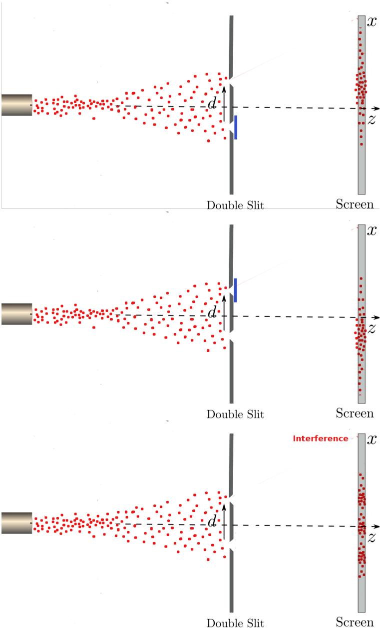
Quantum Mechanics: Introduction

Why Quantum Mechanics?

The first question a student of quantum mechanics might ask is "why do I need quantum mechanics?" Let us first address this question. For this we have to see whether the Newton's Laws of Motion are sufficient to describe everything. If we want to describe the motion of objects, we use Newton's equations. A better word to describe the formalism of Newton's laws is *classical mechanics* - we will use this term to follow convention.

Now if one wants to describe the motion of planets around the sun, one knows that one has to write the Newton's equation taking into account the garvitational force between the sun and a planet. Given the initial postion and velocity (or momentum) of the planet, one can calculate its position and velocity at any future time. What about something smaller than that? Well, classical mechanics can also be used to describe the motion of a football, a cricket ball, a table-tennis ball. It can also be used to describe the motion of tiny bullets fired from an air-gun. The question arises, can classical mechanics describes paticles of any size? What about dust particles, molecules, atoms, electrons?

To answer this question we consider a *gedanken* experiment (thought experiment) with tiny bullets. Suppose that we have an air-gun which can fire tiny bullets onto a screen kept a large distance away. The air-gun, like all other guns, is not hundred percent accurate. One bullet fired in the same direction may go slightly away from another one fired in exactly the same direction. If one fires, say, a hundred bullets on the screen - all of them will not hit the screen at the same spot. One would rather see a spread out blob on the screen. Now suppose one keeps an screen-like obstacle in between the gun and the screen, which has two holes. If one of the holes



A two-slit experiment with electrons.

is blocked, the only bullets which are able to pass through the open hole, and one would see a blob on the screen at a point in line with the gun and the open hole. If one opens the second hole and closes the first one, one gets a blob on the screen at a spot in line with the second hole and the gun.

If now one opens both the holes and again fires lots of bullets, one would see a double blob which will just be the sum of the two blobs obtained in the previous cases. You might say that this is expected because if the bullet goes through one hole, it will land somewhere in the first blob, and if it goes through the second hole, it will land up in the second blob. There is nothing new happening here. Quite true - this is all trivial stuff.

Electron diffraction

Two clever scientists, *Davisson and Germer* tried to repeat this experiment, not with bullets, but with electrons. And they found a weird phenomenon. They found that if either of the two holes is closed, one gets a blob as in the case of bullets, but when both the holes are open one gets a pattern which looks like a long array of blobs. This pattern is not just the sum of the patterns obtaines with only one holes open. *This is the* *most amazing thing one would have ever seen in nature*. Trying to visualize what must be happening, one imagines that an electron fired from the electron gun passes through one of the two holes, and should behave as if only that hole was open. So, the net pattern should be a sum of the two patterns with only one hole open. But this does not happen, which can only mean one of the two things. One, that the electron passes through only one hole, but somehow *knows* that the other hole is open. Second, the electron somehow *passes through both the holes simultaneously*.

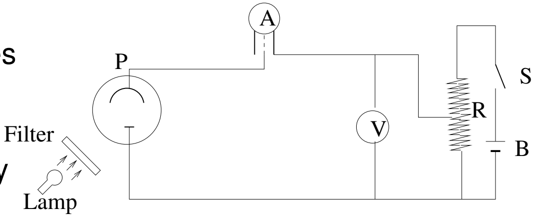
Both these possibilities sound very strange, but that is exactly how nature is seen to work. So, one observes that laws of classical mechanics fail when dealing with electrons. Infact, they mostly fail when applied to particles as tiny as atoms, molecules and subatomic particles.. So there must be new laws of motion which govern the behaviour of electrons. It turns out that these new laws governing the dynamics of atomic scale particles constitute quantum mechanics.

The reader might have noticed a similarity between this experiments with electrons and the *Young's double-slit experiment* that one does with light. There one gets exactly the same pattern as with electrons through the two holes. Light shows this behaviour because of its wave nature. So, the electrons seem to behave like waves.

Photoelectric effect

Let us look at another phenomenon which was observed. Here one looks at a vacuum tube in which one of the electrodes is coated with a metal which can emit electrons if light falls on it.

One observes that if one shines light of low frequency, say infra-red, no electrons are emitted and



Reverse-biased arrangement for studying photo-electric effect.

hence no current flows. One can try to increase the intensity of light to any extent, but still no electrons are ejected. But for light of higher frequency, say blue color, the electrons are emitted and a current flows, even if the intensity is low.

Now the energy of a wave is basically its intensity. The experiment here shows that light is not behaving like a wave, because higher intensity is not able to kick out electrons. On the other hand if we imagine that light is made up of particles, which we can call *photons*, whose energy is $h\nu$, where vu is the frequency of light, one can easily understand the results of this experiment. Higher frequency lights is made up of particles which have higher energy, and so are able to kick out electrons. And if the energy of these *photons* is less than the energy needed to kick out an electron, no electron will be emitted, no matter how many photons one throws at the metal surface. What does this mean? This means that in this experiment, light which is considered normally to be a wave, behaves like particles.

Wave-Particle Duality

So, where do these two experiments leave us? They tell us that particles can behave like waves and waves can behave like particles. Infact, one has to assume that wave and particle are two sides of the same coin. They are two natures of the same entity. In the modern lingo, such quantum objects are called *quantons*. This concept is known as wave-particle duality.

The Stern-Gerlach Experiment

Let us look at another experiment which was performed in 1922 by Stern and Gerlach. They prepared a beam of silver atoms, which are paramagnetic, and passed it through an *inhomogeneous* magnetic field. Before we discuss what they observed, let us try to see what one expects to observe. Suppose each atom has an inherent magnetic moment mu, then the force on it in an inhomogeneous magnetic field is given by

$$F = \nabla(\mu \cdot B)$$

Let us assume that $B_z \gg B_x, B_y$, so that $\mu \cdot B \approx \mu_z B_z$. In this situation, the force will be primarily along the z-axis,

$$F = \mu_z \frac{\partial B_z}{\partial z}\hat{k}$$

where $\hat{k}$ is a unit vector along z-axis. One can see that the deflection of the beam should be proportional to the z-component of the magnetic moment. Now, if one has an unpolarized beam, the z-component of the magnetic moment of different atoms will have all possible values between $-\mu$ and μ.

When the experiment was performed, it was observed that the beam of atoms split into only two beams. This means that the z-component of μ can have only two values! This goes against all physics we have studied till now. We would think that μ is like any ordinary vector, and its z-component can have all possible values between $-\mu$ and μ. But this experiment shows that this is not the case. Our expectation is based on newtonian mechanics, and this experiment seems to indicate that Newton's laws are not valid for angular momentum of atoms.

We need a new theory

All the three experiments described above show that Newtonian mechanics, which is tried and tested for things as small as tiny dust particles to planets and stars, fails miserably when applied to objects which are at the atomic scale. So, obviously we need a new theory. This theory should be able to show that certain quantities can have only restricted (quantized) values, like the angular monentum, and also this new theory should treat waves and particles not as separate objects, but on the same footing. This new theory is called *Quantum Mechanics*

Wave-function and the Schrödinger equation

Because particles seem to behave like waves, one seeks a wave-like theory for particles. Historically, one started from a wave solution

$$\psi(x) = \exp(ikx - i\omega t), \tag{1}$$

where k is the wave vector, ω is the frequency and $\psi(x)$ represents the displacement of whatever is oscillating. For a wave on a stretched string, $\psi(x)$ denotes the amount by which the string is pulled up, at the position x. For a wave generated in a water puddle, $\psi(x)$ denotes the height of the surface of water at the point x. In our theory we do not know what is it that is oscillating, but we know that there is some kind of a wave. So, let us start with that.

Now, de Broglie told us that for a particle with momentum p, there is a wave associated which has a wavelength $\lambda = h/p$. We know that the wave vector is related to the wavelength by the relation $k = 2\pi/\lambda$. Using this we can write write $k = \frac{2\pi p}{h}$. Here we introduce another constant $\hbar = h/2\pi$, and use it to write $k = p/\hbar$. Now we have momentum in the expression, which is what we like because a particle is expected to have quantities like momentum and position. Now the expression for the wave (1), takes the form

$$\psi(x) = \exp\left(\frac{i}{\hbar}px - i\omega t\right) \tag{2}$$

So, what do we do with this expression? Let us differentiate it with respect to x, which gives us

$$\begin{aligned} \frac{\partial\psi(x)}{\partial x} &= \frac{i}{\hbar}p\exp\left(\frac{i}{\hbar}px - i\omega t\right) \\ &= \frac{i}{\hbar}p\psi(x) \end{aligned} \tag{3}$$

Equation (3) indicates that $-i\hbar\frac{\partial}{\partial x}$ plays the role of p. To put it more precisely,

$$p \to -i\hbar\frac{\partial}{\partial x}, \tag{4}$$

which indicates that in our new theory, p is like an **operator** which acts on the function $\psi(x)$. We will see later that this observation is of great importance in quantum mechanics.

Let us now differentiate (2) with respect to t, because it is also a function of time. This yields

$$\begin{aligned}\frac{\partial\psi(x)}{\partial t} &= -i\omega \exp\left(\frac{i}{\hbar}px - i\omega t\right) \\ &= -i\omega\psi(x) \end{aligned} \tag{5}$$

What do we do with ω? We remember that photons, particles of light have energy $E = h\nu = \hbar\omega$. So, we can write $\omega = E/\hbar$. Now that we are dealing with particles, the energy has to be a sum of potential energy and kinetic energy. This leads us to write

$$\omega = \frac{1}{\hbar}\left(\frac{p^2}{2m} + V(x)\right) \tag{6}$$

where $p^2/2m$ denotes the kinetic energy and $V(x)$ represents the potential energy. Using (6), equation (5) takes the form

$$\frac{\partial\psi(x)}{\partial t} = -\frac{i}{\hbar}\left(\frac{p^2}{2m} + V(x)\right)\psi(x) \tag{7}$$

or,

$$i\hbar\frac{\partial\psi(x)}{\partial t} = \left(\frac{p^2}{2m} + V(x)\right)\psi(x) \tag{8}$$

Let us use equation (4) which says that $p = -i\hbar\frac{\partial}{\partial x}$, so that (8) becomes

$$i\hbar\frac{\partial\psi(x)}{\partial t} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x) \tag{9}$$

Equation (9) is known as Schrödinger equation, and is the basic equation of quantum mechanics. This was first constructed by Erwin Schrödinger. It describes how the wave function $\psi(x)$ changes with time, for a particle of mass m in a potential $V(x)$.

What does ψ represent?

From the preceding analysis we conclude that quantum objects act like waves, and the entity which appears to oscillate is the wave function $\psi(x)$. But what does ψ represent, one might ask? In different kinds of waves that we know of, there are different entities which oscillate. In a wave on a stretched string, what oscillates is the displacement of the string in the transverse direction. In the waves on the surface of water, we know that if a leaf falls on the surface, it oscillates. So what oscillates is the surface displacement of the water surface from its mean position. In sound waves, it is the density of air which oscillates, leading to compression and rarifaction. In electromagnetic waves, it is the electric and magnetic field which oscillates. So, what oscillates in our quantum wave? This question confounded people when quantum theory was being formulated. The Schrödinger equation (9) is complex, and in general it admits complex solutions. So, $\psi(x,t)$ is in general complex, and hence cannot represent a measurable quantity which should be real.

Max Born came up with a solution to this problem. He proposed that $\psi(x,t)$ itself has no meaning, but $|\psi(x,t)|^2x = \psi^*(x,t)\psi(x,t)dx$ represents the probability of finding the particle at position x, at a time t. This interpretation of the wave-function is known as the *Born interpretation*, and is known to hold good till now.