

States such as $|R\rangle$ and $|L\rangle$ would be written

$$|R\rangle = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |L\rangle = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (7.6)$$

since, for example, the amplitude for $|R\rangle$ to transition to $|U\rangle$ is $1/\sqrt{2}$ and so on.

Now we can write the vertical S-G operator \hat{S}_z in the form of a matrix

$$\hat{S}_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (7.7)$$

and apply it to the states and see what happens:

$$\hat{S}_z |U\rangle = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 \times 1 + 0 \times 0 \\ 0 \times 1 + (-1) \times 0 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2} |U\rangle \quad (7.8)$$

which is exactly what we wanted to happen. Similarly, we can show that

$$\hat{S}_z |D\rangle = -\frac{\hbar}{2} |D\rangle \quad (7.9)$$

As a matter of completeness, we point out that the other two S-G operators \hat{S}_x and \hat{S}_y can also be written in the form of matrices.

$$\hat{S}_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \hat{S}_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (7.10)$$

Although any operator can be written in the form of a matrix, this is not the same as saying the operator *is* a matrix. There is normally more than one way to represent an operator mathematically and as a matrix is only one example.

The first step in converting an operator into a matrix is to choose the basis that you are going to employ. The same operator will have lots of different matrix representations, depending on the basis set that is being used. To show how this works, let us derive the \hat{S}_z operator using the (UP,DOWN) basis. We should get the result quoted above.

To represent \hat{S}_z as a matrix, such as

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

we need some way of calculating the various elements from this representation. Before we can do this, we have to find a way of writing $\langle U|$ and $\langle D|$ in matrix form as well.

Consider the basic relationship $\langle U | U \rangle = 1$. The rules of matrix multiplication (row x column) show us that the only way to construct something like $\langle U | \psi \rangle$ in matrix form, where

$$|\psi\rangle = \begin{pmatrix} a \\ b \end{pmatrix} \quad (7.11)$$

is to write

$$\begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = (1 \times a + 0 \times b) = a \quad (7.12)$$

as expected. From this result, we must then have

$$\langle U| = \begin{pmatrix} 1 & 0 \end{pmatrix} \quad , \quad \langle D| = \begin{pmatrix} 0 & 1 \end{pmatrix} \quad (7.13)$$

In fact, for any state

$$|\phi\rangle = \begin{pmatrix} a \\ b \end{pmatrix} \quad (7.14)$$

we can write

$$\langle\phi| = \begin{pmatrix} a^* & b^* \end{pmatrix} \quad (7.15)$$

Sticking with UP and DOWN, let's construct a simple calculation along the lines of

$$\langle U|\hat{S}_z|U\rangle = \langle U|\frac{\hbar}{2}|U\rangle = \frac{\hbar}{2}\langle U|U\rangle = \frac{\hbar}{2} \quad (7.16)$$

In matrix form this would be

$$\frac{\hbar}{2} \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2} \quad (7.17)$$

The calculation tells us something more general than that. We have pinned down the top left matrix element.

$$\begin{pmatrix} \langle U|\hat{S}_z|U\rangle & b \\ c & d \end{pmatrix} \quad (7.18)$$

By now it is possible to guess what the overall pattern is going to be, but to be sure, let's try it with one of the other elements. Construct

$$\langle D|\hat{S}_z|U\rangle = \langle D|\frac{\hbar}{2}|U\rangle = \frac{\hbar}{2}\langle D|U\rangle = \frac{\hbar}{2}(0) = 0 \quad (7.19)$$

and then do the same calculation in matrix form:

$$\begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \times 1 + 0 \times 0 \\ 0 \times 1 + (-1) \times 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0 \quad (7.20)$$

Thus, we have found another element

$$\begin{pmatrix} \langle U|\hat{S}_z|U\rangle & b \\ \langle D|\hat{S}_z|U\rangle & d \end{pmatrix} \quad (7.21)$$

In fact, we can fill in the whole matrix

$$\begin{pmatrix} \langle U|\hat{S}_z|U\rangle & \langle U|\hat{S}_z|D\rangle \\ \langle D|\hat{S}_z|U\rangle & \langle D|\hat{S}_z|D\rangle \end{pmatrix} \quad (7.22)$$

as we discussed earlier in the book. The generalization to any other operator is straightforward. If we have some operator \hat{O} and a basis $\{|i\rangle\}$, then the matrix

representing that operator can be written as

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & . & . \\ . & a_{22} & a_{23} & . & . \\ . & . & a_{33} & . & . \\ a_{14} & . & . & a_{44} & . \\ . & . & a_{53} & . & . \end{pmatrix} \quad (7.23)$$

where we have filled in only some of the blanks so that you can see the pattern. The matrix is always going to be square, and the number of rows and columns depends on how many states there are in the basis. The matrix elements, such as a_{11} , a_{12} , and so on, can be calculated from the following rule:

RULE 8:

Matrix elements of operator are calculated from

$$a_{11} = \langle 1 | \hat{O} | 1 \rangle \quad , \quad a_{12} = \langle 1 | \hat{O} | 2 \rangle \quad , \quad a_{ij} = \langle i | \hat{O} | j \rangle \quad (7.24)$$

In fact, physicists call a combination such as $\langle i | \hat{O} | j \rangle$ a *matrix element*.

This method of representing an operator as a matrix works for any operator, but in certain situations a matrix may not be the most convenient form for dealing with the operator. In the case of position and momentum operators, for example, the appropriate bases to use will have an infinite number of basis states as we have seen earlier. As a result, there will be an infinite number of elements in the matrix. We will learn a different way of representing operators in these cases later.

One final point is worth making. An operator can be put into matrix form using any basis and the same operator will have a different matrix representation depending on the basis chosen. However, some choices of basis are more sensible than the others. What happens, for example, when the basis chosen is formed from the eigenstates of the operator concerned? Each matrix element has the form $\langle i | \hat{O} | j \rangle$ and if $|i\rangle$ and $|j\rangle$ are eigenstates, then $\hat{O} |j\rangle = e_j |j\rangle$, e_j is the eigenvalue for the state $|j\rangle$. The matrix element then becomes $e_j \langle i | j \rangle$. Since $|i\rangle$ and $|j\rangle$ are a basis, then $\langle i | j \rangle = 0$ unless $i = j$. The upshot of this is that the matrix is *diagonal*: every element is zero unless it runs down the long diagonal, and the elements on the diagonal are the *eigenvalues* of the operator acting on the basis:

$$\begin{pmatrix} e_1 & 0 & 0 & 0 & . \\ 0 & e_2 & 0 & 0 & . \\ 0 & 0 & e_3 & 0 & . \\ 0 & 0 & 0 & e_4 & . \\ . & . & 0 & . & . \end{pmatrix} \quad (7.25)$$

7.2 First Thoughts about Polarization

We will make a first pass at photon polarization in this section and return to a complete theory later on. Here we will introduce polarization and some of its properties and then discuss some experiments that illustrate the problems with the classical description and the strangeness of quantum phenomena.

Light is really oscillating \vec{E} (electric) and \vec{B} (magnetic) field vectors. In particular, these vectors oscillate in time in a plane (two-dimensional space) perpendicular to the direction of propagation (motion) of the light (called the transverse direction) as shown below.

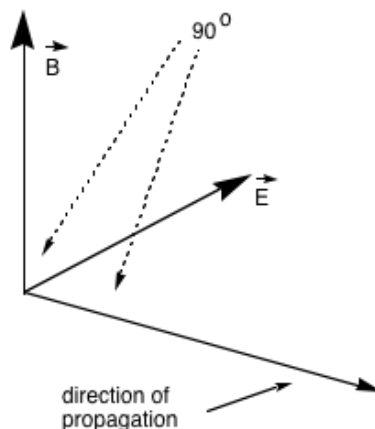


Figure 7.1: Geometry of a plane wave

This is why you are able to see light. Your eye is actually responding to these oscillating electromagnetic fields. The oscillations are of very-high frequency (10^{15} sec^{-1}).

As stated, the electric field vector is oscillating in some direction at any instant of time. Suppose we choose to associate that *instantaneous direction* of the \vec{E} vector with a new quantity called *polarization*.

The \vec{E} vector then defines the *plane* of polarization (orthogonal to direction of propagation) and the *direction* of polarization of the beam of light.

Have you ever observed polarization?

Yes....you all have oriented the aerials of portable radios or FM radios or TV rabbit ears to get the best signal...you were lining them up with the polarization of the electromagnetic waves in each case.

Also, as we shall investigate in much detail shortly, you all have used polaroid sunglasses. These glasses only allow light with polarization in a single direction to get through, thereby cutting down the intensity (amount) of the light reaching your eyes.

Now we can always choose the plane containing the electric and magnetic fields to be the $x-y$ plane and represent the vector as the *sum* of a two vectors, one in the x -direction and the other in the y -direction, such that the \vec{E} vector makes an angle α with the x -axis.

Then we say that the \vec{E} vector is a combination (sum) of an E_x -vector (field) and an E_y -vector (field) as shown below:

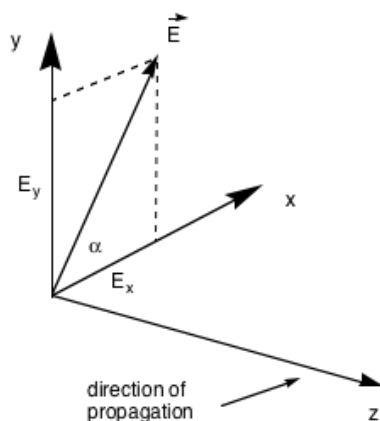


Figure 7.2: Breaking into components

In terms of the polarization, we say that the direction of polarization as represented by the \vec{E} vector is a (linear) combination of two polarizations, one in the x -direction and one in the y -direction, i.e., the polarization *state of a system* is a linear combination of an x -polarized state and a y -polarized state.

Many materials have a property that they will only let light pass through them if the polarization is in a particular direction, i.e., it is in a particular or definite polarization state. We call this axis the *special or preferred or optic axis*. To get through the light must be polarized (have direction of polarization) in a direction *parallel* to the special axis. As I said earlier, you have all seen such material in sunglasses or sheets of *Polaroid* film.

Let us consider some experiments involving polaroid materials, a block of calcite and a laser.

The laser we use produces *unpolarized light* – what does that mean?

It means that if we check(measure) the amount of polarization in any direction(amount of light getting through an oriented polaroid), then we will find the *same amount* of polarization in any directions, i.e., the polarization is equally likely to point in any direction.

Experimental Checks

1. Send the laser beam into a polaroid. Our only observation is that the brightness or intensity decreases (if we carefully measured it it would drop by about $1/2$). If we rotate the polaroid we observe no change, which says that the amount of light in the beam with polarization parallel to the preferred direction is the same no matter how I orient the polaroid(how I point the preferred direction).

The fact that we get the same intensity ($1/2$ of total) no matter what direction we choose.....says that the light coming out of the laser has equal amounts of polarization in the two directions (no matter which you two choose). This is called unpolarized light (we will give a more formal definition later).

Note here that the statement that $1/2$ of the light gets through a polaroid when it oriented in ANY direction just corresponds to the fact that we can use any basis to describe the physical system; they are all equivalent.

When we choose a preferred direction(done when I pick up the polaroid and orient it in the apparatus), then the polarization of any system(the light from the laser in this case - when we set the context for the experiment) we are investigating must be thought of as either be parallel or perpendicular to that chosen direction think about that!

no other cases will occur in the real world in the context(orientation of the polaroid) of this experiment

Again this is true for any direction we might choose.

After passing through the polaroid we say that the light is polarized in a particular direction (parallel to the polaroid preferred axis). All the light with polarization in the orthogonal direction has been removed(that is what the polaroid does).

If this is true, then if I use 2 identical polaroids rotated by 90° with respect to each other, how much light will come out?

The answer must be none!

So we add another polaroid and rotate so that no light comes through. These two polaroids are now oriented at right angles with respect to each

other and since there are only these two possible polarizations with respect to the chosen polaroid directions, no light comes out.

If we rotate the polaroids, keeping their relative orientation fixed no light comes through. This means that there are only two polarizations with respect to the new orientations also and they have cancelled out also.

In this experiment, we choose a preferred direction by bringing the polaroid over - by setting the experimental context. At that point, the light can be thought of as being partly made up of light polarized parallel to the preferred direction and partly of light polarized perpendicular to the preferred direction and the truly amazing result, as we shall see in our later discussions, will be that the system *does not decide* until I bring over the polaroid(until I set the context!).

The act of inserting a polaroid sets the *context* of the experiment!

Think about these statements carefully! They reflect the strange sounding explanations that result when we try to use *words* to describe what is happening. Mathematically, as we shall see later, there will be no confusion about what is happening.

2. Now we send the laser beam into a calcite crystal and we get two beams. Calcite also has an intrinsic(built-in) preferred direction. Calcite causes bending of a light beam where the amount of bending depends on whether the polarization is parallel or perpendicular to the calcite's preferred direction. Since there are only two possible polarizations with respect to the preferred direction of the calcite crystal, we now see two beams.

If I rotate the calcite what will I find?

The same answer with respect to the new preferred direction, of course, i.e., just two beams.

Thus, *the quantum world* seems not to be set until I walk over and make a decision and fix the orientation of the calcite crystal - until I set the *context*.

Again, think about that statement carefully!!! Reflect on the strange explanation in these words. One wonders whether using words can make any sense of these phenomena. The physical world seems to be waiting for the observer to make a decision about what measurement will be made - waiting for the context to be set. This strange idea, which makes no sense in the classical world, is going to get us into a lot of very hot water later in our discussions.

This result is connected to the fact that the act of *measuring or finding out* some property of a system in some way *determines or actualizes* the state of the system being measured.

Now back to the calcite beams.

We check with a polaroid to see that each of the two beams represents light that has a definite polarization by rotating the polaroid.

Using 2 polaroids, where the first cuts out some light and the second cuts out some more, if the rule above is correct and we orient them so that their preferred axes are at right angles, then all light should be stopped. They affect different beams indicating that the beams represent different (orthogonal polarizations).

We note that mirrors have no effect on polarization....they just redirect polarized beams.

3. Now remove the calcite crystal and rotate the pair of polaroids until there is no light intensity. Then rotate the second polaroid 45° . The light intensity returns (actually $1/2$ of the 0° (or parallel) intensity).

Let us see how classical physics explains these polaroid experiments for *intense* (a very large value of photons/sec) beams of light.

Classically, if an incident beam of light is polarized parallel to the special or optic axis, then *all of its energy* gets through the polaroid. If it is polarized orthogonal to the optic axis, then none of its energy will get through the polaroid. If it is polarized at an angle α to the preferred axis, then a fraction $\cos^2 \alpha$ of its energy gets through the polaroid.

Therefore, we can explain polarization experiments when the notion of electric field vectors make sense (when we have intense light or lots of photons/sec) as follows.

Consider 2 polaroids at right angles \rightarrow intensity-out = 0. In pictures we have,

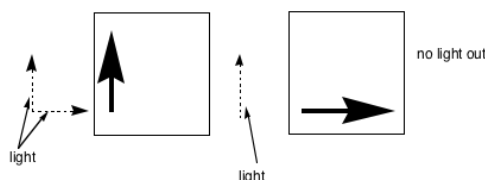


Figure 7.3: Orthogonal polaroids

where the dashed arrows represent the electric field components or polarizations and the solid arrows represent the preferred directions of the polaroids. With components of vectors we have

$$\vec{E}_{in} = E_x \hat{e}_x + E_y \hat{e}_y \rightarrow \vec{E}_{intermediate} = E_y \hat{e}_y \rightarrow \vec{E}_{out} = 0 \quad (7.26)$$

Now 2 polaroids at $45^\circ \rightarrow$ intensity-out $\neq 0$ as shown below.

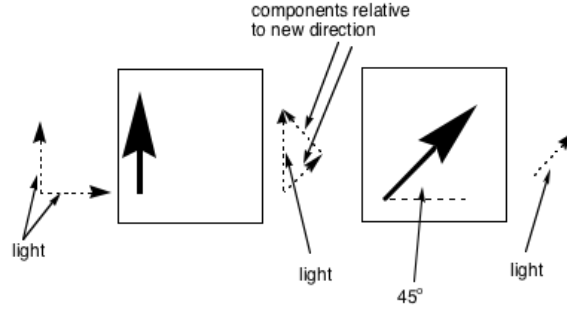


Figure 7.4: 45° polaroids

With components of vectors we can derive the following: we can write the unit vector that makes an angle θ with the x -axis as

$$\hat{n} = \cos \theta \hat{e}_x + \sin \theta \hat{e}_y \quad (7.27)$$

We then have

$$\vec{E}_{in} = E_x \hat{e}_x + E_y \hat{e}_y \quad (7.28)$$

$$\vec{E}_{intermediate} = (\vec{E}_{in} \cdot \hat{e}_y) \hat{e}_y = E_y \hat{e}_y \quad (7.29)$$

since that is what a polaroid does!

$$\begin{aligned} \vec{E}_{out} &= (\vec{E}_{intermediate} \cdot \hat{n}_\theta) \hat{n}_\theta \\ &= ((E_y \hat{e}_y) \cdot (\cos \theta \hat{e}_x + \sin \theta \hat{e}_y)) (\cos \theta \hat{e}_x + \sin \theta \hat{e}_y) \\ &= E_y \sin \theta (\cos \theta \hat{e}_x + \sin \theta \hat{e}_y) \end{aligned} \quad (7.30)$$

Some special cases are:

$\theta = 0^\circ \rightarrow$ orthogonal polaroids

$$\vec{E}_{out} = 0 \quad (7.31)$$

$\theta = 90^\circ \rightarrow$ parallel polaroids

$$\vec{E}_{out} = E_y \hat{e}_y \quad (7.32)$$

$\theta = 45^\circ \rightarrow$ above example

$$\vec{E}_{out} = E_y \sin 45^\circ (\cos 45^\circ \hat{e}_x + \sin 45^\circ \hat{e}_y) = \frac{E_y}{2} (\hat{e}_x + \hat{e}_y) \quad (7.33)$$

So the classical wave theory of electromagnetism seems to be able to explain polarization experiments for intense beams by using *standard vector algebra*.

When there are large numbers of photons in an intense beam the beam behaves as if it had wave properties. Think of water molecules making up a water wave.

Remember, however, light is really composed of individual particles called photons.

4. Now let us add another polaroid to the experiment:

laser + calcite + [2 polaroids at 90 degrees] \rightarrow all gone

[2 polaroids alone at 90 degrees] \rightarrow all gone

This means that first polaroid reduces beams to only one direction which cannot get through the second polaroid (they are the wrong kind... have the wrong direction).

Now that things seem to be making some sort of sense, we disturb this system with another measurement.

- * if we leave the system alone NO light is observed
- * if we add a third polaroid (same orientation as first), then we get same result(no change); there should not be any change because we are not gaining any new information by this *measurement* We already know that half is polarized in each direction.
- * if we add a third polaroid (same orientation as second), then we get same result(no change); again there should not be any change since we are still not gaining any new information We already know that the remaining half are polarized in the other direction.
- * if we add a third polaroid oriented in a different direction \rightarrow different result ... Now some light gets through the 2nd polaroid

What does this mean? Does it mean that we have somehow recreated the other kind of light? Remove the third polaroid and put calcite in its place to see!! It will turn out that it was the act of measurement(inserting a third polaroid to obtain new information) that disturbed the original system and changed the experimental result.

All of the physics contained in the quantum world is in these simple experiments with lasers, polaroids and calcite crystals we just have to pull it out and we will in our later discussions.

Let me illustrate a dilemma.

Let us start with a large number of photons (10^{23}). Since this very intense beam it behaves like a wave. Classical physics should then be able to explain what happens.

Place a polaroid in a laser beam. Half of the light gets through.

Place a second polaroid at right angles. No light gets through.

Place a third polaroid in between at 45° . Half of the light gets through.

This is easy to explain with waves or electric field vectors and vector components as we saw earlier.

Polaroid 1 in y -direction ($\theta = 90^\circ$ direction)

Polaroid 2 in 45° direction (new y' direction or $\theta = 45^\circ$)

Polaroid 3 in x -direction ($\theta = 0^\circ$ direction)

We have the experiment shown below:

$$\begin{array}{ccccccc} \vec{E}_0 & | & \vec{E}_1 & | & \vec{E}_2 & | & \vec{E}_3 \\ \uparrow & & \uparrow & & \uparrow & & \\ \#1 & & \#2 & & \#3 & & \text{polaroids} \end{array}$$

Analyzing with vectors we have:

$$\vec{E}_0 = E_x \hat{e}_x + E_y \hat{e}_y \quad (7.34)$$

$$E_x = E_y \quad (\text{unpolarized light})$$

$$E^2 = E_x^2 + E_y^2 \rightarrow E_x = E_y = \frac{E}{\sqrt{2}}$$

$$\vec{E}_0 = \frac{E}{\sqrt{2}}(\hat{e}_x + \hat{e}_y) \quad (7.35)$$

$$\text{Energy} = E^2 \rightarrow \text{total energy in beam}$$

$$E_x^2 = \frac{E^2}{2} \rightarrow \frac{1}{2} \text{ of energy in } x - \text{ polarized light}$$

$$E_y^2 = \frac{E^2}{2} \rightarrow \frac{1}{2} \text{ of energy in } y - \text{ polarized light}$$

After 1

$$\vec{E}_1 = E_y \hat{e}_y = \frac{E}{\sqrt{2}} \hat{e}_y \rightarrow \text{energy} = \frac{E^2}{2} = \frac{1}{2} \text{ of original energy} \quad (7.36)$$

After 2

$$\begin{aligned} \vec{E}_2 &= \frac{E}{\sqrt{2}} \sin 45^\circ (\cos 45^\circ \hat{e}_x + \sin 45^\circ \hat{e}_y) = \frac{E}{2\sqrt{2}} (\hat{e}_x + \hat{e}_y) \\ \rightarrow \text{energy} &= \frac{E^2}{4} = \frac{1}{4} \text{ of original energy} \end{aligned} \quad (7.37)$$

After 3

$$\vec{E}_3 = \frac{E}{2\sqrt{2}}\hat{e}_x \rightarrow \text{energy} = \frac{E^2}{8} = \frac{1}{8} \text{ of original energy} \quad (7.38)$$

or we get some light!

Now remove the 45 degree polaroid.... We have

Polaroid 1 in y -direction ($\theta = 90^\circ$ direction)

Polaroid 3 in x -direction ($\theta = 0^\circ$ direction)

After 1

$$\vec{E}_1 = E_y\hat{e}_y = \frac{E}{\sqrt{2}}\hat{e}_y \rightarrow \frac{1}{2} \text{ of original energy} \quad (7.39)$$

After 2

$$\vec{E}_3 = 0 \rightarrow \text{energy} = 0 \quad (7.40)$$

or we get no light!

So, again, classical physics has no trouble explaining what is happening for intense beams *where we can talk about dividing the beam energy* between different processes. At each step, the explanation will say that some fraction of the photons or some fraction of the energy does not pass through a particular polaroid and at each stage the intensity of the beam, which is related to the number of photons or the energy, will change in the expected manner.

But what about any *particular* photon in the beam, each of which is polarized at 45° to the preferred axis at polaroid #3?

Now the answer is not clear at all and the fundamental dilemma of the subatomic world rears its ugly head.

Remember, each individual photon cannot be subdivided - its energy cannot be split.

As has become clear during our discussions of quantum mechanics, this question about what will happen to a particular photon under certain conditions is *not very precise* and if we do not ask precise questions, then we should not be surprised that we get confusing answers or answers that seemingly defy reason.

In order for the theory to make clear predictions about experiments, we will have to learn how to ask precise questions. It will take time but we will learn how.

Remember, only questions about the results of experiments have a real significance in physics and it is only such questions that theoretical physics has to

consider. The questions and the subsequent experiments devised to answer the questions must be clear and precise, however.

In this case, we can make the question clear by doing the experiment with a beam containing only one photon(very weak beam) and observe what happens as it arrives at the polaroid.

It was not until the 1980's that experiments of this sort could actually be carried out.

In particular, we make a *simple observation* to see whether or not it passes through the polaroid.

The most important result is that this single photon either passes through the polaroid or it does not. Nothing else happens.

We never observe $1/2$ the energy of a single photon passing through the polaroid. We always observe either no energy or all the energy.

One never observes a part of a photon passing through and a part getting absorbed in the polaroid.

In addition, if a photon gets through, then observation shows that its polarization is in the direction parallel to the optic axis of this particular polaroid (instead of at some arbitrary angle with respect to that axis as it was before it encountered the polaroid). This happens no matter what its polarization was before the polaroid. No matter what its initial polarization, a definite fraction of the photons seem to get through the polaroid.

In a beam of N *identical* photons, each will *behave independently* as the single photon did. *No experiment* can determine which photon will pass through and which will not, even though they are all identical. In each experiment, however, exactly $1/2$ of the total energy and $1/2$ of the photons will pass through polaroid #3.

The only way this result can be interpreted is to say that each photon has a *probability* = $1/2$ of passing through. We are forced into a *probabilistic point of view* by the fact that the energy of the photons in an electromagnetic wave is *quantized (not continuous)*. This is the same result as in other experiments we have discussed.

Quantization forces us to use probability!

We have managed to preserve the indivisibility of the photons(or ultimately the quantization of their energy). We were able to do this *only by abandoning the determinacy* of classical physics with respect to identical objects, i.e., in classical physics if two objects are prepared identically, then they will behave the

same way in identical experiments (within experimental error).

The results in this experiment are not determined by the experimental conditions(initial) under control of the experimenter, as they would have been according to classical ideas.

The most that we will be able to predict in any experiment is a set of possible results, with a probability of occurrence for each.

The experiment described above involving a single photon polarized at an angle to the optic axis, represents the only experimental and theoretical question we can ask.

It is what I shall call a *go-nogo* experiment.

Does the photon go through or is it absorbed? That is the only *legitimate* question we can ask in this case.

So if I arrange my experiment so that only one photon is inside the apparatus at any one time we have a *problem*. Let us redo the experiment with two polaroids at 45° .

What happens as it comes to the first polaroid?

It *either* gets through *or* it does not or **GO-NOGO**.

At the second polaroid(if it got through the first) it is again **GO-NOGO**.

In fact, *at the end*, it either gets through or it does not!

Now send another single photon through. It is identical to the first and is also **GO-NOGO**.

What they do is in no way related to each other.

Wait a century before sending the second photon so the first does its thing long before the second is even created.

What happens after a large number of unpolarized photons are sent through a single polaroid? The answer is that $1/2$ get through!

Just look at the two polaroids in the experiment. If a photon gets through the first polaroid, what happens at the second?

GO-NOGO

But if we send many, then we get exactly $1/2$ of those getting through the first getting through the second(at 45°).

The only interpretation that works here is that after a photon passes through the first, the photon has a probability of $1/2$ of passing through the second.

We do not know and cannot predict what *any* particular photon will do, but we can predict what a *large number* will do.

That is how probability works

As we will see QM will force us to say that between the first and second polaroids the photon is in an unresolved indeterminate state with a 50-50 chance of passing through the second 45° polaroid. As we have said earlier, the photon state is one of latency or propensities waiting to be actualized.

This is once again the mysterious superposition property rearing its ugly head!

We shall see that questions like....

What decides whether a photon goes through?
When does the photon decide whether it will pass through?
How does a photon change its polarization direction?

cannot be answered by experiment and therefore they must be regarded as outside the domain of quantum theory and possibly all of physics and cannot be relevant to any new theory we might develop.

What will our theory of quantum mechanics say about the state of the single photon?

It will be shown that the photon polarized at an angle to the optic axis is in a very *special kind* of state that we will call a *superposition* of being polarized perpendicular to the optic axis and of being polarized parallel to the optic axis.

In this state, there will exist an *extraordinary* kind of relationship between the two kinds(mutually perpendicular directions) of polarization.

The meaning of the word *superposition* follows from the *mathematical formalism and language* we have developed. It represents a new physical connection to mathematics.

This is suggested by an attempt to express the meaning of superposition in ordinary language(words). If we attempt to explain the behavior of the photon polarized at an angle to the optic axis using ordinary language, then we would

have to say something like this

not polarized *parallel* to the optic axis
not polarized *perpendicular* to the optic axis
not simultaneously possessing *both* polarizations
not possessing *neither* polarization

For this experiment with only two possible polarizations, this exhausts all the logical possibilities allowed by ordinary words.

Superposition is something *completely different* than any of the above and it is *not all* of the above. Its physical content will, however, be *precise and clear* in the new mathematical formalism.

When the photon encounters the polaroid, we are observing it. We are observing whether it is polarized perpendicular or parallel to the optic axis of the polaroid. The effect of this measurement will be to end up with the photon having one or the other polarizations. It always makes a *jump* from a state of superposition to a state of a *definite* polarization.

Which of the two states it *jumps* to cannot be predicted. We can, however, predict the probability of each for a large set of identical measurements.

If it "jumps" into the parallel state, it passes through. If it *jumps* into the perpendicular state, it gets absorbed.

We will have a great deal more to say about the two new words, *superposition* and *jump*, as we proceed. We will also have to show that it did not have the property that is observed *after* the polaroid *before* entering the polaroid and that we are not *just finding out* what that prior property was - we will show this later!

7.3 Using Photons and Polarization to Explain How Quantum Mechanics Works?

We now look at photons and polarization in more detail (repeating much of what we just said) and using our mathematical language to understand how quantum mechanics works.

As we said, many experiments indicate that electromagnetic waves have a *vector* property called *polarization*.

Suppose that we have an electromagnetic wave (we will just say *light* from now on) passing through a piece of *polaroid* material.

Remembering our earlier discussion, the polaroid material has the property that

it only allows the light with polarization vector oriented *parallel* to a *preferred* direction in the polaroid (called the *optic axis*) to pass through the material.

Thinking classically once again, if an incident beam of light is polarized *parallel* to the optic axis (as in the figure below), then experiment says that *all* of its energy gets through the polaroid.

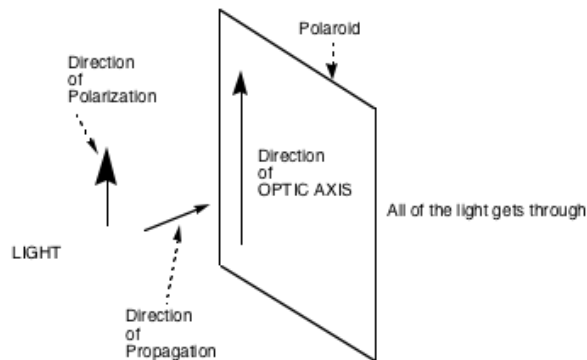


Figure 7.5: Polarized parallel

If, instead, the light is polarized *perpendicular* to the optic axis (as in the figure below), then experiment says that none of its energy gets through the polaroid.

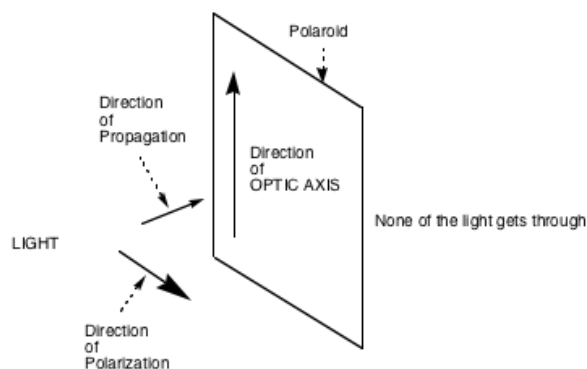


Figure 7.6: Polarized perpendicular

In a more general case, if it is polarized at an *angle* α to the optic axis (as in the figure below), then experiment says that a *fraction* of its energy gets through the polaroid.

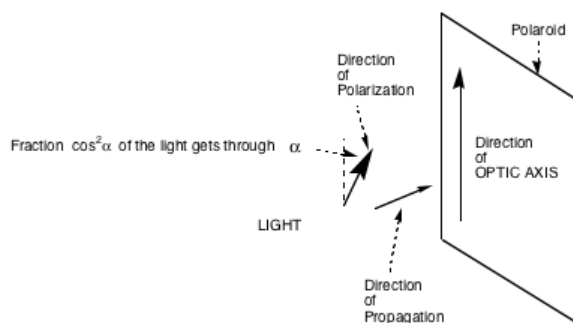


Figure 7.7: Polarized at angle α

By definition, when we specify the polarization of light, we are actually giving the direction of the electric field vector associated with the light. The polarization property or polarization vector of light depends only on the direction of the vector.

Classically, in Maxwell's theory light waves are represented by *plane electromagnetic waves*. This means that the associated electric field vector \vec{E} and the associated magnetic field vector \vec{B} are both perpendicular to the direction of propagation specified by a third vector \vec{k} . According to Maxwell theory, if we choose (arbitrary) the direction of propagation to be the z -axis, which is specified by the unit vector \hat{e}_z , then \vec{E} and \vec{B} lie somewhere in the $x-y$ plane, which is the plane perpendicular to the direction of propagation. \vec{E} and \vec{B} are perpendicular to each other.

Now, any vector in the $x-y$ plane can be specified in terms of a pair of orthonormal vectors (called the basis) in that plane. For light, the pair of orthonormal vectors are called the *basis polarization vectors*.

Two standard sets of orthonormal vectors are often chosen when one discusses polarization. One of the two sets is

$$\hat{e}_x = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \hat{e}_y = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad (7.41)$$

As we will see, they correspond to *plane-polarized* waves.

A second orthonormal set is

$$\hat{\epsilon}_R = \hat{\epsilon}_+ = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix}, \quad \hat{\epsilon}_L = \hat{\epsilon}_- = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix} \quad (7.42)$$

They will correspond to *circularly-polarized waves*.

For classical electromagnetic fields, a light wave propagating in the z -direction is usually described (using one the two orthonormal sets) by electric field vectors of the form given below.

Plane-polarized basis:

$$\vec{E}(\vec{r}, t) = \begin{pmatrix} E_x(\vec{r}, t) \\ E_y(\vec{r}, t) \\ 0 \end{pmatrix} = E_x(\vec{r}, t) \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + E_y(\vec{r}, t) \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = E_x(\vec{r}, t) \hat{\epsilon}_x + E_y(\vec{r}, t) \hat{\epsilon}_y \quad (7.43)$$

Circular-polarized basis:

$$\vec{E}(\vec{r}, t) = \begin{pmatrix} E_x(\vec{r}, t) \\ E_y(\vec{r}, t) \\ 0 \end{pmatrix} = \frac{E_x(\vec{r}, t) + iE_y(\vec{r}, t)}{\sqrt{2}} \hat{\epsilon}_R + \frac{E_x(\vec{r}, t) - iE_y(\vec{r}, t)}{\sqrt{2}} \hat{\epsilon}_L \quad (7.44)$$

By convention and for mathematical simplicity, we represent the field components by

$$\begin{aligned} E_x(\vec{r}, t) &= E_x^0 e^{i(kz - \omega t + \alpha_x)} \\ E_y(\vec{r}, t) &= E_y^0 e^{i(kz - \omega t + \alpha_y)} \end{aligned} \quad (7.45)$$

where $k = 2\pi/\lambda$, λ is the wavelength, ω is the angular frequency, $kz - \omega t + \alpha_x$ and $kz - \omega t + \alpha_y$ are the respective phases, α_x and α_y are the corresponding phases at $x = t = 0$ and E_x^0 and E_y^0 are the (real) amplitudes of the electric field components. This is just the traveling wave formalism we developed earlier.

The actual(physical) electric field components are given by the *real parts* of the complex exponential expressions

$$\begin{aligned} E_x(\vec{r}, t) &= E_x^0 e^{i(kz - \omega t + \alpha_x)} = E_x^0 (\cos(kz - \omega t + \alpha_x) + i \sin(kz - \omega t + \alpha_x)) \\ E_{x,physical}(\vec{r}, t) &= E_x^0 \cos(kz - \omega t + \alpha_x) \end{aligned} \quad (7.46)$$

$$\begin{aligned} E_y(\vec{r}, t) &= E_y^0 e^{i(kz - \omega t + \alpha_y)} = E_y^0 (\cos(kz - \omega t + \alpha_y) + i \sin(kz - \omega t + \alpha_y)) \\ E_{y,physical}(\vec{r}, t) &= E_y^0 \cos(kz - \omega t + \alpha_y) \end{aligned} \quad (7.47)$$

What do these expressions say about the physical electric field vector?

These relations say that in ideal monochromatic light (single wavelength or frequency) the x - and y -components of the electric field vector oscillate with a definite frequency at each point along the direction of propagation.

For simplicity, let us look at position $z = 0$. We have

$$E_x(\vec{r}, t) = E_x^0 \cos(\omega t + \alpha_x) \quad , \quad E_y(\vec{r}, t) = E_y^0 \cos(\omega t + \alpha_y) \quad (7.48)$$

where

$$\begin{aligned} \omega &= 2\pi f \\ f &= \text{frequency} \\ \lambda &= \text{wavelength} \\ c &= \text{speed} = \lambda f \end{aligned}$$

The total electric field vector is a sum or superposition of the two components

$$\vec{E}(\vec{r}, t) = E_x(\vec{r}, t)\hat{\varepsilon}_x + E_y(\vec{r}, t)\hat{\varepsilon}_y \quad (7.49)$$

or it is the resultant effect produced by superposing two independent orthogonal oscillations.

Case #1: The orthogonal oscillations are *initially in phase*, i.e., $\alpha_x = \alpha_y = 0$ for simplicity. We then have

$$\vec{E}(\vec{r}, t) = (E_x^0\hat{\varepsilon}_x + E_y^0\hat{\varepsilon}_y) \cos(\omega t) = \vec{E}_0 \cos(\omega t) \quad (7.50)$$

This says that the electric field vector(the tip) oscillates with the *same* frequency in a *single* direction.

This is called *linearly-polarized or plane-polarized light*.

Case #2: When the orthogonal oscillations are *not initially in phase* the resultant electric vector moves around in an ellipse, i.e., the direction is changing with time.

$$\vec{E}(\vec{r}, t) = E_x(\vec{r}, t)\hat{\varepsilon}_x + E_y(\vec{r}, t)\hat{\varepsilon}_y = E_x^0 \cos(\omega t) \hat{\varepsilon}_x + E_y^0 \cos(\omega t + \alpha) \hat{\varepsilon}_y \quad (7.51)$$

where we have chosen $\alpha_x = 0$, $\alpha_y = \alpha$.

This corresponds to an equation for the vector tip given by

$$\left(\frac{x}{E_x^0}\right)^2 + \left(\frac{y}{E_y^0}\right)^2 - 2 \cos \alpha \frac{x}{E_x^0} \frac{y}{E_y^0} = \sin^2 \alpha \quad (7.52)$$

which looks like

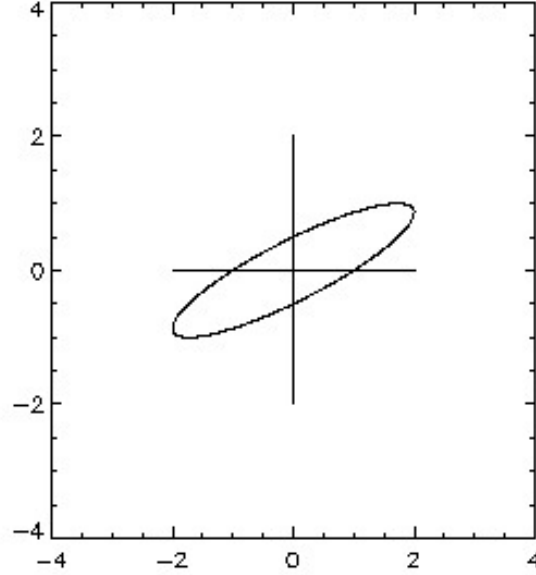


Figure 7.8: Elliptically polarized light

for $E_x^0 = 2.0, E_y^0 = 1.0, \alpha = \pi/6$.

This is called *elliptically-polarized light*. If the ellipse is a circle, then it is called *circularly-polarized light*.

If the tip of the electric field vector when we look at it as the light comes straight toward us, goes around in a counterclockwise direction, the light is right-hand circularly polarized. If it goes clockwise, the light is left-hand circularly polarized.

Mathematically, the relationship between the polarization state of the light and the \vec{E} vector is shown by a few examples below.

- (1) If $E_y = 0$, then the wave is *plane-polarized in the x-direction*

$$\vec{E} = E_x \hat{e}_x = E_x \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad (7.53)$$

- (2) If $E_x = 0$, then the wave is *plane-polarized in the y-direction*

$$\vec{E} = E_y \hat{e}_y = E_y \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad (7.54)$$

(3) If $E_x = E_y$, then the wave is *plane-polarized at 45°*

$$\vec{E} = E_x \hat{e}_x + E_y \hat{e}_y = E_x \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + E_y \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = E_x \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \quad (7.55)$$

(4) If $E_y = -iE_x = e^{-i\pi/2}E_x$, then the y -component lags the x -component by 90° (out of phase by $-\pi/2$) and the wave is *right-circularly polarized*

$$\vec{E} = E_x \hat{e}_R = E_x \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix} \quad (7.56)$$

(5) If $E_y = iE_x = e^{i\pi/2}E_x$, then the y -component leads the x -component by 90° (out of phase by $+\pi/2$) and the wave is *left-circularly polarized*

$$\vec{E} = E_x \hat{e}_L = E_x \begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix} \quad (7.57)$$

This set of polarization properties is almost sufficient for our discussions.

One final case to consider is called *unpolarized light*.

If the initial relative x - and y -phase, i.e., $\alpha_x - \alpha_y$ is not kept fixed, then the electric field vector will oscillate in different directions so that the polarization is constantly changing. In particular, if the polarization direction changes more rapidly than we can detect it, then the light is called unpolarized.

Let us now return to the question - *what is a polaroid?*

In order to understand the answer to this question, we first discuss *birefringence*.

An interesting effect of polarization is that there are substances for which the index of refraction is different for light that is linearly polarized in different directions relative to preferred axes of the material.

Suppose some material consists of long, nonspherical molecules (much longer than they are wide) and suppose that these molecules are arranged in the material with their long axes parallel.

What happens when an oscillating electric field passes through this material?

Suppose that because of the structure of the material, the electrons in the material respond more easily to oscillations in the direction parallel to the long axes of the molecules than they would respond if the electric field tries to push them

perpendicular to the long axes. In this way we expect a different response for polarization in different directions.

The direction parallel to the long axes is called the optic axis. When the polarization is parallel to the optic axis or along the long axes of the molecules, the index of refraction is different then when the polarization is perpendicular to the optic axis. Such a material is called *birefringent*. It has two indices of refraction depending on the direction of the polarization (relative to the optic axis) inside the substance.

The index of refraction affects the electric field as it propagates through the material as shown below:

$$\vec{E}(\vec{r}, t) = \vec{E}_0 \cos(kz - \omega t) = \vec{E}_0 \cos(kz - \omega z/v) = \vec{E}_0 \cos(k - n\omega/c)z \quad (7.58)$$

where n = index of refraction and $v = c/n$ = speed of light in the medium.

What do we expect to happen if we shine polarized light through a plate of birefringent material?

If the polarization is parallel to the optic axis, the light is transmitted with one velocity; if the polarization is perpendicular to the optic axis, the light is transmitted with a different velocity.

What happens when the light is linearly polarized 45° to the optic axis?

Light that is linearly polarized at 45° to the optic axis is represented by the electric field

$$\vec{E} = E_x \hat{e}_x + E_y \hat{e}_y = E_x \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \quad (7.59)$$

or

$$\begin{aligned} \vec{E}(\vec{r}, t) &= E_x^0 \cos((k - n_x \omega/c)z) \hat{e}_x + E_y^0 \cos((k - n_y \omega/c)z) \hat{e}_y \\ &= E^0 \cos 45^\circ \cos((k - n_x \omega/c)z) \hat{e}_x + E^0 \sin 45^\circ \cos((k - n_y \omega/c)z) \hat{e}_y \\ &= \frac{E^0}{\sqrt{2}} (\cos((k - n_x \omega/c)z) \hat{e}_x + \cos((k - n_y \omega/c)z) \hat{e}_y) \end{aligned} \quad (7.60)$$

This corresponds to representing 45° polarization as a superposition of x - and y -polarizations of equal amplitudes, frequency and in phase. Let us assume that we choose the y -axis to line up with the optic axis (x -axis is perpendicular to the optic axis). This choice is always arbitrary. As the light passes through, the phases change at different rates, i.e., at z' the phases will not be equal

$$((k - n_x \omega/c)z') \neq ((k - n_y \omega/c)z') \quad (7.61)$$

Thus, if the two components start out in phase, they will go in and out of phase as they travel through the material. The phase difference is proportional to the depth into the material, i.e.,

$$\Delta(\text{phase}) = \frac{\omega}{c} z' (n_y - n_x) \quad (7.62)$$

If the thickness is just right to introduce a 90° phase shift between the x - and y -components, the linearly polarized (entering material) light will leave the material circularly polarized. A plate with such a thickness is called a *quarter-wave plate*. In this case we have

Entering:

$$\frac{E^0}{\sqrt{2}} (\hat{\varepsilon}_x + \hat{\varepsilon}_y) \cos(\omega t) \quad (7.63)$$

Leaving:

$$\frac{E^0}{\sqrt{2}} (\cos(\omega t) \hat{\varepsilon}_x + \cos(\omega t + \pi/2) \hat{\varepsilon}_y) = \frac{E^0}{\sqrt{2}} (\cos(\omega t) \hat{\varepsilon}_x + \sin(\omega t) \hat{\varepsilon}_y) \quad (7.64)$$

If we send the light through two such quarter-wave plates, then it exits linearly polarized again in a direction at right angles to the original direction. In this case we have

Entering:

$$\frac{E^0}{\sqrt{2}} (\hat{\varepsilon}_x + \hat{\varepsilon}_y) \cos(\omega t) \quad (7.65)$$

Leaving:

$$\frac{E^0}{\sqrt{2}} (\cos(\omega t) \hat{\varepsilon}_x + \cos(\omega t + \pi) \hat{\varepsilon}_y) = \frac{E^0}{\sqrt{2}} (\hat{\varepsilon}_x - \hat{\varepsilon}_y) \cos(\omega t) \quad (7.66)$$

Example: Birefringence of cellophane

Cellophane consists of long, fibrous molecules. It is not isotropic since the fibers lie preferentially in one direction. We create a beam of linearly polarized light by sending unpolarized light through a sheet of polaroid. As we have said earlier, polaroid has the useful property that it transmits light that is linearly polarized parallel to preferred axis of the polaroid with very little absorption, but light polarized perpendicular to the preferred direction is strongly absorbed (not transmitted).

When the unpolarized beam is sent through the polaroid, only that part of the beam (the component of the electric field) that is vibrating parallel to the preferred axis of the polaroid gets through. In this manner, the exiting beam is linearly polarized (in the direction of the preferred axis).

This same property of a polaroid is useful in determining the direction of polarization of any linearly polarized beam or in determining whether the beam is linearly polarized or not.

If the beam is linearly polarized, it will not be transmitted through the sheet when the preferred axis of the polaroid is orthogonal to the direction of the polarization.

If the transmitted beam intensity is independent of the orientation of the polaroid, then the beam is not linearly polarized.

The birefringence of cellophane is illustrated by setup below:

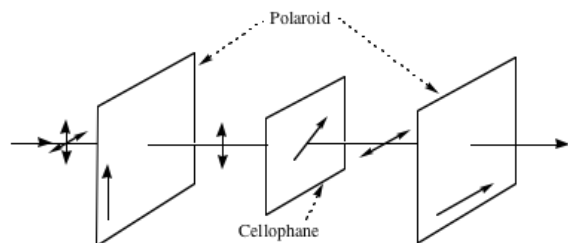


Figure 7.9: Experiment with cellophane

The first polaroid produces a linearly polarized beam (from an entering unpolarized beam). The linearly polarized beam then passes through the cellophane and finally through a second polaroid. The second polaroid detects the effect of the cellophane on the polarization of the beam.

If we initially set the axes of the two polaroids orthogonal to each other, no light is transmitted through the pair (no cellophane present).

We now introduce the cellophane as shown in the diagram. If we rotate the cellophane sheet around the beam axis, we find that some light transmits through the second polaroid. In addition, there are two orthogonal orientations of the cellophane which permit no light to pass through the second polaroid.

These two directions are such that the cellophane has no effect on the linear polarization of the beam so that none gets through the second polaroid. The directions are parallel and perpendicular to the optic axis of the cellophane.

We assume that the light passes through the cellophane with two different speeds in these two different directions, but it is transmitted without changing the direction of polarization. When the cellophane is turned halfway between these two directions (as in the diagram above) we observe that the light passing through the second polaroid is bright.

It turns out that ordinary cellophane is very close to half-wave thickness for most of the colors in white light. Such a sheet will turn the direction of linear polarization through 90° if the incident linearly polarized beam makes an angle of 45° with the optic axis, so that the beam emerging from the cellophane is then vibrating in the right direction to pass through the polaroid sheet.

The cellophane will be a half-wave plate for only one wavelength in the white light and the transmitted light will be that color. The transmitted color depends on the thickness of the cellophane.

Finally we explain polaroids.

Polaroids are materials where not only the index of refraction but also the amount of absorption is different for light polarized in different directions. Polaroid consists of a thin layer of small crystals of herapathite (a salt of iodine and quinine), all aligned with their axes parallel (the optic axis). These crystals absorb light when the polarization is orthogonal to this direction and do not absorb light when the polarization is parallel.

As we said earlier, if we send light into a polaroid so that the light is linearly polarized at an angle θ to the optic axis. What intensity will come through?

We simply resolve the incident light (its electric field) into components parallel($\cos \theta$) and perpendicular($\sin \theta$) to the optic axis. The light that comes out of the polaroid is only the $\cos \theta$ part; the $\sin \theta$ part is absorbed. The amplitude that is transmitted is smaller than the amplitude that entered.

Entering:

$$E^0 (\cos \theta \hat{\epsilon}_x + \sin \theta \hat{\epsilon}_y)$$

Leaving:

$$E^0 \cos \theta \hat{\epsilon}_x$$

The intensity or brightness or energy is: Entering:

$$(E^0 \cos \theta)^2 + (E^0 \sin \theta)^2 = (E^0)^2$$

Leaving:

$$(E^0 \cos \theta)^2 = (E^0)^2 (\cos \theta)^2 < (E^0)^2$$

The absorbed intensity is $(E^0 \sin \theta)^2$.

The interesting experiment, which we have already mentioned is the following. We know that no light will be transmitted through two polaroids if their optic axes are orthogonal.

Now, however, place a third polaroid with its optic axis at with respect to the first polaroid between them. Observations show that some light will now be

transmitted through the second polaroid.

We know that polaroids only absorb light - they do not create light.

Nevertheless, the addition of the third polaroid allows more light get transmitted.

As before, using components of the corresponding electric fields we can explain these results easily.

Only Two Polaroids:

Entering 1st Polaroid:

$$E^0 (\cos \theta \hat{\varepsilon}_{x_1} + \sin \theta \hat{\varepsilon}_{y_1})$$

Leaving 1st Polaroid:

$$E^0 \cos \theta \hat{\varepsilon}_{x_2}$$

Entering 2nd Polaroid:

$$E^0 \cos \theta \hat{\varepsilon}_{x_2}$$

Leaving 2nd Polaroid:

$$0$$

So no energy (no light) gets through.

Three Polaroids:

Entering 1st Polaroid:

$$E^0 (\cos \theta \hat{\varepsilon}_{x_1} + \sin \theta \hat{\varepsilon}_{y_1})$$

Leaving 1st Polaroid:

$$E^0 \cos \theta \hat{\varepsilon}_{x_2}$$

Entering 2nd Polaroid:

$$E^0 \cos \theta (\cos 45^\circ \hat{\varepsilon}_{x_2} + \sin 45^\circ \hat{\varepsilon}_{y_2})$$

Leaving 2nd Polaroid:

$$E^0 \cos \theta \cos 45^\circ \hat{\varepsilon}_{x_2} = \frac{1}{\sqrt{2}} E^0 \cos \theta \hat{\varepsilon}_{x_2}$$

Entering 3rd Polaroid:

$$E^0 \cos \theta \cos 45^\circ (\cos 45^\circ \hat{\varepsilon}_{x_3} + \sin 45^\circ \hat{\varepsilon}_{y_3})$$

Leaving 3rd Polaroid:

$$E^0 \cos \theta \cos 45^\circ \cos 45^\circ \hat{\varepsilon}_{x_3} = \frac{1}{2} E^0 \cos \theta \hat{\varepsilon}_{x_3}$$

In this case, energy = $(E^0 \cos \theta)^2/4$ gets transmitted.

We have assumed that the x -axis for each polaroid is its optic axis.

All of the preceding discussion takes place at the classical level. All the phenomena discussed can be explained with classical physics concepts.

As we have seen, all such explanations fail at the quantum level where ideas like electric fields and components of electric fields will break down.

7.4 The Quantum Theory of Photon Polarization

We now carry out the details of a special case that will illustrate how Quantum Mechanics works and also illustrate the mathematical formalism that we developed earlier. This discussion is more mathematical than the earlier parts of the book, but you have all the tools needed and you will benefit if you persevere and work your way through the material.

As we mentioned earlier, the electric field vector \vec{E} of plane electromagnetic waves lies in a plane perpendicular to the direction of propagation of the wave. Choosing the z -axis as the direction of propagation, we can represent the electric field vector as a 2-dimensional vector in the $x - y$ plane. This means that we will only require *two numbers* to describe the electric field.

Since the polarization state of the light is directly related to the electric field vector, this means that we can also represent the polarization states of the photons by 2-component column vectors or ket vectors of the form

$$|\psi\rangle = \begin{pmatrix} \psi_x \\ \psi_y \end{pmatrix} \quad (7.67)$$

where we assume the normalization condition $\langle\psi | \psi\rangle = 1$. This gives the condition

$$|\psi_x|^2 + |\psi_y|^2 = 1 \quad (7.68)$$

Some examples are:

$$|x\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \rightarrow \text{x - polarized photon (linear or plane polarization)} \quad (7.69)$$

$$|y\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \rightarrow \text{y - polarized photon (linear or plane polarization)} \quad (7.70)$$

$$|R\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} \rightarrow \text{right-circular polarized photon} \quad (7.71)$$

$$|L\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} \rightarrow \text{left-circular polarized photon} \quad (7.72)$$

$$|45\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \rightarrow \text{photon linearly polarized at } 45^\circ \text{ to the x-axis} \quad (7.73)$$

Note that we can write

$$|R\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{i\pi/2} \end{pmatrix} \quad (7.74)$$

so the relative(difference) phase of the components is $\pi/2$ as discussed earlier.

The bra-vector or linear functional corresponding to the ket vector is given by the row vector

$$\langle\psi| = \begin{pmatrix} \psi_x^* & \psi_y^* \end{pmatrix} \quad (7.75)$$

which clearly implies via our inner product rules

$$\langle\psi|\psi\rangle = \begin{pmatrix} \psi_x^* & \psi_y^* \end{pmatrix} \begin{pmatrix} \psi_x \\ \psi_y \end{pmatrix} = |\psi_x|^2 + |\psi_y|^2 = 1 \quad (7.76)$$

In general, for

$$|\varphi\rangle = \begin{pmatrix} \varphi_x \\ \varphi_y \end{pmatrix} \quad (7.77)$$

the inner product rule says

$$\langle\varphi|\psi\rangle = \begin{pmatrix} \varphi_x^* & \varphi_y^* \end{pmatrix} \begin{pmatrix} \psi_x \\ \psi_y \end{pmatrix} = \varphi_x^* \psi_x + \varphi_y^* \psi_y = \langle\psi|\varphi\rangle^* \quad (7.78)$$

We also have

$$\begin{aligned} \langle x|x\rangle &= 1 = \langle y|y\rangle \text{ and } \langle x|y\rangle = 0 = \langle y|x\rangle \rightarrow \text{orthonormal set} \\ \langle R|R\rangle &= 1 = \langle L|L\rangle \text{ and } \langle R|L\rangle = 0 = \langle L|R\rangle \rightarrow \text{orthonormal set} \end{aligned} \quad (7.79)$$

Each of these two sets is a basis for the 2-dimensional vector space of polarization states since any other state vector can be written as a linear combination of them, i.e.,

$$|\psi\rangle = \begin{pmatrix} \psi_x \\ \psi_y \end{pmatrix} = \psi_x \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \psi_y \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \psi_x |x\rangle + \psi_y |y\rangle \quad (7.80)$$

$$|\psi\rangle = \begin{pmatrix} \psi_x \\ \psi_y \end{pmatrix} = \frac{\psi_x - i\psi_y}{2} \begin{pmatrix} 1 \\ i \end{pmatrix} + \frac{\psi_x + i\psi_y}{2} \begin{pmatrix} 1 \\ -i \end{pmatrix} = \frac{\psi_x - i\psi_y}{\sqrt{2}} |R\rangle + \frac{\psi_x + i\psi_y}{\sqrt{2}} |L\rangle \quad (7.81)$$

We can find the components along the basis vectors using

$$\begin{aligned} \langle x|\psi\rangle &= \langle x|(\psi_x |x\rangle + \psi_y |y\rangle) = \psi_x \langle x|x\rangle + \psi_y \langle x|y\rangle = \psi_x \\ \langle y|\psi\rangle &= \langle y|(\psi_x |x\rangle + \psi_y |y\rangle) = \psi_x \langle y|x\rangle + \psi_y \langle y|y\rangle = \psi_y \end{aligned} \quad (7.82)$$

or

$$|\psi\rangle = |x\rangle \langle x|\psi\rangle + |y\rangle \langle y|\psi\rangle \quad (7.83)$$

and similarly

$$|\psi\rangle = |R\rangle \langle R | \psi \rangle + |L\rangle \langle L | \psi \rangle \quad (7.84)$$

Basically, we are illustrating examples of a *superposition principle*, which says that any arbitrary polarization state can be written as a superposition (linear combination) of x - and y -polarization states or equivalently, as a superposition of right- and left-circularly polarized states.

Our earlier discussions of a beam of light passing through a polaroid can now be recast in terms of these polarization states.

Classical physics (and now quantum physics) says that the beam is a superposition of an x -polarized beam and a y -polarized beam and when this beam passes through an x -polaroid, its effect is to remove the y -polarized beam and pass the x -polarized beam through unchanged.

The energy of the beam is given by $|\vec{E}|^2$, which is proportional to $|\psi_x|^2 + |\psi_y|^2$. Thus, the beam energy after passing through an x -polaroid is proportional to $|\psi_x|^2$. The fraction of the beam energy or the fraction of the number of photons in the beam that passes through is given by

$$\frac{|\psi_x|^2}{|\psi_x|^2 + |\psi_y|^2} = |\psi_x|^2 = |\langle x | \psi \rangle|^2 \quad (7.85)$$

Our earlier discussion for the case of a single photon forced us to set this quantity equal to the probability of a single photon in the state $|\psi\rangle$ passing through an x -polaroid or

$$\begin{aligned} &\text{probability of a photon in the state } |\psi\rangle \\ &\text{passing through an } x\text{-polaroid} = |\langle x | \psi \rangle|^2 \end{aligned}$$

This agrees with our earlier mathematical results.

Using earlier discussions, we define $\langle x | \psi \rangle$ as the *probability amplitude* for the individual photon to pass through the x -polaroid.

Another example confirming these results is light passing through a *prism*. A prism passes right-circularly-polarized(RCP) light and rejects (absorbs) left-circularly-polarized(LCP) light.

Since we can write

$$|\psi\rangle = |R\rangle \langle R | \psi \rangle + |L\rangle \langle L | \psi \rangle \quad (7.86)$$

we can generalize the polaroid result to say

Amplitude that a photon in state $|\psi\rangle$
 passes through the prism as a right-circular polarized photon $= \langle R | \psi \rangle$

Amplitude that a photon in state $|\psi\rangle$
 passes through the prism as a left-circular polarized photon $= \langle L | \psi \rangle$

Polaroids and prisms are examples of *go-nogo* devices. Certain photons are passed through while others are absorbed in these devices.

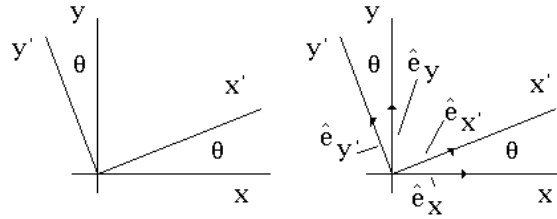
How Many Basis Sets?

We have already seen two examples of basis sets for the 2-dimensional vector space of polarization states, namely,

$$|x\rangle, |y\rangle \quad , \quad |R\rangle, |L\rangle \quad (7.87)$$

In the 2-dimensional vector space there are an infinite number of such orthonormal basis sets related to the $|x\rangle, |y\rangle$ set. They are all equivalent for describing physical systems (they correspond to different orientations of the polaroid in the experimental measurement).

We can obtain the other sets say, $|x'\rangle, |y'\rangle$, by a rotation of the bases (or axes) as shown in the figure on the left below.



We then have in the $x - y$ basis

$$|\psi\rangle = \psi_x |x\rangle + \psi_y |y\rangle = \begin{pmatrix} \psi_x \\ \psi_y \end{pmatrix} = \begin{pmatrix} \langle x | \psi \rangle \\ \langle y | \psi \rangle \end{pmatrix} \quad (7.88)$$

and if we choose to use the equivalent $x' - y'$ basis we have

$$|\psi\rangle = \psi_{x'} |x'\rangle + \psi_{y'} |y'\rangle = \begin{pmatrix} \psi_{x'} \\ \psi_{y'} \end{pmatrix} = \begin{pmatrix} \langle x' | \psi \rangle \\ \langle y' | \psi \rangle \end{pmatrix} \quad (7.89)$$

How are these components related to each other?

We have from earlier that

$$|\psi\rangle = |x\rangle \langle x | \psi \rangle + |y\rangle \langle y | \psi \rangle \quad (7.90)$$

which implies

$$\begin{aligned} \langle x' | \psi \rangle &= \langle x' | x \rangle \langle x | \psi \rangle + \langle x' | y \rangle \langle y | \psi \rangle \\ \langle y' | \psi \rangle &= \langle y' | x \rangle \langle x | \psi \rangle + \langle y' | y \rangle \langle y | \psi \rangle \end{aligned} \quad (7.91)$$

or using matrix multiplication notation

$$\begin{pmatrix} \langle x' | \psi \rangle \\ \langle y' | \psi \rangle \end{pmatrix} = \begin{pmatrix} \langle x' | x \rangle & \langle x' | y \rangle \\ \langle y' | x \rangle & \langle y' | y \rangle \end{pmatrix} \begin{pmatrix} \langle x | \psi \rangle \\ \langle y | \psi \rangle \end{pmatrix} \quad (7.92)$$

So we can transform the basis (transform the components) if we can determine the 2×2 transformation matrix

$$\begin{pmatrix} \langle x' | x \rangle & \langle x' | y \rangle \\ \langle y' | x \rangle & \langle y' | y \rangle \end{pmatrix} \quad (7.93)$$

in the above equation.

It turns out that this result is quite general in the sense that it holds for any two bases, not just the linear polarized bases used to derive it.

For the linear(plane) polarized case, we can think of an analogy to unit vectors along the axes in ordinary space as shown in the above figure on the right. Then we have(by analogy)

$$\begin{aligned} \hat{e}_x \cdot \hat{e}_{x'} &= \cos \theta = \langle x' | x \rangle, & \hat{e}_{x'} \cdot \hat{e}_y &= \sin \theta = \langle x' | y \rangle \\ \hat{e}_x \cdot \hat{e}_{y'} &= \cos \theta = \langle y' | y \rangle, & \hat{e}_{y'} \cdot \hat{e}_x &= -\sin \theta = \langle y' | x \rangle \end{aligned} \quad (7.94)$$

or

$$\begin{aligned} |x\rangle &= \langle x | x' \rangle |x'\rangle + \langle x | y' \rangle |y'\rangle = \cos \theta |x'\rangle - \sin \theta |y'\rangle \\ |y\rangle &= \langle y | x' \rangle |x'\rangle + \langle y | y' \rangle |y'\rangle = \sin \theta |x'\rangle + \cos \theta |y'\rangle \end{aligned} \quad (7.95)$$

or

$$\begin{pmatrix} \langle x' | \psi \rangle \\ \langle y' | \psi \rangle \end{pmatrix} = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} \langle x | \psi \rangle \\ \langle y | \psi \rangle \end{pmatrix} = \hat{R}(\theta) \begin{pmatrix} \langle x | \psi \rangle \\ \langle y | \psi \rangle \end{pmatrix} \quad (7.96)$$

with the transformation matrix, $\hat{R}(\theta)$ given by

$$\hat{R}(\theta) = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \quad (7.97)$$

There are two equivalent ways to interpret these results.

First, we could say it tells us the components of $|\psi\rangle$ in the rotated basis (we keep the vector fixed and rotate the axes).

Second, we can rotate the vector and keep the axes fixed (rotate in the opposite direction). In this case, we regard

$$\begin{pmatrix} \langle x' | \psi \rangle \\ \langle y' | \psi \rangle \end{pmatrix} \quad (7.98)$$

as the new vector $|\psi'\rangle$ whose components in the fixed $x-y$ basis are the same as the components of $|\psi\rangle$ in the $x-y$ basis or

$$\langle x' | \psi \rangle = \langle x | \psi' \rangle, \langle y' | \psi \rangle = \langle y | \psi' \rangle \quad (7.99)$$

For real ψ_x and ψ_y , $|\psi'\rangle$ is the vector rotated clockwise by θ or, regarding $\hat{R}(\theta)$ as a linear operator in the vector space we have

$$|\psi'\rangle = \hat{R}(\theta) |\psi\rangle \quad (7.100)$$

It is a transformation of vectors and is a unitary operator. We can see this as follows:

$$\hat{R}^{-1}(\theta) = \hat{R}(-\theta) = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} = \hat{R}^T(\theta) = \hat{R}^\dagger(\theta) \quad (7.101)$$

Transformation operators are unitary because they transform state vectors which must not change lengths (otherwise probability ideas are messed up). This follows from the fact that unitary transformations preserve inner products (and so they preserve lengths)

$$\begin{aligned} |\psi'\rangle &= \hat{R}(\theta) |\psi\rangle, \quad |\varphi'\rangle = \hat{R}(\theta) |\varphi\rangle \\ \langle \varphi' | \psi' \rangle &= \langle \varphi | \hat{R}^\dagger(\theta) \hat{R}(\theta) | \psi \rangle = \langle \varphi | \hat{R}^{-1}(\theta) \hat{R}(\theta) | \psi \rangle = \langle \varphi | \hat{I} | \psi \rangle = \langle \varphi | \psi \rangle \end{aligned} \quad (7.102)$$

Since $\hat{R}(\theta)$ is a unitary transformation operator for rotations a very general theorem (beyond the scope of this book) says that we can express it as an exponential operator involving the angular momentum operator with respect to the axis of rotation (z -axis), \hat{J}_z , of the form

$$\hat{R}(\theta) = e^{i\theta \hat{J}_z / \hbar} \quad (7.103)$$

PROOF (for the mathematically inclined): We can rewrite $\hat{R}(\theta)$ as

$$\begin{aligned} \hat{R}(\theta) &= \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} = \cos \theta \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + i \sin \theta \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ &= \cos \theta \hat{I} + i \sin \theta \hat{Q} \end{aligned}$$

where

$$\hat{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \text{Identity operator}, \quad \hat{Q} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (7.104)$$

and the physical meaning of the operator \hat{Q} is yet to be determined.

We now show that $\hbar\hat{Q} = \hat{J}_z$. Expanding the exponential in a power series we have

$$\begin{aligned}\hat{R}(\theta) &= e^{i\theta\frac{\hat{J}_z}{\hbar}} = \hat{I} + (i\frac{\hat{J}_z}{\hbar})\theta + \frac{(i\frac{\hat{J}_z}{\hbar})^2}{2!}\theta^2 + \frac{(i\frac{\hat{J}_z}{\hbar})^3}{3!}\theta^3 + \frac{(i\frac{\hat{J}_z}{\hbar})^4}{4!}\theta^4 + \dots \\ &= \hat{R}(0) + \frac{1}{1!}\left.\frac{d\hat{R}(\theta)}{d\theta}\right|_{\theta=0}\theta + \frac{1}{2!}\left.\frac{d^2\hat{R}(\theta)}{d\theta^2}\right|_{\theta=0}\theta^2 + \frac{1}{3!}\left.\frac{d^3\hat{R}(\theta)}{d\theta^3}\right|_{\theta=0}\theta^3 + \frac{1}{4!}\left.\frac{d^4\hat{R}(\theta)}{d\theta^4}\right|_{\theta=0}\theta^4 + \dots\end{aligned}\quad (7.105)$$

Using $\hbar\hat{Q} = \hat{J}_z$, we have $\hat{J}_z^2 = \hbar^2\hat{Q}^2 = \hbar^2\hat{I}$ so that we can write

$$\begin{aligned}\hat{R}(\theta) &= e^{i\theta\frac{\hat{J}_z}{\hbar}} = \hat{I} + (i\frac{\hat{J}_z}{\hbar})\theta + \frac{(i\frac{\hat{J}_z}{\hbar})^2}{2!}\theta^2 + \frac{(i\frac{\hat{J}_z}{\hbar})^3}{3!}\theta^3 + \frac{(i\frac{\hat{J}_z}{\hbar})^4}{4!}\theta^4 + \dots \\ &= \left(1 - \frac{\theta^2}{2!} + \frac{\theta^4}{4!} - \dots\right)\hat{I} + i\left(\frac{\theta}{1!} - \frac{\theta^3}{3!} + \dots\right)\hat{Q} \\ &= \cos\theta\hat{I} + i\sin\theta\hat{Q}\end{aligned}\quad (7.106)$$

which agrees with the earlier result. Thus, we have

$$\hat{J}_z = \hbar\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\quad (7.107)$$

must be the matrix representing the angular momentum operator \hat{J}_z in the $|x\rangle, |y\rangle$ basis. This completes the proof.

Returning to our discussion, we now work out the eigenvectors and eigenvalues of $\hat{R}(\theta)$, which are given by the equation

$$\hat{R}(\theta)|\psi\rangle = \cos\theta + \frac{i}{\hbar}\hat{J}_z|\psi\rangle = c|\psi\rangle\quad (7.108)$$

where c = the eigenvalue corresponding to the eigenvector $|\psi\rangle$. Since all vectors are eigenvectors of the identity operator \hat{I} , we only need to find the eigenvectors and eigenvalues of \hat{J}_z in order to solve the problem for $\hat{R}(\theta)$ (they have the same eigenvectors since they only differ by the identity operator). We let

$$\hat{J}_z|\psi\rangle = \lambda|\psi\rangle\quad (7.109)$$

Now, since $\hat{J}_z^2 = \hbar^2\hat{I}$, i.e.,

$$\hat{J}_z^2 = \hbar^2\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \hbar^2\hat{I}\quad (7.110)$$

we have

$$\hat{J}_z^2|\psi\rangle = \lambda^2|\psi\rangle = \hbar^2\hat{I}|\psi\rangle = \hbar^2|\psi\rangle\quad (7.111)$$

which says that

$$\lambda^2 = \hbar^2 \quad \rightarrow \quad \lambda = \pm\hbar = \text{eigenvalues of } \hat{J}_z\quad (7.112)$$

We can find the corresponding eigenvectors by inserting the eigenvalues into eigenvalue/eigenvector equation

$$\hat{J}_z |J_z = \hbar\rangle = \hbar |J_z = \hbar\rangle \quad (7.113)$$

We assume that

$$|J_z = \hbar\rangle = \begin{pmatrix} a \\ b \end{pmatrix} \quad \text{where} \quad |a|^2 + |b|^2 = 1 \quad (7.114)$$

to get

$$\hbar \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \hbar \begin{pmatrix} -ib \\ ia \end{pmatrix} = \hbar \begin{pmatrix} a \\ b \end{pmatrix} \quad (7.115)$$

This gives the result $ia = b$, which together with the normalization condition says that $a = 1/\sqrt{2}$. We have arbitrarily chosen a to be real since only the relative phase between components will be important in quantum mechanics. This then gives $b = i/\sqrt{2}$. Finally we have the eigenvector

$$|J_z = \hbar\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} = |R\rangle \quad (7.116)$$

Similarly, we get

$$|J_z = -\hbar\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} = |L\rangle \quad (7.117)$$

So the eigenvectors of \hat{J}_z and hence of $\hat{R}(\theta)$ are the RCP and LCP basis states. We then have

$$\begin{aligned} \hat{R}(\theta) |R\rangle &= (\cos \theta \hat{I} + i \sin \theta \frac{\hat{J}_z}{\hbar}) |R\rangle = (\cos \theta + i \sin \theta) |R\rangle = e^{i\theta} |R\rangle \\ \hat{R}(\theta) |L\rangle &= e^{-i\theta} |L\rangle \end{aligned} \quad (7.118)$$

Physically, this says that the $|R\rangle$ and $|L\rangle$ states are only changed by an overall phase factor under rotation of the basis. This allows us to specify what happens to an arbitrary vector $|\psi\rangle$ under rotations.

First, we expand the arbitrary vector in the $|R\rangle, |L\rangle$ basis.

We then apply the rotation operator to obtain

$$\begin{aligned} \hat{R}(\theta) |\psi\rangle &= \hat{R}(\theta) |R\rangle \langle R | \psi \rangle + \hat{R}(\theta) |L\rangle \langle L | \psi \rangle \\ &= e^{i\theta} |R\rangle \langle R | \psi \rangle + e^{-i\theta} |L\rangle \langle L | \psi \rangle \end{aligned} \quad (7.119)$$

or the RCP component is multiplied by the phase factor $e^{i\theta}$ and the LCP component is multiplied by a *different* phase factor $e^{-i\theta}$.

Thus, rotations change the *relative* phase of the components, which is a *real physical change* (as opposed to an overall phase change of the state vector).

Now, it is an experimental fact that if a photon traveling in the z -direction is absorbed by matter, then the z -component of the angular momentum of the absorber increases by \hbar or decreases by \hbar . It never remains the same, nor does it change by any value other than $\pm\hbar$.

We interpret these results to say that the RCP photon is in a state which is an eigenvector of \hat{J}_z with an eigenvalue \hbar for that the photon in that state has spin $= \hbar$. Similarly, an LCP photon has spin $= -\hbar$.

One cannot predict, for any single photon, whether the change will be $+\hbar$ or $-\hbar$. We can, however, predict the probability of either value occurring. In particular, according to our probability formalism, we must have

$$\begin{aligned} |\langle R | \psi \rangle|^2 &= \text{probability of } +\hbar \\ |\langle L | \psi \rangle|^2 &= \text{probability of } -\hbar \end{aligned} \quad (7.120)$$

and the average value of the z -component of the angular momentum is

$$\langle \hat{J}_z \rangle = \sum_{\text{all possibilities}} (\text{eigenvalue}) \times (\text{probability of the eigenvalue}) \quad (7.121)$$

or

$$\langle \hat{J}_z \rangle = \hbar |\langle R | \psi \rangle|^2 - \hbar |\langle L | \psi \rangle|^2 \quad (7.122)$$

In general, a photon is neither pure RCP nor pure LCP and the angular momentum does not have a definite value.

We can still talk in terms of probabilities, however.

The *discreteness* of the angular momentum spectrum once again forces a probabilistic interpretation on us.

We can easily see how all of this works using our mathematical formalism as follows:

$$\begin{aligned} \langle \hat{J}_z \rangle &= \langle \psi | \hat{J}_z | \psi \rangle \\ | \psi \rangle &= | R \rangle \langle R | \psi \rangle + | L \rangle \langle L | \psi \rangle \end{aligned} \quad (7.123)$$

$$\begin{aligned} \langle \hat{J}_z \rangle &= (\langle R | \psi \rangle^* \langle R | + \langle L | \psi \rangle^* \langle L |) \hat{J}_z (| R \rangle \langle R | \psi \rangle + | L \rangle \langle L | \psi \rangle) \\ &= \langle R | \hat{J}_z | R \rangle |\langle R | \psi \rangle|^2 + \langle L | \hat{J}_z | L \rangle |\langle L | \psi \rangle|^2 \\ &\quad + \langle R | \hat{J}_z | L \rangle \langle R | \psi \rangle^* \langle L | \psi \rangle + \langle L | \hat{J}_z | R \rangle \langle L | \psi \rangle^* \langle R | \psi \rangle \\ &= \hbar |\langle R | \psi \rangle|^2 - \hbar |\langle L | \psi \rangle|^2 \end{aligned} \quad (7.124)$$

as above.

Let us return for a moment to the matrix representation of the operator. We have found the following results:

$$\hat{J}_z | R \rangle = +\hbar | R \rangle \quad , \quad \hat{J}_z | L \rangle = -\hbar | L \rangle \quad (7.125)$$

Thus, in the $\{|R\rangle, |L\rangle\}$ basis, these relations imply the matrix representation

$$\hat{J}_z = \begin{pmatrix} \langle R | \hat{J}_z | R \rangle & \langle R | \hat{J}_z | L \rangle \\ \langle L | \hat{J}_z | R \rangle & \langle L | \hat{J}_z | L \rangle \end{pmatrix} = \hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (7.126)$$

which is the standard form of \hat{J}_z in terms of one of the so-called *Pauli matrices*, namely,

$$\hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \rightarrow \hat{J}_z = \hbar \hat{\sigma}_z \quad (7.127)$$

Now

$$|x\rangle = \frac{1}{\sqrt{2}} (|R\rangle + |L\rangle) \quad , \quad |y\rangle = \frac{i}{\sqrt{2}} (|R\rangle - |L\rangle) \quad (7.128)$$

and, therefore, in the $\{|x\rangle, |y\rangle\}$ basis, we have the matrix representation

$$\hat{J}_z = \begin{pmatrix} \langle x | \hat{J}_z | x \rangle & \langle x | \hat{J}_z | y \rangle \\ \langle y | \hat{J}_z | x \rangle & \langle y | \hat{J}_z | y \rangle \end{pmatrix} = \hbar \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (7.129)$$

which is the same form as derived earlier.

Projection Operators

Let us now look at *projection* operators in the context of photon polarization.

The projection operator $|\psi\rangle\langle\varphi|$ can be represented by a 2×2 matrix in the polarization state vector space. It is constructed using the mathematical object called an *outer product*.

$$\hat{P} = |\psi\rangle\langle\varphi| = \begin{pmatrix} \psi_x \\ \psi_y \end{pmatrix} \begin{pmatrix} \varphi_x^* & \varphi_y^* \end{pmatrix} = \begin{pmatrix} \psi_x \varphi_x^* & \psi_x \varphi_y^* \\ \psi_y \varphi_x^* & \psi_y \varphi_y^* \end{pmatrix} \quad (7.130)$$

or *equivalently*, by choosing a basis and finding the matrix representation

$$\hat{P} = \begin{pmatrix} \langle x | \hat{P} | x \rangle & \langle x | \hat{P} | y \rangle \\ \langle y | \hat{P} | x \rangle & \langle y | \hat{P} | y \rangle \end{pmatrix} = \begin{pmatrix} \langle x | \psi \rangle \langle \varphi | x \rangle & \langle x | \psi \rangle \langle \varphi | y \rangle \\ \langle y | \psi \rangle \langle \varphi | x \rangle & \langle y | \psi \rangle \langle \varphi | y \rangle \end{pmatrix} = \begin{pmatrix} \psi_x \varphi_x^* & \psi_x \varphi_y^* \\ \psi_y \varphi_x^* & \psi_y \varphi_y^* \end{pmatrix} \quad (7.131)$$

In particular, we have in the $\{|x\rangle, |y\rangle\}$ basis

$$\begin{aligned} |x\rangle\langle x| &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad , \quad |x\rangle\langle y| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\ |y\rangle\langle x| &= \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad , \quad |y\rangle\langle y| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned} \quad (7.132)$$

From these results, we easily see that

$$|x\rangle\langle x| + |y\rangle\langle y| = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \hat{I} \quad (7.133)$$

and

$$|\psi\rangle = \hat{I}|\psi\rangle = |x\rangle\langle x|\psi\rangle + |y\rangle\langle y|\psi\rangle = \begin{pmatrix} \psi_x \\ \psi_y \end{pmatrix} \quad (7.134)$$

as we specified in our earlier mathematical discussions.

Similarly, we have

$$\hat{I} = |R\rangle\langle R| + |L\rangle\langle L| \quad (7.135)$$

which leads to

$$\hat{J}_z = \hat{J}_z \hat{I} = \hat{J}_z |R\rangle\langle R| + \hat{J}_z |L\rangle\langle L| = \hbar |R\rangle\langle R| - \hbar |L\rangle\langle L| \quad (7.136)$$

which is the expansion of the operator \hat{J}_z in terms of eigenvalues and 1-dimensional subspace projection operators (eigenvectors) that we discussed earlier.

The action of a polarizer can be considered as a measurement. What are the operators representing such measurements? Clearly, the operators for x - and y -polarizers are given by

$$\hat{O}_x = |x\rangle\langle x| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad , \quad \hat{O}_y = |y\rangle\langle y| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad (7.137)$$

since

$$\hat{O}_x |\psi\rangle = \hat{O}_x (a|x\rangle + b|y\rangle) = (|x\rangle\langle x|)(a|x\rangle + b|y\rangle) = a|x\rangle \quad (7.138)$$

and so on.

If light is polarized at an angle θ from the x -axis, it is in the state

$$|\theta\rangle = \cos\theta|x\rangle + \sin\theta|y\rangle = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \quad (7.139)$$

The operator representing the polarizer at angle θ is (in the $x-y$ basis)

$$\hat{O}_\theta = |\theta\rangle\langle\theta| = \begin{pmatrix} \cos^2\theta & \sin\theta\cos\theta \\ \sin\theta\cos\theta & \sin^2\theta \end{pmatrix} \quad (7.140)$$

Note that the probability of measuring x -polarization when in a θ state is

$$\langle x|\hat{O}_\theta|x\rangle = \langle x|\theta\rangle\langle\theta|x\rangle = |\langle x|\theta\rangle|^2 = \cos^2\theta \quad (7.141)$$

A result we have seen several times in earlier discussions.

7.4.0.1 Amplitudes and Probabilities

The *probability interpretation* we have been making follows from the concept of *superposition*.

The superposition idea says that we can write any arbitrary photon state as a linear combination of basis states

$$|\psi\rangle = |R\rangle \langle R | \psi \rangle + |L\rangle \langle L | \psi \rangle \quad (7.142)$$

and then interpret $|\langle R | \psi \rangle|^2$ as the probability that the photon in the state $|\psi\rangle$ will behave as a RCP photon in the state $|R\rangle$.

Generalizing this statement, we say that a system in a state $|\psi\rangle$, in Quantum Mechanics, has a probability $|\langle \varphi | \psi \rangle|^2$ of behaving like it was in the state $|\varphi\rangle$.

You might now conclude, from the experimental fact that only $\pm\hbar$ is transferred to matter, that photons are *always* either in the state $|R\rangle$ with probability α or in the state $|L\rangle$ with probability $1 - \alpha$.

This cannot be correct, however, as we can see by the following arguments.

FACT: An x -polarized photon *never* passes through a y -polaroid.

PROBLEM: If, the above interpretation of being either $|R\rangle$ or $|L\rangle$ was true, then

- (a) an x -polarized photon has a probability $|\langle R | x \rangle|^2$ of being RCP and a RCP photon has a probability $|\langle y | R \rangle|^2$ of being a y -polarized photon and thus passing through a y -polaroid.
- (b) an x -polarized photon has a probability $|\langle L | x \rangle|^2$ of being LCP and a LCP photon has a probability $|\langle y | L \rangle|^2$ of being a y -polarized photon and thus passing through a y -polaroid.

This means that the total probability that an x -polarized photon would get through a y -polaroid in this interpretation is

$$\text{total probability} = |\langle R | x \rangle|^2 |\langle y | R \rangle|^2 + |\langle L | x \rangle|^2 |\langle y | L \rangle|^2 = \frac{1}{2} \quad (7.143)$$

However, as we stated, it *NEVER HAPPENS*. What is wrong?

SOLUTION: When we think of an x -polarized photon being a RCP photon or a LCP photon with equal probability, we are ruling out the possibility of any *interference* effects between the RCP and LCP amplitudes.

We give meaning to the word *interference* here in this way.

The correct calculation of the probability, which lays the groundwork for all of the amplitude mechanics in Quantum Mechanics, goes as follows:

- (a) The probability amplitude of an x -polarized photon passing through a y -polaroid $= \langle y | x \rangle = 0$, which implies that the probability $= |\langle y | x \rangle|^2 = 0$ also.

- (b) If we say that the x -polarized photon is in a superposition of $|R\rangle$ and $|L\rangle$ (we make no statement about probabilities at this point), this implies that

$$|x\rangle = |R\rangle\langle R|x\rangle + |L\rangle\langle L|x\rangle \quad (7.144)$$

which gives

$$\langle y|x\rangle = \langle y|R\rangle\langle R|x\rangle + \langle y|L\rangle\langle L|x\rangle \quad (7.145)$$

or the amplitude for an x -polarized photon to pass through a y -polaroid is the sum of two amplitudes, namely, that it passes through as a RCP photon $\langle y|R\rangle\langle R|x\rangle$ and that it passes through as a LCP photon $\langle y|L\rangle\langle L|x\rangle$. This does not say that it has actually done either!

- (c) The probability of passing through is then the absolute square of the total amplitude

$$\begin{aligned} \text{probability} &= |\langle y|R\rangle\langle R|x\rangle + \langle y|L\rangle\langle L|x\rangle|^2 \\ &= (\langle y|R\rangle^*\langle R|x\rangle^* + \langle y|L\rangle^*\langle L|x\rangle^*)(\langle y|R\rangle\langle R|x\rangle + \langle y|L\rangle\langle L|x\rangle) \\ &= |\langle y|R\rangle|^2|\langle R|x\rangle|^2 + |\langle y|L\rangle|^2|\langle L|x\rangle|^2 \\ &\quad + \langle y|R\rangle\langle R|x\rangle\langle y|L\rangle^*\langle L|x\rangle^* + \langle y|R\rangle^*\langle R|x\rangle^*\langle y|L\rangle\langle L|x\rangle \end{aligned} \quad (7.146)$$

- (d) The first two terms are the same as the incorrect calculation done earlier. The last two terms represent interference effects between the two amplitudes (RCP way and LCP way). A simple calculation shows that the interference terms exactly cancel the first two terms and that the probability equals zero in agreement with experiment!!

INTERPRETATION: The way to interpret this result is as follows:

$\langle y|R\rangle\langle R|x\rangle$ = probability amplitude for an x -polarized photon to pass through a y -polaroid as a RCP photon

$\langle y|L\rangle\langle L|x\rangle$ = probability amplitude for an x -polarized photon to pass through a y -polaroid as a LCP photon

These are *indistinguishable* ways for the process to occur, i.e., no measurement exists that can tell us whether it passes through as an RCP photon or as a LCP photon without destroying the interference, i.e., without radically altering the experiment.

To get the correct total probability, we add all the amplitudes for indistinguishable ways and then square the resulting total amplitude.

In the incorrect calculation, we found the probability for each indistinguishable way and then added the probabilities.

In one case, we eliminated the interference effects and got the wrong result and,

in the other case, we included the interference effects and obtained the correct result.

Summarizing, we have these *rules for amplitude mechanics and probabilities* in Quantum Mechanics:

- (1) The probability amplitude for two successive events is the *product* of the amplitudes for each event, i.e., the amplitude for the x -polarized photon to pass through the y -polaroid as a RCP polarized photon is the product of the amplitude for x -polarized photon to be a RCP photon $\langle R|x\rangle$ and the amplitude for a RCP photon to be a y -polarized photon $\langle y|R\rangle$

$$\langle y|R\rangle\langle R|x\rangle \quad (7.147)$$

- (2) The total amplitude for a process that can take place in several *indistinguishable* ways is the *sum* of the amplitudes for each individual way, i.e.,

$$\langle y|x\rangle = \langle y|R\rangle\langle R|x\rangle + \langle y|L\rangle\langle L|x\rangle \quad (7.148)$$

We note here that this is merely a reflection of the property of projection operators that

$$\hat{I} = |R\rangle\langle R| + |L\rangle\langle L| \quad (7.149)$$

which says that

$$\langle y|x\rangle = \langle y|\hat{I}|x\rangle = \langle y|R\rangle\langle R|x\rangle + \langle y|L\rangle\langle L|x\rangle \quad (7.150)$$

Thus, the mathematical sum over all projection operators being equal to the identity operator is physically equivalent to the sum over all possible intermediate states and it turns into a sum over all the amplitudes for indistinguishable ways in this interpretation.

- (3) The total probability for the process to occur is the absolute square of the total amplitude.

So, in classical physics, we

- (1) find amplitudes and probabilities of each way separately
- (2) add all probabilities to get total probability

We get *NO* interference effects!!

In Quantum Mechanics, we

- (1) find the amplitudes for each indistinguishable way the process can occur
- (2) add all the amplitudes to get a total amplitude
- (3) square the total amplitude to get the total probability

We get interference effects!!

The important result here is that we must consider *ALL INDISTINGUISHABLE WAYS* in step (2).

An indistinguishable way is characterized as follows:

- (1) If two ways are indistinguishable, then there exists *no measurement* that can decide which of the two ways actually happened without altering the experiment.
- (2) In particular, if we attempt to find out, then the interference effects will disappear and we will return to the classical result obtained by adding probabilities.

What actually happens is that during any measurement trying to distinguish the ways, the relative phase of the components in the superposition becomes completely uncertain and this will wash out the interference.

This happens as follows: instead of

$$|x\rangle = |R\rangle \langle R | x\rangle + |L\rangle \langle L | x\rangle \quad (7.151)$$

if we attempted to add a measurement to determine if the x -polarized photon was RCP or LCP, we would have

$$|\tilde{x}\rangle = e^{i\alpha_R} |R\rangle \langle R | x\rangle + e^{i\alpha_L} |L\rangle \langle L | x\rangle \quad (7.152)$$

The probability calculation then gives

$$\begin{aligned} \text{total probability} &= |\langle y | R\rangle|^2 |\langle R | x\rangle|^2 + |\langle y | L\rangle|^2 |\langle L | x\rangle|^2 \\ &\quad + 2\text{Real}[\langle y | R\rangle \langle R | x\rangle e^{i(\alpha_R - \alpha_L)} \langle y | L\rangle^* \langle L | x\rangle^*] \end{aligned} \quad (7.153)$$

The observed probability, which is the result of many *identical* measurements in the laboratory, is an average over all values of the extra phases(they are random).

This involves integrating over the relative phase,i.e.,

$$\frac{1}{2\pi} \int_0^{2\pi} e^{i(\alpha_R - \alpha_L)} d(\alpha_R - \alpha_L) = 0 \quad (7.154)$$

It is clear that the interference term averages to zero and we get the classical result!!

7.4.1 Useful Digression: The Density Operator

We now present an alternate way of representing quantum states. It is an open question whether this alternative is a simple mathematical convenience or a

more ontologically *true* representation. Either way, it has a key role to play in modern interpretations of quantum theory and also some possible solutions to the measurement problem. This discussion is more mathematical than the rest of these notes, but you will benefit if you persevere and work your way through the material. **It is important.**

7.4.1.1 Great Expectations

Earlier, we introduced the *expectation value* - the average of a set of measurement results taken from a collection of systems in the same state. A straightforward calculation of the expectation value takes the following form, with \hat{O} being an operator representing the measurement of a specific physical variable and $|\phi\rangle$ the state of each system in the collection:

$$\langle \hat{O} \rangle = \langle \phi | \hat{O} | \phi \rangle \quad (7.155)$$

If we choose a basis $\{|i\rangle\}$, we can expand $|\phi\rangle$ and $\langle\phi|$

$$|\phi\rangle = \sum_i a_i |i\rangle \quad , \quad \langle\phi| = \sum_j a_j^* \langle j| \quad (7.156)$$

and plug the expansions into our formula for the expectation value:

$$\langle \hat{O} \rangle = \sum_j \left(\sum_i [a_j^* a_i \langle j | \hat{O} | i \rangle] \right) \quad (7.157)$$

To take the next step, we need to remember that $a_i = \langle i | \phi \rangle$ and $a_j^* = \langle \phi | j \rangle$, which can be used to replace the a 's in the formula giving

$$\langle \hat{O} \rangle = \sum_j \left(\sum_i [\langle \phi | j \rangle \langle i | \phi \rangle \langle j | \hat{O} | i \rangle] \right) = \sum_j \left(\sum_i [\langle i | \phi \rangle \langle \phi | j \rangle \langle j | \hat{O} | i \rangle] \right) \quad (7.158)$$

where in the last step all we have done is change the order of the terms in the square bracket.

This formula looks a bit cluttered, but if we examine it closely we find the *matrix element* of \hat{O} hiding in there, $\langle j | \hat{O} | i \rangle$, and also the combination $\langle i | \phi \rangle \langle \phi | j \rangle$. This second combination is the one that interests us at the moment. It can also be interpreted as a matrix element, provided we remember $|\phi\rangle \langle\phi|$ is an operator.

Clearly, it transforms a state into another state as required by any operator....

$$(|\phi\rangle \langle\phi|) |\psi\rangle = |\phi\rangle \langle\phi | \psi\rangle = \alpha |\phi\rangle \quad (7.159)$$

Let us give it the name *density operator* and its own special abbreviation $\hat{D} = |\phi\rangle \langle\phi|$. The expectation value of our original operator \hat{O} can now be converted into

$$\langle \hat{O} \rangle = \sum_j \left(\sum_i [\langle i | \hat{D} | j \rangle \langle j | \hat{O} | i \rangle] \right) \quad (7.160)$$

At the core of this, still rather complicated looking expression, is the combination $\langle i | \hat{D} | j \rangle \langle j | \hat{O} | i \rangle$: the product of two matrix elements. It makes sense to think that this product must represent an element of a single matrix formed by multiplying the other two together. To make this clear, let us strip away the various states and write the product as $D_{ij}O_{ji}$. Putting the first (inner one) of the SUMs back we have

$$\sum_i [D_{ij}O_{ji}] = D_{1j}O_{j1} + D_{2j}O_{j2} + D_{3j}O_{j3} + \dots \quad (7.161)$$

To see what this is, let's just think about the product of two matrices for a moment. Following the rule we set out earlier in these notes, when we multiply matrix A by matrix B , we get

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & \dots \\ a_{21} & a_{22} & a_{23} & \dots \\ a_{31} & a_{32} & a_{33} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} b_{11} & b_{12} & b_{13} & \dots \\ b_{21} & b_{22} & b_{23} & \dots \\ b_{31} & b_{32} & b_{33} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} = \begin{pmatrix} a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31} + \dots & a_{11}b_{12} + a_{12}b_{22} + a_{13}b_{32} + \dots & \dots & \dots \\ a_{21}b_{11} + a_{22}b_{21} + a_{23}b_{31} + \dots & a_{21}b_{12} + a_{22}b_{22} + a_{23}b_{32} + \dots & \dots & \dots \\ \dots & \dots & a_{31}b_{13} + a_{32}b_{23} + a_{33}b_{33} + \dots & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \quad (7.162)$$

where we only started to fill in the elements of the product. We are especially interested in the diagonal elements. The top left diagonal element term is

$$a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31} + \dots \quad (7.163)$$

which looks just like the $D_{1j}O_{j1}$ part of the expectation value since each term starts with a "1" and ends with a "1". If we put the sum over j back in, we can build the entire summation.

Equally, the second term on the diagonal of the AB matrix is

$$a_{21}b_{12} + a_{22}b_{22} + a_{23}b_{32} + \dots \quad (7.164)$$

which could be $D_{2j}O_{j2}$ if we put the sum over j back in as well. In other words, the full calculation of the expectation value is

$$\begin{aligned} \langle \hat{O} \rangle &= \sum_j \left(\sum_i [\langle i | \hat{D} | j \rangle \langle j | \hat{O} | i \rangle] \right) = \sum_j (D_{1j}O_{j1} + D_{2j}O_{j2} + D_{3j}O_{j3} + \dots) \\ &\quad [(D_{11}O_{11} + D_{12}O_{21} + D_{13}O_{31} + \dots) + (D_{21}O_{12} + D_{22}O_{22} + D_{23}O_{32} + \dots) \\ &\quad (D_{31}O_{13} + D_{32}O_{23} + D_{33}O_{33} + \dots)] \end{aligned} \quad (7.165)$$

and each separate term is on the diagonal of the matrix $\hat{D}\hat{O}$. The expectation value is the sum of the diagonal elements of the matrix $\hat{D}\hat{O}$.

Mathematicians have a name for adding up the diagonal elements of a matrix - it is called the *trace* of the matrix as we saw earlier. Using this name we can write

$$\langle \hat{O} \rangle = \text{Trace}(\hat{D}\hat{O}) = \text{Tr}(\hat{D}\hat{O}) \quad (7.166)$$

Why Bother?

The real power of the density operator approach comes to the fore when we have to deal with a situation in which we cannot be sure what state the system is in.

Imagine that we have a whole collection of identical systems, some of which are in state $|\phi_1\rangle$, some in $|\phi_2\rangle$, etc. We might not know which system is in which state, and we might not even know how many systems are in any one given state. As a practical example, think about a beam of electrons that has not passed through any Stern-Gerlach(S-G) magnets. Chances are that the spin states of the electrons are completely random. Perhaps the best we can know is the probability of finding an electron in each state.

$$P_1 = \text{Prob}(|\phi_1\rangle) \quad , \quad P_2 = \text{Prob}(|\phi_2\rangle) \quad , \quad P_3 = \text{Prob}(|\phi_3\rangle) \quad , \quad \dots \quad (7.167)$$

These probabilities have nothing to do with quantum theory as such; they simply represent our ignorance of the details of what is happening. They are not related to any amplitudes.

Given a situation like this, we should to be able to make some useful calculations. For example, we could work out the expectation value of any measurement. After all, if we can calculate the expectation value of each individual state, then the overall expectation value is simply

$$\langle \hat{O} \rangle = P_1 \langle \phi_1 | \hat{O} | \phi_1 \rangle + P_2 \langle \phi_2 | \hat{O} | \phi_2 \rangle + P_3 \langle \phi_3 | \hat{O} | \phi_3 \rangle + \dots + P_n \langle \phi_n | \hat{O} | \phi_n \rangle \quad (7.168)$$

To see this, think back to the original definition of the expectation value: it represents the average value of a measurement. What we have done here is put together a weighted average of the average value for each state.

Now if we construct a density operator that looks like this,

$$\hat{D} = P_1 |\phi_1\rangle \langle \phi_1| + P_2 |\phi_2\rangle \langle \phi_2| + P_3 |\phi_3\rangle \langle \phi_3| + \dots + P_n |\phi_n\rangle \langle \phi_n| \quad (7.169)$$

we can still calculate the expectation value by taking

$$\langle \hat{O} \rangle = \text{Tr}(\hat{D}\hat{O}) \quad (7.170)$$

which is rather neat.

Fans of the density operator call $\hat{D} = |\phi\rangle \langle \phi|$ a *pure state*, and $\hat{D} = P_1 |\phi_1\rangle \langle \phi_1| + P_2 |\phi_2\rangle \langle \phi_2| + P_3 |\phi_3\rangle \langle \phi_3| + \dots + P_n |\phi_n\rangle \langle \phi_n|$ an *unpure state*.

We called a combination of states such as

$$\frac{1}{\sqrt{2}}(|U\rangle + |D\rangle) \quad (7.171)$$

a mixed state, which is also a pure state. A little confusing, but that is convention.

7.4.1.2 More about Pure States, Unpure States and Density Operators

If the photon were in the state $|x\rangle$, then we would have, for some linear operator \hat{A} , the expectation value or average value given by

$$\langle \hat{A} \rangle = \langle x | \hat{A} | x \rangle \quad (7.172)$$

We defined a property of an operator called the *trace* as

$$Tr \hat{Q} = \sum_j \langle q_j | \hat{Q} | q_j \rangle = \text{sum of diagonal matrix elements} = \sum_j (\hat{Q})_{jj} \quad (7.173)$$

that is, the sum over the diagonal matrix elements.

Some Properties of the Trace:

$$\begin{aligned} Tr(\hat{A}\hat{B}) &= Tr(\hat{B}\hat{A}) \\ Tr(c\hat{B}) &= cTr(\hat{B}) \\ Tr(c(\hat{A} + \hat{B})) &= Tr(c\hat{A}) + Tr(c\hat{B}) = cTr(\hat{A}) + cTr(\hat{B}) \end{aligned} \quad (7.174)$$

General Definition: A *density operator* is a *positive, Hermitian operator* \hat{W} with a discrete eigenvalue spectrum such that, given *any* orthonormal basis set $\{|\varphi_k\rangle\}$, we have

$$Tr \hat{W} = 1 = \sum_k W_{kk} = \sum_k \langle \varphi_k | \hat{W} | \varphi_k \rangle \quad (7.175)$$

where W_{kk} is the diagonal matrix element(in the basis) of the density operator \hat{W} .

Quantum theory assumes(equivalent postulates):

- (1) A density operator *exists* for every real physical system (in the same way that every physical system can be represented by a state vector or ket).
- (2) The expectation value of an operator \hat{A} is given by

$$\langle \hat{A} \rangle = Tr(\hat{W}\hat{A}) \quad (7.176)$$

Let us choose a simple example of a density operator to get some handle on what this postulate is saying. In particular, let us choose as our density operator \hat{W} the projection operator for some vector(this is a pure state)

$$\hat{W} = |\psi\rangle \langle \psi| \quad (7.177)$$

This is called an *idempotent* operator since

$$\hat{W}^2 = (|\psi\rangle\langle\psi|)(|\psi\rangle\langle\psi|) = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = \hat{W} \quad (7.178)$$

and thus has eigenvalues $w_k = 0, 1$ only, i.e.,

$$\begin{aligned} \hat{W}|\beta\rangle &= \beta|\beta\rangle \rightarrow \hat{W}^2|\beta\rangle = \hat{W}\beta|\beta\rangle = \beta^2|\beta\rangle = \hat{W}|\beta\rangle = \beta|\beta\rangle \\ &\rightarrow (\beta^2 - \beta)|\beta\rangle = 0 \rightarrow \beta^2 - \beta = 0 \rightarrow \beta = 0, 1 \end{aligned} \quad (7.179)$$

Assume that the eigenvector corresponding to eigenvalue 1 is $|\alpha\rangle$.

Properties of the Density Operator

$$\begin{aligned} \sum_k w_k &= 0 + 1 = 1 = Tr \hat{W} \\ \langle a | \hat{W} | a \rangle &= |\langle a | \alpha \rangle|^2 \geq 0 \end{aligned} \quad (7.180)$$

so that all required properties for a density operator are, in fact, satisfied by the assumed form.

If we denote the eigenvalues of \hat{W} by w_k and the corresponding eigenvectors by $|w_k\rangle$ so that

$$\hat{W}|w_k\rangle = w_k|w_k\rangle \quad (7.181)$$

then, since \hat{W} has a discrete spectrum, we can write \hat{W} in terms of its eigenvalues and eigenvectors as

$$\hat{W} = \sum_k w_k |w_k\rangle\langle w_k| \quad (7.182)$$

Since \hat{W} is Hermitian, its eigenvectors must form an orthonormal basis where

$$\langle w_k | w_j \rangle = \delta_{kj} \quad (7.183)$$

We now derive some other properties of this density operator object.

The spectrum of \hat{W} is the discrete set of numbers $\{w_k\}$. We then have

$$\begin{aligned} Tr \hat{W} &= 1 = \sum_j \langle w_j | \hat{W} | w_j \rangle = \sum_j \langle w_j | w_j \rangle w_j = \sum_j w_j \langle w_j | w_j \rangle \\ &\rightarrow \sum_j w_j = 1 \end{aligned} \quad (7.184)$$

Since \hat{W} is Hermitian, we have

$$\hat{W} = \hat{W}^+ \quad (7.185)$$

which implies that the eigenvalues are real numbers

$$w_k = w_k^* \quad (7.186)$$

Using the fact that \hat{W} is defined to be a positive operator, we then have

$$\langle a | \hat{W} | a \rangle = \langle a | \sum_k w_k | w_k \rangle \langle w_k | a \rangle = \sum_k w_k \langle a | w_k \rangle \langle w_k | a \rangle = \sum_k w_k |\langle a | w_k \rangle|^2 \geq 0 \quad (7.187)$$

for any vector $|a\rangle$. This can only be true, in general, if

$$w_k \geq 0 \quad (7.188)$$

for all k .

The results

$$w_k \geq 0 \quad , \quad \sum_k w_k = 1 \quad (7.189)$$

imply that

$$0 \leq w_k \leq 1 \quad (7.190)$$

Returning to the simple case of a pure state $\hat{W} = |\psi\rangle \langle \psi|$, we then have

$$\begin{aligned} \langle \hat{B} \rangle &= \langle \psi | \hat{B} | \psi \rangle = \langle \psi | \hat{B} \hat{I} | \psi \rangle \\ &= \langle \psi | \hat{B} \left(\sum_k | w_k \rangle \langle w_k | \right) | \psi \rangle = \sum_k \langle \psi | \hat{B} | w_k \rangle \langle w_k | \psi \rangle \\ &= \sum_k \langle w_k | \psi \rangle \langle \psi | \hat{B} | w_k \rangle = \sum_k \langle w_k | (|\psi\rangle \langle \psi|) \hat{B} | w_k \rangle \\ &= \sum_k \langle w_k | \hat{W} \hat{B} | w_k \rangle = Tr(\hat{W} \hat{B}) \end{aligned}$$

Since the important quantities for connection to experiment will be these expectation values, we see that the state represented by \hat{W} is equally well represented by the state vector $|\psi\rangle$ in this case. The density operator and the state vector are equivalent ways of representing a physical system in this simple case.

The most important way of distinguishing whether a state is pure or not follows from the following property of density operators:

The density operator for a **pure state** cannot be written as a linear combination of the density operators of other states, but the density operator for a **nonpure** state can always be so written.

This is illustrated below with some examples.

Using the $|x\rangle, |y\rangle$ basis we have

$$\begin{aligned} \langle \hat{A} \rangle &= \langle x | \hat{A} | x \rangle + \langle y | \hat{A} | y \rangle = Tr(\hat{W} \hat{A}) = \langle x | \hat{W} \hat{A} | x \rangle + \langle y | \hat{W} \hat{A} | y \rangle \\ &= \langle x | \hat{W} \hat{I} \hat{A} | x \rangle + \langle y | \hat{W} \hat{I} \hat{A} | y \rangle \\ &= \langle x | \hat{W} | x \rangle \langle x | \hat{A} | x \rangle + \langle x | \hat{W} | y \rangle \langle y | \hat{A} | x \rangle + \langle y | \hat{W} | x \rangle \langle x | \hat{A} | y \rangle + \langle y | \hat{W} | y \rangle \langle y | \hat{A} | y \rangle \end{aligned} \quad (7.191)$$

This implies that

$$\langle x | \hat{W} | x \rangle = 1 \quad , \quad \langle x | \hat{W} | y \rangle = \langle y | \hat{W} | x \rangle = \langle y | \hat{W} | y \rangle = 0 \quad (7.192)$$

or

$$\hat{W} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = |x\rangle\langle x| \quad (7.193)$$

which is a linear combination (one item in this case) of density operators and says that is a *pure state*.

Now suppose that the photon is in the state

$$|\psi\rangle = \frac{e^{i\alpha_x}}{\sqrt{2}} |x\rangle + \frac{e^{i\alpha_y}}{\sqrt{2}} |y\rangle \quad (7.194)$$

where we know that the phases are equal, $\alpha_x = \alpha_y$ (the relative phase between the components is known exactly in this state) so that

$$|\psi\rangle = e^{i\alpha_x} \left(\frac{1}{\sqrt{2}} |x\rangle + \frac{1}{\sqrt{2}} |y\rangle \right) \quad (7.195)$$

The terms $e^{i\alpha_x}$, etc, are called phase factors.

But, since all states must have length 1, we can ignore the overall phase factor and write

$$|\psi\rangle = \frac{1}{\sqrt{2}} |x\rangle + \frac{1}{\sqrt{2}} |y\rangle \quad (7.196)$$

This says that the probability = 1/2 that the photon behaves like $|x\rangle$ and the probability = 1/2 that the photon behaves like $|y\rangle$.

In this case, we have

$$\begin{aligned} \langle \hat{A} \rangle &= \langle \psi | \hat{A} | \psi \rangle = \frac{1}{2} [\langle x | \hat{A} | x \rangle + \langle x | \hat{A} | y \rangle + \langle y | \hat{A} | x \rangle + \langle y | \hat{A} | y \rangle] \\ &= Tr(\hat{W} \hat{A}) = \langle x | \hat{W} \hat{A} | x \rangle + \langle y | \hat{W} \hat{A} | y \rangle = \langle x | \hat{W} \hat{I} \hat{A} | x \rangle + \langle y | \hat{W} \hat{I} \hat{A} | y \rangle \\ &= \langle x | \hat{W} | x \rangle \langle x | \hat{A} | x \rangle + \langle x | \hat{W} | y \rangle \langle y | \hat{A} | x \rangle + \langle y | \hat{W} | x \rangle \langle x | \hat{A} | y \rangle + \langle y | \hat{W} | y \rangle \langle y | \hat{A} | y \rangle \end{aligned} \quad (7.197)$$

which implies that

$$\langle x | \hat{W} | x \rangle = \frac{1}{2} = \langle x | \hat{W} | y \rangle = \langle y | \hat{W} | x \rangle = \langle y | \hat{W} | y \rangle \quad (7.198)$$

or

$$\hat{W} = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \end{pmatrix} = |\psi\rangle\langle\psi| \quad (7.199)$$

So, again we have a pure state.

But what happens if we *only know* that the probability = 1/2 that the photon behaves like $|x\rangle$ and the probability = 1/2 that the photon behaves like $|y\rangle$.

This says that the state vector is

$$|\psi\rangle = a|x\rangle + b|y\rangle \quad (7.200)$$

where we only know that $|a|^2 = |b|^2 = 1/2$. Let us choose

$$a = \frac{e^{i\alpha_a}}{\sqrt{2}} \quad , \quad b = \frac{e^{i\alpha_b}}{\sqrt{2}} \quad (7.201)$$

We do not have any phase information in this case. In addition, the phases values could be different in each separate experiment. This means that we must average over the relative phase $\alpha_x - \alpha_y$ when computing the probabilities and thus all interference effects will vanish as shown below.

When we calculate the expectation value we have

$$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle = \frac{1}{2} \left[\langle x | \hat{A} | x \rangle + e^{-i(\alpha_a - \alpha_b)} \langle x | \hat{A} | y \rangle + e^{i(\alpha_a - \alpha_b)} \langle y | \hat{A} | x \rangle + \langle y | \hat{A} | y \rangle \right] \quad (7.202)$$

and when we average over the relative phase we obtain

$$\langle \hat{A} \rangle = \frac{1}{2} \langle x | \hat{A} | x \rangle + \frac{1}{2} \langle y | \hat{A} | y \rangle \quad (7.203)$$

Again, we must have

$$\begin{aligned} \langle \hat{A} \rangle &= Tr(\hat{W} \hat{A}) = \langle x | \hat{W} \hat{A} | x \rangle + \langle y | \hat{W} \hat{A} | y \rangle = \langle x | \hat{W} \hat{I} \hat{A} | x \rangle + \langle y | \hat{W} \hat{I} \hat{A} | y \rangle \\ &= \langle x | \hat{W} | x \rangle \langle x | \hat{A} | x \rangle + \langle x | \hat{W} | y \rangle \langle y | \hat{A} | x \rangle + \langle y | \hat{W} | x \rangle \langle x | \hat{A} | y \rangle + \langle y | \hat{W} | y \rangle \langle y | \hat{A} | y \rangle \end{aligned} \quad (7.204)$$

which implies that

$$\langle x | \hat{W} | x \rangle = \frac{1}{2} = \langle y | \hat{W} | y \rangle \quad , \quad \langle y | \hat{W} | x \rangle = \langle x | \hat{W} | y \rangle = 0 \quad (7.205)$$

or

$$\hat{W} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2} |x\rangle \langle x| + \frac{1}{2} |y\rangle \langle y| = \text{probability}(x) |x\rangle \langle x| + \text{probability}(y) |y\rangle \langle y| \quad (7.206)$$

This is a *nonpure state*.

So, we have a pure state only if the relative phase information is known exactly.

Unpolarized Light

Consider the following experiment: We have a beam of monochromatic light that is composed of photons from two sources which output photons in the states $|\psi_1\rangle$ or $|\psi_2\rangle$, respectively. The sources emit the photons randomly and are independent of each other, which implies that we cannot tell which source a particular photon comes from.

We assign these probabilities

$$\begin{aligned} p_1 &= \text{probability that a photon comes from source \#1} \\ p_2 &= \text{probability that a photon comes from source \#2} \end{aligned}$$

where $p_1 + p_2 = 1$. Now the probability that a particular observed photon transfers $+\hbar$ is

$$p_+ = p_1 |\langle R | \psi_1 \rangle|^2 + p_2 |\langle R | \psi_2 \rangle|^2 \quad (7.207)$$

and the probability that it transfers $-\hbar$ is

$$p_- = p_1 |\langle L | \psi_1 \rangle|^2 + p_2 |\langle L | \psi_2 \rangle|^2 \quad (7.208)$$

This implies that the average value of the angular momentum transfer for the beam of photons is

$$\begin{aligned} \langle \hat{J}_z \rangle &= \hbar p_+ - \hbar p_- = \hbar p_1 |\langle R | \psi_1 \rangle|^2 + \hbar p_2 |\langle R | \psi_2 \rangle|^2 - \hbar p_1 |\langle L | \psi_1 \rangle|^2 - \hbar p_2 |\langle L | \psi_2 \rangle|^2 \\ &= p_1 \left[\hbar |\langle R | \psi_1 \rangle|^2 - \hbar |\langle L | \psi_1 \rangle|^2 \right] + p_2 \left[\hbar |\langle R | \psi_2 \rangle|^2 - \hbar |\langle L | \psi_2 \rangle|^2 \right] \\ &= p_1 \langle \hat{J}_z \rangle_1 + p_2 \langle \hat{J}_z \rangle_2 \end{aligned} \quad (7.209)$$

or, the average value of the angular momentum transfer for the beam of photons = sum over the average value in each beam weighted by the probability that photon comes from that beam.

Let me emphasize at this point that it is important to realize that the statement *the photon is either in the state but we do not know which* is *NOT* the same statement as *the photon is in a state which is a superposition of* $|\psi_1\rangle$ and $|\psi_2\rangle$.

In the second case, we are saying the relative phase is known as in the state

$$|\psi\rangle = \frac{1}{\sqrt{2}} |x\rangle + \frac{1}{\sqrt{2}} |y\rangle \quad (7.210)$$

which we found to be a pure state.

Being in a superposition implies that we know the relative phase of the components.

In the first case, however, we are saying that the relative phase is unknown and,

as we have seen, interference effects will vanish.

In pure states, we have superpositions and the probability amplitude rules apply. In nonpure or mixed states, where the system is in one of several states with definite probabilities, we find weighted averages (weighted with the state probabilities) of the value in each state. We use addition of probabilities with no interference effects, which as we have seen, is equivalent to saying the relative phase is unknown.

Unpolarized light has equal probability of being in any polarization state. It is just a special nonpure or mixed state. No relative phase information is known for unpolarized light.

7.5 How Does the Polarization State Vector Change in Physical Systems?

Up to now we have been considering devices such as polaroids and prisms, which are *go-nogo* devices. Some photons get through and some do not for these devices depending on their polarization state.

We now consider devices where all the photons get through no matter what their polarization state is, but the device changes the incident polarization state in some way.

In particular, we consider the example of a *birefringent* crystal, such as calcite. A calcite crystal has a *preferred* direction called the *optic axis*. The crystal has a different index of refraction for light polarized parallel to the optic axis than it has for light polarized perpendicular to the optic axis. We assume that the optic axis is in the x-y plane and send a beam of photons in the z-direction. Photons polarized perpendicular to the optic axis are called *ordinary* and are in the state $|o\rangle$ and photons polarized parallel to the optic axis are called *extraordinary* and are in the state $|e\rangle$.

The set of states $\{|o\rangle, |e\rangle\}$ forms an orthonormal basis and general photon states interacting with a calcite crystal are written as superpositions of these basis states.

This is an example of a *general rule in quantum mechanics*.

If we are doing an experiment using a particular measuring device that measures the observable \hat{Q} , then we should use as the basis for all states, the eigenvectors of \hat{Q} . As we shall see, this requirement pushes us to ask the correct experimental questions (those that quantum mechanics can answer). This particular basis is called the *home space* for the experiment.

Now, as we saw earlier, the phase of a light wave with wavelength λ as it propagates through a medium in the z -direction is given by the quantity $\varphi = e^{ikz}$ with

$$k = \frac{2\pi}{\lambda} = \frac{n\omega}{c} \quad (7.211)$$

where n = index of refraction, $\omega = 2\pi\nu$, ν = frequency and c = speed of light.

Since the phase depends on the index of refraction, the effect of passing through a calcite crystal is to change the relative phase of the $|o\rangle$ and $|e\rangle$ components making up the superposition.

We assume that the state of the photon entering the calcite crystal is

$$|\psi_{in}\rangle = |e\rangle \langle e | \psi_{in} \rangle + |o\rangle \langle o | \psi_{in} \rangle \quad (7.212)$$

The two components have different indices of refraction n_e and n_o , respectively.

If the beam passes through a length ℓ of calcite, then the state upon leaving is given by inserting phase changes for each component and remembering that the component phases change differently.

$$|\psi_{out}\rangle = e^{ik_e\ell} |e\rangle \langle e | \psi_{in} \rangle + e^{ik_o\ell} |o\rangle \langle o | \psi_{in} \rangle = \hat{U}_\ell |\psi_{in}\rangle \quad (7.213)$$

where

$$\hat{U}_z = e^{ik_e z} |e\rangle \langle e| + e^{ik_o z} |o\rangle \langle o| \quad (7.214)$$

is a *time development* operator of some sort since ℓ = distance traveled in a time t .

Now we define two new quantities which are very important throughout the study of Quantum Mechanics.

For transitions between two states (*in* and *out* in this case)

- (1) the transition amplitude for a photon to enter the calcite in state $|\psi_{in}\rangle$ and leave in state $|\phi\rangle = \langle\phi | \psi_{out}\rangle = \langle\phi | \hat{U}_\ell |\psi_{in}\rangle$
- (2) the transition probability $|\langle\phi | \psi_{out}\rangle|^2 = |\langle\phi | \hat{U}_\ell |\psi_{in}\rangle|^2$

To proceed any further, we need to find out more about \hat{U}_z . Now

$$|\psi_z\rangle = \text{state of the photon after traveling distance } z \text{ in calcite} = \hat{U}_z |\psi_{in}\rangle \quad (7.215)$$

From the form of \hat{U}_z we have

$$\begin{aligned} \hat{U}_{z+\varepsilon} &= e^{ik_e(z+\varepsilon)} |e\rangle \langle e| + e^{ik_o(z+\varepsilon)} |o\rangle \langle o| \\ &= (e^{ik_e\varepsilon} |e\rangle \langle e| + e^{ik_o\varepsilon} |o\rangle \langle o|)(e^{ik_e z} |e\rangle \langle e| + e^{ik_o z} |o\rangle \langle o|) \end{aligned} \quad (7.216)$$

or

$$\hat{U}_{z+\varepsilon} = \hat{U}_\varepsilon \hat{U}_z \quad (7.217)$$

This is a general result for all time development operators, namely,

$$\hat{U}_{t+t'} = \hat{U}_{t'} \hat{U}_t \quad (7.218)$$

This implies that

$$|\psi_{z+\varepsilon}\rangle = \hat{U}_{z+\varepsilon} |\psi_{in}\rangle = \hat{U}_\varepsilon \hat{U}_z |\psi_{in}\rangle = \hat{U}_\varepsilon |\psi_z\rangle \quad (7.219)$$

Now let $\varepsilon \rightarrow 0$ such that $k_0\varepsilon \ll 1$ and $k_e\varepsilon \ll 1$ and we can write (to 1st order)

$$\begin{aligned} \hat{U}_\varepsilon &= e^{ik_e\varepsilon} |e\rangle \langle e| + e^{ik_o\varepsilon} |o\rangle \langle o| \\ &= (1 + ik_e\varepsilon) |e\rangle \langle e| + (1 + ik_o\varepsilon) |o\rangle \langle o| \\ &= \hat{I} + i\varepsilon \hat{K} \end{aligned} \quad (7.220)$$

where

$$\hat{I} = |e\rangle \langle e| + |o\rangle \langle o| \quad , \quad \hat{K} = k_e |e\rangle \langle e| + k_o |o\rangle \langle o| \quad (7.221)$$

Now, the relation

$$\hat{K} = k_e |e\rangle \langle e| + k_o |o\rangle \langle o| \quad (7.222)$$

is an expansion of an operator in terms of its eigenvalues and the corresponding projection operators (eigenvectors). It says that the eigenvectors of \hat{K} are $|e\rangle$ and $|o\rangle$ with eigenvalues k_e and k_o , respectively.

This illustrates the *awesome power* in these methods!!

We then have

$$|\psi_{z+\varepsilon}\rangle = (\hat{I} + i\varepsilon \hat{K}) |\psi_z\rangle \quad (7.223)$$

or

$$|\psi_{z+\varepsilon}\rangle - |\psi_z\rangle = i\varepsilon \hat{K} |\psi_z\rangle \quad (7.224)$$

or

$$\lim_{\varepsilon \rightarrow 0} \frac{|\psi_{z+\varepsilon}\rangle - |\psi_z\rangle}{\varepsilon} = i\hat{K} |\psi_z\rangle \quad (7.225)$$

which gives the differential equation for the *time* development of the state vector

$$\frac{d}{dz} |\psi_z\rangle = i\hat{K} |\psi_z\rangle \quad (7.226)$$

It is clearly similar to the differential equation we obtained earlier for the time development operator. If we follow the analogy, then we should have

$$\hat{K} = \text{hermitian operator} \quad , \quad \hat{U}_z = \text{unitary operator} \quad (7.227)$$

Let us derive some important results. We have, using the $x - y$ basis

$$\begin{aligned} \langle x | \psi_{z+\varepsilon} \rangle - \langle x | \psi_z \rangle &= i\varepsilon \langle x | \hat{K} | \psi_z \rangle = i\varepsilon \langle x | \hat{K} \hat{I} | \psi_z \rangle \\ &= i\varepsilon \langle x | \hat{K} | x \rangle \langle x | \psi_z \rangle + i\varepsilon \langle x | \hat{K} | y \rangle \langle y | \psi_z \rangle \end{aligned} \quad (7.228)$$

or the change in the x -component of $|\psi_z\rangle$ as we move an infinitesimal amount ε has one part proportional to the x -component of $|\psi_z\rangle$ and a second part y -component of $|\psi_z\rangle$.

Similarly, we have

$$\begin{aligned}\langle y | \psi_{z+\varepsilon} \rangle - \langle y | \psi_z \rangle &= i\varepsilon \langle y | \hat{K} | \psi_z \rangle = i\varepsilon \langle y | \hat{K} \hat{I} | \psi_z \rangle \\ &= i\varepsilon \langle y | \hat{K} | x \rangle \langle x | \psi_z \rangle + i\varepsilon \langle y | \hat{K} | y \rangle \langle y | \psi_z \rangle\end{aligned}\quad (7.229)$$

Now, since *no photons are lost* as we pass through, we must have

$$\langle \psi_{z+\varepsilon} | \psi_{z+\varepsilon} \rangle = 1 = \langle \psi_z | \psi_z \rangle \quad (7.230)$$

for all z . We then get

$$\begin{aligned}\langle \psi_{z+\varepsilon} | \psi_{z+\varepsilon} \rangle &= \langle \psi_z | \psi_z \rangle + i\varepsilon [\langle x | \hat{K} | x \rangle - \langle x | \hat{K} | x \rangle^*] |\langle x | \psi_z \rangle|^2 \\ &\quad + i\varepsilon [\langle y | \hat{K} | y \rangle - \langle y | \hat{K} | y \rangle^*] |\langle y | \psi_z \rangle|^2 \\ &\quad + i\varepsilon [\langle x | \hat{K} | y \rangle - \langle x | \hat{K} | y \rangle^*] \langle y | \psi_z \rangle \langle x | \psi_z \rangle^* \\ &\quad + i\varepsilon [\langle y | \hat{K} | x \rangle - \langle y | \hat{K} | x \rangle^*] \langle x | \psi_z \rangle \langle y | \psi_z \rangle^*\end{aligned}\quad (7.231)$$

which says that we must have

$$\begin{aligned}\langle x | \hat{K} | x \rangle &= \langle x | \hat{K} | x \rangle^* & , & & \langle y | \hat{K} | y \rangle &= \langle y | \hat{K} | y \rangle^* \\ \langle x | \hat{K} | y \rangle &= \langle x | \hat{K} | y \rangle^* & , & & \langle y | \hat{K} | x \rangle &= \langle y | \hat{K} | x \rangle^*\end{aligned}\quad (7.232)$$

This says that \hat{K} is a Hermitian operator. Finally, one can show that $\hat{U}_z^\dagger \hat{U}_z = \hat{I}$ so that \hat{U}_z is unitary as expected for a time transformation operator. From our earlier discussion we identify

$$\begin{aligned}\hat{U}_z &= \text{transformation operator} \\ \hat{K} &= \text{generator of the transformation}\end{aligned}\quad (7.233)$$

Calculating the Transition Probability

We defined the transition probability as

$$T(z) = |\langle \varphi | \psi_{z,out} \rangle|^2 = |\langle \varphi | \hat{U}_z | \psi_{in} \rangle|^2 \quad (7.234)$$

Using

$$\hat{U}_z = e^{ik_\varepsilon z} |e\rangle \langle e| + e^{ik_o z} |o\rangle \langle o| \quad , \quad |\psi_{in}\rangle = a |o\rangle + b |e\rangle \quad (7.235)$$

where $|a|^2 + |b|^2 = 1$, we get

$$\begin{aligned}T(z) &= |\langle \varphi | (e^{ik_\varepsilon z} |e\rangle \langle e| + e^{ik_o z} |o\rangle \langle o|) (a |o\rangle + b |e\rangle) |^2 \\ &= |\langle \varphi | (be^{ik_\varepsilon z} |e\rangle + ae^{ik_o z} |o\rangle) |^2 = |be^{ik_\varepsilon z} \langle \varphi | e\rangle + ae^{ik_o z} \langle \varphi | o\rangle|^2\end{aligned}\quad (7.236)$$

Now let us ask a *specific* question.

Suppose $a = -ib = 1/\sqrt{2}$, which means the that photon entering the calcite crystal is an LCP photon. What is the probability that it will exit as a RCP photon? This means we choose

$$|\varphi\rangle = |R\rangle = \frac{1}{\sqrt{2}}|o\rangle + \frac{i}{\sqrt{2}}|e\rangle \quad (7.237)$$

or

$$\langle\varphi|e\rangle = \frac{i}{\sqrt{2}} \quad , \quad \langle\varphi|o\rangle = \frac{1}{\sqrt{2}} \quad (7.238)$$

We then get

$$\begin{aligned} T(z) &= \left| be^{ik_e z} \langle\varphi|e\rangle + ae^{ik_o z} \langle\varphi|o\rangle \right|^2 = \left| \frac{i}{\sqrt{2}} e^{ik_e z} \frac{i}{\sqrt{2}} + \frac{1}{\sqrt{2}} e^{ik_o z} \frac{1}{\sqrt{2}} \right|^2 \\ &= \frac{1}{4} \left| e^{ik_o z} - e^{ik_e z} \right|^2 = \frac{1}{4} \left(1 + 1 - e^{i(k_o - k_e)z} - e^{-i(k_o - k_e)z} \right) \\ &= \frac{1}{2} (1 - \cos(k_o - k_e)z) \end{aligned} \quad (7.239)$$

If we choose $(k_o - k_e)z = \pi$, the $T = 1$ and *all* the LCP photons are turned into RCP photons by a calcite crystal of *just the right length*.

This simple example clearly exhibits the power of these techniques.

7.6 Problems

7.6.1 Polaroids

Imagine a situation in which a photon in the $|x\rangle$ state strikes a vertical polaroid. Clearly the probability of the photon getting through the vertical polaroid is 0. Now consider the case of two polaroids with the photon in the $|x\rangle$ state striking a polaroid at 45° and then striking a vertical polaroid.

- (a) Show that the probability of the photon getting through both polaroids is $1/4$.

Consider now the case of three polaroids with the photon in the $|x\rangle$ state striking a polaroid at 30° first, then a polaroid at 60° and finally a vertical polaroid.

- (b) Show that the probability of the photon getting through all three polaroids is $27/64$.

7.6.2 Calcite

A photon is polarized at an angle θ to the optic axis is sent in the z direction through a slab of calcite 10^{-2} cm thick in the z direction. Assume that the

optic axis lies in the $x - y$ plane. Calculate, as a function of θ , the transition probability for the photon to emerge left circularly polarized. Sketch the result. Let the frequency of the light be given by $c/\omega = 5000\text{\AA}$, and let $n_o = 1.50$ and $n_e = 1.65$ for the calcite.

7.6.3 Photons and polarizers

A photon polarization state for a photon propagating in the z -direction is given by

$$|\psi\rangle = \sqrt{\frac{2}{3}} |x\rangle + \frac{i}{\sqrt{3}} |y\rangle$$

- (a) What is the probability that a photon in this state will pass through a polaroid with its transmission axis oriented in the y -direction?
- (b) What is the probability that a photon in this state will pass through a polaroid with its transmission axis y' making an angle ϕ with the y -axis?
- (c) A beam carrying N photons per second, each in the state $|\psi\rangle$, is totally absorbed by a black disk with its normal to the surface in the z -direction. How large is the torque exerted on the disk? In which direction does the disk rotate? REMINDER: The photon states $|R\rangle$ and $|L\rangle$ each carry a unit \hbar of angular momentum parallel and antiparallel, respectively, to the direction of propagation of the photon.

7.6.4 Quarter-wave plate

A beam of linearly polarized light is incident on a quarter-wave plate (changes relative phase by 90°) with its direction of polarization oriented at 30° to the optic axis. Subsequently, the beam is absorbed by a black disk. Determine the rate angular momentum is transferred to the disk, assuming the beam carries N photons per second.

Chapter 8

Some Thoughts on the Collapse Postulate

8.1 The Measurement Process

Based on the unitary operator time evolution postulate, a system consisting of a quantum system (Q-system) and a measurement system (M-system), would necessarily evolve in this way

$$|initial\rangle = (a|+\rangle_Q + b|-\rangle_Q)|0\rangle_M \rightarrow |final\rangle = a|+\rangle_Q|+1\rangle_M + b|-\rangle_Q|-1\rangle_M \quad (8.1)$$

which is a superposition of Q-states and M-states. The M-states represent macroscopic pointer locations on some meter.

What we are saying is that if the meter, which was initially off (state $|0\rangle_M$) was turned on when the system was in the $|+\rangle_Q$ state then the combined system evolves to

$$|+\rangle_Q|0\rangle_M \rightarrow |+\rangle_Q|+1\rangle_M \quad (8.2)$$

that is the meter (assuming it is a good meter) reads +1.

Similarly, if the meter was turned on when the system was in the $|-\rangle_Q$ state then the combined system evolves to

$$|-\rangle_Q|0\rangle_M \rightarrow |-\rangle_Q|-1\rangle_M \quad (8.3)$$

that is the meter (assuming it is a good meter) reads -1.

This says that *measurement*, within the framework of the standard four postulates, *CORRELATES* or *ENTANGLES* the *dynamical* variable (Q-system) to be measured and the *macroscopic* (M-system) indicator that can be directly (macroscopically) observed.

Derivation: Suppose that the meter has eigenvectors (labelled by eigenvalues)

$$\begin{aligned} |+\rangle_M &\Rightarrow \text{meter on : reading } +1 \\ |-\rangle_M &\Rightarrow \text{meter on : reading } -1 \\ |0\rangle_M &\Rightarrow \text{meter off} \end{aligned}$$

and the system has eigenvectors (labelled by eigenvalues)

$$\begin{aligned} |+\rangle_Q &\Rightarrow \text{value} = +1 \\ |-\rangle_Q &\Rightarrow \text{value} = -1 \end{aligned}$$

The initial state is

$$|initial\rangle = (a|+\rangle_Q + b|-\rangle_Q)|0\rangle_M \quad (8.4)$$

which represents the system in a superposition state and the meter off.

We are interested in the evolution of this state according to quantum mechanics.

If, instead of the above initial state, we started with the initial state

$$|A\rangle = |+\rangle_Q |0\rangle_M \quad (8.5)$$

or

$$|B\rangle = |-\rangle_Q |0\rangle_M \quad (8.6)$$

and then turn on the meter, the states *must* evolve into

$$|A'\rangle = |+\rangle_Q |+\rangle_M \quad (8.7)$$

or

$$|B'\rangle = |-\rangle_Q |-\rangle_M \quad (8.8)$$

respectively, indicating that the meter has measured the appropriate value (that is the definition of a *good* meter) since the system is in an eigenstate and has a definite value with certainty.

If the system is in the initial state corresponding to a superposition, however, then the *linearity* of quantum mechanics says that it must evolve into

$$|final\rangle = a|+\rangle_Q |+\rangle_M + b|-\rangle_Q |-\rangle_M \quad (8.9)$$

8.2 Interpreting the state vector: Two models....

- (A) Pure state $|\psi\rangle \rightarrow$ a *complete* description of an individual Q-system. This corresponds to the statement that a dynamical variable \hat{P} has the value p in the state $|\psi\rangle$ if and only if $\hat{P}|\psi\rangle = p|\psi\rangle$.
- (B) Pure state $|\psi\rangle \rightarrow$ the *statistical* properties of an *ensemble of similarly prepared systems*.

Interpretation (A) is the standard interpretation espoused by 90% of all physicists. It assumes that, because the state vector plays the most important role in the mathematical formalism of QM, it must have an equally important role in the interpretation of QM, so that

$$\text{Properties of world} \Leftrightarrow \text{Properties of } |\psi\rangle$$

Interpretation (A) by itself is not consistent with the unitary evolution postulate, that is, the state $|final\rangle$ is not equal to an eigenvector of any indicator (macroscopic pointer) variable. This means that the pointer (of the meter) will *flutter* since the states could be macroscopically separated in space. Since we never observe this flutter, any interpretation of $|final\rangle$ as a description of an individual system cannot be reconciled with both observation and unitary time evolution.

Interpretation (B) has no such difficulties. $|\psi\rangle$ is just an abstract mathematical object which implies the probability distributions of the dynamical variables of an ensemble. It represents a *state of knowledge*.

Physicists that believe interpretation (A) are forced to introduce a new postulate at this point to remove these difficulties. This is the so-called **reduction/collapse** of the state vector postulate, which says that during any measurement we have a *new real process* which causes the *transition*

$$|final\rangle \rightarrow a|+\rangle_Q|+1\rangle_M \quad \text{or} \quad b|-\rangle_Q|-1\rangle_M \quad (8.10)$$

or we end up with an eigenvector of the indicator variable and thus there will be no flutter.

Various *reasons* are put forth for making this assumption, i.e.,

measurements are repeatable

Since this experiment (where the repeated measurement takes place immediately after the first measurement) is rarely realized in the laboratory, I do not know what to make of a requirement like this one. In addition, in many experiments (like those involving photons), the system is destroyed by the measurement (photon is absorbed) making it silly to talk about a repeatable measurement.

In addition, the *reduction* process has never been observed in the laboratory, so I do not understand in what sense it can be thought of as a real physical process.

It is important to note that this difficulty only arises for interpretation (A) where statements are made about state vectors representing individual systems.

8.3 Some Proposed Mechanisms for the Reduction

- (1) **The reduction process is caused by an unpredictable and uncontrollable disturbance of the object by the measuring apparatus (a non-unitary process).**

This means that the energy of the system must take the form

$$E = E_Q + E_M + E_{QM} \quad , \quad E_{QM} \rightarrow \text{disturbance} \quad (8.11)$$

which means, however, that it is already built into the standard unitary time evolution operator and, thus, the disturbance terms can only lead to a final state that is still a superposition of indicator variable states. *IT DOES NOT WORK* unless one do not specify what is meant by *unpredictable and uncontrollable disturbance*!

- (2) **The observer causes the reduction process when she reads the result of the measurement from the apparatus.**

This is just a variation of (1). Here, the observer is just another indicator device. The new final state becomes

$$|final\rangle = a|+\rangle_Q|+1\rangle_M|sees + 1\rangle_O + b|-\rangle_Q|-1\rangle_M|sees - 1\rangle_O \quad (8.12)$$

which is still a superposition and thus is *NO HELP*. It also introduces *consciousness* into QM and that is just silly! All that happens is the observer gets entangled also.

- (3) **The reduction is caused by the environment (called decoherence), where by environment is meant the rest of the universe other than the Q-system and the M-system.**

In this model, the environment is a very large system with an enormous number of degrees of freedom (physical variables). We do not have any information about most of the degrees of freedom and thus must *average* over them. This causes pure states to *change* into nonpure states in a *non-unitary* process.

Why do many physicists think an individual Q-system must have its own state vector or wave function and then assume the collapse postulate?

IT WORKS for doing calculations!

This view has survived so long because it does not lead to any serious errors in most situations. Why?

In general, predictions in quantum mechanics are derived from $|\psi\rangle$ which gives

the wave function and which, in turn, gives the probabilities. The operational significance of a probability is a relative frequency so that the experimentalist has to invoke an ensemble of similar systems to make any comparisons with theory that is independent of any particular interpretation of the wave function. So that interpretation (B) is being used in the end anyway.

Does this mean that we should stop worrying about the interpretation of the wave function? NO! But that is the subject of another (more advanced) book.

What about interpretation (B)? It says that

**A pure state describes the statistical
properties of an ensemble of similarly
prepared systems.**

This means that we must use a density operator $\hat{\rho}$ as the fundamental mathematical object of quantum mechanics instead of the state vector.

It turns out that some systems only have a density operator $\hat{\rho}$ and do not have a *legitimate* state vector $|\psi\rangle$.

For example, consider a box containing a very large number of electrons, each having spin = $1/2$. As we shall see later, this means the spin can have a measurable component = $\pm 1/2$ along any direction. A Stern-Gerlach device measures these spin components.

Now, suppose the box has a hole so that electrons can get out and go into a Stern-Gerlach device oriented to measure z -components (an arbitrary choice). We will find the results

$$+1/2 \text{ 50\% of the time and } -1/2 \text{ 50\% of the time} \quad (8.13)$$

We then ask the question - what are the properties of the electrons in the box?

There are two possibilities:

- (1) *Each individual* electron has the state vector

$$|\psi\rangle_Q = \frac{1}{\sqrt{2}} | +1/2 \rangle + \frac{1}{\sqrt{2}} | -1/2 \rangle = |\psi\rangle_{BOX} \quad (8.14)$$

or

- (2)

$1/2$ of the electrons have $+1/2$
 $1/2$ of the electrons have $-1/2$

so that

$$\begin{aligned} |\psi\rangle_Q &= | +1/2 \rangle \text{ or } | -1/2 \rangle \\ |\psi\rangle_{BOX} &= \frac{1}{\sqrt{2}} | +1/2 \rangle + \frac{1}{\sqrt{2}} | -1/2 \rangle \end{aligned} \quad (8.15)$$

which seems to be the same state $|\psi\rangle_{BOX}$ as in (1), but it is really *NOT* a superposition state in this case.

Therefore, it seems that we will not be able to tell which possibility is the correct one!

It turns out, however, that

$$|x - comp = +1/2\rangle = \frac{1}{\sqrt{2}} | +1/2\rangle + \frac{1}{\sqrt{2}} | -1/2\rangle \quad (8.16)$$

so that, in case (1), if we orient the Stern-Gerlach device to measure x -components we would find *all* the electrons are in the same state $|x - comp = +1/2\rangle$, that is, they are all the same!

On the other hand, in case (2) since

$$|z = \pm 1/2\rangle = \frac{1}{\sqrt{2}} |x = +1/2\rangle \pm \frac{1}{\sqrt{2}} |x = -1/2\rangle \quad (8.17)$$

we would find that $1/2$ give the $|x = +1/2\rangle$ result and $1/2$ give the $|x = -1/2\rangle$ result.

Therefore, the *states are not the same*! If we try to write a state vector for case (2) we have to write

$$|\psi\rangle_Q = \frac{1}{\sqrt{2}} | +1/2\rangle + \frac{e^{i\alpha}}{\sqrt{2}} | -1/2\rangle \quad (8.18)$$

instead of

$$|\psi\rangle_{BOX} = \frac{1}{\sqrt{2}} | +1/2\rangle + \frac{1}{\sqrt{2}} | -1/2\rangle \quad (8.19)$$

where α is a *completely unknown relative phase factor*, which must be averaged over during any calculations since it is different for each separate measurement (each member of the ensemble). With that property for α , this is not a legitimate state vector in my opinion.

If we use density matrices we have a different story. For a pure state we can always write

$$\hat{\rho} = |\psi\rangle \langle\psi| \quad (8.20)$$

for some state vector $|\psi\rangle$.

In fact, case (1) gives

$$\hat{\rho} = \frac{1}{2} (|1/2\rangle \langle 1/2| + |1/2\rangle \langle -1/2| + |1/2\rangle \langle -1/2| + |-1/2\rangle \langle -1/2|) \Rightarrow \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \quad (8.21)$$

where the diagonal matrix elements represent probabilities and the off-diagonal matrix elements imply that we will observe quantum interference effects in this system.

Clearly, any pure state density operator cannot be written as the sum of pure state projection operators.

In case (2), however, we have

$$\hat{\rho} = \frac{1}{2} (|1/2\rangle\langle 1/2| + |-1/2\rangle\langle -1/2|) \Rightarrow \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (8.22)$$

which clearly is the sum of pure state projection operators. This corresponds to a *nonpure* state. Note that the off-diagonals are zero so that this density operator cannot lead to any quantum interference effects.

If we treat case (2) as a pure state with the extra relative phase factor we would obtain

$$\hat{\rho} = \frac{1}{2} \begin{pmatrix} 1 & e^{i\alpha} \\ e^{-i\alpha} & 1 \end{pmatrix} \quad (8.23)$$

which becomes

$$\hat{\rho} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (8.24)$$

when we average over α .

The so-called **decoherence process** has this effect

$$\hat{\rho} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \xrightarrow[\text{reduction}]{\text{environment}} \begin{pmatrix} a & 0 \\ 0 & d \end{pmatrix} \quad (8.25)$$

or a pure state turns into a nonpure state! Here, environment reduction means averaging over the unknown degrees of freedom.

Are any of these ideas correct? This is not yet determined!

In the two-path experiment discussed earlier we had the following discussion:

What if we put a wall into the soft path at the point (x_3, y_1) ?

The wall stops the time evolution of part of the state, so that the state at t_4 would be

$$\frac{1}{\sqrt{2}} |h\rangle |x_5, y_4\rangle - \frac{1}{\sqrt{2}} |s\rangle |x_3, y_1\rangle \quad (8.26)$$

In this case, the state remains nonseparable or entangled with respect hardness/color and coordinate-space properties at t_4 .

If a measurement of position of this electron were to be carried out at (if, say, we were to look and see whether the electron had emerged from the black box), the probability of finding it at (x_5, y_4) would be $1/2$, and if it were found there it would be hard, and if its color were measured, it would be *equally likely to be green or magenta*. That is exactly what we said in our earlier discussions.

The difference here is the the state of the system is a mixture and not a superposition. The reason is that a measurement has been performed and this collapses the original superposition state into a mixture state.

We will have more to say about these difficulties later in the book.

Chapter 9

More Formalism

Earlier we discussed free particle amplitudes using the position representation. We now shift our attention to a very different topic that we need to understand and then return to the earlier discussion.

9.1 Identical Particles

When quantum theory was being put together, one principle was found to be useful from time to time - the notion that quantum physics should, under the correct circumstances, reduce to classical physics. Some aspects of the quantum world, for all their strange detail, slide rather comfortably into the classical world when we consider large enough systems. Other aspects are totally alien and have no classical equivalent. We're now going to discuss one of these *other* aspects - identical particles. When we talk rather glibly about identical things in the classical world, we acknowledge the fact that they cannot be absolutely identical. Some details will differ. This is not true in the quantum world. For example, two electrons are absolutely identical and furthermore their identity has experimental consequences. We will now find out what those consequences are and how quantum theory deals with them.

Some Opening Thoughts

An atom consists of a nucleus, containing protons and neutrons, and electrons. The electrons, which are negatively charged, are attracted to the positively charged protons, and so the atom exists as a stable bound system.

Although atoms are very complicated objects, there are certain situations in which they can be treated as simple lumps of matter. Their internal structure has no relevance to the details of what is happening. This sort of situation is exemplified by experiments in which atoms are deliberately smashed into one another. Such experiments provide an ideal starting point for a study of the

quantum physics of identical particles.

Experimental physics is a complicated business. One must handle a wide range of details if an experiment is to work properly and give good data. Even after the experiment is completed there's generally a long period of further work during which the data have to be processed into a form that makes a clear understanding possible. There is also a danger at this point of consciously or unconsciously forcing the data to agree/disagree with theoretical predictions.

For our purposes, these details are not important. They distract from the physics that we want to extract from a given experiment. Thus, we will often be sketchy about how an experiment is actually carried out. We will not, however, leave out anything important.

One simple-looking experiment involves atomic collisions. To set up this experiment, we have to produce two beams containing atoms moving at a precise speed oriented so that a significant proportion of the atoms actually collide. You also need a way of detecting these atoms after they have collided and, at the same time, the ability to identify which one of them has arrived at a given detector. Such an experiment is illustrated schematically in the figure below.

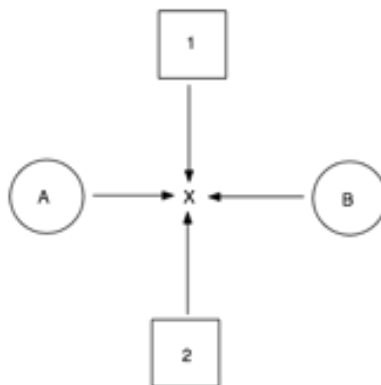


Figure 9.1: Atom-atom collision experiment

A and B represent sources for producing beams of atoms. The two beams collide at location X and the atoms scatter off one another to be detected at either 1 or 2 where the type of atom arriving can be recorded.

It turns out to be impossible to control the experiment precisely enough to enable us to predict with certainty which atom ends up at 1 or 2. If atoms are of different types (say hydrogen and helium), then we can tell which one went where once they have arrived, but we cannot predict that this hydrogen produced at A will end up at 1. This is not only because we don't have enough tight control of the energy and direction of flight of the atoms, but we also have

to face the random nature inherent in quantum events of this type.

Such an experiment can measure the probability that an atom produced at A, will end up at 1, and the probability that it will end up at 2, as shown below

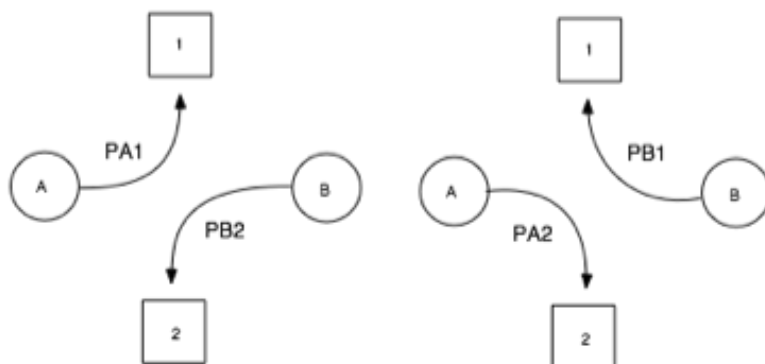


Figure 9.2: Two possible experimental results

where some of the possibilities for how atoms might travel from source to detector are shown.

If we repeat the experiment with a large number of atoms, counting the numbers that arrive at 1 and 2, then the probabilities are given by

$$PA1 = \frac{\text{number of atoms arriving at 1}}{\text{total number of collisions}}$$

$$PA2 = \frac{\text{number of atoms arriving at 2}}{\text{total number of collisions}}$$
(9.1)

Suppose we run this experiment, but choose not to worry about which atom ends up at 1 and which ends up at 2. We just want to measure the probability that one of the atoms arrives at 1 and the other arrives at 2. This is not a simple exercise (e.g., cannot keep track of all atoms) since the atoms might fly off at some angle and miss 1 or 2, but that is an experimental detail which we can ignore!

As a result of this experiment, we can measure the probability of an atom arriving at 1 and an atom arriving at 2, which we will call Prob(1,2).

Theoretically, we would want to check that our predictions agree with the experimental measurements of Prob(1,2). Fortunately Prob(1,2) is easy to calculate from the other probabilities PA1 and PA2, etc. Below we list all the probab-

ities:

$$\begin{aligned}
 PA1 &= \text{probability of A going to 1} \\
 PA2 &= \text{probability of A going to 2} \\
 PB1 &= \text{probability of B going to 1} \\
 PB2 &= \text{probability of B going to 2}
 \end{aligned}$$

Frequently we have to combine probabilities to calculate an overall probability for an event. We discussed this earlier, but let us repeat the rules for a better understanding. The general rule is that you multiply probabilities when you want events 1 *AND* 2 to happen and you add the probabilities when it is event 1 *OR* 2, where *OR* means either 1 happens, or 2 happens, or *both* happen.

In this first experiment, we are interested in one atom arriving at 1 and the other arriving at 2. It might be that A has ended up at 1, which we write as $A \rightarrow 1$ while B has gone to 2, $B \rightarrow 2$. The probability for this would be

$$(PA1 \text{ AND } PB2) = (PA1 \wedge PB2) = PA1 \times PB2 \quad (9.2)$$

However, it could be that $A \rightarrow 2$ and $B \rightarrow 1$. The probability for this would be $PA2 \times PB1$. Since we are not bothered about which atom ends up where, we have to combine these results to get the overall probability.

$$\text{Prob}(1, 2) = (A \rightarrow 1 \text{ AND } B \rightarrow 2) \text{ OR } (A \rightarrow 2 \text{ AND } B \rightarrow 1) \quad (9.3)$$

So,

$$\text{Prob}(1, 2) = PA1 \times PB2 + PA2 \times PB1 \quad (9.4)$$

To go any further, we need to calculate $PA1$, $PB2$, etc.

Now A and B are simply labels for atom sources. Provided that we have constructed these things well enough, they should run in an identical manner. Hence, the experiment would work just as well if we changed the labels around, i.e., interchanged A and B. That being the case, $PA1 = PB1$ and $PA2 = PB2$. So we can write

$$PA1 \times PB2 = PA2 \times PB1 = P \quad (9.5)$$

and thus

$$\text{Prob}(1, 2) = PA1 \times PB2 + PA2 \times PB1 = 2P \quad (9.6)$$

Now remember that when running this experiment we deliberately choose to ignore information available to us about what type of atom ends where and so we don't know from which source a detected atom started out.

Of course, it would be perfectly possible to run the experiment so that A and B were producing the same type of atom (say, both hydrogen). In this case, the information at 1 and 2 would be of no use. Finding a hydrogen atom at 1 does not tell us if it came from A or B. Would this affect our probabilities?

Classically, the *answer is clearly no*. If the atoms are different we can potentially tell which source they started from (hydrogen is A and helium is B); if both of them are the same, then we don't have this ability. However, if we choose not to record what type of atom arrives at a detector, the two experiments are surely the same; Prob(1,2) must be the same in both cases. Of course, you can do the experiment and find out, and you will be disappointed. Using hydrogen atoms coming from both A and B we find that

$$\text{Prob}(1,2) = 4P \quad (9.7)$$

for identical atoms. The probability is twice what it was before. Not being able to tell which atom is which has made a *fundamental and measurable* difference to the result.

Emphasizing the Weird

To make absolutely clear how weird this result is, let's translate the argument into a story involving billiard balls. Imagine that we have a bag that contains two white billiard balls and two black ones. The balls are numbered 1-4, with 1 and 2 being white and 3 and 4 being black. We dip our hand into the bag and pull out one of the balls, note its color and number and return it to the bag. After this we do the same thing again to find and replace a second billiard ball. It is easy enough to calculate the probability of picking out a white ball and a black ball. To make the calculation clear we can consider all the various possibilities. Picking out two balls one after the other means there are 16 possibilities in total, which have been listed below.

1W,1W	1W,2W	<u>1W,3B</u>	<u>1W,4B</u>
2W,1W	2W,2W	<u>2W,3B</u>	<u>2W,4B</u>
<u>3B,1W</u>	<u>3B,2W</u>	3B,3B	3B,4B
<u>4B,1W</u>	<u>4B,2W</u>	4B,3B	4B,4B

The process of picking billiard balls is straightforward. In this list 1W means ball number 1 which happens to be white; 3B is ball three that is black, etc. As we are replacing the balls after picking them out, it is always possible to pick the same ball again on the second draw (i.e., 1W,1W or 3B,3B).

In this list, we have underlined the pairings that correspond to one white ball and one black ball. There are eight of these, so the chance of picking one white and one black is $8/16 = 0.5$ (i.e., a 50% probability - half the time we will get a black and white pair).

From the details of this simple calculation, it should be clear that the numbers on the balls are quite significant. It's the numbers that make it possible to tell which white ball, for example, has been selected.

To connect this with the atom-scattering experiment we have to imagine that the color of the ball identifies which detector the atom ended up in (say white balls represent atoms that ended up at 1 and black balls stand for atoms arriving at 2). The number on the ball would then stand for the types of atoms; it's just in this case we are dealing with four different *types of atom*. Aside from these details, this calculation has used exactly the same logic as we applied to the atoms. Now if we wipe the numbers off the balls it becomes impossible to say which white ball is which. In the case of billiard balls this would not make a difference - we can still tell them apart. Various things such as size, smoothness, and so on, are bound to make a difference.

But this seems not to be so for atoms. If we *wipe off the numbers* (i.e., use identical atoms), then the experiment tells us that there is no way of distinguishing the balls (even in principle), so the various possibilities reduce to

$$W,W \quad W,B \quad B,B \quad (9.8)$$

which, if it could be true for billiard balls, would show us that the probability of getting a white ball and a black ball is only 1/3.

Of course, we are not saying that this is what really happens with billiard balls. Quantum rules do not apply to such objects. However, they do apply to atoms and it happens!

The atomic measurements seem to be hinting at a very important quantum rule:

If we cannot tell the difference between two
situations, then they are not really two situations.
They are actually just one event!

An attempt at illustrating this is shown below.

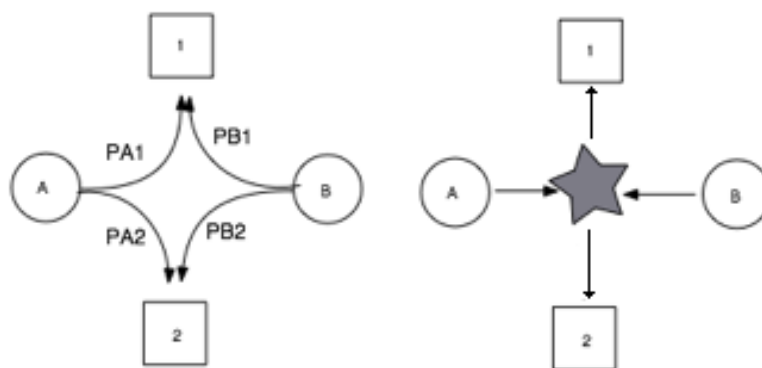


Figure 9.3: Two versions

The left-hand side of the figure shows the classical version of the experiment

with identical atoms. If an atom ends up at 1, this could be due to one of two separate events. Either $(A \rightarrow 1, B \rightarrow 2)$ or $(A \rightarrow 2, B \rightarrow 1)$ will do the job. The quantum world works differently, atoms from A and B go into the mix and then emerge heading towards 1 and 2. *They lose their identity in the middle of the experiment.*

In a classical world (where billiard balls live) we would think about the chance of getting an atom to 1 as well as another to 2 like the left-hand side of the figure. - even if the atoms were of the same type; atoms, however, do not live in this world. The experimental results tell us that the probability is rather different - as if A going to 1 and B going to 1 were the *same* event.

The Meaning of the Story

When we are dealing with atoms (and the particles from which they are made), there is something more to being *identical* than is true for larger-scale objects. Atoms of the same type are really identical - measurably identical - which can make a considerable difference in some experiments.

Clearly quantum theory has to take account of the nature of identical particles as they come up from time to time in the atomic and subatomic worlds (electrons being an example).

Before proceeding with an expanded discussion of identical particles, let us see how quantum theory deals with states that contain more than one particle, identical or otherwise.

States of More Than One Particle - Discussion #1

In the majority of real world situations, the systems that quantum theory will have to describe contain more than one particle. So far we have discussed only single-particle states. Adding even one more particle to the mix can produce significant complications and at the same time expose some of the more interesting aspects of the theory.

As a starting point, consider a very simple universe (a toy universe if you like) in which particles, such as electrons, can exist in one of two different states. According to quantum theory, there is an amplitude for the particle to exist in each of the states.

The amplitudes form a sequence of complex numbers (A_1, A_2) representing the presence of the electron in each state in turn. The probability of finding an electron in a state i is then given by $A_i^* A_i = |A_i|^2$ according to our standard procedure.

Now we introduce a second particle into the toy universe. For the sake of ar-

gument let us say that the particle is a neutron, then there will be no trouble telling the particles apart and we can assume that there's little or no interaction between them. In this case, the probability of a particle being in a state is not affected by the presence of the other particle anywhere in our toy universe. There will be another set of complex amplitudes (B_1, B_2) representing the probability of finding the second particle in the various states. Consequently, the amplitude for finding an electron and a neutron in state 1 would be $A_1 B_1$; for finding an electron in state 1 and a neutron in state 2 it would be $A_1 B_2$, etc. The state of the electron can be written down as

$$|\phi\rangle = A_1 |e1\rangle + A_2 |e2\rangle \quad (9.9)$$

by expanding it over a basis where $|e1\rangle, |e2\rangle$ represent states in which the electron is found in state 1 and state 2.

We can use a similar basis to expand the state of the neutron.

$$|\psi\rangle = B_1 |N1\rangle + B_2 |N2\rangle \quad (9.10)$$

Note that the basis $\{|Nn\rangle\}$ is *not* the same as the basis $\{|en\rangle\}$; this is an important point.

The next step is to consider what form of basis is suitable for expanding a combined state for two particles $|\Psi\rangle$. The easiest possible way of doing this would be a simple combination of the two separate bases so that we get

$$|\Psi\rangle = |\phi\rangle |\psi\rangle = A_1 B_1 |e1\rangle |N1\rangle + A_1 B_2 |e1\rangle |N2\rangle + A_2 B_1 |e2\rangle |N1\rangle + A_2 B_2 |e2\rangle |N2\rangle \quad (9.11)$$

with $4 = 2 \times 2$ terms in the expansion.

This is a most *straightforward extension* to the scheme.

If the particles are allowed to interact with one another, we have to be more careful. It might be that $|\phi\rangle$ describes the state of the first particle in the absence of the second, and $|\psi\rangle$ describes the second particle in the absence of the first, but we cannot now rely on $|\phi\rangle$ and $|\psi\rangle$ working when they are both present. We cannot be sure that $|\phi\rangle |\psi\rangle$ will adequately represent the state of both particles. It is far more likely that we will need to employ a new state $|\Phi\rangle$ where

$$|\Phi\rangle = C_{11} |e1\rangle |N1\rangle + C_{12} |e1\rangle |N2\rangle + C_{21} |e2\rangle |N1\rangle + C_{22} |e2\rangle |N2\rangle \quad (9.12)$$

with C_{11} being the amplitude for the first particle to be in box 1 and the second in state 1 also; C_{21} has the first in state 2 and the second in state 1, etc. Note that we use the same basis in both cases. But importantly, $C_{21} \neq A_2 B_1$, etc, i.e., the earlier straightforward guess cannot be assumed to work. In other words,

$$|\Phi\rangle \neq |\phi\rangle |\psi\rangle \quad (9.13)$$

$|\Phi\rangle$ is a genuine multi-particle state that *cannot be factored* into a product of separate particle states - it is called **inseparable**. Such states produce some of the most interesting physical manifestations of quantum theory as we will see later.

As we will see, multi-particle states contain a lot more information than single-particle states; there is a richness in the physics that such states can contain.

Identical Particles

Earlier, we demonstrated how identical particles in quantum physics are very identical. It is completely impossible to tell them apart, giving rise to some surprising experimental consequences. Following this result we might expect that $|\Phi\rangle$ will be different if the two particles that it represents are identical. In fact, the identity of the particles serves to place an extra constraint on the amplitudes. In the expansion

$$|\Phi\rangle = C_{11} |e1\rangle |N1\rangle + C_{12} |e1\rangle |N2\rangle + C_{21} |e2\rangle |N1\rangle + C_{22} |e2\rangle |N2\rangle \quad (9.14)$$

C_{12} must be linked with C_{21} . After all, for identical particles, we are unable to distinguish between [**particle 1 in state 1 with particle 2 in state 2**] and [**particle 2 in state 1 with particle 1 in state 2**]. The probability can only be [**a particle in state 1 and another in state 2**], that is, $C_{12}C_{12}^* = C_{21}C_{21}^*$. However, there are two ways in which this can be the case, either $C_{12} = C_{21}$ (hence $C_{12}^* = C_{21}^*$) or $C_{12} = -C_{21}$ (hence $C_{12}^* = -C_{21}^*$). So either $C_{12} = C_{21}$ giving

$$\begin{aligned} |\Phi\rangle_S &= C_{11} |e1\rangle |N1\rangle + C_{12} |e1\rangle |N2\rangle + C_{12} |e2\rangle |N1\rangle + C_{22} |e2\rangle |N2\rangle \\ &= C_{11} |11\rangle + C_{12} |12\rangle + C_{12} |21\rangle + C_{22} |22\rangle \end{aligned} \quad (9.15)$$

or $C_{12} = -C_{21}$ giving

$$\begin{aligned} |\Phi\rangle_A &= C_{11} |e1\rangle |N1\rangle + C_{12} |e1\rangle |N2\rangle - C_{12} |e2\rangle |N1\rangle + C_{22} |e2\rangle |N2\rangle \\ &= C_{11} |11\rangle + C_{12} |12\rangle - C_{12} |21\rangle + C_{22} |22\rangle \end{aligned} \quad (9.16)$$

But there is a potential problem in the second case. If we're saying that $C_{12} = -C_{21}$, then what are we to do about the numbers C_{11} and C_{22} ?

If we're to apply the rule strictly then we have the apparent contradiction that $C_{11} = -C_{11}$. The way out of this is to apply the same rule to all the amplitudes in the state $|\Phi\rangle_A$, which requires that the amplitudes $C_{11} = C_{22} = 0$; then $C_{11} = -C_{11}$ makes sense since saying $0 = -0$ makes sense (although it is a poor mathematical expression). There is an important physical significance to this, as we will see later.

The expression for the state $|\Phi\rangle_A$ now looks like

$$|\Phi\rangle_A = C_{12} |12\rangle - C_{12} |21\rangle = C (|12\rangle - |21\rangle) \quad (9.17)$$

This form shows clearly that the state is *antisymmetric* (changes sign) under the exchange of particles 1 and 2.

If we suddenly decide to call particle 1 particle 2 instead (and obviously particle 2 is renamed particle 1) we also need to swap all references to 1 and 2 in the state representation. What we then find is that the state expansion has changed. It becomes the negative of what it was $|\Phi_{12}\rangle_A = -|\Phi_{21}\rangle_A$. This is what we mean by antisymmetric(subscript A). We can show this in the following way:

$$\begin{aligned} |\Phi_{12}\rangle_A &= C(|12\rangle - |21\rangle) \\ |\Phi_{21}\rangle_A &= C(|21\rangle - |12\rangle) = -C(|12\rangle - |21\rangle) = -|\Phi_{12}\rangle_A \end{aligned} \quad (9.18)$$

A similar argument shows that $|\Phi\rangle_S$ (S for symmetric) is symmetric under interchange of the two particles, so that $|\Phi_{12}\rangle_S = |\Phi_{21}\rangle_S$.

All of this manipulation has come from a simple observation. With a set of two identical particles, the probability of particle 1 being in state i and particle 2 being in state j must be $C_{ij}C_{ij}^* = C_{ji}C_{ji}^*$, which can be true if either $C_{ij} = C_{ji}$ (symmetric) or $C_{ij} = -C_{ji}$ (antisymmetric).

Amazingly, this has led to two physically distinguishable situations, for if our combination of identical particles is in an antisymmetric state, then we can *never find both particles in the same state* ($C_{ii} = 0$). This remarkable observation is found to exist in nature for a whole class of particles called *fermions* (the electron is a fermion). Particles whose states are symmetric under an interchange in the labels are called *bosons* (the photon is a boson).

States in the Real World

Suppose now that consider a situation where the single particle states are again written as $|\phi\rangle$ and $|\psi\rangle$. As before we have four possibilities for constructing a multiparticle state, namely,

$$\begin{aligned} &|\phi_1\rangle|\psi_2\rangle \\ &|\phi_2\rangle|\psi_1\rangle \\ &\frac{1}{\sqrt{2}}(|\phi_1\rangle|\psi_2\rangle + |\phi_2\rangle|\psi_1\rangle) \\ &\frac{1}{\sqrt{2}}(|\phi_1\rangle|\psi_2\rangle - |\phi_2\rangle|\psi_1\rangle) \end{aligned} \quad (9.19)$$

However, if the two particles are identical bosons, we cannot be sure which is in state $|\psi\rangle$ and which is in $|\phi\rangle$, so only the third possibility is viable - it is the only one that is symmetric under an interchange between 1 and 2. We note that the $1/\sqrt{2}$ factor in front of the state is there to make sure that the overall

(combined) state is properly normalized to 1, i.e.,

$$\begin{aligned}
\langle \Phi | \Phi \rangle &= \frac{1}{\sqrt{2}} (\langle \phi_1 | \langle \psi_2 | + \langle \phi_2 | \langle \psi_1 |) \times \frac{1}{\sqrt{2}} (|\phi_1\rangle |\psi_2\rangle + |\phi_2\rangle |\psi_1\rangle) \\
&= \frac{1}{2} \left[\underbrace{\langle \phi_1 | \phi_1 \rangle}_{=1} \underbrace{\langle \psi_2 | \psi_2 \rangle}_{=1} + \underbrace{\langle \phi_1 | \phi_2 \rangle}_{=0} \underbrace{\langle \psi_2 | \psi_1 \rangle}_{=0} + \underbrace{\langle \phi_2 | \phi_1 \rangle}_{=0} \underbrace{\langle \psi_1 | \psi_2 \rangle}_{=0} + \underbrace{\langle \phi_2 | \phi_2 \rangle}_{=1} \underbrace{\langle \psi_1 | \psi_1 \rangle}_{=1} \right] \\
&= \frac{1}{2} \left[\underbrace{\langle \phi_1 | \phi_1 \rangle}_{=1} \underbrace{\langle \psi_2 | \psi_2 \rangle}_{=1} + \underbrace{\langle \phi_2 | \phi_2 \rangle}_{=1} \underbrace{\langle \psi_1 | \psi_1 \rangle}_{=1} \right] = \frac{1}{2} [1 + 1] = 1 \quad (9.20)
\end{aligned}$$

as required.

If the two particles concerned are identical fermions, then we need to ensure that the combined particle state is antisymmetric when we interchange 1 and 2. There is only one way of making a combination that will do this.

$$|\Phi\rangle_A = \frac{1}{\sqrt{2}} (|\phi_1\rangle |\psi_2\rangle - |\phi_2\rangle |\psi_1\rangle) \quad (9.21)$$

We easily see that if the two states happen to be the same ($|\psi\rangle = |\phi\rangle$), then the overall state will vanish. Thus, once again we see that identical fermions cannot be in the same state. However, there is an even stronger constraint than this. It turns out this is equivalent to stating that two identical fermions cannot be found at the same position (provided we assume the only physical property the fermions have is *position*). This is not true for identical bosons.

If they have another physical property, say S-G variables, then only the overall state must be antisymmetric, which we can do as shown below (one particle in and other $|U\rangle$ and the other in $|D\rangle$)

$$|\Phi\rangle_A = \frac{1}{\sqrt{2}} (|\phi_1\rangle |\psi_2\rangle + |\phi_2\rangle |\psi_1\rangle) - \frac{1}{\sqrt{2}} (|U_1\rangle |D_2\rangle - |U_2\rangle |D_1\rangle) \quad (9.22)$$

Switching the particles involves switching the S-G states as well, so that the state is still antisymmetric overall although the spatial part happens to be symmetric (so that the particles can now be at the same position).

Another point about a combined state of this form, whether symmetric or antisymmetric, is that we cannot definitely say that the particle is in one of the single states. This is another *inseparable state*.

Some Final Thoughts

The following is in no particular order of importance.

- (1) It is in the nature of fermions (like electrons) to always be in an antisymmetric state. Likewise it is in the nature of bosons (such as photons) to

always be in a symmetric state. This leads to some very different physical consequences for the two classes of particles.

- (2) The difference between fermions and bosons exploits a mathematical *loop hole* in the relationship between amplitudes and probabilities, which seems to be an example of a definite quantum *rule of thumb*: **anything goes unless it's forbidden**. Nature might have chosen to recognize only the $C_{ij} = C_{ji}$ possibility, for example. However, it is probably a good job that she explored all the possibilities open to her, as fermions and bosons represent the two most obvious aspects of reality as we will see.
- (3) Given that the physical differences between fermions and bosons arise from different properties of their amplitudes, one might be tempted to construct an argument that the amplitudes are in some sense *real*.
- (4) Sooner or later you are going to end up asking yourself what it is that prevents two identical fermions from being in the same place. The answer is rather unnerving. Normally, this would be a signal that some force of some kind as acting to keep the particles apart. Unfortunately, this does not work for various reasons (no obvious force that can do the job, the effect being independent of how far apart the particles are, etc). The identical fermions simply avoid one another like polite strangers on the street. In the end, one ends up dabbling with the rather Zen-like answer that it is **symmetry** (or rather antisymmetry) that is keeping them apart!

9.2 Spin

We now attempt to draw together several of our ongoing discussions. In particular, we want to connect the Stern-Gerlach(S-G) experiments and identical particles. What ties these two things together is the concept of spin - a piece of quantum physics that has *no exact counterpart* in classical physics.

Fermions, Bosons and Stern-Gerlach Magnets

We have a couple of loose ends lying around. For one thing, we have yet to explain why it is that an electron passing through an S-G magnet can take only two paths. Up to now we have assumed that there's some physical property belonging to the electron that determines which path it will take through the S-G magnetic field. Since this is a quantum mechanical property, we have seen that the behavior of the electron depends on the context of the experiment as well.

Earlier we looked at the properties of multiparticle states and discovered that states composed of identical particles could be either symmetric under interchange of any two particles, or antisymmetric. We called the particles that

belong to symmetric multiparticle states bosons, and those that have antisymmetric states fermions. However, we have not said what it is that makes a boson behave differently from a fermion.

Now we are going to start to pull these ideas together by introducing a new physical property called spin. Then we will look at fermion states in general and see how they behave under particle exchanges.

What distinguishes a fermion from a boson is its spin property. An electron's spin gives it a tiny magnetic field, which interacts with the S-G field, causing the electrons to be deflected. Despite this classical sounding picture, spin is a quantum physical property with no exact classical equivalent. Any attempt to build a picture of what spin is, based on classical ideas, will ultimately fail, as no classical picture can capture everything to do with spin. But, we have to start somewhere and as good a place as any is with the classical properties of *angular momentum*.

Angular Momentum

Ordinary (linear) momentum (mass \times velocity) plays a very important role in classical mechanics. The total (linear) momentum in the world is conserved (meaning that the sum for all objects is a fixed quantity), and the change in momentum per second experienced by an object is a measure of the force applied to it - that is Newton's second law of mechanics for the motion of objects.

Angular momentum takes a very similar role in the classical mechanics of rotating objects. It is also a conserved quantity, and its rate of change per second is a measure of the turning force (*torque*) applied.

Calculating angular momentum is very straightforward, at least in the case of a point mass moving around in a circular path, the magnitude (L) of the angular momentum (it is a vector quantity) is $L = mrv$, where r is the radius of the path (the magnitude of the position vector) and mv the magnitude of the momentum of the mass.

If we have a more complicated situation, such as a spinning top, we imagine that the top is constructed of a collection of point masses and add up the angular momentum (vector addition) of each to get the angular momentum of the whole object. So, angular momentum has a much more general application (any objects) than the simple example of a point mass in a circular path.

As stated above, angular momentum (vector) has a direction as well as a magnitude. This might seem odd; after all having a particle moving around a circular path means that its direction is continually changing. Well, the direction of the angular momentum is not the same as that of the moving particle. In fact, the angular momentum has a direction at right angles to the plane of the orbit as

shown below.

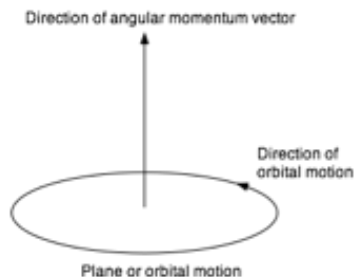


Figure 9.4: Direction of angular momentum

where for a point mass moving in a circular path, the angular momentum is given a direction (vertical arrow) as shown which is at right angles to the plane of the orbit. The head of the arrow always points away from the plane and toward your eye if you are looking down from above and the orbit is anticlockwise from that perspective.

Of course, for real world objects, the angular momentum would be a 3-dimensional vector, so it would have x , y , and z components. In classical physics we say

$$L^2 = L_x^2 + L_y^2 + L_z^2 \quad (9.23)$$

with L being the total angular momentum (symbolized by the length of the arrow in the figure below) and L_x , L_y , and L_z the components in the three reference directions.

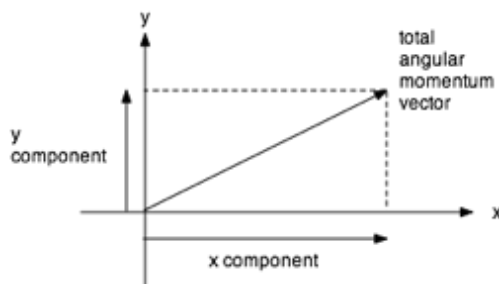


Figure 9.5: 2-dimensional example

where an angular momentum (large arrow) is shown with the x and y components of that angular momentum.

Angular momentum in 3-dimensions is a very tricky subject and has to be handled carefully. Fortunately, we don't need to explore this in any detail. To help you visualize angular momentum in 3-dimensions, we give an example in the figure below.

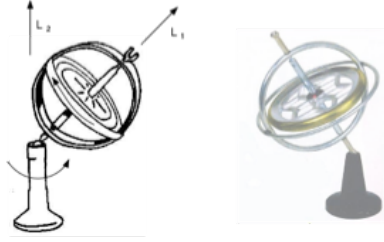


Figure 9.6: Gyroscope

A gyroscope can spin about its own axis, giving it an angular momentum with direction at right angles to the wheel part of the gyroscopes (L_1 in the figure). In addition, they can be set to precess about the point of contact with the stand, which is a bit similar to a point mass following a circular path. This second angular momentum is L_2 in the diagram. The total angular momentum in the system is the sum(vectors) of these two angular momenta.

Angular Momentum in Quantum Theory

To represent angular momentum in quantum mechanics, we have to replace L with a suitable operator \hat{L} . Using the classical definition, we will just write down the components and the operator for the total angular momentum. Their derivation is not important to our discussion - it is only important that they exist and have certain properties. Details beyond that are beyond this book.

$$\begin{aligned}\hat{L}_x &= \hat{y}\hat{p}_z - \hat{z}\hat{p}_y & \hat{L}_y &= \hat{z}\hat{p}_x - \hat{x}\hat{p}_z & \hat{L}_z &= \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \\ \hat{L}^2 &= \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2\end{aligned}\quad (9.24)$$

Eigenstates of \hat{L}^2 have a definite predictable value of total angular momentum, so you would think that such states would also be eigenstates of the three components. Not so. It turns out that you can only have an eigenstate of \hat{L}^2 and one of the three components at any one time(the components are not compatible observables). This surprising feature is the key piece needed to explain what is happening in the S-G experiment.

We cannot be any more specific at this point because exact mathematical forms for the \hat{p} and \hat{r} operators and have not been developed yet.

The eigenstates of angular momentum are given by the relations

$$\hat{L}^2 |\ell, m_\ell\rangle = \hbar^2 \ell(\ell + 1) |\ell, m_\ell\rangle \quad , \quad \hat{L}_z |\ell, m_\ell\rangle = \hbar m_\ell |\ell, m_\ell\rangle \quad (9.25)$$

You can construct simultaneous eigenstates of \hat{L}^2 and any one of the three component operators, but we will generally work with \hat{L}^2 and L_z when we discuss angular momentum. An eigenstate of these operators $|\ell, m_\ell\rangle$ is characterized by two numbers ℓ and m_ℓ . Both of these have to be integers, but m_ℓ can be negative. They are related to one another by the rules

$$\ell = 0, 1, 2, 3, \dots, \quad m_\ell = 0, \pm 1, \pm 2, \dots, \pm \ell \quad (9.26)$$

Consequently, for every ℓ value there is a collection of states with the same ℓ value but with different m_ℓ values.

$$|0, 0\rangle \quad |1, 1\rangle, |1, 0\rangle, |1, -1\rangle \quad |2, 2\rangle, |2, 1\rangle, |2, 0\rangle, |2, -1\rangle, |2, -2\rangle \quad (9.27)$$

The behavior of angular momentum eigenstates $|\ell, m_\ell\rangle$ is such that for each ℓ , the total angular momentum takes on the value $\hbar\sqrt{\ell(\ell+1)}$. There are a collection of states with the same ℓ value, which have different z -components as illustrated below.

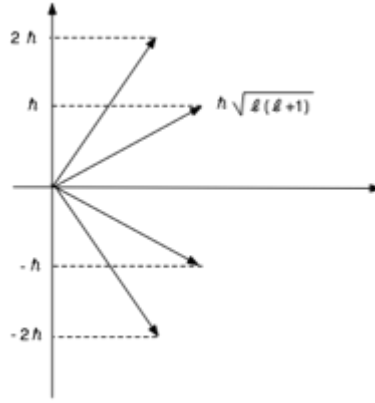


Figure 9.7: Allowed z -component values

Remember, in quantum physics a system cannot have a definite value of \hat{L}^2 with more than one component at the same time.

These results are valid for so-called *orbital* angular momentum, which classically would correspond to standard particle motion in orbit. There is, as mentioned above, a second kind of angular momentum in quantum mechanics, namely, spin. It does not have anything to do with something spinning in a classical sense. However, the operators representing it have the same properties, i.e.,

$$\begin{aligned} \hat{S}^2 &= \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2 \\ \hat{S}^2 |s, m_s\rangle &= \hbar^2 s(s+1) |s, m_s\rangle, \quad \hat{S}_z |s, m_s\rangle = \hbar m_s |s, m_s\rangle \\ s &= 0, 1/2, 1, 3/2, 2, 5/2, 3, \dots, \quad m_s = -s, -s+1, \dots, s-1, s \end{aligned} \quad (9.28)$$

Note that we have not written down expression for the spin-components in terms of position and momentum components because the spin has no dependence on

position and momentum. Note the appearance of half-integer value of spin. Orbital angular momentum values can only be integers. The appearance of half-integers will be very important.

Magnetic Moments

The original S-G experiment was performed with a beam of silver atoms rather than electrons. Stern and Gerlach expected the beam to be deflected by their nonuniform magnetic field since they knew that silver atoms had their own small magnetic field (actually arising from the electrons in the atom).

Any moving object with an electric charge will produce a magnetic field. A crude (pre-quantum mechanical) picture of the hydrogen atom has an electron moving in a circular orbit around the nucleus(a proton). As the electron is a moving charge, it will produce a magnetic field.

An moving charged electron in orbit can be compared with a single loops of wire carrying current. This configuration produces a magnetic field passing through the plane of the orbit or the loop of wire.

The direction of the field is determined by the sense in which the current (electron) travels. If the electron is moving in an counterclockwise(anticlockwise) sense when viewed from above, then the magnetic field will be pointing upward.

More complicated atoms often do not have an overall magnetic field since the fields due to the various electrons circulating around manage to cancel out each other. Silver was selected for the S-G experiment as it was easier to work with than hydrogen and had an “unpaired” electron in its outermost orbit and so had a magnetic field to work with. The size of the field resulting from the orbital motion is related to the orbital angular momentum of the orbiting electron via the magnetic moment μ .

A simple bar magnet has a magnetic moment defined by $\mu = pd$ where p is the strength of its magnetic poles and d is the distance between them. The magnetic moment for a charged object moving in a circular path(orbit) is given by

$$\mu = \frac{qL}{2m} \quad (9.29)$$

where L is the orbital angular momentum of the orbiting object, q its charge, and m its mass.

By measuring the deflection of an atom through an S-G magnet’s field, physicists can work backwards and calculate the magnetic moment of the atom and so figure out something about the orbital angular momentum.

The Magnetic Moment of an Electron

Given that electrons are deflected when passing through an S-G magnet, it seems sensible to suggest that the electron must have a tiny magnetic field of its own and hence a magnetic moment. If we could carry out an S-G type experiment with electrons in reality rather than as a thought experiment as we have been doing, we could calculate an electron's magnetic moment from the deflection produced.

From the results of S-G experiments for atoms with unpaired electrons, but no orbital magnetic field (no orbital angular momentum contribution), we know that the electron's magnetic moment is

$$\mu_e = \frac{e\hbar}{2m_e} \quad (9.30)$$

This is an interesting result. If you look back at the formula above for the magnetic moment of an orbiting charge, then we can compare this with the electron's magnetic moment and decide that the electron must have an *intrinsic* (not due to its orbital motion) angular momentum. Here is how it works.

Electron's own magnetic moment

$$\mu_e = \frac{e\hbar}{2m_e} \quad (9.31)$$

Orbital motion magnetic moment

$$\mu = \frac{qL}{2m} \quad (9.32)$$

As both e and q are charges and m and m_e are masses in both cases, this would suggest that the angular momentum of an electron is $L = \hbar$.

Actually, for a variety of technical reasons, we have not quite gotten this correct. Certain effects due to relativity alter the calculation. The S-G measurement is correct, but it is not correct to compare it directly with an orbital magnetic moment, instead we must use

$$\mu = g \frac{qL}{2m} \quad (9.33)$$

where $g = g_\ell = 1$ in the orbital case and $g = g_e = 2$ in the electron (intrinsic) case so that we must compare

$$\mu_e = g_e \frac{e\hbar}{2m_e} \quad (9.34)$$

and

$$\mu = g_\ell \frac{qL}{2m} \quad (9.35)$$

which gives the result $L = \hbar/2$ for the intrinsic (non-orbital) angular momentum.

We have used the following thought sequence:

- (1) Since they have a magnetic field(moment), atoms get deflected by S-G magnets.
- (2) This field comes from orbiting electrons.
- (3) Electrons themselves get deflected by S-G magnets.
- (4) Electrons must have their own magnetic field, even if they are not in atoms.
- (5) Electrons must have their own angular momentum.

Intrinsic Angular Momentum

So, what sort of angular momentum is intrinsic angular momentum, or spin as it is actually called?

Well, this is where we start to get into trouble. It's very easy to try to compare an electron to some sort of classical objects that has intrinsic angular momentum, for example, a spinning top. If we think of an electron as a tiny ball of charge spinning about some axis, we can believe that it would have a magnetic field. After all, the rotation of the charge will generate a magnetic field.

Unfortunately, it can't be that simple. Since the radius of the electron, coupled with its rate of rotation, would determine the intrinsic angular momentum and hence the magnetic field we get in trouble because given any reasonable size for an electron, it edges would have to be moving faster than the speed of light to generate the measured magnetic field, which is in clear contradiction to Einstein's theory of special relativity.

Another reason why the simple picture won't work goes back to the S-G experiment. There seems to be no reason why a classically rotating ball should not spin about any axis. As the magnetic field is aligned with the spin axis, we ought to be able to have the electron's magnetic field in any given direction, which is not in accord with the S-G experiment. After all, if a general S-G state $|\phi\rangle$ collapses into either $|U\rangle$ or $|D\rangle$, it implies that the electron's magnetic field can be pointing only *UP* or *DOWN* and not at any intermediate angle. Following on from this, we can have the electron's axis of spin pointing only *UP* or *DOWN*. **That is not very classical behavior!**

Finally, the classical picture cannot explain why all the electrons have exactly the same spin. We know this must be the case, as all of them are deflected by the same amount in the S-G field (it might be upward or downward, but it's the same deflection). We could alter the angular momentum of a spinning sphere in a number of ways. All we have to do is apply a suitable force to speed it up or slow it down. However, nothing of this sort affects the electron's spin.

Given these difficulties, it might be better to give up the idea that the electron's

magnetic field was related to any sort of angular momentum and try to find some different physics to explain what is going on. However, there are independent pieces of evidence that point to electrons having angular momentum of their own.

When an electron orbits an atomic nucleus, the magnetic field it sets up interacts with the electron magnetic field, a process known as spin-orbit coupling. This interaction influences the energy of the atom and thus appears in the observed light that is emitted by the atoms.

In addition, a thorough analysis of the possible orbital motions shows we cannot conserve angular momentum for the atom as a whole just by using the orbital angular momentum, the spin has to be taken into account as well.

Also, the operators introduced earlier to describe the S-G measurement process, \hat{S}_x , \hat{S}_y and \hat{S}_z turn out to have exactly the same mathematical properties as \hat{L}_x , \hat{L}_y and \hat{L}_z as we mentioned above, strongly suggesting that the S-G operators must represent some form of angular momentum as well.

So we are left with a very odd situation. On the one hand, electrons appear to behave as if they have an intrinsic angular momentum leading to a magnetic moment, but on the other hand any attempt to work out a theory in which the electron is spinning like a top, leads to absurd conclusions.

Physicists have now resigned themselves to the notion that spin is a purely quantum mechanical effect that has no direct correspondence to anything that we see in the large-scale world - there does not exist a classical model for a spinning electron that works!.

Spin Operators

Earlier, we wrote down an operator corresponding to the (UP,DOWN) S-G measurement situation and gave it eigenvalues $\pm\hbar/2$.

$$\hat{S}_z |U\rangle = +\frac{\hbar}{2} |U\rangle \quad , \quad \hat{S}_z |D\rangle = -\frac{\hbar}{2} |D\rangle \quad (9.36)$$

As we said, \hat{S}_z forms a set with \hat{S}_x and \hat{S}_y and $\hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2$ with exactly the same mathematical properties as the angular momentum operators from earlier. This means we ought to be able to construct sets of eigenstates with properties similar to those for orbital angular momentum as we indicated above. In other words,

Spin Eigenstates

$$\hat{S}^2 |s, m_s\rangle = \hbar^2 s(s+1) |s, m_s\rangle \quad , \quad \hat{S}_z |s, m_s\rangle = \hbar m_s |s, m_s\rangle \quad (9.37)$$

All we need now is a clue from the experiment to help figure out what s and m_s should be (we indicated that half-integer values appear - now let us see how and why).

Earlier we said the measured value of the electron's angular momentum was $\hbar/2$.

Now we have to be careful. We cannot interpret this as being the value of the total spin angular momentum because actually what the S-G experiment tells us is that there are two components $+\hbar/2$ and $-\hbar/2$ corresponding to $|U\rangle$ and $|D\rangle$, respectively. What we have actually found here is that

$$\hat{S}_z |s, 1/2\rangle = +\frac{\hbar}{2} |s, 1/2\rangle \quad , \quad \hat{S}_z |s, -1/2\rangle = -\frac{\hbar}{2} |s, -1/2\rangle \quad (9.38)$$

If we stick to the same pattern as with the orbital angular momentum eigenstates, where the maximum value of m_s is s , then we must have $s = 1/2$, which is the only possibility for the electron, i.e., maximum value of $m_s = 1/2$ and that implies $s = 1/2$ with m_s values $\pm 1/2$.

Thus, we finally make the connection

$$|U\rangle = \left| \frac{1}{2}, \frac{1}{2} \right\rangle \quad , \quad |D\rangle = \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \quad (9.39)$$

So, the eigenvalues of \hat{S}_z are $\pm\hbar/2$ as we indicated. Note that there are only two values of m_s which corresponds to the fact that only two beams are observed to come out of the S-G device!

9.3 Fermions and Bosons

The picture that we have built up is one that describes electrons as particles with a *system property* (does not change) called spin, which has the value $\hbar\sqrt{s(s+1)}$ with $s = 1/2$, and a *state property* (can change), the component of spin, which has eigenvalues $\hbar_s = \pm\hbar/2$ along any direction that we point the S-G magnet. This is shown in the figure below.

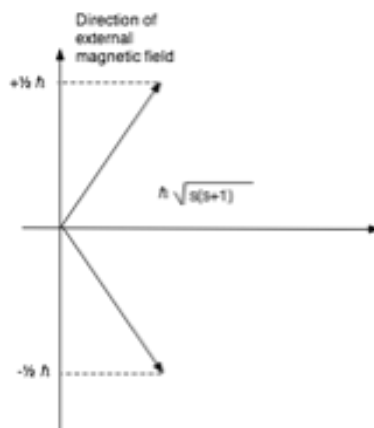


Figure 9.8: Allowed spin component values

The figure depicts the following situation. In the presence of a magnetic field, a spin $1/2$ particle aligns itself so that the component of spin is either $+\hbar/2$ or $-\hbar/2$. This happens irrespective of the direction in which the magnetic field is pointing. The arrows represent the direction of the axis about which the particle is spinning. In truth, these arrows could be pointing in any direction around a cone of the correct angle. The actual magnitude of the spin is given by the formula $\hbar\sqrt{s(s+1)}$ where $s = 1/2$ in this case.

Fermion States

We now want to show how the spin of a particle is related to the symmetry of a state.

Exchange and Rotation

Earlier we suggested that identical fermion multiparticle states are antisymmetric under an interchange of two of the particles. Let us explore this idea further.

Although we have not mentioned it so far, the antisymmetry of fermion states presents us with a puzzle. After all, if the particles are identical we are not supposed to be able to tell the difference between them. Yet, exchanging does make a difference to the state. How does the state then *know* that the exchange has taken place? Put it in a different way: if the particles are identical the physical situation after the exchange would appear to be identical to that beforehand, yet the state is different. How has that change come about? Although these are interesting questions as formulated it turns out they are not the correct questions in quantum theory - quantum systems do not “know” things - that is a classical, macro world idea.

Exchanging two particles is a simple thing in symbolic terms; all we have to do is rub out some letters and write in some different ones instead. In practice, however, the process is not simply snapping our fingers and watching particles teleport from place to place. We would have to pick one particle up and move it to a new place and move the other one back again.

In the figure below we have linked two clips by a ribbon and laid the whole thing out on a table (left part of figure). For the purpose of this argument, the clips are supposed to represent two identical particles in a multiparticle state. The ribbon is a rather more abstract thing representing the *geometrical connection* between the particles (this is an idea that will build as we proceed with this discussion).



Figure 9.9: Exchanging identical particles

In the next step, we have picked up one particle (clip) and moved it across to the other and pushed the first one across into its place. In other words, we have swapped (exchanged) the position of the two particles. This has obviously put a loop into the ribbon (see middle part of above figure). Now we just grab the bottom of the loop and pull it tight; the figure above on the right becomes remarkably similar to what we had to start with; we have just gained a twist in the ribbon under the right-hand side particle (compare (left part) and (right part) above).

Given that the clips are supposed to represent identical particles, if we just look at the clips, we can't tell the difference between the (left part) and the (right part) of the figure.

However, the connecting ribbon tells another story. Something has happened, as now the ribbon has a twist in it beneath the right-hand side particle. This twist is the record of the switch having taken place.

The same effect could have been achieved by leaving all the clips in place and simply twisting the ribbon under the right-hand side one, a twist can be generated by rotating the right-hand side clip through 360° on the spot.

This is an extraordinary prediction: switching two identical particles has the same physical effect as leaving them where they are and rotating one of them 360° on the spot.

There is no easy way of imagining this without the aid of the last figure. The best we can do is to remind you that any switch in practice would have to be done by moving and sliding particles about, something that would distort their connections with their surroundings and one another. Geometrically we have shown that this sort of distortion is the same as a single rotation.

We can take the prediction further. After all we have already seen that exchanging fermions causes a multiparticle state $|\phi\rangle$ to go to $-|\phi\rangle$ (phase inversion), so we can conclude that the same thing must happen if we simply rotate one of the particles through 360° .

Furthermore, as any change made as a result of the rotation must be localized to one of the particles, it would follow that a 360° rotation of any *single-particle* fermion state would invert the phase (multiply by -1) of the state.

Rotational Symmetry of States

There are two surprising aspects to this result. The first we have already mentioned: switching two particles is the same as rotating one on the spot. The other is to do with rotations.

Sometimes when you rotate an object through an angle less than 360° , things look just the same as they did before. This is called *rotational symmetry*. The basic idea is illustrated in the figure below, which shows two different types of playing cards. The ace of diamonds has 180° rotational symmetry, that is, if we rotate the card by 180° about one corner it will look exactly the same. No smaller rotation than this will work; if we turn it through 90° it will look completely different. Of course, bigger rotations can work; 360° is just as good, since that is just two 180° rotations in sequence. Basically any integer multiple of 180° will be fine.

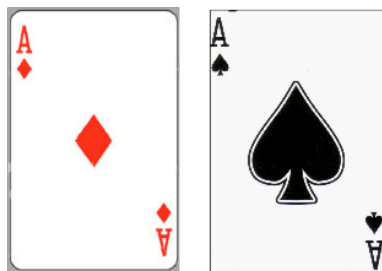


Figure 9.10: Examples of rotational symmetry

However, the ace of spades does not have 180° rotational symmetry, as the center of the card is decorated by a large spade symbol, which looks different when upside down. This ace has 360° rotational symmetry.

You might think that every single object you come across has 360° rotational symmetry. Indeed, most do, but surprisingly it is possible to set up a situation where a rotation through 720° is the smallest one required to restore an object. We will see a 3-D example using a coffee mug and ribbons later.

The fermion situation is even more puzzling. After all, we are supposed to be dealing with a particle that is so small it can be treated as an infinitesimal point. Yet, according to our earlier argument, if we rotate a fermion through 360° its state will change. Physically something is different. To see how this can come about, we need to think more about what is the real nature of rotations. However, before we get to that point, we want to demonstrate that this prediction is correct and to do that we need an experiment.

Reversing the Polarity of Neutron Flow

The Stern-Gerlach (S-G) experiment demonstrated the basic technique that will be needed for this experiment. Electrons are deflected because the tiny magnetic field they generate interacts with the S-G magnet's field. Of course, the poles of the S-G magnet were specially shaped to generate the correct sort of nonuniform field that would produce a path deflection; however, in the presence of any magnetic field, the electrons would try to align themselves so that their own magnetic field would point in the same direction as the external field as shown below.

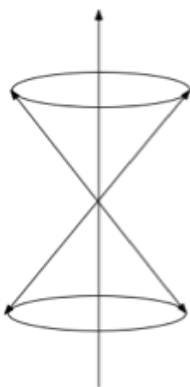


Figure 9.11: Aligning with the field

The vertical arrow represents an externally applied magnetic field. In the presence of such a field, the magnetic axis of a particle (which is the same as its spin axis) rotates around the magnetic field direction (on the cone); this is called precession.

So, if we can construct a magnetic field that changes over a distance, we can hope to alter the alignment of an electron that happens to be passing through the field and rotate the electron (or its spin) in the process.

We have illustrated one way of doing this in the figure below.



Figure 9.12: Rotating an electron spin

The dotted arrow indicates the orientation of an electron's magnetic field as it moves left to right through an externally applied combination of two magnetic fields (black arrows). The electron field will try to align itself with the two fields, but more toward the direction of the stronger field (longer arrow). By varying the strength of the two fields as the electron passes through, we can force it to rotate about a vertical axis. In this case, we have shown a 180° rotation about a vertical axis (perpendicular to the page as we look at it).

Here we are rotating an electron in a magnetic field. The dotted arrow represents the magnetic field direction of an electron. The two thick lines are externally applied fields, which change strengths along the sequence.

Actually, this sort of experiment proves to be rather impractical with electrons. They have a small mass, which makes them very sensitive to variations in the magnetic field. In fact, the magnetic field of the earth can influence them enough to spoil the experiment. Fortunately, the principle can be effectively demonstrated using a more massive fermion, namely, the neutron.

At first sight, this seems to be an odd choice since neutrons don't have an electric charge and you might think that, consequently, they don't have a magnetic field either. However, neutrons are composed of quarks that do have electric charge and the residual effects of the quark charge gives the neutron a magnetic field.

The first experimental results confirming the rotational behavior of fermion states was published in 1975. The experiment used a specially developed crystal of silicon to split a beam of neutrons coming from a nuclear reactor. The beams were then reflected by a second crystal so that they merged again creating an interference setup(just like classic interference experiments discussed earlier).

To demonstrate the phase shift, one neutron beam passed through a magnetic field which rotated the orientation of the neutrons. Varying the strength of the magnetic field gives control over the amount of rotation. Finally a detector measured the intensity of the combined beams as the rotation of the neutrons in path I was changed. See figure below.

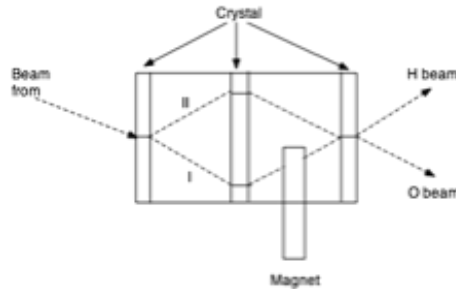


Figure 9.13: Neutron interference experiment

Here the experimental arrangement for the neutron phase-shift experiment is viewed from above. A crystal splits a neutron beam from a reactor along paths I and II. A second chunk of crystal reflects the split beams back toward one another. A magnet rotates the state in path I, whereas path II is unaffected. The O and H beams are formed from the interference of the I and II beams in the final piece of crystal. Finally, the intensity of both beams is measured as the magnetic field varies. The results(below) show that as the magnetic field changes, the intensity of both beams varies but out of phase with one another.

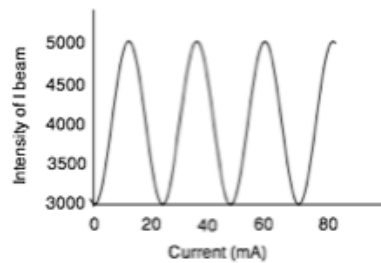


Figure 9.14: Experimental results

These are typical results from the neutron-interferometer experiment. The vertical scale shows the intensity of the O beam at a fixed point along its path after the two beams (I and II) have interfered. and the horizontal scale on this graph is not the distance along the detector as one might expect for an interference experiment, but the strength of the magnetic field, which is equivalent to the rotation angle for the neutron state. Clearly, the combined intensity varies in a periodic manner as the magnetic field is increased. A 360° change in neutron state rotation brings a minimum intensity to a maximum and vice versa. The measured periodicity from the experiment was $(704 \pm 38^\circ)$. More modern and more sophisticated experiments now give a result much closer to 720° .

Of course we already know that a 360° rotation is supposed to send a fermion state such as $|U\rangle$ into $-|U\rangle$, but what about rotations of a different size? If we multiply a state $|U\rangle$ by an amplitude that has magnitude 1 and phase θ , we will not change the probability, but we will alter the way in which that state will interfere with another state. The interference pattern clearly shows how the rotation of the neutrons is causing a continuous change in the phase of their state.

When the magnetic field is changed sufficiently, a 360° rotation comes about, which sends the phase to -1 and destructive interference is produced. Increasing the field further, so that a second 360° rotation takes place, sending the phase back again to +1 and the interference state goes back to what it was.

This is a truly remarkable result, which, once again, raises questions about the nature of quantum states. In all cases, everyday physical objects look exactly the same if we rotate them through 360° . Yet the quantum state of a fermion is not the the same, but in a curious way. Any probability that we calculate from the state is unchanged since $A^*A = (-A^*)(-A)$, but as we have seen from the results of the neutron experiment, the state is different in a physically meaningful way. Perhaps there is something *real* about complex amplitudes.

Coffee Mugs and Quantum States

When we talk about rotating an object, such as a particle, or exchanging two particles, we must have some fixed points of reference or we can't tell what happened. Normally, we use the system of coordinates or positions set up as a background to our whole theory. However, in more general terms, the mathematical consequences of what we are doing can't depend on the specific system of reference we have chosen.

To give a concrete example, imagine that we have a coffee mug, floating in empty space far away from any mass, so there is no background that we can use to orient ourselves. We go away for a moment and return to find that a colleague claims to have rotated the mug through 360° about its vertical axis.

How can we tell? Do we care?

A mathematician would suggest the following. Imagine that we have used a set of ribbons to attach the coffee mug to a collection of fixed reference points a long way away. These ribbons represent the abstract mathematical links between an object and its fixed reference environment that allow us to judge its motion and orientation. As such, the ribbons can be bent, and twisted - provided the anchor points stay fixed to the mug and the reference points. We are not allowed to cut the ribbons. Think of them as being like the grid on a graph paper: not physically real, but allowing us to chart the position of an object by referring to its coordinates on the grid. The difference is that more general connections do not have to rely on straight lines or right angles on the grid.

If the mug is rotated about its vertical axis through 360° , a twist is placed in all ribbons, which cannot be removed no matter how we fiddle with things. The only way of untwisting them is to rotate the mug back again. The *connections* between the mug and its surroundings or the reference coordinate system have been distorted by the rotation and retain a *memory* of what happened. The figures below of the captive coffee mug show the connection between an object and its surroundings.

A coffee mug has been anchored to a reference point by a ribbon.



The mug is then rotated through 360° about its vertical axis.



The ribbon wraps itself around the mug, but can then slip down to reveal



a ribbon with a single twist in its length



Doing this again produces a double-twisted ribbon. However, in this case the twist can be removed by



looping the ribbon over the top of the mug



So we see that if the mug is rotated again by 360° in the same direction, we now have a double twist, which can be removed by taking the ribbon over the top of the mug. We are allowed this maneuver, as the anchor points stay fixed. All it does is display how the double twisted ribbons are in fact *connectively* the same as untwisted ribbons.



Figure 9.15: Twisting and untwisting

Here then is a concrete example of a 3-D situation in which a 360° rotation doesn't bring things back to the starting arrangement. The twist in the ribbon prevents that. However, a second 360° rotation in the same sense changes things to a situation that can then be easily returned to the starting configuration.

Although we've been talking about a coffee mug, the same sort of argument

can easily be applied to a particle such as an electron. As we have seen, a 360° rotation of a fermion makes a physical difference to its state, and a second 360° rotation puts things back again.

So, although it looks as if an object has 360° rotational symmetry, there may be some internal physics that is able to tell the difference. In particular, you have to be careful about 360° rotations and keep track of how many of them have happened.

Spin, Symmetry, and Exchanges

Now we have the following three pieces of information about fermions:

- (1) They have half-integer spin; electrons are spin $1/2$.
- (2) Their identical multiparticle states are antisymmetric under an exchange of any two particles.
- (3) The phase of a fermion state is inverted by a 360° rotation.

All of these features are related to one another. We have already demonstrated the connection between the phase inversion on rotation and the antisymmetry of the multiparticle state, but we have not connected this to spin.

A full understanding of the link between spin and rotation would require some very sophisticated mathematics and the theory of relativity. It is one of the most beautiful results in theoretical physics.

We can, however, get a rough understanding of how this works using a somewhat *hand-waving*, but nevertheless subtly beautiful argument.

Time

Time is one of the great mysteries in physics. It has also confounded philosophical understanding for centuries. For the purposes of this argument, however, we need to have only the loose understanding of time that we all carry around on a daily basis.

One of the deepest mysteries connected with time is its, apparent, one-way flow. Time marches on relentlessly from the past toward the future. This has occasionally led physicists to speculate about what might happen if you could reverse the flow of time. Mathematically this is very easy to do; you just replace t with $-t$ and see what happens. In quantum physics we have an operator to do this job.

Let us now consider what happens to the spin components of a fermion when we imagine reversing the flow of time.

To do that, we have to work with the dangerously classical idea that electrons have spin because they are tiny rotating spheres of charge.

I know that we have already shown how this picture cannot account for all the quantum properties of spin and indeed that spin is purely a quantum property without a classical analog. The fact is, though, that unless we try to do relativistic quantum theory, we will not proceed any further without using this simplistic picture. It turns out that we do not get into any trouble in this case - we get the same result as we would have gotten by applying the full theory!

To make the idea of reversing the flow of time clearer, let's imagine that we can film the rotation of an electron at a fast enough rate that we can see the electron turning from one movie frame to the next. Then we try to visualize what it would look like if we played the film back in the opposite direction.

Earlier we found that the angular momentum has a direction at right angles to the plane of an orbit. We can use the same trick with a rotating sphere, drawing the angular momentum arrow in the same direction as that for a point particle orbiting in the same sense as the sphere is spinning as shown below.

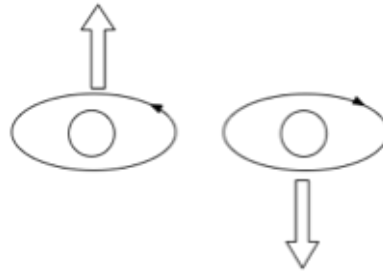


Figure 9.16: Angular momentum directions

The electron on the left-hand side is **spin UP** ($+\hbar/2$) and is **spin DOWN** ($-\hbar/2$) on the right. As the figure shows, playing the film backward will make the electron appear to be rotating in the opposite direction, so it will turn a **spin UP** electron into a **spin DOWN** electron. In terms of the basis used to describe spin states, we can write this as follows:

$$\hat{T}|U\rangle = |D\rangle \quad , \quad \hat{T}|D\rangle = |U\rangle$$

with \hat{T} being the symbol used for the operator that acts to *reverse the direction of time in the following state*.

Actually, we have moved too quickly with these two equations. Since there is no physical difference between one state and a copy that has been multiplied by an amplitude of magnitude 1 and fixed phase, we should allow the possibility

that \hat{T} will do exactly that to one or the other of the states:

$$\hat{T}|U\rangle = |D\rangle \quad , \quad \hat{T}|D\rangle = k|U\rangle$$

where k is a complex number of magnitude 1 and phase θ , i.e., $k = e^{i\theta}$.

What we need to do now determine k (or θ). A good way of doing that is to consider what happens when we reverse the time flow on a different state such as $|L\rangle$ or $|R\rangle$. We start by writing $|L\rangle$ and $|R\rangle$ in terms of $|U\rangle$ and $|D\rangle$

$$|L\rangle = \frac{1}{\sqrt{2}}(|U\rangle - |D\rangle) \quad , \quad |R\rangle = \frac{1}{\sqrt{2}}(|U\rangle + |D\rangle)$$

and then apply the time-reversal procedure

$$\hat{T}|L\rangle = \frac{1}{\sqrt{2}}(\hat{T}|U\rangle - \hat{T}|D\rangle) = \frac{1}{\sqrt{2}}(|D\rangle - k|U\rangle)$$

Given what we said about time reversing the $|U\rangle$ and $|D\rangle$ states, we might guess that

$$\hat{T}|L\rangle = |R\rangle$$

(at least to within a constant). Therefore, we must have

$$\frac{1}{\sqrt{2}}(|D\rangle - k|U\rangle) = \frac{1}{\sqrt{2}}(|U\rangle + |D\rangle)$$

which implies that $k = -1$ (or $\theta = \pi$). We can check that this works as follows:

$$\begin{aligned} \hat{T}|R\rangle &= \frac{1}{\sqrt{2}}(\hat{T}|U\rangle + \hat{T}|D\rangle) = \frac{1}{\sqrt{2}}(|D\rangle + k|U\rangle) \\ &= \frac{1}{\sqrt{2}}(|D\rangle - |U\rangle) = -|L\rangle \end{aligned}$$

as we would expect.

As one final point, consider the following quick calculation:

$$\hat{T}[\hat{T}|U\rangle] = \hat{T}|D\rangle = -|U\rangle \quad , \quad \hat{T}[\hat{T}|D\rangle] = \hat{T}[-|U\rangle] = -|D\rangle$$

and similarly for the $|L\rangle$ and $|R\rangle$ states

$$\hat{T}[\hat{T}|L\rangle] = -|L\rangle \quad , \quad \hat{T}[\hat{T}|R\rangle] = -|R\rangle$$

It would appear that double time reversals have the same effect on fermion states as 360° rotations.

This is just as puzzling as the 360° phase flip. After all, you would expect that reversing the flow of time and then reversing it back again would put things back just the way they were. In this case, evidently not.

Our argument, however, is not done. What we want to do is use the effect of double time reversals to explain the 360° rotation phase flip. To do that we have to show that a double time reversal is the same as a 360° rotation.

Spinning Things Round

There is a branch of mathematics called topology, which is a sort of generalization of geometry. In geometry one studies the properties of points, lines shapes and angles. Topology takes this a step further by looking at how regions of space are connected to one another. In topology any shape that can be deformed into another without cutting or tearing is regarded as being the same. To a topologist there would be no difference between a circle and a square as one can be changed into the other with a bit of twisting but without actually breaking any of the lines. However, it would not be possible to change a sphere into a doughnut shape as getting the hole in the middle would require breaking the surface; a sphere and a donut are *not* topologically equivalent.

Recently physicists have taken an interest in topology as it provides the right sort of mathematics to describe space-time and how particles relate to one another within that space-time.

If we mark the progress of a particle through space and time by a series of *points* (or more properly *events*) and then connect them together, the result is known as a *worldline*. Now imagine an electron proceeding along in a straight line. The worldline of this electron would be something like the tape in (upper-left) of the figure below in which we take the progress of time to be vertically up the table and the x -direction in space to be horizontally across the table.

If the electron were to go through two time reversals in sequence, then the tape would change to look something like that in (upper-right). If you now take either end of the tape and pull it out gently as in (lower-left), then at its full extension the tape has a 360° twist in it as in (lower-right). What this rather curious demonstration shows is that a double time reversal is (topologically) equivalent to the electron proceeding along and rotating through 360° on its way.

Another way to think about this is to imagine that the electron has *tendrils* spreading out into space which are its connections to other parts of the universe(same as earlier). The continuity of the tape in the above figure illustrates this to some extent as this is modeling the electron's worldline as a continuous thing, not a collection of disconnected points. Double time reversing the electron's path will inevitably put *twists* in these tendrils in a manner similar to the electron spiraling through space.

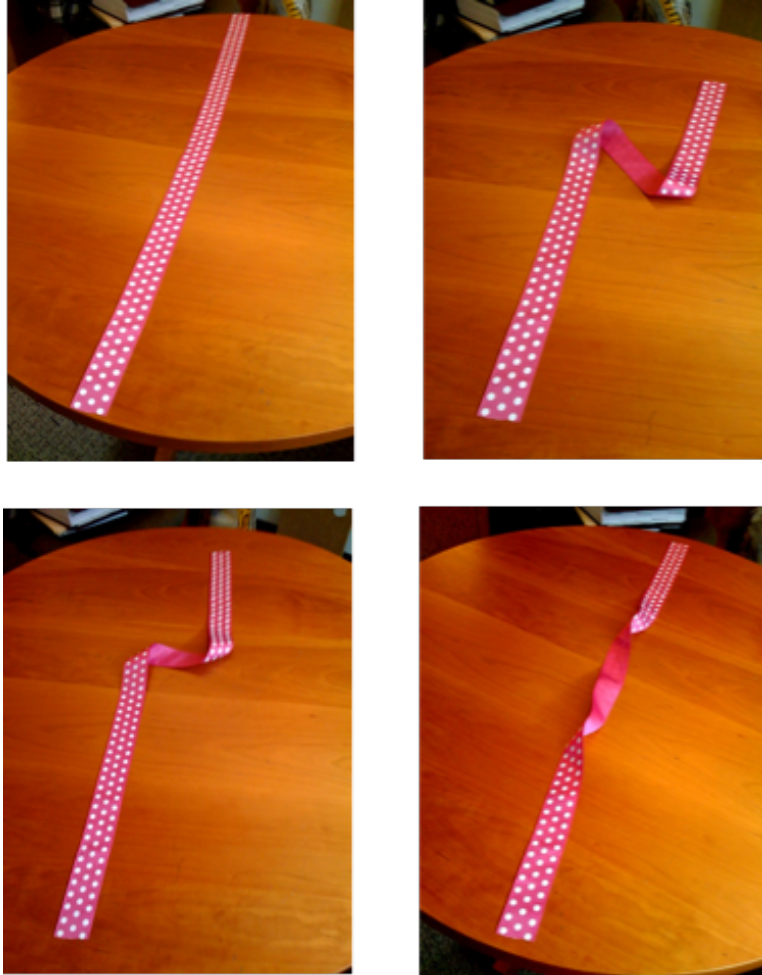


Figure 9.17: Double time reversal

So, the conclusion to this argument is that double time reversal in the world line of an electron produces the same effect as rotating the electron through 360° . In terms of the state of the electron, we can then write (as we saw in the last section):

$$\hat{R}(360^\circ) |U\rangle = \hat{T}\hat{T} |U\rangle = -|U\rangle \quad (9.40)$$

using an obvious notation where $R(\theta)$ is the operator that carries out the process **rotate the following state through angle θ** .

Some Important Points

- (1) Switching particles in an identical multiparticle state has the same effect on the state as rotating one of them through 360°

- (2) A 360° rotation is the same as a double time reversal
- (3) Double time reversal applied to an example set of fermion states ($|U\rangle$ and $|D\rangle$) causes a phase flip in the states
- (4) Hence, switching fermions in an identical multiparticle state must cause a phase flip; fermion multiparticle states are antisymmetric
- (5) If identical multiparticle states are antisymmetric, then no two fermions of the same type can ever be in exactly the same state

This is the link between spin and fermion nature. The weak point in the argument is point (3). How do we know that double time reversals do not do the same thing for bosons?

Boson Spin States

A spin 1 charged particle passing through an S-G apparatus produces three emerging beams. As with the spin 1/2 case, one beam would be deflected upward (but with more of a deflection) and one beam downward. The big difference from the spin 1/2 example is the presence of the third beam that proceeds straight through without being deflected.

The existence of three beams follows directly from what we were saying about angular momentum earlier. For a spin 1 particle, we have $s = 1$ and thus $m_s = 0, \pm 1$ which gives three emerging beams corresponding to the states

$$|1, 1\rangle, |1, 0\rangle, |1, -1\rangle \quad (9.41)$$

We are going to abbreviate these states as

$$|+1\rangle, |0\rangle, |-1\rangle \quad (9.42)$$

respectively. In addition to this we need to be able to indicate the direction of the S-G apparatus, which will be either vertical or horizontal. This was easy in the spin 1/2 case as we could use (UP,DOWN) or (LEFT,RIGHT). Now we need something a little more subtle, such as

$$|V, +1\rangle, |V, -1\rangle, |V, 0\rangle \quad , \quad |H, +1\rangle, |H, -1\rangle, |H, 0\rangle \quad (9.43)$$

where clearly V is for vertical and H is for horizontal.

The semiclassical interpretation of these states follows from our picture of the spin 1/2 components (see earlier discussion) and is illustrated below.

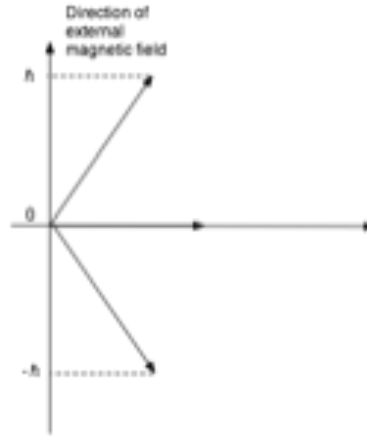


Figure 9.18: Allowed component values

where we illustrate that a spin 1 object can have three possible components with respect to an applied magnetic field.

Now imagine that we have a particle, which we know to be in the state $|V, 0\rangle$, approaching a horizontally aligned S-G apparatus. To deal with such a situation we would have to write the $|V, 0\rangle$ state in terms of the three horizontal states that act as a basis. In other words, we would write

$$|V, 0\rangle = a|H, +1\rangle + b|H, 0\rangle + c|H, -1\rangle$$

where a , b , and c are the complex amplitudes determining the relative probabilities of the three possible outcomes.

Actually, we are not all that interested in the actual values of a , b , and c as we want to try to figure out why it is that spin 1 particles (and by extension bosons, in general) don't flip their signs under exchange - why their state vectors are symmetric. We can do this by considering what happens to the states when we apply the time-reversal argument as before without any specific numbers a, b, c being involved.

More on Time Reversal

Before we can pursue what happens to boson states when they are *time reversed* we need to clarify the effect of \hat{T} being applied to a general state multiplied by an amplitude. As an illustration of this, consider a free-particle momentum eigenstate

$$|\Psi\rangle = \sum_x \left[A \exp \left[\frac{2\pi i}{h} (p_x x - Et) \right] |x\rangle \right] \quad (9.44)$$

where p_x is the momentum of the particle and E is its energy.

Applying time reversal to the amplitude must have some effect. We might imagine that x does not change (the precise point where we might find the particle is not altered) and neither does E . However, $p_x \rightarrow -p_x$ since the *tape played backward* would show the particle traveling in the opposite direction. Of course, the other alteration is $t \rightarrow -t$. The result of all of this would be

$$\begin{aligned}
\hat{T}|\Psi\rangle &= \hat{T} \sum_x \left[A \exp \left[\frac{2\pi i}{h} (p_x x - Et) \right] |x\rangle \right] \\
&= \sum_x \left[\hat{T} \left(A \exp \left[\frac{2\pi i}{h} (p_x x - Et) \right] \right) |x\rangle \right] \\
&= \sum_x \left[\left(A \exp \left[\frac{2\pi i}{h} (-p_x x + Et) \right] \right) \hat{T}|x\rangle \right] \\
&= \sum_x \left[A \exp \left[-\frac{2\pi i}{h} (p_x x - Et) \right] \hat{T}|x\rangle \right]
\end{aligned} \tag{9.45}$$

Looking back at our discussion of complex numbers we have that

$$\exp(-i\theta) = (\exp(i\theta))^* \tag{9.46}$$

so that applying \hat{T} to an amplitude A changes it to A^* . Although we have demonstrated this only for a single example of the free particle, the general rule holds true

$$\hat{T}(A|\phi\rangle) = A^* \hat{T}|\phi\rangle \tag{9.47}$$

Time-Reversed Boson States

Now that we have a slightly deeper understanding of how \hat{T} works on a state, we can now consider the simplest of boson states - that of a spin 1 particle in a state with no vertical spin component.

It makes reasonable sense to propose that

$$\hat{T}|V, 0\rangle = k|V, 0\rangle \tag{9.48}$$

on the grounds that filming a particle spinning *on its side* and playing the film backward will show a particle that is spinning *on its side*.

To be sure, the direction of the spin will be reversed in this process, but in terms of the component of the spin (see last figure) it will still be $|V, 0\rangle$. The number k has been introduced to remind us that although the state may be the same, the process of applying \hat{T} can always multiply a state by an amplitude of magnitude 1 and any phase.

So, following this argument through, we should have

$$\hat{T}|V, 0\rangle = k|V, 0\rangle = k[a|H, +1\rangle + b|H, 0\rangle + c|H, -1\rangle] \tag{9.49}$$

where we have expanded the $|V, 0\rangle$ state in terms of the set of states appropriate for a horizontal spin measurement (a , b , and c being the appropriate amplitudes for this expansion).

It seems reasonable to further suggest that

$$\hat{T}|H, +1\rangle = A|H, -1\rangle \quad , \quad \hat{T}|H, 0\rangle = B|H, 0\rangle \quad , \quad \hat{T}|H, -1\rangle = C|H, +1\rangle \quad (9.50)$$

following from an argument similar to that applied when we considered spin 1/2 states that had been time reversed. Here A , B , and C are the phases introduced into the states, as k was earlier.

The next step needs to be carried out carefully.

$$\begin{aligned} \hat{T}|V, 0\rangle &= \hat{T}[a|H, +1\rangle + b|H, 0\rangle + c|H, -1\rangle] \\ &= a^*\hat{T}|H, +1\rangle + b^*\hat{T}|H, 0\rangle + c^*\hat{T}|H, -1\rangle \\ &= a^*A|H, -1\rangle + b^*B|H, 0\rangle + c^*C|H, +1\rangle \end{aligned} \quad (9.51)$$

Earlier we argued that $\hat{T}|V, 0\rangle = k|V, 0\rangle$; thus,

$$a^*A|H, -1\rangle + b^*B|H, 0\rangle + c^*C|H, +1\rangle = k[a|H, +1\rangle + b|H, 0\rangle + c|H, -1\rangle] \quad (9.52)$$

If this is to work, then we must have

$$kc = a^*A \quad , \quad kb = b^*B \quad , \quad kc = c^*C \quad (9.53)$$

from which we can deduce that

$$A = \frac{kc}{a^*} \quad , \quad B = \frac{kb}{b^*} \quad , \quad C = \frac{ka}{c^*} \quad (9.54)$$

Now we are nearly where we want to be as the next step is to consider what happens if we double time reverse the various states. We have

$$\begin{aligned} \hat{T}\hat{T}|H, +1\rangle &= \hat{T}[A|H, -1\rangle] = A^*\hat{T}|H, -1\rangle = A^*C|H, +1\rangle \\ &= \left(\frac{kc}{a^*}\right)^* \left(\frac{ka}{c^*}\right) |H, +1\rangle = k^*k|H, +1\rangle \end{aligned} \quad (9.55)$$

and similarly for the other states. For all of them, applying $\hat{T}\hat{T}$ produces k^*k times the original state.

One thing must be true about k^*k or indeed any complex number times its conjugate) is that it must be positive. There is no state flip for any of the spin 1 states. Furthermore, applying $\hat{T}\hat{T}$ to any expansion of states such as

$$|V, 0\rangle = a|H, +1\rangle + b|H, 0\rangle + c|H, -1\rangle \quad (9.56)$$

multiplies each part of the expansion by k^*k , shifting the phase of each by the same amount, which is not physically relevant.

Hence, since a double time reversal is the same as a 360° rotation and a 360° rotation is the same as a swap between two particles, we end up demonstrating that swapping two particles in a boson state does not produce a sign flip. Multiparticle boson states are symmetric.

What Just Happened?

The previous argument was rather mathematical and, understandably, could have left you with the feeling that you have not gotten to the root of the problem.

Why is it that bosons behave differently than fermions? The key difference between the boson and fermion states is the presence of the the 0 component states (e.g., $|V, 0\rangle$ and $|H, 0\rangle$). These states are, in principle, present in any expansion of another state, yet do not change when time reversal is applied. What this does is to *lock in place* the phase relationships between the other states, which in turn fixes the exchange behavior.

The relationship between spin and rotation is one of the deepest results in quantum theory. None of the arguments we have used here are very rigorous as they stand, but they can be replaced by more formal mathematical proofs with the same end results.

9.4 Wave Functions - Approach #1

We now deal with continuous physical variables such as position and momentum in the context of a mathematical object called the wave function, which will satisfy the famous Schrödinger equation. This part of the notes expands on topics we discussed earlier and we will discuss this topic in more detail later for those of you who are more mathematically inclined.

Representations

To write down a complete expression for the state of a system in any circumstance, we need a list of all its physical variables. For a free electron this would be energy, momentum, position and spin. A complete expansion of the state would then be

$$|\Phi\rangle = \sum_x \left[A \exp \left[\frac{i}{\hbar} (px - Et) \right] |x\rangle \right] \otimes [a|U\rangle + b|D\rangle] \quad (9.57)$$

To a mathematician, the funny symbol \otimes has a specific meaning (they call it the *tensor product*). For us, it simply indicates that two independent aspects of the state have to be combined to get the full picture. In general terms one could write

$$|\Phi\rangle = |\Psi\rangle \otimes |S\rangle \quad (9.58)$$

with $|S\rangle$ being the spin state of the system and $|\Psi\rangle$ the *spatial state*, the part that deals with energy, momentum, etc. The spin information is not contained within the spatial state; that has to be dealt with separately. We note that this does not say they do not influence each other, i.e., spin component values determine deflection angles(spatial properties) in S-G experiments.

Clearly, $|S\rangle$ can be expanded over (UP,DOWN) or (LEFT, RIGHT) or any other pair of directions oriented at some angle. These would be different representations of the spin state. Equally $|\Psi\rangle$ could, in general, be expanded over position states as above) or momentum states or energy states, each would be a different *representation*.

In some circumstances a state can be an eigenstate of more than one physical variable. The free particle expansion over $|x\rangle$ is an example. This is an eigenstate of energy and momentum. However, it is never possible to be in an eigenstate of position and momentum at the same time. Position and momentum are said to be *conjugate variables(incompatible)*. The various spin and angular momentum components are also conjugate variables, which is why we can't construct an eigenstate of both the total angular momentum and more than one of its components.

Mathematically, it is perfectly possible to switch between representations, provided we can expand one representation over the basis of another. Dirac(of bra-ket notation fame) worked out the mathematical rules required to do this. We have used these rules already. Earlier we used a procedure based on Dirac's rules to get from the (UP,DOWN) basis to the (LEFT,RIGHT).

Infinite Expansions

When we take a position basis and set out to expand a state over a range of possible positions, we must remember that we are dealing with an infinite expansion even if we choose the smallest range of possible positions. After all, something like a particle has a very small size and we can, in principle, specify its exact position very precisely. Actually quantum theory treats particles as if they are point-like objects of no size at all.

Now this presents us with a slightly tricky problem. If we need to expand a state $|\phi\rangle$ over an infinite number of possible positions, $|x\rangle$, exactly how do we do the sum? In practice nobody can add up an infinite number of things. Fortunately there is a mathematical way out of this dating back to Newton's time(the integral that we discussed earlier). Let us take a region of space such as L in the figure below and cut it up into many chunks of equal size Δx . One such chunk is the rectangular box in the figure.

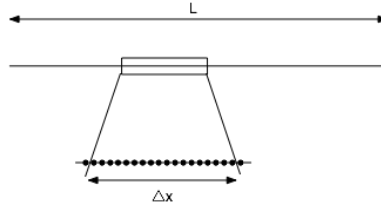


Figure 9.19: Chopping up a line

If we make these chunks small enough, we will find that the amplitude for detecting a particle at any point within the *range* of a chunk is roughly the same for each point - it is approximately constant over the small box. We can keep using smaller chunks until we find this to be the case for any degree of accuracy we fancy.

Consequently the overall amplitude for finding a particle *somewhere* inside Δx is actually the amplitude for finding it at *any* point inside Δx multiplied by the length Δx , at least to the level of approximation we need in this book.

Using this trick we can always get a rough answer to an infinite sum by dividing it up into a finite series of chunks and adding up the chunks. In other words, we can take the expansion of the state $|\phi\rangle$ and break it down as follows:

$$\begin{aligned}
 |\phi\rangle = \sum_x [a(x)|x\rangle] &\approx a(x_1)\Delta x_1|x_1\rangle + a(x_2)\Delta x_2|x_2\rangle + a(x_3)\Delta x_3|x_3\rangle \\
 &+ \dots + a(x_n)\Delta x_n|x_n\rangle + \dots
 \end{aligned}
 \tag{9.59}$$

where x_1 is a point inside Δx_1 , x_2 is a point inside Δx_2 , x_3 is a point inside Δx_3 , etc; and a state such as $|x_1\rangle$ represents a particle being found within a region Δx_1 wide about a point x_1 . Of course, this doesn't give us an exact answer: the sum of the chunks is not the same as the original sum because the approximation glosses over the differences between points inside a chunk. However, what we can do is repeat the sum using a smaller Δx and see how the answer changes; and then we do it again, and again each time, reducing the size of Δx to see how the overall sum changes.

Remarkably(as we saw in our discussion of calculus earlier) when we do this in practice we find that as we reduce the size of Δx , the overall sum changes by smaller amounts. Our approximation to the *real* sum gets better and better. So, although we can never actually do the real infinite sum, we can see what the answer will be as our approximation clearly gets closer to a value which must be that of the real sum.

Isaac Newton worked out exactly how to do this process in a formal mathematical way. He needed to develop this new mathematics called integration(calculus

- see Section 5.3 of this book) to help him deal with the laws of motion that he was developing. For example, take the distance you travel on a journey. To estimate the distance you can just multiply your average speed by the time the journey took. However, that might not be good enough: at any time your speed might be quite different than the overall average. A better approximation would be to divide the journey up into shorter chunks of time and use the average within each chunk. Then you have to add up the distance traveled within each chunk of time to get the overall journey. Clearly, if you are going to do this exactly you will need an infinite number of infinitesimal chunks. This is just the same sort of problem as the one we are dealing with in our quantum case.

Using our modern mathematical terminology, we could write the quantum expansion(infinite) as:

$$|\phi\rangle = \sum_x [a(x)|x\rangle] = \int_0^L a(x)|x\rangle dx \quad (9.60)$$

The symbol \int is called an integral sign and the integration element dx has replaced Δx .

The part $(0, L)$ of \int is telling us that position x ranges from 0 to L on the distance line. What an integral does, in formal mathematical way, is to carry out the infinite sum by breaking it into chunks and summing those and then letting the chunk size get progressively smaller. Of course, you will get a different answer depending on $a(x)$ that you need to use. Over the years, mathematicians have worked out many standard integrals using common forms of $a(x)$.

We are not going to do any integrals in this book, but we will switch to using the correct notation from now on when the SUM should be infinite, for example,

$$|\phi\rangle = \int_0^L a(x)|x\rangle dx \text{ expansion over position eigenstates} \quad (9.61)$$

$$|\phi\rangle = \int_{-P}^P a(p_x)|p_x\rangle dp_x \text{ expansion over momentum eigenstates} \quad (9.62)$$

In the momentum expansion, we have set the *limits* on the integration as P and $-P$ to show that the state might represent a particle going in either direction.

Wave Functions and State Functions

Buried inside the expansion of position states is the slightly mysterious term $a(x)$. As we explained earlier, $a(x)$ is a mathematical notation for the phrase *a is a number whose value depends on the choice of another number x*. Mathematicians also say that *a is a function of x*. We can carry this terminology

more or less straight over into physics, except that we have to remember that x is a quantity (number and unit) rather than simply a number, and so $a(x)$ might be as well.

As it stands, $a(x)$ doesn't tell us very much. It is a statement claiming a direct link between a and x , but without any indication of the precise rule that links the two. The rule might be *take x and add one to it* so that $a(x) = x + 1$. Equally, the rule could be *take x and square it, then add 7* so that $a(x) = x^2 + 7$. Of course, in the case of our specific application of $a(x)$, we are dealing with amplitudes, which are complex numbers. This does not alter the point, though, which is that without the precise rule, $a(x)$ is just a phrase. Clearly in quantum mechanics we need something else that allows us to pick out the specific rule $a(x)$ that applies in a given physical situation. We need the equations of quantum theory to help us do that.

Before we go further down this road, which eventually leads to the Schrödinger equation, we would like to tidy up some terminology.

The expansion of position states now runs

$$|\phi\rangle = \int_0^L a(x) |x\rangle dx \quad (9.63)$$

and we want to pick out a particular position X ; we do this by multiplying by the bra $\langle X|$. Using the fact that $\langle X|x\rangle = 0$ unless X is the same as x (in which case $\langle x|x\rangle = \langle X|X\rangle = 1$), we get

$$\langle X|\phi\rangle = \int_0^L a(x) \langle X|x\rangle dx = a(X) \quad (9.64)$$

In other words, we kill off all the terms in the sum aside from the specific one where X is x . We will see how to do this in a more rigorous mathematical fashion shortly.

What this simple argument reveals is nothing more than the notational point $a(x) = \langle x|\phi\rangle$ (the switch to lowercase x being of no significance other than it looks nicer...). Historically, $a(x)$ is more often written as $\phi(x) = \langle x|\phi\rangle$ and has been called the *state function*.

In many situations the expansion will have both position and time, in which case $\phi(x)$ will turn out to be $\Psi(x, t)$. We call $\Psi(x, t)$ a *wave function*.

In the early quantum theoretical work on the wave nature of electrons, physicists were searching for a physical wave that could either guide (de Broglie) or be (Schrödinger) the *true* nature of the electron. By a physical wave we mean

something existing in space, spread out or condensed in some region, with a physically real amplitude rather like the height of a water wave. Although they had no idea what this physical wave might be, they called it a wave function, gave it the symbol Ψ and searched for an equation that would govern its behavior.

Schrödinger was the first person to write down an equation for extracting the specific rule $\Psi(x, t)$ that applied in a given situation. His great triumph was to use the equation to derive $\Psi(x, t)$ for the electron orbiting a hydrogen nucleus and then show how many of the known properties of hydrogen (such as the spectrum of light it emits) could be explained from this wave function.

Meanwhile, working in parallel, Dirac was developing his theory of states and amplitudes based on some of Heisenberg's early work. In turn, Heisenberg, together with Born and Jordan, had been expanding his early ideas using matrices.

With all this work going on in parallel and providing similar results, it was inevitable that people would look to see links between the different approaches. Schrödinger started this off with an outline of how his own *wave mechanics* and the Heisenberg/Jordan/Born *matrix mechanics* could relate to one another. Despite this breakthrough, Schrödinger still felt that using $\Psi(x, t)$ was a more significant approach and that the wave function was a physical wave of some form. He continued to search for an appropriate meaning for Ψ .

The decisive step was actually taken by Max Born who demonstrated how quantum theory could be placed on an entirely consistent footing by interpreting

$$|\Psi(x, t)|^2 \Delta x \quad (9.65)$$

as representing the probability of finding a particle within Δx of x at time t .

In many ways, Ψ is no more significant than any other amplitude that we have talked about. It happens to be the subject of the Schrödinger equation and so tends to be the amplitude function we reach for first in a given situation. Once we are armed with $\Psi(x, t)$ we can use Dirac's rules to transfer to any other related basis.

Many physicists hardly talk about states in a formal way. They work with the wave function on its own and do not tie it to state expansions, and the like. We, however, believe that the state approach (ala Dirac) is the best approach and will continue to use that in this book.

Observables

One of the most mysterious aspects of quantum theory is the association between physical variables and operators.

So far we have mentioned some operators that relate directly to physical variables (such as $\hat{S}_x, \hat{S}_y, \hat{S}_z, \hat{p}$ for momentum, and \hat{E} for energy) and one that evolves a quantum state into the future \hat{U} . However, we have not discussed why it is that physical variables must be treated in this manner in quantum physics. To discuss this we are going to start with a consideration of momentum.

The Problem of Momentum

In classical physics, the momentum of an object in a given direction has a strict definition, which is clearly related to observable properties, i.e.,

$$p_x = m \left[\frac{x_2 - x_1}{t_2 - t_1} \right] \quad (9.66)$$

where p_x is the momentum in the x -direction, m is the mass of the object, x_1 is the position at time t_1 , and x_2 is the position at time t_2 . From this definition it's easy to imagine how you might conduct a simple set of measurements to measure momentum. One suitable procedure would involve taking two photographs at times t_1 and t_2 to observe the position of the object against some prearranged length scale (ruler).

How can we translate such a procedure so that it could work for a quantum object such as an electron?

Well, the start would have to be a collection of identical objects in the same state $|\phi\rangle$, which is presumably not an eigenstate of position. Then we would carry out the first position measurement on each one at exactly the same time t_1 . This produces a set of measured positions $\{x_i\}$ with each possible value appearing a certain number of times depending on the probability of the position being measured.

The catch is that after this first measurement we no longer have a collection of particles in the same state.

The position measurement has collapsed the state $|\phi\rangle$ into $|x_i\rangle$ with a subcollection of particles in each possible state.

What can we do next?

One possibility would be to take only particles with a specific position, say x_1 , and do a repeated position measurement on them. However, as we have seen previously, a position eigenstate cannot be a momentum eigenstate. We can, if we wish, take a second position measurement on the subcollection of particles and then employ the formula

$$p_x = m \left[\frac{x_2 - x_1}{t_2 - t_1} \right] \quad (9.67)$$

to calculate something; but what have we calculated? Our second position measurement, carried out only on the particles with state $|x_1\rangle$ after the first, will yield another range of possible positions $\{x_2\}$, so we will get a wide variation of p values at the end of this calculation. And lest we forget, we have used only a fraction of the particles that we started with. What can we say about the momentum of the others?

At the root of the problem here is, once again, the inappropriateness of trying to say that a quantum particle has a definite path.

Yet, there has to be some way of dealing with momentum; after all we have been talking about it throughout this book. The problem does not lie with the *idea* of momentum, but with the *classical definition* as given by the above formula.

We need a quantum reinterpretation of what we mean by momentum.

A suitable working definition comes from the de Broglie relationship $p_x = \hbar/\lambda$. Now, to take the next step, we need to reintroduce the amplitude for a free particle.

$$|\Psi\rangle = \sum_x \left[A \exp \left[\frac{i}{\hbar} (p_x x - Et) \right] |x\rangle \right] \quad (9.68)$$

After all, this is a momentum eigenstate: what better state can be used to find out something about momentum?

Using this state, we can find the amplitude for a particle to be at any chosen x .

$$\Psi(x, t) = \langle x | \Psi \rangle = A \exp \left[\frac{i}{\hbar} (p_x x - Et) \right] \quad (9.69)$$

In other words, this is the *wave function* for a particle in this state and there we have, right in the middle, the momentum p_x .

Obtaining Momentum

When we first introduced the free particle wave function (without calling it that) earlier, we showed how the amplitude progressed along a line x at a fixed time. This figure is reproduced below. The wavelength, if you remember, is defined as the distance along x that you need to travel to see the phase turn through a complete rotation as shown in the diagram.

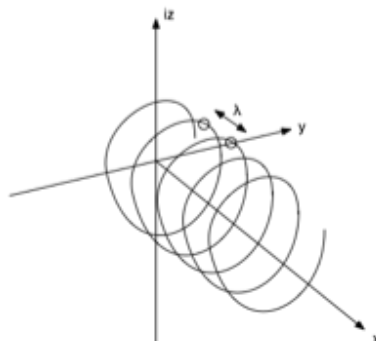


Figure 9.20: Free particle amplitude

Now we can see that this rotation is *driven* by the momentum of the particle. Since the phase of the wave function is given by

$$\frac{1}{\hbar} (p_x x - Et) \quad (9.70)$$

comparing two points on the x -axis separated by a distance of 1 meter we will see a phase difference of p_x/\hbar (provided we look at the two of them at the same time). It would be appropriate to say that the *rate* at which the phase changes with distance is given by p_x/\hbar .

Now you might not be familiar with this way of using the term *rate*. In everyday speech *rate* is normally used in a context where something is changing with time. Mathematicians never leave a good idea alone if they can generalize it; to them a rate refers to how one quantity changes as you vary something else. In this case we're looking at the change in phase as we pick different points on the x -axis. Remember though, that this comparison between different points is going to work only if we look at them at the same time, otherwise the Et part of the phase is going to get in the way. This fixed time condition helps to point out that our use of *rate* can in no way refer to a time change.

To go along with this use of *rate*, mathematicians have an operator that calculates how one quantity change with another; it is called the *gradient operator* and is denoted as follows:

$$\text{Rate of change of } \phi \text{ with } x = \nabla_x(\phi) \quad (9.71)$$

where the operator is the ∇_x part that *acting on* ϕ . Of course, it is entirely possible that we may want to find out the rate of change of something with time; we then use the operator ∇_t .

We can use this operator to *extract* from the wave function information about

the momentum. After all if *the rate of change of phase with x is p_x/\hbar* , then

$$\hat{p}_x/\hbar = \nabla_x \Rightarrow \hat{p}_x = \hbar \nabla_x \quad (9.72)$$

Actually, this is not quite right. A mathematical nicety to do with the fact that the phase is part of a complex number means that the true momentum operator is written as follows:

Momentum Operators

$$\hat{p}_x = -i\hbar \nabla_x \text{ momentum in the } x \text{ - direction} \quad (9.73)$$

$$\hat{p}_y = -i\hbar \nabla_y \text{ momentum in the } y \text{ - direction} \quad (9.74)$$

$$\hat{p}_z = -i\hbar \nabla_z \text{ momentum in the } z \text{ - direction} \quad (9.75)$$

Do not worry about the minus sign, which just comes from manipulating the i 's that go into the formula. We will derive this result rigorously later.

Operators and Representations

The job of an operator such as \hat{p}_x is to *extract* the eigenvalue from one of its eigenstates.

$$\hat{p}_x |p_1\rangle = p_1 |p_1\rangle \quad (9.76)$$

This is rather an abstract task, after all states do not have specific mathematical forms and the operator \hat{p}_x is not given a structure in this equation. However, we can perform a simple trick since

$$\hat{p}_x |p_1\rangle = p_1 |p_1\rangle \Rightarrow \langle x | (\hat{p}_x |p_1\rangle) = \langle x | (p_1 |p_1\rangle) = p_1 \langle x | p_1 \rangle \quad (9.77)$$

Hence

$$\langle x | \hat{p}_x |p_1\rangle = p_1 \langle x | p_1 \rangle = -p_1 \phi_{p_1}(x) \quad (9.78)$$

As we will show later this gives

$$\hat{p}_x \phi_{p_1}(x) = p_1 \phi_{p_1}(x) \quad (9.79)$$

which shows the momentum operator *acting on a momentum space eigenstate that has been written in a position representation*. Just to be absolutely clear, $\phi_{p_i}(x)$ is the state function, corresponding to the position state expansion of a momentum eigenstate

$$|p_1\rangle = \int \phi_{p_1}(x) |x\rangle dx \quad (9.80)$$

Since the \hat{p}_x operator is acting here on the position representation of a state function, it better have a position representation as well. Of course, we found what it was:

$$\hat{p}_x = -i\hbar \nabla_x \quad (9.81)$$

The point we are trying to make here is all to do with representations. Any state of a system can be written in various representations, meaning that the

state can be expanded over any suitable basis. If it is a position basis, then we have a position representation of the state. Operators that represent physical variables have to be able to act on a state and get the same results no matter what representation the state is in. Hence the same operator must have different representations as well.

So far we have shown only the position representation of \hat{p}_x . The other commonly used representation involves expanding over momentum eigenstates.

$$|\phi\rangle = \int A(p_x) |p_x\rangle dp_x \quad (9.82)$$

It's possible to convert operators in one representation into those in another. The mathematics is beyond this book so we will just quote the operator representation.

Operator	Position Representation	Momentum Representation
\hat{x}	$x \times$	$-i\hbar \nabla_p$
\hat{p}_x	$-i\hbar \nabla_x$	$p_x \times$

We have included the position operator \hat{x} in this table although we have not talked about it much up to now. As you can see there is a nice symmetry between the representations of \hat{x} and \hat{p}_x .

So What Can We Do with \hat{p}_x ?

Well, one thing that we can do is

$$\begin{aligned} \hat{p}_x \left[A \exp \left[\frac{i}{\hbar} (p_x x - Et) \right] \right] &= -i\hbar \nabla_x \left[A \exp \left[\frac{i}{\hbar} (p_x x - Et) \right] \right] \\ &= p_x A \exp \left[\frac{i}{\hbar} (p_x x - Et) \right] \end{aligned} \quad (9.83)$$

extracting the momentum information for this state (you will have to trust me that $-i\hbar \nabla_x$ has been correctly applied). In a sense, though, this does not really do much. After all, arguably if p_x is in the wave function we already *know* what's going on.

Things are a bit different, though, if we're dealing with a state that's not a momentum eigenstate. There is no definite value of momentum to pull out; the best we can do is work with an expectation value.

Rule 7 sets out the role of operators, \hat{O} , in representing physical variables and how the operator can be used to calculate the expectation values, $\langle \phi | \hat{O} | \phi \rangle$, of a series of measurements made on a collection of systems in the same state $|\phi\rangle$. However, we have not yet seen in detail how such a calculation is done. We can now do just that, at least for one specific example \hat{p}_x .

This is going to be a two-step process. The first step is to expand our state $|\phi\rangle$ over a basis. Let's be adventurous in our choice and go for $\{|x\rangle\}$ so that

$$\begin{aligned}\langle\phi|\hat{p}_x|\phi\rangle &= \left(\sum_{x_1}\phi^*(x_1)\langle x_1|\right)\hat{p}_x\left(\sum_{x_2}\phi(x_2)|x_2\rangle\right) \\ &= \left(\int\phi^*(x_1)\langle x_1|dx_1\right)\hat{p}_x\left(\int\phi(x_2)|x_2\rangle dx_2\right)\end{aligned}\quad (9.84)$$

The second step is to simplify this ghastly looking expansion.

$$\begin{aligned}\langle\phi|\hat{p}_x|\phi\rangle &= \left(\int\phi^*(x_1)\langle x_1|dx_1\right)\hat{p}_x\left(\int\phi(x_2)|x_2\rangle dx_2\right) \\ &= \int\int dx_1dx_2\langle x_1|x_2\rangle\phi^*(x_1)[-i\hbar\nabla_x\phi(x_2)] \\ &= \int dx\phi^*(x)[-i\hbar\nabla_x\phi(x)]\end{aligned}\quad (9.85)$$

which is as far as we can get without a specific $\phi(x)$ to deal with. In this derivation we have used the result

$$\int dx'\langle x|x'\rangle f(x') = f(x) \quad (9.86)$$

which we will show in detail later. Everything we have done applies equally well to other operators.

Position Operator

The momentum operator is a tool used to extract momentum information from a state. Equally, there is an operator that can be used in a similar fashion to extract position information, namely, \hat{x} . Fortunately, in the position representation \hat{x} has a particularly simple form $x\times$, that is, multiply by x .

Straight away we can write down the expectation value of position for a set of measurements carried out on objects in the same state $|\phi\rangle$

$$\langle\phi|\hat{x}|\phi\rangle = \int dx\phi^*(x)x\phi(x) \quad (9.87)$$

By now you may be feeling a certain state of confusion. After all, we have liberally used x and p to mean position and momentum *inside* our wave functions, and now we are using operators \hat{x} and \hat{p}_x to act on the wave functions. Why do the same ideas appear to have two separate mathematical expressions in the same theory?

These are actually very deep waters and I am not sure that quantum physics, in the end, has a satisfactory answer to give. Modern day quantum theories of gravity undermine our view of space so as to make us puzzle over what we mean by x anyway, so that might be in the end what rescues us from our question.

However, the question deserves something of an answer, so let us make a first attempt.

When we use terms such as x , p_x , E , and t inside wave functions we take them to mean possible values or outcomes of a measurement. The operators \hat{x} , \hat{p}_x and \hat{E} (there is no \hat{t} , but that is beyond this book) are more like mathematical tools that allow us to extract information of a given sort out of the state. In some ways we should think of them representing the *process* of measurement, rather than the actual results of that measurement. More about this subject later.

Energy Operator

Earlier, we used the general notion of rate of change to argue that the momentum was related to the rate of change of phase with position and hence the position representation of the momentum operator was $-i\hbar\nabla_x$.

At the time, you may have been wondering what was going to happen with the Et/\hbar part of the free-particle phase. If the momentum is determining the rate of change of phase with distance, then one could equally say that the energy is determining the rate of change of phase with time. We also said that the normal use of the term rate, as in how something changes with time, translates mathematically into the operator ∇_t . So, we can use this operator to extract energy information just the way we used ∇_x to extract the momentum.

The quantum theoretical energy operator is as follows:

$$\hat{E} = i\hbar\nabla_t \quad (9.88)$$

The Equations of Quantum Theory

In classical physics, if you want to calculate what's going to happen in a given situation, you basically have two options open to you. You can carefully specify the positions and momenta of all the particles involved, list the forces acting, and then plug into Newton's laws of motion and calculate away. Alternatively, you can inspect all the kinetic energies, potential energies, and any other form of energy involved and work through a calculation based on the conservation of energy.

Every form of energy that we come across in mechanics (particles in motion) can be related back to position or momentum. For example, take the kinetic energy. The formula for kinetic energy is $KE = mv_x^2/2$ (object is traveling in the x -direction), or as momentum $p_x = mv_x$, we can write $KE = p_x^2/2m$. Potential energies come in various forms. Gravitational potential energy is mass x strength of gravity x height above the ground, mgh , and h can be expressed in terms of position. The elastic potential energy stored in a stretched spring is $kx^2/2$, where k is the strength of the spring and x the amount of stretch (position

again). All of which illustrate the basic notion that mechanical energies depend on position and momentum. This is very important, as we already have quantum mechanical operators for position and momentum, so we should be able to build operators for any energy we want to use.

In classical mechanics, it is useful to construct an expression that totals up the energies involved in a given situation.

$$H = \frac{p_x^2}{2m} + V(x) \quad (9.89)$$

where we are using the expression $V(x)$ to denote all the forms of potential energy possessed by the particle. This expression is called the *Hamiltonian*.

Hamiltonians have proven to be very useful in making the change from the way in which classical mechanics describes a situation to the quantum mechanical version. After all, if we can represent momentum and position in terms of operators, then we ought to be able to write down an operator for the Hamiltonian.

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \hat{V}(x) \quad (9.90)$$

In this expression, the operator $\hat{V}(x)$ works like the position operator: you multiply by $V(x)$. This just leaves us to worry about the meaning of \hat{p}_x^2 .

When we are dealing with ordinary numbers, x^2 is simply $x \times x$; thus, it would be sensible to think of \hat{p}_x^2 as $\hat{p}_x \times \hat{p}_x$, which is the same as applying the operator twice in a row. Ultimately, the way we can tell if we are right about this is to see the results we obtain correspond to experimental measurements.

So now we have this Hamiltonian. what can we do with it? Clearly if we act on a state that is an eigenstate of the Hamiltonian, we ought to get one of the eigenvalues.

$$\hat{H} |E_n\rangle = E_n |E_n\rangle \quad (9.91)$$

where E_n is one of the energy eigenvalues of the system (possible results of measurement of the energy).

As we have a specific form of \hat{p}_x and \hat{x} in the position representation, we can write the Hamiltonian operator as:

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \hat{V}(x) = \frac{(-i\hbar\nabla_x) \otimes (-i\hbar\nabla_x)}{2m} + \hat{V}(x) \quad (9.92)$$

When we use this operator to act on a state function, we obtain the so-called *time-independent Schrödinger equation*

$$\frac{(-i\hbar\nabla_x) \otimes (-i\hbar\nabla_x)}{2m} \phi_n(x) + \hat{V}(x) \phi_n(x) = E_n \phi_n(x) \quad (9.93)$$

where $\{\phi_n(x)\}$ is the collection of energy eigenstate functions for the system. Solutions to this equation gives us the state function for a given situation - specified by the specific form of $V(x)$ corresponding to the physics of the system. We will derive this result later.

The time-independent Schrödinger equation is very useful in certain specific situations when we know that the system has to be in an energy eigenstate. However, there has to be another similar equation to deal with more general situations, for example, when the potential energy depends on time as well as position.

It will have occurred to you that we now have two energy operators, \hat{H} as above and $\hat{E} = i\hbar\nabla_t$ from earlier. Clearly if things are to go well, we must get the same answer when we apply both operators to the same state. In other words,

$$\hat{H}|\Psi\rangle = \hat{E}|\Psi\rangle \quad (9.94)$$

which, when written in full in the position representation gives the *time-dependent Schrödinger equation*

$$\frac{(-i\hbar\nabla_x) \otimes (-i\hbar\nabla_x)}{2m}\psi(x, t) + \hat{V}(x, t)\psi(x, t) = i\hbar\nabla_t\phi_n(x)\psi(x, t) \quad (9.95)$$

Solving this equation for a given $\hat{V}(x, t)$ will produce the wave function for a system in that state. For example, if we plug in the appropriate $\hat{V}(x, t)$ for an electron in an atom, we can solve the time-dependent Schrödinger equation to get the wave function of an electron in orbit around that atom, something of vital importance in atomic physics and chemistry.

\hat{E} and \hat{H}

I want to make a couple of remarks about the different roles of \hat{E} and \hat{H} in quantum theory.

The Hamiltonian \hat{H} is a model of the system constructed specifically by considering a particular potential energy function $\hat{V}(x, t)$. This model may only be an approximate one as the details are too difficult to include. However, if the model is reasonably correct and we set $\hat{H}|\Psi\rangle = \hat{E}|\Psi\rangle$, which is effectively the time-dependent Schrödinger equation, then we can solve this to give the wave function $\Psi(x, t)$ for that model of that system. Using the wave function we can make various predictions about what the system is likely to do and pass them on to the experimental experts. If their results agree with our predictions, then our model is correct.

Put another way: \hat{E} is the total energy of the system, and \hat{H} is the list of what we think that total energy is made up of. If we have got this list correct, then $\hat{H}|\Psi\rangle = \hat{E}|\Psi\rangle$.

Stationary States

The discovery of the Schrödinger equation was a key moment in the history of quantum physics. Up to its announcement, calculations in quantum theory had been cumbersome and required the use of mathematical techniques that were not familiar to most physicists. The Schrödinger equation had a familiar mathematical form and quite conventional techniques could be applied to solve it in various situations.

There is one crucial point though. None of the steps we used to produce, either the time-dependent or time-independent versions of the Schrödinger equation, were forced on us. There is no logically compelling way of deriving either equation. We can argue for plausibility, but after that it is down to using them to make predictions which are then checked against reality. Their successful application is their only compelling justification. Of course, the same is true for all the laws of nature.

However, we do seem to have an embarrassment of riches: when do we use one of these equations and when the other?

A key point in answering this is to see that the time-dependent equation will convert into the time-independent equation when

$$i\hbar\nabla_t\Psi(x,t) = E_n\Psi(x,t) \tag{9.96}$$

that is, $\Psi(x,t)$ is the position representation of an eigenstate of \hat{E} . Physically, this will mean that the repeated energy measurements on the state bring the same value. The energy is not changing with time. The system is in a *stationary state*. If a system is going to change its energy, then it can only do this by leaking some energy into (or from) its surroundings, so the only chance of producing and maintaining a stationary state is to isolate the system from its surroundings.

Chapter 10

Schrödinger Equation

These topics are for the more mathematically inclined students.

10.1 The Dirac δ -Function

(You need calculus for this section - see Section 5.3)

History

In the development of quantum mechanics by P. Dirac, the following sequence of ideas occurred

- (1) Observable = measurable quantity = Hermitian operator
- (2) Physical states are linear combinations of the eigenvectors [requires complete orthonormal basis]
- (3) Possible measurements are represented by the eigenvalues [must be real numbers]

$$\hat{O}|\lambda\rangle = \lambda|\lambda\rangle \quad , \quad |\lambda\rangle = \text{eigenvector} \quad , \quad \lambda = \text{eigenvalue} \quad (10.1)$$

- (4) Some observables have a discrete spectrum [finite number or denumerably infinite number]. Then have for eigenvectors

$$\langle \lambda' | \lambda \rangle = \delta_{\lambda'\lambda} \quad (10.2)$$

In this case, for different eigenvalues this is a well-defined statement.

- (5) Other observables have a continuous spectrum [non-denumerably infinite number of eigenvalues]. For example, the position operator \hat{X} , which we have discussed and will discuss further shortly, is such that

$$\hat{X}|x\rangle = x|x\rangle \quad , \quad |x\rangle = \text{eigenvector} \quad , \quad x = \text{eigenvalue} \quad (10.3)$$

We now ask the question, what is $\langle x' | x \rangle$? Dirac assumed that

$$\langle x' | x \rangle \equiv \delta_{x'x} \equiv \delta(x - x') \quad (10.4)$$

where he proposed the definitions

$$\int_{-\infty}^{\infty} \delta(x - x') dx' = 1 \quad (10.5)$$

$$\delta(x - x') = 0 \text{ if } x' \neq x \quad (10.6)$$

$$\int_{-\infty}^{\infty} f(x') \delta(x - x') dx' = f(x) \quad (10.7)$$

Although, this new mathematical object assumed by Dirac did not fit in with any mathematics known at the time (1929), the assumption gives the correct physical theory in the sense that all predictions agree with experiment.

Eventually (1960) the mathematicians, who initially vehemently disputed Dirac's assumption of this new "function", caught up to the physicists and proved all of its properties in the Theory of Distributions.

Here is how Dirac(in his own words) introduced this function:

Our work in Chapter 10 led us to consider quantities involving a certain kind of infinity. To get a precise notation for dealing with these infinities, we introduce a quantity $\delta(x)$ depending on a parameter x satisfying the conditions

$$\int_{-\infty}^{\infty} \delta(x) dx = 1 \quad (10.8)$$

$$\delta(x) = 0 \text{ for } x \neq 0 \quad (10.9)$$

To get a picture of $\delta(x)$, take a function of the real variable x which vanishes everywhere except inside a small domain, of length ϵ say, surrounding the origin $x = 0$, and which is so large inside this domain that its integral over the domain is unity. The exact shape of the function inside this domain does not matter, provided there are no unnecessary wild variations (for example provided the function is always of order $1/\epsilon$). Then in the limit $\epsilon \rightarrow 0$ this function will go over into $\delta(x)$.

$\delta(x)$ is not a function of x according to the usual mathematical definition of a function, which requires a function to have a definite value for each point in its domain, but is something more general, which we may call an "improper function" to show up

the difference from a function defined by the usual definition. Thus $\delta(x)$ is not a quantity which can be generally used in mathematical analysis like an ordinary function, but its use must be confined to certain simple types of expressions for which it is obvious that no inconsistency can arise.

Properties for Complicated Arguments

(1) Consider

$$\begin{aligned} \int_{0-}^{0+} dt' \delta(-t') f(t') &= - \int_{-0-}^{-0+} dt' \delta(t') f(-t') = - \int_{0+}^{0-} dt' \delta(t') f(-t') \\ &= \int_{0-}^{0+} dt' \delta(t') f(-t') = f(0) \end{aligned} \quad (10.10)$$

which implies that $\delta(-t) = \delta(t)$ in the sense of using integrals, i.e.,

$$f(0) = \int \delta(-t) f(t) dt = \int \delta(t) f(t) dt \quad (10.11)$$

(2) Consider

$$\int_{0-}^{0+} dt' \delta(at') f(t') = \frac{1}{|a|} \int_{0-/a}^{0+/a} dt'' \delta(t'') f(t''/a) = \frac{1}{|a|} f(0) \quad (10.12)$$

which implies that

$$\delta(at) = \frac{1}{|a|} \delta(t) \quad (10.13)$$

in the sense of using integrals, i.e.,

$$\frac{1}{|a|} f(0) = \int \delta(at) f(t) dt = \frac{1}{|a|} \int \delta(t) f(t) dt \quad (10.14)$$

(3) Consider

$$\int_{0-}^{0+} dt' t' \delta(t') f(t') = f(0)(0) = 0 \quad (10.15)$$

If $f(0) \neq 0$, then this implies that $t\delta(t) = 0$

(4) Consider

$$\int_{-L}^L f(x) \delta(x^2 - b^2) dx = \int_{-L}^0 f(x) \delta(x^2 - b^2) dx + \int_0^L f(x) \delta(x^2 - b^2) dx \quad (10.16)$$

Now near $x = -b$, we can write

$$x^2 - b^2 = -2b(x + b) \quad (10.17)$$

and near $x = b$, we can write

$$x^2 - b^2 = 2b(x - b) \quad (10.18)$$

Therefore we have

$$\begin{aligned} \int_{-L}^L f(x) \delta(x^2 - b^2) dx &= \int_{-L}^0 f(x) \delta(-2b(x + b)) dx + \int_0^L f(x) \delta(2b(x - b)) dx \\ &= -\frac{1}{2|b|} f(-b) + \frac{1}{2|b|} f(b) \end{aligned} \quad (10.19)$$

or

$$\delta(x^2 - b^2) = \frac{\delta(x - b) + \delta(x + b)}{2|b|} \quad (10.20)$$

- (5) Now consider a function $g(x)$ which has a single zero at $x = x_0$. This implies that near x_0 we have

$$g(x) = (x - x_0)g'(x_0) \quad (10.21)$$

In this case we can write

$$\int_{-\infty}^{\infty} f(x) \delta(g(x)) dx = \int_{-\infty}^{\infty} f(x) \frac{\delta(x - x_0)}{|g'(x_0)|} dx = \frac{f(x_0)}{|g'(x_0)|} \quad (10.22)$$

and we have

$$\delta(g(x)) = \sum_{i=1}^N \frac{\delta(x - x_i)}{|g'(x_i)|} \quad (10.23)$$

EXAMPLES:

$$\int_{-\infty}^{\infty} e^{-x} \delta(x^2 - a^2) dx = \int_{-\infty}^{\infty} e^{-x} \frac{\delta(x - a) + \delta(x + a)}{2a} dx = \frac{e^{-a} + e^a}{2a} = \frac{\cosh(a)}{a} \quad (10.24)$$

$$\begin{aligned} \int_{-\infty}^{\infty} e^{-x^2} \delta(\sin x) dx &= \int_{-\infty}^{\infty} e^{-x^2} \sum_{n=-\infty}^{\infty} \frac{\delta(x - n\pi)}{|(\cos n\pi)|} dx \\ &= \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-x^2} \delta(x - n\pi) dx = \sum_{n=-\infty}^{\infty} e^{-n^2 \pi^2} \end{aligned} \quad (10.25)$$

10.2 Introduction to the Schrödinger Equation in One Dimension

(This is difficult stuff but rewarding when done)

Time Evolution

One way of doing quantum calculations is called the Schrödinger Picture and involves the Schrödinger equation for determining the wavefunctions corresponding to energy eigenstates and for specifying the time evolution of physical quantities.

In this picture:

- (a) states are represented by ket vectors that depend on time t , $|\psi(t)\rangle$
- (b) operators \hat{Q} representing observables or measurable quantities are independent of time

We then get a time-dependent expectation value of the form

$$\langle \hat{Q}(t) \rangle = \langle \psi(t) | \hat{Q} | \psi(t) \rangle \quad (10.26)$$

Now let t be a continuous parameter. We consider a family of unitary operators $\hat{U}(t)$, with the following properties

$$\hat{U}(0) = \hat{I} \quad , \quad \hat{U}(t_1 + t_2) = \hat{U}(t_1)\hat{U}(t_2) \quad (10.27)$$

Transformations such as displacements, rotations and Lorentz boosts satisfy these properties and it make sense to require them in general.

As we will see, this operator is the time development operator whose existence was one of our postulates and whose form we specified earlier.

Now we consider infinitesimal t . We can then write the infinitesimal version of the unitary transformation (using a Taylor series) as

$$\hat{U}(t) = \hat{I} + \left. \frac{d\hat{U}(t)}{dt} \right|_{t=0} t + O(t^2) \quad (10.28)$$

Since the unitary operator must satisfy the unitarity condition

$$\hat{U}\hat{U}^\dagger = \hat{I} \quad (10.29)$$

for all t , we have

$$\begin{aligned} \hat{U}\hat{U}^\dagger &= \hat{I} = \left(\hat{I} + \left. \frac{d\hat{U}(t)}{dt} \right|_{t=0} t + \dots \right) \left(\hat{I} + \left. \frac{d\hat{U}^\dagger(t)}{dt} \right|_{t=0} t + \dots \right) \\ &= \hat{I} + \left[\left. \frac{d\hat{U}(t)}{dt} + \frac{d\hat{U}^\dagger(t)}{dt} \right] \right|_{t=0} t + \dots \end{aligned} \quad (10.30)$$

which implies that

$$\left[\frac{d\hat{U}(t)}{dt} + \frac{d\hat{U}^+(t)}{dt} \right] \Big|_{t=0} = 0 \quad (10.31)$$

If we define

$$\frac{d\hat{U}(t)}{dt} \Big|_{t=0} = -i\hat{H} \quad (10.32)$$

then the condition becomes

$$-i\hat{H} = +(i\hat{H})^+ = -i\hat{H}^+ \quad (10.33)$$

or

$$\hat{H} = \hat{H}^+ \quad (10.34)$$

which says that \hat{H} is a Hermitian operator. It is called the *generator* of the family of transformations $\hat{U}(t)$ because it determines these operators uniquely.

Now consider the property

$$\hat{U}(t_1 + t_2) = \hat{U}(t_1)\hat{U}(t_2) \quad (10.35)$$

A *partial derivative* is defined by

$$\frac{\partial f(x, y, z)}{\partial x} = \frac{df(x, y, z)}{dx} \Big|_{y, z = \text{constants}} \quad (10.36)$$

For example, if $f(x, y, z) = x^3y + xy^7z + x^2\sin(z)$, then

$$\begin{aligned} \frac{\partial f}{\partial x} &= 3x^2y + y^7z + 2x\sin(z) \\ \frac{\partial f}{\partial y} &= x^3 + 7xy^6z \\ \frac{\partial f}{\partial z} &= xy^7 + x^2\cos(z) \end{aligned} \quad (10.37)$$

Using the partial derivative we have

$$\frac{\partial}{\partial t_1} \hat{U}(t_1 + t_2) \Big|_{t_1=0} = \frac{d}{dt} \hat{U}(t) \Big|_{t=t_2} = \left(\frac{d}{dt_1} \hat{U}(t_1) \right) \Big|_{t_1=0} \hat{U}(t_2) = -i\hat{H}\hat{U}(t_2) \quad (10.38)$$

which is the same as the equation for arbitrary t

$$i \frac{d\hat{U}(t)}{dt} = \hat{H}\hat{U}(t) \quad (10.39)$$

This equation is satisfied by the unique solution

$$\hat{U}(t) = e^{-i\hat{H}t} \quad (10.40)$$

which gives us an expression for the time development operator in terms of the Hamiltonian. Formally, this result is called *Stone's theorem*. This is the same

form as we specified earlier for the time-development operator.

The *Schrödinger picture* follows directly from this discussion of the $\hat{U}(t)$ operator.

Suppose we have some physical system that is represented by the state vector $|\psi(0)\rangle$ at time $t = 0$ and represented by the state vector $|\psi(t)\rangle$ at time t .

We ask this question. How are these state vectors related to each other? We make the following assumptions:

- (1) *every vector* $|\psi(0)\rangle$ such that $\langle\psi(0)|\psi(0)\rangle = 1$ represents a *possible state* at time $t = 0$
- (2) *every vector* $|\psi(t)\rangle$ such that $\langle\psi(t)|\psi(t)\rangle = 1$ represents a *possible state* at time t
- (3) *every Hermitian operator* represents an *observable* or *measurable* quantity
- (4) the properties of the physical system determine the state vectors to *within a phase factor* since $|\varphi\rangle = e^{i\alpha}|\psi\rangle$ implies that

$$\langle\varphi|\varphi\rangle = \langle\psi|e^{-i\alpha}e^{i\alpha}|\psi\rangle = \langle\psi|\psi\rangle = 1 \quad (10.41)$$

- (5) $|\psi(t)\rangle$ is *determined* by $|\psi(0)\rangle$

Now, if $|\psi(0)\rangle$ and $|\phi(0)\rangle$ represent two possible states at $t = 0$ and $|\psi(t)\rangle$ and $|\phi(t)\rangle$ represent the *corresponding* states at time t , then

$|\langle\varphi(0)|\psi(0)\rangle|^2$ = probability of finding the system in the state represented by $|\phi(0)\rangle$ given that the system is in the state $|\psi(0)\rangle$ at $t = 0$

$|\langle\varphi(t)|\psi(t)\rangle|^2$ = probability of finding the system in the state represented by $|\phi(t)\rangle$ given that the system is in the state $|\psi(t)\rangle$ at t

- (6) it makes *physical sense* to assume that these two probabilities should be the same

$$|\langle\varphi(0)|\psi(0)\rangle|^2 = |\langle\varphi(t)|\psi(t)\rangle|^2 \quad (10.42)$$

Wigner's theorem (linear algebra) then says that there exists a unitary, linear operator $\hat{U}(t)$ such that

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle \quad (10.43)$$

and an expression of the form

$$|\langle\alpha|\hat{U}(t)|\beta\rangle|^2 \quad (10.44)$$

gives the probability that the system is in state $|\alpha\rangle$ at time t given that it was in the state $|\beta\rangle$ at time $t = 0$.

We assume that this expression is a continuous function of t . As we have already showed, we then have $\hat{U}(t)$ satisfying the equation

$$i \frac{d\hat{U}(t)}{dt} = \hat{H} \hat{U}(t) \quad (10.45)$$

or

$$\hat{U}(t) = e^{-i\hat{H}t} \quad (10.46)$$

and thus,

$$|\psi(t)\rangle = \hat{U}(t) |\psi(0)\rangle = e^{-i\hat{H}t} |\psi(0)\rangle \quad (10.47)$$

which implies the following equation of motion for the state vector

$$i \frac{d\hat{U}(t)}{dt} |\psi(0)\rangle = \hat{H} \hat{U}(t) |\psi(0)\rangle \quad (10.48)$$

$$i \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \quad (10.49)$$

which is the *abstract form* of the famous Schrödinger equation. We will derive the standard form of this equation shortly.

As we said earlier, the operator $\hat{U}(t) = e^{-i\hat{H}t}$ is called the *time evolution operator*.

Finally, we can write a time-dependent expectation value as

$$|\psi(t)\rangle = \hat{U}(t) |\psi(0)\rangle = e^{-i\hat{H}t} |\psi(0)\rangle \quad (10.50)$$

$$\langle \hat{Q}(t) \rangle = \langle \psi(t) | \hat{Q} | \psi(t) \rangle \quad (10.51)$$

This is the *Schrödinger picture* where *state vectors change with time and operators are constant in time*.

We note that the Schrödinger picture is *not the same* as the Schrödinger equation. The Schrödinger equation involves a mathematical object called the *wave function* which is *one particular representation* of the state vector, namely the *position representation*, as we shall see later. Thus, the Schrödinger equation is applicable *only* to Hamiltonians that describe operators dependent on *external degrees* of freedom like position and momentum. The Schrödinger picture, on the other hand, works with *both internal and external degrees of freedom* and can handle a much wider class of physical systems, as we shall see.

The Schrödinger Wave equation in the Coordinate Representation - Wave functions: Approach #2

To form a *representation* of an abstract linear vector space we must carry out these steps:

- (1) Choose a complete, orthonormal set of basis vectors $\{|\alpha_k\rangle\}$

- (2) Construct the identity operator \hat{I} as a sum over the one-dimensional subspace projection operators $|\alpha_k\rangle\langle\alpha_k|$

$$\hat{I} = \sum_k |\alpha_k\rangle\langle\alpha_k| \quad (10.52)$$

- (3) Write an arbitrary vector $|\psi\rangle$ as a linear combination or superposition of basis vectors using the identity operator

$$|\psi\rangle = \hat{I}|\psi\rangle = \left(\sum_k |\alpha_k\rangle\langle\alpha_k|\right)|\psi\rangle = \sum_k \langle\alpha_k|\psi\rangle |\alpha_k\rangle \quad (10.53)$$

It is clear from this equation, that knowledge about the behavior (say in time) of the expansion coefficients $\langle\alpha_k|\psi\rangle$ will tell us the behavior of the state vector $|\psi\rangle$ and allow us to make predictions. Remember also, that the expansion coefficient is the probability amplitude for a particle in the state $|\psi\rangle$ to behave like it is in the state $|\alpha_k\rangle$.

A particular representation that has become very important in the study of many systems using Quantum Mechanics is formed using the eigenstates of the position operator as a basis. It is called the *coordinate or position representation*. We will restrict our attention to one dimension for simplicity.

The eigenstates $\{|x\rangle\}$ of the position operator \hat{x} satisfy

$$\hat{x}|x\rangle = x|x\rangle \quad (10.54)$$

where the eigenvalues x are continuous variables in the range $[-\infty, \infty]$. They form the *basis of the coordinate representation*.

Expanding our earlier discussions, in this case, the summations become integrals and we have

$$\hat{I} = \int |x\rangle\langle x| dx \quad (10.55)$$

$$|\psi\rangle = \hat{I}|\psi\rangle = \int (|x\rangle\langle x|)|\psi\rangle dx = \int \langle x|\psi\rangle |x\rangle dx \quad (10.56)$$

The expansion coefficient in the coordinate representation is given by

$$\psi(x) = \langle x|\psi\rangle \quad (10.57)$$

Since the inner product is defined for all states $|x\rangle$, this new object is clearly a function of the eigenvalues x . It will be the *probability amplitude* for finding the particle to be at the point x in 1-dimensional space if it is in the (abstract) state vector $|\psi\rangle$. It is called the *wave function*.

The bra vector corresponding to $|\psi\rangle$ is

$$\langle\psi| = \langle\psi|\hat{I} = \int \langle\psi|x\rangle\langle x| dx = \int \langle x|\psi\rangle^* \langle x| dx \quad (10.58)$$

The normalization condition takes the form

$$\begin{aligned}\langle \psi | \psi \rangle &= 1 = \langle \psi | \hat{I} | \psi \rangle = \int \langle \psi | x \rangle \langle x | \psi \rangle dx \\ &= \int |\langle x | \psi \rangle|^2 dx = \int |\psi(x)|^2 dx = \int \psi^*(x) \psi(x) dx\end{aligned}\quad (10.59)$$

The probability amplitude for a particle in the state $|\psi\rangle$ to behave like it is in the state $|\phi\rangle$, where

$$|\phi\rangle = \hat{I} |\phi\rangle = \int (|x\rangle \langle x|) |\phi\rangle dx = \int \langle x | \phi \rangle |x\rangle dx \quad (10.60)$$

is given by

$$\begin{aligned}\langle \phi | \psi \rangle &= \left(\int \langle x | \phi \rangle^* \langle x | dx \right) \left(\int \langle x' | \psi \rangle |x'\rangle dx' \right) \\ &= \int dx \int dx' \langle x | \phi \rangle^* \langle x' | \psi \rangle \langle x | x' \rangle\end{aligned}\quad (10.61)$$

In order to evaluate this, we need the normalization condition $\langle \vec{x} | \vec{x}' \rangle$. We have

$$|\psi\rangle = \int \langle x' | \psi \rangle |x'\rangle dx' \quad (10.62)$$

$$\langle x | \psi \rangle = \int \langle x' | \psi \rangle \langle x | x' \rangle dx' \quad (10.63)$$

$$\psi(x) = \int \psi(x') \langle x | x' \rangle dx' \quad (10.64)$$

which implies that

$$\langle \vec{x} | \vec{x}' \rangle = \delta(\vec{x} - \vec{x}') \quad (10.65)$$

where

$$\delta(x - a) = \begin{cases} \text{undefined} & x \neq a \\ 0 & \text{otherwise} \end{cases} \quad (10.66)$$

and

$$\int_{-\infty}^{\infty} f(x) \delta(x - a) dx = f(a) \quad (10.67)$$

for any function $f(x)$. This “function” is called the *Dirac delta function*. Putting this into the above equation for $\psi(x)$, we have

$$\psi(x) = \int \psi(x') \langle x | x' \rangle dx' = \int \psi(x') \delta(x - x') dx' \quad (10.68)$$

which is just the defining integral.

Thus, the delta function normalization follows from the completeness property of the projection operators.

Using this result we get

$$\begin{aligned}\langle \varphi | \psi \rangle &= \int dx \int dx' \langle x | \varphi \rangle^* \langle x' | \psi \rangle \delta(x - x') \\ &= \int \langle x | \varphi \rangle^* \langle x | \psi \rangle dx = \int \varphi^*(x) \psi(x) dx\end{aligned}\quad (10.69)$$

We formally write the \hat{x} operator using the expansion in eigenvalues and projection operators as

$$\hat{x} = \int x |x\rangle \langle x| dx \quad (10.70)$$

We will also need the properties of the linear momentum operator. The eigenstates $\{|p\rangle\}$ of the momentum operator \hat{p} satisfy

$$\hat{p} |p\rangle = p |p\rangle \quad (10.71)$$

where the eigenvalues p are continuous variables in the range $[-\infty, \infty]$. They form the basis of the *momentum representation*.

As before, we have

$$\hat{I} = \frac{1}{2\pi\hbar} \int |p\rangle \langle p| dp \quad (10.72)$$

$$|\psi\rangle = \hat{I} |\psi\rangle = \frac{1}{2\pi\hbar} \int (|p\rangle \langle p|) |\psi\rangle dp = \frac{1}{2\pi\hbar} \int \langle p | \psi \rangle |p\rangle dp \quad (10.73)$$

The expansion coefficient in the momentum representation is

$$\Psi(p) = \langle p | \psi \rangle \quad (10.74)$$

It is the probability amplitude for finding the particle with momentum p if it is in state $|\psi\rangle$.

The bra vector corresponding to $|\psi\rangle$ is

$$\langle \psi | = \langle \psi | \hat{I} = \frac{1}{2\pi\hbar} \int \langle \psi | p \rangle \langle p| dp = \frac{1}{2\pi\hbar} \int \langle p | \psi \rangle^* \langle p| dp \quad (10.75)$$

The normalization condition takes the form

$$\begin{aligned}\langle \psi | \psi \rangle &= 1 = \langle \psi | \hat{I} |\psi\rangle = \frac{1}{2\pi\hbar} \int \langle \psi | p \rangle \langle p | \psi \rangle dp = \frac{1}{2\pi\hbar} \int |\langle p | \psi \rangle|^2 dp \\ &= \frac{1}{2\pi\hbar} \int |\Psi(p)|^2 dp = \frac{1}{2\pi\hbar} \int \Psi^*(p) \Psi(p) dp\end{aligned}\quad (10.76)$$

The probability amplitude for a particle in the state $|\psi\rangle$ to behave like it is in the state $|\phi\rangle$, where

$$|\phi\rangle = \hat{I} |\phi\rangle = \frac{1}{2\pi\hbar} \int (|p\rangle \langle p|) |\phi\rangle dp = \frac{1}{2\pi\hbar} \int \langle p | \phi \rangle |p\rangle dp \quad (10.77)$$

is given by

$$\begin{aligned}\langle \varphi | \psi \rangle &= \left(\frac{1}{2\pi\hbar} \int \langle p | \varphi \rangle^* \langle p | dp \right) \left(\frac{1}{2\pi\hbar} \int \langle p' | \psi \rangle |p'\rangle dp' \right) \\ &= \frac{1}{(2\pi\hbar)^2} \int dp \int dp' \langle p | \varphi \rangle^* \langle p' | \psi \rangle \langle p | p' \rangle\end{aligned}\quad (10.78)$$

The normalization condition follows from

$$|\psi\rangle = \frac{1}{2\pi\hbar} \int \langle p' | \psi \rangle |p'\rangle dp' \quad (10.79)$$

$$\langle p | \psi \rangle = \frac{1}{2\pi\hbar} \int \langle p' | \psi \rangle \langle p | p' \rangle dp' \quad (10.80)$$

$$\Psi(p) = \frac{1}{2\pi\hbar} \int \psi(p') \langle p | p' \rangle dp' \quad (10.81)$$

which implies that

$$\frac{1}{2\pi\hbar} \langle p | p' \rangle = \delta(p - p') \quad (10.82)$$

Using this result we get

$$\begin{aligned}\langle \varphi | \psi \rangle &= \frac{1}{2\pi\hbar} \int dp \int dp' \langle p | \varphi \rangle^* \langle p' | \psi \rangle \delta(p - p') \\ &= \frac{1}{2\pi\hbar} \int \langle p | \varphi \rangle^* \langle p | \psi \rangle dp = \frac{1}{2\pi\hbar} \int \Phi^*(p) \Psi(p) dp\end{aligned}\quad (10.83)$$

We formally write the \hat{p} operator using the expansion in eigenvalues and projection operators as

$$\hat{p} = \frac{1}{2\pi\hbar} \int p |p\rangle \langle p| dp \quad (10.84)$$

We will now derive the connections between the two representations. We need to determine the quantity $\langle \vec{x} | \vec{p} \rangle$. This is, in fact, the key result. It will enable us to derive the Schrödinger equation. We will find that

$$\langle \vec{x} | \vec{p} \rangle = e^{i\vec{p} \cdot \vec{x} / \hbar} \quad (10.85)$$

Derivation:

A representation of the Dirac delta function is

$$\frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{ip(x-x')} dp = \delta(x - x') \quad (10.86)$$

By representation it is implied that we can show that

$$\int_{-\infty}^{\infty} f(x) \left[\frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{ip(x-a)} dp \right] dx = f(a) \quad (10.87)$$

for any function $f(x)$. This result follows from Fourier transform theory.

Now we can rewrite the equation in another way

$$\begin{aligned}
\frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{ip(x-x')} dp &= \delta(x-x') = \langle x | x' \rangle = \langle x | \hat{I} | x' \rangle \\
&= \langle x | \left[\int_{-\infty}^{\infty} |p\rangle \langle p| dp \right] | x' \rangle = \int_{-\infty}^{\infty} \langle x | p \rangle \langle p | x' \rangle dp \\
&= \int_{-\infty}^{\infty} \langle x | p \rangle \langle x' | p \rangle^* dp
\end{aligned} \tag{10.88}$$

which is clearly satisfied by

$$\langle \vec{x} | \vec{p} \rangle = e^{i\vec{p} \cdot \vec{x} / \hbar} \tag{10.89}$$

It is not a unique choice, however. It is the choice, however, that allows Quantum mechanics to *make predictions that agree with experiment*.

We might even say that this choice is *another postulate*.

Now, we can use these results to determine the expectation values of operators involving the position and momentum operators.

Since we are interested in the coordinate representation we need only determine the following relationships.

The position operator calculations are straightforward

$$\langle x | \hat{x} | \psi \rangle = x \langle x | \psi \rangle \quad , \quad \langle x | f(\hat{x}) | \psi \rangle = f(x) \langle x | \psi \rangle \tag{10.90}$$

For the momentum operator we write

$$\begin{aligned}
\langle x | \hat{p} | \psi \rangle &= \frac{1}{2\pi\hbar} \int dp \langle x | \hat{p} | p \rangle \langle p | \psi \rangle \\
&= \frac{1}{2\pi\hbar} \int dp \langle x | p | p \rangle \langle p | \psi \rangle = \frac{1}{2\pi\hbar} \int p dp \langle x | p \rangle \langle p | \psi \rangle
\end{aligned} \tag{10.91}$$

Using

$$\langle x | p \rangle = e^{ipx/\hbar} \tag{10.92}$$

we have

$$p \langle x | p \rangle = -i\hbar \frac{d}{dx} \langle x | p \rangle = \langle x | \hat{p} | p \rangle \tag{10.93}$$

and

$$\begin{aligned}
\langle x | \hat{p} | \psi \rangle &= \frac{1}{2\pi\hbar} \int dp \langle x | \hat{p} | p \rangle \langle p | \psi \rangle \\
&= \frac{1}{2\pi\hbar} \int dp \langle x | p | p \rangle \langle p | \psi \rangle = \frac{1}{2\pi\hbar} \int dp \left[-i\hbar \frac{d}{dx} \langle x | p \rangle \right] \langle p | \psi \rangle \\
&= \frac{-i}{2\pi} \frac{d}{dx} \int dp \langle x | p \rangle \langle p | \psi \rangle = -i\hbar \frac{d}{dx} \langle x | \psi \rangle
\end{aligned} \tag{10.94}$$

We can also show that

$$\langle \hat{x} | \hat{p}^2 | \psi \rangle = - \left(-i\hbar \frac{d}{dx} \right)^2 \langle \hat{x} | \psi \rangle = -\hbar^2 \frac{d^2}{dx^2} \langle \hat{x} | \psi \rangle \quad (10.95)$$

Using these equations, we can now derive the Schrödinger wave equation.

The Schrödinger wave equation in one dimension is the differential equation that corresponds to the eigenvector/eigenvalue equation for the Hamiltonian operator or the energy operator.

The resulting states are the energy eigenstates. We already saw that energy eigenstates are stationary states and thus have simple time dependence. This property will allow us to find the time dependence of amplitudes for very complex systems in a straightforward way.

We have

$$\hat{H} |\psi_E\rangle = E |\psi_E\rangle \quad (10.96)$$

where E is a number and

$$\begin{aligned} \hat{H} &= \text{energy operator} \\ &= (\text{kinetic energy} + \text{potential energy}) \text{ operators} \\ &= \frac{\hat{p}^2}{2m} + V(\hat{x}) \end{aligned} \quad (10.97)$$

We then have

$$\langle x | \frac{\hat{p}^2}{2m} + V(\hat{x}) | \psi_E \rangle = E \langle x | \psi_E \rangle \quad (10.98)$$

$$\langle x | \frac{\hat{p}^2}{2m} | \psi_E \rangle + \langle x | V(\hat{x}) | \psi_E \rangle = E \langle x | \psi_E \rangle \quad (10.99)$$

$$- \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \langle x | \psi_E \rangle + V(x) \langle x | \psi_E \rangle = E \langle x | \psi_E \rangle \quad (10.100)$$

$$- \frac{\hbar^2}{2m} \frac{d^2 \psi_E(x)}{dx^2} + V(x) \psi_E(x) = E \psi_E(x) \quad (10.101)$$

which is the *time-independent Schrödinger wave equation* in one dimension. The quantity

$$\psi_E(x) = \langle x | \psi_E \rangle \quad (10.102)$$

is the *wave function* or the *energy eigenfunction* in the *position representation* corresponding to energy E .

The quantity

$$|\psi_E(x)|^2 = |\langle x | \psi_E \rangle|^2 \quad (10.103)$$

represents the probability density to find a particle at coordinate x if it is in the state represented by the vector $|\psi_E\rangle$.

Now the energy eigenfunctions have a simple time dependence, as we can see from the following.

Since

$$\hat{U}(t) |\psi_E\rangle = e^{-i\frac{\hat{H}}{\hbar}t} |\psi_E\rangle = e^{-i\frac{E}{\hbar}t} |\psi_E\rangle \quad (10.104)$$

we have

$$\langle x | \hat{U}(t) |\psi_E\rangle = \psi_E(x, t) = e^{-i\frac{E}{\hbar}t} \langle x | \psi_E\rangle \quad (10.105)$$

$$\psi_E(x, t) = e^{-i\frac{E}{\hbar}t} \psi_E(x, 0) \quad (10.106)$$

Therefore,

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_E(x, t)}{dx^2} + V(x) \psi_E(x, t) = E \psi_E(x, t) \quad (10.107)$$

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_E(x, t)}{dx^2} + V(\vec{x}) \psi_E(x, t) = i\hbar \frac{\partial}{\partial t} \psi_E(x, t) \quad (10.108)$$

which is the *time-dependent Schrödinger wave equation*.

Clearly, systems change in time. One change is the collapse process, which is discontinuous (and non-unitary). We have also developed (from postulate #4) a deterministic (unitary) time evolution between measurements.

Between measurements states evolve according to the equation

$$|\psi(t)\rangle = \hat{U}(t) |\psi(0)\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle \quad (10.109)$$

For energy eigenstates we find that

$$|\psi_E(t)\rangle = \hat{U}(t) |\psi_E(0)\rangle = e^{-i\frac{\hat{H}}{\hbar}t} |\psi_E(0)\rangle = e^{-i\frac{E}{\hbar}t} |\psi_E(0)\rangle \quad (10.110)$$

that is, they only change by a phase factor.

Let us look at a simple example to illustrate the process.

We consider a particle with the hardness property but now we place it in an external force that makes the system have a higher energy when the particle is in the hard state $|h\rangle$ than when it is in the soft state $|s\rangle$. We define these two energies to be $+E_0$ for $|h\rangle$ and $-E_0$ for $|s\rangle$. These energies are just the corresponding energy eigenvalues for these two states. Therefore, the energy operator (in the hard-soft basis) is given by

$$\hat{H} = \begin{pmatrix} +E_0 & 0 \\ 0 & -E_0 \end{pmatrix} \quad (10.111)$$

Thus, we have

Case #1

$$|\psi(0)\rangle = |h\rangle \quad (10.112)$$

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |h\rangle = e^{-iE_0t/\hbar} |h\rangle \quad (10.113)$$

and

Case #2

$$|\psi(0)\rangle = |s\rangle \quad (10.114)$$

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |s\rangle = e^{iE_0t/\hbar} |s\rangle \quad (10.115)$$

In either case, if we measure the hardness of this particle at time t , it still has the same value as at $t = 0$, that is, for case #1

$$|\langle h | \psi(t) \rangle|^2 = |\langle h | e^{-iE_0t/\hbar} |h\rangle|^2 = |\langle h | h \rangle|^2 = 1 \quad (10.116)$$

$$|\langle s | \psi(t) \rangle|^2 = |\langle s | e^{-iE_0t/\hbar} |h\rangle|^2 = |\langle s | h \rangle|^2 = 0 \quad (10.117)$$

or the hardness of the particle does not change in time if it starts out in a state of definite hardness (they are energy eigenstates).

When the initial state is not an energy eigenstate, that is, when it is a superposition of hard and soft states, then it will change with time. The change will be in the *relative phase* between the components.

We illustrate this below:

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}} (|h\rangle + |s\rangle) \rightarrow |g\rangle \quad (10.118)$$

$$\begin{aligned} |\psi(t)\rangle &= e^{-i\hat{H}t/\hbar} |\psi(0)\rangle = \frac{1}{\sqrt{2}} e^{-i\hat{H}t/\hbar} (|h\rangle + |s\rangle) = \frac{1}{\sqrt{2}} (e^{-i\hat{H}t/\hbar} |h\rangle + e^{-i\hat{H}t/\hbar} |s\rangle) \\ &= \frac{1}{\sqrt{2}} (e^{-iE_0t/\hbar} |h\rangle + e^{iE_0t/\hbar} |s\rangle) \end{aligned} \quad (10.119)$$

so that the relative phase is $e^{2iE_0t/\hbar}$. This state is not an eigenstate of hardness or color! What is the probability of measuring various results?

Initially:

$$|\langle h | \psi(0) \rangle|^2 = \frac{1}{2} = |\langle s | \psi(0) \rangle|^2 \quad (10.120)$$

$$|\langle g | \psi(0) \rangle|^2 = 1 \quad , \quad |\langle m | \psi(0) \rangle|^2 = 0 \quad (10.121)$$

At time t :

$$|\langle h | \psi(t) \rangle|^2 = \left| \langle h | \left(\frac{1}{\sqrt{2}} (e^{-iE_0 t/\hbar} |h\rangle + e^{iE_0 t/\hbar} |s\rangle) \right) \right|^2 = \left| \frac{1}{\sqrt{2}} e^{-iE_0 t/\hbar} \right|^2 = \frac{1}{2} \quad (10.122)$$

$$|\langle s | \psi(t) \rangle|^2 = \left| \langle s | \left(\frac{1}{\sqrt{2}} (e^{-iE_0 t/\hbar} |h\rangle + e^{iE_0 t/\hbar} |s\rangle) \right) \right|^2 = \left| \frac{1}{\sqrt{2}} e^{iE_0 t/\hbar} \right|^2 = \frac{1}{2} \quad (10.123)$$

$$\begin{aligned} |\langle g | \psi(t) \rangle|^2 &= \left| \langle g | \left(\frac{1}{\sqrt{2}} (e^{-iE_0 t/\hbar} |h\rangle + e^{iE_0 t/\hbar} |s\rangle) \right) \right|^2 \\ &= \left| \frac{1}{\sqrt{2}} e^{-iE_0 t/\hbar} \langle g | h \rangle + \frac{1}{\sqrt{2}} e^{iE_0 t/\hbar} \langle g | s \rangle \right|^2 \\ &= \left| \frac{1}{2} e^{-iE_0 t/\hbar} + \frac{1}{2} e^{iE_0 t/\hbar} \right|^2 = \cos^2 \frac{2E_0 t}{\hbar} \end{aligned} \quad (10.124)$$

$$\begin{aligned} |\langle m | \psi(t) \rangle|^2 &= \left| \langle m | \left(\frac{1}{\sqrt{2}} (e^{-iE_0 t/\hbar} |h\rangle + e^{iE_0 t/\hbar} |s\rangle) \right) \right|^2 \\ &= \left| \frac{1}{\sqrt{2}} e^{-iE_0 t/\hbar} \langle m | h \rangle + \frac{1}{\sqrt{2}} e^{iE_0 t/\hbar} \langle m | s \rangle \right|^2 \\ &= \left| \frac{1}{2} e^{-iE_0 t/\hbar} - \frac{1}{2} e^{iE_0 t/\hbar} \right|^2 = \sin^2 \frac{2E_0 t}{\hbar} \end{aligned} \quad (10.125)$$

So the probability of measuring the hardness of this particle that was originally in the green state remains $1/2$ (as it was at $t = 0$) since they are energy eigenstates or stationary states. But much more interesting is the fact that the probability for measurements of color oscillates between probability =1 for green and probability = 1 for magenta.

So the procedure is the following:

- (1) Find the energy operator for the physical system.
- (2) Express the initial state as a superposition of energy eigenstates.
- (3) Insert the simple time dependence of the energy eigenstate to obtain the time dependence of the state of the system.
- (4) Determine probability for final measurements by taking appropriate inner products.

Chapter 11

Simple Systems

Again, these topics are for the more mathematically inclined students.

11.1 One-Dimensional Quantum Systems

The Schrodinger equation in 1-dimension is

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_E(x)}{dx^2} + V(x)\psi_E(x) = E\psi_E(x) \quad (11.1)$$

The solutions $\psi_E(x)$ are the energy eigenstates (eigenfunctions). As we have seen, their time dependence is given by

$$\psi_E(x, t) = e^{-i\frac{E}{\hbar}t} \psi_E(x, 0) \quad (11.2)$$

where

$$\psi_E(x, 0) = \langle x | E \rangle \quad (11.3)$$

and

$$\hat{H} |E\rangle = E |E\rangle \quad (11.4)$$

where

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \quad (11.5)$$

We are thus faced with solving an ordinary differential equation with boundary conditions.

Since $\psi_E(x)$ is physically related to a probability amplitude and hence to a measurable probability, we *assume* that $\psi_E(x)$ is continuous.

Using this fact, we can determine the general continuity properties of $d\psi_E(x)/dx$.

The continuity property at a particular point, say $x = x_0$, is derived as follows: we have

$$\begin{aligned} \int_{x_0-\varepsilon}^{x_0+\varepsilon} \frac{d^2\psi_E(x)}{dx^2} dx &= \int_{x_0-\varepsilon}^{x_0+\varepsilon} d\left(\frac{d\psi_E(x)}{dx}\right) \\ &= -\frac{2m}{\hbar^2} \left[E \int_{x_0-\varepsilon}^{x_0+\varepsilon} \psi_E(x) dx - \int_{x_0-\varepsilon}^{x_0+\varepsilon} V(x) \psi_E(x) dx \right] \end{aligned} \quad (11.6)$$

Taking the limit as $\varepsilon \rightarrow 0$

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \left(\frac{d\psi_E(x)}{dx} \Big|_{x=x_0+\varepsilon} - \frac{d\psi_E(x)}{dx} \Big|_{x=x_0-\varepsilon} \right) \\ = -\frac{2m}{\hbar^2} \left[E \lim_{\varepsilon \rightarrow 0} \int_{x_0-\varepsilon}^{x_0+\varepsilon} \psi_E(x) dx - \lim_{\varepsilon \rightarrow 0} \int_{x_0-\varepsilon}^{x_0+\varepsilon} V(x) \psi_E(x) dx \right] \end{aligned} \quad (11.7)$$

or

$$\Delta \left(\frac{d\psi_E(x)}{dx} \right) = \frac{2m}{\hbar^2} \lim_{\varepsilon \rightarrow 0} \int_{x_0-\varepsilon}^{x_0+\varepsilon} V(x) \psi_E(x) dx \quad (11.8)$$

where we have used the continuity of $\psi_E(x)$ to set

$$\lim_{\varepsilon \rightarrow 0} \int_{x_0-\varepsilon}^{x_0+\varepsilon} \psi_E(x) dx = 0 \quad (11.9)$$

This makes it clear that whether or not $d\psi_E(x)/dx$ has a discontinuity depends directly on the potential energy function.

If $V(x)$ is continuous at $x = x_0$, i.e., if

$$\lim_{\varepsilon \rightarrow 0} [V(x_0 + \varepsilon) - V(x_0 - \varepsilon)] = 0 \quad (11.10)$$

then

$$\Delta \left(\frac{d\psi_E(x)}{dx} \right) = \frac{2m}{\hbar^2} \lim_{\varepsilon \rightarrow 0} \int_{x_0-\varepsilon}^{x_0+\varepsilon} V(x) \psi_E(x) dx = 0 \quad (11.11)$$

and $d\psi_E(x)/dx$ is continuous.

If $V(x)$ has a finite discontinuity (jump) at $x = x_0$, i.e.,

$$\lim_{\varepsilon \rightarrow 0} [V(x_0 + \varepsilon) - V(x_0 - \varepsilon)] = \text{finite} \quad (11.12)$$

then

$$\Delta \left(\frac{d\psi_E(x)}{dx} \right) = \frac{2m}{\hbar^2} \lim_{\varepsilon \rightarrow 0} \int_{x_0-\varepsilon}^{x_0+\varepsilon} V(x) \psi_E(x) dx = 0 \quad (11.13)$$

and $d\psi_E(x)/dx$ is continuous.

Finally, if $V(x)$ has an infinite jump at $x = x_0$, then we have two choices

- (1) if the potential is infinite over an extended region of x , then we must force $\psi_E(x) = 0$ in that region and use only the continuity of $\psi_E(x)$ as a boundary condition at the edge of the region.
- (2) if the potential is infinite at a single point, i.e., $V(x) = \delta(x - x_0)$, then we would have

$$\begin{aligned}\Delta\left(\frac{d\psi_E(x)}{dx}\right) &= \frac{2m}{\hbar^2} \lim_{\varepsilon \rightarrow 0} \int_{x_0-\varepsilon}^{x_0+\varepsilon} V(x)\psi_E(x)dx \\ &= \frac{2m}{\hbar^2} \lim_{\varepsilon \rightarrow 0} \int_{x_0-\varepsilon}^{x_0+\varepsilon} \delta(x - x_0)\psi_E(x)dx \\ &= \frac{2m}{\hbar^2} \lim_{\varepsilon \rightarrow 0} \psi_E(x_0) = \frac{2m}{\hbar^2} \psi_E(x_0)\end{aligned}\quad (11.14)$$

and, thus, $d\psi_E(x)/dx$ is discontinuous.

The last thing we must worry about is the validity of our probability interpretation of $\psi_E(x)$, i.e., $\psi_E(x) = \langle x | \psi_E \rangle$ = probability amplitude for the particle in the state $|\psi_E\rangle$ to be found at x , which says that we must also have

$$\langle \psi_E | \psi_E \rangle = \int_{-\infty}^{\infty} |\psi_E(x)|^2 dx < \infty \quad (11.15)$$

This means that we must be able to normalize the wave functions and make the total probability that the particle is somewhere on the x -axis equal to one.

A wide range of interesting physical systems can be studied using 1-dimensional potential energy functions.

11.2 Quantized Energy Levels in the Infinite Square Well Potential

We now consider the potential energy function

$$V(x) = \begin{cases} 0 & -a/2 \leq x \leq a/2 \\ \infty & |x| \geq a/2 \end{cases} \quad (11.16)$$

This is the so-called *infinite square well* shown in the figure below. We consider the three regions labeled I, II, III.

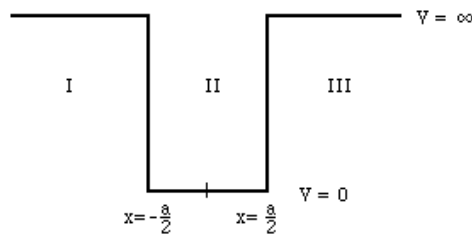


Figure 11.1: Infinite square well potential energy function

This is an example of a potential that is infinite in an extended region. Therefore, we must require that the wave function $\psi(x) = 0$ in these regions or the Schrodinger equation makes no sense mathematically. In this case we have

$$\psi_I(x) = 0 \quad , \quad \psi_{III}(x) = 0 \quad (11.17)$$

Digression: Second-Order ODEs

The solution technique we will use in most cases is called *exponential substitution*.

Exponential Substitution

This method is applicable to all differential equations of the form

$$A \frac{d^2 y}{dt^2} + B \frac{dy}{dt} + Cy = 0 \quad (11.18)$$

where A , B and C are constants.

Definitions:

2nd-order = order of highest derivative

linear = no squares or worse

homogeneous = right-hand side = 0

constant coefficients = A, B, C

Therefore this equation is a 2nd-order, homogeneous, linear differential equation with constant coefficients.

The Simple Harmonic Motion equation(spring) has this form,

$$M \frac{dv}{dt} = -kx \Rightarrow M \frac{d}{dt} \left(\frac{dx}{dt} \right) = -kx \Rightarrow M \frac{d^2 x}{dt^2} + kx = 0 \quad (11.19)$$

so that $A = M$, $C = k$ and $B = 0$.

The 1-dimensional Schrodinger equation will also take this form in different regions as we shall see.

The Method: Consider a typical equation of the form

$$\frac{d^2y}{dt^2} + 3\frac{dy}{dt} + 2y = 0 \quad (11.20)$$

We make the exponential substitution

$$y = e^{\alpha t} \quad (11.21)$$

into the ODE. This will convert the diffeQ into an algebraic equation for α . We have

$$\frac{d^2y}{dt^2} = \frac{d^2e^{\alpha t}}{dt^2} = \alpha^2 e^{\alpha t} \quad (11.22)$$

$$\frac{dy}{dt} = \frac{de^{\alpha t}}{dt} = \alpha e^{\alpha t} y = e^{\alpha t} \quad (11.23)$$

which gives the result

$$(\alpha^2 + 3\alpha + 2) e^{\alpha t} = 0 \Rightarrow \alpha^2 + 3\alpha + 2 = 0 \quad (11.24)$$

since $e^{\alpha t} \neq 0$.

The solutions of this algebraic equation tell us the *allowed* values of α that give *valid* solutions to the ODE. In particular in this case we get

$$\alpha = -1, -2 \quad (11.25)$$

as solutions to the quadratic equation. This result means that $y = e^{-t}$ and $y = e^{-2t}$ satisfy the original ODE as can be seen by direct substitution.

If there is more than one allowed value of (as in this case), then the most general solution will be a linear combination of all possible solutions (because this is a linear diffeQ). Since, in this case, the allowed values of α are $\alpha = -1, -2$, the most general solution of the ODE is

$$y(t) = ae^{-t} + be^{-2t} \quad (11.26)$$

where a and b are constants to be determined by the *initial conditions*.

The number of arbitrary constants that need to be determined by the initial conditions is equal to the order (highest derivative $\rightarrow 2$ in this case) of this ODE.

Suppose the initial conditions are

$$y = 0 \quad , \quad \frac{dy}{dt} = 1 \quad (11.27)$$

at $t = 0$. Then we have

$$y(t) = ae^{-t} + be^{-2t} \quad (11.28)$$

$$y(0) = 0 = a + b \quad (11.29)$$

$$\frac{dy}{dt} = -ae^{-t} - 2be^{-2t} \quad (11.30)$$

$$\frac{dy}{dt}(0) = -a - 2b = 1 \quad (11.31)$$

which gives $a = -b = 1$ and thus

$$y(t) = e^{-t} - e^{-2t} \quad (11.32)$$

One can easily substitute this solution into the original equation and see that it works and has the correct initial conditions!!

Although this method is very powerful as described, we can make it even more powerful by defining a new mathematical quantity called the *complex exponential*. This will allow us to use the method for the SHM case.

Complex Exponentials - Alternative Very Powerful Method

Remember the exponential function has the power series expansions:

$$e^{\alpha x} = 1 + \alpha x + \frac{\alpha^2}{2!}x^2 + \frac{\alpha^3}{3!}x^3 + \frac{\alpha^4}{4!}x^4 + \dots = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!}x^n \quad (11.33)$$

Similarly the sine and cosine functions are given by:

$$\sin \alpha x = \sum_{n=0}^{\infty} (-1)^n \frac{\alpha^{2n+1}}{(2n+1)!}x^{2n+1} = \frac{\alpha}{1!}x - \frac{\alpha^3}{3!}x^3 + \dots \quad (11.34)$$

$$\cos \alpha x = \sum_{n=0}^{\infty} (-1)^n \frac{\alpha^{2n}}{(2n)!}x^{2n} = 1 - \frac{\alpha^2}{2!}x^2 + \frac{\alpha^4}{4!}x^4 + \dots \quad (11.35)$$

We then showed the neat result that

$$e^{\pm i\alpha t} = \cos \alpha t \pm i \sin \alpha t \quad (11.36)$$

which is very useful in physics. It is called Euler's formula.

From these results we also derived the relations

$$\sin \omega t = \frac{e^{i\omega t} - e^{-i\omega t}}{2i} \quad , \quad \cos \omega t = \frac{e^{i\omega t} + e^{-i\omega t}}{2} \quad (11.37)$$

Finally, we can use these results to solve the SHM equation

$$M \frac{d^2 y}{dt^2} + ky = 0 \rightarrow \frac{d^2 y}{dt^2} + \omega^2 y = 0 \quad , \quad \omega^2 = \frac{k}{M} \quad (11.38)$$

using the exponential substitution method. We have

$$\frac{d^2 y}{dt^2} + \omega^2 y = 0 \quad (11.39)$$

Substituting $y = e^{\alpha t}$ we get the algebraic equation

$$\alpha^2 + \omega^2 = 0 \quad (11.40)$$

which has solutions (allowed values of α) of $\alpha = \pm i\omega$ so that the most general solution takes the form

$$y(t) = Ae^{i\omega t} + Be^{-i\omega t} \quad (11.41)$$

Suppose now that the initial conditions are

$$y = y_0 \quad , \quad \frac{dy}{dt} = 0 \quad (11.42)$$

at $t = 0$. Then we have

$$y(t) = Ae^{i\omega t} + Be^{-i\omega t} \quad (11.43)$$

$$y(0) = y_0 = A + B \quad (11.44)$$

$$\frac{dy}{dt} = i\omega Ae^{i\omega t} - i\omega Be^{-i\omega t} \quad (11.45)$$

$$\frac{dy}{dt}(0) = i\omega A - i\omega B = 0 \rightarrow A - B = 0 \quad (11.46)$$

or

$$A = B = \frac{y_0}{2} \quad (11.47)$$

and

$$y(t) = y_0 \frac{e^{i\omega t} + e^{-i\omega t}}{2} = y_0 \cos \omega t \quad (11.48)$$

Alternatively, if the initial conditions are

$$y = 0 \quad , \quad \frac{dy}{dt} = v_0 \quad (11.49)$$

at $t = 0$, then we have

$$y(t) = Ae^{i\omega t} + Be^{-i\omega t} \quad (11.50)$$

$$y(0) = 0 = A + B \quad (11.51)$$

$$\frac{dy}{dt} = i\omega Ae^{i\omega t} - i\omega Be^{-i\omega t} \quad (11.52)$$

$$\frac{dy}{dt}(0) = i\omega A - i\omega B = v_0 \rightarrow A - B = v_0/i\omega \quad (11.53)$$

or

$$A = -B = \frac{v_0}{2i\omega} \quad (11.54)$$

and

$$y(t) = \frac{v_0}{\omega} \left(\frac{e^{i\omega t} - e^{-i\omega t}}{2i} \right) = \frac{v_0}{\omega} \sin \omega t \quad (11.55)$$

and in general we have for the initial conditions

$$y = y_0 \quad , \quad \frac{dy}{dt} = v_0 \quad (11.56)$$

at $t = 0$, then we have

$$y(t) = Ae^{i\omega t} + Be^{-i\omega t} \quad (11.57)$$

$$y(0) = y_0 = A + B \quad (11.58)$$

$$\frac{dy}{dt} = i\omega Ae^{i\omega t} - i\omega Be^{-i\omega t} \quad (11.59)$$

$$\frac{dy}{dt}(0) = i\omega A - i\omega B = v_0 \rightarrow A - B = v_0/i\omega \quad (11.60)$$

or

$$A = \frac{1}{2} \left(y_0 + \frac{v_0}{i\omega} \right) \quad , \quad B = \frac{1}{2} \left(y_0 - \frac{v_0}{i\omega} \right) \quad (11.61)$$

and

$$\begin{aligned} y(t) &= Ae^{i\omega t} + Be^{-i\omega t} = \frac{1}{2} \left(y_0 + \frac{v_0}{i\omega} \right) e^{i\omega t} + \frac{1}{2} \left(y_0 - \frac{v_0}{i\omega} \right) e^{-i\omega t} \\ &= y_0 \frac{e^{i\omega t} + e^{-i\omega t}}{2} + \frac{v_0}{\omega} \frac{e^{i\omega t} - e^{-i\omega t}}{2i} = y_0 \cos \omega t + \frac{v_0}{\omega} \sin \omega t \end{aligned} \quad (11.62)$$

Returning to the infinite square well Schrodinger equation:

Now in region II, the Schrodinger equation becomes

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_{II}}{dx^2} = E\psi_{II} \quad , \quad E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \quad (11.63)$$

which has a general solution(using the above method) given by

$$\psi_{II}(x) = Ae^{ikx} + Be^{-ikx} \quad (11.64)$$

where k is some parameter to be determined.

The continuity of the wavefunction at $x = \pm a/2$ says that we must have

$$\psi_{II}\left(-\frac{a}{2}\right) = Ae^{-i\frac{ka}{2}} + Be^{i\frac{ka}{2}} = 0 \quad (11.65)$$

$$\psi_{II}\left(\frac{a}{2}\right) = Ae^{i\frac{ka}{2}} + Be^{-i\frac{ka}{2}} = 0 \quad (11.66)$$

which imply that

$$\frac{B}{A} = -e^{-ika} = -e^{ika} \quad (11.67)$$

This is an equation for the allowed values (values corresponding to a valid solution) of the parameter k .

The equation is

$$e^{2ika} = 1 \quad (11.68)$$

The allowed values of k form a discrete spectrum of energy eigenvalues (quantized energies) given by

$$2k_na = 2n\pi \rightarrow k_n = \frac{n\pi}{a} \rightarrow E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2}, \quad n = 1, 2, 3, 4, \dots \quad (11.69)$$

The corresponding wave functions are

$$\begin{aligned} \psi_{II}^{(n)}(x) &= A_n(e^{ik_n x} - e^{-ik_n a} e^{-ik_n x}) = A_n e^{-i \frac{k_n a}{2}} \left(e^{ik_n(x + \frac{a}{2})} - e^{-ik_n(x + \frac{a}{2})} \right) \\ &= \tilde{A}_n \sin k_n \left(x + \frac{a}{2} \right) \end{aligned} \quad (11.70)$$

where \tilde{A}_n is determined by the normalization condition

$$\int_{-\frac{a}{2}}^{\frac{a}{2}} |\psi_n(x)|^2 dx = 1 \quad (11.71)$$

Substituting the value of k_n we get

$$\psi_{II}^{(n)}(x) = \tilde{A}_n \sin \frac{n\pi}{a} \left(x + \frac{a}{2} \right) \quad (11.72)$$

or

$$\psi_{II}^{(1)}(x) = \tilde{A}_1 \sin \frac{\pi}{a} \left(x + \frac{a}{2} \right) = \tilde{A}_1 \sin \left(\frac{\pi x}{a} + \frac{\pi}{2} \right) = \tilde{A}_1 \cos \left(\frac{\pi x}{a} \right) \quad (11.73)$$

$$\psi_{II}^{(2)}(x) = \tilde{A}_2 \sin \frac{2\pi}{a} \left(x + \frac{a}{2} \right) = \tilde{A}_2 \sin \left(\frac{2\pi x}{a} + \pi \right) = \tilde{A}_2 \sin \left(\frac{2\pi x}{a} \right) \quad (11.74)$$

$$\psi_{II}^{(3)}(x) = \tilde{A}_3 \sin \frac{3\pi}{a} \left(x + \frac{a}{2} \right) = \tilde{A}_3 \sin \left(\frac{3\pi x}{a} + \frac{3\pi}{2} \right) = \tilde{A}_3 \cos \left(\frac{3\pi x}{a} \right) \quad (11.75)$$

or

$$\psi_{II}(x) = \begin{cases} \sin \left(\frac{n\pi x}{a} \right) & n \text{ even} \\ \cos \left(\frac{n\pi x}{a} \right) & n \text{ odd} \end{cases} \quad (11.76)$$

We have mathematically solved the ordinary differential equation problem, now what is the physical meaning of these results?

We find a *discrete spectrum* of allowed energies corresponding to *bound states* of the Hamiltonian. The energy is *quantized*. Bound states designate states which are localized in space, i.e., the probability is large only over restricted regions of space and goes to zero far from the potential region.

The *lowest* energy value or lowest energy *level* or *ground state* energy is

$$E_1 = \frac{\pi^2 \hbar^2}{2ma^2} > 0 \quad (11.77)$$

with

$$\psi_1(x) = \begin{cases} A \cos\left(\frac{\pi x}{a}\right) & |x| \leq a/2 \\ 0 & |x| \geq a/2 \end{cases}$$

This minimum energy is not zero because of the Heisenberg uncertainty principle. Since the particle has a nonzero amplitude for being in the well, we say that it is localized such that $\Delta x \approx a$ and thus

$$\Delta p \geq \frac{\hbar}{\Delta x} \approx \frac{\hbar}{a} \quad (11.78)$$

This says that the kinetic energy (or energy in this case because the potential energy equals zero in region II) must have a minimum value given approximately by

$$E_{\min} = K_{\min} \approx \frac{(\Delta p)^2}{2m} \approx \frac{\hbar^2}{2ma^2} \quad (11.79)$$

The integer $n-1$ corresponds to the number of nodes (zeros) of the wave function (other than the well edges).

The solutions also have the property

$$\psi(-x) = \psi(x) \quad n \text{ odd} \quad (11.80)$$

$$\psi(-x) = -\psi(x) \quad n \text{ even} \quad (11.81)$$

The above discrete transformation of the wave function corresponds to the *parity* operator \hat{p} where we have

$$\hat{p}\psi(x) = \psi(-x) = \psi(x) \rightarrow \text{even parity} \quad (11.82)$$

$$\hat{p}\psi(x) = \psi(-x) = -\psi(x) \rightarrow \text{odd parity} \quad (11.83)$$

Let us look more generally at the parity operation. Suppose that the potential energy function obeys the rule $V(\vec{x}) = V(-\vec{x})$ and let $\psi(\vec{x})$ be a solution of the Schrodinger equation with energy E . Then

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}) \right) \psi(\vec{x}) = E\psi(\vec{x}) \quad (11.84)$$

Now let $\vec{x} \rightarrow -\vec{x}$ to get the equation

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V(-\vec{x}) \right) \psi(-\vec{x}) = E\psi(-\vec{x}) \quad (11.85)$$

or

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}) \right) \psi(-\vec{x}) = E\psi(-\vec{x}) \quad (11.86)$$

This says that, if $\psi(\vec{x})$ is a solution of the Schrodinger equation with energy E , then $\psi(-\vec{x})$ is also a solution of the *same* Schrodinger equation and hence with the *same* energy E . This says that $\psi(\vec{x}) \pm \psi(-\vec{x})$ are also solutions of the same Schrodinger equation with the same energy E . Now

$$\psi(\vec{x}) + \psi(-\vec{x}) \rightarrow \text{even parity solution} \quad (11.87)$$

$$\psi(\vec{x}) - \psi(-\vec{x}) \rightarrow \text{odd parity solution} \quad (11.88)$$

This says that if $V(\vec{x}) = V(-\vec{x})$, then we can always choose solutions that have a definite parity (even or odd).

We formally define the *parity operator* by the relation

$$\langle \vec{x} | \hat{p} | \psi \rangle = \langle -\vec{x} | \psi \rangle \quad (11.89)$$

Since

$$\langle \vec{x} | \hat{p}^2 | \psi \rangle = \langle -\vec{x} | \hat{p} | \psi \rangle = \langle \vec{x} | \psi \rangle \quad (11.90)$$

we must have $\hat{p}^2 = \hat{I}$, which means the eigenvalues of \hat{p} are ± 1 as we indicated earlier.

We can show

$$[\hat{H}, \hat{p}] = 0 \quad (11.91)$$

for symmetric potentials by

$$\hat{p} \hat{H} |E\rangle = \hat{p} E |E\rangle = E \hat{p} |E\rangle = \pm E |E\rangle \quad (11.92)$$

$$\hat{H} \hat{p} |E\rangle = \pm \hat{H} |E\rangle = \pm E |E\rangle \quad (11.93)$$

$$\Rightarrow (\hat{p} \hat{H} - \hat{H} \hat{p}) |E\rangle = 0 \quad (11.94)$$

$$\Rightarrow [\hat{H}, \hat{p}] = 0 \quad (11.95)$$

since $|E\rangle$ is an arbitrary state. This commutator relationship says that \hat{H} and \hat{p} share a common set of eigenfunctions and that

$$\hat{H} \hat{p} = \hat{p} \hat{H} \quad (11.96)$$

$$\hat{p} \hat{H} \hat{p} = \hat{p}^2 \hat{H} = \hat{H} \quad (11.97)$$

$$\hat{p}^{-1} \hat{H} \hat{p} = \hat{H} \quad (11.98)$$

which means that \hat{H} is invariant under the \hat{p} transformation. We have used $\hat{p}^2 = \hat{I}$ in this derivation. It also says that

$$\hat{H} (\hat{p} |E\rangle) = \hat{p} (\hat{H} |E\rangle) = E (\hat{p} |E\rangle) \quad (11.99)$$

or $\hat{p} |E\rangle$ is an eigenstate of \hat{H} with energy E as we stated. The concept of parity invariance and the fact that \hat{H} and \hat{p} share a common set of eigenfunctions can greatly simplify the solution of the Schrodinger equation in many cases.

11.3 Tunneling through a Potential Barrier

We now change the potential energy function so that we have a barrier. The new potential energy function is shown in the figure below.

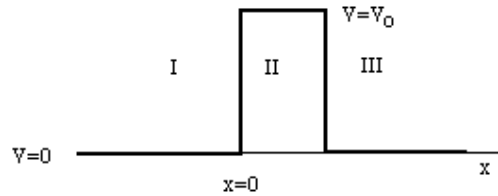


Figure 11.2: Square barrier potential energy function

The interesting physical case for quantum systems corresponds to when $E < V_0$.

In the classical case, there is no probability of the particle appearing on the right side of the barrier if it started out on the left side of the barrier. In order to appear on the right side of the barrier, the particle would some how have to pass through region II where

$$E < V_0 \rightarrow T = \frac{1}{2}mv^2 < 0 \quad (11.100)$$

Classically, the kinetic energy cannot be negative, which means there would have to be a violation of conservation of energy if the classical particle appeared on the right side of the barrier.

As we shall see, it turns out that a real traveling wave can appear on the other side of the barrier (even though it started on the left side and there are no sources of particles on the right side) in this case. This is called *quantum tunneling*. Let us see how it works.

We have three regions I, II and III to consider as shown in the figure. We get

three equations in the three regions

$$x \leq 0 \quad -\frac{\hbar^2}{2m} \frac{d^2\psi_I}{dx^2} = E\psi_I \quad (11.101)$$

$$\psi_I = A_1 e^{ikx} + B_1 e^{-ikx} \quad , \quad E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \quad , \quad k \text{ real} \quad (11.102)$$

$$0 \leq x \leq a \quad -\frac{\hbar^2}{2m} \frac{d^2\psi_{II}}{dx^2} + V_0 \psi_{II} = E\psi_{II} \quad (11.103)$$

$$\psi_{II} = C e^{\gamma x} + D e^{-\gamma x} \quad , \quad V_0 - E = \frac{\hbar^2 \gamma^2}{2m} \quad , \quad \gamma \text{ real} \quad (11.104)$$

$$x \geq a \quad -\frac{\hbar^2}{2m} \frac{d^2\psi_{III}}{dx^2} = E\psi_{III} \quad (11.105)$$

$$\psi_{III} = A_2 e^{ikx} + B_2 e^{-ikx} \quad , \quad E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \quad , \quad k \text{ real} \quad (11.106)$$

A term of the form $A_1 e^{ikx}$ corresponds physically to a particle traveling towards $+x$ (to the right) and a term of the form $B_1 e^{-ikx}$ corresponds physically to a particle traveling towards $-x$ (to the left).

If we set up the experiment so that there are particles moving towards $+x$ (on the left) at the start, then later we expect particles also to be traveling to towards $-x$ (on the left). Hence, we expect both coefficients A_1 and B_1 to be nonzero. On the other hand, there are no particle sources on the right and thus, the only way particles can be on the right is if they came from the left side and therefore must be traveling towards $+x$. We therefore assume that the coefficient $B_2 = 0$.

We have two sets of continuity equations (at $x = 0$ and $x = a$). At $x = 0$ we get

$$\psi_I(0) = \psi_{II}(0) \rightarrow A_1 + B_1 = C + D \quad (11.107)$$

$$\frac{d\psi_I(0)}{dx} = \frac{d\psi_{II}(0)}{dx} \rightarrow ik(A_1 - B_1) = \gamma(C - D) \quad (11.108)$$

and at $x = a$ we get

$$\psi_{II}(a) = \psi_{III}(a) \rightarrow C e^{\gamma a} + D e^{-\gamma a} = A_2 e^{ika} \quad (11.109)$$

$$\frac{d\psi_{II}(a)}{dx} = \frac{d\psi_{III}(a)}{dx} \rightarrow \gamma(C e^{\gamma a} - D e^{-\gamma a}) = ik A_2 e^{ika} \quad (11.110)$$

The reflection and transmission probabilities are given by

$$R = \frac{|B_1|^2}{|A_1|^2} \quad , \quad T = \frac{|A_2|^2}{|A_1|^2} \quad (11.111)$$

Algebra shows $R+T = 1$ as it must in order to conserve probability (or particles). Evaluating horrible algebra, we get the expression for T

$$T = \frac{1}{1 + \frac{V_0^2 \sinh^2 \gamma a}{4E(V_0 - E)}} \quad , \quad \gamma^2 = (V_0 - E) \frac{2m}{\hbar^2} \quad (11.112)$$

The fact that $T > 0$ for $E < V_0$ implies the existence of *tunneling*. The probability amplitude *leaks through the barrier*.

It is important to realize that the fact that $T > 0$ *DOES NOT* say that particles passed through the barrier.

No measurement can be done on the system that will allow us to observe a particle in the region $0 < x < a$ with $E < V_0$, since this would violate energy conservation.

It is *ONLY* probability that is leaking through.

If this causes the probability amplitude and hence the probability to be nonzero on the other side of the barrier, than it *must be possible for us to observe* the particle on the other side, i.e., we can observe the particle on the left side of the barrier with $E < V_0$ and later in time on the right side of the barrier with $E < V_0$, but we can never observe it in the region of the barrier with $E < V_0$. That is what is being said here. That is the way quantum mechanics works!

11.4 The Finite Square Well

We now consider the potential energy function

$$V(x) = \begin{cases} -V_0 & |x| \leq a/2 \\ 0 & |x| \geq a/2 \end{cases}$$

This is the so-called *finite square well* shown in the figure below.

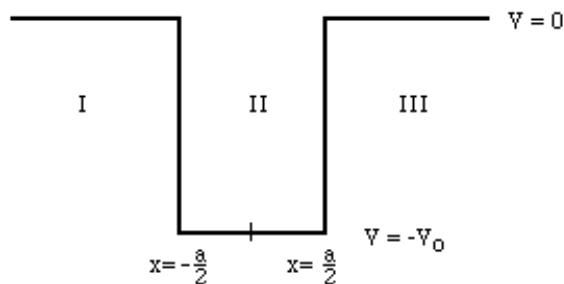


Figure 11.3: Finite square well potential energy function

The solutions are:

Region I:

$$x < -\frac{a}{2} \quad , \quad -\frac{\hbar^2}{2m} \frac{d^2\psi_I}{dx^2} = E\psi_I \quad (11.113)$$

$$0 \geq E \geq -V_0 \quad , \quad \hbar^2 k^2 = 2m|E| \quad , \quad E = -|E| \quad (11.114)$$

$$\psi_I(x) = Ae^{-kx} + Be^{kx} \quad (11.115)$$

Since $x = -\infty$ is included in this region, we must exclude the e^{-kx} term by choosing $A = 0$ (otherwise the wave function cannot be normalized), which gives

$$\psi_I(x) = Be^{kx} \quad x < -\frac{a}{2} \quad (11.116)$$

Region II:

$$\frac{a}{2} \geq x \geq -\frac{a}{2} \quad , \quad -\frac{\hbar^2}{2m} \frac{d^2\psi_{II}}{dx^2} - V_0\psi_{II} = E\psi_{II} \quad (11.117)$$

$$0 \geq E \geq -V_0 \quad , \quad \hbar^2 k^2 = 2m|E| \quad (11.118)$$

$$E = -|E| \quad , \quad p^2 = 2m(V_0 - |E|) \quad (11.119)$$

$$\psi_{II}(x) = Ce^{ipx/\hbar} + De^{-ipx/\hbar} \quad (11.120)$$

Region III:

$$x > \frac{a}{2} \quad , \quad -\frac{\hbar^2}{2m} \frac{d^2\psi_{III}}{dx^2} = E\psi_{III} \quad (11.121)$$

$$0 \geq E \geq -V_0 \quad , \quad \hbar^2 k^2 = 2m|E| \quad , \quad E = -|E| \quad (11.122)$$

$$\psi_{III}(x) = Fe^{kx} + Ge^{-kx} \quad (11.123)$$

Since $x = +\infty$ is included in this region, we must exclude the e^{kx} term by choosing $F = 0$ (otherwise the wave function cannot be normalized), which gives

$$\psi_{III}(x) = Ge^{-kx} \quad x > \frac{a}{2} \quad (11.124)$$

This represents a general solution to the problem. There seems to be 4 unknown constants, namely, B , C , D , and G . However, since $V(x) = V(-x)$, parity is conserved and we can choose even and odd solutions, or solutions of definite parity.

Even parity implies $\psi(x) = \psi(-x)$ or $G = B$ and $C = D$. This solution is

$$\psi_{even}(x) = \begin{cases} C \cos \frac{px}{\hbar} & |x| \leq a/2 \\ Be^{-kx} & x > a/2 \\ Be^{kx} & x < -a/2 \end{cases} \quad (11.125)$$

Odd parity implies $\psi(x) = -\psi(-x)$ or $G = -B$ and $D = -C$. This solution is

$$\psi_{odd}(x) = \begin{cases} C \sin \frac{px}{\hbar} & |x| \leq a/2 \\ Be^{-kx} & x > a/2 \\ -Be^{kx} & x < -a/2 \end{cases} \quad (11.126)$$

Thus, by using parity we reduce the number of unknowns in the problem to two for each type of solution. We now impose the continuity conditions of the wave function and its derivative only at $x = a/2$ for both solutions. Since these are definite parity solutions the continuity condition at $x = -a/2$ will give no new information and is not needed.

Even Parity

$$A \cos \frac{pa}{2\hbar} = C e^{-\frac{ka}{2}} \quad , \quad -\frac{p}{\hbar} A \sin \frac{pa}{2\hbar} = -k C e^{-\frac{ka}{2}} \quad (11.127)$$

$$\frac{C}{A} = e^{\frac{ka}{2}} \cos \frac{pa}{2\hbar} = \frac{p}{\hbar k} e^{\frac{ka}{2}} \sin \frac{pa}{2\hbar} \quad (11.128)$$

$$p \tan \frac{pa}{2\hbar} = \hbar k \quad (11.129)$$

This last equation is a *transcendental equation* for k and its solutions determine the allowed E values for the even parity states for this potential energy function. These E values are the even parity energies or energy levels of a particle in the finite square well potential.

Odd Parity

$$A \sin \frac{pa}{2\hbar} = C e^{-\frac{ka}{2}} \quad , \quad \frac{p}{\hbar} A \cos \frac{pa}{2\hbar} = -k C e^{-\frac{ka}{2}} \quad (11.130)$$

$$\frac{C}{A} = e^{\frac{ka}{2}} \sin \frac{pa}{2\hbar} = -\frac{p}{\hbar k} e^{\frac{ka}{2}} \cos \frac{pa}{2\hbar} \quad (11.131)$$

$$p \cot \frac{pa}{2\hbar} = -\hbar k \quad (11.132)$$

Again, this last equation is a transcendental equation for k and its solutions determine the allowed E values for the odd parity states for this potential energy function. These E values are the odd parity energies or energy levels of a particle in the finite square well potential.

In general, at this stage of the solution, we must either devise a clever numerical or graphical trick to find the solutions of the transcendental equations or resort to a computer.

The first thing one should always do is change variables to get rid of as many extraneous constants as possible. In this case we let

$$\beta = ka = \frac{a}{\hbar} \sqrt{2m|E|} \quad , \quad \alpha = \gamma a = \frac{p}{\hbar} a = \frac{a}{\hbar} \sqrt{2m(V_0 - |E|)} \quad (11.133)$$

The first useful equation we can derive is

$$\alpha^2 + \beta^2 = \frac{2mV_0a^2}{\hbar^2} \quad (11.134)$$

which is a constant for a given well. This is the equation of a circle or radius

$$\sqrt{\frac{2mV_0a^2}{\hbar^2}} \quad (11.135)$$

With these new variables the two transcendental equations are

$$\beta = \alpha \tan \frac{\alpha}{2} \text{ even parity} \quad , \quad \beta = -\alpha \cot \frac{\alpha}{2} \text{ odd parity} \quad (11.136)$$

We can find solutions graphically by plotting as shown below for the case (effectively a choice of the quantity $V_0 a^2$)

$$\text{circle radius} = \sqrt{\frac{2mV_0 a^2}{\hbar^2}} = \frac{5\pi}{2} \quad (11.137)$$

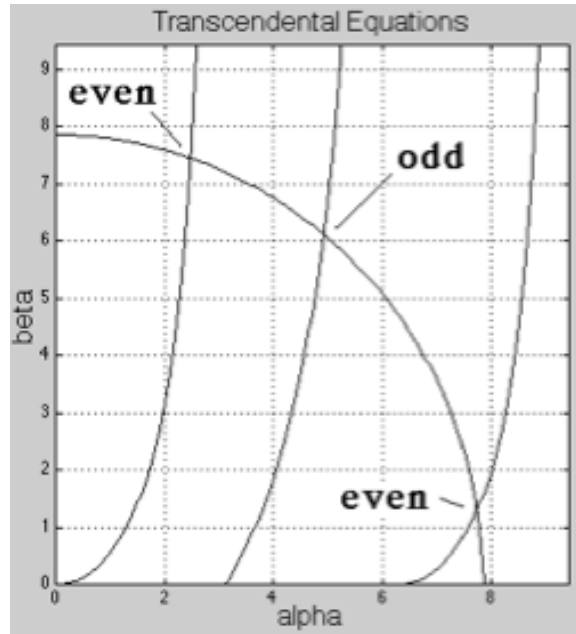


Figure 11.4: Graphical solution for finite square well energies

The solutions correspond to the intersections of the circle (fixed for a given well) and the curves represented by the two transcendental equations. It is shown in the figure.

For the choice of potential well shown in the figure we have 2 even parity solutions and 1 odd parity solution. These correspond to the allowed energy levels for this particular well and the corresponding wave functions and energies represent bound states of the well.

We can also do a straight numerical solution for even parity by rearranging the

equations as follows:

$$\alpha^2 + \beta^2 = \frac{2mV_0a^2}{\hbar^2} \quad , \quad \beta = \alpha \tan \frac{\alpha}{2} \quad (11.138)$$

$$\alpha^2 \left(1 + \tan^2 \frac{\alpha}{2}\right) = \frac{\alpha^2}{\cos^2 \frac{\alpha}{2}} = \frac{2mV_0a^2}{\hbar^2} \quad (11.139)$$

$$\alpha^2 - \frac{2mV_0a^2}{\hbar^2} \cos^2 \frac{\alpha}{2} = 0 \quad (11.140)$$

For the case

$$\sqrt{\frac{2mV_0a^2}{\hbar^2}} = \frac{5\pi}{2} \quad (11.141)$$

we have

$$\alpha^2 - \frac{25\pi^2}{4} \cos^2 \frac{\alpha}{2} = f(\alpha) = 0 \quad (11.142)$$

The numerical solution of this equation can be carried out by any standard technique (Newton-Raphson method, for instance) for finding the zeros of the function $f(\alpha)$. For this case we get

$$\alpha = 2.4950 \quad , \quad 7.1416 \quad (11.143)$$

which is clearly in agreement with the graphical result.

11.5 Delta-Function Potentials

We now consider the potential energy function

$$V(x) = A\delta(x - a) \quad (11.144)$$

where

$$\delta(x - a) = 0 \quad x \neq a \quad (11.145)$$

$$\int_{-\infty}^{\infty} f(x)\delta(x - a)dx = f(a) \quad (11.146)$$

and solve the corresponding Schrodinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \quad (11.147)$$

As we discussed earlier the wave function $\psi(x)$ is assumed to be continuous for physical reasons relating to the probability interpretation. The derivative of the wave function, however, is not continuous at $x = a$ for this potential. We can see this as follows. We have

$$-\frac{\hbar^2}{2m} \int_{a-\varepsilon}^{a+\varepsilon} \frac{d^2\psi}{dx^2} dx + A \int_{a-\varepsilon}^{a+\varepsilon} \delta(x - a)V(x)\psi(x)dx = E \int_{a-\varepsilon}^{a+\varepsilon} \psi(x)dx \quad (11.148)$$

In the limit $\varepsilon \rightarrow 0$, using the continuity of $\psi(x)$, we get

$$-\frac{\hbar^2}{2m} \left[\left. \frac{d\psi}{dx} \right|_{a+\varepsilon} - \left. \frac{d\psi}{dx} \right|_{a-\varepsilon} \right] = E\psi(a) \int_{a-\varepsilon}^{a+\varepsilon} dx - A\psi(a) \quad (11.149)$$

$$\text{discontinuity} \left(\frac{d\psi}{dx} \right)_{x=a} = \Delta \left(\frac{d\psi}{dx} \right) = \frac{2mA}{\hbar^2} \psi(a) \quad (11.150)$$

For simplicity we choose $a = 0$. We have two regions to consider

$$\text{region I } x < 0 \quad , \quad \text{region II } x > 0 \quad (11.151)$$

and the derivative is discontinuous at $x = 0$.

Transmission Problem

We first carry out the calculation of the transmission and reflection probabilities. We assume that $V > 0$ (we have a delta function barrier), $E > 0$ and an incident wave of unit intensity coming in from the left.

In region I we have

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_I}{dx^2} = E\psi_I \rightarrow \psi_I(x) = e^{ikx} + Be^{-ikx} \quad , \quad E = \frac{\hbar^2 k^2}{2m} > 0 \quad (11.152)$$

We have *both* an incident and a reflected wave.

In region II we have

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_{II}}{dx^2} = E\psi_{II} \rightarrow \psi_{II}(x) = Ce^{ikx} \quad , \quad E = \frac{\hbar^2 k^2}{2m} > 0 \quad (11.153)$$

There is *only* a transmitted wave.

The boundary conditions (at $x = 0$) give

$$\psi_I(0) = \psi_{II}(0) \rightarrow 1 + B = C \quad (11.154)$$

$$\frac{d\psi_{II}(0)}{dx} - \frac{d\psi_I(0)}{dx} = \frac{2mA}{\hbar^2} \psi_{II}(0) \rightarrow ikC - ik(1 + B) = \frac{2mA}{\hbar^2} C \quad (11.155)$$

The solutions are

$$C = \frac{ik}{ik - \frac{mA}{\hbar^2}} \quad , \quad B = \frac{\frac{mA}{\hbar^2}}{ik - \frac{mA}{\hbar^2}} \quad (11.156)$$

We then have

$$T = \text{transmission probability} = |C|^2 = \frac{1}{1 + \frac{mA^2}{2\hbar^2 E}} \quad (11.157)$$

and

$$R = \text{reflection probability} = |B|^2 = \frac{1}{1 + \frac{2\hbar^2 E}{mA^2}} \quad (11.158)$$

We note that $R + T = 1$ as it must for the probability interpretation to make sense.

It turns out that the energy values of the poles (zeros of the denominator) of the transmission probability correspond to the bound state energies for the delta function well problem ($A < 0$), i.e., for the single delta function potential, T has a pole at

$$E = -\frac{mA^2}{2\hbar^2} \quad (11.159)$$

Bound-State Problem

We let $A \rightarrow -A$, $A > 0$. In region I we have

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_I}{dx^2} = -|E|\psi_I \rightarrow \psi_I(x) = Be^{\alpha x} \quad , \quad E = -|E| = -\frac{\hbar^2\alpha^2}{2m} < 0 \quad (11.160)$$

We have excluded the negative exponential term since it would diverge in region I as $x \rightarrow -\infty$.

In region II we have

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_{II}}{dx^2} = -|E|\psi_{II} \rightarrow \psi_{II}(x) = Ce^{-\alpha x} \quad , \quad E = -|E| = -\frac{\hbar^2\alpha^2}{2m} < 0 \quad (11.161)$$

We have excluded the positive exponential term since it would diverge in region II as $x \rightarrow +\infty$.

The boundary conditions give

$$\psi_I(0) = \psi_{II}(0) \rightarrow B = C \quad (11.162)$$

$$\frac{d\psi_{II}(0)}{dx} - \frac{d\psi_I(0)}{dx} = -\frac{2mA}{\hbar^2}\psi_I(0) \rightarrow -\alpha C - \alpha B = -\frac{2mA}{\hbar^2}B \quad (11.163)$$

The resulting equation for α gives the allowed the bound state energies. We have

$$\alpha = \frac{mA}{\hbar^2} \rightarrow \text{only 1 solution only} \rightarrow 1 \text{ bound state} \quad (11.164)$$

$$E = -|E| = -\frac{\hbar^2\alpha^2}{2m} = -\frac{mA^2}{2\hbar^2} \quad (11.165)$$

which is the *same* value as we obtained from the pole of the transmission probability.

We also note that the solution has definite parity (even) since $\psi(x) = \psi(-x)$. This must occur since $V(x) = V(-x)$ and hence parity commutes with the Hamiltonian. As we also saw in the square well case, if only one solution exists then it is always an even parity solution.

Chapter 12

Uncertainty

The Heisenberg Uncertainty Principle lies at the center of quantum theory - in some senses guaranteeing the consistency of our view of the microscopic world. Yet there is a puzzle with Heisenberg's discovery: is it a statement of epistemological limitations (what we can measure about the world) or an ontological limit written into the world itself?

12.1 Expectation is Not Enough

If we take a collection of quantum objects, all of which are in the same state $|\phi\rangle$ and measure the value of a given physical property for each of them (call it O), then we will get a collection of values $\{o_i\}$. We will find the average value of all these measurements will be equal to the expectation value of the operator \hat{O} associated with the property O in this state.

The expectation value, however, does not tell the whole story. We also need to know how widely spaced the range of values are. In one instance the collection $\{o_i\}$ could all be very close to the average value and in another, some of the measurements might produce values considerably different from the average, not because of some experimental mistake, just due to the nature of the state.

Whenever physicists think about a perfect set of experimental values, they dream of something called the normal distribution curve, as shown in the figure below.

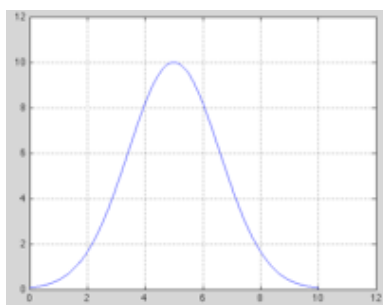


Figure 12.1: Normal distribution

In this case we are supposed to imagine that the figure represents the results of identical measurements made on a collection of objects. We are not just talking about quantum systems being measured here. The normal distribution applies to the experimental results found in classical physics as well, although for different physical reasons.

The x -axis tells us the values of the results obtained and the y -axis the number of times that value turned up. As we can see in this case, the result 5 was obtained 10 times. Also, as seems evident, the average value over all readings was 5. However, there were quite a few times when a value significantly different from 5 was obtained.

Now consider the figure below.

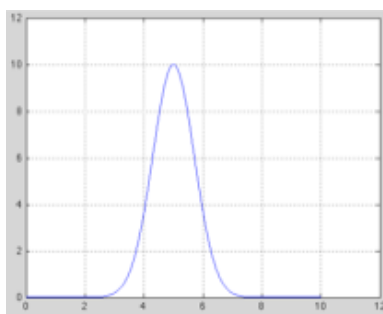


Figure 12.2: Normal distribution - narrower spread of values

Here we have a normal distribution curve, but with a much narrower spread of values (peak value still 5, average value still 5). On this curve a much higher proportion of the results are closer to the average than before.

To tell the full story of a set of measurement results, we need more than simply the average. Conventionally, we deal with the width of the distribution as well.

This has a technical definition in statistics, but we do not have to worry about that. Suffice to say the width is obtained by taking each value, working how far it is from the average in some manner and then averaging the results.

Mathematicians call this the standard deviation, but to be consistent with quantum theory, we will use the term uncertainty. See the figure below.

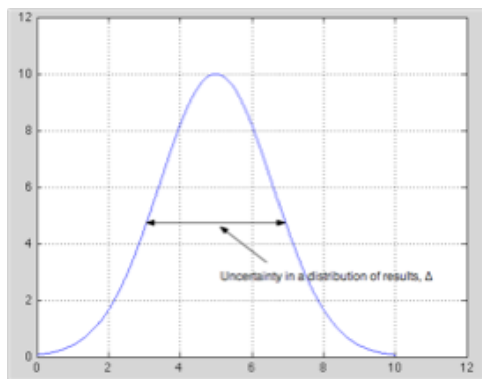


Figure 12.3: Normal distribution - standard deviation or uncertainty

In classical physics, the width, spread, or uncertainty in a set of experimental results is generally attributable to the normal experimental variations one finds, due to small differences in the objects being tested. Alternatively, they can be attributed to variations in the apparatus used or environmental factors.

Experiments in quantum physics suffer from all the same sort of variations, but in addition we have to face what happens when the objects being tested are not in eigenstates of the variables being measured. Taking position as an example, once again, we can start with a state $|\phi\rangle$ given by

$$|\phi\rangle = \int \phi(x) |x\rangle dx \quad (12.1)$$

in which case making position measurements on a set of particles in this state we will find a range of values, with each possible x value occurring according to the probability

$$\phi^*(x)\phi(x) = |\phi(x)|^2 \quad (12.2)$$

Plotting the results and the number of time that we find each value will then produce a curve, on the same lines as that in the last figure, with a corresponding width or uncertainty Δx . In other words, the measurement distribution will draw out $|\phi(x)|^2$ for us.

The uncertainty then becomes a direct measure of the range of x values over which the amplitude, or state function, $\phi(x)$ is significant - meaning the range of x values that are highly likely to occur when you make a measurement.

Just as there is a formula in quantum theory to calculate the expectation value, so a similar calculation will yield the uncertainty.

$$\langle \phi | \hat{x} | \phi \rangle = \langle x \rangle = \int \phi^*(x) x \phi(x) dx \quad \text{expectation value} \quad (12.3)$$

$$\Delta x = \sqrt{\int \phi^*(x) x^2 \phi(x) dx - \left(\int \phi^*(x) x \phi(x) dx \right)^2} \quad \text{uncertainty} \quad (12.4)$$

You're right to think that the second formula is rather messy; I've presented it here to show that Δx is as much a property of the state as $\langle x \rangle$ is.

Of course, the same state could equally well be expanded over a momentum basis $|p_x\rangle$, and the experimental results of momentum measurements also plotted to reveal the uncertainty in this variable Δp_x .

What about in the case of an eigenstate? Well, if we happen to start with such a state then we can predict with absolute certainty what the result of a measurement of that variable will be. A plot of the results will then show no width (aside from fluctuations that you can't avoid in experiments), giving $\Delta p_x = 0$. However, there is a catch. As we have already said, a momentum eigenstate cannot also be a position eigenstate and vice versa. When you expand a momentum eigenstate over a position basis you have to take, in principle, an infinite number of possible positions, leading to $\Delta x = \infty$. So, it would appear that if $\Delta p_x = 0$, then $\Delta x = \infty$.

12.2 Heisenberg's Principle

All this is very good, but what about those states (surely in the majority) that are neither position nor momentum eigenstates? Well, given such a state $|\phi\rangle$ we can have

$$|\phi\rangle = \int \phi(x) |x\rangle dx \Rightarrow \langle x \rangle, \Delta x \quad (12.5)$$

$$|\phi\rangle = \int \psi(p_x) |p_x\rangle dp_x \Rightarrow \langle p_x \rangle, \Delta p_x \quad (12.6)$$

i.e., the position representation yielding an expectation value $\langle x \rangle$ and uncertainty Δx and the momentum representation yielding an expectation value $\langle p_x \rangle$ and uncertainty Δp_x . Things do not stop there though; as it's the same state being expanded in both representations there is a connection between Δx and Δp_x . This connection was first demonstrated by Heisenberg and is now named after him.

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$$\Delta x \Delta p_x \geq \frac{\hbar}{2} \quad (12.7)$$

For a given state, the smaller the range of probable x values involved in a position expansion, the larger the range of p_x values involved in a momentum expansion, and vice versa.

The key part of this expression is the \geq sign, which is telling us that the product $\Delta x \Delta p_x$ cannot be less than $\hbar/2$. In some situations, the measurement results might be such that $\Delta x \Delta p_x$ is much greater than $\hbar/2$, which is fine; but you can never find a situation where $\Delta x \Delta p_x$ is less than $\hbar/2$. Quantum theory places a limit on how precise our two sets of measurements can be.

Putting it in a different way: Δx is telling us the range of x values over which $\phi(x)$ is significantly large, if we expand the state over a position basis, and Δp_x the corresponding range of $\Psi(p_x)$, if you expand the same state over a momentum basis. The uncertainty principle is relating the range of $\phi(x)$ to that of $\Psi(p_x)$. If you choose to make a position measurement you will most likely get a value within Δx of the expectation value $\langle x \rangle$. If you make a momentum measurement *instead* (not after), then you will most likely get a value within Δp_x of $\langle p_x \rangle$.

That last statement is important. If you make a position measurement, then you will collapse the state into something close to a position eigenstate, which needs a different momentum expansion than the original state. The uncertainty principle relates Δx and Δp_x for the same state.

You may immediately be having some questions about this principle. What about an object that is not moving? Is it not sitting perfectly still (precise momentum, zero) at a precise spot? Well, putting to one side the notion that nothing can be perfectly still (we are after all orbiting the sun), the immediate point is that the uncertainty principle *prevents* such a state from happening in the microworld.

So What?

People were not afraid of drawing philosophical conclusions from the uncertainty principle, almost from the moment the paper was published. Heisenberg himself launched one of the earliest efforts, his target being the *principle of causality*.

Classical physics leads quite naturally to the view that a sufficiently powerful computer, fed with detailed information about the positions, momenta, and forces at work on every particle in the universe, could subsequently predict as accurately as you want the future of the universe. Such thinking easily leads one to doubt such things as free will, the human mind, morality, and pretty

much the whole ball game in the end. Heisenberg's attack on this rather bleak view was quite simple. The uncertainty principle prevents one from knowing both the position and the momentum of any particle with sufficient accuracy, rendering prediction impossible.

Causality, the notion that everything that happens has been caused by something happening previously, has been central to physics for hundreds of years. Experiments in the quantum world started to undermine this thinking with their apparently unpredictable outcomes (earlier discussions) and then came the uncertainty principle undermining the basis of physics: our ability to measure. To the physicist this was outrageous. Nature seemed to be built on a set of principles completely contrary to the approach that had served science well for generations. It was almost like a betrayal.

Actually the more modern theory of chaos deals a more significant blow to our predicting computer. It would be possible to regard the quantum challenge as being mounted in the world of the small, of no relevance to the big world in which we live. However, the study of chaotic systems has shown us that small effects do not necessarily lead to small consequences and that no measurement (quantum or otherwise) can, even in principle, yield sufficiently accurate results to do the job.

Putting aside all the philosophical debate, the uncertainty principle can still be quite alarming when you first come across it as a physicist. Our basic education points to the vital role that measurement and precision take in science. A measurement has to be a faithful rendering of what is really out there, or there is no point in the exercise. Realism to me is the natural state of a physicist; it is only when you run into quantum physics that you begin to doubt these instincts (surely it cannot *really* be like that).

I'm Not Sure What Uncertainty Means...

There is a serious point here. Many paragraphs of text have been written about the meaning and significance of the uncertainty principle. As you might expect, it all depends on what side of the realist/instrumentalist divide you stand and on exactly what shade of interpretation you favor. However, to my mind the most important aspect of the uncertainty principle, from a philosophical point of view, is whether you take it to be a limitation on what we can know about the world or an inherent limitation in the world. In philosophical speak, is it an epistemological statement, or is it ontological?

Whatever Heisenberg may have thought, one of the first arguments that he used to demonstrate the uncertainty principle had an epistemological tinge. This is the famous *gamma ray microscope*.

Heisenberg envisaged a microscope constructed to use gamma rays rather than

light waves. Such a microscope could be used to determine the position of something as small as an electron by detecting the gamma rays that have scattered off it. The path of the rays would help pinpoint its location. The snag is the wavelength of the gamma rays.

As is well known in optics, there is a limitation on the detail that can be seen by a microscope. This limitation depends on the wavelength of the waves being used. To view a level of detail sufficient to locate something as small as an electron, quite high-energy gamma rays (very short wavelength) are needed. Such a gamma ray scattering off an electron would be bound to transfer a significant amount of energy. This would cause the electron to recoil in an unspecified direction, hence affecting its momentum. There would be no way of determining the energy transferred and the subsequent disturbance in the electron's momentum. If you wanted to do that, you would have to measure the gamma ray before it hit and that process would be bound to disturb the gamma ray.

The key point is this: the gamma ray microscope argument assumes that the electron *has* a position and a momentum; the problem is that the interaction with the measuring device means we cannot accurately *determine* what these quantities are.

Every time a measuring device makes a measurement it must interact with the thing it is measuring. In classical physics the scale of these interactions is either too small to worry us or can be calculated and accounted for in a sensible way. That cannot be said in quantum physics. The scale of the interaction is too great and causes profound changes to the properties of the object being measured. Also the interaction is inherently unpredictable. Any attempt to stick another measuring device in to judge the scale of the interaction will not work as the second instrument will itself have to interact in a manner that cannot be detected. An infinite regression follows, which like most infinite regressions gets us nowhere.

This is an important argument, as it cuts once again to the nature of a quantum state. If an electron happens to be in an eigenstate of position (or momentum) we can say with certainty what the result of measuring that position (momentum) will be. If the electron is not in eigenstate then what can we say? We can predict various values that might be revealed by a measurement, and their relative probabilities, but what does that tell us? What is the position (or momentum) of an electron in this situation?

If you take the view that states refer to collections of objects, rather than individuals, then the way forward is quite clear. Inside this collection, the electrons must be identical with one another, within the limitations laid down by the nature of the quantum state. However, there could be *hidden variables* - variables we do not know yet how to measure - which take different values in the collection. When a measurement is made, these variables determine the outcome, but

because we do not know what they are it all looks random to us. The electrons have perfectly well-determined positions and momenta, but we cannot know in advance what they will be as we cannot access the physics that determines the values.

Of course, the gamma ray microscope example runs contrary to this way of thinking. That argument is clearly dealing with single electrons, not collections. However, it does assume that positions and momenta are really there, just partially hidden from us.

Such a *hidden variable* type view would have the uncertainty principle as expressing the *epistemological limits* of current science. Heisenberg himself took the view that the uncertainty principle was an *ontological* thing, at least in his later writings.

To him the uncertainty principle expressed the limits to which classical *ideas* of momentum, or position, can be applied in a given situation. This harks back to our earlier argument about how the classical definition of momentum cannot be applied in quantum physics. If we take this view, then we have to say that an object that is not in an eigenstate of position simply *does not have a position*. The concept has no meaning in such a state. Heisenberg would have said that the position of the particle was *latent* or a potential property. When a measurement takes place, this latency becomes an actuality and our classical ways of thinking can now be applied.

This is very much a realistic view but acknowledges that our assumptions about what should be classified as real may have to be enlarged. To Heisenberg latent properties should be given some points for being real.

The gamma ray microscope was used by Heisenberg as a way of introducing the uncertainty principle. However, he held back from stating that it was an ontologically valid description of what would actually happen.

Yet More Uncertainty

I have tried to show how the uncertainty principle arises as a natural consequence of our ability to expand a state in various bases. Although I have illustrated this with position and momentum, there are clearly lots of other physical variables with basis sets that we can expand a state over. Unless position and momentum have some special significance, there must be versions of the uncertainty principle that apply to other physical variables as well.

The basic rule is this: if you choose to expand a state over a pair of bases, and the physical variables involved happen to be conjugate variables, then you are going to end up with an uncertainty principle. A state cannot be an eigenstate of two conjugate variables at the same time, in which you cannot get a definite

value from measuring either variable, and an uncertainty relationship must apply.

Non-Compatibility

If an operator acts on an eigenstate, the result is that the state remains the same, but is now multiplied by the eigenvalue.

$$\hat{p}|p_1\rangle = p_1|p_1\rangle \quad , \quad \hat{x}|x_1\rangle = x_1|x_1\rangle \quad (12.8)$$

If the state is not an eigenstate, then funny things happen instead.

Now, let's consider two physical variables represented by operators \hat{O}_1 and \hat{O}_2 , which happen to be compatible. Then the state $|\phi\rangle$ can be an eigenstate of both. What happens when we use both operators on the state, one after the other?

$$\hat{O}_1|\phi\rangle = o_1|\phi\rangle \quad (12.9)$$

$$\hat{O}_2 o_1|\phi\rangle = o_1 \hat{O}_2|\phi\rangle = o_1 o_2|\phi\rangle \quad (12.10)$$

Equallywell, we could do things the other way around

$$\hat{O}_2|\phi\rangle = o_2|\phi\rangle \quad (12.11)$$

$$\hat{O}_1 o_2|\phi\rangle = o_2 \hat{O}_1|\phi\rangle = o_2 o_1|\phi\rangle \quad (12.12)$$

which says that

$$\hat{O}_2 \hat{O}_1|\phi\rangle = \hat{O}_1 \hat{O}_2|\phi\rangle \quad (12.13)$$

or

$$[\hat{O}_2 \hat{O}_1 - \hat{O}_1 \hat{O}_2]|\phi\rangle = 0 \quad (12.14)$$

The bracket is regarded as being so important in quantum theory that it is given its own name:

THE COMMUTATOR

$$Commutator(\hat{O}_2, \hat{O}_1) = [\hat{O}_2, \hat{O}_1] = [\hat{O}_2 \hat{O}_1 - \hat{O}_1 \hat{O}_2] \quad (12.15)$$

If two operator *commute*, then $[\hat{O}_2, \hat{O}_1] = 0$, and they *can* (not must) have simultaneous eigenstates. If they don't commute, simultaneous eigenstates are not possible and an uncertainty relationship follows.

RULE 9:

Non-compatible physical variables are represented by operators that do not commute and so have to be linked by an uncertainty principle.

$$\Delta O_1 \Delta O_2 \geq \frac{1}{2} \langle i [\hat{O}_2, \hat{O}_1] \rangle \quad (12.16)$$

Time Again....

There is another uncertainty relationship that does not follow directly from these arguments, namely,

ENERGY/TIME UNCERTAINTY

$$\Delta E \Delta \tau \geq \frac{\hbar}{2} \quad (12.17)$$

where τ is related to the characteristic development time of the system, i.e., it is given by

$$\tau = \frac{\langle A \rangle}{d\langle A \rangle/dt} \quad (12.18)$$

for any physical variable of the system. Let us see how this works.

Rule 7 states the link between operators and the measurement of physical variables. We have seen several examples of such operators and learned how they are used to calculate expectation values.

However, where things start to go weird is over the \hat{t} operator. After all, you can measure position, momentum, energy, etc, but how do you measure time?

Let us be clear about this: you can measure a *duration* (e.g., with a stopwatch) but what physical measurement tells you the actual *time*?

The issues involved here are very subtle, and not every quantum mechanic would agree with what I am about to say, but here goes.

The drama of conventional quantum mechanics is acted out on a stage formed from three directions in space and one universal time (x, y, z, t) . Think of the space arena as a giant spider's web; with the threads so closely woven the web appears to be a continuous disk. The spider is able to crawl around and so occupies a position at any moment on the web. The position of the spider is a physical variable - a property of the spider's state that can be measured. In quantum mechanics, the position would be represented by an operator \hat{x} . In some accounts, the position operator is denoted as \hat{q} to make it clear that this is not the same as the x -value, which is *part of the web*, not part of the *spider's state*.

Time is evidently rather different from this. If we can picture it at all, we think of it as a line stretching out to infinity in both directions. The spider on this line would not be stationary, but sliding along this line as time passes. In most instances we cannot conceive of an experiment that would enable us to *measure* the spider's position on the time line. Time itself is not a property of the spider's state; hence there is no time operator.

But what of a system that is changing with time, a falling ball, for example? Here the momentum of the ball increases as time passes, suggesting that it is a “time variable”. However, in this case, the physical variable that is changing does not change at a uniform rate (the momentum increases at an increasing rate), and in any case when it hits the ground, time as measured by the momentum would stop, although t continues.

Of course, there are some systems in which a physical variable corresponds in a more satisfactory way with the passage of time. We tend to call them clocks. The second hand of an analog clock has an angular position θ , which changes with time. Measuring this angle gives us a measure of time for that system. In any real clock there will also be an energy, which will tend to depend on θ so that we can define an energy operator \hat{E} and a time operator $\hat{\theta}$, which will not commute and so lead to an uncertainty relationship. However, θ is only a physical variable of that clock and so cannot be applied as a *time operator* to any other system.

Energy/Time Uncertainty

Let us ask the question: how can we tell if something has changed?

A physical system will have various properties that can be measured. If we suspect that something has happened to change the system’s state, we’ll have to go through a new set of measurements to see what’s going on. How do we do this in quantum physics? Every measurement we make will collapse the state into an eigenstate, so we can’t necessarily repeat measurements of the same state. If we do lots of measurements on a collection of identical systems in the same state, how do we tell if the values we are getting are different because of some change affecting all systems in the collection, or it is just the normal spread of measurements that come with a state that is not an eigenstate to begin with?

In a nutshell, we are trying to distinguish between a range of values caused by the inherent uncertainty in the state itself and a range caused by some causal evolution ($\hat{U}(t)$) taking place in the systems.

The way to tell this is to compare the expectation value $\langle O \rangle$ with the uncertainty ΔO . If we do a remeasure on a collection of systems and see that the difference between the new expectation value $\langle O' \rangle$ and the old one is greater than ΔO (i.e., $(\langle O' \rangle - \langle O \rangle) \geq \Delta O$), then we can be quite sure that the system’s state has changed. It then becomes a question of how long we have to leave a system to evolve, in a given situation, before the change can be appreciated in this manner.

We can work this out if we employ the rate of change with time operator, ∇_t . In elementary physics, the distance traveled by a moving object is the rate at which it is traveling (speed) multiplied by the time it travels for ($d = s \times t$).

Equally, if we know the rate at which any quantity is changing and multiply by the time period, we will produce the amount by which the quantity has changed in that time. If the quantity happens to be an expectation value then $\nabla_t \langle O \rangle \Delta t$ is the amount by which the expectation value has changed in the *time duration* Δt . Our condition for a measurable change then becomes

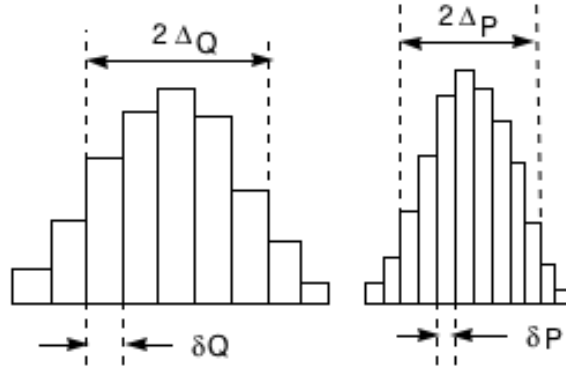
$$\nabla_t \langle O \rangle \Delta t \geq \Delta O \quad \text{or} \quad \Delta t \geq \frac{\Delta O}{\nabla_t \langle O \rangle} \quad (12.19)$$

Although we do not quite have all the theory needed to close the loop yet, this is how we should interpret the Δt in the energy-time uncertainty relationship. It represents the duration of time that you have to wait to be sure that the energy has changed by an amount at least equal to ΔE .

The Meaning of the Indeterminacy Relations

What is the significance of indeterminacy relations in the world of experimental physics?

Consider the experimental results shown below:



These are frequency distributions for the results of independent measurements of Q and P on an ensemble of similarly prepared systems, i.e., on each of a large number of similarly prepared systems one performs a single measurement (either Q or P). The histograms are the statistical distribution of the results.

The standard deviations (variances) as shown must satisfy (according to the theory) the relation

$$\Delta_Q \Delta_P \geq \frac{\hbar}{2}$$

They must be distinguished from the resolution of the individual measurements, δQ and δP .

Let me emphasize these points:

- (1) The quantities Δ_Q and Δ_P are *not* errors of measurement. The *errors* or preferably the *resolutions* of the Q and P measuring instruments are δQ and δP . They are logically unrelated to Δ_Q and Δ_P and to the uncertainty relations except for the practical requirement that if

$$\delta Q > \Delta_Q \quad (\text{or } \delta P > \Delta_P)$$

then it will not be possible to determine Δ_Q (or Δ_P) in the experiment and the experiment cannot test the uncertainty relation.

- (2) The experimental test of the indeterminacy relation *does not* involve simultaneous measurements of Q and P , but rather it involves the measurement of one or the other of these dynamical variables on each independently prepared representative of the particular state being studied.

Why am I being so picky here?

The quantities Δ_Q and Δ_P as defined here are often misinterpreted as the errors of individual measurements. This probably arises because Heisenberg's original paper on this subject, published in 1927, was based on an early version of quantum mechanics that predates the systematic formulation and statistical interpretation of quantum mechanics as it exists now. The derivation, as carried out here was not possible in 1927!

Final Thoughts

We have now reached a critical point in our development of quantum theory. We have discussed all the theoretical ideas needed. Hopefully, you now have a reasonable understanding of states, wave functions, amplitudes, operators, and the general machinery of how quantum theory works.

We now proceed to tackle some of the more philosophical aspects such as what quantum theory might actually mean.

Before proceeding, however, let us do a couple of interesting derivations.

The following topics are for the more mathematically inclined students.

12.3 Derivation of the Uncertainty Relations in General

Given two Hermitian operators \hat{A} and \hat{B} and a state vector $|\psi\rangle$, we define the two new operators

$$\hat{D}_A = \hat{A} - \langle \hat{A} \rangle \quad , \quad \hat{D}_B = \hat{B} - \langle \hat{B} \rangle \quad (12.20)$$

where $\langle \dots \rangle$ equals the average or expectation value in the state $|\psi\rangle$.

In the statistical analysis of data, we use a quantity called the standard or mean-square deviation as a measure of the uncertainty of an observed quantity. It is defined, for a set of N measurements of the quantity q by

$$\begin{aligned} (\Delta q)^2 &= (\text{standard deviation})^2 = \frac{1}{N} \sum_{i=1}^N (q_i - q_{\text{average}})^2 \\ &= \frac{1}{N} \sum_{i=1}^N (q_i)^2 - \frac{1}{N} \sum_{i=1}^N (q_i q_{\text{average}}) - \frac{1}{N} \sum_{i=1}^N (q_{\text{average}} q_i) + \frac{1}{N} \sum_{i=1}^N (q_{\text{average}})^2 \\ &= (q^2)_{\text{average}} - (q_{\text{average}})^2 \end{aligned} \quad (12.21)$$

where we have used

$$q_{\text{average}} = \frac{1}{N} \sum_{i=1}^N q_i \quad (12.22)$$

In analogy, we define the mean-square deviations for \hat{A} and \hat{B} as

$$(\Delta \hat{A})^2 = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2 = \langle (\hat{A} - \langle \hat{A} \rangle)^2 \rangle = \langle \hat{D}_A^2 \rangle \quad (12.23)$$

$$(\Delta \hat{B})^2 = \langle \hat{B}^2 \rangle - \langle \hat{B} \rangle^2 = \langle (\hat{B} - \langle \hat{B} \rangle)^2 \rangle = \langle \hat{D}_B^2 \rangle \quad (12.24)$$

We then have

$$(\Delta \hat{A})^2 (\Delta \hat{B})^2 = \langle \hat{D}_A^2 \rangle \langle \hat{D}_B^2 \rangle \quad (12.25)$$

Now we assume that

$$[\hat{D}_A, \hat{B}] = [\hat{A}, \hat{B}] = [\hat{D}_A, \hat{D}_B] = i\hat{C} \quad (12.26)$$

where \hat{C} is also a Hermitian operator and we let

$$|\alpha\rangle = \hat{D}_A |\psi\rangle = (\hat{A} - \langle \hat{A} \rangle) |\psi\rangle \quad , \quad |\beta\rangle = \hat{D}_B |\psi\rangle = (\hat{B} - \langle \hat{B} \rangle) |\psi\rangle \quad (12.27)$$

we have

$$\begin{aligned} (\Delta \hat{A})^2 &= \langle \hat{D}_A^2 \rangle = \langle \psi | \hat{D}_A^2 | \psi \rangle = (\langle \psi | \hat{D}_A) (\hat{D}_A | \psi \rangle) = \langle \alpha | \alpha \rangle \\ (\Delta \hat{B})^2 &= \langle \hat{D}_B^2 \rangle = \langle \psi | \hat{D}_B^2 | \psi \rangle = (\langle \psi | \hat{D}_B) (\hat{D}_B | \psi \rangle) = \langle \beta | \beta \rangle \end{aligned} \quad (12.28)$$

The Schwarz inequality says that for any two vectors we must have the relation

$$\langle \alpha | \alpha \rangle \langle \beta | \beta \rangle \geq |\langle \alpha | \beta \rangle|^2 \quad (12.29)$$

We therefore have

$$\begin{aligned} (\Delta \hat{A})^2 (\Delta \hat{B})^2 &= \langle \hat{D}_A^2 \rangle \langle \hat{D}_B^2 \rangle = \langle \alpha | \alpha \rangle \langle \beta | \beta \rangle \geq |\langle \alpha | \beta \rangle|^2 \\ &= |\langle \psi | \hat{D}_A \hat{D}_B | \psi \rangle|^2 = |\langle \hat{D}_A \hat{D}_B \rangle|^2 \end{aligned} \quad (12.30)$$

This gives

$$(\Delta \hat{A})^2 (\Delta \hat{B})^2 \geq |\langle \hat{D}_A \hat{D}_B \rangle|^2 \quad (12.31)$$

$$\begin{aligned} |\langle \hat{D}_A \hat{D}_B \rangle|^2 &= |\langle \Delta \hat{A} \Delta \hat{B} \rangle|^2 = \left| \left\langle \frac{1}{2} [\Delta \hat{A}, \Delta \hat{B}] + \frac{1}{2} \{\Delta \hat{A}, \Delta \hat{B}\} \right\rangle \right|^2 \\ &= \left| \left\langle \frac{1}{2} [\hat{A}, \hat{B}] + \frac{1}{2} \{\hat{A}, \hat{B}\} \right\rangle \right|^2 \end{aligned} \quad (12.32)$$

$$[\hat{A}, \hat{B}]^\dagger = -[\hat{A}, \hat{B}] \rightarrow \text{anti-hermitian} \rightarrow \text{expectation value is imaginary} \quad (12.33)$$

$$\{\hat{A}, \hat{B}\}^\dagger = \{\hat{A}, \hat{B}\} \rightarrow \text{hermitian} \rightarrow \text{expectation value is real} \quad (12.34)$$

Therefore,

$$(\Delta \hat{A})^2 (\Delta \hat{B})^2 \geq \left| \left\langle \frac{1}{2} [\hat{A}, \hat{B}] + \frac{1}{2} \{\hat{A}, \hat{B}\} \right\rangle \right|^2 \quad (12.35)$$

$$(\Delta \hat{A})^2 (\Delta \hat{B})^2 \geq \frac{1}{4} |\langle i\hat{C} \rangle + a|^2 \quad (12.36)$$

where a = a real number. We then have

$$(\Delta \hat{A})^2 (\Delta \hat{B})^2 \geq \frac{1}{4} |\langle i\hat{C} \rangle + a|^2 = \frac{1}{4} |a|^2 + \frac{1}{4} |\langle \hat{C} \rangle|^2 \quad (12.37)$$

$$(\Delta \hat{A})^2 (\Delta \hat{B})^2 \geq \frac{1}{4} |\langle \hat{C} \rangle|^2 \quad (12.38)$$

since $|a|^2/4 \geq 0$.

If

$$[\hat{A}, \hat{B}] = i\hat{C} = 0 \quad (12.39)$$

we then get

$$(\Delta \hat{A})^2 (\Delta \hat{B})^2 \geq 0 \quad (12.40)$$

and we have no uncertainty relation between the observables.

On the other hand, if $\hat{A} = \hat{x}$ and $\hat{B} = \hat{p}_x$, we have

$$[\hat{x}, \hat{p}_x] = i\hbar = \hat{C} \quad (12.41)$$

which means that

$$(\Delta \hat{A})^2 (\Delta \hat{B})^2 \geq \frac{\hbar^2}{4} \quad (12.42)$$

or

$$\Delta \hat{x} \Delta \hat{p}_x \geq \frac{\hbar}{2} \quad (12.43)$$

which is the Heisenberg uncertainty principle. It is simply the Schwarz inequality!! Hopefully, that removes any *mysticism* associated with the principle!

12.4 Time-Energy Uncertainty Relations

The use of time-energy uncertainty relations in most textbooks is simply incorrect. Let us now derive the most we can say about such relations.

We need to derive the time-dependence of expectation values. We have

$$\langle \hat{Q} \rangle = \langle \psi(t) | \hat{Q} | \psi(t) \rangle \quad (12.44)$$

so that

$$\begin{aligned} \frac{d\langle \hat{Q} \rangle}{dt} &= \frac{d}{dt} \langle \psi(t) | \hat{Q} | \psi(t) \rangle = \frac{d}{dt} \langle \psi(0) | e^{i\hat{H}t/\hbar} \hat{Q} e^{-i\hat{H}t/\hbar} | \psi(0) \rangle \\ &= \langle \psi(0) | \frac{d}{dt} \left(e^{i\hat{H}t/\hbar} \hat{Q} e^{-i\hat{H}t/\hbar} \right) | \psi(0) \rangle \\ &= \langle \psi(0) | \left(\frac{i\hat{H}}{\hbar} e^{i\hat{H}t/\hbar} \hat{Q} e^{-i\hat{H}t/\hbar} \right) | \psi(0) \rangle - \langle \psi(0) | \left(e^{i\hat{H}t/\hbar} \hat{Q} \frac{i\hat{H}}{\hbar} e^{-i\hat{H}t/\hbar} \right) | \psi(0) \rangle \\ &= \langle \psi(0) | e^{i\hat{H}t/\hbar} \frac{i}{\hbar} [\hat{H}, \hat{Q}] e^{-i\hat{H}t/\hbar} | \psi(0) \rangle = \frac{i}{\hbar} \langle \psi(t) | [\hat{H}, \hat{Q}] | \psi(t) \rangle \end{aligned} \quad (12.45)$$

or

$$\frac{d\langle \hat{Q} \rangle}{dt} = \frac{1}{i\hbar} \langle [\hat{Q}, \hat{H}] \rangle \quad (12.46)$$

We consider the dynamical state of the system at a given time t . Let $|\psi\rangle$ be the vector representing that state. Call ΔQ , ΔE the root-mean-square deviations of \hat{Q} and \hat{H} , respectively. Applying the Schwarz inequality (as above) to the vectors

$$(\hat{Q} - \langle \hat{Q} \rangle) |\psi\rangle \quad , \quad (\hat{H} - \langle \hat{H} \rangle) |\psi\rangle \quad (12.47)$$

and carrying out the same manipulations as (as above) we find after some calculations

$$\Delta Q \Delta E \geq \frac{1}{2} | \langle [\hat{Q}, \hat{H}] \rangle | \quad (12.48)$$

the equality being realized when $|\psi\rangle$ satisfies the equation

$$(\hat{Q} - \alpha) |\psi\rangle = i\gamma(\hat{H} - \varepsilon) |\psi\rangle \quad (12.49)$$

where α , γ and ε are arbitrary real constants (as above). Putting everything together we get

$$\frac{\Delta Q}{\left| \frac{d\langle \hat{Q} \rangle}{dt} \right|} \Delta E \geq \frac{\hbar}{2} \quad (12.50)$$

or

$$\tau_Q \Delta E \geq \frac{\hbar}{2} \quad (12.51)$$

where we have defined

$$\tau_Q = \frac{\Delta Q}{\left| \frac{d\langle \hat{Q} \rangle}{dt} \right|} \quad (12.52)$$

τ_Q appears as a time characteristic of the evolution of the expectation value of \hat{Q} . It is the time required for the center $\langle \hat{Q} \rangle$ of the statistical distribution of \hat{Q} to be displaced by an amount equal to its width ΔQ . In other words, the time necessary for this statistical distribution to be appreciably modified. In this way we can define a characteristic evolution time for each dynamical variable of the system.

Let τ be the shortest of the times thus defined. τ may be considered as the characteristic time of evolution of the system itself, that is, whatever the measurement carried out on the system at an instant of time t' , the statistical distribution of the results is essentially the same as would be obtained at the instant t , as long as the difference $|t - t'|$ is less than τ .

According to the above derivation, this time τ and the energy spread ΔE satisfy the time-energy uncertainty relation

$$\tau \Delta E \geq \frac{\hbar}{2} \quad (12.53)$$

If, in particular, the system is in a stationary state where

$$\frac{d\langle \hat{Q} \rangle}{dt} = 0 \quad (12.54)$$

no matter what \hat{Q} , and consequently τ is infinite, then $\Delta E = 0$. That is the meaning of a stationary state.

Ordinary time t is just a parameter in non-relativistic QM and not an operator! Our derivation does not say that

$$\Delta t \Delta E \geq \frac{\hbar}{2} \quad (12.55)$$

which is an equation that has no meaning!

Chapter 13

Entanglement, EPR and Bell

There will be two threads running through this part of the book. The first stems from Einstein's desire to discredit quantum physics as a fundamental theory of reality: which in the end led to some of the most impressive and far-reaching confirmations of the quantum view. The second derives from Schrödinger who introduced the term *entanglement* to the physics community and showed how entangled states lead to very bizarre features of the quantum world.

I will make multiple passes through each topic so that the reader can see different derivations, discussions and points of view. Hopefully this enhances understanding!

13.1 Is Quantum Theory Complete?

Despite being responsible for a number of key developments in the theory, Einstein was never happy with the final form of quantum theory. At first he objected to the uncertainty principle and tried to conjure up some thought experiments designed to show how you could get around its limitations. In each case Bohr and Heisenberg found a counter-argument and the uncertainty principle and quantum theory prevailed.

Einstein then switched from trying to show that quantum theory was *inconsistent* (did not always give the same answer in similar cases) to proving that it was *incomplete* (that there were some situations not covered by the theory).

In 1935 Einstein thought that he had found a way to discredit quantum theory. In a famous paper published in collaboration with Boris Podolsky and Nathan Rosen (now known as the EPR paper), Einstein constructed an argument that he felt demonstrated the need for a deeper (more deterministic) theory to replace quantum mechanics.

The paper titled **Can a quantum mechanical description of physical reality be considered complete?** starts by defining exactly what is meant by a complete physical theory. According to the authors if a theory is to be complete then, *every element of the physical reality must have a counterpart in the physical theory*. This seems entirely reasonable, provided you can decide what you mean by an *element of the physical reality*.

That is not very straightforward however. According to the authors, we cannot guess or try to figure out the elements of physical reality. They have to be *found by an appeal to the results of experiments and measurements*. The workings of the world are too subtle and surprising for us to guess correctly. We need some experiments to lead the way and tell us *it must be like this*.

Even then it is not quite as simple as it sounds. Experiments produce huge amounts of data, some of which are important and some of which are random *noise*. We need some way of separating out the key features of the information from the random (experimental) fluctuations that always happen. The EPR answer to this ties theory with experiment. They suggest that the following condition must be met:

if, without in any way disturbing the system, we can predict with certainty the value of a physical quantity then there exists an element of physical reality corresponding to this physical quantity.

The part about **disturbing the system** is there to set a trap for quantum theory.

In the next stage of the paper, the EPR team apply their condition for reality to a specific case. They remind us that quantum theory employs a state $|\psi\rangle$ (actually they use the wave function ψ) to represent a system and operators \hat{O} to represent physical variables.

If $|\psi\rangle$ happens to be an eigenstate of \hat{O} , then

$$\hat{O}|\psi\rangle = a|\psi\rangle \quad (13.1)$$

where a is the corresponding eigenvalue. We know that we can say with certainty that a measurement of the physical variable linked to \hat{O} will give us the value a (this is one of our quantum postulates or rules). Then, by the EPR condition, the physical variable represented by \hat{O} must be an element of reality (in that state).

However, if we choose to measure some other physical variable, linked to an operator \hat{Q} , for example, for which $|\psi\rangle$ is not an eigenstate, then we cannot predict with certainty what a measurement will produce. We would have to expand $|\psi\rangle$ over the basis of eigenstates of \hat{Q} and calculate the expectation value for a set of

results, or the probability of a given result. The only way to predict with 100% certainty what a measurement will give us is to *disturb the system* by turning $|\psi\rangle$ into one of the eigenstates of \hat{Q} . Thus, by the EPR condition, \hat{Q} cannot be an element of physical reality, or, at least, it cannot be at the same time as \hat{O} .

Specifically, we could have an electron in state $|p\rangle$, an eigenstate of the momentum operator, \hat{p} , in which case momentum is part of the electron's reality. However, in this state, position cannot be an element of the electron's reality as $|p\rangle$ is not an eigenstate of \hat{x} .

The whole basis of the EPR argument is the philosophical view that we cannot create reality by bending an electron (or something) to fit the words “*disturb the system*”. We should be able to find a set of physical variables and a theory that allows us to predict them with certainty, as reality must be *out there* for us to find, not something we can create.

Having set up their conditions for reality and illustrated them for a simple quantum mechanical case, the EPR team then spring their trap by describing a situation in which it appears that quantum theory fails to describe every element of a system's reality.

13.2 The EPR Argument

Consider two particles, A and B, which interact with one another and then separate in opposite directions. After a while, they are so far apart that they cannot interact with one another anymore (at least during the duration of the subsequent experiments due to the finite speed of light which, as we know, is the maximum speed of signal transfer according to Einstein's theory of relativity). The combined state of the two particles can now be written as a product of the separate states:

$$|\psi\rangle = |A\rangle |B\rangle \quad (13.2)$$

It is very likely that the particles will be separating in momentum eigenstates, as one factor that is always conserved in any interaction is the total momentum. See figure below.

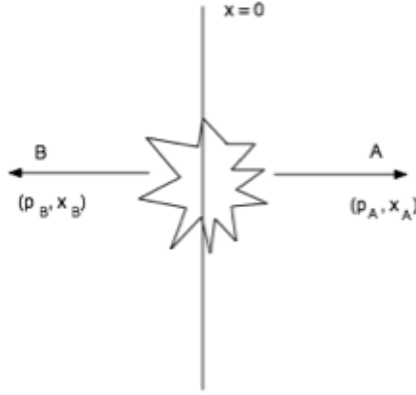


Figure 13.1: Two particles interacting and then separating

Here, two particles interact and separate as part of the EPR argument. The vertical line is drawn through the point where the interaction (the cloud) takes place.

So, the states of the two particles might well be

$$|A\rangle = \exp\left(\frac{i}{\hbar} (p_A x_A)\right) |p_A\rangle \quad (13.3)$$

$$|B\rangle = \exp\left(\frac{i}{\hbar} (-p_B x_B)\right) |-p_B\rangle \quad (13.4)$$

Note that x_B is the distance traveled, not the coordinate, so it doesn't need to be negative as is the case with the momentum, where the sign gives the direction of motion.

The total state must now be

$$\begin{aligned} |\Psi\rangle &= \sum_{p_A} \sum_{p_B} \left[\exp\left(\frac{i}{\hbar} (p_A x_A)\right) |p_A\rangle \exp\left(\frac{i}{\hbar} (-p_B x_B)\right) |-p_B\rangle \right] \\ &= \int \int \exp\left(\frac{i}{\hbar} (p_A x_A)\right) |p_A\rangle \exp\left(\frac{i}{\hbar} (-p_B x_B)\right) |-p_B\rangle dp_A dp_B \end{aligned} \quad (13.5)$$

We have summed over p_A and p_B since we don't know what the momentum is going to be. So by Rule 3, we have to add up the amplitudes for all possibilities. The second line is just the same thing in integral form, as the momentum is continuous. The states are not normalized here since that will not be important in this argument.

We can be a bit cleverer than this, however. The momentum of one particle must be equal in size, but opposite in direction, to that of the other (conservation of momentum). We have already taken care of the direction bit as one of the

expressions inside brackets has a p_A and the other one $-p_B$. Now, we can get rid of the distinction between p_A and p_B and just call them p as they have to be equal in size. In other words, $p_A = p$ and $p_B = p$, so we can get away with just one sum over p :

$$\begin{aligned} |\Psi\rangle &= \sum_p \left[\exp\left(\frac{i}{\hbar}(px_A)\right) |p\rangle \exp\left(\frac{i}{\hbar}(-px_B)\right) |-p\rangle \right] \\ &= \int \exp\left(\frac{i}{\hbar}(x_A - x_B)p\right) |p\rangle |-p\rangle dp \end{aligned} \quad (13.6)$$

where we remember that the first ket (from the left) refers to the state of particle A, and the second one to that of particle B.

Now we get to the real core of the EPR argument. If we measure the momentum of particle A, giving us some value P , then state $|A\rangle$ must collapse to the eigenstate with eigenvalue P . That is fine, we have disturbed the state $|A\rangle$ so its momentum cannot really be called an element of reality. But we know straight away that the momentum of particle B, if we chose to measure it, would be $-P$ since we have already said that they are equal and opposite. Note, though, that we have not *disturbed system B*. We can predict the value of B's momentum with absolute certainty without disturbing B, so its momentum must be an *element of reality*.

The next step in the argument is to think what might happen if we choose to measure the *position* of particle A instead of its momentum. To figure out what happens, we have to change the basis states of particle A from $|p\rangle$ to $|x\rangle$ - go to the HOME space!. This looks a bit complicated, but its nothing new. We have done such things before.

The starting point is the expansion of momentum states in terms of position eigenstates.

$$|p\rangle = \int \langle x | p \rangle |x\rangle dx \quad (13.7)$$

Next we put this into the formula for $|\Psi\rangle$ to give

$$|\Psi\rangle = \int \exp\left(\frac{i}{\hbar}(x_A - x_B)p\right) \left[\int \langle x_A | p \rangle |x_A\rangle dx_A \right] |-p\rangle dp \quad (13.8)$$

where we have expanded over x_A states.

Now let us measure particle A's position to reveal the value X . This collapses the sum over x in the expression inside the square bracket and picks out the ket $|x_A = X\rangle$ from among the $|x\rangle$ s. The expression inside the square bracket simply becomes $|x_A = X\rangle$ and the value of x_A in the integral becomes X .

$$\begin{aligned} |\Psi'\rangle &= \int \exp\left(\frac{i}{\hbar}(X - x_B)p\right) |-p\rangle dp \\ &= \left[\int \exp\left(\frac{i}{\hbar}(X - x_B)p\right) |-p\rangle dp \right] |x_A = X\rangle \end{aligned} \quad (13.9)$$

We are interested in the term inside the square bracket. We have seen something like this before: it's a complete expansion over momentum eigenstates, and so it must be a position eigenstate for B. In fact, it is the state $|x_B = X\rangle$.

$$\int \exp\left(\frac{i}{\hbar}(X - x_B)p\right) | -p \rangle dp = |x_B = X\rangle \quad (13.10)$$

and hence

$$|\Psi'\rangle = |x_B = X\rangle |x_A = X\rangle \quad (13.11)$$

In other words, particle B has also traveled a distance X , but in the opposite direction. That's exactly what we would expect, as they both have the same momentum and have been traveling for the same amount of time.

Now the trap closes.

Note what we have done. Measuring the position of particle A has *disturbed the state* of A, because we have interacted with it. We have not interacted with B, so we cannot have disturbed its state. However, collapsing the state A has allowed us to predict B's position with certainty, so that must be a part of B's physical reality.

Hang on a moment though. Previously we argued that the momentum must be part of B's physical reality, now we are saying the position is as well. The uncertainty principle forbids us to be certain of both position and momentum at the same time. *Something has gone wrong.*

This is the EPR argument. If we choose to measure A's momentum we can be sure of B's momentum without measuring it, so it must be part of B's reality. If we measure A's position instead, we can be sure of B's position so it must be part of B's reality as well. Whatever we choose to measure that belongs to A, we have not *disturbed the state* of B, so we must be finding out true things about B that have not changed due to the measurement of A. Yet this breaks one of the fundamental rules of quantum theory. The theory doesn't allow us to construct a state with a fixed value of position and momentum at the same time.

The theory must be incomplete. It cannot deal with this situation.

Toward the end of their short paper the authors comment that they *would not arrive at their conclusion if one insisted that two ... physical quantities can be regarded as simultaneous elements of reality only when they can be simultaneously measured or predicted ... This [simultaneous predictability] makes the reality of [the momentum of B] and [the position of B] depend upon the process of measurement carried out on the first system which does not disturb the second system in any way. No reasonable definition of reality could be expected to permit this.*

Or could it

Follow-Up by David Bohm

There is an air of *slight of hand* about the EPR argument, as it depends on starting with a very specific state. Some commentators have questioned how realistic the initial state is in practice. Fortunately, there is another version put together by David Bohm using spin states, which cannot be subjected to the same criticism.

To see this argument at work, we need to start by thinking about possible combined states of two spin 1/2 particles, for example, two electrons. To describe the combined system we need a collection of basis states.

$$|U\rangle|U\rangle \quad , \quad |D\rangle|D\rangle \quad , \quad |U\rangle|D\rangle \quad , \quad |D\rangle|U\rangle \quad (13.12)$$

where we assume that the first ket refers to the first particle in each case.

When you combine two spin-1/2 particles, the quantum rules governing how you add together angular momentum dictate two possible results: spin-1 or spin-0.

The spin-0 case is quite straightforward; the overall state of the two electrons will be

$$|singlet\rangle = \frac{1}{\sqrt{2}} (|U\rangle|D\rangle - |D\rangle|U\rangle) \quad (13.13)$$

It's called a singlet state as this is the only combination that adds up to spin 0 overall.

The spin-1 combination is slightly trickier. Earlier we discussed the three z -component spin states for a spin-1 particle. The same reasoning applies to a combined system of spin-1/2 particles with an overall spin-1. There must be three state functions corresponding to three z components.

$$|triplet\ 1\rangle = |U\rangle|U\rangle = |V, +1\rangle \quad (13.14)$$

$$|triplet\ 2\rangle = \frac{1}{\sqrt{2}} (|U\rangle|D\rangle + |D\rangle|U\rangle) = |V, 0\rangle \quad (13.15)$$

$$|triplet\ 3\rangle = |D\rangle|D\rangle = |V, -1\rangle \quad (13.16)$$

Bohm's EPR argument starts with a pair of electrons that have been prepared in the singlet (spin 0) combined state. The electrons are flying off in different directions. One of the electrons reaches a Stern-Gerlach (S-G) magnet, which measures its vertical spin component. This has the effect of collapsing its state.

If the first measurement reveals the first electron to be spin UP, the state collapses to the first pairing in the singlet state and so the other electron must

have spin DOWN. If the measurement reveals the first electron to be DOWN that picks out the second pairing and then the other electron is spin UP.

$$|\text{singlet}\rangle = \frac{1}{\sqrt{2}} (|U\rangle |D\rangle - |D\rangle |U\rangle) \xrightarrow[\text{if first particle measures as } |U\rangle]{\text{collapses into}} |U\rangle |D\rangle \quad (13.17)$$

$$|\text{singlet}\rangle = \frac{1}{\sqrt{2}} (|U\rangle |D\rangle - |D\rangle |U\rangle) \xrightarrow[\text{if first particle measures as } |D\rangle]{\text{collapses into}} |D\rangle |U\rangle \quad (13.18)$$

The upshot is that measuring the spin of one electron allows us to predict with certainty the spin of the other. By the EPR condition of reality, the vertical spin component of the second electron must be a *real* physical property with two possible values (UP,DOWN).

But, what happens if you choose to measure the horizontal spin component? To see what happens we must switch bases in the singlet state using $|L\rangle$ and $|R\rangle$ instead, Taking

$$|U\rangle = \frac{1}{\sqrt{2}} (|L\rangle + |R\rangle) \quad , \quad |D\rangle = \frac{1}{\sqrt{2}} (|L\rangle - |R\rangle) \quad (13.19)$$

and plugging into the singlet state, we get

$$\begin{aligned} |\text{singlet}\rangle &= \frac{1}{\sqrt{2}} (|U\rangle |D\rangle - |D\rangle |U\rangle) \\ &= \frac{1}{\sqrt{2}} \left[\frac{1}{\sqrt{2}} (|L\rangle + |R\rangle) \frac{1}{\sqrt{2}} (|L\rangle - |R\rangle) - \frac{1}{\sqrt{2}} (|L\rangle - |R\rangle) \frac{1}{\sqrt{2}} (|L\rangle + |R\rangle) \right] \\ &= \frac{1}{\sqrt{2}} \left[\begin{array}{l} \frac{1}{2} (|L\rangle |L\rangle - |L\rangle |R\rangle + |R\rangle |L\rangle - |R\rangle |R\rangle) \\ - \frac{1}{2} (|L\rangle |L\rangle + |L\rangle |R\rangle - |R\rangle |L\rangle - |R\rangle |R\rangle) \end{array} \right] \\ &= \frac{1}{\sqrt{2}} [|R\rangle |L\rangle - |L\rangle |R\rangle] \end{aligned} \quad (13.20)$$

showing that in the (LEFT,RIGHT) basis we have a singlet state as well.

Now that we have the state in the (LEFT,RIGHT) basis we can put together the second part of the EPR argument.

Measuring the *horizontal* component of electron 1 will collapse the overall state so that an exact prediction can be made of electron 2's spin (if 1 is LEFT, 2 must be RIGHT, and vice versa). EPR would then argue that the horizontal spin is a real property of electron 2. However, we said a moment ago that electron 2 must have a precise value of its vertical spin state. Quantum theory, however, does not allow us to put together a state with precise values of *both* horizontal and vertical spins and so it must be incomplete.

The importance of Bohm's version of the EPR argument stems from its comparative simplicity; the initial state involved can be achieved in practice and we

can conduct an experiment to test the EPR argument.

We will look at such experiment later on, once we have seen how John Bell developed this line of thought. Meanwhile, I want to consider one of the most important responses made to the EPR argument that came from Bohr.

13.3 Locality, EPR and Bell - Another Presentation

States of More Than One Particle - Discussion #2

Before proceeding into this discussion, let us present multi-particle states for a second time, i.e., let us figure out the properties of quantum states (vectors) when *more than one particle* is present in a particular state. In this book, we will only need to look at the case of two particles.

Imagine two particles (1 and 2) in states $|a_1\rangle$ (eigenstate of operator \hat{A}) and $|b_1\rangle$ (eigenstate of operator \hat{B}) respectively. We write the state describing the situation where particle 1 is in state $|a_1\rangle$ and particle 2 is in state $|b_1\rangle$ as

$$|a_1\rangle_1 |b_1\rangle_2 \rightarrow |a_1, b_1\rangle \quad (13.21)$$

and these symbols represent a vector in the state-space of the two-particle system.

What are the properties of these vectors, *especially* with respect to probabilities?

If the two particles *do not interact* with each other, then their probabilities are independent. That means that the probability that particle 1 has \hat{A} measured as a_3 and particle 2 has \hat{B} measured as b_4 , is given by

$$|({}_1\langle a_3 | {}_2\langle b_4 |) (|a_1\rangle_1 |b_1\rangle_2)|^2 = |{}_1\langle a_3 | a_1\rangle_1|^2 |{}_2\langle b_4 | b_1\rangle_2|^2 \quad (13.22)$$

or that the joint probability that $A = a_3$ and $B = b_4$ is simply the product of the probability for $A = a_3$ and the probability for $B = b_4$.

Our basis set of vectors for the 2-particle universe is given by

$$|a_i\rangle_1 |b_j\rangle_2 \rightarrow |a_i, b_j\rangle \rightarrow |i, j\rangle \quad (13.23)$$

for all possible a_i, b_j values, which means that the dimension of the space is

$$(\text{dim of space of 1-basis}) \times (\text{dim of space of 2-basis}) \quad (13.24)$$

The basis set is *orthonormal*, i.e.,

$$({}_1 \langle a_i | {}_2 \langle b_k |) (|a_j\rangle_1 |b_m\rangle_2) = {}_1 \langle a_i | a_j \rangle_1 {}_2 \langle b_k | b_m \rangle_2 = \begin{cases} 1 & i = j \text{ and } k = m \\ 0 & i \neq j \text{ and/or } k \neq m \end{cases} \quad (13.25)$$

This means that any linear combination of basis vectors

$$|Q\rangle = c_{11} |1, 1\rangle + c_{12} |1, 2\rangle + c_{21} |2, 1\rangle + c_{22} |2, 2\rangle + \dots \quad (13.26)$$

will also be a vector, and hence another physical state, in the two-particle state space.

Now for something very interesting!

It turns out that a two-particle state $|Q\rangle$ (one of many such examples) as given below

$$|Q\rangle = \frac{1}{\sqrt{2}} |1, 2\rangle - \frac{1}{\sqrt{2}} |2, 1\rangle \quad (13.27)$$

which is a superposition of two-particle state vectors where particle 1 is in a superposition of states $|1\rangle_1$ and $|2\rangle_1$ and particle 2 is *simultaneously* in a superposition of states $|1\rangle_2$ and $|2\rangle_2$, *cannot be decomposed* into a state of the form $|r, s\rangle$ (for some values of r, s), that is, a separately well-defined state of particle 1 and a separately well-defined state of particle 2.

That means that states like $|Q\rangle$ cannot possibly be described by propositions of the form

the state of particle 1 is such - and - such
and
the state of particle 2 is so - and - so

In other words, in such a state, no measurable property of particle 1 alone, and no measurable property of particle 2 alone, *has any definite value*. We saw this type of state in the hardness/color two-path experiment and the Mach-Zehnder experiment, although these were not two-particle states..

These are called *nonseparable or entangled* 2-particle states. *Nonseparability or entanglement* along with *superposition* and *incompatibility* are the ways in which quantum theory *differs* most from classical physics.

Now consider the state:

$$|\alpha\rangle = \frac{1}{\sqrt{2}} |x_1 = 5\rangle |x_2 = 7\rangle - \frac{1}{\sqrt{2}} |x_1 = 9\rangle |x_2 = 11\rangle \quad (13.28)$$

where

$$\hat{X}_1 |x_1\rangle = x_1 |x_1\rangle \quad , \quad \hat{X}_2 |x_2\rangle = x_2 |x_2\rangle \quad (13.29)$$

i.e., the particle states are eigenvectors of the position operators in each space.

In this state, neither the position of particle 1, nor the position of particle 2, nor anything else about them separately, has any definite value here.

On the other hand, the difference in their positions does have a definite value because:

$$(\hat{X}_2 - \hat{X}_1)|\alpha\rangle = 2|\alpha\rangle \quad (13.30)$$

i.e., it is an eigenvector of the $(\hat{X}_2 - \hat{X}_1)$ operator with eigenvalue 2, which implies that the difference in the positions (in this state) is equal to 2 with *certainty* or probability = 1.

Two interesting cases will illustrate how we deal with probability and collapse for these states.

First, suppose that the state of the 2-particle system is $|\beta\rangle$, and that \hat{A} and \hat{B} , which are observables of particles 1 and 2 respectively, are measured. The probability that the outcomes of those experiments will be $A = a$ and $B = b$, is given by

$$|\langle a, b | \beta \rangle|^2 \quad (13.31)$$

which is just one of our original postulates.

Now, suppose that *only* \hat{A} is measured.

The probability that the outcome of the measurement will be $A = a_1$ is given by a sum over probability amplitudes squared as shown below:

$$P = |\langle a_1, b_1 | \beta \rangle + \langle a_1, b_2 | \beta \rangle + \langle a_1, b_3 | \beta \rangle + \dots|^2 \quad (13.32)$$

where \hat{B} is any observable of particle 2 and the sum ranges over all the eigenvalues $\{b_i\}$ of \hat{B} (all possible measured values of \hat{B}) since \hat{B} is not measured, which is just another of our postulates.

We say it as follows:

The probability amplitude that $A = a_1$ is equal to sum of the probability amplitudes of all the various different and indistinguishable ways it is possible for \hat{A} to be a_1 , i.e., independent of the values of \hat{B} , which was not measured, and the actual probability is the square of the resulting total amplitude.

Classically we would have the very different result

$$P = |\langle a_1, b_1 | \beta \rangle|^2 + |\langle a_1, b_2 | \beta \rangle|^2 + |\langle a_1, b_3 | \beta \rangle|^2 + |\langle a_1, b_4 | \beta \rangle|^2 + \dots \quad (13.33)$$

that is, *the sum of the squares of the individual amplitudes (individual probabilities) and the possibility of any interference would vanish (no cross-terms and no interference).*

Now let us elaborate the principle(postulate) of collapse for a two-particle state.

Suppose that the state of a certain 2-particle system just prior to the time t_1 is $|\delta\rangle$ and suppose that at t_1 the observable \hat{A} (of particle 1) is measured, and suppose that the outcome of that measurement is $A = a_5$ (one of the eigenvalues of \hat{A}).

Here is how to calculate how the state of the 2-particle system is changed(collapsed) by the \hat{A} measurement.

Start with state $|\delta\rangle$ expressed in terms of eigenstates of \hat{A} and \hat{B}

$$|\delta\rangle = d_{11} |1, 1\rangle + d_{12} |1, 2\rangle + d_{21} |2, 1\rangle + d_{22} |2, 2\rangle + \dots \quad (13.34)$$

where

$$d_{ij} = \langle i, j | \delta \rangle \quad , \quad |i, j\rangle = |a_i, b_j\rangle \quad (13.35)$$

Then, throw away all the terms where $A \neq a_5$ (that is what the measurement $A = a_5$ does according to the postulates). This leaves

$$|\delta\rangle = d_{51} |5, 1\rangle + d_{52} |5, 2\rangle + d_{53} |5, 3\rangle + d_{54} |5, 4\rangle + \dots \quad (13.36)$$

Renormalize the new vector to 1 (one of our postulates) and the resulting vector is the new state vector of the system after the measurement.

Note that it has only one value of \hat{A} , but *many, possibly all*, values of \hat{B} .

If the original state had only one component with $A = a_5$, then \hat{B} would necessarily have the value in that state. So if the state is

$$|\alpha\rangle = \frac{1}{\sqrt{2}} |x_1 = 5\rangle |x_2 = 7\rangle - \frac{1}{\sqrt{2}} |x_1 = 9\rangle |x_2 = 11\rangle \quad (13.37)$$

and we measure $X_1 = 5$, then we *necessarily* have $X_2 = 7$ (particle 2 must be in this state) due to our collapse postulate, *even though we did not measure \hat{X}_2* .

This is a most important point! We state that $X_2 = 7$ even though we have not measured it; this is called a **counterfactual** statement. We are saying stuff about property B without actually measuring \hat{B} !

With these properties of 2-particle states, we can continue our discussions.

E(instein)P(odolsky)R(osen) - Version #2

A famous attempt to escape from the standard (Copenhagen) way of thinking about quantum mechanics was initiated in the 1930s by Einstein, Podolsky and Rosen, and had a surprising aftermath, in the 1960s, in the work of John Bell.

We first discuss the escape attempt itself and then delve into the most fundamental work of Bell. In 1935, Einstein, Podolsky and Rosen (EPR) produced an argument, which was supposed to open the way to an escape from the standard way of thinking about quantum mechanics.

First, they define *completeness*:

A description of the world is complete (for EPR) if nothing that is true about the world, nothing that is an element of the reality of the world is left out of the description.

EPR never actually presented a prescription for determining what all the elements of reality are (made it very difficult to challenge them because they could always say.....“you must have missed one”).

Instead, they did something much narrower (which was sufficient for the purposes of their argument). They wrote down a condition for a measurable property of a certain system at a certain moment to be an element of the reality of that system at that moment.

The condition is that:

if, without in any way disturbing a system, we can predict with certainty (with probability = 1) the value of a physical quantity, then there exists an element of reality corresponding to this physical quantity.

Let us see what this condition means. Consider the following question:

If a measurement of a particular observable \hat{O} of a certain particular physical system S were to be carried out at a certain particular future time T , what would the outcome be?

Suppose that there is a method available to me so that I can, prior to time T , answer that question with certainty.

Also, suppose that the method I used involves no disturbance of the system S whatsoever.

Then(according to EPR) there must *now* already be some definite information(*hidden away somewhere*) about what the outcome of the future \hat{O} measurement on S would be at time T .

Some Examples:

Suppose we have just measured the color of some particular electron. Having done that (and since measurements of color are repeatable) we are in a position

to predict with certainty what the outcome of a later color measurement will be, if such a measurement were to be carried out. Making such a prediction need not involve any further interaction with the electron at all. So the EPR reality condition says that color must, at that moment, be an element of the reality of this electron.

This is identical to any statements we might make in the standard way of thinking!

Suppose, on the other hand, that I had just now measured the hardness of an electron. In order to be able to predict with certainty what the outcome of a future measurement of the color of that electron would be (if we made such a measurement), I would need to measure the color of *that* electron (I would need to *interact* with it and potentially disturb it).

The EPR reality condition does not say that the color of the electron is an element of the reality of *this* electron at that moment.

Again this agrees completely with the standard way of thinking!

So what EPR want to argue is the following:

If the predictions of quantum mechanics are correct, then there must be elements of reality of the world which have no corresponding elements in the quantum-mechanical *description* of the world.

They are attempting to use quantum mechanics against itself. They are saying that quantum mechanics is missing something!

Their argument goes something like this:

Consider a system consisting of two electrons. Electron 1 is located at position 1, and electron 2 is located at position 2.

Assume that the color-space state of these two electrons is (note that it is a nonseparable or entangled state)

$$|A\rangle = \frac{1}{\sqrt{2}} |green\rangle_1 |magenta\rangle_2 - \frac{1}{\sqrt{2}} |magenta\rangle_1 |green\rangle_2 \quad (13.38)$$

The state $|A\rangle$, like any state in the space, is necessarily an eigenstate of some observable (Hermitian operator) of this pair of electrons, say \hat{O} , where $\hat{O}|A\rangle = +1|A\rangle$ (eigenvalue = +1). Now we have written $|A\rangle$ in the color basis. Let us convert it to the hardness basis.

Remember

$$|green\rangle = \frac{1}{\sqrt{2}}|hard\rangle + \frac{1}{\sqrt{2}}|soft\rangle \quad (13.39)$$

$$|magenta\rangle = \frac{1}{\sqrt{2}}|hard\rangle - \frac{1}{\sqrt{2}}|soft\rangle \quad (13.40)$$

Substituting we get

$$|A\rangle = \frac{1}{\sqrt{2}}|soft\rangle_1|hard\rangle_2 - \frac{1}{\sqrt{2}}|hard\rangle_1|soft\rangle_2 \quad (13.41)$$

It takes the *same nonseparable* form in both bases (in fact, it would do so in any basis we might use!).

Now suppose we carry out a measurement of the color of electron 1 (in the state in the color basis). The outcome of the measurement will be either *green* or *magenta* with equal probability (using our two-particle state probability rules).

Moreover, quantum mechanics says (and it is experimentally confirmed) that in the event that the outcome of the measurement is *green*, then the outcome of any subsequent measurement of the color of electron 2 will necessarily be *magenta* and in the event that the outcome of the measurement is *magenta*, then the outcome of any subsequent measurement of the color of electron 2 will necessarily be *green*.

Both of these statements *follow directly* from the collapse postulate for two-particle states.

EPR assumed (this is the *only assumption* (it is called *locality*) they make on top of the basic assumption that the predictions of quantum mechanics are correct) that things could in principle be set up in such a way as to guarantee that the measurement of the color of electron 1 produces no physical disturbance whatsoever in electron 2.

To them it was a *self-evident* statement!

What influence could there be???

There seemed to be any number of ways for them satisfy this condition.

You could separate the two electrons by some immense distance (nothing we have said so far says that any of the properties of quantum mechanics changes with electron separation). Then the two measurement events are such that according to special relativity they could not influence each other (they are called *spacelike* separated).

Or you could insert an impenetrable wall between them (nothing we have said

so far say that any of the properties of quantum mechanics depends on what happens to be located in between the electrons).

Or we could set up any array of detectors you like in order to verify that no measurable signals pass from one of the electrons to the other in the course of the experiment (since quantum mechanics predicts that no such array, in such circumstances, whatever sort of signals it may be designed to detect, will ever register anything).

This is a very important point.

The locality assumption says that

I cannot punch you in the nose unless my fist gets to the place where your nose is (in space and time)

Of course, something I do with my fist far from where your nose is can cause some other fist which is near your nose to punch your nose (i.e., something I do with my fist might signal somebody else to punch you in the nose). Their seemingly obvious assumption is just this:

if my fist never gets anywhere near your nose then I cannot punch you in the nose directly. If you got punched in such an arrangement, then it cannot be my fist that punched you

If something I do with my fist far from your nose is the cause of your getting punched in the nose, then necessarily some *causal sequence of events at contiguous points in space and at contiguous points in time* (the propagation of some signal for instance) stretches all the way without a break from whatever it was I did with my fist to your being punched in the nose.

The important thing about the sequence of events is that it must necessarily require some finite time(exact amount depends on what is along the path in space and time) to completely unfold. The shortest time possible would occur if the signal(s) travel with the speed of light in a straight line (the maximum speed of propagation of information).

So summarizing their assumption:

Locality

Measurement of color 1 has no effect on measurement of color 2 if measurements are spacelike separated.

Returning to the color basis entangled state

$$|A\rangle = \frac{1}{\sqrt{2}} |green\rangle_1 |magenta\rangle_2 - \frac{1}{\sqrt{2}} |magenta\rangle_1 |green\rangle_2 \quad (13.42)$$

it is clear that we can predict with certainty, if *locality* is true, without disturbing electron 2, what outcome of subsequent measurement of color 2 will be.

Measure color 1 \rightarrow know outcome of measurement of color 2 *opposite* of outcome of measurement of color 1 or *we know color 2 without measuring it!*

The reality condition then says that color is element of the reality of electron 2. The color of 2 has a definite value when in state $|A\rangle$.

So both 1 and 2 have definite color values!

Now switch to the hardness basis so we can talk about hardness measurements.

$$|A\rangle = \frac{1}{\sqrt{2}} |soft\rangle_1 |hard\rangle_2 - \frac{1}{\sqrt{2}} |hard\rangle_1 |soft\rangle_2 \quad (13.43)$$

Using the same arguments in hardness basis we find that both 1 and 2 have definite *hardness* values!

Since we actually can prepare states like $|A\rangle$ in the real world, EPR say the standard interpretation must be false.

EPR conclude both color and hardness are elements of reality of electron 2, even though the two observables are *supposed to be incompatible* according to quantum mechanics.

So the formalism must be *incomplete*, since some elements of the physical reality of world have no corresponding elements in Quantum Mechanics.

There must exist *hidden facts*(*not in the postulates*) about color and hardness of 2, when in state $|A\rangle$.

Is there way out of the EPR proposed dilemma?

Nothing in QM formalism allows both the color/hardness of electron 2 to be predicted with certainty simultaneously.

Similar arguments hold for electron 1.

EPR were clearly very clever!

If true, the statement that system is in state $|A\rangle$ then constitutes an incomplete description of state of pair of electrons - there are some *hidden variables* somewhere.

EPR say QM predicts *everything* correctly, but is *wrong*.

EPR noticed something very odd about collapse postulate for two-particle systems.

It was *nonlocal*.

If two particles are initially in nonseparable state, then a measurement carried out on one can cause changes, *instantaneously*, in the quantum mechanical description of the other, no matter how far apart two particles are or what lies in between.

Suppose that a pair of electrons is initially in state $|A\rangle$ and a measurement of color 1 carried out. The outcome of the measurement is either green or magenta, with equal probabilities. The collapse postulate for a two-particle systems says as soon as the measurement is over, the state of 2 will be either $|magenta\rangle$ (if 1 was green) or $|green\rangle$ (if 1 was magenta) *depending on what happened in the measurement*.

EPR said nonlocality is *disposable artifact* of particular mathematical formalism, of a particular procedure for calculating statistics of outcomes of experiments and that there must be other (*as yet undiscovered*) procedures, which give rise to some statistical properties, but are local (no infinite speeds necessary).

30 years later, Bell showed that their suspicion was wrong!

Bell's work, as we shall see, is taken as a proof that any attempt to be realistic about values of observables of pair of electrons in state $|A\rangle$, must necessarily be *nonlocal*.

Things are actually even more serious than that!!

Bell actually gives a proof that there is genuine nonlocality in the actual workings of nature, *however* we attempt to describe it.

Nonlocality is feature of quantum mechanics, and via Bell's theorem is necessarily a feature of every possible manner of calculating (*with or without superpositions*) which produces same probability predictions (which are experimentally correct) as quantum mechanics.

What is this quantum nonlocality?

First, in state $|A\rangle$, statistics(probabilities) of outcomes of *measurements* on 2 depend nonlocally on outcomes of measurements on 1, and vice versa. But do statistics of outcomes of measurements on 2, when system in state $|A\rangle$, depend nonlocally on *whether* a measurement is *actually carried out on 1* (and vice versa)?

Let us figure it out.

Suppose the system is in state $|A\rangle$, and suppose we measure color 2. Using $|A\rangle$ in the color basis plus the standard quantum-mechanical rules for calculating probabilities of measurement outcomes implies the outcome of the measurement is *equally likely* to be green or magenta.

Suppose the system is in state $|A\rangle$ and we measure color 1, and *then* measure color 2. The measurement of color 1 is *equally likely* to be green or magenta. If green, the collapse postulate says a subsequent measurement of color 2 will be magenta, and if magenta, the collapse postulate says that subsequent measurement of color 2 will be green.

So, when system is in state $|A\rangle$, the outcome of a measurement of color 2 is equally likely to be green or magenta *whether or not* measurement of color 1 carried out first.

Suppose the system is in state $|A\rangle$ and we measure hardness 1, and then measure color 2. Using $|A\rangle$ in hardness basis plus probability rules says the outcome of hardness measurement on 1 equally likely to be hard or soft.

If the outcome of first measurement is soft, the collapse postulate plus probability rules say outcome of second measurement (color 2) is equally likely to be green or magenta. The same result is true if outcome of first measurement is hard.

So here is where we are:

When the system is in state $|A\rangle$, the outcome of a measurement of color 2 is equally likely to be green or magenta, whether

measurement of color 1 is carried out first

or

measurement of hardness 1 is carried out first

or

no measurement on 1 is carried out

The probabilities of various outcomes of measurement on 2 do not depend in any way on whether or not a measurement is made on 1 first.

Since the predictions of QM are correct, there must be non-local influences in nature and they must be of a particularly *subtle* kind.

The outcomes of measurements do sometimes depend non-locally on outcomes

of other, distant measurements, but outcomes of measurements invariably *do not* depend non-locally on *whether* any other distant measurements actually get carried out.

Another way (tricky...must think about this one) to say this:

Non-local influences are so subtle (they surely exist) that they cannot be used to transmit any signal containing information, non-locally, between two distant points. They cannot encode information you want to send in decision to make a measurement or not to make one, or in a decision about which measurement to make, since no such decisions can have detectable non-local effects.

Let us look at a simple experiment (actually done in 1980 with photons) that refutes EPR and agrees with Bell's results (which we will derive shortly). We will discuss this experiment again later with more detail and mathematical rigor.

Consider a pair of electrons in an entangled state like $|A\rangle$ where we use the observable spin(up/down in any direction).

$$|A\rangle = \frac{1}{\sqrt{2}} |z-up\rangle_1 |z-down\rangle_2 - \frac{1}{\sqrt{2}} |z-down\rangle_1 |z-up\rangle_2 \quad (13.44)$$

The electrons separate in physical space without changing this state vector. We end up with two separated electron beams. Each beam has equal numbers of z -up and z -down electrons (since probability = 1/2 for each in each component).

Each electron in one beam is correlated with a partner in other beam since if measure electron in one beam z -up, then partner in other beam is z -down due to entanglement and vice versa.

This nonseparable state remains nonseparable no matter what basis (direction we measure spin) we use.

We define the direction(orientation of S-G magnet) of measurement by the angle θ it makes with an arbitrarily chosen z -axis direction. The original states($\theta = 0$, i.e., we chose the z -axis). So we can write

$$|A\rangle = \frac{1}{\sqrt{2}} |z(0)-up\rangle_1 |z(0)-down\rangle_2 - \frac{1}{\sqrt{2}} |z(0)-down\rangle_1 |z(0)-up\rangle_2 \quad (13.45)$$

A state in an arbitrary direction basis is

$$|A\rangle = \frac{1}{\sqrt{2}} |z(\theta)-up\rangle_1 |z(\theta)-down\rangle_2 - \frac{1}{\sqrt{2}} |z(\theta)-down\rangle_1 |z(\theta)-up\rangle_2 \quad (13.46)$$

where (in original basis)

$$|z(\theta) - up\rangle = \cos \frac{\theta}{2} |z(0) - up\rangle + \sin \frac{\theta}{2} |z(0) - down\rangle \quad (13.47)$$

$$|z(\theta) - down\rangle = -\sin \frac{\theta}{2} |z(0) - up\rangle + \cos \frac{\theta}{2} |z(0) - down\rangle \quad (13.48)$$

Does this make sense? Stand on your head $\rightarrow \theta = 180^\circ \rightarrow$

$$|z(180) - up\rangle = |z(0) - down\rangle \quad (13.49)$$

$$|z(180) - down\rangle = |z(0) - up\rangle \quad (13.50)$$

as expected.

Suppose we measure beam 1 in a direction θ_1 and beam 2 in a direction θ_2 and count number of times

beam 1 up **and** beam 2 up

or

= a MATCH

beam 1 down **and** beam 2 down

and count the number of times

beam 1 up **and** beam 2 down

or

= a MISS

beam 1 down **and** beam 2 up

Quantum mechanics says the experimental results depend only on the angle difference

$$\varphi = \theta_2 - \theta_1 \quad (13.51)$$

and *not separately* on θ_1 and θ_2 . These results are confirmed experimentally no matter where two detectors are located...in same room, or on opposite sides of city or wherever!!!!.

Suppose we code the results coming from two detectors as follows.

If $\varphi = 0$, the z -axes of the 2 detectors are in the same direction and we get

$$beam\ 1 \rightarrow \uparrow\downarrow\uparrow\downarrow\downarrow\uparrow\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\downarrow\uparrow\downarrow\downarrow\uparrow \dots\dots\dots$$
$$beam\ 2 \rightarrow \downarrow \uparrow \downarrow \uparrow \uparrow \downarrow \uparrow \uparrow \uparrow \downarrow \downarrow \uparrow \downarrow \uparrow \uparrow \downarrow \dots\dots\dots$$

i.e., *ALL MISSES* (remember if 1 is up, 2 is down). We get two opposite *binary data* sequences in the two detectors

1010010001101001.....

0101101110010110.....

If $\varphi = 180^\circ$, the z -axes of the 2 detectors are in opposite directions and we get *ALL MATCHES*, i.e.,

$$\begin{aligned} \text{beam 1} &\rightarrow \uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow \dots\dots\dots \\ \text{beam 2} &\rightarrow \uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow \dots\dots\dots \end{aligned}$$

(up in 1 is in opposite direction to up in 2 or up in 2 is down in 1). We would get the same binary sequences in this case.

Quantum mechanics predicts the number of *MATCHES* varies like

$$[\#MATCHES] = [\#ELECTRONS] \sin^2 \frac{\varphi}{2} \quad (13.52)$$

$$[\#MISSES] = [\#ELECTRONS] \cos^2 \frac{\varphi}{2} \quad (13.53)$$

$$[\#MATCHES + \#MISSES] = [\#ELECTRONS] [\sin^2 \frac{\varphi}{2} + \cos^2 \frac{\varphi}{2}] \quad (13.54)$$

$$= [\#ELECTRONS] \quad (13.55)$$

as it should!

We now set the angle between the detector axes to be $\varphi = 120^\circ$. Quantum mechanics predicts

$$[\#MATCHES] = \frac{3}{4} \#ELECTRONS \quad (13.56)$$

What would EPR say?

If $\varphi = 60^\circ$, then

$$[\#MATCHES] = \frac{1}{4} \#ELECTRONS \quad (13.57)$$

(this is same as the quantum mechanical prediction - check it!).

So now EPR align the detectors ($\varphi = 0^\circ$). They then rotate detector 1 such that $\varphi = 60^\circ$ and get 1/4 *MATCHES*.

So now EPR re-align the detectors ($\varphi = 0^\circ$). They then rotate detector 2 (opposite direction) such that $\varphi = -60^\circ$ and also get 1/4 *MATCHES*.

The EPR version of reality (*locality*) says rotating detector 1 can *ONLY* change sequence of ups/downs at detector 1 and rotating detector 2 can *ONLY* change sequence of ups/downs at detector 2.

That is their **LOCALITY** assumption

Now they rotate detector 1 by $\varphi = 60^\circ$ from the aligned direction and rotate the detector 2 by $\varphi = -60^\circ$ from the aligned direction (for a total angle between

= 120°).

EPR then predict

$$\frac{1}{4} + \frac{1}{4} = \frac{1}{2} \text{ MATCHES (not } \frac{3}{4} \text{)} \quad (13.58)$$

Experiment says answer is 3/4!! Quantum mechanics is correct!

The local view of reality due to EPR cannot be correct.

Somehow information seems to be *flowing* between detectors 1 and 2 *NO MATTER WHAT WE DO*. The speed of information flow(if there is a signal) might even be infinite(best measurement so far $\approx 10^7 c = 3 \times 10^{15} m/sec$).

It is important to emphasize that we have not observed any non-local interactions directly, but only indirectly demonstrated the need for them.

Each measurement is separately local, i.e., we measure any spin direction in either detector and always get 50-50 up and down no matter what the other detector is doing. It is the sequences that differ(in a random way) as we change the angles. This means, as before, that we cannot transmit any messages.

We only find out the sequences(messages) when we bring them together, which takes some time.

So, it seems in QM, that my QM fist can punch your QM nose without being at your QM nose!!

13.4 Bohr and EPR - Discussion #1

A criterion of reality like that proposed by the named authors contains ... an essential ambiguity when it is applied to the actual problems with which we are here concerned - Neils Bohr

Bohr produced a reply to the EPR paper within 2 months of its publication. His counterargument uses the *contextuality* of quantum theory and the principle of *complementarity* to punch a hole in EPR's definition of reality. We have seen these arguments already in our discussion.

13.4.1 Complementarity

We are suspended in language in such a way we cannot say what is up and what is down. The word **reality** is also a word, a word which we must learn to use correctly - Neils Bohr

Bohr had a unique, deeply thought out, and very subtle view on the nature of science and the interpretation of quantum theory. As such it defies easy and

compact summary. Some of his writings read rather like an instrumentalist viewpoint, but this would be an oversimplification.

In essence, Bohr was convinced that humans could never picture the inner mechanisms of the atoms. This follows from the nature of our language. As a result of our daily experience, the sort of ideas and concepts that we deal with comfortably and express in language are restricted to the classical world; they may not extend easily into the quantum world, hence the need to abandon classical thinking and try to develop new concepts.

However, there is a snag. The experiments that we carry out rely on gathering together instruments and equipment that are clearly very much bigger than atomic scales and are, consequently, described by our everyday language (including the obvious need to add technical terms for brevity). All the various measurements that we make on atoms and particles in that end come down to numbers read from dials (or similar) on a measuring apparatus. It is essential to the success of science that the equipment we use be described in relatively ordinary terms, which makes it possible for others to understand and reproduce the experiment.

So we are caught in a dilemma. The experiments we carry out should not only be capable of being described, essentially, in everyday language, but they *must* also be so to make science possible. Yet, when we try to gather the results of our experiments together to make a description of the atomic world, we find that the same everyday language and ideas start to fail. Photons seem to act as particles in some circumstances and as waves in others. We can find appropriate mathematics to describe the situation, but that does not help us visualize or speak about photons.

Bohr hoped to find a way out of this trap by developing the *principle of complementarity*. He accepted that there were two completely contradictory pictures of the photon that could not be tied together into one picture, but that did not matter, as you never did an experiment that required the use of both pictures at the same time. It was acceptable to employ a form of “double think” using one of the pairs of complementary views at any one time, depending on what was most appropriate. The actual *true* nature of the photon would never be expressible in language, which is essentially an instrument to describe the classical world, but you could represent what was going on by keeping complementary pictures in mind:

The two views of the nature of light are rather to be considered as different attempts at an interpretation of experimental evidence in which the limitation of classical concepts is expressed in complementary ways ... In fact, here again we are not dealing with contradictory but with complementary pictures of the phenomena, which only together offer a natural generalization of the classical

modes of description.

Heisenberg also expressed a similar view:

Light and matter are both single entities, and the apparent duality arises in the limitations of our language. It is not surprising that our language should be incapable of describing processes occurring within atoms, for, as has been remarked it was invented to describe the experiences of daily life, and these consist only of processes involving exceedingly large numbers of atoms. Furthermore, it is very difficult to modify our language so that it will be able to describe these atomic processes, for words can only describe things of which we can form mental pictures, and this ability, too, is a result of daily experience. Fortunately, mathematics is not subject to this limitation, and it has been possible to invent a mathematical scheme - the quantum theory - which seems entirely adequate for the treatment of atomic processes; for visualization, however, we must content ourselves with two incomplete analogies - the wave picture and the corpuscular picture.

Following from this it is clear that concepts such as position, momentum, frequency, energy, and so on, can be defined only in the context of the experiment to measure them. If you want to talk about the frequency of light (wave picture) then you need to do an experiment in which the wave picture is appropriate. If you want to talk about the momentum of a photon (particle picture) then you need to do a totally different sort of experiment. By insisting on this, Bohr ensured that concepts such as momentum, energy, frequency, and so on, remained rooted in the classical world, while at the same time acknowledging that they would have only a limited application in the quantum world. Bohr wrote that quantum theory *forces us to adopt a new mode of description designated as complementary in the sense that any given application of classical concepts precludes the simultaneous use of other classical concepts which in a different connection are equally necessary for the elucidation of the phenomena.*

The emphasis on relating the meaning of theoretical terms to the experiment in which they are measured is what gives Bohr's thinking an instrumental tinge. However, a careful reading of his writings confirms that Bohr retained the ambition of a realist tempered by his conviction that the atomic world could not be described by limited human experience and language.

These two key aspects of Bohr's thinking, that experiments in the end had to be described by classical physics and that complementary classical ideas may have to be used in tandem, formed the cornerstones of what has become known as the Copenhagen interpretation of quantum mechanics. We will discuss this interpretation later.

13.4.2 Extensions

Bohr came to feel that the principle of complementarity would have a useful application in other branches of thought. Examples that Bohr considered were mind/matter and living/nonliving.

Let us consider the second one. Bohr was quite convinced that organisms were comprised of just the same forms of matter as nonliving things. There is no extra *vital spark* present in life. Equally, living creatures are subject to the same laws of nature as the rest of the material world (Bohr, however, did believe in freedom of the will) and can be studied in the same way. Of course, though, there is a snag. How do we find out what it is about life that makes it alive? The standard scientific approach would be to study the organisms in terms of the fundamental chemical processes at work within it, in the hope of finding out what it was that made them special. In other words, one would rely on the normal scientific process of *reductionism*.

Reductionism works like this. Imagine that you wanted to find out how an old-fashioned mechanical clock worked. You would take it apart until you had a collection of pieces that could not be broken down any further, springs pendulums, gears, etc. By carefully studying each piece you could find out what it was and what it did. Then you would know exactly how the parts could interconnect with one another and gradually trace how the whole mechanism worked. Such is the way that science tackles complicated wholes by analyzing their parts.

The key assumption behind this process is that the properties of the parts are just the same outside the mechanism as they are when part of the mechanism. *The whole does not affect the part.*

Now, generally this is taken as stated, and undoubtedly part of the reason for the great success of science is the application of reductionism. In general, it works. However, it pays to remember that it is an assumption. Some physicists have certainly speculated that the *contextuality* of quantum theory and the nature of entangled states might signal an eventual failure of reductionism.

So, coming back to what Bohr had to say about life, if we were to carry out the procedure of dismantling an organism we would undoubtedly kill it in the process. If reductionism is right, then this should not matter. But, if there is some way that the context of being in a living organism affects the way in which the parts work, then the process of dismantling will not show that up. Given what we have found about the *contextuality* of quantum theory, Bohr was sounding a warning. He felt that living/nonliving might be complementary concepts in the same way that wave/particle ideas are. Similar thinking might be applied to mind/matter.

Here we are now touching on an area in which quantum-type thinking can lead to the greatest abuse: the quantum hype that abounds in endless bad books about the subject. Complementarity, and with it the uncertainty principle, does not provide a license for lazy thinking. There is a great temptation to take a couple of ideas that we do not understand, bolt them together, call them complementary, and justify pairing them as quantum physicists say you can do things like that. Look out for this when evaluating potential quantum hype.

The ideas that Bohr linked in a complementary fashion were forced on him by *experiments*. He always stressed that complementarity arises when two classical concepts, which seem opposite to one another and cannot be reconciled, are nevertheless required together to get a full grasp of what is going on. By full grasp, of course, we mean as full as we can get, given the necessarily classically limited nature of our language and thinking.

It may be that complementarity is a helpful way forward in other branches of science; but if that is going to be the case it will arise from a scientist's struggle to reconcile what seems to be impossible to reconcile, yet is clearly indicated by experiment.

13.4.3 Bohr's Reply to the EPR Argument

In essence, Bohr's point is that the measurement of particle A may not physically disturb the state of particle B, but it does *set up the context* for any information about B.

To measure the momentum of A we have to build a specific device. In essence we have to let it interact with something with a pre-determined momentum and see what change it makes. Of course, if we want to measure the momentum of the device, we find that the uncertainty principle gets in the way. Accurately measuring the momentum of the device destroys any information about where exactly it is. In which case, *it cannot act as a position reference point as well*. This applies to both particles. A measurement of position needs a fixed reference point to work from. When we set up equipment to measure the momentum of particle A, we automatically prevent that equipment from forming a precise reference point for a position measurement of A.

Let us say we then set out to measure the position of particle B. We cannot compare the position of B with anything to do with particle A as we cannot fix the position of the equipment at B's end relative to us. We have effectively blurred the position of particle B by measuring the momentum of particle A. As Bohr puts it: *If we choose to measure the momentum of one of the particles, we lose through the uncontrollable displacement inevitable in such a measurement any possibility of deducing from the behavior of this particle the position of the ... apparatus, and have thus no basis whatever for predictions regarding the location of the other particle.*

A similar argument applies if we choose to measure the position of A instead. Accurate position measurements rely on fixed objects to act as reference points. When particle A collides with a device designed to record its position, there is bound to be an exchange of momentum between the device and the particle. We have interacted with the measuring device. With the device fixed in place we cannot measure that momentum exchange. Any attempt to measure the momentum of the measuring device, to figure out how much it has been changed, is bound to run into uncertainty problems. We need an accurate fix of the position of the device to measure the position of A, so we cannot be sure of the momentum of the device. This ruins any potential momentum measurement we might try to make of B. Momentum can only be known relative to some object. A cup of tea on a table in front of us may be stationary to us, but as we are on a train passing through a station the tea will be in rapid motion compared with those standing on the platform. If we set up a momentum measurement of B, we have no basis to compare it with A. Bohr explains this in the following way: *By allowing an essentially uncontrollable momentum to pass from the first particle into the mentioned support, however, we have by this procedure cut ourselves off from any future possibility of applying the law of conservation of momentum to the system consisting of two particles, and therefore have lost our only basis for an unambiguous application of the idea of momentum in predictions regarding the behavior of the second particle.*

The key difference between the philosophical positions expressed by EPR and Bohr hinges on *without disturbing the system*. To Bohr a property, such as momentum or position, has a meaning only in the context of the experimental equipment used to measure it. Particle B may not come in contact with the equipment at all; in such a case any information we have about it is useless as there is nothing we can do with it. If we would like to use the information, say to predict where the second particle will be after a while and check that information experimentally, then the second particle has to come into contact with the measuring equipment, or some other stuff has to be linked to it.

As far as complementarity is concerned, Bohr insisted that the concepts of momentum and position work only within a specific experimental context. The two particles can live either in the same context, in which case limited comparisons of the same properties can be made, or not, in which case we have two separate bundles of information that cannot be related to one another.

13.4.4 Einstein and Bohr

These two great physicists were never able to reach a common ground; their philosophical viewpoints were entirely different.

Einstein maintained as a point of principle that the probabilities in quantum mechanics were unacceptable in a fundamental theory. He had himself pioneered the use of statistics in calculating the behavior of large numbers of particles (e.g.,

Brownian motion), but this was different. The assumption had always been that the particles involved had properties such as position and momentum; it was just that there were so many of them that individual calculations could not be done, hence the need to average and use statistics.

Bohr and his followers believed that the probability in quantum theory was fundamental, not a consequence of our inability to measure or calculate.

Einstein was quite convinced that there would be another layer of theory underneath quantum mechanics and that the *hidden variables* of this theory would remove the need to use probability. In this sense, quantum mechanics had to be incomplete.

In 1905, Einstein, in a letter to Schrödinger, wrote, *the fundamentally statistical character of the theory is simply a consequence of the incompleteness of the description ... it is not surprising that the fellows struggle against admitting it (even to themselves)*.

13.5 Schrödinger Introduces Entanglement

It is rather discomfoting that the theory should allow a system to be steered or directed into one or the other type of state at the experimenter's mercy in spite of his having no access to it.

Erwin Schrödinger

The term **entanglement** probably entered the physics vocabulary in an essay by Schrödinger, which he read to the Cambridge Philosophical Society in 1935. At the start of the article, Schrödinger argues that the state of a system of two particles that have interacted generally cannot be written as a product of individual states for each particle.

$$|\text{Particle A interacting with B}\rangle \neq |A\rangle |B\rangle \quad (13.59)$$

Such a state would be an *entanglement* of individual states in which you cannot say with certainty which particle is in which state. A state such as

$$|\text{singlet}\rangle = \frac{1}{\sqrt{2}} (|U\rangle |D\rangle - |D\rangle |U\rangle) \quad (13.60)$$

is an entangled state as the first particle could be in either $|U\rangle$ or $|D\rangle$. Of course, there is an even more general situation in which the amplitude function relates to both sets of physical variables in one function $\phi(x_1, x_2, x_3, \dots, x_n)$.

The basis of the EPR argument, and the Bohm variation, is that the system starts in an entangled state. Schrödinger saw entanglement as the defining

characteristic of quantum mechanics: the thing that made it totally different from classical physics. To emphasize this he discussed the disentanglement that happens when a measurement is made. Measuring the spin of particle A allows us to deduce the spin of B if they are in the singlet state. We have collapsed the combined state into one of the two entangled possibilities. In Schrödinger's view this disentanglement is of key (he used the word *sinister*) importance as it is involved in every act of measurement.

13.5.1 Entanglement and Measurement

We now repeat an argument we made earlier about measurement and collapse on entangled states.

The possible vertical spin states of an electron moving toward an S-G magnet are $|U\rangle$ and $|D\rangle$. If we use quantum theory to describe the S-G magnet itself, its possible states are going to be $|\phi_n\rangle$ (n for neutral, the resting state of the apparatus), $|\phi_U\rangle$ (U for UP showing the apparatus is registering the UP state of the electron), and $|\phi_D\rangle$ (D for DOWN registering the DOWN state of the electron).

We might know that the electron is in the state $|U\rangle$ before it reaches the S-G magnet (as we have passed it through one beforehand), in which case the state of the combined system before the interaction of the electron and the S-G magnet must be $|U\rangle|\phi_n\rangle$. After the interaction, if the measuring device is any good, the state will have evolved into $|U\rangle|\phi_U\rangle$ - a process governed entirely by the equations of quantum theory (the Schrödinger equation or the $\hat{U}(t)$ operator).

$$|U\rangle|\phi_n\rangle \xrightarrow{\text{evolves into}} |U\rangle|\phi_U\rangle \quad \text{or} \quad |U\rangle|\phi_U\rangle = \hat{U}(t)(|U\rangle|\phi_n\rangle) \quad (13.61)$$

Note that no collapse of the state has taken place, just the evolution of the state of the S-G apparatus from $|\phi_n\rangle$ to $|\phi_U\rangle$ during the interaction.

For the first time we are treating the measuring device as something that can be described by quantum theory as well, rather than the incomplete statements made earlier that the measuring device collapses the state.

If we take quantum theory seriously as the underlying theory of all reality, we surely have to describe measuring device, such as S-G magnets, in a quantum way as well. Yet if we do this, a state does not collapse when a measurement takes place; it simply entangles with the states of the equipment.

To see why this happens let us look at how things pan out if we do not know the initial state of the electron. In such a case, we have to write its state as

$$|\psi\rangle = a|U\rangle + b|D\rangle \quad (13.62)$$

where $|a|^2 + |b|^2 = 1$.

The initial joint state of the electron and the S-G devices is

$$|\psi\rangle|\phi_n\rangle = (a|U\rangle + b|D\rangle)|\phi_n\rangle \quad (13.63)$$

Based on the linearity property of QM this should evolve into

$$(a|U\rangle + b|D\rangle)|\phi_n\rangle \Rightarrow a|U\rangle|\phi_U\rangle + b|D\rangle|\phi_D\rangle \quad (13.64)$$

and now we have an entangled state to deal with.

The state still has not collapsed. So what are we to do now? Well, one reasonably obvious suggestion is to consider what happens when a passing physicist comes to the apparatus to *read off* the measurement results. If we consider ourselves as part of the same universe as everyone else (and I do, no matter what any of you might think), we presumably have to be described by quantum theory as well. We must have states such as

$$|\text{physicist has not looked yet}\rangle, |\text{physicist sees UP}\rangle, |\text{physicist sees DOWN}\rangle \quad (13.65)$$

To record the results, we have to interact with the apparatus so that

$$\begin{aligned} (a|U\rangle|\phi_U\rangle + b|D\rangle|\phi_D\rangle)|\text{physicist has not looked yet}\rangle \Rightarrow \\ a|U\rangle|\phi_U\rangle|\text{physicist sees UP}\rangle + b|D\rangle|\phi_D\rangle|\text{physicist sees DOWN}\rangle \end{aligned} \quad (13.66)$$

and we become part of the entanglement as well. See the discussion of the *Wigner's friend* later.

This is probably why Schrödinger felt that entanglement was so sinister: there seems to be no way to stop it from spreading until the whole universe is part of a stupendous entangled state. This process is called an *infinite regression*. We will have more to say about this later.

13.5.2 That Damned Cat

One can even set up quite ridiculous cases. A cat penned up in a steel chamber, along with the following device (which must be secured against direct interference by the cat): in a Geiger counter there is a tiny bit of radioactive substance, so small, that perhaps in the course of one hour one of the atoms decays, but also, with equal probability perhaps none; if it happens, the counter tube discharges and through a relay releases a hammer which shatters a small flask of hydrocyanic acid. If one has left this entire system to itself for an hour, one would say that the cat still lives if no atom has decayed. The wave function of the entire system would express this by having in it the living and dead cat (pardon the expression) mixed or smeared out in equal parts.

The sorry tale of Schrödinger's cat has assumed the status of a quantum mechanical fairy story. It is amazing how thoroughly this cat has entered the quantum zeitgeist when you consider that this quoted paragraph above is the only reference to the unfortunate creature in the whole of Schrödinger's written output. See figure below.

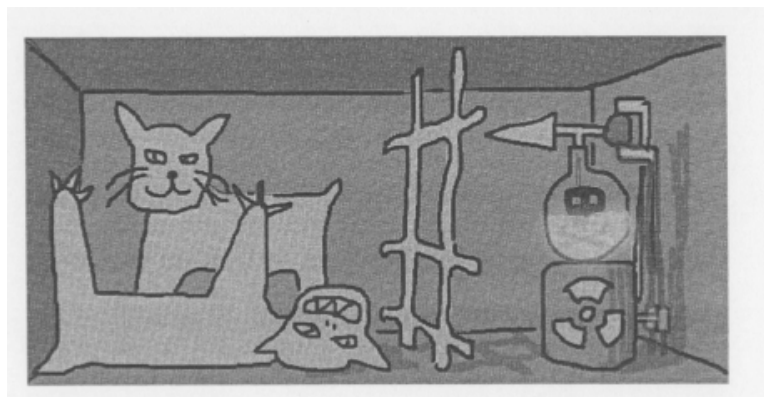


Figure 13.2: Schrödinger cat setup

In the standard Schrödinger's cat experiment a small radioactive device is linked to a trigger controlling the release of a poison gas. After a period of time, the quantum state of the radioactive device is a superposition of states

$$|\text{decayed}\rangle + |\text{not decayed}\rangle \quad (13.67)$$

The state of the gas and ultimately the state of the cat are entangled with this, so that it is not possible to tell in the quantum description if the cat is alive or dead.

Schrödinger brought the cat to our attention as a means of illustrating the bizarre nature of entanglement and the superposition of quantum states. It is worth remembering that when we introduced superposition, the fact that quantum states can be combinations of states that would not make sense classically, it was because we needed it to describe quantum systems. Entanglement follows directly from this. Schrödinger's cat illustrates the problem of scale. At what scale do classically forbidden combinations stop being allowed? Experimentally we see that a photon seems to be able to travel in two directions at once, but surely a cat cannot be alive and dead at the same time.

Trying to look inside the experiment to see if the cat is alive or dead doesn't improve the situation. As we saw earlier, our state would become entangled with things as well.

This discussion is once again dabbling with the measurement problem, which

is a crucial issue for any interpretation of quantum theory. We will see later in these notes that Bohr dissolved the problem by insisting that at some point a measuring device or cat or person has to be described classically, breaking the chain of entanglement.

13.5.3 Schrödinger's Cat and Wigner's Friends

According to the Copenhagen interpretation, the state vector for 2-particle quantum state does not disentangle as particles separate in space-time. Instead of changing into two separate vectors, one associated with each particle, the state vector remains entangled and, when a measurement is made, the state collapses instantaneously no matter how large the separation distance.

EPR's view of physical reality says that if two particles are isolated from each other, then they are no longer described by single state vector when a measurement is made.

The reality they are referring to is called *local reality* and the ability of particles to separate into 2 locally real independent physical entities is called *Einstein separability*.

In the EPR experiment, the Copenhagen interpretation or standard view of quantum theory (which we will discuss in detail later) denies that the 2 particles are Einstein separable and thus denies they are locally real until a measurement is made on one or other, at which point both become localized and real (the so-called collapse process).

13.5.4 Entangled States and Schrödinger's Cat - Another Presentation

Schrödinger proposed a most famous QM paradox.

In our earlier discussions, the notion of the collapse of a state vector was presented without reference to the point in the measurement process at which the collapse occurs.

One might assume that collapse occurs at the moment a microscopic quantum system interacts with macroscopic measuring device.

Is this assumption justified?

A macroscopic measuring device is composed of microscopic entities - molecules, atoms, protons, neutrons and electrons. Interactions takes place on microscopic level, which should use quantum mechanics for their description.

Suppose a microscopic quantum system described by state vector $|\psi\rangle$ interacts

with measuring instrument (any device which responds to an interaction with a quantum system producing macroscopic results like pointers or dials) with two measurement eigenstates $|\psi_+\rangle$ and $|\psi_-\rangle$.

These eigenstates combine with macroscopic device to reveal one of 2 possible outcomes of a measurement, deflection of pointer to left (+ result) or right (- result).

Recognizing that the instrument itself consists of quantum particles, we describe the state of instrument before measurement by a state vector $|\varphi_0\rangle$, corresponding to central pointer position.

The total state of the quantum system+measuring instrument before the measurement is made described by state vector $|\Phi_0\rangle$, is given by

$$|\Phi_0\rangle = |\psi\rangle |\varphi_0\rangle = \frac{1}{\sqrt{2}} (|\psi_+\rangle + |\psi_-\rangle) |\varphi_0\rangle = \frac{1}{\sqrt{2}} (|\psi_+\rangle |\varphi_0\rangle + |\psi_-\rangle |\varphi_0\rangle) \quad (13.68)$$

where $|\psi\rangle$ has been expressed in terms of its measurement eigenstates (we assume that they form an orthonormal basis as usual) and where

$$\langle\psi_-|\psi\rangle = \langle\psi_+|\psi\rangle = \frac{1}{\sqrt{2}} \quad (13.69)$$

i.e., both final pointer results are equally probable.

Here is a description of what happens if we treat the macroscopic measuring instrument as quantum object. We are repeating this discussion again because it is so important.

First, how does $|\Phi_0\rangle$ evolve in time during act of measurement?

From earlier discussions, we know the application of a time evolution operator \hat{U} allows us to calculate the state vector at later time, which we denote by $|\Phi\rangle$, as

$$|\Phi\rangle = \hat{U} |\Phi_0\rangle \quad (13.70)$$

or

$$|\Phi\rangle = \frac{1}{\sqrt{2}} (\hat{U} |\psi_+\rangle |\varphi_0\rangle + \hat{U} |\psi_-\rangle |\varphi_0\rangle) \quad (13.71)$$

What is effect of \hat{U} on these states?

If the instrument interacts with a quantum system which is already present in one of measurement eigenstates ($|\psi_+\rangle$ say), then the total system (quantum system+instrument) must evolve into product quantum state $|\psi_+\rangle |\varphi_+\rangle$, i.e.,

$$\hat{U} |\psi_+\rangle |\varphi_0\rangle = |\psi_+\rangle |\varphi_+\rangle \quad (13.72)$$

or, in other words, if the quantum system is in a state (with probability = 1) corresponding to a definite pointer position, then the measuring device state must evolve into a state where the pointer is pointing to the proper place. This is what happens in the laboratory.

Similarly, we must have

$$\hat{U} |\psi_{-}\rangle |\varphi_0\rangle = |\psi_{-}\rangle |\varphi_{-}\rangle \quad (13.73)$$

Using these special case results, we then have for the evolution of any arbitrary state the result

$$|\Phi\rangle = \frac{1}{\sqrt{2}} (|\psi_{+}\rangle |\varphi_{+}\rangle + |\psi_{-}\rangle |\varphi_{-}\rangle) \quad (13.74)$$

where the measuring device states $|\varphi_{+}\rangle$ and $|\varphi_{-}\rangle$ correspond to the pointer ending up at + or - , respectively.

This result suggests that the measuring instrument evolves into superposition state in which pointer has equal probability to point either to the left or right, but *not into a definite pointer state*.

Thus, neither quantum system nor pointer has a definite value.

This state will remain a superposition (pointer does not point) *unless we allow for collapse* so that the pointer can point (take on a definite value)!

If this were the final state of the system, then the pointer should never settle down and point somewhere! It has even been suggested that it would have to *flutter* back and forth between the two macroscopically different pointer positions.

Collapsing the state vector of system + measuring-device seems to require a further measurement.

But then whole argument can be repeated ad infinitum and we keep getting larger and larger superpositions (the infinite regression mentioned earlier).

Are we therefore locked into an endless chain of measuring processes?

At what point does chain stop or at what point does the state vector collapse so we see the pointer actually pointing?

This problem is created by our inability to obtain collapse of state vector using a continuous, deterministic equation of motion from which the time evolution operator is derived.

Schrödinger called state vector $|\Phi\rangle$ given above *entangled* because, once generated, it is impossible to separate into constituent parts except by invoking some

kind of nondeterministic collapse - some discontinuous process - some non-unitary time evolution.

Such a collapse is not accounted for in equations of orthodox quantum theory ... we had to add it as a fifth postulate.

The paradox of Schrödinger's cat (another repeat) is designed to show up this apparent absurdity by shifting focus from microscopic world of sub-atomic particles to the macroscopic world of cats and human observers.

A cat is placed in steel chamber together with radioactive source, a detector, a hammer mounted on pivot and bottle of prussic acid. The chamber is closed. From the amount of radioactive material in the source and the known time for its decay(half-life), it is expected that within one hour the probability is $1/2$ that one atom has disintegrated (decayed). If an atom does disintegrate, then the detector is triggered sending a signal to release the hammer that smashes the bottle releasing prussic acid which kills the cat. The essential ingredients are shown in the figures below

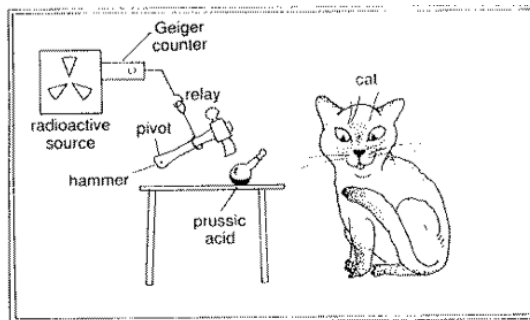


Figure 13.3: Cat alive

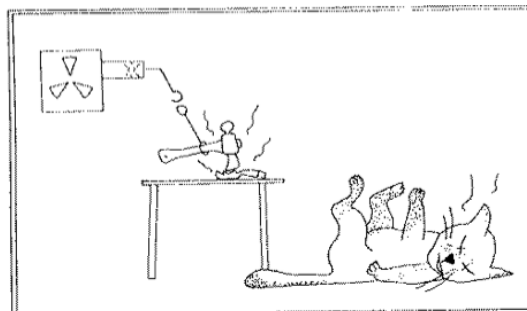


Figure 13.4: Cat dead

Prior to actually measuring a disintegration, the state vector of the radioactive atom must be expressed as linear superposition of measurement eigenstates, corresponding to the physical states of undecayed atom and decayed atom.

However, as seen above, treating the measuring instrument as quantum object and using the equations of quantum mechanics leads to a superposition of two possible outcomes of measurement.

But what about cat?

These arguments seem to suggest that we should express the state vector of (system + cat) as linear superposition of products of state vectors describing disintegrated atom and dead cat and of state vectors describing intact atom and live cat, i.e.,

$$|\Phi\rangle = \frac{1}{\sqrt{2}} (|\text{no decay}\rangle |\text{live cat}\rangle + |\text{decay}\rangle |\text{dead cat}\rangle) \quad (13.75)$$

where the state vector of the dead cat is shorthand for the state corresponding to triggered detector, released hammer, smashed bottle, released prussic acid and dead cat.

Prior to the measurement, the physical state of cat is therefore *blurred* - neither alive nor dead but some peculiar combination of *both alive and dead* states. We can perform a measurement on the (system+cat) by opening the chamber and determining its physical state.

Do we suppose at that point (system+cat) collapses and we record the observation that cat is alive or dead as appropriate?

What happens?

The only result that QM predicts is that if we set up N (N large) similar systems, then when we open the N boxes after 1 hour we will find 1/2 the cats alive and 1/2 the cats dead.

That is what actually happens experimentally.

Millions of measurements and probability always wins!

Although obviously intended to be somewhat tongue-in-cheek, Schrödinger's paradox nevertheless brings our attention to important difficulty we must confront.

The Copenhagen interpretation will say elements of empirical reality are defined by the nature of experimental apparatus we construct to perform measurements on a quantum system. It insists we resist temptation to ask what physical state

a particle (or a cat) was actually in prior to measurement as this question is without any meaning within this interpretation of QM.

This positivist interpretation sits uncomfortably with some scientists, particularly those with a special fondness for cats.

Some have accepted the EPR argument that quantum theory is incomplete. They have set about searching for an alternative theory, one that allows us to attach physical significance to properties of particles without need to specify the nature of measuring instrument, that allow us to define independent reality and that reintroduces strict causality.

Even though searching for such a theory might be engaging in meaningless metaphysical speculation, they believe that it is a search that has to be undertaken.

These are the *hidden variables* people! They have not succeeded with this approach and as we will see shortly the Bell/EPR arguments say that this is a futile search.

13.5.5 Wigner's friend - Another Entanglement Strangeness

Now we investigate the influence of *consciousness*(*the human brain*) on quantum mechanics. In the early 1960s, physicist Eugene Wigner addressed this problem using an argument based on a measurement made through the agency of a second observer. This argument is known as *paradox of Wigner's friend*.

Wigner reasoned as follows:

Suppose a measuring device is constructed which produces a flash of light every time a quantum particle is detected to be in particular eigenstate $|\psi_+\rangle$. The corresponding state of the measuring device (the one giving the flash of light) is $|\varphi_+\rangle$. The particle can be detected in one other eigenstate, $|\psi_-\rangle$, for which corresponding state of measuring device (no flash of light) is $|\varphi_-\rangle$.

Initially, the quantum particle in a superposition state

$$|\psi\rangle = c_+ |\psi_+\rangle + c_- |\psi_-\rangle \quad (13.76)$$

The combination (particle in state $|\psi_+\rangle$, light flashes) is given by the product state $|\psi_+\rangle |\varphi_+\rangle$. Similarly the combination (particle in state $|\psi_-\rangle$, no flash) is given by the product state $|\psi_-\rangle |\varphi_-\rangle$.

If we treat the combined system - (particle+measuring device) - as single quantum system, then we must express the state vector of this combined system as

$$|\Phi\rangle = c_+ |\psi_+\rangle |\varphi_+\rangle + c_- |\psi_-\rangle |\varphi_-\rangle \quad (13.77)$$

as earlier.

Thus, Wigner can discover the outcome of next quantum measurement by waiting to see if the light flashes.

However, he chooses not to do so.

Instead, he steps out of laboratory and asks a friend to observe the result.

A few moments later, Wigner returns and asks his friend if she saw a light flash.

How should Wigner analyze situation before his friend speaks?

If he considers his friend to be part of larger measuring *device* with states $|\varphi'_+\rangle$ and $|\varphi'_-\rangle$, then total system of (particle + measuring device + friend) is represented by the superposition state

$$|\Phi'\rangle = c_+ |\psi_+\rangle |\varphi'_+\rangle + c_- |\psi_-\rangle |\varphi'_-\rangle \quad (13.78)$$

Wigner can therefore anticipate there will be probability $|c_+|^2$ that his friend will answer **Yes** and probability $|c_-|^2$ she will answer **No**.

If his friend answers **Yes**, then as far as Wigner is concerned the state vector $|\Phi'\rangle$ collapses at that moment and probability that the alternative result was obtained is zero. Wigner therefore infers that particle was detected in eigenstate $|\psi_+\rangle$ and that the light flashed.

Wigner probes his friend a little further. He asks:

What did you *feel* about flash before I asked you?

To which friend replies: I told you already, I did[did not] see the flash.

Wigner concludes (not unreasonably) that his friend had made up her mind about measurement before she was asked about it.

Wigner wrote that state vector $|\Phi'\rangle = \dots\dots$ involving a superposition of $|\varphi'_+\rangle$ and $|\varphi'_-\rangle$ appears absurd at this point because it implies that his friend was in state of suspended animation before she answered his question.

And yet we know that if replace Wigner's friend with simple physical system such as a single atom, capable of absorbing light from the flash, then the mathematically correct description is in terms of the superposition $|\Phi'\rangle$, and not either of collapsed states $|\psi_+\rangle |\varphi'_+\rangle$ or $|\psi_-\rangle |\varphi'_-\rangle$.

It follows, according to Wigner, that a being with consciousness must have a different role in quantum mechanics than an inanimate measuring device like

an atom.

Of course, there is nothing in principle to prevent Wigner from assuming this friend was indeed in state of suspended animation before answering the question. However, to deny existence of the consciousness of his friend to this extent is surely an unnatural attitude.

This is **solipsism** - a view that all information delivered to your conscious mind by your senses is a figment of your imagination, i.e. *nothing exists but your consciousness*.

Wigner was, therefore, led to argue that state vector collapses when it interacts with first conscious mind it encounters.

Are cats conscious beings?

If they are, then Schrödinger's cat might be spared the discomfort of being both alive and dead: its fate has already been decided by its own consciousness before a human observer lifts lid of box.

Conscious observers, therefore, appear to violate physical laws which govern the behavior of inanimate objects.

Wigner calls up a second argument in support of his view.

Nowhere in physical world is it possible physically to act on an object without some kind of reaction.

Should consciousness be any different?

Although small, the action of a conscious mind in collapsing the state vector must produce an immediate reaction – the knowledge of the state of system is irreversibly generated in the mind of observer.

This reaction may lead to other physical effects, such as the writing of the result in a laboratory notebook or publication of research paper.

In this hypothesis, an influence of matter over mind is balanced by an influence of mind over matter.

We will have more to say of these kind of concepts later.

13.5.6 John Bell and Bohm's EPR

Einstein believed in a layer of reality underneath quantum theory that contains *hidden variables* - properties of particles that we have not yet discovered. Think

of it like this. When you look at an old-fashioned mechanical clock face, you can see the hands going around, but you may not be able to see the hidden mechanisms driving them. A careful study of the hands as they move might enable us to figure out the properties of the clock, but we would have a much better understanding if we could get inside to see the workings. In Einstein's view quantum mechanics is a theory of the hands; we need another theory that looks inside the mechanism. At the moment we cannot see the *mechanism* inside quantum systems, as we've not discovered the *hidden variables* involved.

As we do not have a technique for measuring these hidden variables (if they exist), we cannot make definite predictions about the outcome of experiments. When we repeat experiments, we are effectively averaging over the various (unknown) possible values of these variables, which is why we end up using probability in quantum theory.

In 1964, John Bell demonstrated to the physics community that any hidden variable theory that could reproduce EPR-type entangled states would have to break another of Einstein's most cherished assumptions about the way the world works, namely, *local causality*.

Take causality, the view that everything happening in the world is due to something else (the cause) happening first, and glue it to the assumption that nothing can travel faster than light (central to Einstein's theory of relativity), and you have *local causality*.

When particles interact with one another, they can potentially influence one another's properties. For example, if we measure the spin state of particle A, it's possible that the result of the measurement can influence the properties of particle B: but there has to be a time delay. Whatever the connection between A and B, information can flow between them only at speeds less than that of light. So, if we measure A and then B somewhere far enough away, the fact that A has been measured will not have reached B yet and so can have no influence on the measurement we make of B. This is what we mean by local causality. Particle A can only influence other particles that happen to be in its locality.

Bell wondered if a local hidden variable theory could properly reproduce all the results of quantum theory, especially when dealing with EPR-type entangled states. To bring this out, let's look at a Bohm-type EPR experiment using spin states.

Let's imagine that there's some set of hidden variables determining the results of spin measurements on particles. If we create two particles in a singlet state (as shown below), then these hidden variables must have opposite values in each particle.

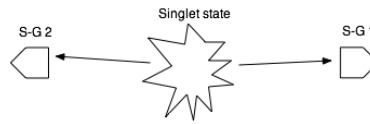


Figure 13.5: Bohm-EPR spin state experimental setup

In this experiment two particles, created in a singlet state, are heading toward a pair of S-G magnets. The right-hand side S-G magnet is much closer to the place where the particles were created.

If we could read these values we would know that particle A was UP (say) and particle B was DOWN. As we don't know the values, we have to mix both possibilities for each particle into an entangled state. Of course, if we took a series of repeated measurements and found A always UP and B always DOWN, then we could avoid using the entangled state. As we do not see that happening in these experiments, we have to assume that the values of the hidden variables are randomly determined when the particles are created. The spins are always opposite, but which value each one has comes out randomly.

Particle A now reaches S-G 1, a magnet set to some arbitrary angle. As a result of the measurement we either get UP along this S-G angle or DOWN. The probability of each would not be 50:50 unless the S-G angle happens to be vertical.

If we wanted to calculate the probability of UP along the S-G angle, we would have to look at the angle between the S-G 1's axis and the vertical. That's a standard quantum theoretical calculation and the details are not important here.

The point is this. While the particles are able to interact with one another, it's possible that the values of the hidden variables in one can alter the values in the other. When A is measured the interaction between A and S-G 1 might alter its hidden variables, and that information could be communicated to B and so have some influence on what happens when we measure B.

If we set things up so that S-G 1 and S-G 2 are far apart, there is not time enough for any information to travel from S-G 1 to S-G 2 before particle B reaches S-G 2. So the only things that can influence what happens when particle B reaches S-G 2 are the values of its hidden variables, which were supposedly set when the particles were created.

Compare this with what will happen from the quantum mechanical point of view. When the first measurement takes place at S-G 1, the entangled state of both particles will collapse producing a 50:50 UP:DOWN result *no matter*

what the angle of S-G 1 is. If you remember we showed that a vertical singlet state was also a horizontal singlet state. At that moment the spin direction of particle A manifests along the line of the magnetic field in S-G 1 and at the same moment the spin direction of B must manifest itself opposite to that. If S-G 1 records UP, the the particle B arrives at S-G 2 in the DOWN state *along the axis of S-G 1*. If S-G 2 is pointing along the same axis, then it is bound to record DOWN for particle B, if not, then it will get UP and DOWN along its axis according to how it is oriented with respect to S-G 1.

Crucial to this is the collapse of the state affecting both particles at the same time(if in fact we can continue to think of them as separate particles when they are in an entangled state).

If a hidden variable theory is going to match the effects of state collapse, the information from one measurement has to get to the other and if we set up the experiment correctly, it will have to do so faster than the speed of light.

By assuming that a hidden variable theory had to obey the rule of local causality, Bell was able to derive a formula to compare the results of each measurement over a long run of trials.

An experiment can then test Bell's formula to see if the quantum description is correct or if local hidden variables can work.

13.5.7 Bell's Formula

Many versions of Bell's formula have been produced since his original article in 1964. Earlier in section 13.3 we presented a simple version of Bell's idea. We will now present several different versions of Bell's idea each with increasing complexity. We will first present the following argument due to d'Espagnat.

At the start we build an experiment so that the S-G magnets can be set to one of three angles 0° , 45° and 90° . We also allow the magnets to switch between the angles randomly as the experiment goes on. Then we simply sit back and watch singlet states pass through both magnets and count up the results.

If the results from the two magnets have no influence on one another, then we should find that

$$N[\text{S-G1}(0^\circ)\text{UP}, \text{S-G2}(45^\circ)\text{DOWN}] + N[\text{S-G1}(45^\circ)\text{UP}, \text{S-G2}(90^\circ)\text{DOWN}] \geq N[\text{S-G1}(0^\circ)\text{UP}, \text{S-G2}(90^\circ)\text{DOWN}] \quad (13.79)$$

In this formula, N is the number of pairs of particles counted satisfying a set of conditions [...], the conditions being inside the square brackets. For example, in

$$N[\text{S-G1}(0^\circ)\text{UP}, \text{S-G2}(45^\circ)\text{DOWN}] \quad (13.80)$$

N is the number of times particle A registered spin UP in S-G1 when it was set to 0° along with particle B registering as DOWN when S-G2 was set at 45° .

Although the formula looks rather complicated, we can see how it works with the aid of the figure below, which shows how Bell's formula

$$N(A, \bar{B}) + N(B, \bar{C}) \geq N(A, \bar{C}) \quad (13.81)$$

is derived. Note that in the formula, if A means passes test A , then \bar{A} means fails test A .

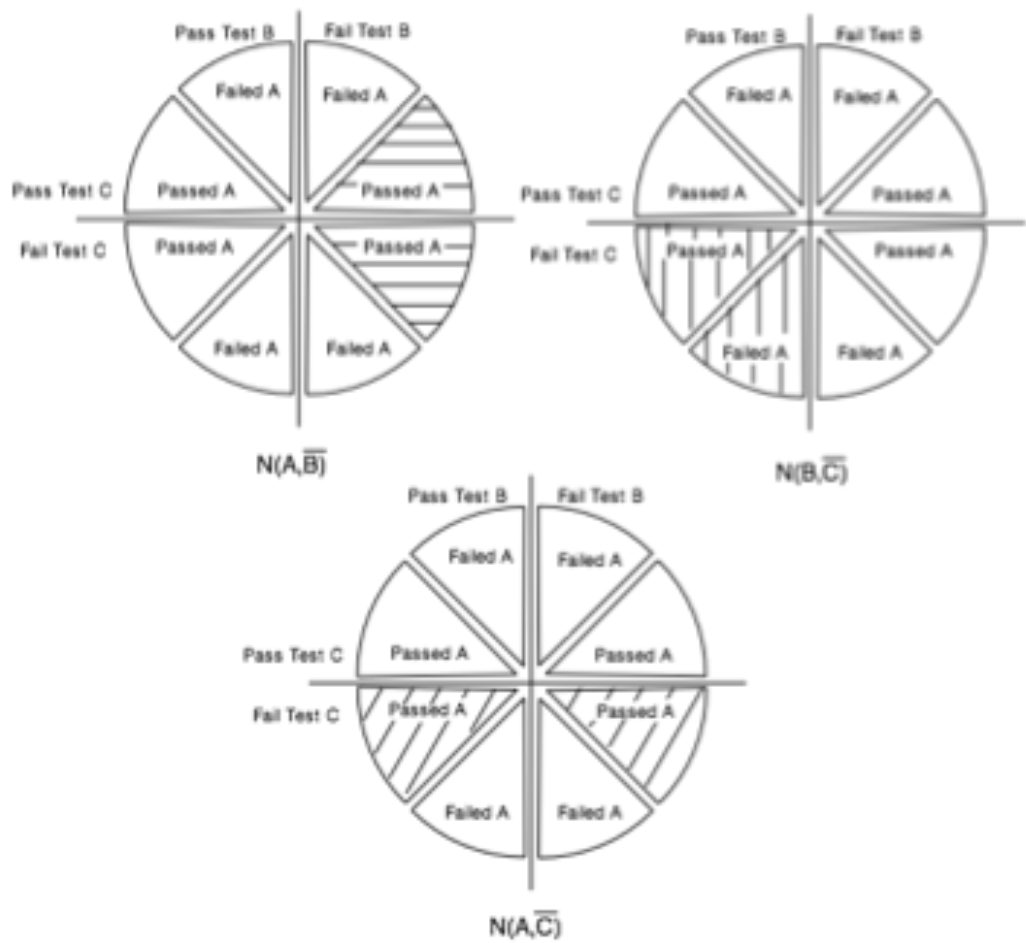


Figure 13.6: Proof of Bell's formula

To make things easier, forget about particles for the moment. Replace the idea of measuring particle spins with that of passing or failing different tests - A , B , and C . The different tests are going to stand for different angles of the S-G magnets. Passing means spin UP and failing means spin DOWN along that angle. The first test we set up will be the equivalent of a measurement at S-G1 and a second measurement at S-G2. We're also going to assume that the result of one test has no effect on the next.

A symbol like $N(A, \bar{C})$ is going to stand for the number of times we pass test A first and then fail (\bar{C}) test C , or in experimental terms the number of pairs that were spin UP in S-G 1 set to angle A and spin DOWN in S-G 2 set to angle C .

Now look at the figure. The figure is broken up into three pie charts, each of which stands for one part of the formula. Each pie chart is divided by vertical and horizontal lines. The left-hand side of each vertical line stands for passing test B , the right-hand side for failing test B . Above the horizontal line stands for passing test C and below for failing test C . Scattered around the segments of the pie charts are passing and failing tests A . All three possibilities are equally represented in the pie charts.

In the top left chart, the lined segments represent the times that test A was passed and test B failed: $N(A, \bar{B})$. In the top right chart, the lined segments are the number of occasions that B was passed and C failed: $N(B, \bar{C})$. Finally, in the bottom chart the lined segments are passing A but failing C : $N(A, \bar{C})$.

Now if we look closely and compare the three charts, we see that the checked segments in the bottom chart have already been covered by the dotted regions in the other two charts, but with area to spare. So,

$$N(A, \bar{B}) + N(B, \bar{C}) \geq N(A, \bar{C}) \quad (13.82)$$

which is d'Espagnat's version of the Bell formula.

The startling thing about this demonstration is that it shows how few assumptions need to be used in deriving Bell's formula and that it is a simple property of numbers and standard logic.

The formula itself has nothing to do with quantum theory. It's simply a relationship between numbers that fall (using standard logic) into certain categories.

Amazingly, quantum physics **does not obey** this formula.

13.5.8 Aspect's Experiment

Although d'Espagnat's version of Bell's formula might be relatively easy to demonstrate, it is not easy to test in an experiment. Generally, a different

formula is used, which we will quote here but not derive:

$$|E(a, b) - E(a, b')| + E(a', b) + E(a', b') \leq 2 \quad (13.83)$$

for a local hidden variable theory ($E(a, b)$ is defined below).

The terms in the expression directly relate to the experimental arrangement in the figure below which shows Aspect's experiment to test Bell's formula.

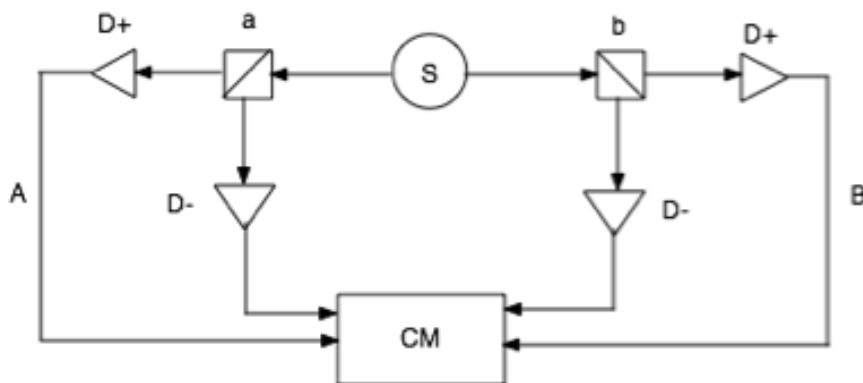


Figure 13.7: Aspect's experimental setup

The vertical lines in the first term simply mean that we always take the positive value of the quantity. For example, if $E(a, b)$ was 0.5 and $E(a, b')$ was 0.7, then

$$|E(a, b) - E(a, b')| = |0.5 - 0.7| = |-0.2| = 0.2 \quad (13.84)$$

By the way, the collection of terms on the left-hand side is often called the S parameter, so a simplified version would be $S \leq 2$.

The idea of the experiment is to measure the S value and see if it fits the quantum theoretical description which has $S > 2$.

In 1982 Alain Aspect's team at the Institute for Optics in Paris performed a significant test of Bell's formula since it was the first experiment that allowed the detector angles to be changed while the particles were in flight (see above figure).

Source S produces a pair of photons in a combined singlet state. Either side of the source are the equivalents of S-G magnets for photons (polarizers). These devices, labelled A and B, check the polarization of the photons (their equivalent of spin).

If a photon entering device A is *spin UP* along the device's angles, it is detected by D+, if not it is picked up by D-. The same is true on the right-hand side

in device B . The devices can be set to different angles: the left-hand one can be set to either angle a or a' , the right-hand one to b or b' . Each of the four detectors feeds into a *coincidence monitor* (CM), which counts the number of times we get each possibility (*in coincidence=simultaneously*):

N_{++} which is UP at A and UP at B
 N_{--} which is DOWN at A and DOWN at B
 N_{+-} which is UP at A and DOWN at B
 N_{-+} which is DOWN at A and UP at B

The experiment is run while allowing A and B to switch their angles between a and a' and b and b' , respectively. Finally we use these counts to construct

$$E(a, b) = \frac{(N_{++} + N_{--}) - (N_{+-} + N_{-+})}{N_{++} + N_{--} + N_{+-} + N_{-+}} \quad (13.85)$$

which is a sort of expectation value for the results.

Aspect's experiment was conducted with the angles $a = 0^\circ$, $a' = 45^\circ$, $b = 22.5^\circ$, and $b' = 67.5^\circ$; a combination predicted by the quantum mechanical calculation to break Bell's formula by the largest amount.

In all this detail, it is important not to lose sight of the purpose of the experiment and the significance of Bell's formula. If the experimental information fits Bell's formula, so that $S \leq 2$, then quantum mechanics is wrong and could possibly be replaced by a hidden variable theory subject to the condition of local causality. If $S > 2$ the local causality is broken and it seems that the results of one measurement can influence the results of another, although a signal traveling at the speed of light would not have a chance to reach the second measurement in time.

The experiment represents a crucial step in our understanding of quantum reality. Working with the angles used in Aspect's experiment, quantum theory predicts $S = 2.828$. This value has to be *massaged* slightly to take into account the detector's efficiency (sometimes they miss things), which reduces S to 2.70. Aspect's team measured $S = 2.697 \pm 0.015$, clearly in agreement with quantum theory and breaking Bell's formula. Not only that, but the measured results also coincided exactly with the quantum theory predictions for the separate terms in Bell's formula.

Since Aspect's pioneering experiment, other teams have tried to check these results and in every case quantum theory has come out correct. In 2001, a team from the University of Innsbruck used two detectors (Alice and Bob) 400 m apart to check the formula. Their detection efficiency was such that the quantum mechanical prediction was $S = 2.74$ and they measured $S = 2.73 \pm 0.02$. The conditions of the 2001 experiment place an even greater restriction on things,

since the choice of angle at each detector was truly random, the angles set after the photons had left the source and the results stored at each detector and compared only after the experiment had been completed. All of these totally rule out any communication between the two photons, or even the two detectors, that could explain the results.

13.5.9 Implications

Einstein could not have seen where the EPR argument would lead: from Bohm's simpler and more practical version, to Bell's analysis in terms of local hidden variables to Aspect's experiment and the results that have been produced since.

Quantum theory has survived every test thrown at it and thanks to Bell's argument, it now seems impossible that it will ever be replaced by a local hidden variable theory. Of course, the option of a hidden variable theory that does not obey local causality is still on the table. The experimental results showing correlations between the two detectors could be explained by *communication* between the two particles traveling faster than the speed of light, something that would hardly have made Einstein feel any better about things.

Quantum theory survives Bell's test because entangled states collapse at the first measurement. Remarkably this collapse affects both particles in the entangled state no matter how far apart they may be. Bohr simply shrugged this off as a consequence of having to use the same experimental context for both particles, an argument that is logically compelling but does not seem to do justice to the remarkable properties of entangled states.

Bell's formula is broken by an entangled state, so if we want to take a realistic view of what's happening, state collapse has to be a real physical change happening everywhere at once. Perhaps we ought to stop thinking of the two entangled particles as being separate at all.

13.5.10 BELL'S THEOREM - Alternative Presentation

Bell demonstrated that under certain conditions quantum theory and local hidden variable theories *predict different results* for the same experiments on pairs of correlated particles.

This difference, which is intrinsic to *all* local hidden variable theories and is *independent* of the exact nature of the theory, is summarized in Bell's derived inequalities.

This proof *forced* questions about hidden variables to immediately change character.

They were no longer *academic questions* about philosophy but *practical ques-*

tions of profound importance for quantum theory.

The choice between quantum theory and local hidden variable theories was no longer matter of *taste*, but matter of *correctness*.

Bertlmann's Socks

Let us derive Bell's theorem with help of a famous Dr Bertlmann (this whimsical story is by Bell himself). We will do a more mathematical derivation later.

Any philosopher in the street, who has not suffered through a course in quantum mechanics, is quite unimpressed by the Einstein-Podolsky-Rosen correlations.

She can point to many examples of similar correlations in everyday life. The case of *Dr. Bertlmann's socks* is often cited.

Dr. Bertlmann likes to wear two socks of different colors.

Which color he will have on given foot on given day is quite unpredictable. But when you see the first sock is pink you are sure the second sock will not be pink. Observation of first, and experience with Dr. Bertlmann, gives immediate information about second. There is no mystery in such correlations.

Isn't this EPR business just the same sort of thing?

Dr. Bertlmann happens to be physicist who is very interested in physical characteristics of his socks. He has secured a research grant from a leading sock manufacturer to study how his socks stand up to the rigors of prolonged washing at different temperatures.

Bertlmann decides to subject his left socks (socks A from now on) to 3 different tests:

test a washing for 1 hour at $0.0^\circ C$

test b washing for 1 hour at $22.5^\circ C$

test c washing for 1 hour at $45.0^\circ C$

He is particularly concerned about numbers of socks A that survive intact (a + result) or are destroyed (a - result) by prolonged washing at these different temperatures.

He denotes the number of socks that pass test a and fail test b as

$$n[a + b-] \tag{13.86}$$

Being a theoretical physicist, he knows that he can discover simple relationships between such numbers without actually performing tests using real socks and

real washing machines. This makes his study inexpensive and more attractive to his research sponsors.

He reasons as follows: $n[a + b-]$ can be written as the sum of the numbers of socks belonging to two subsets, one where individual socks pass test a , fail b and pass c and one where socks pass test a , fail b and fail c , i.e.,

$$n[a + b-] = n[a + b - c+] + n[a + b - c-] \quad (13.87)$$

This works because

$$P(C) + P(\text{not } C) = 1 \quad (13.88)$$

so that the above equation just says that

$$n[a + b-] = (P[c+] + P[c-])n[a + b-] \quad (13.89)$$

Similarly, we get

$$n[b + c-] = n[a + b + c-] + n[a - b + c-] \quad (13.90)$$

where individual socks pass test b , fail c and pass a and one where socks pass test b , fail c and fail a and

$$n[a + c-] = n[a + b + c-] + n[a + b - c-] \quad (13.91)$$

where individual socks pass test a , fail c and pass b and another one where socks pass test a , fail c and fail b .

From the first equation it follows that

$$n[a + b-] \geq n[a + b - c-] \quad (13.92)$$

since all the numbers involved are ≥ 0 .

Similarly, from the second equation it follows that

$$n[b + c-] \geq n[a + b + c-] \quad (13.93)$$

Adding these last two equations gives the result

$$n[a + b-] + n[b + c-] \geq n[a + b - c-] + n[a + b + c-] = n[a + c-] \quad (13.94)$$

or

$$n[a + b-] + n[b + c-] \geq n[a + c-] \quad (13.95)$$

At this stage, Dr. Bertlmann notices flaw in reasoning, which all of you will, *of course*, have spotted right at the beginning.

Subjecting one of socks A to test a will necessarily change irreversibly its physical characteristics such that, even if it survives the test, it may not give the result

for test b that might be expected of brand new sock.

And, of course, if sock fails test b , it will simply not be available(destroyed) for test c .

Thus, the numbers like $n[a + b-]$, etc, have no practical (we cannot measure them in real world) relevance.

Bertlmann now remembers his socks always come in pairs.

He assumes that, apart from differences in the color, the physical characteristics of each sock in a pair are identical.

Thus, a test performed on the right sock (sock B) can be used to predict what the result of same test would be if the test had been performed on left sock(sock A), even though the test on A is *not actually carried out* - remember this is a counterfactual statement!.

He must further assumes that whatever test he chooses to perform on B in no way affects the outcome of any other test he might perform on A , *but this seems so obviously valid that he does not give it any thought whatsoever*. Can you figure out where we are in the EPR argument?

Bertlmann now devises three different sets of experiments to be carried out on three samples each containing the *same total number* of pairs of socks.

In experiment 1, for each pair, sock A is subjected to test a and sock B is subjected to test b . If sock B fails test b , this implies that sock A would also have failed test b had it been performed on sock A .

Thus, the number of pairs of socks for which sock A passes test a and sock B fails test b , which we denote by

$$N_{+-}(a, b) \quad (13.96)$$

must be equal to the (hypothetical) number of socks A which pass test a and fail test b , i.e.,

$$N_{+-}(a, b) = n[a + b-] \quad (13.97)$$

In experiment 2, for each pair, sock A is subjected to test b and sock B is subjected to test c . The same kind of reasoning allows Bertlmann to deduce that

$$N_{+-}(b, c) = n[b + c-] \quad (13.98)$$

where $N_{+-}(b, c)$ denotes the number of pairs of socks for which sock A passes test b and sock B fails test c .

Finally, in experiment 3, for each pair, sock A is subjected to test a and sock B

is subjected to test c . In a similar manner, Bertlmann deduces that

$$N_{+-}(a, c) = n[a + c -] \quad (13.99)$$

where $N_{+-}(a, c)$ denotes the number of pairs of socks for which sock A passes test a and sock B fails test c .

The experimental arrangements are summarized below. Bertlmann, now using

Experiment	Sock A Test	Sock B Test
1	a	b
2	b	c
3	a	c

the revised calculations, concludes that we must have the inequality

$$N_{+-}(a, b) + N_{+-}(b, c) \geq N_{+-}(a, c) \quad (13.100)$$

to represent experiments. Bertlmann generalizes this result for any batch of pairs of socks by dividing each number by the total number of pairs of socks (which was same for each experiment) to arrive at frequencies with which each joint result was obtained.

He identifies these frequencies with probabilities for obtaining results for experiments to be performed on any batch of pairs of socks that, statistically, have same properties.

Thus, he finds that

$$P_{+-}(a, b) + P_{+-}(b, c) \geq P_{+-}(a, c) \quad (13.101)$$

This is **Bell's inequality** for this experiment.

Now we follow the above arguments again, replacing

- (1) socks with photons
- (2) pairs of socks with pairs of entangled photons
- (3) washing machines with polarization analyzers
- (4) temperatures with polarizer orientations

and we will still arrive at Bell's inequality, i.e., we only change the words in our description of the experiments and not the conclusions!

Our three tests now refer to polarization analyzers set with their vertical(optic) axes oriented at $a \rightarrow 0.0^\circ$, $b \rightarrow 22.5^\circ$, and $c \rightarrow 45.0^\circ$.

Experiment	Photon A Angle	Photon B Angle	Angle Difference Δ
1	$a = 0.0^\circ$	$b = 22.5^\circ$	22.5°
2	$b = 22.5^\circ$	$c = 45.0^\circ$	22.5°
3	$a = 0.0^\circ$	$c = 45.0^\circ$	45.0°

The different experimental arrangements are summarized as follows: The probabilities predicted by quantum theory for a given angle difference Δ between the polaroids in each test are given by

$$P = \frac{1}{2} \sin^2 \Delta \quad (13.102)$$

i.e., remember the matches and misses arguments.

Putting the angles above into the Bell inequality we get

$$\frac{1}{2} \sin^2 22.5^\circ + \frac{1}{2} \sin^2 22.5^\circ \geq \frac{1}{2} \sin^2 45.0^\circ \quad (13.103)$$

or

$$0.1464 \geq 0.2500 \quad (13.104)$$

which is **obviously incorrect!**

Thus, for these particular arrangements of polarization analyzers, the probability formula from quantum theory predicts results that violate Bell's inequality.

However, the quantum mechanical probability formula results agrees with experimental observations!!

The comparison of quantum mechanics and the Bell inequality is shown in the figure below:

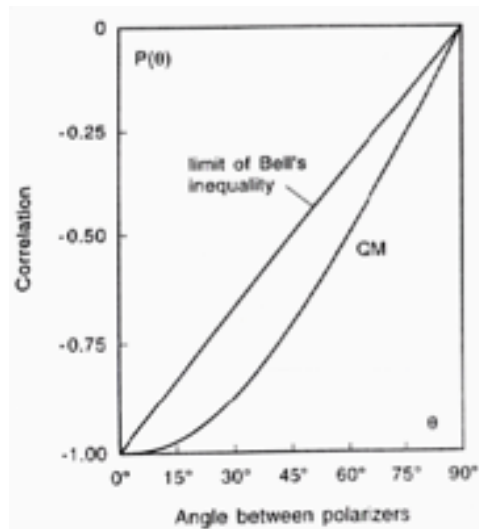


Figure 13.8: The violation of Bell's formula

The experimental demonstration of the violation of the Bell inequality on the spin correlation of proton pairs is shown below.

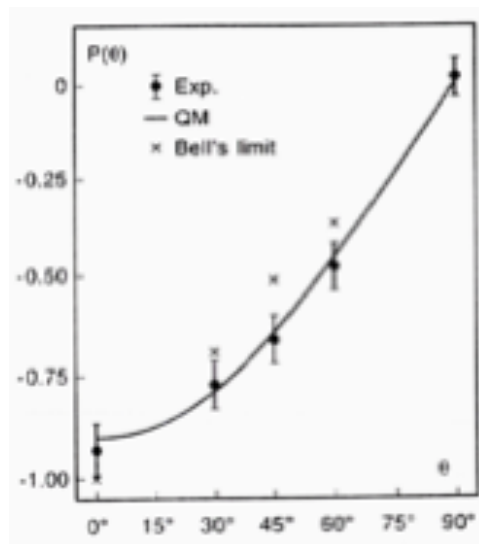


Figure 13.9: First experimental results

Clearly, quantum mechanics is correct.

The most important assumption made in the reasoning which led to the inequality was Einstein separability or local reality of the photons(or socks).

The inequality is quite independent of nature of any local hidden variable theory that could be devised.

The conclusion is inescapable.

Quantum theory is incompatible with any local hidden variable theory and hence incompatible with any form of local reality.

This means that any theory that has the same probabilistic predictions as quantum mechanics must be nonlocal.

We should not, perhaps, be too surprised by this result.

The predictions of quantum theory are based on the properties of a 2-particle state vector which, before collapsing into one of *measurement eigenstates*, is *delocalized or entangled* over the whole experimental arrangement.

The 2 particles are, in effect, always in *contact* prior to measurement and can therefore exhibit a degree of correlation impossible for 2 Einstein separable (locally realistic) particles.

Bell's inequality provides us with a straightforward test. If experiments like those described here are actually performed, the results allow us to make a choice between quantum theory and a whole range of theories based on local hidden variables and hidden variable theories are ruled out conclusively.

Bohr once declared when he was asked whether the quantum mechanical algorithms could be considered as somehow mirroring an underlying quantum reality: He said :

There is no quantum world.

There is only an abstract quantum mechanical description.

It is wrong to think that the task of physics is to find out how Nature is.

Physics is concerned only with what we *can* say about Nature.

Heisenberg said:

In the experiments about atomic events we have to do with things and facts, with phenomena that are just as real as any phenomena in daily life. But the atoms or the elementary particles are not as

real; they form a world of *potentialities or possibilities* rather than one of real things or facts.

Jordan declared:

That observations not only *disturb* what has to be measured, they *produce* it. In a measurement of position of an electron, the electron is forced to a decision.

We compel it to *assume a definite position*; previously it was, in general, *neither here nor there*; it had not yet *made its decision about a definite position*.

In the next chapter, we will do a more mathematically rigorous derivation of the EPR/Bell phenomena.

Then we will move on to a discussion of this new *quantum reality*.

Prior to doing this, however, we need to digress and look back at our earlier discussion of the density operator. This will set the stage for our later discussions.

13.6 The Density Operator

13.6.1 Useful Digression

We now present an alternate way (based on the density operator introduced earlier) of in which quantum states can be represented. It is an open question whether this alternative is a simple mathematical convenience or a more ontologically *true* representation. Either way, it has a key role to play in modern interpretations of quantum theory and also some possible solutions to the measurement problem. We first repeat the material in section 7.4.1 and then take the discussion further. This discussion is even more mathematical than the rest of these notes, but you will benefit if you persevere and you work your way through the material. **It is important.**

13.6.1.1 Great Expectations

Earlier, we introduced the *expectation value* - the average of a set of measurement results taken from a collection of systems in the same state. A straightforward calculation of the expectation value takes the following form, with \hat{O} being an operator representing the measurement of a specific physical variable and $|\phi\rangle$ the state of each system in the collection:

$$\langle \hat{O} \rangle = \langle \phi | \hat{O} | \phi \rangle \quad (13.105)$$

If we choose a basis $\{|i\rangle\}$, we can expand $|\phi\rangle$ and $\langle\phi|$

$$|\phi\rangle = \sum_i a_i |i\rangle \quad , \quad \langle\phi| = \sum_j a_j^* \langle j| \quad (13.106)$$

and plug the expansions into our formula for the expectation value:

$$\langle \hat{O} \rangle = \sum_j \left(\sum_i [a_j^* a_i \langle j | \hat{O} | i \rangle] \right) \quad (13.107)$$

To take the next step, we need to remember that $a_i = \langle i | \phi \rangle$ and $a_j^* = \langle \phi | j \rangle$, which can be used to replace the a 's in the formula giving

$$\langle \hat{O} \rangle = \sum_j \left(\sum_i [\langle \phi | j \rangle \langle i | \phi \rangle \langle j | \hat{O} | i \rangle] \right) = \sum_j \left(\sum_i [\langle i | \phi \rangle \langle \phi | j \rangle \langle j | \hat{O} | i \rangle] \right) \quad (13.108)$$

where in the last step all we have done is change the order of the terms in the square bracket.

This formula looks a bit cluttered, but if we examine it closely we find the *matrix element* of \hat{O} hiding in there, $\langle j | \hat{O} | i \rangle$, and also the combination $\langle i | \phi \rangle \langle \phi | j \rangle$. This second combination is the one that interests us at the moment. It can also be interpreted as as a matrix element, provided we remember $|\phi\rangle \langle \phi|$ is an operator.

Clearly, it transforms a state into another state as required by any operator....

$$(|\phi\rangle \langle \phi|) |\psi\rangle = |\phi\rangle \langle \phi | \psi \rangle = \alpha |\phi\rangle \quad (13.109)$$

Let us give it the name *density operator* and its own special abbreviation $\hat{D} = |\phi\rangle \langle \phi|$. The expectation value of our original operator \hat{O} can now be converted into

$$\langle \hat{O} \rangle = \sum_j \left(\sum_i [\langle i | \hat{D} | j \rangle \langle j | \hat{O} | i \rangle] \right) \quad (13.110)$$

At the core of this, still rather complicated looking expression, is the combination $\langle i | \hat{D} | j \rangle \langle j | \hat{O} | i \rangle$: the product of two matrix elements. It makes sense to think that this product must represent an element of a single matrix formed by multiplying the other two together. To make this clear, let us strip away the various states and write the product as $D_{ij} O_{ji}$. Putting the first (inner one) of the SUMs back we have

$$\sum_i [D_{ij} O_{ji}] = D_{1j} O_{j1} + D_{2j} O_{j2} + D_{3j} O_{j3} + \dots \quad (13.111)$$

To see what this is, let's just think about the product of two matrices for a moment. Following the rule we set out earlier in these notes, when we multiply

matrix A by matrix B , we get

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & \dots \\ a_{21} & a_{22} & a_{23} & \dots \\ a_{31} & a_{32} & a_{33} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} b_{11} & b_{12} & b_{13} & \dots \\ b_{21} & b_{22} & b_{23} & \dots \\ b_{31} & b_{32} & b_{33} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} = \begin{pmatrix} a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31} + \dots & a_{11}b_{12} + a_{12}b_{22} + a_{13}b_{32} + \dots & \dots & \dots \\ a_{21}b_{11} + a_{22}b_{21} + a_{23}b_{31} + \dots & a_{21}b_{12} + a_{22}b_{22} + a_{23}b_{32} + \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \quad (13.112)$$

where we only started to fill in the elements of the product. We are especially interested in the diagonal elements. The top left diagonal element term is

$$a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31} + \dots \quad (13.113)$$

which looks just like the $D_{1j}O_{j1}$ part of the expectation value since each term starts with a "1" and ends with a "1". If we put the sum over j back in, we can build the entire summation.

Equally, the second term on the diagonal of the AB matrix is

$$a_{21}b_{12} + a_{22}b_{22} + a_{23}b_{32} + \dots \quad (13.114)$$

which could be $D_{2j}O_{j2}$ if we put the sum over j back in as well. In other words, the full calculation of the expectation value is

$$\begin{aligned} \langle \hat{O} \rangle &= \sum_j \left(\sum_i [\langle i | \hat{D} | j \rangle \langle j | \hat{O} | i \rangle] \right) = \sum_j (D_{1j}O_{j1} + D_{2j}O_{j2} + D_{3j}O_{j3} + \dots) \\ &= [(D_{11}O_{11} + D_{12}O_{21} + D_{13}O_{31} + \dots) + (D_{21}O_{12} + D_{22}O_{22} + D_{23}O_{32} + \dots) \\ &\quad (D_{31}O_{13} + D_{32}O_{23} + D_{33}O_{33} + \dots)] \end{aligned} \quad (13.115)$$

and each separate term is on the diagonal of the matrix $\hat{D}\hat{O}$. The expectation value is the sum of the diagonal elements of the matrix $\hat{D}\hat{O}$.

Mathematicians have a name for adding up the diagonal elements of a matrix - it is called the *trace* of the matrix as we saw earlier. Using this name we can write

$$\langle \hat{O} \rangle = \text{Trace}(\hat{D}\hat{O}) = \text{Tr}(\hat{D}\hat{O}) \quad (13.116)$$

Why Bother?

The real power of the density operator approach comes to the fore when we have to deal with a situation in which we cannot be sure what state the system is in.

Imagine that we have a whole collection of identical systems, some of which are in state $|\phi_1\rangle$, some in $|\phi_2\rangle$, etc. We might not know which system is in which state, and we might not even know how many systems are in any one given state. As a practical example, think about a beam of electrons that has not passed through any Stern-Gerlach(S-G) magnets. Chances are that the spin states of the electrons are completely random. Perhaps the best we can know is the probability of finding an electron in each state.

$$P_1 = \text{Prob}(|\phi_1\rangle) \quad , \quad P_2 = \text{Prob}(|\phi_2\rangle) \quad , \quad P_3 = \text{Prob}(|\phi_3\rangle) \quad , \quad \dots \quad (13.117)$$

These probabilities have nothing to do with quantum theory as such; they simply represent our ignorance of the details of what is happening. They are not related to any amplitudes.

Given a situation like this, we should to be able to make some useful calculations. For example, we could work out the expectation value of any measurement. After all, if we can calculate the expectation value of each individual state, then the overall expectation value is simply

$$\langle \hat{O} \rangle = P_1 (\langle \phi_1 | \hat{O} | \phi_1 \rangle) + P_2 (\langle \phi_2 | \hat{O} | \phi_2 \rangle) + P_3 (\langle \phi_3 | \hat{O} | \phi_3 \rangle) + \dots + P_n (\langle \phi_n | \hat{O} | \phi_n \rangle) \quad (13.118)$$

To see this, think back to the original definition of the expectation value: it represents the average value of a measurement. What we have done here is put together a weighted average of the average value for each state.

Now if we construct a density operator that looks like this,

$$\hat{D} = P_1 |\phi_1\rangle \langle \phi_1| + P_2 |\phi_2\rangle \langle \phi_2| + P_3 |\phi_3\rangle \langle \phi_3| + \dots + P_n |\phi_n\rangle \langle \phi_n| \quad (13.119)$$

we can still calculate the expectation value by taking

$$\langle \hat{O} \rangle = \text{Tr}(\hat{D} \hat{O}) \quad (13.120)$$

which is rather neat.

Fans of the density operator call $\hat{D} = |\phi\rangle \langle \phi|$ a *pure state*, and $\hat{D} = P_1 |\phi_1\rangle \langle \phi_1| + P_2 |\phi_2\rangle \langle \phi_2| + P_3 |\phi_3\rangle \langle \phi_3| + \dots + P_n |\phi_n\rangle \langle \phi_n|$ an *unpure state*.

We called a combination of states such as

$$\frac{1}{\sqrt{2}} (|U\rangle + |D\rangle) \quad (13.121)$$

a mixed state, which is also a pure state. A little confusing, but that is convention.

13.6.2 Density Operator and EPR/Bohm Experiments

To see how all of this works in practice, let's consider a specific example.

A team of scientists gets funding to carry out a very large Einstein-Podolsky-Rosen(EPR) experiment of the type suggested by Bohm. They place one detector (Alice) on the Moon and another (Bob) on Earth. A space station placed much nearer to the Moon than the Earth is the source of particles in a spin 0 singlet state that fly off in opposite directions. Alice is set up to measure the vertical spin component. As the space station is nearer to the Moon, particles will arrive first at Alice, causing the state to collapse, before they arrive at Bob. However, there isn't enough time for the results of the Alice experiment to be sent to Earth before the other particle arrives at Bob.

Since we know that the particles start off in a singlet state, it's clear that if Alice measures $|U\rangle$, then the particle flying toward Bob must be in state $|D\rangle$. If Alice measures $|D\rangle$, we know that a $|U\rangle$ particle is on the way to Bob. Of course, in truth, Bob does not actually know any of this, as he does not get the results of Alice's measurement before the particle arrives on Earth.

From Bob's point of view, the experimental situation requires him to build a density operator or matrix to represent the particle heading toward him. Again, as the combination started out in a singlet state, we know that Alice has a 50:50 chance of measuring $|U\rangle$ or $|D\rangle$, so the density operator must be

$$\hat{D} = 0.5 |U\rangle \langle U| + 0.5 |D\rangle \langle D| \quad (13.122)$$

Let us use a specific representation for $|U\rangle$ and $|D\rangle$

$$|U\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |D\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (13.123)$$

$$\langle U| = \begin{pmatrix} 1 & 0 \end{pmatrix}, \quad \langle D| = \begin{pmatrix} 0 & 1 \end{pmatrix} \quad (13.124)$$

which makes our density matrix

$$\begin{aligned} \hat{D} &= 0.5 |U\rangle \langle U| + 0.5 |D\rangle \langle D| \\ &= 0.5 \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} + 0.5 \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0.5 & 0 \\ 0 & 0.5 \end{pmatrix} \end{aligned} \quad (13.125)$$

using the rules of matrix multiplication.

Note that the *off-diagonal* elements in the matrix are zero. This is by no means always the case. In some matrix representations of the density operator these elements will not be zero, but that does not matter as the expectation value is always given by tracing over the density operator multiplied by the operator.

For example, since the z component spin operator \hat{S}_z can also be written as a matrix

$$\hat{S}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (13.126)$$

the expectation value for vertical spin on the Earth is

$$\begin{aligned}\langle \hat{S}_z \rangle &= \text{Tr}(\hat{D} \hat{S}_z) = \text{Tr} \left(\begin{pmatrix} 0.5 & 0 \\ 0 & 0.5 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right) \\ &= \text{Tr} \left(\begin{pmatrix} 0.5 & 0 \\ 0 & -0.5 \end{pmatrix} \right) = 0\end{aligned}\quad (13.127)$$

which is exactly what you would expect given a 50:50 chance of UP/DOWN at the Earth end of the experiment.

So far this is all rather mundane and you might be wondering why we have bothered to introduce the density operator at all. If you can be patient for a moment longer, we will get to the point.

13.6.2.1 Representing a State

Let us look at a slightly different situation: Alice does not measure vertical spin; the S-G magnet on the Moon has been set to some other angle, say horizontal for convenience.

However, we are expecting vertical eigenstates to arrive on Earth, as we assume that's how Alice's experiment has been set up.

Half the time, Alice will measure $|R\rangle$ and so we get $|L\rangle$ on Earth. Since we do not know this, we carry on and make a vertical spin measurement of the $|L\rangle$ state, giving us $|U\rangle$ and $|D\rangle$ with equal chance.

However, if Alice measures $|L\rangle$, then we get $|R\rangle$ and the vertical measurement comes up 50:50 $|U\rangle$ and $|D\rangle$ again.

Overall, we will get half $|U\rangle$ and half $|D\rangle$, no matter what Alice comes up with. In other words, the density operator is still the same. In fact, no matter what angle Alice chooses, we get the correct expectation value using the *original density operator*.

In a fit of pure rebellion, the Alice team decides to point its magnet along some other angle α between vertical and horizontal. Half the time they will get spin UP along this angle, which we call $|\alpha+\rangle$, and half the time spin DOWN, $|\alpha-\rangle$. In terms of a vertical basis, let us assume that at angle

$$|\alpha+\rangle = \frac{1}{\sqrt{3}} (|U\rangle + \sqrt{2}|D\rangle) \quad (13.128)$$

$$|\alpha-\rangle = \frac{1}{\sqrt{3}} (\sqrt{2}|U\rangle - |D\rangle) \quad (13.129)$$

This is just choosing a particular angle!

So, half the time Alice will measure $|\alpha+\rangle$, which means that we get $|\alpha-\rangle$. On $1/3$ of those occasions, our measurement of the vertical spin axis will give us $|D\rangle$ and for the other $2/3$ of the time we get $|U\rangle$. However, if Alice measures $|\alpha-\rangle$, we get $|\alpha+\rangle$ and on $1/3$ of those occasions we measure $|U\rangle$ and the rest of the time ($2/3$) we measure $|D\rangle$. Overall, we get $|U\rangle$ and $|D\rangle$ 50% of the time each.

The density operator is correct again.

If you stop to think about it for a moment, no measurement made on Earth will tell us what angle the Alice team has chosen. This fits, as otherwise we would have invented a way of sending information faster than the speed of light. It would be like the post office on the space station sending out two letters, one to Alice and one to Bob. When the scientists of the Alice team read their letter, they find a *speeling mistook* that they correct. This collapses the state and corrects the spelling in the letter to Earth while it is still on the way. That would be faster than light signaling, something that is apparently forbidden in our universe.

The density operator is popular among some physicists as the true representation of a quantum state. They point to its ability to catch all the information that can be extracted from a quantum system. If we follow this line, we would be effectively saying there was no physical difference between $|\alpha+\rangle$ and $|\alpha-\rangle$ as far as Bob on Earth was concerned. Since Bob has not set to angle α , he cannot tell what is coming in his direction. Indeed, even if the Bob team decided to rebel and set its S-G magnet to angle α by pure luck, they will only see 50% UP along this angle and 50% DOWN, just as they would with any other angle.

It is a fair point, the density operator tells us everything that we can possibly know, but it may be pushing us further from a realistic view of quantum reality.

Chapter 14

EPR and Bell - Details

This section of the book is more technical and mathematical.

Let us first rethink some quantum mechanical ideas in a context needed for this discussion. This review will hopefully reinforce the ideas you have learned so far.

14.1 Single-Photon Interference

All good discussions on quantum mechanics present a long and interesting analysis of the double slit experiment. The crux of the discussion comes when *the light intensity is reduced sufficiently for photons to be considered as presenting themselves at the entry slit one by one.*

For a long time this point was very contentious, because correlations between two successive photons cannot be ruled out **a priori**.

Since 1985, however, the situation has changed. An experiment was performed by Grangier, Roger and Aspect. It was an interference experiment with only a single photon. They used a light source devised for an EPR experiment which guarantees that photons arrive at the entry slit singly. The experiment is difficult to do in practice, but is very simple in principle and it provides an excellent experimental introduction to the concepts of quantum mechanics.

The light source is a beam of calcium atoms, excited by two focused laser beams having wavelengths $\lambda' = 406\text{ nm}$ and $\lambda'' = 581\text{ nm}$, respectively.

Two-photon excitation produces a state having the angular momentum quantum number(value) $J = 0$. When it decays, this state emits two monochromatic photons having the wavelengths $\lambda_1 = 551.3\text{ nm}$ and $\lambda_2 = 422.7\text{ nm}$, respectively, in a cascade of two electronic transitions from the initial $J = 0$ level to the final

$J = 0$ state, passing through an intermediate $J = 1$ state. The figure below shows the excitation and decay of the calcium atom.

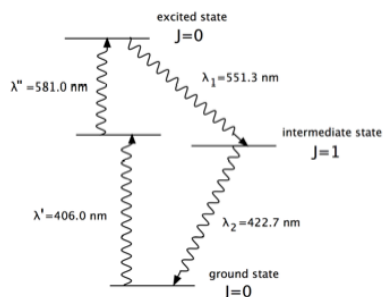


Figure 14.1: Excitation and decay of calcium atom

The mean lifetime of the intermediate state is 4.7 ns . To simplify the terminology, we shall call the $\lambda_1 = 551.3 \text{ nm}$ light *green* and the $\lambda_2 = 422.7 \text{ nm}$ light *violet*.

Next we describe the experiment, exhibiting its three stages which reveal the complications of the apparatus in progressively greater detail (next three figures).

1. The first stage is a trivial check that the apparatus is working properly; nevertheless it is already very instructive (figure below).

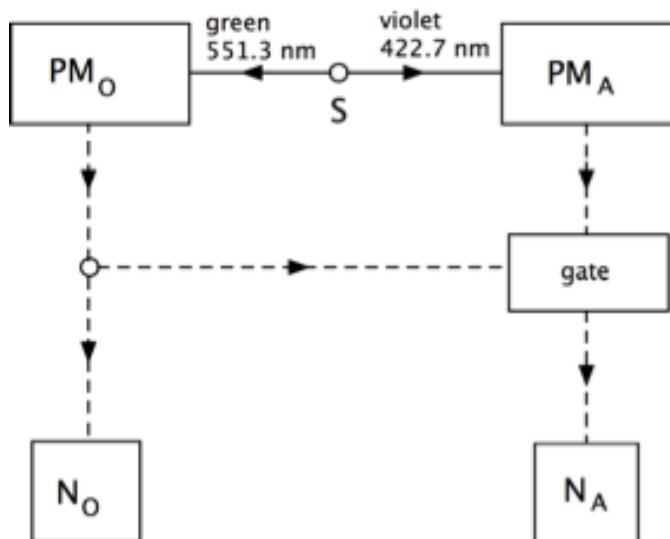


Figure 14.2: Experiment - first stage

Here we have interference with a single photon (first stage). In this sketch, solid lines are optical paths and dashed lines are electrical connections.

On either side of the source S one positions two photomultiplier tubes PM_O and PM_A . These are very sensitive, and can detect the arrival of a single photon. Detection proceeds through photoelectric absorption, followed by amplification which produces an electric signal proportional to the energy of the incident photon. The associated electronic logic circuits can identify the photons absorbed by each detector: the channel PM_O responds only to green light, and the channel PM_A responds only to violet light. The electronic gate is opened (for 9 ns - this is twice the mean lifetime and corresponds to an 85% probability that the photon has been emitted) when green light is detected by PM_O . If, while the gate is open, violet light is emitted by the same atom towards(not all of the violet photons go towards the source) PM_A , then PM_A detects this photon, producing a signal that passes through the gate and is counted in N_A . The counter N_O registers the number of green photons detected by PM_O . It turns out that $N_A \ll N_O$. As the observation period becomes very long(approximately 5 hours), the ratio N_A/N_O tends to a limit that is characteristic of the apparatus. It represents the probability of detecting a violet photon in PM_A during the 9 ns following the detection of a green photon by PM_O .

The purpose of this arrangement is to use a green photon in order to open a 9 ns time window, in which to detect a violet photon emitted by the same atom. As we will see, there is only an extremely small probability of detecting another violet photon emitted by a different atom within the same window .

We will assume that a second observer is in the lab. This observer always feels compelled to present what he thinks are *simple-minded truths* using ordinary words. We will called this second observer Albert. Albert, as we shall see, has a tendency to use, one after another, the three phrases, **I observe**, **I conclude**, and **I envisage**.

Consulted about the above experiment, Albert states, with much confidence

I observe that the photomultiplier PM_A detects violet light when the source S is on, and that it ceases to detect anything when the source is off. I conclude that the violet light is emitted by S , and that it travelled from S to PM_A .

I observe that energy is transferred between the light and the photomultiplier PM_A always in the same amount, which I will call a quantum.

I envisage the quanta as particles, emitted by the source, propagating freely from S to PM_A , and absorbed by the detector. I shall call this quanta photons.

Albert stops talking at this point.

2. The second stage of the experiment introduces the concept of individual photons (see figure below)

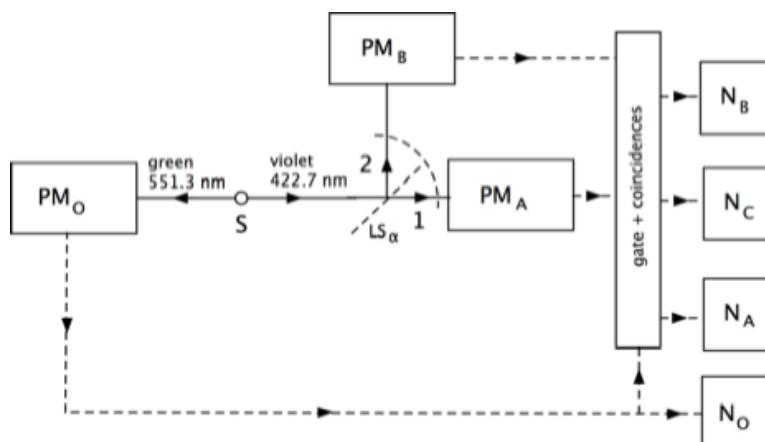


Figure 14.3: Experiment - second stage

Here we have interference with a single photon (second stage). In this sketch, solid lines are optical paths and dashed lines are electrical connections.

Across the path of the violet light one places a half-silvered mirror LS_α , which splits the primary beam into two secondary beams (equal intensity), one transmitted and detected by PM_A , the other reflected and detected by PM_B . As in the first stage, the gate is opened for $9ns$, by PM_O . While it is open, one registers detection by either PM_A (counted as N_A) or by PM_B (counted as N_B) or both, which we call a coincidence (counted as N_C). The experiment runs for 5 hours again and yields the following results:

- (a) The counts N_A and N_B are both of the order of 10^5 . By contrast, N_C is much smaller, being equal to 9.
- (b) The sequence of counts from PM_A is random in time, as is the sequence of counts from PM_B .
- (c) The very low value of N_C shows that counts in PM_A and PM_B are mutually exclusive (do not occur at same time).

The experimenters analyzed the value of N_C in depth; their reasoning can be outlined as follows:

- (a) Suppose two different atoms each emit a violet photon, one being transmitted to PM_A and the other reflected to PM_B , with both arriving during the 9 ns opening of the gate; then the circuitry records a coincidence. In the regime under study, and for a run of 5 hours, quantum theory predicts that the number of coincidences should be $N_C = 9$. The fact that this number is so small means that, in practice, any given single photon is either transmitted or reflected.
- (b) If light is considered as a wave, split into two by LS_α and condensed into quanta on reaching PM_A and PM_B , then one would expect the photon counts to be correlated in time, which would entail $N_C \gg 9$. Classically speaking this would mean that we cannot have a transmitted wave without a reflected wave.
- (c) Experiment yields $N_C = 9$; this quantum result differs from the classical value by 13 standard deviations; hence the discrepancy is very firmly established, and allows us to assert that we are indeed dealing with a source of individual photons.

Albert leaves such logical thinking to professionals. Once he notes that N_C is very small, he is quite prepared to treat it as if it were zero. He therefore says

I observe that light travels from the source to PM_A or to PM_B , because detection ceases when the source is switched off.

I observe the counts N_A and N_B correspond to a game of heads or tails, in that the two possibilities are mutually exclusive, and that the counts are random.

I observe that the optical paths 1 and 2 are distinguishable, because the experiment allows me to ascertain, for each quantum, whether it has travelled path 1 (detection by PM_A) or path 2 (detection by PM_B).

I envisage that, on arrival at the half-silvered mirror, each photon from the source is directed at random either along path 1 or along path 2; and I assert that it is the nature of photons to play heads or tails.

14.1.0.2 Digression: The Mach-Zehnder Interferometer

The next experiment uses a Mach-Zehnder interferometer. We have used this type of interferometer before. Let us look a little more carefully as to

how it operates.

Background information: Consider a single photon incident on a 50-50 beam splitter (that is, a partially transmitting, partially reflecting mirror, with equal coefficients). Whereas classical electromagnetic energy divides equally, the photon is indivisible. That is, if a photon-counting detector is placed at each of the output ports (see figure below), only one of them clicks. Which one clicks is completely random (that is, we have no better guess for one over the other).



Figure 14.4: 50-50 beam splitter

The input-output transformation of the waves incident on 50-50 beam splitters and perfectly reflecting mirrors are shown in the figure below.

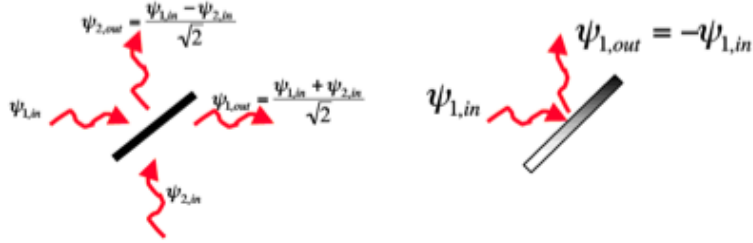


Figure 14.5: Input-output transformations

It turns out that with these rules, there is a 50-50 chance of either of the detectors shown in the first figure above to click. We show this below.

According to the rules given

$$\psi_{1,out} = \frac{1}{\sqrt{2}}\psi_{in} \quad , \quad \psi_{2,out} = \frac{1}{\sqrt{2}}\psi_{in} \quad (14.1)$$

since nothing enters port #2.

By our probability postulate (called the Born rule) the probability to find a photon at position 1 or 2 is

$$\left. \begin{aligned} P_{1,out} &= \int |\psi_{1,out}|^2 dx = \frac{1}{2} \int |\psi_{in}|^2 dx = \frac{1}{2} \\ P_{2,out} &= \int |\psi_{2,out}|^2 dx = \frac{1}{2} \int |\psi_{in}|^2 dx = \frac{1}{2} \end{aligned} \right\} \Rightarrow 50 - 50\% \text{ chance} \quad (14.2)$$

Note: As we see from the experimental discussion below, the photon is found at one detector or the other, never both. The photon is indivisible. This contrasts with classical waves where half of the intensity goes one way and half the other; an antenna would also receive energy. We interpret this as the mean value of a large number of photons.

Now we set up a Mach-Zehnder interferometer(shown below):

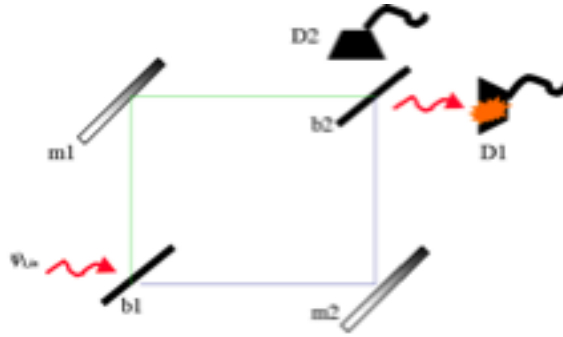


Figure 14.6: Mach-Zehnder interferometer

The wave is split at beam-splitter b1, where it travels either path b1-m1-b2(call it the green path) or the path b1-m2-b2 (call it the blue path). Mirrors are then used to recombine the beams on a second beam splitter, b2. Detectors D1 and D2 are placed at the two output ports of b2.

Assuming the paths are perfectly balanced (that is equal length), the probability for detector D1 to click is 100% - no randomness! We can show this as follows:

To find the wavefunctions impinging on detectors D1 and D2 let us apply the transformation rules sequentially.

(1) Beamsplitter #1

$$\psi_{1,out} = \frac{1}{\sqrt{2}}\psi_{in} \quad , \quad \psi_{2,out} = \frac{1}{\sqrt{2}}\psi_{in} \quad (14.3)$$

(2) Propagation a distance $L/2$ along each path mean that the phase of the wavefunction changes by $e^{ikL/2}$ so that the wavefunctions are

$$\psi_{1,at-mirror} = \frac{1}{\sqrt{2}}e^{ikL/2}\psi_{in} \quad , \quad \psi_{2,at-mirror} = \frac{1}{\sqrt{2}}e^{ikL/2}\psi_{in} \quad (14.4)$$

(3) Reflection off mirrors means wavefunctions become

$$\psi_{1,after-mirror} = -\frac{1}{\sqrt{2}}e^{ikL/2}\psi_{in} \quad , \quad \psi_{2,after-mirror} = -\frac{1}{\sqrt{2}}e^{ikL/2}\psi_{in} \quad (14.5)$$

(4) Propagation a distance $L/2$ along each path mean that the phase of the wavefunction changes by e^{ikL} so that the wavefunctions are

$$\psi_{1,at-b2} = \frac{1}{\sqrt{2}}e^{ikL}\psi_{in} \quad , \quad \psi_{2,at-b2} = \frac{1}{\sqrt{2}}e^{ikL}\psi_{in} \quad (14.6)$$

(5) After beamsplitter #2

$$\psi_{out,1} = \frac{\psi_{1,at-b2} + \psi_{2,at-b2}}{\sqrt{2}} = e^{ikL}\psi_{in} \quad , \quad \psi_{out,2} = \frac{\psi_{1,at-b2} - \psi_{2,at-b2}}{\sqrt{2}} = 0 \quad (14.7)$$

Therefore,

$$P_{1,out} = \int |\psi_{out,1}|^2 dx = \int |\psi_{in}|^2 dx = 1 \quad (14.8)$$

$$P_{2,out} = \int |\psi_{out,2}|^2 dx = 0 \quad (14.9)$$

Thus, we have a 100% chance of detector D1 firing and a 0% chance of detector D2 firing. There is no randomness.

Classical logical reasoning would predict a probability for D1 to click given by

$$P_{D1} = P(\text{transmission at } b1|\text{green path})P(\text{green path}) \\ + P(\text{reflection at } b2|\text{blue path})P(\text{blue path}) \quad (14.10)$$

Let us calculate this and compare it to the quantum result and explain what is happening.

Classical reasoning

$$P_{D1} = \frac{P(\text{transmission at } b2|\text{green})P(\text{green})}{(\text{probability of transmission at } b2 \text{ given green path}) \times (\text{probability green path was taken})} \\ + \frac{P(\text{reflection at } b2|\text{blue})P(\text{blue})}{(\text{probability of transmission at } b2 \text{ given blue path}) \times (\text{probability blue path was taken})} \quad (14.11)$$

Now we know that there is a 50-50 probability for the photon to take the blue or green path which implies that

$$P(\text{green}) = P(\text{blue}) = 1/2 \quad (14.12)$$

Also with the particle incident at b2 along the green path there is a 50% chance of transmission and similarly for reflection of the blue path.

Therefore,

$$P(\text{transmission at b2}|\text{green}) = P(\text{reflection at b2}|\text{blue}) = 1/2 \quad (14.13)$$

and

$$P_{D1} = \frac{1}{2} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{2} \quad (14.14)$$

so that classical reasoning implies a 50-50 chance of D1 firing, that is, it is *completely random*!

The quantum case is different because the two paths which lead to detector D1 interfere. For the two paths leading to D1 we have

$$\psi_{total} = \frac{\frac{1}{\sqrt{2}}e^{ikL}\psi_{in} + \frac{1}{\sqrt{2}}e^{ikL}\psi_{in}}{\sqrt{2}} \quad (14.15)$$

$$P_{D1} = \int |\psi_{total}|^2 dx = P_{D1} = \frac{1}{2} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{2} = 1 \quad (14.16)$$

where the last two terms are the so-called interference terms. Thus, $P_{D1} = 1$. The paths that lead to detector D2 destructively interfere so that

$$P_{D2} = 0 \quad (14.17)$$

How would we set up the interferometer so that detector D2 clicked with 100% probability? How about making them click at random? Let us do this leaving the *basic geometry the same*, that is, we will not change the direction of the beam splitters or the direction of the incident light.

We now want constructive interference for the paths leading to D2 and destructive interference for D1.

We can achieve this by changing the relative phase of the two paths by moving the mirror so that the path lengths are not the same.

Suppose we move the mirror on the green path (at an angle of 45°) so that the path length in the green path is both changed to $L + \Delta L$. We then have

$$\psi_{out,1} = \frac{\frac{1}{\sqrt{2}}e^{ik(L+\Delta L)} + \frac{1}{\sqrt{2}}e^{ikL}}{\sqrt{2}} = \psi_{in} \quad (14.18)$$

$$\psi_{out,2} = \frac{\frac{1}{\sqrt{2}}e^{ik(L+\Delta L)} - \frac{1}{\sqrt{2}}e^{ikL}}{\sqrt{2}} = \psi_{in} \quad (14.19)$$

and

$$\begin{aligned}
P_{D1} &= \int dx |\psi_{2,out}|^2 = \frac{1}{4} \int dx |\psi_{in}|^2 |e^{ikL}|^2 |e^{ik\Delta L} + 1|^2 \\
&= \frac{1}{4} (e^{ik\Delta L} + 1) (e^{ik\Delta L} + 1)^* = \frac{1}{4} (e^{ik\Delta L} + 1) (e^{-ik\Delta L} + 1) \\
&= \frac{1}{4} (2 + e^{ik\Delta L} + e^{-ik\Delta L}) = \frac{1 + \cos(k\Delta L)}{2} = \cos^2\left(\frac{k\Delta L}{2}\right) \quad (14.20)
\end{aligned}$$

Similarly we have

$$\begin{aligned}
P_{D2} &= \int dx |\psi_{1,out}|^2 = \frac{1}{4} \int dx |\psi_{in}|^2 |e^{ikL}|^2 |e^{ik\Delta L} - 1|^2 \\
&= \frac{1}{4} (e^{ik\Delta L} - 1) (e^{ik\Delta L} - 1)^* = \frac{1}{4} (e^{ik\Delta L} - 1) (e^{-ik\Delta L} - 1) \\
&= \frac{1}{4} (2 - e^{ik\Delta L} - e^{-ik\Delta L}) = \frac{1 - \cos(k\Delta L)}{2} = \sin^2\left(\frac{k\Delta L}{2}\right) \quad (14.21)
\end{aligned}$$

Therefore, to achieve $P_{D1} = 0$ and $P_{D2} = 1$ we choose

$$k\Delta L = m\pi \quad (m \text{ odd}) \Rightarrow \Delta L = m \frac{\pi}{k} = m \frac{\lambda}{2} \quad (14.22)$$

We can make the both random if

$$\cos^2\left(\frac{k\Delta L}{2}\right) = \sin^2\left(\frac{k\Delta L}{2}\right) = \frac{1}{2} \Rightarrow \frac{k\Delta L}{2} = p \frac{\pi}{4} \quad (p \text{ odd}) \quad (14.23)$$

$$\Delta L = p \frac{\pi}{2k} = p \frac{\lambda}{4} \quad (14.24)$$

3. The third stage consists of an interference experiment as shown in the figure below.

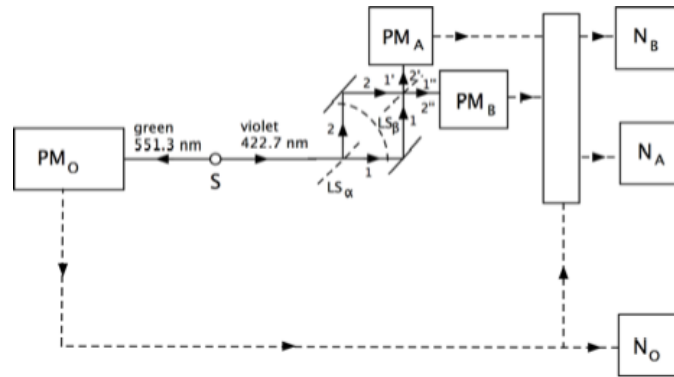


Figure 14.7: Experiment - third stage

Here we have interference with a single photon (third stage). In this sketch, solid lines are optical paths and dashed lines are electrical connections.

A so-called Mach-Zehnder interferometer is used, allowing one to obtain two interference profiles. The beam of violet light from the source S is split into two by the mirror LS_α . After reflection from two different mirrors, these secondary beams meet on a second half-silvered mirror LS_β . Here, each secondary beam is further split into two; thus one establishes two interference regions, region $(1', 2')$ where one places PM_A , and region $(1'', 2'')$ where one places PM_B .

A very high precision piezoelectric system allows one of the mirrors to be displaced so as to vary the path difference between the two arms of the interferometer. In this way one can shift the pattern of interference fringes by regular steps, without moving the detectors PM_A and PM_B ; the standard step corresponds to a change of $\lambda/50$ in the difference between the two optical paths.

A sweep, taking 15 sec for each standard step, yields two interference plots corresponding, respectively, to the paths $(1', 2')$ and $(1'', 2'')$; the fringes have good contrast (difference in intensity between maxima and minima), and their visibility

$$\frac{(N_{A,\max} - N_{A,\min})}{(N_{A,\max} + N_{A,\min})} \quad (14.25)$$

was measured as 98% as shown in the figure below:

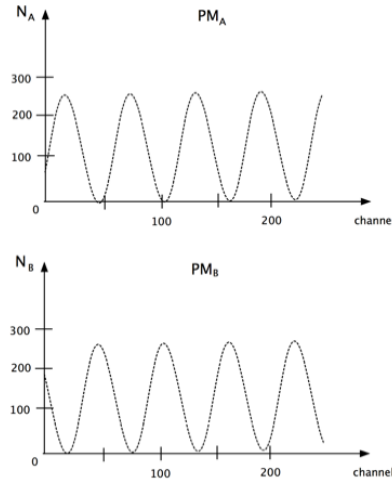


Figure 14.8: Experimental results

These are the two interference plots obtained with the Mach-Zehnder interferometer. Note that the maximum counting rates in PM_A correspond to minima in PM_B , indicating a relative displacement of $\lambda/2$ between the two interference patterns.

If we recall that we are reasoning in terms of photons, and that the photons are being processed individually, then we must admit that the interference does not stem from any interaction between successive photons, but that each photon interferes with itself.

What would Albert have to say? He seems exasperated but is still polite. His statements are brief:

I observe that the optical paths differ in length between LS_α and LS_β and are then coincident over $(1', 2')$ and over $(1'', 2'')$.

In PM_A I observe a process that seems perfectly natural to me, namely

$$light + light \rightarrow light$$

In PM_B I observe a process that I find astounding, namely

$$light + light \rightarrow darkness$$

Such superposition phenomena with light I shall call interference, constructive in PM_A and destructive in PM_B .

In the situation considered before, I envisaged light as consisting of particles called photons, which travelled either along path 1 or along path 2. In the present situation I want to know for each individual photon which path it has travelled; to this end I should like to ask you to close off path 2, since this will ensure that the photons travel by path 1.

Clearly Albert is perturbed. He awaits the new experimental results with some anxiety.

On closing either path, whether 1 or 2, one observes that all interference phenomena disappear. For instance, instead of a very high count N_A and a very low count N_B , we now obtain essentially equal counts from PM_A and PM_B .

Albert is visibly displeased and now very wary. He then continues with his analysis of the experiment:

I observe that in order to produce interference phenomena it is necessary to have two optical paths of different lengths, both open.

Whenever a photon is detected, I note my inability to ascertain

whether the light has travelled by path 1 or by path 2, because I have no means for distinguishing between the two cases.

If I were to suppose that photons travel only along 1, then this would imply that path 2 is irrelevant, which is contrary to what I have observed. Similarly, if I were to suppose that photons travel only along 2, then this would imply that path 1 is irrelevant, which is also contrary to my observations.

If I envisage the source S as emitting particles, then I am forced to conclude that each individual photon travels simultaneously along both paths 1 and 2; but this result contradicts the results of the previous experiment (second stage), which compelled me to envisage that every photon chooses, at random, either path 1 or path 2. I conclude that the notion of particles is unsuited to explaining interference phenomena.

I shall suppose instead that the source emits a wave; this wave splits into two at LS_α , and the two secondary waves travel one along path 1 and the other along path 2. They produce interference by mutual superposition on LS_β constructively in $(1', 2')$ and destructively in $(1'', 2'')$. At the far end of $(1', 2')$ or of $(1'', 2'')$ I envisage each of the waves condensing into particles, which are then detected by the photomultipliers (essentially by PM_A since the contrast is 98% means only very few photons are detected by PM_B).

It seems to me that I am beginning to understand the situation. I envisage light as having two complementary forms: depending on the kind of experiment that is being done, it can manifest itself either as a wave, or as a particle, but never as both simultaneously and in the same place. Thus, in the experiment where the path followed by the light cannot be ascertained (third stage), light behaves first like a wave, producing interference phenomena; but it behaves like a particle when, afterwards, it is detected through the photoelectric effect. I conclude that light behaves rather strangely, but nevertheless I have the impression that its behavior can be fully described once one has come to terms with the idea of wave-particle duality.

Albert leaves the room slowly, hesitantly, even reluctantly. He might be impressed by all the completeness of all that he has just described or maybe he is worried that more needs to be said.

In fact, something does remain to be said, since the problem of causality remains open. Let us look carefully at the experimental layouts in the second and third stages: we see that they have LS_α in common, and that they differ only beyond some boundary (indicated by the dashed circle downstream from

LS_α). We have stated that light behaves like a particle or like a wave depending on whether or not one can ascertain the path it takes through the apparatus; but in the two experiments under consideration, the choice between the alternatives must be decided on LS_α , *before* the light has crossed the crucial boundary, that is, at a stage where nothing can as yet distinguish between the two kinds of apparatus, since they differ only beyond the point of decision. It is as if the light *chose* whether to behave like a wave or like a particle before *knowing* whether the apparatus it will pass through will elicit interference phenomena or the photoelectric effect. Hence the question of causality is indeed opened up with vengeance.

Albert comes back abruptly. He is disconcerted and wearily says:

Originally I supposed that light would behave like a wave or like a particle, depending on the kind of experiment to which it was being subjected.

I observe that the choice must be made on the half-silvered mirror LS_α , before the light reaches that part of the apparatus where the choice is actually implemented; this would imply that the effect precedes the cause.

I know that both waves and particles obey the principle of causality, that is, that cause precedes effect.

I conclude that light is neither wave nor particle; it behaves neither like waves on the sea, nor like projectiles fired from a gun, nor like any other kind of object that I am familiar with.

I must ask you to forget everything I have said about this experiment, which seems to me to be thoroughly mysterious.

Albert leaves, but quickly returns with a contented smile, and his final statement is not without a touch of malice.

I observe in all cases that the photomultipliers register quanta when I switch on the light source.

I conclude that *something* has travelled from the source to the detector. This *something* is a quantum object, and I shall continue to call it a photon, even though I know that it is neither a wave nor a particle.

I observe that the photon gives rise to interference when one cannot ascertain which path it follows; and that interference disappears when it is possible to ascertain the path.

For each detector, I observe that the quanta it detects are randomly distributed in time.

If I repeat the experiment several times under identical conditions, then I observe that the photon counts registered by each photomultiplier are reproducible in a statistical sense. For example, suppose that in the first and in the second experiments PM_A registers N'_A and N''_A respectively; then one can predict that N''_A has a probability of 0.68 of being in the interval $N'_A \pm \sqrt{N'_A}$.

Thus, these counts enable me to determine experimentally, for any kind of apparatus, the probability that a given detector will detect a quantum, and it is precisely such probabilities that constitute the results of experiments. I assert that the function of a physical theory is to predict the results of experiments.

What I expect from theoretical physicists is a theory that will enable me to predict, through calculation, the probability that a given detector will detect a photon. This theory will have to take into account the random behavior of the photon, and the absence or presence of interference phenomena depending on whether the paths followed by the light can or cannot be ascertained.

Albert leaves, wishing the physicists well in their future endeavors.

Physicists have indeed worked hard and the much desired theory has indeed come to light, namely, quantum mechanics, as we have seen in our discussions. As we have seen, it applies perfectly not only to photons, but equally well to electrons, protons, neutrons, etc; in fact, it applies to all the particles of microscopic physics. For the last 75 years it has worked to the general satisfaction of physicists.

Meanwhile, it has produced two very interesting problems of a philosophical nature.

1. Chance as encountered in quantum mechanics lies in the very nature of the coupling between the quantum object and the experimental apparatus. No longer is it chance as a matter of ignorance or incompetence: it is **chance quintessential and unavoidable**.
2. Quantum objects behave quite differently from the familiar objects of our everyday experience: whenever, for pedagogical reasons, one allows an analogy with macroscopic models like waves or particles, one always fails sooner or later, because the analogy is never more than partially valid. Accordingly, the first duty of a physicist is to force her grey cells, that is her concepts and her language, into unreserved compliance with quantum mechanics (as we have been attempting to do); eventually this

will lead her to view the actual behavior of microsystems as perfectly normal. As a teacher of physics, our duties are if anything more onerous still, because we must convince the younger generations that quantum mechanics is not a branch of mathematics, but an expression of our best present understanding of physics on the smallest scale; and that, like all physical theories, it is predictive.

In this context, let us review the basic formalism of quantum mechanics as we have developed it so far.

14.2 Review of Basic Formalism

We will introduce the elements of quantum mechanics as axioms. Physicists have devised a new mathematical tool. The transition amplitude from initial to final state, and it is this amplitude that enables one to calculate the needed probabilities.

- (1) For the experiment where the photon travels from the source S to the detector PM_A (see figure (a) below), we write the transition amplitude from S to PM_A as

$$\langle \text{photon arriving at } PM_A | \text{photon leaving } S \rangle \quad (14.26)$$

The figure shows the three arrangements sufficient to determine the transition amplitude: (a) a single optical path; (b) two paths, allowing us to ascertain which path has actually been taken; (c) two paths, not allowing us to ascertain which path has actually been taken.

As we know, this is a complex number and it is read from right to left. We write it more symbolically as $\langle f | i \rangle$, which simply means the transition amplitude from initial to final state.

The transition probability from the initial state $|i\rangle$ to the final state $|f\rangle$ is given by

$$|\langle f | i \rangle|^2 \quad (14.27)$$

- (2) If the photon emitted by the source can take either of two paths, and if it is, in principle, possible to ascertain which path it actually does take (figure (b) above) then there are two transition amplitudes:

$$\langle \text{photon arriving at } PM_A | \text{photon leaving } S \rangle \quad (14.28)$$

$$\langle \text{photon arriving at } PM_B | \text{photon leaving } S \rangle \quad (14.29)$$

which we symbolize simply as

$$\langle f_1 | i \rangle \quad , \quad \langle f_2 | i \rangle \quad (14.30)$$

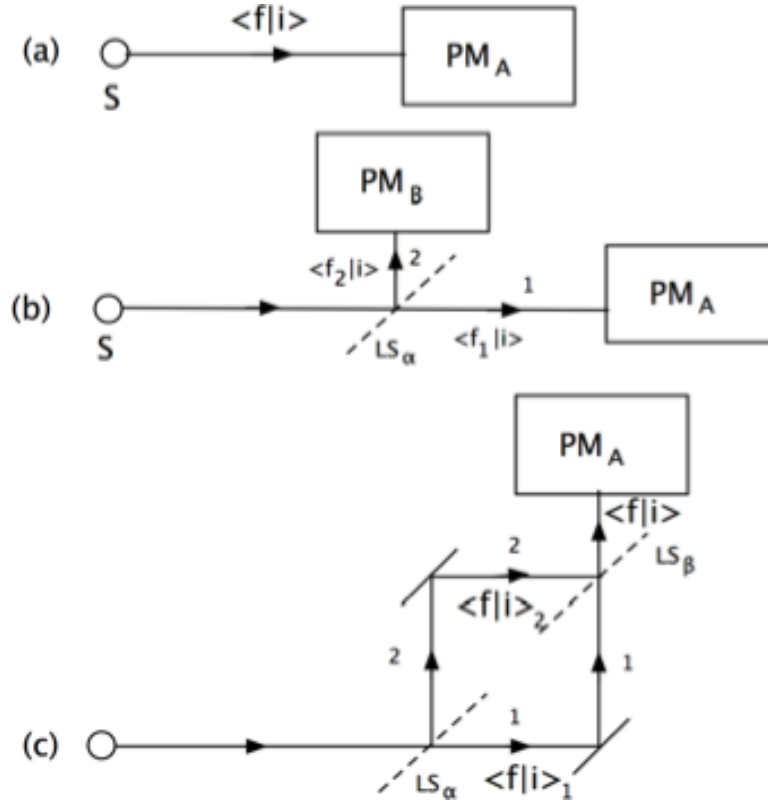


Figure 14.9: Three experiments

In this case there are two probabilities:

$$|\langle f_1 | i \rangle|^2, \quad |\langle f_2 | i \rangle|^2 \quad (14.31)$$

The total probability is their sum:

$$|\langle f_1 | i \rangle|^2 + |\langle f_2 | i \rangle|^2 \quad (14.32)$$

More generally, we would write

$$|\langle f | i \rangle|^2 = \sum_k |\langle f_k | i \rangle|^2 \quad (14.33)$$

where the sum is over all possible paths

- (3) If a photon is emitted by the source S can take either of two paths, but it is impossible to ascertain which path it does take (figure (c) above), then there are again two transition amplitudes:

$$\langle \text{photon arriving at } PM_A | \text{photon leaving } S \rangle_{\text{along path 1}} \quad (14.34)$$

$$\langle \text{photon arriving at } PM_A | \text{photon leaving } S \rangle_{\text{along path 2}} \quad (14.35)$$

which we symbolize simply as

$$\langle f | i \rangle_1 \quad , \quad \langle f | i \rangle_2 \quad (14.36)$$

To allow for interference, we assert that in this case it is the amplitudes that must be added; the total amplitude reads

$$\langle f | i \rangle = \langle f | i \rangle_1 + \langle f | i \rangle_2 \quad (14.37)$$

The total probability is:

$$|\langle f | i \rangle_1 + \langle f | i \rangle_2|^2 \quad (14.38)$$

More generally, we would write

$$\text{total amplitude: } \langle f | i \rangle = \sum_k \langle f | i \rangle_k \quad (14.39)$$

$$\text{total probability: } |\langle f | i \rangle|^2 = \left| \sum_k \langle f | i \rangle_k \right|^2 \quad (14.40)$$

where the sums are over all possible paths.

- (4) If one wants to analyze the propagation of the light more closely, one can take into account its passage through the half-silvered mirror LS_α , considering this as an intermediate state (figure (b) above). The total amplitude for path 1 is

$$\langle \text{photon arriving at } PM_A | \text{photon leaving } S \rangle \quad (14.41)$$

However, it results from two successive intermediate amplitudes:

$$\langle \text{photon arriving at } LS_\alpha | \text{photon leaving } S \rangle \quad (14.42)$$

$$\langle \text{photon arriving at } PM_A | \text{photon leaving } LS_\alpha \rangle \quad (14.43)$$

Here we consider the total amplitude as the product of the successive intermediate amplitudes; symbolically, labeling the intermediate state as ν , we have

$$\langle f | i \rangle = \langle f | \nu \rangle \langle \nu | i \rangle \quad (14.44)$$

Finally, consider a system of two mutually independent photons. If photon 1 undergoes a transition from a state i_1 to a state f_1 , and photon 2 from a state i_2 to a state f_2 , then

$$\langle f_1 f_2 | i_1 i_2 \rangle = \langle f_1 | i_1 \rangle \langle f_2 | i_2 \rangle \quad (14.45)$$

The four rules just given suffice to calculate the detection probability in any possible experimental situation. They assume their present form as a result of a long theoretical evolution; but they are best justified **a posteriori**, because in 75 years they have never been found to be wrong. Accordingly, we may

consider them as the basic principles governing the observable behavior of all microscopic objects, that is, objects whose action on each other are of order \hbar (Planck's constant). From these principles (they are equivalent to our earlier postulates - just look different because we are using the amplitude instead of the state vector as the fundamental mathematical object in the theory) one can derive all the requisite formalism, that is, all of quantum mechanics.

Quantum mechanics as we have described it earlier and also above, works splendidly, like a well-oiled machine. It, and its basic principles, might therefore be expected to command the assent of every physicist; yet it has evoked, and on occasion continues to evoke, reservations both explicit and implicit. For this there are two reasons:

- (1) Quantum mechanics introduces unavoidable chance, meaning that its characteristic randomness is inherent in the microscopic phenomena themselves.
- (2) It attributes to microscopic objects properties so unprecedented that we cannot represent them through any macroscopic analogs or models.

Both features are revolutionary, and it is natural that they should have provoked debate. On the opposite sides of this debate we find two great physicists, Neils Bohr and Albert Einstein, and we will now discuss how the debate evolved from its beginnings in 1927 to its conclusion in 1983 (that is 56 years!).

14.3 Inseparable Photons (the EPR Paradox)

Though ornithologists have known about inseparable parrots for a long time, to physicists the existence of inseparable photons has been brought home only during the last two decades, through a beautiful series of experiments by Alain Aspect and his research group at Orsay Laboratory in Paris. The experiments are exemplary, in virtue both of the difficulties they had to overcome and the results achieved, which are exceptionally clear-cut. In fact, the significance of the experiments extends beyond the strict confines of physics, because they provide the touchstone for settling a philosophical debate that has divided physicist for 75 years. The division dates back to the appearance of two mutually contradictory interpretations of quantum mechanics at the Como conference in 1927. To sketch the debate, we start with a brief summary of the philosophy of physics.

14.3.1 The Philosophical Stakes in the Debate

Our summary is best presented diagrammatically as shown in the figure below:

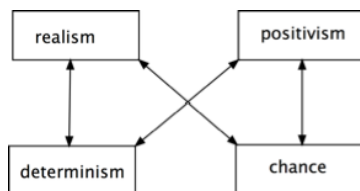


Figure 14.10: The philosophical elements

which shows the philosophical elements in a debate between physicists.

- (1) For the physicist who is a **realist**, a physical theory reflects the behavior of real objects, whose existence is not brought into question.
- (2) For the physicist who is a **positivist**, the purpose of a physical theory is to describe the relations between measurable quantities. The theory does not tell one whether anything characterized by these quantities really exists, nor even whether the question makes sense.
- (3) For the physicist who is a **determinist**, exact knowledge of the initial conditions and of the interactions allows the future to be predicted exactly. Determinism is held to be a universal characteristic of natural phenomena, even about those which we know, as yet, little or nothing. In this framework, any recourse to chance merely reflects our own ignorance.
- (4) For the physicist who is a **probabilist**, chance is inherent in the very nature of microscopic phenomena. To her, determinism is a consequence, on the macroscopic level, if the laws of chance operating on the microscopic level; it is appropriate to measurements of mean values of quantities whose relative fluctuations are very weak.

From these four poles, realism, positivism, determinism, and chance, the physicist chooses two, one on each axis. Though sometimes the choice is made in full awareness of what it entails, most often it is made subconsciously. In our description of quantum mechanics, we might adopt without reservations, the point of view of the elementary particle physicist. For a start, she believes firmly in the existence of particles, since she spends her time in accelerating, deflecting, focusing, and detecting them. Even though she has never seen or touched them, to her their objective existence is not in any doubt. Next she observes that they impinge on the detectors quite erratically, whence she has no doubts, either, that their behavior is random. Accordingly, the elementary particle experimentalist has chosen realism and chance, most often without realizing that she has made choices at all.

There are other philosophical options that can be adopted with eyes fully open: realism and determinism are the choices of Albert Einstein; positivism and chance are those of Niels Bohr. They are well acquainted and each thinks very

highly of the other: which is no bar to their views being incompatible, nor to the two men representing opposite poles of the debate.

14.3.1.1 From Como to Brussels (1927-30)

On September 26, 1927, in Como, Niels Bohr delivered a memorable lecture. His stance is that of an enthusiastic champion of the new quantum mechanics. He puts special weight on the inequalities proved by Heisenberg the year before:

$$\Delta x \Delta p_x \geq \frac{1}{2} \hbar \quad , \quad \Delta t \Delta E \geq \frac{1}{2} \hbar \quad (14.46)$$

They imply that it is impossible to define exact initial conditions for a microscopic object, which automatically makes it impossible to construct, on the microscopic scale, a deterministic theory patterned on classical mechanics. Only a probabilistic theory is possible, and that theory is quantum mechanics.

Einstein disagrees with this point of view, and his opposition to Bohr's theses becomes public at the Brussels conference in 1930: he adopts the role of a dissenter who knows precisely how to press home the most difficult questions. Deeply shocked by the retreat from determinism, he tries to show via his thought (gedanken) experiments he can contravene the Heisenberg inequalities.

At the cost of several sleepless nights devoted to analyzing the objections of his adversary, Bohr refutes all of Einstein's criticisms, and emerges from the conference as the undoubted winner.

14.3.1.2 From Brussels to the EPR Paradox (1930-35)

Having lost the argument at Brussels, Einstein tries to define his objections with ever greater precision. Believing as he does that position and momentum exist *objectively and simultaneously*, he considers quantum mechanics to be incomplete and merely provisional. The points of view of the two antagonists at this stage of the debate can be spelled out as follows.

For Einstein, a physical theory must be a deterministic and a complete representation of the objective reality underlying the phenomena. It features known variables that are observable, and others, unknown as yet, called *hidden variables*. Because of our provisional ignorance of the hidden variables, matter at the microscopic level appears to us to behave arbitrarily, and we describe it by means of a theory that is incomplete and probabilistic, namely by quantum mechanics.

For Bohr, a physical theory makes sense only as a set of relations between observable quantities. Quantum mechanics supplies a correct and complete description of the behavior of objects at the microscopic level, which means that the theory itself is likewise complete. The observed behavior is probabilistic,

implying that chance is inherent in the nature of the phenomena.

Between chance as a matter of ignorance, as advocated by Einstein, and chance unavoidable, as advocated by Bohr, the debate does not remain merely philosophical. Quite naturally it returns to the plane of physics with the thought experiment proposed by Einstein, Podolsky and Rosen in 1935, which in their view proves that quantum mechanics is indeed incomplete. Their thought experiment is published as a paper in the Physical Review, but it is so important that it reverberates as far as the New York Times. Physicists call the proposal the EPR paradox, after its proponents. It will take fifty years to untangle the question, first in theory and then by experiment. We will not, of course, follow these fifty years blow by blow; instead, we confine attention to three decisive stages reached respectively in 1952, 1964, and 1983. But we start with an illustration that helps one see what the EPR paradox actually is.

14.3.1.3 Elementary Introduction to the EPR Paradox (using cards this time instead of gloves)

Consider two playing cards, one red(diamond) and one black(spade) as shown below:

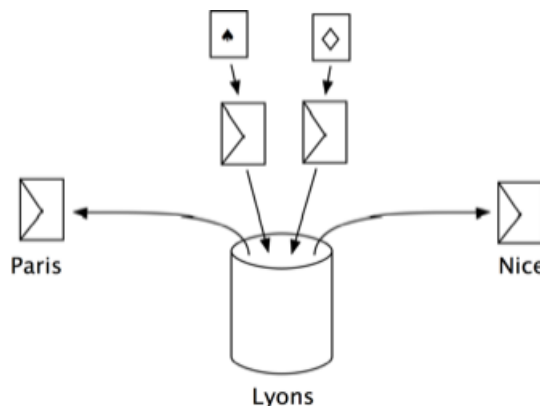


Figure 14.11: Replacing quantum gloves with quantum cards

An experimenter in Lyons puts them into separate envelopes which she then seals. She is thus provided with two envelopes looking exactly alike, and she puts both into a container. She shakes the container so as to *shuffle the pack*, and the system is ready for the experiment.

At 8:00, two travelers, one from Paris and one from Nice, come to the container (in Lyons), take one envelope each, and then return to Paris and Nice, respectively. At 14:00 they are back at their starting points; each opens her envelope, looks at the card, and telephones to Lyons reporting the color. The experiment

is repeated every day for a year, and the observer in Lyons keeps a careful record of the results. At the end of the year the record stands as follows:

1. The reports from Paris are *red* or *black*, and the sequence of these reports is random. The situation is exactly the same as in a game of heads or tails, and probability of each outcome is $1/2$.
2. The reports from Nice are *red* or *black*, and the sequence of these reports is random. Here too probability of each outcome is $1/2$.
3. When Paris reports *red*, Nice reports *black*; when Paris reports *black*, Nice reports *red*. One sees that there is perfect(anti) correlation between the report from Paris and the report from Nice.

Accordingly, the experiment we have described displays two features:

- (1) It is *unpredictable* and thereby random at the level of individual observations in Paris and Nice.
- (2) It is *predictable*, by virtue of the correlation, at the level where one observes the Paris and the Nice results simultaneously.

Einstein and Bohr might have interpreted the correlation as follows.

According to Einstein, the future of the system is decided at 8:00 when the envelopes are chosen, because he believes that the contents of the two envelopes differ. Suppose, for instance, that Paris has (without knowing it) drawn a red card, and Nice the black. The colors so chosen exist in reality, even though we do not know them. The two cards are moved, separately, by the travelers between 8:00 and 14:00, during which time they do not influence each other in any way. The results on opening the envelopes read “red” in Paris and “black” in Nice. Since the choice at 8:00 was made blind, the opposite outcome is equally possible, but the results at 14:00 are always correlated (either red/black or black/red). This correlation at 14:00 is determined by the separation of the colors at 8:00, and we say the theory proposed by Einstein is *realist, deterministic, and separable(or local)*, by virtue of a hidden variable, namely, the color.

According to Bohr, there is a crucial preliminary factor, inherent in the preparation of the system. On shaking the container with the two envelopes, one loses information regarding the colors. Afterwards, one only knows that each envelope contains either a red card (probability $1/2$) or a black card (probability $1/2$). We will therefore say that a given envelope is in a *brown state*, which is a superposition of a red state and of a black state having equal probabilities. At 8:00 the two envelopes are identical: both are in a *brown state*, and the future of the system is still undecided. There is no solution until the envelopes are opened at 14:00, since it is only the action of opening them that makes the colors observable. The result is probabilistic. There is a probability $1/2$ that in Paris the envelope will be observed to go from the “brown state” to the red,

while the envelope in Nice is observed to go from the “brown state” to the black; there is the same probability $1/2$ of observing the opposite. But the results of the observations on the two envelopes are always correlated, which means that there is a mutual influence between them, in particular at 14:00; in fact it is better to say that, jointly, they constitute a single and non-separable system, even though one is in Paris and the other is in Nice. Accordingly, the theory proposed by Bohr is *positivist, probabilistic (non-deterministic) and non-separable(non-local)*, interrelating as it does the colors that are actually observed.

Einstein’s view appears to be common sense, while it must be admitted that Bohr’s is very startling; however, the point of this macroscopic example is, precisely, to stress how different the quantum view is from the classical.

Proceeding with impeccable logic but from different premises, both theories predict the same experimental results. Can we decide between them? At the level considered here it seems we cannot: for even if the envelopes were opened prematurely while still in Lyons, one would merely obtain the same results at a different time, and without affecting the validity of either interpretation. The solution to the problem must be looked for at the atomic level, by studying the true EPR set-up itself.

14.3.1.4 The EPR Paradox (1935-52)

Albert Einstein, Boris Podolsky, and Nathan Rosen meant to look for an experiment that could measure, indirectly but simultaneously, two mutually exclusive quantities like position and momentum. Such results would contravene the predictions of quantum mechanics, which allows the measurement of only one such quantity at any one time; that is why the thought experiment is called the EPR paradox.

In 1952, David Bohm showed that the paradox could be set up not only with continuously varying quantities like position and momentum, but also with discrete quantities like spin. This was the first step towards any realistically conceivable experiment. Meanwhile, objectives have evolved, and nowadays it is more usual to talk of the EPR scenario, meaning some sensible experiment capable of discriminating between quantum theory and hidden-variable theories. Such a set-up is sketched in the figure below.

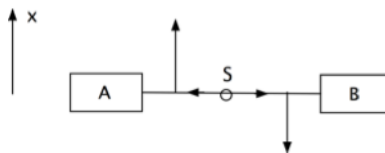


Figure 14.12: David Bohm EPR setup

which shows the simplest EPR scenario.

A particle with spin 0 decays, at S , into two particles of spin $1/2$, which diverge from S in opposite directions. Two Stern-Gerlach type detectors A and B measure the x -components of the spins. Two types of response are possible:

- (1) *spin up* at A , *spin down* at B , a result denoted by $(+1, -1)$
- (2) *spin down* at A , *spin up* at B , a result denoted by $(-1, +1)$

Thus far everyone is agreed, but the interpretation is yet to come.

Einstein reasons that if pairs of particles produced at S elicit different responses $(+1, -1)$ and $(-1, +1)$ from the detector system A, B , then the pairs must have differed already at S , immediately after the decay. It must be possible to represent this difference by a hidden variable λ , which has an objective meaning, and which governs the future of the system. After the decay the two particles separate without influencing each other any further, and eventually they trigger the detectors A and B .

Bohr reasons that all the pairs produced at S are identical. Each pair constitutes a non-separable system right up to the time when the photons reach the detectors A and B . At that time we observe the response of the detectors, which is probabilistic, admitting two outcomes $(+1, -1)$ and $(-1, +1)$.

To sum up, Einstein restricts the operation of chance to the instant of decay (at S), whose details we ignore, but which we believe creates pairs whose hidden variables λ are different. By contrast, Bohr believes that chance operates at the instant of detection, and that it is inherent in the very nature of the detection process: this chance is unavoidable. We are still in the realms of thought, and stay there up to 1964.

In 1964, the landscape changes: John Bell, a theorist at CERN, shows that it is possible to distinguish between the two interpretations experimentally. The test applies to the EPR scenario; it is refined by Clauser, Horne, Shimony, and Holt, whence it is called the BCHSH inequality after its five originators.

14.3.1.5 The BCHSH Inequality (1964)

To set up an EPR scenario, one first needs a source that emits particle pairs. Various experimental possibilities have been explored:

- (1) atoms emitting two photons in cascade
- (2) electron-positron annihilation emitting two high-energy photons
- (3) elastic proton-proton scattering

It is solution (1) that has eventually proved the most convenient; it has been exploited by Alain Aspect at the Institute for Optics in Paris, in particular.

Next one needs detectors whose response can assume one of two values, represented conventionally by $+1$ and -1 . Such a detector might be

- (1) for spin $1/2$ particles, a Stern-Gerlach apparatus responding to *spin up* or *spin down*
- (2) for photons, a polarizer responding to *parallel polarization* or *perpendicular polarization*

Our sketch of the EPR scenario can now be completed as in the figure below.

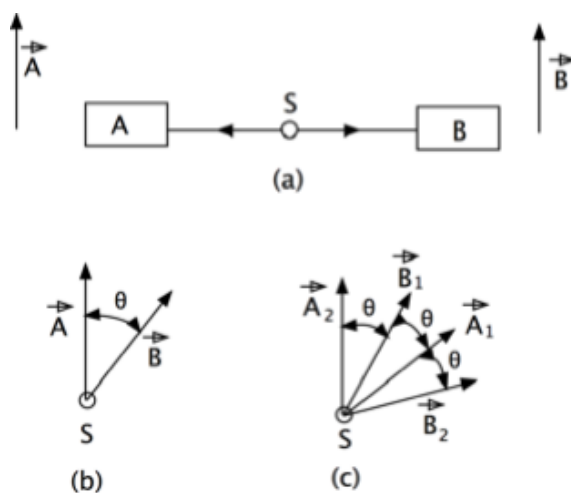


Figure 14.13: EPR scenario

This represents the most general EPR scenario. We have

- (a) views the apparatus perpendicularly to axis, showing the two detectors A and B , with their polarizing directions denoted as \vec{A} and \vec{B} .
- (b) views the apparatus along its axis, and shows that the analyzing directions of the two detectors are not parallel, but inclined to each other at an angle θ
- (c) also a view along the axis of the apparatus, and shows the actual settings chosen by Aspect: two orientations are allowed for each detector, \vec{A}_1 or \vec{A}_2 for one, and \vec{B}_1 or \vec{B}_2 for the other.

We adopt the following conventions:

- (1) $\alpha = \pm 1$ is the response of detector A when oriented along \vec{A}
- (2) $\beta = \pm 1$ is the response of detector B when oriented along \vec{B}

Since each detector has two possible orientations, called 1 and 2, we shall denote their responses as α_1, α_2 and β_1, β_2 , respectively.

Now consider the quantity $\langle \gamma \rangle$ defined by

$$\langle \gamma \rangle = \langle \alpha_1 \beta_1 \rangle + \langle \alpha_1 \beta_2 \rangle + \langle \alpha_2 \beta_1 \rangle - \langle \alpha_2 \beta_2 \rangle \quad (14.47)$$

where the symbol $\langle \dots \rangle$ denotes the mean value over very many measured events. We call $\langle \gamma \rangle$ the *correlation function* of the system.

The BCHSH inequality then reads

$$-2 \leq \langle \gamma \rangle \leq 2 \quad (14.48)$$

Its authors have proved that it must be satisfied if mechanics at the microscopic level constitutes a theory that is realist, deterministic, and separable: or in other words if the theory contains a hidden variable. A sketch of the a proof is shown below.

14.3.1.6 A Proof of Bell's Inequality

Suppose that the pair a, b emerging from S can be characterized by a hidden variable λ . The responses of the detectors A, B are $\alpha(\vec{A}, \lambda)$ and $\beta(\vec{B}, \lambda)$ respectively as shown in the figure below.

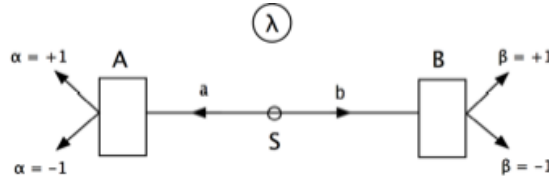


Figure 14.14: Setup to prove Bell's inequality

We assume a theory that is deterministic and separable.

- (1) **deterministic**, because the results are determined by the hidden variables plus the settings \vec{A} and \vec{B}
- (2) **separable**, because the response of A is independent of the response of B , and vice versa

Since the value of λ is unknown and different for each pair, the responses of A and B seem random. Lacking information about λ , we characterize it by choosing a statistical distribution $\rho(\lambda)$, which then allows us to derive the distribution of the responses $\alpha(\vec{A}, \lambda)$ and $\beta(\vec{B}, \lambda)$, which can be compared with experiment.

Bell's inequalities have the great virtue that they apply to any hidden variable

theory, irrespective of the choice of $\rho(\lambda)$.

Theorem1: Consider the four numbers α_1 , α_2 , β_1 , and β_2 , each of which can assume only the values 1 or -1 . Then the combination

$$\gamma = \alpha_1\beta_1 + \alpha_1\beta_2 + \alpha_2\beta_1 - \alpha_2\beta_2 \quad (14.49)$$

can assume only the values 2 and -2 .

To prove the theorem, one constructs a truth table for all 16 possibilities, which shows that 2 and -2 are indeed the only possible values of γ .

α_1	α_2	β_1	β_2	γ
1	1	1	1	2
1	1	1	-1	2
1	1	-1	1	2
1	1	-1	-1	2
1	-1	1	1	2
1	-1	1	-1	2
1	-1	-1	1	2
1	-1	-1	-1	2
-1	1	1	1	2
-1	1	1	-1	2
-1	1	-1	1	2
-1	1	-1	-1	2
-1	-1	1	1	2
-1	-1	1	-1	2
-1	-1	-1	1	2
-1	-1	-1	-1	2

Theorem 2: Consider very many sets of four numbers $(\alpha_1, \alpha_2, \beta_1, \beta_2)$. The mean value of γ lies in the range $[-2, 2]$. In other words,

$$-2 \leq \langle \gamma \rangle \leq 2 \quad (14.50)$$

This is obvious, because every value of γ lies in this range, and so therefore must the mean. The endpoints are included in order to allow for limiting cases.

Note that both theorems are purely mathematical, neither involves any assumptions about physics.

14.3.1.7 The BCHSH Inequality (or Bell's inequality in the real world)

Within the framework of a theory that is realist, deterministic, and separable, we can describe the photon pair in detail. Realism leads us to believe that polarization is an objective property of each member of the pair, independent

of any measurements that may be made later. Determinism leads us to believe that the polarizations are uniquely determined by the decay cascade, and that they are fully specified by the hidden variable λ , which governs the correlation of the polarizations in A and B . Finally, separability leads us to believe that the measurements in A and B do not influence each other, which means in particular that the response of detector A is independent of the orientation of detector B . Now consider a pair of photons a, b , characterized by a hidden variable λ . The response of the apparatus in its four settings would be as follows:

$$\begin{aligned} \alpha_1 \text{ and } \beta_1 &\text{ in the orientation } (\vec{A}_1, \vec{B}_1) \\ \alpha_2 \text{ and } \beta_2 &\text{ in the orientation } (\vec{A}_2, \vec{B}_2) \\ \alpha'_1 \text{ and } \beta'_2 &\text{ in the orientation } (\vec{A}_1, \vec{B}_2) \\ \alpha'_2 \text{ and } \beta'_1 &\text{ in the orientation } (\vec{A}_2, \vec{B}_1) \end{aligned}$$

Recall that the variables α and β can only take on the values 1 and -1 .

It is impossible in practice to make four measurements on one and the same pair of photons, because each photon is absorbed in the first measurement made on it; that is why we have spoken conditionally, that is, **of what results would be (a COUNTERFACTUAL statement)**. But if we believe that the photon correlations are governed by a theory that is realist, deterministic, and separable, then we are entitled to assume that the responses, of type α or type β , depend on properties that the photons possess before the measurement, so that the responses correspond to some objective reality. In such a framework we can appeal to the principle of separability, which implies, for instance, that detector A would give the same response to the orientations (\vec{A}_1, \vec{B}_1) and (\vec{A}_1, \vec{B}_2) , because the response of A is independent of the orientation of B . Mathematically, this is expressed by the relation

$$\alpha_1 = \alpha'_1 \quad (14.51)$$

Similarly one finds

$$\alpha_2 = \alpha'_2, \beta_1 = \beta'_1, \beta_2 = \beta'_2 \quad (14.52)$$

Thus, we have shown that, for a given pair of photons, all possible responses of the apparatus in its four chosen settings can be specified by means of only four two-valued variables $\alpha_1, \alpha_2, \beta_1$, and β_2 .

This reduction from eight to four variables depends on the principle of separability. In this way, we are led to a situation covered by Theorem 2, and therefore $-2 \leq \langle \gamma \rangle \leq 2$.

By making many measurements for each of the four settings we can determine the four mean values $\langle \alpha_1 \beta_1 \rangle, \langle \alpha_1 \beta_2 \rangle, \langle \alpha_2 \beta_1 \rangle, \langle \alpha_2 \beta_2 \rangle$ and thus the mean value of the correlation

$$\langle \gamma \rangle = \langle \alpha_1 \beta_1 \rangle + \langle \alpha_1 \beta_2 \rangle + \langle \alpha_2 \beta_1 \rangle - \langle \alpha_2 \beta_2 \rangle \quad (14.53)$$

Otherwise, i.e., according to quantum mechanics (which is positivist, probabilistic, and non-separable), there are cases where the BCHSH inequality is violated.

In particular, one can show that for photons in the configuration chosen by Aspect quantum mechanics yields

$$\langle \gamma \rangle = 3 \cos 2\theta - \cos 6\theta \quad (14.54)$$

This leads to values well outside the interval $[-2, 2]$, for example to $\langle \gamma \rangle = 2\sqrt{2}$ when $\theta = 22.5^\circ$ and to $\langle \gamma \rangle = -2\sqrt{2}$ when $\theta = 67.5^\circ$.

Proof: The laboratory reference frame $Oxyz$ serves to specify the orientations of detectors and polarizers as shown in the figure below:

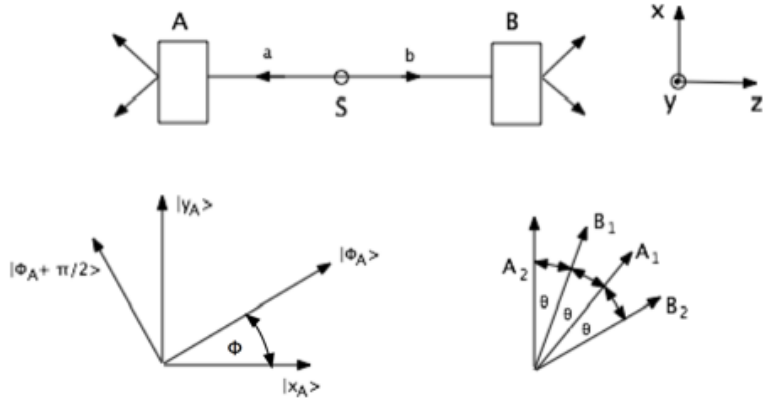


Figure 14.15: Theoretical and experimental setup

Before any measurements have been made, the photon pair a, b forms a non-separable entity, represented by the vector

$$|\Phi\rangle = \frac{1}{\sqrt{2}} (|x_A, x_B\rangle + |y_A, y_B\rangle) \quad (14.55)$$

The act of measurement corresponds to passage to the φ -basis. Hence, we require the transition amplitudes from the two states $|x_A, x_B\rangle, |y_A, y_B\rangle$ to the four states $|\varphi_A, \varphi_B\rangle, |\varphi_A, \varphi_B + \pi/2\rangle, |\varphi_A + \pi/2, \varphi_B\rangle, |\varphi_A + \pi/2, \varphi_B + \pi/2\rangle$.

In the φ -basis we have

$$|\Phi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \cos(\varphi_B - \varphi_A) |\varphi_A, \varphi_B\rangle - \sin(\varphi_B - \varphi_A) |\varphi_A, \varphi_B + \pi/2\rangle \\ + \sin(\varphi_B - \varphi_A) |\varphi_A + \pi/2, \varphi_B\rangle \\ + \cos(\varphi_B - \varphi_A) |\varphi_A + \pi/2, \varphi_B + \pi/2\rangle \end{pmatrix} \quad (14.56)$$

The square of each amplitude featured here represents the detection probability. For example, the probability if simultaneously detecting photon a polarized at

the angle φ_A and the photon b polarized at the angle φ_B is

$$\left(\frac{1}{\sqrt{2}} \cos(\varphi_B - \varphi_A) \right)^2 = \frac{1}{2} \cos^2(\varphi_B - \varphi_A) \quad (14.57)$$

By convention, we write the responses of detector A to a photon in state $|\varphi_A\rangle$ (respectively $|\varphi_A + \pi/2\rangle$) as $\alpha = 1$; similarly with β for detector B .

Let us analyze the four possible responses:

- (1) $|\varphi_A, \varphi_B\rangle$ gives $\alpha = 1, \beta = 1$ so that $\alpha\beta = 1$; the probability is

$$P_{++} = \frac{1}{2} \cos^2(\varphi_B - \varphi_A) \quad (14.58)$$

- (2) $|\varphi_A, \varphi_B + \pi/2\rangle$ gives $\alpha = 1, \beta = -1$ so that $\alpha\beta = -1$; the probability is

$$P_{+-} = \frac{1}{2} \sin^2(\varphi_B - \varphi_A) \quad (14.59)$$

- (3) $|\varphi_A + \pi/2, \varphi_B\rangle$ gives $\alpha = -1, \beta = 1$ so that $\alpha\beta = -1$; the probability is

$$P_{-+} = \frac{1}{2} \sin^2(\varphi_B - \varphi_A) \quad (14.60)$$

- (4) $|\varphi_A + \pi/2, \varphi_B + \pi/2\rangle$ gives $\alpha = -1, \beta = -1$ so that $\alpha\beta = 1$; the probability is

$$P_{--} = \frac{1}{2} \cos^2(\varphi_B - \varphi_A) \quad (14.61)$$

The mean value of $\langle\alpha\beta\rangle_{AB}$ follows immediately as

$$\langle\alpha\beta\rangle_{AB} = P_{++} - P_{+-} - P_{-+} + P_{--} = \cos 2(\varphi_B - \varphi_A) \quad (14.62)$$

The settings chosen by Aspect are as shown in the above figure. Corresponding to it we have the four terms

$$\langle\alpha_1\beta_1\rangle = \langle\alpha\beta\rangle_{A_1B_1} = \cos 2(\varphi_{B_1} - \varphi_{A_1}) = \cos 2\theta \quad (14.63)$$

$$\langle\alpha_1\beta_2\rangle = \langle\alpha\beta\rangle_{A_1B_2} = \cos 2(\varphi_{B_1} - \varphi_{A_2}) = \cos 2\theta \quad (14.64)$$

$$\langle\alpha_2\beta_1\rangle = \langle\alpha\beta\rangle_{A_2B_1} = \cos 2(\varphi_{B_2} - \varphi_{A_1}) = \cos 2\theta \quad (14.65)$$

$$\langle\alpha_2\beta_2\rangle = \langle\alpha\beta\rangle_{A_2B_2} = \cos 2(\varphi_{B_2} - \varphi_{A_2}) = \cos 6\theta \quad (14.66)$$

For comparison with Bell's inequality, we introduce the correlation function $\langle\gamma\rangle$:

$$\langle\gamma\rangle = \langle\alpha_1\beta_1\rangle + \langle\alpha_1\beta_2\rangle + \langle\alpha_2\beta_1\rangle - \langle\alpha_2\beta_2\rangle = 3 \cos 2\theta - \cos 6\theta \quad (14.67)$$

Thus, the BCHSH test turns the EPR scenario into an arena for rational confrontation between the two interpretations; it remains only to progress from thought experiments to experiments conducted in the laboratory.

14.3.2 The Beginnings of the Experiment at Orsay (1976)

Alain Aspect's experiment studies the correlation between the polarizations of the members of photon pairs emitted by calcium. We now present the details we left out in our earlier discussions.

The light source is a beam of calcium atoms, excited by two focused laser beams having wavelengths $\lambda' = 406\text{ nm}$ and $\lambda'' = 581\text{ nm}$, respectively.

Two-photon excitation produces a state having the angular momentum quantum number(value) $J = 0$. When it decays, this state emits two monochromatic photons having the wavelengths $\lambda_1 = 551.3\text{ nm}$ and $\lambda_2 = 422.7\text{ nm}$, respectively, in a cascade of two electronic transitions from the initial $J = 0$ level to the final $J = 0$ state, passing through an intermediate $J = 1$ state. The figure below shows the excitation and decay of the calcium atom.

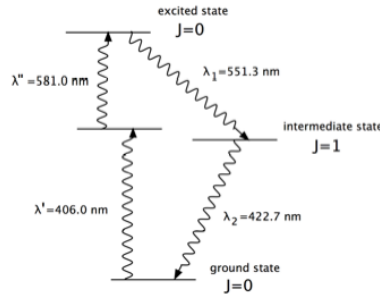


Figure 14.16: Photon source

The mean lifetime of the intermediate state is 4.7 ns . To simplify the terminology, we shall call the $\lambda_1 = 551.3\text{ nm}$ light *green* and the $\lambda_2 = 422.7\text{ nm}$ light *violet*.

The polarizer, which works like a Wollaston prism shown below

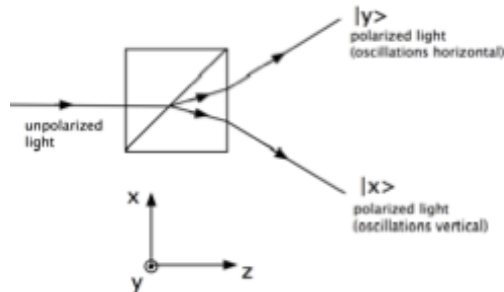


Figure 14.17: Wollaston prism as a polarizer

The figure shows the two-valued response of a Wollaston prism. It is made of quartz or calcite. It splits an incident beam of natural (unpolarized) light into two beams of equal intensity, polarized at 90° to each other. If only a single unpolarized photon is incident, it emerges either in the state $|x\rangle$, with probability $1/2$, or in the state $|y\rangle$, with probability $1/2$. Thus, the response of the system is two-valued.

The photon is detected by the photomultiplier tubes (PM) downstream from the prism. Every electric pulse from these detectors corresponds to the passage of a photon, allowing the photons to be counted. The experimental layout of the first Orsay experiment is sketched in the figure below.

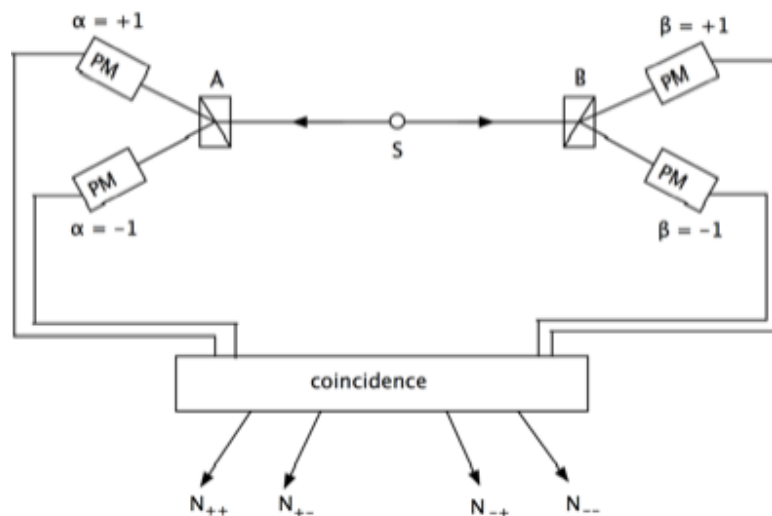


Figure 14.18: The Orsay experiment

It uses a coincidence circuit which registers an event whenever two photons are detected in cascade. In this way four separate counts are recorded simultaneously, over some given period of time. In the EPR scenario envisaged by Bohm, where $\theta = 0^\circ$, the only possible responses are $(+1, -1)$ or $(-1, +1)$ (in the situation realized by Aspect, the angle θ is non-zero, and four different responses are possible).

- (1) N_{++} , the number of coincidences corresponding to $\alpha = 1$ and $\beta = 1$, that is, to $\alpha\beta = 1$
- (2) N_{+-} , the number of coincidences corresponding to $\alpha = 1$ and $\beta = -1$, that is, to $\alpha\beta = -1$
- (3) N_{-+} , the number of coincidences corresponding to $\alpha = -1$ and $\beta = 1$, that is, to $\alpha\beta = -1$

- (4) N_{--} , the number of coincidences corresponding to $\alpha = -1$ and $\beta = -1$, that is, to $\alpha\beta = 1$

The resolving time of the coincidence circuit is 10 ns , meaning that it reckons two photons as coincident if they are separated in time by no more than 10 ns . The mean life of the intermediate state of the calcium atom is 4.7 ns . Therefore, after a lapse of 10 ns , that is more than twice the mean lifetime, almost all the atoms have decayed (actually 88%). In other words, the efficiency of the coincidence counter is very high.

The experiment consists in counting, over some given time interval, the four kinds of coincidence: N_{++} , N_{+-} , N_{-+} , and N_{--} . The total number of event is

$$N = N_{++} + N_{+-} + N_{-+} + N_{--} \quad (14.68)$$

Accordingly, the different kinds of coincidence have probabilities

$$\begin{aligned} P_{++} &= N_{++}/N && \text{corresponding to } \alpha\beta = 1 \\ P_{+-} &= N_{+-}/N && \text{corresponding to } \alpha\beta = -1 \\ P_{-+} &= N_{-+}/N && \text{corresponding to } \alpha\beta = -1 \\ P_{--} &= N_{--}/N && \text{corresponding to } \alpha\beta = 1 \end{aligned}$$

and the measured average of $\alpha\beta$ is

$$\langle\alpha\beta\rangle = \frac{N_{++} - N_{+-} - N_{-+} + N_{--}}{N} \quad (14.69)$$

Each set of four coincidence counts corresponds to one particular setting of \vec{A} , \vec{B} , and yields a mean value $\langle\alpha\beta\rangle$. But in order to determine the correlation function $\langle\gamma\rangle$ used in the BCHSH inequality, we need four mean values $\langle\alpha\beta\rangle$. Therefore, we choose, in succession four different settings as shown in figure(c) on page 553; four counting runs then yield the four mean values $\langle\alpha_1\beta_1\rangle, \langle\alpha_1\beta_2\rangle, \langle\alpha_2\beta_1\rangle, \langle\alpha_2\beta_2\rangle$, which then determine the value of $\langle\gamma\rangle$ via

$$\langle\gamma\rangle = \langle\alpha_1\beta_1\rangle + \langle\alpha_1\beta_2\rangle + \langle\alpha_2\beta_1\rangle - \langle\alpha_2\beta_2\rangle \quad (14.70)$$

14.3.2.1 The Results of the First Experiment at Orsay

These results are shown in the figure below. The angle θ which specifies the setting of the polarizers is plotted horizontally, and the mean value $\langle\gamma\rangle$ vertically. It is drawn as the solid curve on the graph (the curve has been corrected for instrumental effects, which explains why its ends are not precisely at 2 and -2). The correlation function predicted by quantum mechanics reads

$$\langle\gamma\rangle = 3 \cos 2\theta - \cos 6\theta \quad (14.71)$$

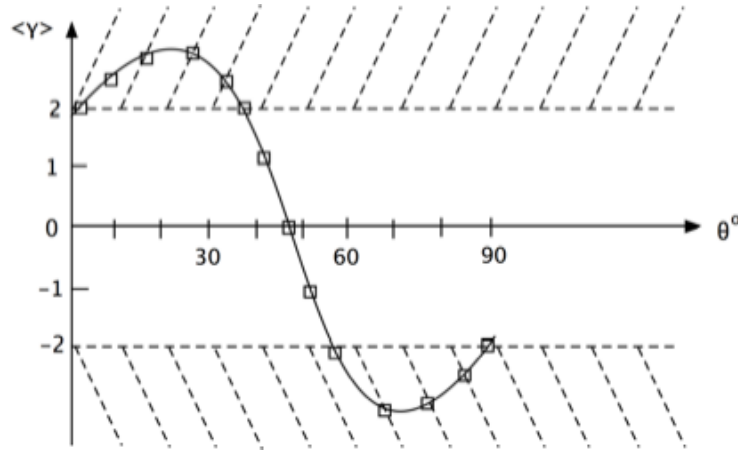


Figure 14.19: Theory and experiment compared

According to the BCHSH inequality

$$-2 \leq \langle \gamma \rangle \leq 2 \quad (14.72)$$

so that hidden-variable theories exclude the cross-hatched regions of the plane, which correspond to $\langle \gamma \rangle > 2$ or $\langle \gamma \rangle < -2$.

The experimental results from 17 different values of θ are indicated on the figure by squares, where the vertical size of the square gives plus or minus one standard deviation (a measure of the experimental error).

Clearly, there can be no doubt that the BCHSH inequality is violated; many of the experimental points fall outside the interval $[-2, 2]$. At the point where the violation is maximal ($\theta = 22.5^\circ$), one finds

$$\langle \gamma \rangle = 2.70 \pm 0.015 \quad (14.73)$$

which represents a departure of over 40 standard deviations from the extreme value of 2. What is even more convincing is the precision with which the experimental points lie on the curve predicted by quantum mechanics.

Quite evidently, for the EPR scenario one must conclude not only that hidden-variable theories fail, but also that quantum mechanics is positively the right theory for describing the observations.

14.3.3 The Relativistic Test

The EPR experiment just described shows that the measurements in A and B are correlated. What is the origin of the correlations?

According to quantum theory, before the measurement each particle pair constitutes a single system extending from A to B , whose two parts are non-separable and correlated. This interpretation corresponds to a violation of Bell's inequality and agreement with experiment.

According to hidden-variables theories, the particle pair is characterized, at the instant of decay, by its hidden variable λ , which determines the correlation between the polarizations measured in A and B . This interpretation satisfies Bell's inequality but disagrees with experiment.

Accordingly, the Orsay experiment supports the quantum interpretation (in terms of the correlation between two parts A and B of a single system).

However, to clinch this conclusion, one must ensure *that no influence is exerted* in the ordinary classical sense through some interaction propagated between the two detectors A and B , that is, no influence which might take effect after the decay at S , and which might be responsible for the correlation actually observed.

Let us therefore examine the Orsay apparatus in more detail as in the figure below.

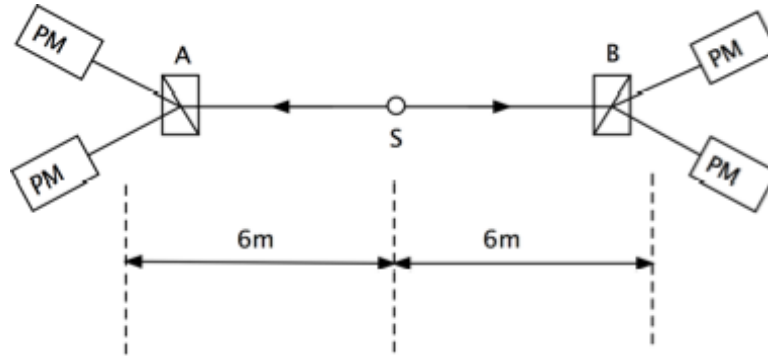


Figure 14.20: Orsay apparatus in detail

We are interested here in the idea of Einsteinian non-separability.

When the detectors at A and B record a coincidence, this means that both have been triggered within a time interval of at most $10ns$, the resolving time of the circuit. Could it happen that, within this interval, A sends to B a signal capable of influencing the response of B ? In the most favorable case, such a signal would travel with the speed of light in vacuum, which according to relativity theory is the upper limit on the propagation speed of information, and thereby of energy. To cover the distance AB , which is $12m$ in the figure, such a signal would need $40ns$. This is too long by at least $30ns$, and rules out any causal links between A and B in the sense of classical physics. One says that *the interval between A*

and B is space-like.

One of the advantages of the Orsay experiment is that it uses a very strong light-source, allowing sufficient distance between the detectors A and B while still preserving reasonable counting rates. By increasing the distance AB step by step, Aspect could check that the correlation persists, even when the interval between A and B becomes space-like. This is the check that guarantees that the two-photon system is non-separable irrespective of the distance AB .

It has become the custom to speak of *the principle of Einsteinian separability* in order to denote the absence of correlations between two events separated by a space-like interval. This is the principle that the Orsay experiment invites us to reconsider, even though our minds, used to the world at the macroscopic level, find it difficult to conceive of two *microscopic* photons 12m apart as a single indivisible object.

14.3.3.1 The Final Stage of the Experiment at Orsay (1983)

Though the results of the first Orsay experiment are unarguable and clear-cut, the conclusion they invite is so startling that one should not be surprised at the appearance of a last-ditch objection, which as it happens gave the experimenters a great deal of trouble. In the preceding section we discussed the possible role of interactions between A and B operating after the decay at S , and duly eliminated the objection. But one can also ask whether correlations might be introduced through an interaction operating *before* the decay. We could imagine that the decay itself is preconditioned by the setting of detectors A and B , such influences taking effect through the exchange of signals between the detectors and the source. No such mechanism is known *a priori*, but we do know that, if there is one, then Einsteinian non-separability would cease to be a problem, because the mechanism could come into action long before the decay, removing any reason for expecting a minimum 30ns delay. Though such a scenario is very unlikely, the objection is a serious one and must be taken into account; to get around it, the experimenter must be able to choose the orientation of the detectors A and B at random after the decay has happened at S . In more picturesque language, we would say that the two photons must leave the source without knowing the orientations of the polarizers A and B . Briefly put, this means that it must be possible to change the detector orientations during the 20ns transits over SA and SB .

The solution adopted at Orsay employs periodic switching every 10ns. These changes are governed by two independent oscillators, one for channel A and one for channel B . The oscillators are stabilized, but however good the stabilization it cannot eliminate small random drifts that are different in the two channels, seeing that the oscillators are independent. This ensures that the changes of orientation are random even though the oscillations are periodic, provided the experiment lasts long enough (1 to 3 hours).

The key element of the second Orsay experiment is the optical switch shown in the figure below.

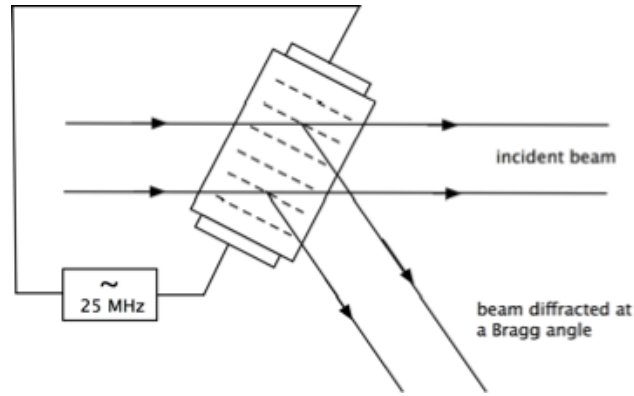


Figure 14.21: Optical switch - Acousto-optical modulator - Pockel cell

In a water tank, a system of standing waves is produced by electro-acoustic excitation at a frequency of 25 MHz (corresponds to 10 ns between switchings).

The fluid keeps changing from a state of perfect rest to one of maximum agitation and back again. In the state of rest, the light beam is simply transmitted, In the state of maximum agitation, the fluid arranges itself into a structure of parallel and equidistant plane layers, alternately stationary (nodal planes) or agitated (antinodal planes). Thus, one sets up a lattice of net-like diffracting planes; the diffracted intensity is maximum at the so-called Bragg angles, just as in scattering from a crystal lattice. Here the light beam is deviated through 10^{-2} radians (the angles in the figure are exaggerated for effect). The two numerical values, 25 MHz and 10^{-2} radians, suffice to show the magnitude of the technical achievement. With the acoustic power of 1 watt , the system functions as an ideally efficient switch.

The second Orsay experiment (using optical switches) is sketched in the figure below.

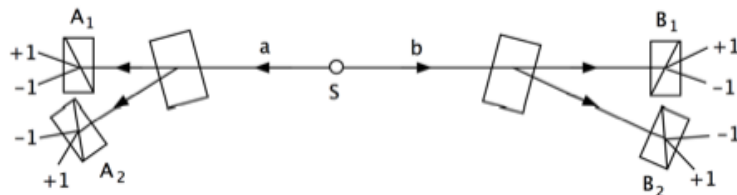


Figure 14.22: 2nd Orsay experiment - relativistic test

In this set-up, the photons a and b leave S without *knowing* whether they will

go, the first to A_1 or A_2 , and second to B_1 or B_2 .

The second experiment is less precise than the first, because the light beams must be very highly collimated in order to ensure efficient switching. Nevertheless, its results exhibit an unambiguous violation of Bell's inequality, reaching 5 standard deviations at the peak; moreover the results are entirely compatible with the predictions of quantum mechanics.

14.3.3.2 The Principle of Non-Separability

Experiment has spoken. Half a century after the Como conference, Bohr's interpretation once again beats Einstein's, in a debate more subtle and also more searching. There were two conflicting theories: The violation of the BCHSH in-

Einstein	Bohr
hidden variables	quantum mechanics
realist	positivist
deterministic	probabilistic
separable	non-separable

equality argues for Bohr's interpretation, all the more so as the measured values of $\langle \gamma \rangle$ are in close agreement with the predictions of quantum mechanics.

It remains to ask oneself just why hidden-variable theories do fail. Of the three basic assumptions adopted by such theories, namely realism, determinism, and separability, at least one must be abandoned. In the last resort, it is separability that seems to be the most vulnerable assumption. Indeed, one observes experimentally that the violation of the BCHSH inequality is independent of the distance between the two detectors A and B , even when this distance is $12m$ or more. There are still die-hard advocates of determinism, who try to explain non-separability through non-local hidden variables. Such theories, awkward and barely predictive, are typically ad hoc, and fit only a limited number of phenomena. They are weakly placed to defend themselves against interpretations furnished by quantum mechanics, which have the virtues of simplicity, elegance, efficiency, and generality, and which are invariably confirmed by experiment.

The principle of Einsteinian separability asserts that *there are no correlations between two phenomena separated by a space-like interval*. In other words, no interaction can propagate faster than light in vacuum. In an EPR scenario this principle must be abandoned, and replaced by a principle asserting non-separability:

In a quantum system evolving free of external perturbations, and from well-defined initial conditions, all parts of the system remain correlated, even when the interval between them is space-like

This assertion reflects the properties of the state vector of a quantum system. For an EPR system, the state vector after the decay of the source reads

$$|\Phi\rangle = \frac{1}{\sqrt{2}} (|x_A, x_B\rangle + |y_A, y_B\rangle) \quad (14.74)$$

This expression combines the elements A and B in a non-separable manner, which is what explains the observed correlations. The truth is that all this has been well known ever since the beginnings of quantum mechanics, with the concept of the electron cloud as the most telling illustration. It is for instance hard to imagine separability between the 92 electrons of a uranium atom. What is new is that quantum mechanics, considered hitherto as a microscopic theory applicable on the atomic scale, is now seen to apply to a two-particle system macroscopically, on the scale of meters. The truly original achievement of Aspect's experiment is the demonstration of this fact.

Quantum objects have by no means exhausted their capacity to astonish us by their difference from the properties of the macroscopic objects in our everyday surroundings. In the preceding sections we saw that a photon can interfere with itself and we have shown that two photons 12 m apart constitute but a single object. Thus, it becomes ever more difficult to picture a photon through analogies with rifle bullets, surface waves in water, clouds in the sky, or with any other object of our familiar universe. Such partial analogies fail under attempts to make them more complete, and through their failure we discover new properties pertaining to quantum objects. The only fruitful procedure is to follow the advice of Niels Bohr, namely, to bend one's mind to the new quantum concepts until they become habitual and thereby intuitive. Earlier generations of physicists have had to face similar problems. They had to progress from Aristotle's mechanics to Newton's, and then from Newton's to Einstein's. The same effort is now required of us, at a time favorable in that, by mastering the EPR paradox, quantum mechanics has passed a particularly severe test with flying colors.

From this point of view, the principle of non-separability seems as important as the principle of special relativity, and Aspect's experiment plays the same role now that the Michelson-Morley experiment played then.

Chapter 15

Erasers and Pots

15.1 Quantum Erasers (Complementarity and Entanglement)

In our earlier discussions, we saw that closing the locality loophole involved switching between different analyzer orientations while the emitted photons were still in flight. The choice between the nature of the measurement was therefore delayed with respect to the transitions that originally created the photons.

Is it possible to make this a delayed choice between measuring devices of a more fundamental nature?

For example, in our discussion of the double-slit measurements, we found that if we allow a sufficient number of photons individually to pass through the slits, one at a time, an interference pattern will be built up. This observation suggests that the passage of each photon is governed by wave interference so that it has a greater probability of being detected (producing a spot on the screen) in the region of a bright fringe. It would seem that the photon literally passes through both slits and interferes with itself. As we noted earlier, the skeptical physicist who places a detector over one of the slits to show that the photon passes through one or the other does indeed prove their point - the photon is detected, or not detected, at one slit. But then the interference pattern can no longer be observed.

Advocates of local hidden variable theories could argue that the photon is somehow affected by the way we choose to set up our measuring device. It thus adopts a certain set of physical characteristics (owing to the existence of hidden variables) if the apparatus is set up to show particle-like behavior, and adopts a different set of characteristics if the apparatus is set up to show wave interference. However, if we design an apparatus that allows us to choose between these totally different kinds of measuring device, we could delay our choice un-

til the photon was (according to the local hidden variable theory) *committed* to showing one type of behavior. We suppose that the photon cannot change its *mind* **after** it has passed through the slits, when it discovers which kind of measurement is being made (whatever this last sentence may actually mean!!)

15.1.1 Delayed Choice or Quantum Eraser Experiment

As we said, QM says systems can change behavior depending on measurements made on them or in response to a decision that has not yet been made. One part of an entangled pair can affect properties of its partner instantaneously, no matter where in the universe partner happens to be.

A so-called *quantum eraser* experiment has now been done...it dramatizes several aspects of quantum strangeness at once.

These experiments dramatically show the non-local effects, i.e., the ability of an experiment in one place to influence the outcome of another regardless of time or distance—but without transmitting any signals.

The idea behind a quantum eraser is to make paths(like those in a 2-slit system) distinguishable, which eliminates the interference effect, but then erase the *which-path* information just before the light reaches the screen where we actually observe the interference pattern.

QM predicts that the interference pattern should then reappear and it does.

A quantum mystery of the following sort. A photon approaching slits will need to know whether or not there is an eraser further down the path(in its future), so that it can decide whether to pass through slits as a superposition of all possibilities (paths are indistinguishable) and produce an interference pattern later on the screen or that it should behave as a *particle* (paths are distinguishable) and produce no interference pattern **later** on the screen!!

An early eraser experiment can be visualized as a two-slit experiment as shown in the diagram below:

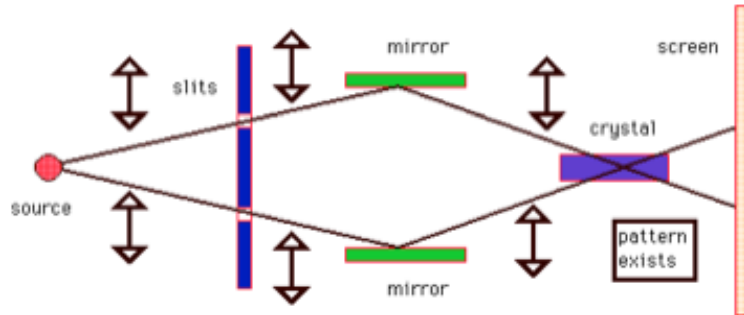


Figure 15.1: Simple eraser experiment

Photons passing through a double slit are all vertically polarized (indistinguishable paths). They can get to a recombination crystal by two paths as shown, which remakes a beam that produces an interference pattern on the screen, i.e., if paths are indistinguishable, then we have a superposition of all possible paths (2 paths in this case) and we get an interference pattern.

Now we insert a polarization rotator on one path only

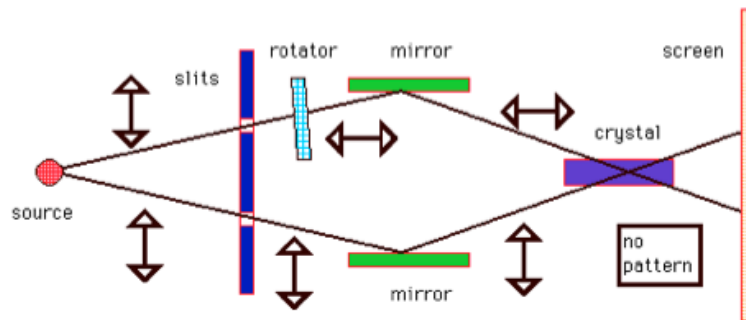


Figure 15.2: Adding a polarization rotator

and rotate the polarization of the photons to horizontal in that path. Since the paths now produce distinguishable photons, we get *particle like* behavior and the interference should disappear. It does! Now we add a quantum eraser after recombination (a polaroid at 45°)

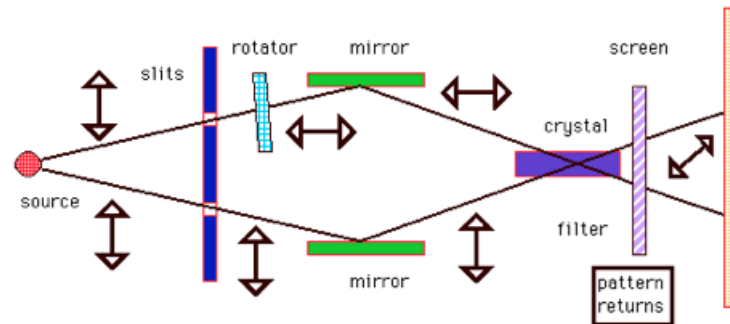


Figure 15.3: Adding a quantum eraser

The polaroid filter produces equal numbers of photons with both vertical and horizontal polarization (with respect to new direction).

Half of the new vertically polarized photons come from the horizontal polarized photons of the top path and half of the new vertically polarized photons come from the vertical polarized photons of the bottom path (similarly for the new horizontally polarized photons). It is impossible to tell whether a photon was vertically or horizontally polarized before the eraser. Thus, the two paths are once again indistinguishable. If the interference pattern reappears, then a photon approaching the slits somehow needs to *know* whether or not there is an eraser down the line so it can decide whether to pass through the slits as a superposition(wave) and produce interference effects or as a mixture(particle) and produce no interference. The pattern reappears immediately confirming the quantum mechanical prediction. The filter erases the which-path information caused by the rotator.

A truly astounding result.

What does this say about the classical idea that it is the two-slit system that is the *real* cause of the interference pattern?

Worry: Experimenters, knowing the fundamental importance of these results, wanted to leave no possible source of controversy intact. In the above version of the experiment, there is a potential problem because the which-path information is carried by the same photons that interfere, making the experiment difficult to interpret.

A new version of experiment... Here which-path information is not carried by what one would naively call the interfering photon. Instead, it is carried by 2nd photon and along way it also demonstrates the striking non-local effects of QM. The experiment looks like:

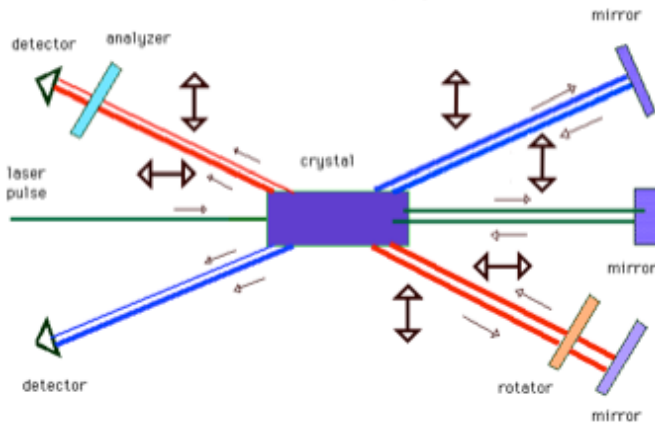


Figure 15.4: Separating the paths

High intensity laser photons are sent into parametric down-conversion non-linear crystal such as lithium iodate. The crystal converts some incoming photons (green) into pairs of identical photons with lower energy and vertical polarization moving at an angle to the original direction. The photons are produced as entangled partners. A measurement on one photon automatically tells us about the other with no direct measurement on the 2nd photon necessary.

Twin beams exit crystal at an angle to the original path. These are the thick red and blue lines.

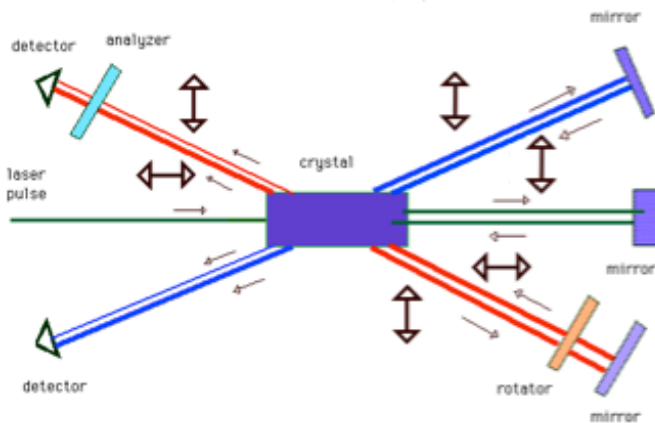


Figure 15.5: All the beams

They are reflected back towards the crystal by mirrors and pass straight through it to detectors (the intensity is now too weak to cause down-conversion). These are the thick red and blue lines.

However, not all the laser light gets converted on 1st pass.

Some goes straight through the crystal to another mirror(green) and is reflected back into crystal(still high intensity) where the crystal creates more photon pairs which then follow same path as other beams to detectors. These are the thin red and blue lines.

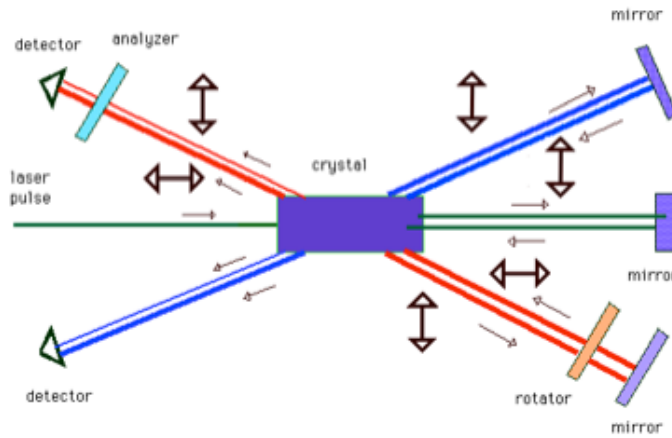


Figure 15.6: More details

As a result, we have two different beams heading towards each detector each having follow different paths.

Each pair of beams corresponds to a separate double slit experiment.

If there is no way to distinguish the photons created on first pass through crystal from those created on 2nd pass(and there is not), both detectors should have interference patterns and they do!!

We now make one returning beam in one leg distinguishable from other by inserting a polarization rotator into red path(as shown below) converting vertical polarization to horizontal polarization in that leg.

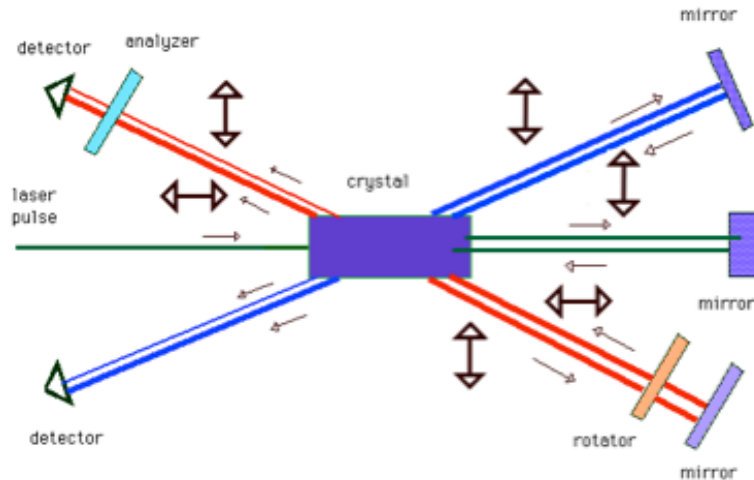


Figure 15.7: Adding polarization rotator

The interference pattern in the top detector vanishes instantly as it should since the two (interfering) beams now have distinguishable paths.

Now, however, we also find that interference pattern disappears in left detector!!!!!!

Why?

We have done nothing to disturb these beams so that the beams in the bottom detector still correspond to indistinguishable paths and photons!!!!

Remember, however, that the photons are created in entangled pairs, so when the red-path photons become labeled with which path info, the same info becomes available to blue-path photons, no matter where they are!!!

This is *non-locality* at work.

To erase the *which-path* info, we now add a 45° polaroid in red path, just in front of detector.

The interference pattern immediately reappears in top detector as it should (same as previous experiment).

It seemed however, that pattern did not reappear in bottom detector. One might imagine this is so because erasing red-path photon information does not

erase any information from blue path.

In addition, if it did reappear immediately, then we would be able to send signals faster than light with such an eraser.

However, as in EPR experiment we find, if we bring two data sets back together and compare them, the pattern had, in fact, been restored along both paths (need both data sets) to see correlations among the individual photons. Alternatively, one can do a coincidence measurement, which only looks at those photons counted in each detector simultaneously and one can see the interference pattern return directly, that is, the *which way* and interference effects are being recorded for *single* photons.

Thus, inserting or removing which-path information transforms the behavior of light throughout the entire system simultaneously demonstrating the amazing quantum eraser and the dramatic non-local behavior of QM.

This experiment makes it clear that there is a direct relationship between tests of complementarity and tests of quantum non-locality. Interference effects are the direct manifestation of non-local behavior. These effects can be *encoded* in the mathematical structure of quantum entanglement - in this case, entanglement of the states responsible for interference with the state used to detect "which way" information. These states cannot be disentangled without forcing the system to reveal one type of behavior or the other. They cannot be disentangled to reveal both types of behavior simultaneously.

Though still a subject for debate, a consensus is building that complementarity - and hence non-locality and entanglement - is the mechanism for the mutual exclusivity in the dual wave-particle nature of quantum objects, what Richard Feynman described as the *central mystery* at the heart of quantum mechanics.

15.2 Watching the Quantum Pot

Consider a *pot* consisting of a few thousand Be ions (one electron removed). Such charged ions can be corralled by an electric-field into *ion trap = the quantum pot*.

This model is just like water molecules in pot on stove.

Now we want to make the pot of Be ions boil and see if watching them while they are trying to boil can stop boiling and demonstrate the collapse process, i.e., *can we actually see collapse process*.

At the start, the ions are all in same quantum energy level 1 of a 3-level system.

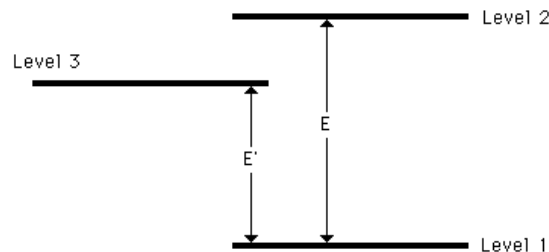


Figure 15.8: Ion energy levels

We apply a burst of radio waves with particular energy (frequency)

$$E = E_2 - E_1$$

for exactly 256 msec , which causes *all* the ions to make a transition up to the higher energy level 2.

The upward transition is so rapid and the downward transition so slow that any ions that get to level 2 effectively remain there for duration of experiment.

this ion trap + radio waves = boiling pot

On a stove, heating supplies energy and boiling is the process of raising all molecules to higher energy (higher velocity) states which then allows them to escape from surface as steam.

The picture we just described happens if *do not measure the system at all*.

Now we ask how and when do the ions actually make a transition from one quantum state to other?

Remember, they only decide what state(choose among probabilities) they are in when that state is measured – when an observer takes look at the ions, according to quantum mechanics.

Quantum mechanics says the transition is *GO-NOGO* process, an all or nothing affair; either the ion does or does not(via probabilities) change levels.

256 msec is the characteristic time in system when there is almost exactly 100% probability that any individual ion will have made the transition to level 2.

At 128 msec , there is exactly a 50-50 probability that any ion has made transition to level 2 or remained in level 1.

At any time in interval $0 - 256\text{ msec}$, the system is in superposition of states with an appropriate mixture of probabilities

$$|\text{pot at time } t\rangle = \cos\left(\frac{2\pi t}{1.024}\right)|\text{not boiled}\rangle + \sin\left(\frac{2\pi t}{1.024}\right)|\text{boiled}\rangle$$

i.e.,

$$\begin{aligned} P(\text{not boiled}) &= \cos^2\left(\frac{2\pi t}{1.024}\right) \\ P(\text{boiled}) &= \sin^2\left(\frac{2\pi t}{1.024}\right) \end{aligned}$$

When it is observed, we must always find the quantum system in definite state; we never see a superposition of states.

If could look at ions at 128 msec , theory says would have to choose between two possible states, just like Schrodinger's cat had to be dead or alive.

With equal probabilities, $1/2$ choose level 1 and $1/2$ choose level 2. This agrees with experiment.

NIST experimenters devised a neat technique for looking at the ions while they were making up their *minds* about which state to be in.

They sent a very brief pulse of laser light into quantum pot with photon energy

$$E' = E_3 - E_1$$

This laser burst interacts with the ions in pot so that the ions in level 2 are unaffected and all the ions remaining in level 1 are excited up to different higher energy level 3.

From level 3, they immediately ($\Delta t < 10^{-7}\text{ sec}$) go back to level 1.

As they jump back, they emit characteristic photons of energy E' . These fixed energy photons are detected and counted.

The number of photons counted tells us number of ions that were in level 1 when this special pulse was sent into pot.

When the ions were looked at once by the laser pulse after 128 msec , half were found in level 1.

This is what we should see according to quantum mechanics.

If the experimenters peeked 4 times during the 256 msec at equal intervals, at end of the experiment $5/8$ of the ions were still in level 1 not all in level 2 as was true when they did not look.

As stated earlier, at any arbitrary time t the state of the system is

$$|\text{pot at time } t\rangle = \cos\left(\frac{2\pi t}{1.024}\right)|\text{not boiled}\rangle + \sin\left(\frac{2\pi t}{1.024}\right)|\text{boiled}\rangle$$

In particular, this says that

$$\begin{aligned} |\text{pot at time} = 0\rangle &= |\text{not boiled}\rangle \\ |\text{pot at time} = 256\rangle &= |\text{boiled}\rangle \end{aligned}$$

The probabilities are non-linear functions of time. This means that the transition rates are not constant in time, i.e., it varies depending where we are in the interval $0 - 256 \text{ msec}$.

Luckily, for us, the collapse mechanism intervenes to simplify the problem!

If we make 4 measurements each separated by 64 msec , then here is what happens. At 64 msec if we found a particle in state 1 (not boiled) then the collapse process resets the clock to $t = 0$ and to 256 msec if particle is found in state 2.

In particular, the probability of making a transition to state 2(boiled) during a time interval $= 256/n =$ time between peeks, if it was in 1 at the beginning of interval, is given by

$$\sin^2\left(\frac{\pi}{2n}\right)$$

and hence probability of it remaining in state 1 (unboiled) is

$$1 - \sin^2\left(\frac{\pi}{2n}\right) = \cos^2\left(\frac{\pi}{2n}\right)$$

Similar arguments can be given for probabilities associated with starting in level 2.

If one uses quantum mechanics to calculate what happens after n measurements one finds the prediction for probability of finding it in 2 after n measurements is given by

$$P(n) = \frac{1}{2} \left(1 - \cos\left(\frac{\pi}{2n}\right) \right)$$

which corresponds to $P = 3/8$ for $n = 4$ or $5/8$ are still unboiled.

If they peeked 64 times (once every 4 msec), almost all ions were in level 1 at the end. In fact it goes like

n	$P(n)$
2	0.500
4	0.375
6	0.289
8	0.235
10	0.197
16	0.133
32	0.072
64	0.037
128	0.029

So, even though the radio waves were doing their best to boil the pot of ions, the watched quantum pot refused to boil. WHY?

The reason is that after 4 msec , the probability that a single ion will have made transition to level 2 is about 0.01%, so laser *finds* 99.99% of ions in level 1

It has, however, done more than that.

The act of looking at ions(measuring where they are) has collapsed the system back to level 1 quantum state as if ? since that is where we found them.

Now the state(all in level 1 again) begins to once again try to become a mixture but 4 msec later we look again and collapse it again. At end of experiment ions have had no opportunity to make transition to level 2 without being observed and thus collapsed even though we are continuously supplying proper energy!!!

We are saying.....

The exact agreement with quantum theory shows that if it were possible to monitor the ions all time then none of them would ever change. If, as quantum mechanics suggests(according to some physicists), the world only exists because it is being observed, then it is also true that world only changes because it is not being observed all the time.

Chapter 16

Interpretations

We are now going to look at the various dominant interpretations of quantum theory and what they have to say about the nature of quantum reality. Prior to doing this, however, we must discuss what is at stake.

16.1 What is an Interpretation?

Before going into the philosophical quagmire, we need to establish what it is that we're looking for. What is an interpretation of quantum theory and how will we know when we have the correct one?

Every physical theory needs a form of interpretation. When we write down a string of mathematical formulas there has to be some link between the symbols on the page and the measurements that we make. This is one of the jobs an interpretation is designed to do.

While we have been doing classical physics there was no real problem involved; the association between mathematics and measurements was so close that a formal interpretation wasn't really needed. With quantum theory, things have changed: the intimate link between mathematics and measurements has been broken. We have a successful set of mathematical rules allowing us to manipulate symbols such as $|\phi\rangle$, but that still leaves us free to argue over what $|\phi\rangle$ *means*.

Not every mathematical symbol used in the theory needs a direct link to measurement. We associate the operator \hat{p} (in its position representation) with momentum and calculate $\langle\phi|\hat{p}|\phi\rangle$ to get the average value of momentum observed. However, \hat{p} *itself* is not in any sense *measured* and it could well be (as some physicists think) that $|\phi\rangle$ is nothing more than a mathematical convenience used to get us from one set of results to another without representing anything in the real world. After all, we divide the surface of the Earth up with lines of

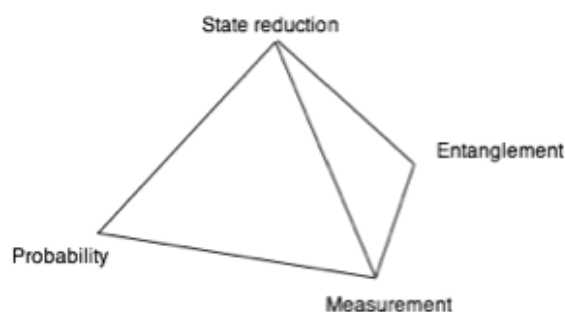
latitude and longitude to help us find our way about, but we don't expect to find the lines actually drawn on the ground.

I think that there's something more to an interpretation than just a formal link between symbols and measurements. An interpretation should provide us with a picture of the world. Not a literal picture like a drawing, but something that we can glimpse in our minds as to the *shape* of what is out there. This is partly done by links between symbols and measurements, but as in the poem **The Blind Man and the Elephant** by John Godfrey Saxe, we still want to see what the whole elephant looks like.

If you take this view of interpretation, it is clear that *instrumentalism* is not an interpretation in that sense. An instrumentalist is either not bothered at all about a picture of the world or not fixed to one rather than any other. They are content to use whichever picture make the current problem easier. This is certainly a very practical approach; you can get on with doing science this way. It's an example of *shut up and calculate*. However, I cannot believe that such a view gets many people interested in science in the first place. Surely a scientist's basic ambition is to be a realist, otherwise why bother?

A Collection of Problems

In his influential book on quantum theory, Chris Isham has usefully drawn attention to four key issues (see figure below)



that any realistic interpretation of quantum theory has to face:

- (1) The nature of probability
- (2) The role of measurement
- (3) The reduction of the state vector
- (4) Entanglement

This diagram shows Chris Isham's collection of four linked problems in the interpretation of quantum theory. They are drawn at the four corners of a

tetrahedron to emphasize how they are interconnected.

One way of distinguishing between various interpretations is to categorize how they approach these four issues. We will take them one by one and draw together various threads using each one as a context.

16.1.1 The Nature of Probability

Probability is one of those annoying ideas that get harder to understand the more you think about them. This problem comes partly from *probability* being a blanket word that refers to a collection of closely related ideas that people sometimes get confused.

If you're a betting person, you will have a good idea of what *odds* are all about. When we're told that the odds of Swarthmore beating Haverford in some event are 60:40, we must imagine that the event is allowed to happen 100 times in identical fashion (same weather, same teams, same phase of the moon, etc), in which case Swarthmore will win 60 of these events and Haverford 40 of them. Of course, we cannot actually run the event 100 times in this way, so the estimation of odds is not based on any reliable scientific measuring process. The odds have been obtained by some estimation that is supposed to refer to the physical attributes and the abilities of the teams, but the odds themselves are not an objective property of people or things. We cannot *measure the odds*. To what extent then do these odds *exist*? Do they correspond to anything in the world, or are they simply something that we have cooked up to make our lives a little more entertaining?

Another example of probability is the tossing of a fair coin. If this (mythical) object is tossed 100 times its supposed to come up heads 50 times and tails 50 times. Of course, in practice this happens very rarely, and what are we to deduce from that?

If it comes up heads 80 times, we may well suspect the *fairness* of the coin. If it comes up heads 53 times we'll probably say that's just the way things are: after all it is a random process.

In truth with this small number of trials we probably cannot tell which of these possibilities is the right one. If it was 1000 trials coming up 800 heads and 200 tails then we will be more inclined to doubt the coin.

In either case, we are assuming that the coin has some reliable property that determines, at least to some extent, the outcome of the toss. The way the coin is made, the extent to which the metal is distributed across its width, etc., will all help to fix how the coin lands, along with other factors to do with the forces applied during the toss. Small variations from toss to toss mean that we can never fully see the coin's nature; it just becomes clearer when we make more

tosses, or at least that is the assumption. By trying a large number of coin tosses we're hoping that these fluctuations in the toss balance out: there will be as many occasions when an uneven toss tips the coin one way as the other, so overall these effects will smear out.

In this situation we estimate the probability using

$$Prob(heads) = \frac{\text{number of times heads comes up}}{\text{total number of tosses}}$$

without really thinking about it too much. However, there are some difficulties involved here.

Let us say that we toss the coin 100 times and get 57 heads. Our estimate of the probability of a head is 57/100 or 0.57. But what does this refer to? Is it an estimation of some probability that exists even before we *measure it*. Is it a measure of some property of the coin? Or is it simply a probability that refers to that particular collection of 100 tosses with limited use of validity outside of that collection?

We generally assume that our probability estimation is of use outside the collection of results used to obtain it; we use the number to make further predictions.

OK then, but what if we take the same coin and toss it 1000 times so that 578 heads come out? Now we have a probability estimate of 0.578. This might be a more accurate estimation of the "underlying" probability, or it might just simply refer to the collection of 1000 tosses. After all, it would be possible to do another 1000 tosses with the same coin and end up with 643 heads. Does this mean our original estimation was wrong? Of course we tend to think not, and assume that the more often we toss the coins the closer we get to the underlying probability (aside from statistical flukes like the 643 result). In other words,

$$\text{Probability estimation} \xrightarrow{\text{greater number of tosses}} \text{actual probability}$$

which implies that there is a *real*, objective right answer.

All of this might be starting to sound like the debate over the *real* nature of the quantum state, which is possibly no coincidence.

Moving into an area more directly related to classical physics, the most obvious use of probability comes when we start to work with very large numbers of particles, as in a gas. The huge number of particles involved in even the smallest volume of gas makes trying to calculate exactly what is happening based on the motion of every single particle a hopeless task. Instead, we work out what is probably going to happen.

The figure below shows the Maxwell-Boltzmann speed distribution for molecules

in a gas at three different temperatures. The distributions have been calculated for one million particles at each temperature, based on a statistical calculation of the relative probabilities for each speed.

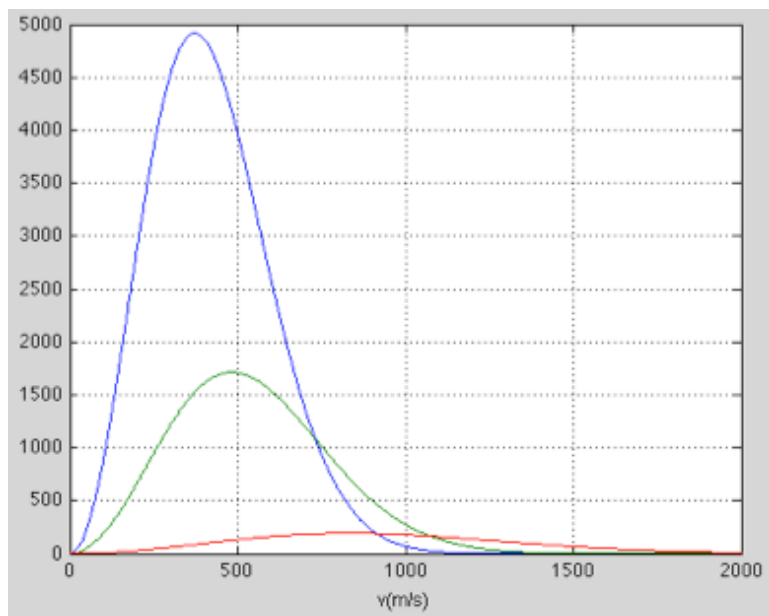


Figure 16.1: Maxwell-Boltzmann speed distributions

The figure shows the Maxwell-Boltzmann distribution of speeds within a gas at three different temperatures -100 , 20 , and 600°C . The horizontal axis is speed in meters per second and the vertical axis shows the number of particles at a given speed. Each distribution contains a total of one million particles.

If we pick a single particle out of the gas, these theoretical calculations tell us the probability that the particle will have a given speed. Now this probability can't really be called a property of the particle. After all, each particle has a speed whereas the probability distribution refers to every speed that a randomly chosen particle might have.

Effectively, we are dividing the particles into groups, each group containing just those particles with a given speed (or within a small amount of a given speed). Then when we say that x is the probability of a selected particle having a specific speed, we mean that the chances of it having come from a given group is x . We can calculate this theoretical probability using laws of nature and standard statistical techniques. Then we experiment on a real gas to see how well it corresponds to the theory.

In this sort of situation, probability is being used to cover up our ignorance

about the fine details of what is going on. However, we talk as if this probability exists in some objective way and that all the real gases measure up against this standard to some extent.

In quantum theory, probability pops up in two different ways. First, we may not know exactly what state the quantum system is in. We may have a collection of systems some of which are in state $|\phi_1\rangle$, some in $|\phi_2\rangle$, or in $|\phi_3\rangle$ $|\phi_n\rangle$, etc; or we may have one system and just not be sure what state it is in. In either case, we construct a density operator to summarize our information about the state

$$\hat{D} = \sum_n [p_n |\phi_n\rangle \langle \phi_n|] \quad (16.1)$$

where p_n is the probability of finding the system in state $|\phi_n\rangle$. We either *estimate* this probability by counting systems or *calculate* it based on some knowledge of how the systems are made. In either case, the probability is being used in the same way as we did with the gas particle. We'll call this a *classical probability*.

However, even if we know that the system is in state $|\phi\rangle$ we have a probability associated with the results of a measurement. If $|\phi\rangle$ is an eigenstate of some physical variable, we can be 100% sure that the measurement will reveal the eigenvalue. If not, then the probability of some value a_n is calculated from $|\langle a_n | \phi \rangle|^2$. Is this the same sort of probability as before? We will call this quantum probability to distinguish it from the classical probability named earlier. One of the challenges that any interpretation of quantum theory faces is to explain where quantum probabilities come from and illuminate their relationship to classical probabilities (if there is one).

16.1.2 State Reduction

Throughout this book we have tended to use expressions such as *the state of a system* or *the system is in state $|\phi\rangle$* . These are inherently realistic things to say. Indeed, one could argue that the pivot point between realism and instrumentalism reflects the extent to which you are willing to relate the quantum state to an individual system, rather than a collection of them.

We have used this sort of expression because the language is smoother, not to bang a realistic drum. However, we have to acknowledge that some physicists deny that quantum states refer to individuals at all. They would claim that the state refers to a collection of identical systems, something that is often called an *ensemble* of systems. After all, to measure the expectation value of any physical property we have to make a series of measurements on identical systems. The expectation value belongs to the *collection*, so why not the state?

The ensemble view does however leave open an important question regarding the physical properties of systems. Do the individuals in the ensemble have physical properties with fixed values?

Let us imagine that we have a collection of identical systems and that we know that the quantum states from the set $\{|\phi_n\rangle\}$ are involved. A realist would say that each system is in a state and that we can divide an ensemble of systems into several piles (subensembles) with all the systems in a pile having the same state. Someone with a less-realistic viewpoint would prefer to say that the systems are divided into piles and the state refers to the pile as a whole. Some might even say until you divide the systems up into piles, the systems do not have a definite state!

In either of the first two cases, we would describe the ensemble of states by the density operator

$$\hat{D} = \sum_n [p_n |\phi_n\rangle \langle \phi_n|] \quad (16.2)$$

Now imagine that we perform a measurement, or a collection of measurements, that allows us to divide the systems into their respective piles and that we concentrate only on the pile with systems associated with the state $|\phi_3\rangle$. To do any further work with the *subpile* $|\phi_3\rangle$, we need to use

$$\hat{D}_3 = |\phi_3\rangle \langle \phi_3| \quad (16.3)$$

if we want to stay in density operator language. We have *reduced the state* from \hat{D} to \hat{D}_3 .

$$\hat{D} = \sum_n [p_n |\phi_n\rangle \langle \phi_n|] \Rightarrow \hat{D}_3 = |\phi_3\rangle \langle \phi_3| \quad (16.4)$$

There is nothing especially mysterious in this; it just reflects a change in how much we know about what is going on.

As a next step, let's imagine making a further measurement of some physical property represented by the operator \hat{O} with eigenstates $|a_m\rangle$ and that $|\phi_3\rangle$ is not one of these eigenstates. After the measurement the pile of states $|\phi_3\rangle$ has been converted into a collection of smaller piles, one for each $|a_m\rangle$. The number of systems in each of these smaller piles is directly related to $|\langle a_m | \phi_3 \rangle|^2$. In fact,

$$\begin{aligned} & (\text{Number of systems in pile } |a_m\rangle) \\ &= |\langle a_m | \phi_3 \rangle|^2 \times (\text{number of systems in pile } |\phi_3\rangle) \end{aligned} \quad (16.5)$$

where $|\langle a_m | \phi_3 \rangle|^2$ is a quantum probability.

When we describe what has happened here, we talk in terms of the state $|\phi_3\rangle$ having *reduced or collapsed* into one of the $|a_m\rangle$; $|\phi_3\rangle \Rightarrow |a_m\rangle$. A realist regards this as a physical change of some form in the system itself, as each state is connected with an individual. In this case, the quantum probability must be a measure of how likely this physical change is and so presumably related to the extent of the change, that is, how different the two states are.

For those who are more instrumentalist in thinking, there is no physical change

in any system. We are, once again, focussing on a smaller number of systems that come under the collective state of $|a_m\rangle$.

However, there is a catch. Imagine that we have performed this measurement on each systems in the collection $|\phi_3\rangle$ so that the systems have been subdivided into piles of $|a_m\rangle$ and that we then get some colleagues to make a further series of measurements without telling them the results of what we have done. They are allowed to know that we have made a measurement of \hat{O} , so they know they are dealing with a collection of states $\{|a_m\rangle\}$ but won't know which system is which. How will they describe the collection of systems? They will have to use the density operator

$$\hat{D}_O = \sum_m [p_m |a_m\rangle \langle a_m|] \quad (16.6)$$

But we can go a little further than this. We can tell them that the systems started off in the state $|\phi_3\rangle$ so that the various probabilities p_m in their density operator are actually $|\langle a_m | \phi_3 \rangle|^2$.

$$\hat{D}_O = \sum_m [|\langle a_m | \phi_3 \rangle|^2 |a_m\rangle \langle a_m|] \quad (16.7)$$

So now, here is the tricky bit. When we construct such a density operator, we say that the p_m 's are *classical probabilities*, but we have just identified the $|\langle a_m | \phi_3 \rangle|^2$ as *quantum probabilities*.

- (1) Have they converted from one type to another?
- (2) How can \hat{D}_O be a different sort of density operator than \hat{D} ?
- (3) Is there actually any difference between quantum and classical probabilities?
- (4) Can we keep up a distinction between

$$\hat{D} = \sum_n [p_n |\phi_n\rangle \langle \phi_n|] \Rightarrow \hat{D}_3 = |\phi_3\rangle \langle \phi_3|$$

and

$$|\phi_3\rangle \Rightarrow |a_m\rangle$$

if the probabilities are the same?

These are all issues that a realistic interpretation must attempt to resolve.

16.1.3 Entanglement

An entangled state is a state of more than one system that cannot be broken down into a combination of unique states for each system. The existence of entangled states in quantum theory is remarkable, not just for the amazing physical properties that they show, but also for the fact that they potentially cut across one of the basic assumptions behind much of Western philosophy.

A particularly Western approach to the study of the world is the use of **reductionism**: the notion that any system can be understood by examining the parts from which it is made. If this is to work at all, we have to assume that the parts behave in exactly the same fashion when they are members of the whole as they do when they are on their own. The problem with entangled states is that they bury the distinction between part and whole.

At one level of approximation, two electrons can be treated separately and the behavior of one has no influence on the other. However, in detail, every electron is in an entangled state with all the other electrons in the universe, just from the fact that they are all identical fermions. Allow them to take part in an EPR-type experiment and they become even more deeply entangled. With a combined state such as

$$\frac{1}{\sqrt{2}} [|\phi_A\rangle |\Psi_B\rangle - |\phi_B\rangle |\Psi_A\rangle]$$

we can no longer say with any certainty that electron A is in state $|\phi\rangle$ while electron B is in state $|\Psi\rangle$. So, can we consistently think of the electrons existing as separate parts within the whole any more?

At one level, entanglement presents us with a philosophical challenge, one that threatens to pick away at our notion of what a *thing* is. At another level, entanglement presents us with a practical problem:

Why does anything happen at all?

As we have seen, the interaction between a particle and a measuring device necessarily entangles the states of the particle with those of the measuring device (provided we accept that the measuring device can be described by quantum theory)

$$|\Psi\rangle |\phi_n\rangle = [a|U\rangle + b|D\rangle] |\phi_n\rangle \Rightarrow a|U\rangle |\phi_U\rangle + b|D\rangle |\phi_D\rangle$$

where $|\phi_n\rangle$, $|\phi_U\rangle$, and $|\phi_D\rangle$ represent the neutral, recording UP, and recording DOWN states of the measuring device, respectively. While the entanglement exists, neither the particle nor the measuring device can be said to be in one state or another. If we take a literal interpretation of this, the measuring device (like Schrödinger's cat) is in an intermediate form of existence that we certainly do not observe in practice.

It is not just a measurement interaction that will entangle states. Any interaction between two quantum systems will entangle their states together. Consequently, the entanglement spreads like an infectious disease.

Entanglement is governed by the $\hat{U}(t)$ operator constructed from the Hamiltonian specifying the energy of interaction between device and particle. As we have argued before, $\hat{U}(t)$ cannot produce a state collapse, so how do we see anything happen?

16.1.4 Measurement

This brings us to the measurement problem. There are two questions we have to answer if the measurement problem is to be solved.

- (1) What makes a measurement interaction any different from an ordinary interaction?
- (2) What causes a state to collapse, if indeed it happens at all?

Going back to our earlier discussion on probability, it should be clear that if we relate states only to collections of systems, then there is no real measurement problem. The state $|\phi\rangle$ refers to the big pile of systems and the state $|a_m\rangle$ to one of the smaller subpiles within the big pile. No physical change has taken place, just a shift in our focus or a change in our knowledge or information. So, this disposes of the measurement problem in one sense, but replaces it with another.

How do we know which systems go into which pile? If we do this on the basis of making a set of measurements, are we not verging on saying that the systems have values of properties *before* we make a measurement of them? This sounds somewhat like the sorting of electrons that we tried earlier and it didn't work. An ensemble-type view of state collapse follows if we accept the limitations of instrumentalism, but in turn it raises its own fundamental problems.

A realistic view of state collapse seems part and parcel of a realistic approach to the measurement problem, as without a state collapse of some form the state of a system are hopelessly entangled with those of the measuring device. If state collapse actually happens, then quantum probabilities must exist and so amplitudes seem to have some sort of reality.

Carnegie Hall - There's an old joke in which a tourist in New York asks a cab driver how to get to Carnegie Hall (a famous concert venue); the helpful reply comes "well, I wouldn't start from where you are".

The fact is that if we want to be scientists with a realistic view of what we do, then quantum theory is not the best place to start. But it's not like we have a choice. Quantum theory was not invented as a way for physicists to give philosophers migraines; it has come from our attempts to describe the world revealed by sets of experiments. That being the case, We believe that we have to fight to retain a realistic interpretation of quantum theory, albeit one that forces us to modify our views of what the world is like.

16.2 The Copenhagen Interpretation

We now take a look at the so-called **standard interpretation** of quantum theory, namely, the Copenhagen interpretation. However, there is actually no

single clear statement of the Copenhagen interpretation, and many of the originators differed in the details of their beliefs. What modern physics regards as the Copenhagen interpretation is actually an amalgam of ideas. Because of this, we will focus on the thinking of three key players, each of them contributed something important to the overall view of what the Copenhagen interpretation says about reality.

16.2.1 Bohr's Influence

Undoubtedly standing at the center of it all was Niels Bohr, working out of his institute in Copenhagen. Bohr had a profound personal and scientific influence on a generation of physicists. However, his writing on the philosophy of physics is notoriously unclear, which caused some debate about the interpretation of Bohr.

With this sort of confusion among his close colleagues, it is surprising that Bohr had the range of influence that he did. Perhaps this was due to his personal magnetism and conviction. As Pauli pointed out: *Bohr himself integrated, in lectures at international congresses and at those carefully planned conferences in Copenhagen, the diverse scientific standpoints and epistemological attitudes of the physicists, and thereby imparted to all participants in these conferences, the feeling of belonging, in spite of all their dissensions, to one large family.*

The picture below shows Niels Bohr and Albert Einstein during the Solvay international conference on quantum theory.



Figure 16.2: Bohr and Einstein

The picture below shows all of the participants at the Solvay Conference, 1927.

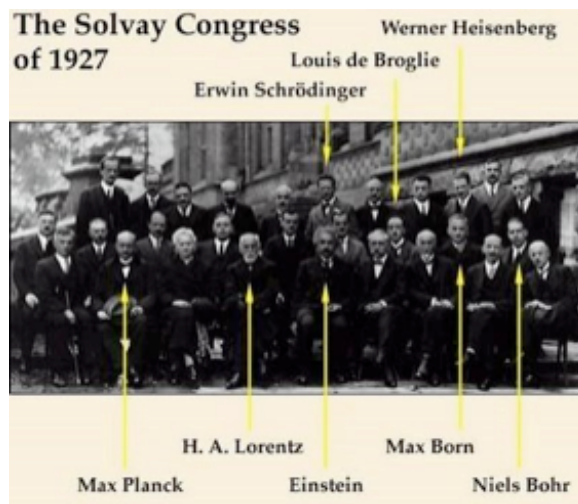


Figure 16.3: Solvay Conference

Bohr took very little interest in the mathematical development of quantum theory, preferring instead to focus on the concepts and the description of atomic events in ordinary language. As Heisenberg once said, Bohr was *primarily a philosopher and not a physicist*. As a result some physicists at the time felt Bohr had sorted out all the philosophical aspects of the theory, although they found his ideas hard to follow, for example, *complementarity*. As we mentioned earlier, Bohr introduced this notion to deal with the apparently contradictory experimental results that were cropping up. Complementarity became part of the physics vocabulary so that everyone could discuss about it, even if all of them thought it meant something slightly different. With Bohr's stamp of approval behind it, there had to be something to it, so people bought into the idea.

Unfortunately, Bohr wrote very little about state reduction and measurement. He made only one written comment about the measurement problem, and that is so obscure that we are not even going to quote it to you. As far as state reduction is concerned Bohr seems to have treated this as *nothing more than the necessary change in mathematical description when you move from one experimental context to another*. He regarded such issues as being related to the mathematical formalism, not the physical interpretation. He thought that all of the stuff about Schrödinger equation, wave functions, states, operators, and the like, was only a set of abstract rules that meant nothing unless they were anchored to classical concepts in experiments. When talking about the Schrödinger equation in 1958, Bohr said, *we are dealing with a purely symbolic*

procedure, the unambiguous physical interpretation of which in the last resort requires a reference to a complete experimental arrangement. Arguably Bohr had an instrumental view of the mathematics of quantum theory and a realistic view of the concepts used to describe events.

Although he cannot help us with two of our most important problems, we need to face up to Bohr's views, as he was undoubtedly one of the most gifted minds of the 20th century. Einstein once commented that Bohr's *thinking* was clear, it was only his *writing* that was obscure. Bohr has left an indelible mark on the history of ideas and any modern interpretation has to directly challenge his thinking.

16.2.2 Bohr's View of Quantum Theory

Some historians of physics take the view that Bohr's thinking developed markedly during the course of his career. In particular, they say that Bohr's ideas had to change in some crucial ways after the Einstein, Podolsky, and Rosen (EPR) paper had been published. I do not go along with this and agree with those historians who say that Bohr's ideas were fully in place before EPR was published (the speed at which he produced the counterargument tends to suggest that he did not need a lot of time to rethink things) and that his reply to EPR helped make his thinking clearer.

As to the nature of Bohr's ideas, experts point to four key ideas that he repeatedly emphasized.

- (1) You are forced to use classical concepts to describe the results of any experiment.
- (2) During a measurement it is impossible to separate a quantum object from the apparatus as you cannot control the interaction between the two.
- (3) You cannot rely on being able to relate the results of one experimental arrangement(context) to another.
- (4) You cannot have an accurate description of an object in terms of its position in space and time as well as an accurate description of its energy and momentum, so the classical way of explaining how the world works has to be replaced by something new.

At various stages, Bohr tried to arrange these ideas into a logical sequence so that he could justify one in terms of another. Unfortunately, he never entirely succeeded in doing this in a satisfactory fashion. Despite this, these four points taken together form an overall picture of both the quantum world and the role of physics. They are an interlocking set of ideas that you have to *accept* as a whole, but to explain them further we have to take them one by one.

16.2.2.1 Classical Concepts

Some statements from Bohr:

It lies in the nature of physical observation, that all experience must ultimately be expressed in terms of classical concepts.

Ultimately, every observation can, of course, be reduced to our sense perceptions.

However far the phenomena transcend the scope of classical physical explanation, the account of all evidence must be expressed in classical terms. The argument is simply that by the word *experiment* we refer to a situation where we can tell others what we have done and what we have learned and that, therefore, the account of the experimental arrangement and of the results of the observations must be expressed in unambiguous language with suitable application of the terminology of classical physics.

Bohr felt that the ultimate purpose of physics was to describe the world in clear language that everyday people could understand. This language, as well as the whole of our thinking, is rooted in the classical world and the basic physics on which it operates. We cannot strip away our very way of thinking and talking, to start again in quantum theory.

Clearly, raw experimental results (pointer readings, photographic films, detector readouts, et.,) are part of the classical world and so they have to be described in classical terms using everyday language (with the obvious technical additions). This arrangement has worked well for generations. However, Bohr's point was more sophisticated than *it's not broke, so don't fix it*. In his view it was not simply practically valid to use classical physics in this way, it was logically necessary as well. It is like the board on which we play the game; classical physics is logically prior to quantum physics, not just historically earlier. Although the overall pattern of results from different experiments may not fit any of our classical theories, we still need to describe each separate experiment using classical concepts.

In this area, Bohr is on slightly shaky ground. First, many would argue that physics achieves its aims by using a mathematical description of the world, and the concepts used in mathematics are perfectly capable of going beyond everyday language. Second, what is wrong with trying to develop new concepts in quantum theory and showing, in some way, how the classical concepts arise from them in the right circumstances?

Bohr was so convinced of the role of classical language and concepts that he shut off any thinking about alternatives: *Not only as far as I can see, have we up to now no clues for such a re-arrangement, but the **old** experimental concepts*

seem to me to be inseparably connected with the foundation of man's power of visualizing. It is easy to suggest that Bohr was being close-minded over this, but actually it is perfectly reasonable to start off from a set of assumptions that cannot be justified other than from the successful theory that develops out of them. As I have suggested, Bohr's key points link together in a mesh and you cannot really change any of the points without unravelling the whole thing.

Interestingly, although we can criticize Bohr over the use of classical concepts, the ultimate need to refer to them was widely accepted at the time. Even Einstein, his strongest critic over quantum theory, seemed to accept this point.

16.2.2.2 You Cannot Separate a Quantum Object from the Equipment during a Measurement

If we set up some equipment to measure the position of an electron at a given time, then we have to make sure that the equipment is *rigidly attached* to the rest of the world; otherwise when the electron hits the equipment, it will cause the equipment to move slightly, ruining our ability to pin down exactly where the electron is. The equipment can be very simple. A single sheet of metal with a small hole in it will do, provided the sheet is fixed to something. If an electron passes through the hole we can get a fix on its position to within the width of the hole. We can make the hole as small as we like, so we can have as good a measurement of position as required. The problem is that in passing through the hole, the electron may well have scattered off one of the edges. We cannot tell if this happened, as we are not measuring the momentum of the electron at the same time, nor are we able to see if the sheet of metal recoiled slightly as it's fixed in place. We might have measured the momentum of the electron before it arrived at the hole, but now that measurement is useless.

In classical physics we do not worry too much about this as we can always assume that any impact between the electron and the edge of the hole is small enough not to matter. According to Bohr, though, this is no longer valid: Planck had shown how energy and momentum are exchanged in finite lumps that can be quite large compared with the original energy and momentum of the electron. Bohr called this the *quantum postulate* and talked in terms of an *unspecified and uncontrollable disturbance* of the particle.

As there is no consistent definition of the quantum postulate, we cannot be sure what Bohr meant. There are certainly circumstances where energy and momentum do not have to be exchanged in quantized lumps. However, the idea that the measuring device interacts with the object being measured in an uncontrollable way is important, so it is good that Bohr was able to justify it on other grounds as well.

Imagine that we try to detect the interaction between a particle and a measuring device. We can do this only by inserting more equipment into the system.

Bohr would then argue that this is a completely new experiment and the results are going to be different (think back to our earlier discussions and the Pockels cell). In any case, the quantum object is going to interact with any device that we use to detect its interaction with the main equipment, so how are we going to deal with that? That is the start of Bohr's explanation of why the behavior of quantum objects is so *context-dependent*.

If we accept that the interaction between a quantum object and a measuring device is not just an *uncontrollable disturbance* but also one that we cannot directly measure either, then we can follow Bohr's suggestion that *an independent reality in the ordinary sense can neither be ascribed to the phenomena nor to the agencies of observation*. In classical mechanics we could talk about the object being studied as if it were separate from the equipment being used to study it, as we could always rely on the interaction between them being small enough not to radically change the object. You cannot chop up the quantum world in such an easy manner. The interaction between measured and measuring knits them together as a whole.

Although this sounds like the entanglement between a quantum system and an experimental apparatus, Bohr was thinking in different terms. We could say that a state $|\phi\rangle$ does not belong to the quantum object, but only to the combined system of quantum object and measuring device linked together by an interaction that cannot be minimized. Bohr is stressing the *contextuality* of quantum theory and the *wholeness* of the object-equipment system.

Bohr went further than this. Given the need to use classical ideas such as energy, momentum, position, and so on, to describe the results of our experiments, and now accepting that we cannot split an object off from the apparatus used to measure it, it follows that quantum objects will have classical properties *in the context of the measurement used*. In other words, the measurement context defines the properties. What we mean by momentum is defined by the equipment that we would use to measure it in a given experiment.

This does two things for us. It gives another reason why we can never get around the problem of interaction between the measuring device and the object being studied. After all, an experiment to measure the position of an electron prevents an accurate *definition* of the energy and momentum of the electron, so even if it does scatter off the edge of a hole we cannot hope to follow the details of what happened in those terms. It also sets up Bohr's reply to the EPR argument, which as we saw earlier is based on the whole experimental arrangement providing a context for what is going on. It is not an interaction between the measuring device and the distant particle that is messing things up; the experimental equipment defines the concepts that can be used consistently: *of course there is in a case like that just considered no question of a mechanical disturbance of the system under investigation during the last critical phase of the measuring procedure. But even at this stage there is essentially the question of*

an influence on the very conditions which define the possible types of predictions regarding the future behavior of the system.

So, the properties of a quantum object have to be described classically and are valid only in the context of the experiment being used. Going back to the uncontrolled disturbance that takes place during a measurement, it is easy to see how this could be related to the uncertainty principle. After all, it is the argument behind Heisenberg's gamma ray microscope discussed earlier. However, for Bohr this was not the root reason for uncertainty. He believed that the uncertainty principle reflected the difficulty in defining the two classical concepts (say position and momentum) at the same time in the same experiment, a point that he convinced Heisenberg to accept and include in a later draft of his uncertainty paper.

Although Bohr stressed the need to use classical ideas to describe experimental equipment and results, from time to time he applied quantum ideas, such as uncertainty, to measuring devices. This was particularly the case at a conference held in Brussels in 1927 (the 5th Solvay Conference) during which Einstein repeatedly presented arguments, using his famous thought experiments, that were intended to show the inconsistency of quantum theory. Heisenberg and Bohr worked together to counter every single argument Einstein came up with by applying the uncertainty principle to parts of the experimental setup Einstein had devised (such as the metal sheet with a hole in it that we mentioned earlier).

Bohr was quite aware that there was a possible inconsistency here. On the one hand he claimed that you had to resort in the end to classical ideas, and on the other hand he was applying a quantum concept such as uncertainty to the equipment. A clarification was required and it came in his reply to the EPR experiment.

Let us say that during an experiment to measure the position of a particle (using a metal sheet with a hole (slit) in it), you want to measure the amount of momentum the sheet gets from the impact of the electron. Well, the sheet has to be treated *as regards its position relative to the rest of the apparatus ... like the particle traversing the slit, as an object of investigation, in the sense that the quantum mechanical uncertainty relations regarding its position and momentum must be explicitly taken into account.* The key part here is the phrase *be treated, like the particle traversing the slit, as an object of investigation.* What Bohr is doing is considering the metal sheet as part of the object being measured, linking it in with the quantum object, something that he can easily justify in terms of the uncontrolled disturbance linking the two. Consequently not only are you able to use the uncertainty principle on the metal sheet, consistency requires that you must.

The position of the metal sheet must be measured relative to the rest of the

equipment, so an uncontrolled disturbance has to take place in that interaction. Where does it all stop? Bohr had an answer to this as well. At some point you have to use a completely classical description of the equipment: *In the system to which the quantum mechanical formalism is applied, it is of course possible to include any intermediate auxiliary agency employed in the measuring process, but some ultimate measuring instruments must always be described entirely on classical lines, and consequently kept outside the system subject to quantum mechanical treatment.*

The question then becomes, at which stage do you draw the line? How do you avoid one device measuring another, etc., *ad infinitum*? Once again, Bohr had the answer. The sequence can stop when you reach *a region where the quantum mechanical description of the process concerned is effectively equivalent with the classical description*, or in more obvious terms *the use, as measuring instruments, of rigid bodies sufficiently heavy to allow a completely classical account of their relative positions and velocities.*

So, the quantum object links to part of the equipment and that part links to another part, etc. At some point you have to draw a line and say on one side of the line you are going to treat everything quantum mechanically and on the other side everything is classical. The best place to do this is when you get to part of the equipment that is so comparatively massive, it can absorb the sort of energy and momentum involved without notably altering its motion (or lack of).

It is hard not to think of this in terms of an entanglement between quantum object and equipment that is broken by a classical dividing line, which is exactly how the Copenhagen interpretation is generally publicized. However, Bohr was not thinking in this way. Entanglement was part of the formal mathematical part of the theory, and so Bohr did not take a great deal of interest in it.

From within Bohr's system, the whole picture makes complete sense; however, some modern physicists feel that this was a *cop out* on Bohr's part. As everything is made of atoms and molecules, including measuring devices, and quantum theory is the appropriate atomic theory, it simply will not do to draw a line across the world and assert that two different theories have to be used either side of the line, with no link between them.

16.2.2.3 You Cannot Relate Results of One Experiment to Another

Bohr made this statement:

The extent to which renunciation of the visualization of atomic phenomena is imposed upon us by the impossibility of their subdivision is strikingly illustrated by the following example to which Einstein very early called attention and often has reverted. If a semi-reflecting

mirror is placed in the way of a photon, leaving two possibilities for its direction of propagation, the photon may be recorded on one, and only one, of two photographic plates situated at great distances in the two directions in question, or else we may, by replacing the plates by mirrors, observe effects exhibiting an interference between the two reflected wave-trains. In any attempt of a pictorial representation of the behavior of the photon we would, thus, meet with the difficulty: to be obliged to say, on the one hand, that the photon always chooses one of the two ways and, on the other hand, that it behaves as if it had passed both ways.

In the preceding quotation, Bohr is drawing attention to the Mach-Zehnder experiment discussed earlier. He is using it as an example to emphasize another of his key ideas: we have to give up any attempt to picture exactly what a quantum object is like.

His argument up to now has been the following: you have to describe experiments in classical terms; you cannot separate a quantum object from the context of the experiment, so you have to describe a quantum object in classical terms appropriate to that experiment. All of which leaves open a very obvious question - why does classical physics not work? Where is the room for a quantum particle to behave in a quantum fashion?

Bohr's answer to this hinges on the *contextuality* of quantum theory. The properties of a quantum object are so context-dependent that we cannot compare one experiment with another. Any attempt to knit together classical ideas to produce a theory of what is going on is bound to fail. There is no firm experimentally independent rock on which to build a structure. The only hope is to adopt the idea of complementarity. Stick to a particular picture in a particular context and accept that you have to use a range of different pictures, which are impossible to relate to one another in terms of a complete classical theory.

As we cannot find a set of classical concepts that work equally well in every single experiment, we are forced to use probability. When we relate one set of experimental results to another, the classical concepts in one will only imperfectly fit in the other. We may need to use a totally different complementary picture in the second experiment. However, we can make a link between them using probabilities.

Bohr made this point while talking about the difference between the wave and photon pictures of light:

In this situation, there could be no question of attempting a causal analysis of radiative phenomena, but only, by a combined use of the contrasting pictures, to estimate probabilities for the occurrence of the individual radiation processes. However, it is most important to realize that the recourse to probability laws under such circum-

stances is essentially different in aim from the familiar application of statistical considerations as a practical means of accounting for the properties of mechanical systems of great structural complexity. In fact, in quantum physics we are presented not with intricacies of this kind, but with the inability of the classical frame of concepts to comprise the peculiar feature of indivisibility, or *individuality*, characterizing the elementary processes.

Here Bohr is making it clear that these are not classical probabilities, but quantum probabilities brought about by trying to fit concepts from one experiment into another. The probabilities measure how well the ideas fit. Bohr talked about a *rupture* in the causal description of a particle when we make a measurement. In other words, poking an object with a measuring device designed to measure its position means that we can no longer be sure of its energy and momentum, and so we have to use probability to figure out what is going to happen next, as we do not have a complete set of accurate classical values on which to base a prediction. This links in well with the final key idea on our list.

16.2.2.4 Classical Explanations

Most popular accounts, and also a few professional ones, talk about Bohr's complementarity solely in terms of wave/particle duality. However, Bohr did not think of wave/particle duality as the most important application of complementarity. When he first introduced the idea, he stressed the complementary roles of a space-time description and a causal one: *the very nature of quantum theory thus forces us to regard the space-time co-ordination and the claim of causality, the union of which characterizes the classical theories, as complementary but exclusive features of the description.*

Classical physics takes various measurements and uses laws of motion to predict the future. With something simple like a bowling ball, you need to measure its position at a given moment and the forces acting on it. Instead of the forces, you can work entirely in terms of energy (kinetic and potential) and momentum and use conservation laws to predict what is going to happen. In any case, you need to know where it is now and the energy/momentum it has now to figure out where it is going to be in the future.

According to Bohr, this is just not going to work any more with quantum objects. If you try to measure the position of an electron at a given time (the *space-time co-ordination* in Bohr's terminology), you will necessarily mess up any information you have about energy and momentum, because the experiment allows an *uncontrolled disturbance* to take place and limits the extent to which energy and momentum can be defined. Without good knowledge of energy and momentum we cannot apply the conservation laws (the causal rules) to predict an outcome. The link between the two, so crucial in classical theory, is broken.

We can talk about energy and momentum or positions in space and time. This

is where quantum objects get the room that they need to behave in a quantum fashion. This is why we need probability to link our experiments together. An exact knowledge of position blurs our knowledge of momentum, via the uncertainty principle (or Bohr's "uncontrolled disturbance" and difficulty of definition), so we can predict only a range of possibilities within the blur.

So, now we will try to draw all the threads together and come up with a concise summary of Bohr's thinking.

When we do experiments on quantum objects, such as electrons and photons, we find that certain traditional classical ideas (such as position) work fine but others (such as momentum) do not seem to fit. When we do a different experiment on the same quantum object, the picture can change (momentum works, but position does not). The reason for this lies in the interaction between the quantum object and the measuring equipment, which we cannot control and know about in detail. This interaction knits the object and equipment together into one whole system.

Consequently, we can only talk about the classical properties of a quantum object within the context of an experiment that actually defines their relevance. We are forced to stick with an attempted classical description, as we do not have another way of thinking. To try and develop specific quantum concepts would be like trying to teach a person blind from birth the difference between red and blue. The problem is that we cannot use classical physics any more as the properties seen in one experiment do not always transfer to another experiment with a different context. The best we can do is link experiments together using states or wave functions, which tell us how likely we are to get a certain fit between results. Our best hope for a physical picture of what is happening is by a complementary *double think*, which flips between classical pictures, each of which is a partial picture of the truth. However, we have to be careful. The unbreakable link between a quantum object and a measuring device also extends the need to apply quantum principles (such as uncertainty) to the equipment. This will get us in trouble, as we cannot necessarily define the properties of the apparatus consistently from one experiment to the next. In the end we are stopped from extending this right across the universe because at some scale the quantum effects are small enough to ignore and we can use a completely classical description.

The Bohr picture is a complete and satisfactory one, provided you stay within the limits it sets out for itself.

16.2.3 Heisenberg and Potentia

It seems that the first person to use the term **Copenhagen interpretation** was Heisenberg in an article on Bohr's contribution to physics that appeared in 1955.

The months which followed Schrödinger's visit were a time of the most intensive work in Copenhagen, from which there finally emerged what is called the *Copenhagen interpretation of quantum theory* From the spring of 1927, therefore, there existed a complete, unambiguous mathematical procedure for the interpretation of experiments on atoms or for predicting their results ... Since the Solvay conference of 1927, the *Copenhagen interpretation* has been fairly generally accepted, and has formed the basis of all practical applications of quantum theory.

Some historians feel that Heisenberg overstates the case that the Copenhagen view was completed in 1927. Perhaps the publication of Bohr's reply to the EPR paper (1935) is a more accurate date for the crystallization of ideas. Be that as it may, it is clear that no one used the term "Copenhagen interpretation" at that time. No matter what Heisenberg might say, recent historical analysis suggests that the picture of one Copenhagen interpretation on which the dust had settled is an oversimplification.

Having said that, Heisenberg was a close friend and collaborator of Bohr's for many years and took great interest in both the mathematical and philosophical sides of the theory. He was very well read in philosophy and talked to representatives of several philosophical schools about the implications of quantum theory. Heisenberg clearly felt that between them Bohr and he had cracked the problems, so we need to examine what Heisenberg has to say on the subject.

In his book **Physics and Philosophy**, Heisenberg devotes an entire chapter to his version of the Copenhagen interpretation. Right from the start, he puts his cards on the table and states his key point that the Copenhagen interpretation *starts from a paradox. Any experiment in physics, whether it refers to the phenomena of daily life or to atomic events, is to be described in the terms of classical physics. The concepts of classical physics form the language by which we describe the arrangements of our experiments and state the results. We cannot and should not replace these concepts by any others.* Clearly, he is in complete agreement with Bohr on this.

Heisenberg differed from Bohr over the relationship between mathematics and language. Heisenberg felt that the mathematics was primary: set up the mathematics and find the language to describe it, rather than get the language(ideas) right and then set up the mathematics. Consequently, Heisenberg took a more objective view of the quantum state and drew conclusions about the nature of quantum objects that Bohr was reluctant to take. Using an idea that dates back to Aristotle, Heisenberg viewed the quantum state as an objective description of an object's *potentia* - the collection of possible or latent properties that come to be when a measurement takes place. To Heisenberg, quantum systems do not have properties until they become manifest in a measurement.

While Bohr's view of state collapse is not entirely clear, Heisenberg regarded it (at least in his later writings) as being a real change in the system brought about by making the *potentia* that exist between measurements *actual* at the time of measurement. As a result it is not possible to say what is *really* happening between one measurement and the next. If a quantum object *exists* at all between measurements, then it is a strange sort of potential existence; not at all like the existence of things that we see in the everyday world: *Therefore, the transition from the possible to the actual takes place during the act of observation.* If we want to describe what happens in an atomic event, we have to realize that the word *happens* can *apply only to the observation, not to the state of affairs between two observations.*

Although Heisenberg certainly went along with the notion of complementarity, there are some subtle differences in his views from those of Bohr. When he talks of the complementarity between a space-time coordinate description of a quantum object and the causal description, he stresses the two forms of state evolution: one governed by $\hat{U}(t)$ and the other by state collapse: He said:

The space-time description of the atomic events is complementary to their deterministic (causal) description. The probability function (wave function or density matrix) obeys an equation of motion ... its change in the course of time is completely determined by the quantum mechanical equation, but it does not allow a description in space and time. The observation, however, enforces the description in space and time but breaks the determined continuity of the probability function by changing our knowledge of the system.

In other words, the normal evolution of a state is determined by $\hat{U}(t)$; but when we make a measurement this is broken and the state collapses into an actuality at a given point in space and time. Undoubtedly Heisenberg was influenced by von Neumann's work on the measurement problem(1932), which we will discuss shortly.

When it comes to the *probability function*, he said:

It should be emphasized, however, that the probability function does not in itself represent a course of events in the course of time. It represents a tendency for events and our knowledge of events. The probability function can be connected with reality only if one essential condition is fulfilled: if a new measurement is made to determine a certain property of the system. Only then does the probability function allow us to calculate the probable result of the new measurement. The result of the measurement again will be stated in terms of classical physics.

This comes back to Heisenberg's realistic view of an objectively existing quantum state, bought at the expense of a very different sort of *reality* which we are

not used to, but which Aristotle may have anticipated.

In another key passage about the probability function (in this context he means density matrix) Heisenberg says that

It contains statements about possibilities or better tendencies (*potentia* in Aristotelian philosophy), and these statements are completely objective, they do not depend on any observer; and it contains statements about our knowledge of the system, which of course are subjective in so far as they may be different for different observers. In ideal cases the subjective element in the probability function may be practically negligible as compared with the objective one. The physicists then speak of a pure case.

The *subjective* statements are what we have called classical probabilities in the density matrix, and the *objective* ones are the quantum probabilities within each state that makes up the density matrix. Clearly he accepts the reality of both forms of probability and the distinction between them. The quantum probability is a reflection of an object's *potentia*.

In another interesting variation on Bohr, Heisenberg saw the contrast between Schrödinger's waves and his matrix mechanics as a mathematical reflection of the complementarity between wave and particle. To him the Schrödinger equation is the wave view and the matrix mechanics the particle view. As Bohr stressed ideas more than mathematics, he felt that you needed both wave and particle pictures in complementary balance to describe a situation, whereas Heisenberg was content that either mathematical view could capture the whole truth (it was just a case of picking the form of math that was most easily applied to a given problem).

If asked to name the key features of the Copenhagen interpretation, most contemporary physicists would probably come up with something similar to Heisenberg's version, rather than pure Bohr. However, there is still one thing missing. I mentioned earlier that von Neumann had influenced Heisenberg's view of state collapse. Von Neumann's treatment of the measurement problem remains a classic piece of work and an important issue that any other interpretation has to deal with. It is the final piece of the Copenhagen interpretation that we need to discuss.

16.2.4 von Neumann and Measurement

John von Neumann was a Hungarian mathematician famous for his important contributions to logic, set theory, game theory, and computer science. He enters the story of the Copenhagen interpretation via his book **Mathematical Principles of Quantum Mechanics** (1932). In this book, von Neumann sets out to present a full mathematical treatment of quantum theory starting from the smallest set of assumptions possible.

When a theory is developed, there are always some important aspects that are not explained within the theory. I am not talking here about something that the theory gets wrong or is not good enough to explain. I am referring to the assumptions that are used to set up the theory. In Newtonian (classical) mechanics, the relationship between force, mass and acceleration (Newton's 2nd law of motion)

$$\text{Force} = \text{mass} \times \text{acceleration}$$

is an obvious example. Classical mechanics does not explain *why* force is linked to mass and acceleration in this way; it takes it as a starting point.

In quantum theory, there are also a set of assumptions as we have seen (postulates and rules). In a more formal mathematical treatment of quantum theory, one would have started by setting out what these assumptions are. The sort of assumptions that we are talking about are things like the following:

- (1) Every system is represented by a quantum state that contains all the information about that system that can be known in a given context.
- (2) Probability = complex square of amplitude.
- (3) If possibilities cannot be distinguished, you add amplitudes and then complex square.
- (4) The time-dependent Schrödinger equation and so on.

The exact list varies between different authors.

Starting from a set of assumptions, von Neumann set out for the first time what is now the standard mathematical approach to quantum mechanics (with a little added terminology from Dirac). His book is a landmark in the development of quantum theory.

Von Neumann's book also contains the first full coverage of measurement, treating the equipment in a quantum theoretical way. As I mentioned earlier, Bohr had applied the uncertainty principle to some experimental arrangements while countering Einstein's arguments against the consistency of quantum theory. He had also acknowledged that experimental equipment should have quantum physical properties, but at some point you had to draw a line when the quantum effects were small enough not to worry about.

Von Neumann took this further. In his account, he shows how quantum theory needs two ways to describe how a state can change over time, if it is to work at all. First, we have to have the *continuous and causal changes in the course of time*, for example, what we have called $\hat{U}(t)$ processes. Second, there are the *discontinuous, non-causal and instantaneously acting experiments or measurements* or state collapses. Crucially, von Neumann was able to demonstrate mathematically that \hat{U} processes cannot lead to state collapse of the sort

required by measurement. Consequently, state collapse is not part of the mathematical structure of the theory. For this reason, it has to be *glued on* to make things work. In his own words *quantum mechanics describes the events that occur in the observed portion of the world, so long as they do not interact with the observing portion, with the aid of the processes (\hat{U}) but as soon as such an interaction occurs, that is, a measurement, it requires the application of a process (of the second kind).*

By *observed portions of the world* von Neumann is clearly referring to a quantum system, but of course it is not *observed* in the true sense of the *world between measurements*; the *observing portion* being the measuring equipment. In this case, I would be very reluctant to link the term *events which occur* to the idea of how a state changes between measurements. I suspect that Heisenberg would not have liked it, and neither would Bohr. Between measurements the quantum state is a collection of evolving possibilities, not a set of actually realized events.

It is this *added on* extra assumption that lies at the heart of many criticisms of the Copenhagen interpretation. Some alternatives try to do without the assumption of state collapse by modifying the equations governing $\hat{U}(t)$ so that they can cause a form of collapse.

Interestingly, von Neumann himself might not have been that committed to the extra assumption he introduced. In conversation with a colleague he accepted that it might be possible to modify quantum theory so that $\hat{U}(t)$ brings about state collapse.

Von Neumann's written output doesn't really contain any statements of his views on realism and instrumentalism, It is also not easy to find any definitive statements about how state collapse comes about, in his view. This is another odd historical quirk, for physicists generally think that von Neumann was the first person to suggest that state collapse happens when an experimental result enters someone's conscious mind.

16.2.5 Mind of the Observer

Von Neumann's book is quite mathematical, even for physicists, and probably would not have the influence it now enjoys had Fritz Wolfgang London and Edmund Bauer not written a book that helped put across von Neumann's ideas in simpler form. Historically, this book appears to be the first written suggestion that the mind of the observer is involved in state collapse.

In contrast to von Neumann's rather cautious approach, London and Bauer come right out and say that a measurement does not actually happen until the result are *registered* in the mind of some observer. The observer has a completely different point of view: for him it is only the object and the apparatus that pertain to the external world, to that which he calls *objective*. By contrast,

he has within himself relations of a very peculiar character For he can immediately give an account of his own state ... namely, to cut the claim of statistical co-ordination ... by saying *I am in state $|a_j\rangle$ and see value a_j for physical variable A .*

Eugene Wigner took up this point in an argument that is now known as *Wigner's friend* as we discussed earlier. In simple terms it goes like this.

Suppose we start off with a system in a state $a_1|1\rangle + a_2|2\rangle$ and ask some friend to observe it. After the observation, the entangled state of the system and friend is

$$a_1|1\rangle|\text{friend sees 1}\rangle + a_2|2\rangle|\text{friend sees 2}\rangle$$

If we now ask the friend "what did you see?" we will get the reply "I saw 1" with probability $|a_1|^2$ and "I saw 2" with probability $|a_2|^2$.

So far, there is nothing remarkable here. But, what if I then ask "what did you see before I asked you?"

Now we have a problem. The answer is going to be "I just told you, I saw 1" or "I just told you, I saw 2", which seems to imply that the state just after my friend looked at the system was either $|1\rangle|\text{friend sees 1}\rangle$ or $|2\rangle|\text{friend sees 2}\rangle$, not the entangled state.

This would be a very different situation if the *friend* was actually some other quantum system.

In Wigner's original argument $|1\rangle$ was related to a light bulb flashing on and $|2\rangle$ to the light bulb remaining off. The friend was then replaced by an atom, which would go into an excited state if it picks up some light from the bulb or obviously not if the bulb did not come on. In this case the correct quantum description is evidently

$$a_1|1\rangle|\text{atom excited}\rangle + a_2|2\rangle|\text{atom in ground state}\rangle$$

which has observably different properties to the mixed state

$$a_1|1\rangle|\text{friend sees 1}\rangle + a_2|2\rangle|\text{friend sees 2}\rangle$$

In Wigner's words:

If the atom is replaced by a conscious being the wave function appears absurd because it implies that my friend was in a state of suspended animation before he answered my question. It follows that the being with a consciousness must have a different role in quantum mechanics than an inanimate measuring device: the atom considered above.

Consciousness causes state collapse.

Among modern day physicists, a few (Henry Stapp) are still following this line of thinking - quantum theory is intimately linked with nature of the mind. Roger Penrose has proposed a modification to quantum theory to explain state collapse and then used this to develop some ideas about how consciousness arises in the brain.

16.2.6 The Deep End

The use of the mind as the ultimate reason why states collapse was not generally accepted by the originators of quantum theory. Heisenberg, for one, specifically rejected this view:

If we want to describe what happens in an atomic event, we have to realize that the word *happens* can apply only to the observation, not to the state of affairs between two observations. It applies to the physical, not the psychical act of observation, and we may say that the transition from the *impossible* to the *actual* takes place as soon as the interaction of the object with the measuring device, and thereby with the rest of the world, has come into play; it is not connected with the act of registration of the result by the mind of the observer.

Nevertheless, the potential use of mind in physics has caught the imagination of some commentators who have used this to support various views of the world. However, it is an approach that has many problems connected with it.

For one, it closes science off in an unsatisfactory manner. If mind lies beyond the reach of physics, then it seems that the crucial role of measurement has been put out to play as far as further research is concerned.

For another, if mind is responsible for collapsing states, what is *going on* when there is no mind to observe thing? As Einstein once asked Bohr "*Do you really think the moon isn't there if you aren't looking at it?*" Extending this we have to face the fact that the universe seems to have existed perfectly well before human beings came along to observe it. If mind is necessary to collapse states, then that would seem to require some *mind* to be permanently present in the universe.

One obvious suggestion, of course, is God.

I do not want to be rude about a suggestion like this, but it seems to me that there are as many *theological* problems with it as there are physical ones. If it is God's continual *observation* that makes things happen, then surely we are quite right to *blame* him for all the evils, both moral and physical, taking place in the world.

16.2.7 Conclusions

It seems a long way from Bohr's struggles with complementarity and language to the participatory universe. In a way this is a measure of the problem facing physics when it comes to constructing an interpretation of quantum theory. You may feel that Wheeler has gone too far in using the mind to bring the past into being. Yet in the next section we will come across other physicists who think that there are an infinite number of parallel universes in existence and if we could travel in time, we would also jump from one universe to the next. When it comes to weighing up these thoughts, we should remember that Bohr produced a completely consistent interpretation of quantum theory 90 years ago. We can criticize his views and try to be more bold in our speculations now, but we should not forget that his ideas have never been shown to be wrong.

16.3 Further Conclusions

It is truly surprising how little difference this all makes. Most physicists use quantum mechanics every day in their working lives without needing to worry about the fundamental problem of its interpretation. Being sensible people with very little time to follow up all the ideas and data in their own specialties and not having to worry about this fundamental problem, they do not worry about it.

A while back, two physicists at the University of Texas were waiting for an elevator and their conversation turned to a young theorist who had been quite promising as a graduate student and who had then dropped out of sight. One asked what had interfered with the ex-student's research. The other shook his head sadly and said, "*He tried to understand quantum mechanics*".

Whether you are an instrumentalist or a realist, you are trying to make a map of the world. The only difference is the seriousness with which you take the map and the job you want to use it for.

I am a realist: I like to think that what I struggle to understand in physics is the world as it really is out there. As I like mathematics and science, I find the map that physics creates challenging, interesting and in the end quite beautiful.

That beauty, however, can be quite beguiling. There is a danger that you come to think of the map physics creates as the only complete map of the world. From time to time we have talked about some wider philosophical issues such as the nature of free will, morality and the mind. In my view, physics gives us only one view of the subject: an important view, but nevertheless a view from a particular angle.

Take free will for example. No matter what our philosophical position might

be on the existence, or not, of free will we all act on a daily basis as if we are free to determine our own fate, even to the point of which breakfast cereal to buy. We have a basic intuition of free will. Classical physics is structured in a very deterministic way. Given a sufficiently detailed knowledge of positions, momenta, and forces for every particle in the universe, classical physics, if it were right, would enable us to predict the future as far ahead as we liked. As a result of this, some philosophers lost nerve and started to doubt their intuitions of free will. To paraphrase John Polkinghorne's memorable phrase, if physics leaves no room for free will, so much the worse for physics.

Quantum physics has relaxed this deterministic stranglehold on the world. As a result, physicists have become more willing to admit that the world is not as gray as they once told us it was. The study of chaotic systems has contributed to this as well. Nowadays, it is the biologists who are more inclined to paint a jaundiced view of humanity. The point, though, remains the same.

We are entitled to judge our scientific theories by their consonance with our basic human experience. Of course, when it comes to things such as black holes, superconductivity, and so on, scientific experiment must have the last word, as human experience has been extended into new areas by suitable experiments. So, what does that leave me with? I tend to agree with state collapse, as an assumption pasted onto quantum theory, is a bit rich. I still think that we have a lot to learn from Bohr, especially when it comes to our use of language and how it can lead us astray. I like Heisenberg's use of *potentia* as a good way of thinking about the quantum state in its potential form before specific aspects become manifest. In the end though, something new has to come along to convert the potential into the manifest. This has to be something linked to the *complexity* of a measuring apparatus compared to the simplicity of a few atoms or particles.

The conscious human mind is not something that we should ignore, nor should we downplay the importance of mind coming to be in the universe, but in cosmic terms it is relatively new on the scene. We have evolved from the dust of the world, and the existence of mind must be exploiting something in the fundamental laws of nature; but it's that way around, not mind making fundamental processes possible.

Decoherence is an important step forward, but diagonalizing the density matrix is not the same as picking out a specific state, so it does not solve the measurement problem. The many other interpretations of quantum theory, that we have not discussed, are even less realistic to many physicists.

In the end, I think that we need something new. There must be some form of active information that is influencing the evolution of quantum states. This information would have to be expressed in some manner, and its effect could easily be linked to matter of scale, so that quantum behavior merges into the

classical world.

Whatever the end result, the exploration of quantum physics still has a great deal to tell us about the world and our place in it.

The ultimate nature of reality is a powerfully absorbing puzzle, which generations of philosophers and physicists have struggled to answer by painting their own individual maps of the world. I come back, though, to one of my earlier points. When the map is constructed, we have to keep a balance between what science tells us and the personal experience of our daily lives. The real lesson of the quantum revolution is that we were too quick to paint ourselves as mindless mechanistic lumps of matter, when physics seemed to suggest a deterministic world. Now that quantum theory has swept away this classical view, there is a danger that anything goes in its place. Hence the rise of quantum hype that I mentioned earlier.

Science is an important tool for viewing the world, but it is not the only road to truth.

Chapter 17

Other Thoughts

17.1 MANY-WORLDS INTERPRETATION - Some Other Thoughts to Help Us Understand

The concept of collapse of the state vector introduced by von Neumann in 1930s and has become integral part of orthodox interpretation of quantum theory.

What evidence do we have that this collapse really takes place?

Well . . . pots and erasers now seem to be direct evidence for collapse.

What if they turn out to have a different explanation? What are the other possibilities?

As we have seen, collapse seems to be necessary to explain how a quantum system initially in linear superposition state before measurement is converted into quantum system existing in only one of measurement eigenstates after measurement process has occurred.

It was introduced into the theory because our experience is that pointers point in only one direction at a time.

17.1.1 Early View

The Copenhagen solution to the measurement problem is to say *there is no solution*.

Pointers point because they are part of a macroscopic measuring device which conforms to laws of classical physics.

Collapse is only way in which *real world* of classical objects can be related to

unreal world of quantum particles.

Is it simply a useful invention, an algorithm, that allows us to predict outcomes of measurements and not a real process. Many point out that if we wish to make collapse a real physical change occurring as a real physical property of quantum system, then we must add something to theory, if only the suggestion that consciousness somehow involved. This is not a satisfactory outcome to many physicists.

So the simplest solution to problem of quantum measurement is to say there is no problem.

Over the last 60 years, quantum theory has proved its worth time and time again in the laboratory. Why change it or add extra bits to it?

Although, it is overtly a theory of the microscopic world, we know that macroscopic objects are composed of atoms and molecules, so why not accept that quantum theory applies equally well to pointers, cats and human observers? Pointers point because of collapse and that is that!!!! That is the standard view!

There is a different interpretation accepted by many. In this interpretation the observer is assumed to split into number of different, non-interacting conscious selves. Each individual self records and remembers a different result, and *all possible results are realized*.

In this interpretation, the act of measurement splits the *entire universe* into a number of branches, with a different result being recorded in each branch.

This is so-called *many-worlds interpretation* of quantum theory.

17.1.2 Relative States

Everett insisted that pure Schrodinger wave mechanics is all that is needed to make a complete theory.

Thus, wavefunction obeys deterministic, time-symmetric equations of motion at all times in all circumstances. Initially, no interpretation is given for wavefunction; rather, the meaning of wavefunction must emerge from formalism itself. Without the collapse of the wavefunction, the measurement process occupies no special place in theory. Instead, the results of the interaction between a quantum system and an external observer are obtained from properties of a larger composite system formed from them.

In complete contrast to special role given to observer in von Neumann's and Wigner's theory of measurement, in Everett's interpretation the observer is

nothing more than an elaborate measuring device.

In terms of the effect on the physics of quantum system, a conscious observer is no different from an inanimate, automatic recording device, which is capable of storing an experimental result in its memory.

The *relative state* formulation is based on properties of quantum systems which are composed of smaller sub-systems. Each sub-system can be described in terms of some state vector which, in turn, can be written as linear superposition of some arbitrary set of basis states. The vector space of composite system is a product of vector spaces of sub-systems. If we consider simple case of 2 sub-systems, then the overall state vector of the composite system is a giant linear superposition of terms involving all parts of both sub-systems.

The end result is a giant entangled state, where every property of one sub-system is entangled with all other properties of the other sub-system.

We can see more clearly what this means by looking at specific example.

Consider once again the interaction between a measuring device and a simple quantum system, which possesses just two eigenstates. The measuring device may, or may not, involve observation by human observer.

From previous discussions, can write the state vector of the composite system (quantum system + measuring device) as

$$|\Phi\rangle = c_+ |\psi_+\rangle |\varphi_+\rangle + c_- |\psi_-\rangle |\varphi_-\rangle \quad (17.1)$$

As before $|\psi_+\rangle$ and $|\psi_-\rangle$ are measurement eigenstates of quantum system and $|\varphi_+\rangle$ and $|\varphi_-\rangle$ are the corresponding states of measuring device (different pointer positions, for example) after interaction has taken place.

Everett's argument is that we can no longer speak of the state of either the quantum system or the measuring device independently.

However, can define states of measuring device *relative* to those of quantum system as follows:

$$|\Phi_{REL}^+\rangle = c_+ |\varphi_+\rangle \quad (17.2)$$

$$|\Phi_{REL}^-\rangle = c_- |\varphi_-\rangle \quad (17.3)$$

and

$$|\Phi\rangle = |\psi_+\rangle |\Phi_{REL}^+\rangle + |\psi_-\rangle |\Phi_{REL}^-\rangle \quad (17.4)$$

The relative nature of the states is made more explicit by writing expansion coefficients c_+ and c_- as amplitudes:

$$c_+ = \langle \psi_+, \varphi_+ | \Phi \rangle \quad , \quad |\Phi_{REL}^+\rangle = \langle \psi_+, \varphi_+ | \Phi \rangle |\varphi_+\rangle \quad (17.5)$$

$$c_- = \langle \psi_-, \varphi_- | \Phi \rangle \quad , \quad |\Phi_{REL}^-\rangle = \langle \psi_-, \varphi_- | \Phi \rangle |\varphi_-\rangle \quad (17.6)$$

where

$$\langle \psi_+, \varphi_+ | = \langle \psi_+ | \langle \varphi_+ | \quad , \quad \langle \psi_-, \varphi_- | = \langle \psi_- | \langle \varphi_- | \quad (17.7)$$

Everett went on to show that the relative states formulation of quantum mechanics is entirely consistent with the way quantum theory is used in its orthodox interpretation to derive probabilities. Instead of talking about simple amplitudes and probabilities, it is necessary to talk about conditional probabilities, which is the probability that a particular result will be obtained in a measurement given certain conditions.

The name is different, but procedure is same.

All this is reasonably straightforward and non-controversial. However, the logical extension of Everett's formulation of quantum theory leads inevitably to conclusion that, once entangled, relative states can *never* be disentangled.

17.1.3 The Branching Universe

In Everett's formulation of quantum theory, there is no doubt as to reality of quantum system. Indeed, the theory is quite deterministic in the way that Schrodinger had originally hoped. Given a certain set of initial conditions, the wavefunction of quantum system develops according to quantum laws of motion. The wavefunction describes the real properties of a real system and its interaction with a real measuring device so that all speculation about determinism, causality, quantum jumps and collapse of wavefunction is unnecessary.

However, restoration of reality in Everett's formalism comes with a fairly large trade-off.

If there is no collapse, each term in the superposition of the total state vector $|\Phi\rangle$ is real, i.e., *all experimental results are realized*.

Each term in the superposition corresponds to a state of the composite system and is an eigenstate of observation. Each describes a correlation of the states of the quantum system and the measuring device (or observer) in the sense that $|\psi_+\rangle$ is correlated with $|\varphi_+\rangle$ and $|\psi_-\rangle$ is correlated with $|\varphi_-\rangle$. Everett argued this correlation indicates that observer perceives only one result, corresponding to a specific eigenstate of observation.

In his July 1957 paper, he wrote:

Thus with each succeeding observation (or interaction), the observed state *branches* into a number of different states. Each branch represents a different outcome of measurement and a *corresponding* eigenstate for [composite] system. All branches exist simultaneously in superposition after any given sequence of observations.

Thus, in the case where an observation is made of the polarization state of a photon known to be initially in a state of 45° polarization, the act of measurement causes universe to split into two separate universes.

In one of these universes, an observer measures and records that photon was detected in a state of vertical polarization. In the other, the same observer measures and records that photon was detected in a state of horizontal polarization. The same observer now exists in two distinct states in two universes.

Looking back at paradox of Schrodinger's cat, we can see that difficulty is now resolved. The cat is not simultaneously alive and dead in the same universe, it is alive in one branch of the universe and dead in the other!

With repeated measurements, the universe, together with observer, continues to split. A repeated measurement for which there are two possible outcomes continually splits the universe. The path followed from beginning of a *tree* to the end of one of its branches corresponds to a particular sequence of results observed in one split universe.

In each branch, the observer records a different sequence of results. Because each particular state of observer does not perceive universe to be branching, the results appear entirely consistent with the notion that wavefunction of the original 45° polarized photon collapsed into one or the other of two measurement eigenstates.

Why does the observer not retain some sensation that the universe splits into two branches at moment of measurement? The answer given by the proponents of the Everett theory is that laws of quantum mechanics simply do not allow the observer to make this kind of observation.

DeWitt argued that if splitting were to be observable, then it should be possible in principle to set up a second measuring device to obtain a result from memory of first device which differs from that obtained by its own direct observation.

Wigner's friend could respond with an answer which differs from one that Wigner could check for himself. This not only never happens (except where a genuine human error occurs) but is also not allowed by the mathematics.

The branching of the universe is unobservable!!! Not very satisfying at all!!

17.2 Decoherence

Although we feel that the principles of quantum mechanics do indeed apply in the large-scale world that we inhabit in our daily lives, their consequences are unobservable.

Interference effects and the uncertainty *jitter* are too small in the everyday world to be observed.

The notion of decoherence, on the other hand, takes exception to this. Proponents of decoherence claim that Schrodinger's cat, and indeed all other macroscopic objects, are effectively not described by superpositions, but rather by something called *mixtures* or *mixed states*. Thus, they claim, Schrodinger's paradox is in fact not a paradox.

What is the difference between a superposition and a mixture?

Suppose a system is in the state

$$|A\rangle = c_1 |a_1, b_1\rangle + c_2 |a_2, b_2\rangle \quad (17.8)$$

where these are states containing information about two observables.

Then the probability that we will measure the value a for the first observable independent of the value of the second observable is different in the two cases of superposition and mixture:

$$P(a)_s = |c_1 + c_2|^2 \quad (17.9)$$

$$P(a)_m = |c_1|^2 + |c_2|^2 \quad (17.10)$$

The only difference is one is the square of the sum and the other is the sum of squares. How can this be so dramatic?

Consider a very special case....

$$c_1 = -c_2 = Q \quad (17.11)$$

$$P(a)_s = 0 \quad (17.12)$$

$$P(a)_m = 2|Q|^2 \quad (17.13)$$

So a superposition allows for the possibility of interference (zeros) and mixtures do not!

The essential element behind decoherence is the recognition that, unless extraordinary precautions are taken in the laboratory, large objects are never isolated

from their environments.

Furthermore, these environments are continually and erratically fluctuating.

Electrons, atoms, and the like can be studied in isolation - they exist in a vacuum, so to speak.

But cats and baseballs are perpetually buffeted about.

As it sits in its box, Schrodinger's cat is ever so slightly shaken by seismic waves from an earthquake in Peru. A tiny breath of wind disturbs the flying baseball's path. Indeed, in this regard even the perpetual microscopic jittering back and forth of the atoms of which large-scale objects are composed can be thought of as part of this continual erratic fluctuation. And the consequence of this fluctuation is that, for all practical purposes, superpositions are converted into mixtures.

A further essential element of the notion of decoherence is that it is to some degree an illusion.

The total system consists of both the cat and its environment - and this total system is truly in a superposition state.

But when we think about the cat, we are thinking of merely part of the total system, and this part is effectively described by a mixture. In this way, the notion of decoherence does not invalidate the general principle that quantum mechanics applies to all things, big as well as little.

How does the incessant fluctuation in an object's environment convert its state from a superposition into a mixture?

The basic ideas behind the process can be understood with the help of a simple illustrative example.....

We will need to remember a few facts about spin states....

The states are only *up or down* in a given direction and the most general state is a superposition of these two.

$$|spin\rangle = \alpha |up\rangle_z + \beta |down\rangle_z \quad (17.14)$$

with

$$|\alpha|^2 + |\beta|^2 = 1 \quad (17.15)$$

Remember α and β are complex numbers and have both a real and an imaginary part

$$\alpha = \alpha_r + i\alpha_i \quad , \quad \beta = \beta_r + i\beta_i \quad (17.16)$$

It can be shown that this superposition state is in fact an eigenstate of the spin along a new direction.

If we specialize to spins restricted to the x - y plane, we can reduce this expression to the form

$$|spin\rangle = A [|up\rangle_z + B |down\rangle_z] \quad (17.17)$$

where

$$|A| = \frac{1}{\sqrt{2}} \quad , \quad |B| = 1 \quad (17.18)$$

Our illustration of decoherence involves a game, which goes as follows.

I have a machine that spits out electrons. They are traveling along the z -axis, and I guarantee that their spins are perpendicular to this axis - that is, their spins point along some direction in the $x - y$ plane. Your task is to find that direction.

How do you do it?

You are equipped with a Stern-Gerlach apparatus that is oriented perpendicularly to the incoming beam of electrons (in the $x - y$ plane). This apparatus splits the beam into two, one whose spins are up along the directional axis of the SG machine, and the other whose spins are down along this axis.

Hold up your measuring device to my beam of electrons and orient it along some randomly chosen direction in the $x - y$ plane. You will find some of the electrons traveling along its upper path and some along the lower.

Now rotate your apparatus to some other randomly chosen axis, making sure that it still lies in the $x - y$ plane. Still you find some electrons taking the upper path and some the lower. But as you continue rotating your apparatus this way and that, eventually you will find one particular direction with the important property that every electron passes along the upper path.

With this last step you have won the game.

The direction you have found is the direction of the spin of the particular spin state we are sending into the apparatus.

It is important to realize that if you continue swinging your apparatus this way and that, you are eventually sure to win - for, as we stated, every superposition state corresponds to an eigenstate pointing purely along some direction.

In order to find it, all you must do is keep trying.

But there is another wrinkle to the game.

Upon my machine a switch is mounted, which so far has been in the *off* position.

Now I flip it to *on*.

(The switch could equally well be labeled *isolated from environment*, and *not isolated from environment*; or alternatively, *superposition* and *mixture*).

Once I do so, no matter how you turn your Stern-Gerlach apparatus, you never find a direction for which all the electrons pass along one of the two paths.

More than that; no matter how you orient it, half the electrons turn out to traverse the upper path and half the lower.

Note that this result is incomprehensible if the state of the electrons emitted by my machine is described by a superposition, for a superposition always corresponds to an eigenstate along some direction.

Thus my machine suddenly seems to be violating the rules of quantum mechanics.

It is not, of course.

Rather it is now converting its output, which used to be a superposition, into a mixture.

Here is how my machine works.

Inside is a gun that emits electrons.

When the switch is *off*, these electrons' spins are invariably oriented along a definite axis in the x-y plane.

But when the switch is *on*, the machine does something more.

Now just prior to emitting each electron, it spins a roulette wheel. The outer rim of this wheel, rather than being marked off in the usual fashion, is labeled in degrees. Thus, when the wheel's marble comes to rest, it does so having randomly specified a certain angle. Call that angle φ . The machine now proceeds to rotate the electron's spin by the angle φ away from its initial position - and it then fires the electron off into space.

Thus, with the switch *off*, my machine emits electrons whose spins all point in the same direction; but with the switch *on*, the spins are random.

It is now easy to see why you found equal numbers of electrons traversing the upper and lower paths of your Stern-Gerlach apparatus when my switch was

on.

Had you happened to guess the angle φ correctly, you would have found all electrons traversing the upper path. But you were equally likely to have guessed 180° away from φ , in which case you would have found all electrons traversing the lower path.

Similarly, had you happened to guess 90° , or 270° away from φ , you would have found equal numbers of electrons traversing the two paths because of A and B .

And finally, had you happened to choose some angle α away from φ , you would have obtained some definite ratio between the upper and lower paths - but had you chosen the complement of α , namely, $\pi - \alpha$, you would have obtained the opposite ratio.

By symmetry, for a random set of guesses on your part, you would have found a random distribution of traversals of the two paths.

Mathematically, there are two ways to describe the state of the electrons emitted by my machine with the switch *on*.

First, this state is described by the superposition, but the angle φ is randomly re-set prior to each emission. We know, however, that each choice of φ corresponds to an eigenstate along the φ axis, so a second way to describe the state is to say that each individual electron is in a quantum state

$$\psi_0, \psi_1 \text{ or } \psi_2 \dots \dots \text{ or } \psi_{359} \quad (17.19)$$

where

ψ_0 is the state where spin is oriented up along the $\varphi = 0^\circ$ axis
 ψ_1 is the state where spin is oriented up along the $\varphi = 1^\circ$ axis
.....

and so on, each with a probability of $1/360$.

This description represents a mixture.

We have reached the following crucial insight:

a superposition with randomly fluctuating coefficients is equivalent to a mixture!!!

This, then, is how decoherence operates: *by continually and erratically changing the coefficients of a superposition.*

But how does it do so - and what has all this to do with interactions between

the system and its environment?

Here is how my roulette wheel works.

It is meant to model the results of the interaction between the electron emitted by my machine and a complex environment. The *environment* is an external magnetic field applied to the electron. Like the real environment, this field is continually and erratically fluctuating.

We know that, because the electron possesses a magnetic moment, it has an interaction with this erratically fluctuating magnetic field.

The two terms in the superposition, the one having spin up and the other spin down, have different interactions with the environment. In particular they will have slightly different energy values. Now, it is a general principle of quantum mechanics that the time-evolution operator depends on the energy of the state. Therefore, the two terms in the superposition evolve in time differently. Furthermore, because the magnetic field is fluctuating erratically, so is the time evolution.

It is by exploiting this randomly fluctuating difference that we can make the coefficients in the superposition fluctuate, so as to turn it into a mixture.

The electron gun emits particles whose spins initially all point along a particular direction.

The exact answer looks like

$$|spin, t\rangle = \frac{1}{\sqrt{2}} e^{-iEt/\hbar} [|up\rangle_z + e^{i\gamma Bt} |down\rangle_z] \quad (17.20)$$

The coefficients of the two terms in the superposition are randomly fluctuating. And because they are doing so, the superposition has been converted into a mixture.

How long does this take?

An illustrative example will make clear that decoherence is a spectacularly rapid process for macroscopic objects.

Consider a body at rest on the surface of the Earth. Imagine that it shifts about ever so slightly. Because it has done so, it has moved to a slightly higher or lower elevation, and so shifted its gravitational potential energy. This will cause the phase factor Et/\hbar , to fluctuate. If the shifting about is random, the resulting fluctuation in this phase will wipe out quantum coherence.

If the mass M shifts its elevation by H , its gravitational potential energy has

changed by MgH , where g is the acceleration due to gravity. Then, after a time $t = \hbar/MgH$, the phase factor has altered significantly.

If the mass M is, say 100 *kilograms*, and H is on the order of the dimensions of a single atom $10^{-10} m$, then this occurs in the extraordinarily short time of 10^{-27} *seconds*!

Thus even the smallest of motions will have an extraordinarily rapid effect.

That is an elementary model of **decoherence**.

Its essential elements are as follows.

- (1) The environment in which any system is embedded is constantly and irregularly fluctuating.
- (2) If a system is described by a superposition, the different terms in this superposition will interact differently with the environment. In particular, they will have different interaction energies.
- (3) Therefore, the time evolution of each of the terms in the superposition is constantly and irregularly fluctuating
- (4) and this is indistinguishable from a mixture.

17.3 Quantum Theory of Measurement: The Infinite Regress

The Schrodinger equation does not describe the collapse of the wave function caused by a measurement.

We now ask what the Schrodinger equation does describe?

We will find an astonishing result: according to the Schrodinger equation **measurements never happen**.

Rather, what happens is an *infinite regress*.

If we attempt to measure the location of a photon by monitoring the upward transition of an atom: what we find is that, rather than telling us about this transition, the Schrodinger equation merely predicts that the atom went into a superposition state of being in both states.

$$|photon\rangle = a|atom_{ground}\rangle + b|atom_{excited}\rangle \quad (17.21)$$

In fact, however, the final state is not a simple superposition but an enormously complex entanglement.

The configuration we usually analyze is a single atom in the presence of a photon. But the configuration we should analyze is an entire collection of atoms - all the atoms in the entire apparatus - together with the photon.

To deal with this problem we need to write down a factor describing the state of the first atom, a second factor describing the state of the second atom, and so on until we have covered every atom in the apparatus and then a final factor describing the photon. If the Schrodinger equation is applied to this problem, it predicts a complex state. The first term of this state consists of

1. a factor describing atom #1 in the superposition state;
2. factors describing all the other atoms in their ground state;
3. a factor describing the photon at the location of atom #1.

Similarly, the second term is

1. a factor describing atom #2 in the superposition state;
2. factors describing all the other atoms in their ground state;
3. a factor describing the photon at the location of atom #2.

and so forth.

Clearly, this final state is an entanglement.

Just as clearly, it is exceedingly difficult to work with.

So, for the purposes of clarity, let us consider an even simpler problem the problem of measuring, not a photon's location, but its energy. The advantage of this shift is that it allows us to work with a detector that really does consist of a single atom, as opposed to an apparatus that consists of many.

In fact, we will consider an even simpler problem: a measurement whose sole function is to tell us whether the photon's energy is very great or very small.

The detection process is an excitation of a particular sort: **an ionization**.

If the photon is of high energy, the atom will be ionized by it; but if the photon's energy is low, the atom will not. What does the Schrodinger equation predict if it is applied to this problem? It predicts that

$$|photon\rangle = a|photon_{low}atom_{neutral}\rangle + b|photon_{high}atom_{ionized}\rangle \quad (17.22)$$

where a and b are coefficients(amplitudes).

This expands the original superposition state.

But all the dissatisfaction with the earlier state that we had applies as well to our new result.

We set out to perform a measurement of a photon's energy - but rather than doing this, the Schrodinger equation has informed us that a peculiar state has developed, a state for which there is no classical analogue, and which hardly seems to have anything to do with a measurement.

But we need not stop here.

We could determine the photon's energy if we could find out whether the atom was ionized or not. So let us turn our attention to this problem. An ionized atom possesses a net electric charge, and charges respond to electric fields. So perhaps we can measure the photon's energy by applying an electric field to the atom and seeing what it does. If the photon had high energy, the atom will be deflected by the field; if it had low energy, the atom will go straight. What does the Schrodinger equation predict?

Perhaps the reader will not be surprised to learn that the Schrodinger equation does not predict anything that we might interpret as a clean measurement.

Rather it predicts a yet larger entanglement—*not* an entanglement of two factors, but of three:

$$\begin{aligned} |photon\rangle = & a |photon_{low}atom_{neutral}atom_{straight}\rangle \\ & + b |photon_{high}atom_{ionized}atom_{deflects}\rangle \end{aligned} \quad (17.23)$$

To determine whether the atom was deflected by the electric field, we can place a detector of atoms in the undeflected beam. If this detector catches an atom, the photon had low energy; and if it does not, the atom had high energy. But, here too, all that develops is a yet larger entanglement:

$$\begin{aligned} |photon\rangle = & a |photon_{low}atom_{neutral}atom_{straight}detector_{catches\ atom}\rangle \\ & + b |photon_{high}atom_{ionized}atom_{deflects}detector_{does\ not\ catches\ atom}\rangle \end{aligned} \quad (17.24)$$

The further we go in our analysis, the larger does the entanglement grow. But at no point does a measurement occur. Rather, what occurs is an infinite regress.

17.3.1 Termination of the Infinite Regress: The Projection Postulate

What would constitute a measurement of the photon's energy? Notice that in the very last step of our analysis, an important transformation has occurred: we have included a macroscopic measuring device. The conundrum presented to us by the quantum theory of measurement is that this device is predicted to

be in an ambiguous state: a superposition. But in reality, we know perfectly well that, if it is working correctly, a detector never behaves in such an obscure fashion. It either detects the atom, or detects its absence.

In order to make this happen, in order to perform a measurement, we need to terminate the infinite regress at some stage, and replace the entanglement by a single term. But this cannot be done by the Schrodinger equation.

It is necessary, therefore, to divide the time evolution of a quantum system into two distinct parts. The first lasts from the instant a quantum state is prepared until the moment just prior to the act of measurement. During this period of time, the system evolves in a precisely specified manner according to the time-dependent Schrodinger equation, in which the forces acting on the system are included through the potential energy function $V(r)$:

$$|t\rangle = \exp\left(-i\frac{\hat{E}}{\hbar}t\right)|t=0\rangle = \exp\left(-\frac{i}{\hbar}\left[\frac{\hat{p}^2}{2m} + V(\hat{r})\right]t\right)|t=0\rangle \quad (17.25)$$

The result is an ever-increasing entanglement.

But the act of measurement stands in sharp-contrast to this orderly time development. No potential energy function, no energy operator, exists for measurement, no equation analogous to the Schrodinger equation describes its evolution in time. Within orthodox quantum mechanics, measurement is an acausal process that, in a very real sense, falls outside the theory.

The mathematician von Neumann described the problem thoroughly in his classic text *Mathematical Foundations of Quantum Mechanics*. From him we have inherited an ad hoc mathematical device to get around the problem of the infinite regress.

In place of the dynamical state, von Neumann described the projection postulate.

This is the postulate that, when a measurement occurs, the entanglement is replaced by a single term. The wave function of the quantum system is *projected onto* the various possibilities provided by the detector, with a probability of projection given by the square of the coefficient multiplying each of the terms of the entanglement.

In the context of the example we have been considering, the projection postulate is that, at the moment of measurement, the state is collapsed either onto

$$|photon_{low}atom_{neutral}atom_{straight}detector_{catches\ atom}\rangle \quad (17.26)$$

with probability $|a|^2$ or onto

$$|photon_{low}atom_{neutral}atom_{straight}detector_{does\ not\ catches\ atom}\rangle \quad (17.27)$$

with probability $|b|^2$.

Notice that, in both states, the detector is left in a perfectly well-defined state - and this is just what we mean by a measurement.

We emphasize that the projection postulate is nothing more than a mathematical statement of our postulate of the collapse of the wave function.

We also emphasize that the projection postulate does not correspond to a real, physical process. Rather it is a purely mathematical procedure, which gets us from the causal language of quantum mechanics to experimental probabilities in a way that agrees with experiment. In so doing, as Heisenberg put it, what was probable becomes actual. But how does this occur? The answer is the subject of much contention.

The projection postulate presents us with a distasteful state of affairs. One dissatisfying feature is that we do not understand how the projection comes about. But a further dissatisfying element is that sometimes the postulate is not needed.

In certain situations the postulate is required in order to make a measurement, but in other situations it is not! We will illustrate this point by returning to our above analysis of a photon whose energy can be either quite large or quite small.

We will discuss three situations.

In the first two, a measurement will occur quite naturally, within the framework of the orderly evolution described by the Schrodinger equation. Only in the third will the Schrodinger equation prove to be insufficient, and the postulate will be required.

How is such a photon produced?

It is produced by the decay of an atom whose energy-level diagram is similar to that illustrated below.

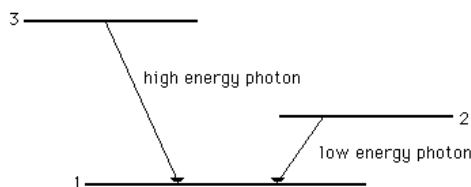


Figure 17.1: Decaying atom energy-level diagram

The decay of such an atom from level 2 to level 1 produces a photon of low energy; that from 3 to 1 produces one of high energy. In case I we prepare a single atom in a well-defined state - either level 2 or level 3. The decay of this atom produces our photon. Via the series of experiments we have outlined above, its energy can be determined. If the photon's energy is low, one state describes the final state; if it is high, the other state does it.

This is very like a classical situation, in which the outcome of a measurement stands in direct correspondence with the state of the system prior to the measurement. The initial state may not be known to us beforehand, but the outcome of the measurement reveals it to us. And finally, notice that at no stage have we been forced to invoke the projection postulate: the measurement has been effected solely as the result of the time-dependent Schrodinger equation.

In case II we prepare a collection of such atoms, some in level 2 and some in level 3. Suppose for the sake of argument that 10% are in 2 and 90% in 3.

Such a collection is, of course, simply the mixture we have already encountered. Once again, we measure the emitted photons, allowing sufficient time for the entire ensemble of atoms to decay. Since each individual atom is described as in the previous case, the result of each measurement is perfectly straightforward, and once again the projection postulate is not required.

We will not be able to predict in advance which energy each particular photon will have, but this is no cause for concern. We simply do not have sufficient information - even in the classical universe, it is seldom possible to predict an event with this kind of certainty. But we do know that we will find 10% of the decay photons to be of low energy and 90% of high energy. Results like this lend support to our conventional understanding of reality as having an independent existence and well-defined attributes, regardless of the act of measurement.

Notice that, in both cases I and II, the initial state of the atom or atoms corresponds directly to one of the eigenstates of the detection apparatus. As long as this is true, measurement in quantum mechanics does not contradict our naive view of reality. However, as we have seen time and time again, the special feature of quantum mechanics is that it allows states other than simple eigenstates. The situation changes dramatically if we consider them.

In case III we prepare a collection of atoms, each one of which is in the superposition state given by

$$|\varphi\rangle = \sqrt{0.1}|atom_{in\ level\ 2}\rangle + \sqrt{0.9}|atom_{in\ level\ 3}\rangle \quad (17.28)$$

The newly observed phenomenon of quantum beats gives clear evidence that even single atoms can be prepared in such states. When such a state decays,

the emitted photon is in a superposition state of its own:

$$|photon\rangle = \sqrt{0.1}|photon_{low}\rangle + \sqrt{0.9}|photon_{high}\rangle \quad (17.29)$$

If we now seek to measure the energy of this photon, the infinite regress we encountered above will result - an infinite regress that can only be terminated by invoking the projection postulate.

Here lies the nub of the problem.

In case III the outcome of the series of measurements we perform will be identical to that produced in case II:

10% of the photons will turn out to be of low energy

and

90% of the photons will turn out to be of low energy

In this case, however, we have no theoretical understanding of how the measurements came about.

Furthermore, what is it that distinguishes the pathological case III from the well-behaved cases I and II?

Only the choice of initial states to be studied!

Those that happen to coincide with the eigenstates of our measuring apparatus will not require the extra projection postulate. Finally, notice that measuring devices exist whose eigenstates are not those of energy, but correspond to more complex superpositions of energy eigenfunctions. And if we substitute these devices for our previous ones, the need for the projection postulate will evaporate. Surely this is a most unsatisfactory state of affairs!

17.4 Attempts to Solve the Measurement Problem

The measurement problem described earlier has received much attention. We turn now to a description of some of the many attempts that have been made to solve it. We caution the reader that there is no general agreement as to where the actual solution lies, so our discussion will not lead to any definite conclusion.

17.4.1 Small Detectors and Big Detectors: Decoherence

Return to our analysis of the infinite regress that develops when we attempt to describe a measurement. Recall our comment that, in going from state where

ionization did or did not take place to state where detector did or did not catch atom,

$$|photon\rangle = a|photon_{low}atom_{neutral}atom_{straight}\rangle + b|photon_{high}atom_{ionized}atom_{deflects}\rangle \quad (17.30)$$

$$|photon\rangle = a|photon_{low}atom_{neutral}atom_{straight}detector_{catches\ atom}\rangle + b|photon_{high}atom_{ionized}atom_{deflects}detector_{does\ not\ catches\ atom}\rangle \quad (17.31)$$

an important new element has entered the situation, namely, **we made a transition from microscopic to macroscopic**.

Recall also from earlier that large objects, unless they are of a very special sort, are subject to the process of decoherence.

A number of workers in the field have argued that this solves the measurement problem. Their claim is that decoherence does away with the need for the projection postulate. We turn now to this claim.

We now re-state the essential points of decoherence, but with one change from our earlier discussion - everywhere we used the word *system* before, we use *macroscopic detector*.

The essential elements of decoherence are as follows:

- (1) The environment in which any macroscopic detector is embedded is constantly and irregularly fluctuating.
- (2) If a macroscopic detector is described by a superposition, the different terms in this superposition will interact differently with the environment. In particular, they will have different interaction energies.
- (3) Therefore, the time evolution of each of the terms in the superposition is constantly and irregularly fluctuating
- (4) and this is indistinguishable from a mixture.

Up to now in our discussion of measurement, we have tacitly assumed the macroscopic detector to behave in the same way as do microscopic objects such as photons and atoms. But the phenomenon of decoherence shows that this assumption was unwarranted. Let us now correct this error.

We imagine a macroscopic measuring device as being composed of two parts. The first part describes all the imperfections of a real measurement process, one made by a large-scale object. The second part consists of the sort of absolutely perfect device we have been considering up to now. We will call the first part a *confuser*, and the second an *ideal detector*. The figure below diagrams the configuration we have in mind.

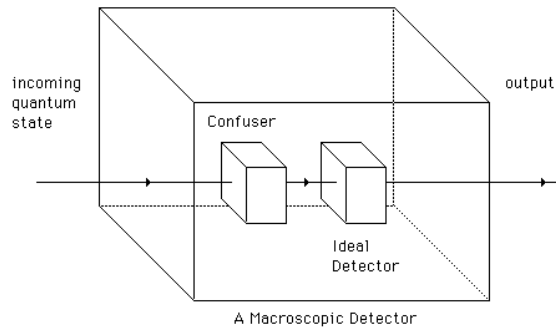


Figure 17.2: Model of measuring device

In this diagram, the confuser represents all the unwanted interactions of the large-scale detector with the environment and with its own internal states, which themselves constitute an irregularly fluctuating intrusion into its behavior (it mimics the coupling between a macroscopic detector and its irregularly fluctuating environment). We have no information about these interactions, which means that they cannot be included in the quantum-mechanical treatment of the detector's behavior. We can only treat them as unknown and uncontrollable perturbations.

How does such a two-part measuring device work?

As before, decay photons are emitted by our atoms into a certain state. This can be any of the states we treated in our three cases above: an eigenstate, a mixture or a superposition. In any event, the state is well-defined. But now these photons enter the confuser, and at this point everything changes. An element of randomness enters our description, arising from the process of decoherence. Recall that the effect of this randomness is to make a superposition indistinguishable from a mixture. And as case II made clear, *if the state being measured is a mixture, the projection postulate is not required.*

No matter what the input state into the confuser, its output will be effectively a mixture. This state now enters the second component of our large-scale measuring device, the perfect detector.

And as we have seen, in this situation we simply do not need the projection postulate. In this way, the argument goes, the phenomenon of decoherence solves the measurement problem by obviating the need for this strange and unsatisfactory postulate.

17.4.2 Does Decoherence Solve the Measurement Problem?

17.4.2.1 The Quantum Eraser

Not all workers in the field agree that decoherence solves the measurement problem. At this time, there is intense debate as to whether the line of argument we have sketched above is valid. There is no debate over the fact that macroscopic detectors are intimately connected to a complex and fluctuating environment; and there is no debate over the fact that a complex, fluctuating superposition state is indistinguishable from a mixture for certain purposes.

But there is much debate as to whether this state is in principle the same thing as a mixture - and the measurement problem is one of principle, not of practice.

Our earlier discussion of decoherence was somewhat equivocal - it was peppered with phrases such as *equivalent to*, *indistinguishable from* and the like, rather than simply *is*. This equivocation reflects the lack of consensus in the field at present.

It will not be possible to do justice to the subtle arguments that have been raised in this debate. But let us go back to the *quantum eraser*, which sheds interesting light on the problem.

We will begin by describing an experiment that embodies it, after which we will point out its relevance to the problem of measurement.

The experimental setup is so complex that we will approach it a different way than before and in stages, reaching the actual design only in the third stage. The first figure below illustrates the first step. It is a simple Mach-Zehnder interferometer. As the phase shifter in one of the paths is varied, the detector D records an interference pattern.

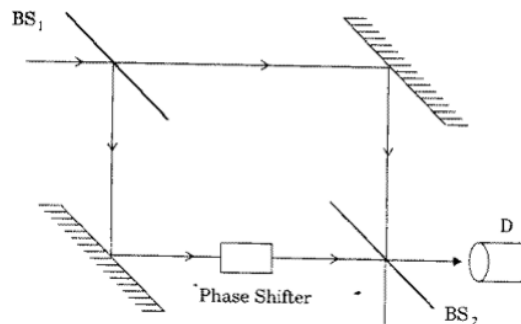


Figure 17.3: Basic Mach-Zehnder interferometer

Now move on to the second stage of the analysis. We insert two nonlinear down-conversion crystals, X_1 and X_2 . Each photon, as it enters a crystal, is split into a pair. These are illustrated in the second figure.

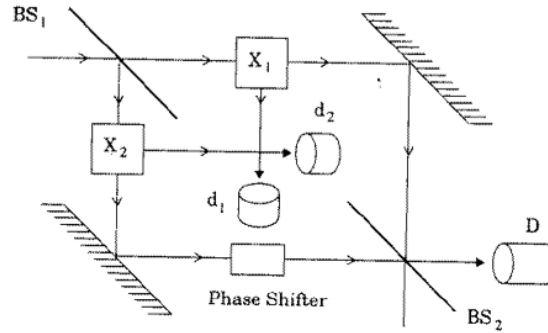


Figure 17.4: Splitting the photons into pairs

In the figure, nonlinear crystals have been placed in the two arms of the interferometer, and their outputs monitored by two additional detectors d_1 and d_2 .

Will the initial detector D still register an interference pattern as the phase shifter is adjusted? The principles of QM say that it will not.

The apparatus illustrated in the second figure is capable of giving us which-path information; therefore it cannot exhibit interference. To see how this comes about, suppose that we send a single photon into the apparatus. We know that it is going to split into two photons, because either path it takes leads to a nonlinear crystal. One of the two additional detectors, d_1 and d_2 , is therefore sure to register a count. And if d_1 clicks, we know the initial photon chose the upper path. Similarly, if d_2 clicks, the initial photon chose the lower path. Thus, whenever D clicks, we ask which of d_1 or d_2 also clicks. The answer gives which-path information.

The essence of Scully's concept of the quantum eraser is that this which-path information can be erased and when it is, the interference pattern can return. This is accomplished in the final stage of the experiment in the third figure below. In this figure, a beam splitter BS_3 erases the which-path information that in the second figure had been provided by the crystals, and a coincidence counter between D and d_2 records an interference pattern, i.e., when we place a third beam splitter into the paths of the secondary photons from X_1 and X_2 . Now we have lost the means of knowing which photon it was that made d_2 register a count. By the principles of QM, since we have no which-path information, an interference pattern can be seen.

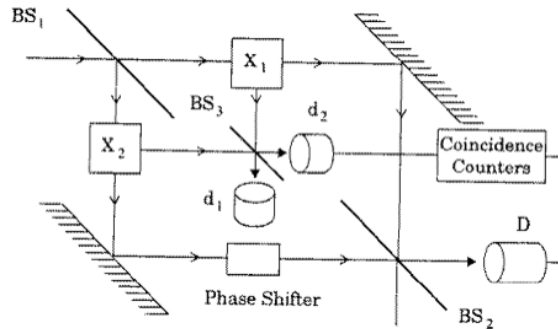


Figure 17.5: Adding a coincidence counter

But, as we emphasized earlier in our discussion of quantum nonlocality, this interference signal does not show up if we record only counts in the detector D . Rather we must connect D and d_2 by a coincidence counter, which fires only if D and d_2 fire simultaneously. It is this coincidence signal that registers an interference pattern as the phase shifter is varied.

The experiment we have described has been performed by Mandel and coworkers at the University of Rochester. Two photon parametric down conversion supplied the secondary photons, in this case twice. Thus, a single ultraviolet photon from a powerful laser was first placed into a one-photon superposition state of the usual kind by passing it through a beam splitter. But then this superposition state passed through two down-conversion crystals, X_1 and X_2 , creating thereby a complex two photon entangled state. Inserting and removing the third beam splitter made this state's interference properties appear and disappear.

What is the relevance of such an experiment to the measurement problem? It lies in the fact that the interference pattern will only be observed if we look at coincidence counts between two detectors. Interference, of course, is the characteristic sign of quantum behavior: *and this quantum behavior will not be seen if we do the wrong experiment*. Looking at only the single detector D is the wrong experiment: it reveals what appears to be classical behavior - the absence of interference.

In the normal single-photon Mach-Zehnder experiment diagrammed in first figure, detector D is *the* detector, and it reveals quantum behavior as the phase shifter is varied. But in the more complex two photon experiment of the third figure it alone does not. We might be tempted to argue that this is because the full experiment makes use of nonlinear crystals, which are macroscopic devices, subject to all the fluctuations of which decoherence treats. The quantum eraser experiment reveals that this, however, is not the case. In reality the full quan-

tum behavior is still present, but it can only be seen by performing a different measurement.

Indeed, the effect of the nonlinear crystals here is not to wipe out quantum coherence. It is to entangle a photon arriving at the detector D with something else - with another photon arriving at d_2 . Similarly, the effect of the incessant, fluctuating interactions to which all macroscopic detectors are subject is also to entangle them with something else. In this case, however, the *something else* is far more complex. It is the rest of the world. The lesson of this experiment is that only if the right experiment could be performed, one which detects all the multitudinous components of this gigantic entangled state, could quantum behavior be seen.

In the decoherence model, the conceptual device that we have termed a *confuser* introduces a complex, random disruption of the quantum state. This leads to a loss of interference. But does the loss of interference mean that quantum coherence (ability to see interference effects) has been lost?

This is the key issue addressed by the eraser experiment. If this disruption truly destroys quantum coherence, destroys it not just in practice but in principle, then it will be impossible ever to recover an interference signal. On the other hand, if the disruption leads rather to the creation of an entanglement, then the state has become more complex but its fundamental nature has not altered. It is a superposition, not a mixture. In the measurement process, the projection postulate will be unnecessary only if the output of the confuser is truly a mixture: nearly a mixture is not good enough. And, at least in this one experiment, it is clear that the quantum behavior has not been destroyed by decoherence.

Comments:

In the real world, the detailed analysis of a detector with its attendant confuser is beyond our reach theoretically. For this reason, it is difficult to be sure how much relevance this simple model has to the measurement problem. Complex and subtle arguments have been brought to bear on this issue, with no general agreement at present.

We close by briefly mentioning three other ideas that have been put forward in an attempt to solve the measurement problem. These are not the only such attempts, nor are they necessarily the most significant. Rather, our goal in selecting them is simply to indicate how wide is the net that has been cast in the debate on the subject.

Everett, as we have seen, has put forward a re-interpretation of quantum mechanics, commonly known as the many-worlds interpretation, in which the state vector does not collapse. The entanglement of system and observer is never resolved. Instead, each measurement multiplies the number of branches that the

system and observer must simultaneously sustain. Each branch represents a real option for the universe. In Everett's interpretation, all universes or worlds are simultaneously present with comparable reality.

Ghirardi, Rimini and Weber, on the other hand, modify standard quantum mechanics in a way that has no effect on microscopic objects while at the same time changing the quantum dynamics of large objects into a stochastic mechanics that displays all the features of classical physics. They accomplish this by introducing a term describing a continually fluctuating field whose effect is to cause superpositions to rapidly evolve into mixtures.

Finally, Wigner has proposed that a measurement occurs, and the state vector collapses, when a person becomes aware of a detector's state. In this view the brain is described by ordinary quantum mechanics, but the mind is not: it stands outside normal physics, and its workings are not subject to physical law.

The great variety of these suggestions, and the absence of agreement on how the measurement problem is to be solved, are all the more remarkable in that the idea of measurement lies at the very heart of quantum mechanics. It lies at the heart of the probability prescription that square of some coefficient evaluated at some point gives the probability that a measurement will find a particle there. It lies at the heart of the prescription we use in QM to calculate the average value of a series of measurements of the an observable. Indeed, the concept is essential to every scientific theory for it is through measurements that theory makes contact with experimental reality.

Finally, it is a commonplace that measurements take place every day in laboratories throughout the world. Indeed, if Wigner's proposal is wrong and consciousness itself flows from the workings of the human brain, and if quantum mechanics applies to the brain just as well as SQUIDS and macroscopic bits of ferritin - then the very act of looking and seeing is a measurement. How can so prosaic an act be so fraught with difficulty for a theory that has proved so wonderfully successful in every other regard?

Chapter 18

Final Thoughts

18.1 A Few Other Interesting Items

18.1.1 Free Will and Determinism

You may have been tempted from time to time during our discussions to cast your mind back to good old Newtonian thinking, where everything seemed to be set on much firmer ground.

Remember our discussion that classical physics was based on the idea of a grand scheme: a mechanical clockwork universe where every effect could be traced back to a cause. Set the clockwork in motion under some precisely known initial conditions and it should be possible to predict its future development in unlimited detail.

However, apart from the reservations we now have about our ability to know the initial conditions with sufficient precision, there are two profound philosophical problems associated with the idea of a completely deterministic universe.

The first is that if every effect must have a cause, then there must have been a *first* cause that brought the universe into existence.

The second is that, if every effect is determined by the behavior of material entities conforming to these physical laws, what happens to the notion of *free will*?

Let us discuss the second(easiest) first.

The Newtonian vision of the world is essentially reductionist:

the behavior of a complicated object is understood in terms of the properties and behavior of its elementary constituent parts

If we apply this vision to the brain and consciousness, we are ultimately led to the modern view that both should be understood in terms of complex, but deterministic, physical and chemical processes occurring in the machinery. Taken to the extreme, this view identifies the mind as the software which programs the hardware of the brain. The proponents of so-called strong AI (Artificial Intelligence) believe that it should one day be possible to develop and program a computer to think.

One consequence of this completely deterministic picture is that our individual personalities, behavior, thoughts, actions, emotions, etc., are effects which we should in principle be able to trace back to a set of one or more material causes. For example, my choice of words in the last sentence is not a matter of my individual freedom of will, it is a necessary consequence of the many physical and chemical processes occurring in my brain. The particular things said were, in principle, dictated by my genetic makeup and physical environment, integrated up to the moment that my *state of mind* led me to *make* my decision.

We should differentiate here between actions that are essentially instinctive (and which are therefore *reactions*) and actions based on an apparent freedom of choice. I would accept that my reaction to pain is entirely predictable, whereas my senses of value, justice, truth and beauty seem to be matters for me to determine as an individual. Ask an individual exhibiting some pattern of conditioned behavior, and she will tell you (somewhat indignantly) that, at least as far as accepted standards of behavior and the law are concerned, she has her own mind and can exercise free will. Is she suffering a delusion?

Before the advent of quantum theory, the answer given by the majority of philosophers would have been **YES**. As we have seen, Einstein himself was a realist and a determinist and consequently rejected the idea of free will. In choosing at some apparently unpredictable moment to light his pipe, Einstein saw this not as an expression of his freedom to will a certain action to take place, but as an effect which has some physical cause. One possible explanation is that the chemical balance of the brain is upset by a low concentration of nicotine, a chemical on which it had come to depend. A complex series of chemical changes takes place which is translated by his mind as a desire to smoke his pipe. These chemical changes therefore cause his mind to will the act of lighting his pipe, and that act of will is translated by the brain into the bodily movements designed to achieve the end result.

If this is the correct view, then we are left with nothing but physics and chemistry!

In fact, is it not true that we tend to analyze the behavior patterns of everyone (with the usual exception of ourselves) in terms of their personalities and the circumstances that lead to their acts.

Our attitude towards an individual may sometimes be irreversibly shaped by a *first impression*, in which we analyze the physiognomy, speech, body language and attitudes of a person we are dealing with. How often do we say - "Of course, that is just what you would expect him to do in those circumstances".

If we analyze our own past decisions carefully, would we not expect to find that the outcomes of those decisions were entirely unpredictable, based on what we know about ourselves and our circumstances at the time? Is anyone truly unpredictable?

Classical physics paints a picture of the universe in which we are nothing but irrelevant cogs in the grand machinery of the cosmos.

However, quantum physics paints a rather different picture and may allow us to restore some semblance of self-esteem.

Out go causality and determinism, to be replaced by the indeterminism embodied in the uncertainty relations. Now the future development of the system becomes impossible to predict except in terms of probabilities. Furthermore, if we accept von Neumann's and Wigner's arguments about the role of consciousness in quantum physics, then our conscious selves become the most important things in the universe. Quite simply, without conscious observers, there would be no physical reality. Instead of tiny cogs forced to grind on endlessly in a reality not of our own design and whose purpose we cannot fathom, we become the *creators* of the universe. We are the masters!

However, we should not get too carried away. Despite this changed role, it does not necessarily follow that we have much freedom of choice in quantum physics. When the state vector collapses (or when Everett's universe splits or when the conscious self splits.....), it does so unpredictably in a manner which would seem to be beyond our control. Although our minds may be essential to the realization of a particular reality, we cannot know or decide in advance what the result of a quantum measurement will be. We cannot choose what kind of reality we would like to perceive beyond choosing the measurement eigenstates (what to measure). In this interpretation of quantum measurement, our only influence over matter is to make it real. Unless we are prepared to accept the possibility of a variety of paranormal phenomena, it would seem that we cannot bend matter to our will.

Of course, the notion that a conscious mind is necessary to sustain reality is not new to philosophers, although it is perhaps a novel experience to see it advocated as a key explanation in one of the most important and successful of the 20th century scientific theories.

Now to return to the first question.

The first is that if every effect must have a cause, then there must have been a *first* cause that brought the universe into existence.

Let us call this discussion - **The Hand of God**

Einstein's comment that *God does not play dice* is one of the most famous of his many remarks on quantum theory and its interpretation.

Is it possible that after centuries of philosophical speculation and scientific research on the nature of the physical world we have, in quantum theory, finally run up against nature's grand architect? Is it possible that the fundamental problems posed by quantum theory in its present form arise from our inability to fathom the mind of God? Are we missing the *ultimate* hidden variable? Could it be that behind every apparently indeterministic quantum measurement we can discern God's guiding hand?

Away from the cut-and-thrust of their scientific research papers, Einstein, Bohr and their contemporaries spoke and wrote freely about God and her designs.

To a limited extent, this habit continues with modern-day scientists. For example, in **A Brief History of Time**, Stephen Hawking writes in a relaxed way about a possible role for God in the creation of the universe and in **The Emperors New Mind**, Roger Penrose writes of *God-given* mathematical truth.

Discovering more about how God created the world was all the motivation Einstein needed for his work. Admittedly, Einstein's was not the traditional medieval God of Judaism or Christianity or Islam or Buddha or any other faith, but an impersonal God *identical* with nature *God or Nature* as described by the 17th century philosopher Baruch Spinoza.

Herein lies a difficulty for all of you. In modern times it is almost impossible to resist the temptation to equate belief in God with an adherence to a religious philosophy or orthodoxy. Scientists are certainly taught not to allow the scientific judgment to be clouded by their personal beliefs. Religious belief entails blind acceptance of so many dogmatic truths that it negates any attempt at detached, rational, scientific analysis(maybe that is what is wanted). I do not in any way downplay the extremely important sociological role that religion plays in providing comfort and identity in an often harsh and brutal world(some brought about by religion itself). But once we accept God without religion, we can ask ourselves the all-important questions with something approaching intellectual rigor. The fact that we may have lost the habit or the need to invoke the existence of God should not prevent us from examining this possibility as a serious alternative to the interpretations of quantum theory already discussed. It is, after all, no less metaphysical or bizarre that some of the other possibilities we have considered so far.

18.1.2 Does God Exist?

There is a timelessness about this question. It has teased the intellects of philosophers for centuries and weaves its way through the entire history of philosophical thought. Even in periods where it may have been generally accepted to be a non-question, it has lurked in the shadows, biding its time.

Thomas Aquinas restored Aristotelian philosophy and science that had all but been forgotten during the dark ages. However, being a scholar of the Roman Catholic church, he carefully weeded out all pagan and heretical elements. The church then elevated Aristotelianism to the exalted status of religious dogma and so pronounced on all matters not only of religious faith, but also of science (witness the Galileo trials).

18.1.2.1 Descartes argument for the existence of God:

Descartes had already established (with certainty) in earlier work that he is a thinking being and that, therefore he exists.

As a thinking being, he recognizes that he is imperfect in many ways, but he can conceive of the *idea* of a supremely perfect being, possessing all possible perfections. Now it goes without saying that a being that is imperfect in any way, is not a supremely perfect being. Descartes assumed that existence is a perfection, in the sense that a being that does not exist is imperfect. Therefore, he reasoned, it is self-contradictory to conceive of God as a supremely perfect being that does not exist and so lacks a perfection. Such a notion is as absurd as trying to conceive of a triangle that has only two angles. Thus, God must be conceived as a being who exists. Hence, God must exist.

There is no dramatic revelation in this argument. Descartes could not have come up with any other answer because he believed God to exist. He wanted to establish a fundamental truth through pure reason. His major contribution was not in the particular proofs, but in the methods he used to derive them.

18.1.2.2 Leibniz Proof of the Existence of God:

The Leibniz argument is based on the principle of *sufficient reason*, which he interpreted to mean that if something exists, then there must be a good reason. Thus, the existence of the world and of the eternal truths of mathematics and logic must have a reason. Something must have caused these things to come into existence. He claimed that there is within the world itself no sufficient reason for its own existence. As time elapses, the state of the world evolves according to certain physical laws of change. It could be argued, then, that the cause of the existence of the world at any one moment is to be found in the existence of the world just a moment before. Leibniz rejected this argument.

The world cannot just *happen* to exist, and whatever (or whoever) caused it

to exist must also exist, since the principle of sufficient reason demands that something cannot come from nothing. Furthermore, the ultimate, or first, cause of the world must exist outside the world. Of course, this first cause is God. God is the only sufficient reason for the existence of the world. The world exists, therefore it is necessary for God to exist.

This type of proof also has modern applicability.

We now have good reason to believe that the world(which in modern context we take to mean the universe) was formed about 15 billion years ago in the big-bang space-time singularity. The subsequent expansion of space-time has produced the universe as we know it today, complete with galaxies, stars, planets and living creatures. Modern theories of physics and chemistry allow us deduce the reasons for the existence of all these things based on the earlier states of the universe. In other words, once the universe was off to a good start, the rest follows from fundamental physical and chemical laws. Scientists are not inclined to suggest that we need to call on God to explain the evolution of the post big-bang universe.

But the universe had a *beginning*; which implies that it must have had a first cause. Do we need to call on God to explain the big bang? Stephen Hawking writes: “*An expanding universe does not preclude a creator, but it does place limits on when she might have carried out the job*”.

To be sure, there are a number of theories that suggest the big bang might not have been the beginning of the universe but only the beginning of the present phase of the universe. These theories invoke endless cycles each consisting of big bang, expansion, contraction of the universe in a *big crunch*, followed by another big bang and so on. It might even be the case that the laws of physics are redefined at each new start (different universes).

However, this does not solve the problem. We still do not know what started the cycles....and so on.

18.1.2.3 God or Nature:

To Spinoza, God is *identical* with nature rather than its external creator. He distinguished between substances that could exist independently of other things and those that could not. The former substances provide in themselves sufficient reason for their existence—they are their own causes—and no two substances can possess the same essential attributes.

Since different substances cannot possess the same set of attributes, it follows logically that if a substance with infinite attributes exists then it must be the only substance that can exist:

Whatever is, is in God

Spinoza felt that God was not omniscient, omnipresent God of Judeo-Christian tradition, who is frequently imagined to be an all-powerful being with many human-like attributes. The God of Spinoza God is the embodiment of everything in nature. The argument is that when we look at the stars, or on the fragile earth and its inhabitants, we are seeing the physical manifestations of the attributes of God. God is not outside nature—she did not shape the fundamental physical laws by which the universe is governed—she is nature. Neither is she a free agent in the sense that she can exercise a freedom of will outside the fundamental physical laws. She is free in the sense that she does not rely on an external substance or being for her existence. She is a deterministic God in that her actions are determined by nature. This is the kind of God that most western scientists would feel comfortable with, if they had to accept that a God exists at all.

Modern physics, which has been so successful in defining the character of physical law, does not reduce the power of the Spinoza arguments. Some scientists feel that science *offers a surer path to God than religion*. Although scientists tend not to refer in papers to God as such, with the advent of modern cosmology and quantum theory, some have argued that the need to invoke a *substance with infinite attributes* is more compelling than ever.

The references by Einstein were to the God of Spinoza. He believed that there must be some divine plan or order to the universe. He strictly adheres to a need for causality and determinism. He expected to find *reason* in nature and was not willing to have the apparent trust in luck suggested by quantum indeterminism.

18.1.2.4 A World Without God:

The final parting of the way between philosophy and theology was achieved by Hume and Kant in the 18th century. Hume demolished both the Descartes and the Leibniz proofs of the existence of God. Hume claimed that there was a limit to what can be rationally claimed through metaphysical speculation and pure reason. He claimed that the earlier proofs fail because too many assumptions are made without justification. Why should existence be regarded as perfection? Why is it necessary for the world to have a cause, whereas God does not (indeed, cannot). Why not simply postulate that the world itself needs no cause, thus eliminating the need for God.

Kant(Critique of Pure Reason) continued where Hume left off. Kant concluded that all metaphysical speculation about God, the soul, and the nature of things cannot provide a path to knowledge. True knowledge can be gained only through experience and, since we appear to have no direct experience of God as a supreme being, we are not justified in claiming she exists.

Unlike Hume, Kant did not want to develop a purely empiricist philosophy, in which all things that we cannot know through experience are rejected. Kant felt that we must *think* of certain things as existing in themselves even though we cannot know their precise natures from the ways in which they appear to us.

Kant did not reject metaphysics totally, but redefined it and placed clear limits on the kind of knowledge to be gained through speculative reasoning. What he left were those things that require an *act of faith*. This is a general statement. It is about the very practical faith which is necessary to make the connection between things as they appear and *things-in-themselves* of which we can have no direct experience.

Kant rejected the proofs of Descartes and Leibniz because their arguments necessarily transcend experience. Any attempt to prove the existence of God requires assumptions that go beyond our conscious experience and cannot therefore be justified. The existence of God requires acts of faith for its justification. This does not make God unnecessary, but does limit what we can know about her.

Logical positivism represents the ultimate development of the kind of empiricism advocated by Hume. The positivist philosophy is based on what we can meaningfully say about what we experience. For the 20th century positivists, philosophy has become an analytical science. Wittgenstein, once remarked that the sole remaining task for philosophy is the analysis of language.

Despite the positivists efforts to eradicate metaphysics from philosophy, the old metaphysical questions escaped virtually unscathed. I find it rather fascinating to observe that although the possibility of the existence of God and the relationship between mind and body no longer form part of the staple diet of the modern philosopher of science, they have become increasingly relevant to discussions on modern quantum physics.

Three centuries of gloriously successful physics have brought us right back to the kind of speculation that it took three centuries of philosophy to reject as meaningless. It may be that the return to metaphysics is really grasping at straws - an attempt to provide a more *acceptable* world view until some time as the further subtleties of nature can be revealed in laboratory experiments and this agonizing over interpretation stopped. But we have no guarantees that future subtleties will be any less bizarre than present day quantum physics.

And what about God? Does quantum theory provide any support for the idea that God is behind it all? This, of course, is a question that cannot be answered here, and I am sure that you are not expecting me to try. Like all the other possible interpretations of quantum theory we have discussed, the God-hypothesis has many things to commend it, but we really have no means(at present) by which to reach a logical, rational preference for one interpretation over the others. If you can draw comfort from the idea that either Spinoza's God or a more

traditional religious God presides over the apparent uncertainty of the quantum world, then that is a matter for your own personal faith.