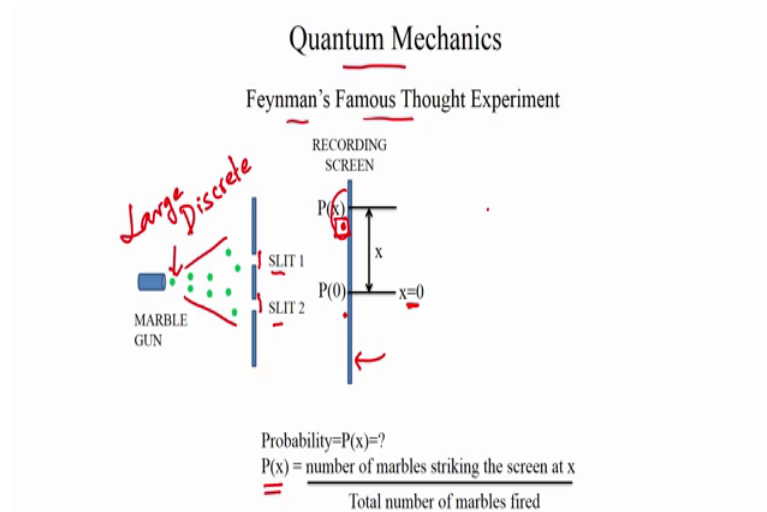


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**Lecture - 01**

**Quantum Mechanics: Concept of Wave Particle, Schrodinger's Equation**

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We will start off with the Fundamentals of Quantum Mechanics, ok. Now, most students are probably at the end of their high school are very familiar with classical mechanics which is governed by the traditional Newtonian laws of physics, which is very commonly taught at the high school level. Now, for students are not been exposed quantum mechanics some of these ideas can turn out to be very strange, and you know sometimes very puzzling, ok. And there is no better way to introduce quantum mechanics at least in my opinion then to look at this famous thought experiment by Richard Feynman, ok. And the experiment starts off you know the discussion on this starts off like this.

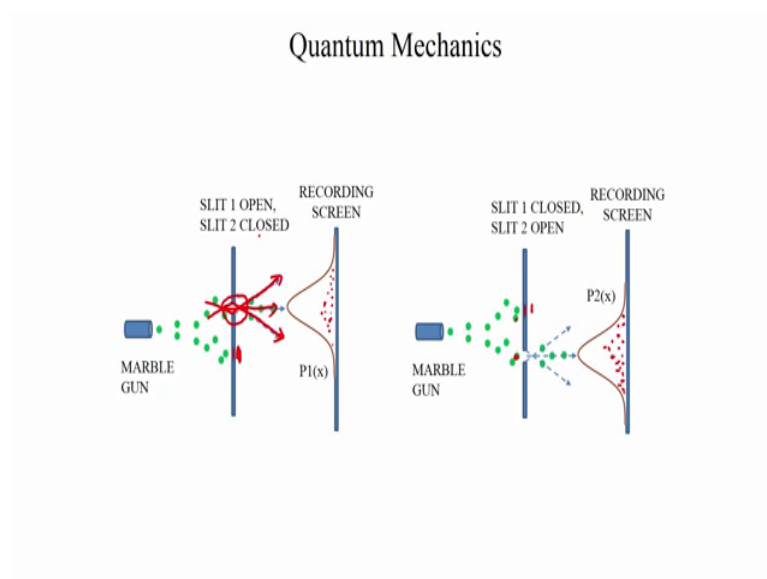
So, many students are familiar with the Young's double slit experiment, but what we are going to do we are going to play around with this experiment and try out different ideas here. So, let us say you have instead of you have a gun, and it is a special kind of a gun which shoots out marbles, ok. So, essentially what I mean by marbles is any large discrete particle, ok. So, it could be marbles or you know it could be bullet us it really

does not matter large discrete particles that cannot break up that are going to come, that are going to remain you know structurally which have got structural integrity throughout this experiment.

And you take this gun and you start firing marbles one at a time, and there is a certain spread to this firing. So, it is not going in a straight line there is a certain spread. And then you place a barrier right in front of this gun, and this barrier has got 2 gaps they got 2 fine gaps through which the marble can get through and we will call these gaps a slit 1 and slit 2, ok. And what we are interested in seeing is we want to know what the pattern of impact is on a screen that is placed behind this barrier. So, we have a recording screen here, and this these little marbles will come and try to stick on to this recording screen, and what we want to find out is how many marbles were collected at some point  $x$  from some reference  $x$  equal to 0.

So, if you define this point on the screen as  $x$  equal to 0 and you vary this distance as  $x$ , I want to know what is the probability, that a marble came and struck the screen at this point and a simple way to estimate this probability is simply by counting the number of marbles that came in impacted the screen at this point divided by the total number of marbles where fired from this gun, it is a very simple way of looking imagining this. So, I need to find out I want to get a distribution of the impact profile on the screen, ok. So, that is that is the simple experiment.

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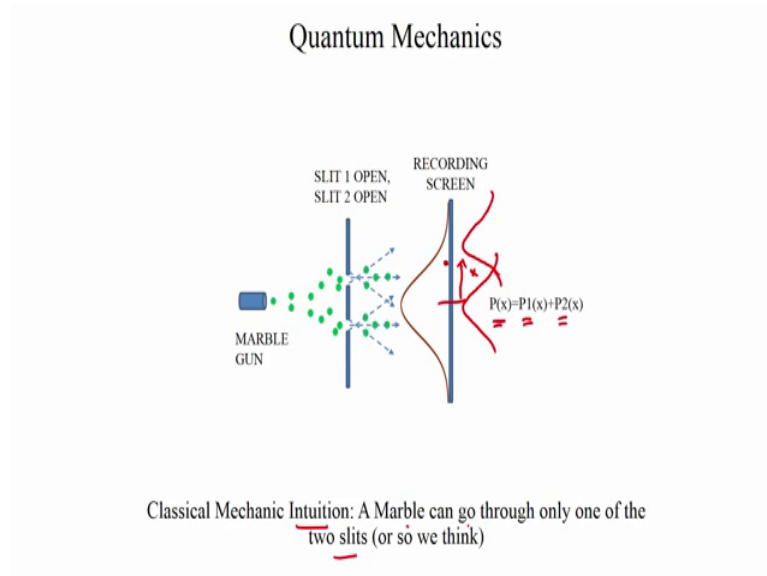
Now, let us try to play around with this. So, let us say we closed one of these gaps, ok. So, this gap is closed. So, slit 2 is closed and slit 1 is open and you fire your marble gun and you will find that all the marbles you know they cannot get through the barrier beyond this point in these regions, and the only possible way to you know impact screen is by travelling through this gap here. So, you will find that the marbles randomly travel through this gap. So, it might go there you know bounce off this edge some of the marbles might bounce off that edge and some of them might just get through and so on.

And what you would expect is you would expect most of the marbles that ever got through this gap to strike the screen at some point here, and there would be some sort of a gradual decrease in this probability that a marble really impacted the screen at the other places. And this is what any this is what say common sense might tell us, ok. And it is a fairly good argument because there is only one entrance to this entire path to the screen.

On the other hand if you were to close slit 1 and keep slit 2 open you would expect the same profile, but the only thing is it shifted in  $x$ , ok. So, you do not expect the profile there because there is no path to strike the screen over there into the marbles are now, going to enter is going to enter this barrier through slit 2 and they are going to impact the screen in this manner you will find a lot of marbles impacting here and very few in the other regions. So, you have some kind of a profile like this.

Now, what is key is to understand that the marbles are going through one marble is going through only one slit, a marble cannot decide to go through both slits together, ok. That is what that is what we feel that is what our intuition is, ok, the reality might be different, ok. So, if you were to go talk to a layman and say you know this marble travel through both slits together it would appear a bit puzzling at least initially, ok. And you with that intuition you do expect this distribution and this is what you might actually see if you were to conduct this experiment.

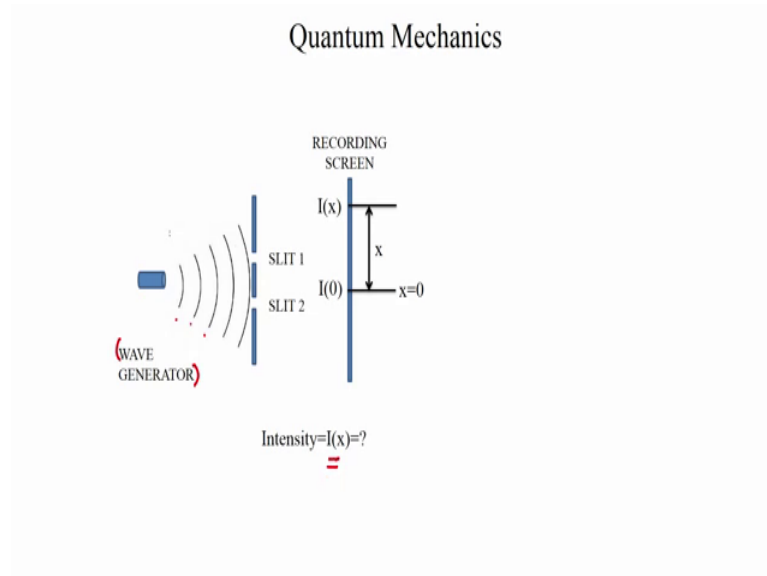
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Now, if you keep both slits open you will find that the marbles are able to go through both slits simultaneously you will see a profile of marbles you know impacting the screen in various paths and you expect the profile to look more or less like this. So, I probably cover it with all my writings, but you would expect the effective profile to be a summation of these two profiles that you see and you would expect something of this kind, ok. And of these slits are very far apart you might you might see a slight dip up here in this.

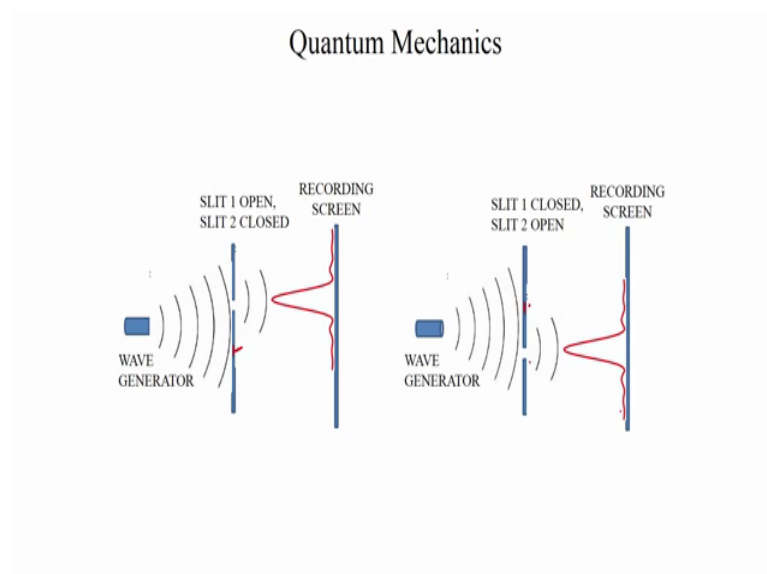
So, essentially the probability of finding a marble the probability that a marble impacted the screen at some point  $x$ , from this reference is let us say  $p$  of  $x$  and that is simply the summation of the probability that the marble came through slit 1 and impact to the screen and that the marble came through slit 2 an impact in the screen. So, it is just a summation of these two probabilities. And what is important is that we have this intuition that a marble can only go through one of the two slits, ok. So, it cannot go through both slits. So, now, that is what the experiment with marbles tell us, ok. So, now, let us change the experiment of it.

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Instead of having a gun which shoots out marbles we will have a wave generator, ok. So, you can think of it as a way a gun that shoots out waves. And these are the wave fronts, so you can conduct this entire experiment in water or oil if you like and these are the wave fronts, of this wave. And this waveform front propagates through and we keep the same barrier that we use in the previous experiment maybe change the sizes a bit, but essentially the idea is the same and once again we need to keep a recording screen and we want to record the intensity of the wave observed on the screen, ok. And we want to find out what is how does the intensity vary with the  $x$ , ok.

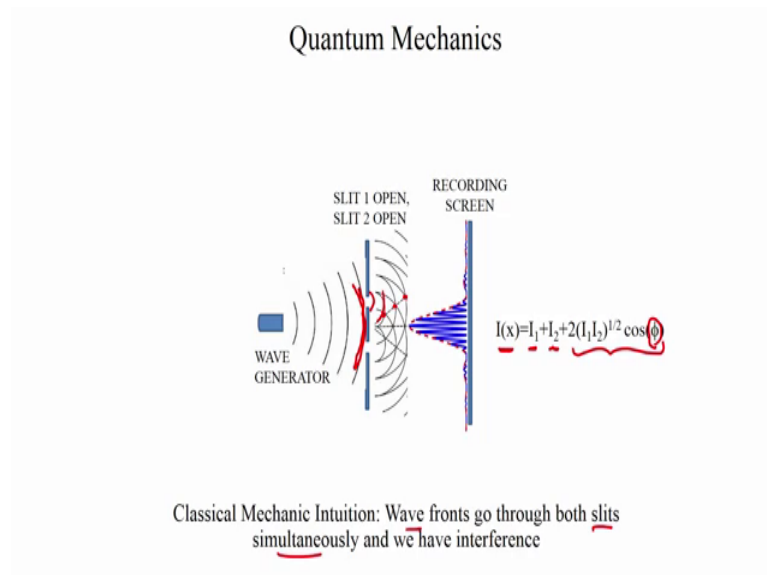
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So, once again if you go back through our thought experiment which is to close the slit and keep that slit open the wave front strikes this barrier and it would sort of diffract through this little opening and it would strike the screen giving you a distribution and intensity distribution that probably looks something like this, ok. And this distribution is very strongly of course, it is very strongly dependent on the size of the slit, but that is not the main point of all this argument, ok. So, you have an intensity distribution that looks like this.

Now, if you were to close that slit and keep this one open you will find another intensity distribution that looks like this.

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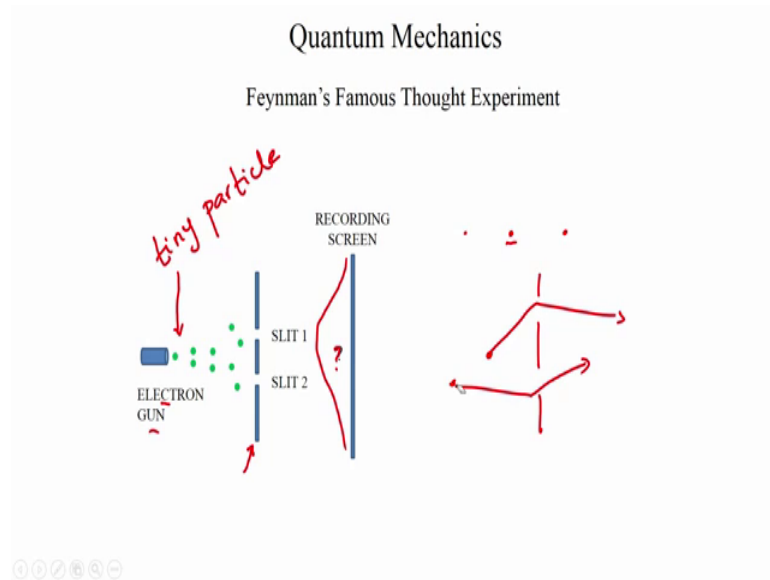


Now, if you were to keep both slits open the wave front enters through both slits at the same time and what you will see is an interference of these two waves. So, you see all these points where both these wave fronts are interfering with each other, ok. So, what you will see is an interference pattern, wherein the effective intensity at some point  $x$  depends on the intensity of the wave coming the intensity 1 which is basically the intensity or the waves coming through slit one and intensity 2 in this manner, and this is the interference term where this is the phase difference between these waves.

So, what is key here is unlike bullet us we imagine the waves to be going through both slits simultaneously and that is why we have interference, ok. Now, the bullet us did not do this, that is what our intuition told us but on the other hand the wave front you see it

approaches both slits simultaneously. And it goes through both of the slits simultaneously and therefore, you have interference. And this is you know sort of very well expected and we have experiments such as the Young's double slit experiment which sort of sort of provides an empirical or an experimental corroboration with all this theory, ok.

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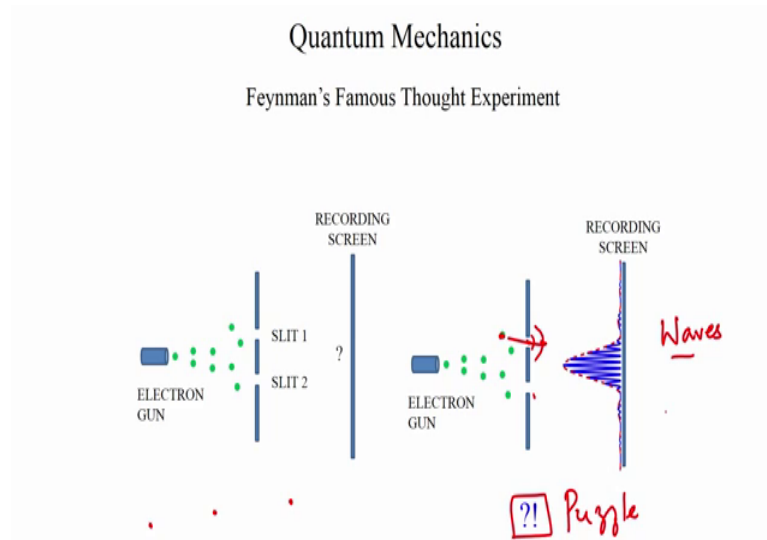
Now, let us come down to a third experiment. And what we do here is we go back to a marble gun, ok, but instead of firing marbles we have to fire electrons, ok. So, we have an electron gun. So, essentially you can imagine these to be very tiny particles. So, what I mean by an electron gun is it has to be very tiny particles, ok. And it is alright at this point think of these particles as discrete, ok. And we perform the same experiment and we fire one electron at a time.

So, let us say you do not had to fire all of them together you do not have to fire you do not have to fire them at any specific rate let us assume that you are firing one electron at a time. So, you have one electron, you wait for some time, you fire a second electron you wait for some time and go on so forth, and you perform the same experiment, you still have your barrier with 2 slits and you have a recording screen. And the question is what do you think will happen here, ok.

Now, if you follow the intuition of the marble if you think of electrons as discrete particles they are very tiny you would expect that the electrons that one particular electron chooses to go through any one slit, right. So, maybe this electron went through

this slit the second electron went through this slit and so on, and what you would expect to see it is a distribution that looks not very different from our experiment on marbles right you would expect to see a distribution that looks like that, but the reality is quite surprising.

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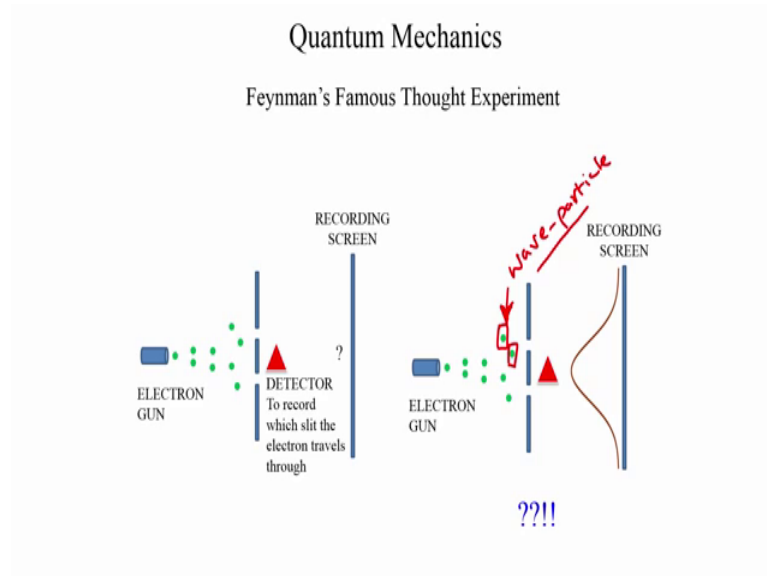


If you were to do this experiment what is expected is you would see a distribution that looks more like what the way more like the manner in which the waves behaved as compared to the bullet us, ok. And that is largely slow because it is not intuitive, and there is this a puzzle because we were to believe that the electron went through only one slit at a time, right. The electron this particular electron decided to either go through this slit or this one it did not go through both slits that was our intuition but that is not what the experiment says.

The experiment is telling you that despite the electrons being fired one at a time you know with even some sufficient space and time between the firings. Each electron has gone through both slits simultaneously much like a wave and not like a particle and that is a big puzzle, ok.



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So, we say that the, this is not quite possible we say that it is impossible for the particle like electron to be behaving like a wave and producing an intensity pattern that is expected when we have waves, ok. And we say that we do not believe the fact that the electron went through both slits simultaneously and therefore, we are now, going to place a detector at this location in order to identify the position of the electron. Or in other words they are going to place this detector that is going to exchange information with electron it is going to ping the electron at the photon let us say and in obtained information with regards to the position of the electron.

And the point placing the detector is to identify the slit through which the electron is going to enter, and then see has to what kind of recording these obtained on the screen. So, let us say we keep the experimental setup the same the recording screen is the same, the position of the slits are the same, the electron gun is the same etcetera and the only difference is the appearance of this detector. So, what kind of pattern do we think that we will see the electrons create on the recording screen? So, when we run the experiment we have a very surprising result. We see that when the experiment is run with the detector and place the electrons produce an intensity pattern that was seen when bullet us were fired or when large particles were fired.

Now, this is even more surprising than the previous experiment. So, what the electrons are saying is that when there is no detector around, we are going to behave very

differently; we are going to behave like waves and create an intensity pattern that is expected of waves. But the moment we identified that a detector is watching us, they are going to behave very differently and we are going to behave like bullet us and create a very different intensity pattern. And this is the puzzle of quantum mechanics, and this is what quantum mechanics tells you which is that the, that at the very basic level you treat every particle as a wave and a particle or a wave particle ok. And from this point on they are going to go ahead and develop this concept and try to understand this idea of a wave particle.

As far as this part of the experiment is concerned, which is the interaction of the detector with the electron, creating the making the electron behave differently it is a very wonderful ground for philosophers to act on and there are a lot of interesting debates, ok. while there is while it is quite at least qualitatively understood that as to what happens, there are a lot of interesting debates between physicists of the twentieth century in trying to argue this factor out. So, it makes so very for some very good reading for the student who is interested.

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**Wave-Particle Duality** ←

Need both the Wave and Particle like treatment to explain Experiments  
 Photons, electrons etc behave as particle and wave

Wavelength of the Particle  $\lambda = h/p$  (De Broglie's Equation)  
 $h = 6.6 \times 10^{-34}$  Js is the Planck's constant

*Planck's const*  
 $\lambda = \frac{h}{p}$   
*wave*

*photo* → *wave*  
*Particle Photoelect*

*Scattering*  
 $P = mv$   
 $E_{kin} = \frac{1}{2}mv^2$

**Example: Electron**  
 Charge =  $-1.6 \times 10^{-19}$  C  
 Mass =  $m = 9.1 \times 10^{-31}$  kg  
 Velocity =  $v =$  say  $1 \times 10^6$  m/s  
 Momentum =  $p = mv = 9.1 \times 10^{-26}$  kg.m/s  
 Kinetic Energy =  $mv^2/2 = p^2/2m = 4.55 \times 10^{-21}$  J =  $(4.55 \times 10^{-21}) (1.6 \times 10^{-19})$  eV = 28.4 meV  
 Wavelength =  $\lambda = h/p = 6.6 \times 10^{-34} / 9.1 \times 10^{-26} = 7.2$  nm

**Example: Tennis Ball**  
 Mass =  $m = 0.058$  kg  
 Velocity =  $v =$  say 50 m/s  
 Momentum =  $p = mv = 2.9$  kg.m/s  
 Kinetic Energy =  $mv^2/2 = p^2/2m = 72.5$  J  
 Wavelength =  $\lambda = h/p = 6.6 \times 10^{-34} / 2.9 = 2.3 \times 10^{-32}$  m

*9.1 x 10<sup>-32</sup> m*

So, let us now try to understand this key concept of quantum mechanics, which is called as the wave particle duality, ok. And the idea of this concept is that both a wave like and particle like treatment is needed to explain electron explain the experiments involving electrons photons or any other tiny particles. So, for example, if you look at the photon

we have, its wave like nature appear in experiments such as the Young's double slit experiment. And we have its particle like nature appear in experiments such as such as the photoelectric effect, ok.

And if you look at the electron, we have its wavelike nature appear in the experiments that we just discussed which was which was like the Young's double slit experiment. And we have its particle like nature appear and experiments which involves a scattering, ok. So, we need both of wave like treatment as well as a particle like treatment to explain the behaviour of these entities, and coming to the electron you know, which are basically the particles of interest with regards to this course of course, it is not that the photon is not of interest, but we would like to elect understand the electron very well.

So, coming to the coming to the electron just like how you know its particle like aspect can be defined with the with terms like the momentum, which is say the mass into the velocity and terms like the kinetic energy, which is half into the mass into the velocity square. Just like how you can define say the particle attributes of the electron we need to also identify the wavelike attributes of the electron. So, what is the wave length of an electron? And this relation between the wavelike nature and particle like nature is defined by the De Broglie's equation. So, it is a very very essential idea or essential concept, which connects the wavelength of the wave particle to the momentum of the wave particle.

So, we say that  $\lambda$  which is the wavelength is defined as  $h$  by  $p$ , where  $h$  is a constant and it is called as a Planck's constant and it is got a value of this. It is the same constant that is used to define the energy of a photon. So, the energy of a photon is  $h$  times  $\nu$ , where  $\nu$  is the frequency of photon, we are talking about the same Planck's constant and  $p$  is the momentum of the electron. So, if you know the momentum of the electron.

So, let us say the electron is fired from a gun with a certain amount of energy kinetic energy. So, we know the kinetic energy of the electron which is nothing, but the momentum squared by  $2m$ , where  $m$  is the mass of the electron and therefore, we know the momentum of the electron and if we know the momentum of the electron we know the wavelength of the electron via the De Broglie's equation. So, let us get some numbers and some estimates and you know try to see as to how we can use this equation. So, the

electron has got all these properties it is got a charge of minus  $1.6 \times 10^{-19}$  coulombs, it is got a mass of  $9.1 \times 10^{-31}$  kilograms. So, that is a rest mass of the electron.

Now, let us say the electron is fired from an electron gun you know for the purpose of this example, we say that it is got a velocity of  $10^5$  meters per second, and therefore, it is got a momentum of mass into velocity which is about  $9.1 \times 10^{-26}$  kg meter per second. And therefore, it has got a kinetic energy and this kinetic energy can be represented in Joules, but by dividing it by  $q$ , which is the magnitude of the charge of the electron.

We can also represent energy in terms of a unit called as electron volts. So, if you have energy in Joules, so let us say you have 1 Joule in order to get this energy in electron volt units electron volts is a unit of energy in order to get this into electron volts units you take  $E$  and divide it by the magnitude of an electron charge, which is 1 joule divided by  $1.6 \times 10^{-19}$ , and you have the energy in electron volts. So, joule is a large it is a huge amount of electron volts. And since we talk about very small numbers in semiconductors its useful to have this unit of electron volts.

And therefore, the terms potential and potential energy are all in some sense connected, ok, the terms potential and terms energy are all interrelated because of this neat connection. And since you have this being the energy what is the wavelength of the electron? The wavelength of the electron is given by the De Broglie equation and  $\lambda$  is  $h$  by  $p$  which is about 7.2 nanometres in this case. So, you see that the electron fired off with the velocity  $10^5$  meters per second has a wavelength of about 7.2 nanometres.

Now, let us take just for just for the sake of argument, ok. So, let us say we have a very large particle, and I have taken example for tennis ball and a tennis ball is not a single particle its composed of many little particles, but let us say that is not the case and it is we are talking about one very large particle. And this particle has got a mass of about 58 grams and it is got a velocity about 50 meters per second, I have used values which are typically used for a tennis ball and therefore, it is got a momentum of this much. And what is the wavelength? The wavelength is  $h$  by  $p$  and since the momentum is very very large the wavelength is extremely small its  $9.1 \times 10^{-32}$  meters.

So, you can compare the wavelength of a large particle or a heavy particle with the wavelength of a very tiny particle or a light particle. And you see that the difference is quite immense, ok. So, this is an example just to illustrate what mass does to the wavelength or what momentum does to the wavelength of an object.

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Useful Relations to Note

$k = \text{wave vector} = 2\pi/\lambda$   
*(k also used for the Boltzmann's coefficient later on, please note the context.)*

$\lambda = h/p$   
 $p = h/\lambda = (h/2\pi)(2\pi/\lambda) = \hbar k$   
 'h bar' is the reduced Planck's constant  $\hbar = h/2\pi \approx 1.05 \times 10^{-34} \text{ Js}$

Energy of a photon  
 $h\nu = hc/\lambda$   
 $h\nu = (h/2\pi)(2\pi\nu) = \hbar\omega$

*Handwritten notes:*  
 $k = \text{Wave number} = \frac{2\pi}{\lambda}$   
 $\lambda = \frac{h}{p} \Rightarrow p = \frac{h}{\lambda}$   
 $p = \frac{h}{\lambda} \left( \frac{2\pi}{\lambda} \right) = \hbar k$   
 $\frac{h\nu}{2\pi} = \hbar\omega$   
 $\frac{h}{2\pi} = \hbar$

So, here I have summarized some useful relations that would serve as well in this course we have the first variable which is k, which we will be using in the context to the wave vector or a wave number, and which is given by 2 pi by lambda it is got a value of 2 pi or its got an amplitude of 2 pi by lambda or a magnitude of 2 pi by lambda the lambda as the wavelength. Now, k is also, later on in the course k is also used to define the Boltzmann's coefficient, and I hope that this will not be a matter of confusion because the context will be quite clear and I believe and I hope that this will not create any confusion.

The other important relation is the De Broglie's relation which is  $\lambda = h/p$  which says that lambda is equal to the Planck's constant divided by the momentum. And the momentum therefore, can be written in terms of the terms of the wavelength as p is equal to h by lambda. Now, if you were to take this relation and you divide and multiply by 2 pi, you say h by 2 pi into 2 pi by lambda is equal to your p we see that this is nothing but k,  $h/2\pi$  by lambda is k and this term which is h by 2 pi is given a new definition, ok. It is called h bar or its also known as the reduced Planck's constant, ok.

So, the term  $h$  by  $2\pi$  is also denoted by  $\hbar$ , which is called the reduced Planck's constant and it is got a value of about  $1 \times 10^{-34}$  Joule seconds and therefore, the momentum can also be expressed as  $\hbar k$ .

The energy of a photon is already well known which is  $h\nu$  which is a Planck's constant into  $\nu$  and since we can write  $h$  as  $\hbar$  we can say  $h$  is  $\hbar$  by  $2\pi$  and  $\nu$  as  $\omega/2\pi$  and you multiply  $2\pi$  before  $\nu$  you find that the energy of photon is also equal to  $\hbar\omega$ , by the  $\omega$  as the angular frequency where  $\nu$  is in hertz and  $\omega$  as in say radians per second, ok. So, these are some very useful definitions that would serve us in this course.

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**Heisenberg's Uncertainty Principle**

Cannot measure position and momentum – both – absolutely accurately.  
(Equivalently, error in energy and error in time of measurement)  
If  $\Delta x$  is the error in determining position and  $\Delta p$  the error in determining momentum,  $\Delta p \Delta x \geq \hbar/2$

In general a signal in time/space  $\leftrightarrow$  frequency will have this restriction

Momentum well defined  
(eg. energy of the electron gun is known)  
Position not defined

$p_x \sim h/\lambda; d \sin(\Delta\theta) = \lambda \Rightarrow \Delta\theta \sim \lambda/d$   
 $\Delta y \sim d; \Delta p_y \sim p_x \Delta\theta \sim h/d \sim h/\Delta y; \Delta p_y \Delta y \sim h$

ELECTRON GUN

Moving on another key idea behind in quantum mechanics is something called as the Heisenberg's uncertainty principle. And the essence of this idea can be very nicely understood for a person who is got some experience in signal processing or let us say who is who understands the idea of a Fourier transform. But just to summarize just to you know introduce this concept let us say that we are looking at a signal, that is going to occur or an event that is going to occur at some point in time. So, let us say we have the time or space domain it really does not matter.

So, first let us look at time and we say that, there is a signal that is going to occur at some point in time. So, let us say there is a signal that occurred at this point in time if at if somebody asked us as to when the signal occurred the answer is very very clear we say

that yes the signal occurred at this moment in time that is a very clear question and we have a very clear answer. But if now, somebody asked us as to what is the frequency of the signal, what is the wavelength of the signal.

Now, that question seems a bit absurd because the signal had a very it was not periodic firstly, it had it occurred at just one moment in time and that was it. And therefore, the only way one can determine the wavelength or the frequency of the signal is by taking a Fourier transform and we find that the Fourier transform is wideband signal, right. It is got its got frequencies in from minus infinite from frequencies from 0 to infinite, ok. And therefore, the frequency enhance the wavelength of the signal is not very clear and therefore, we feel that the question on what the frequency of the signal is not a very clear question because the signal is a wideband signal.

Now, let us take the example of another signal, and we say that this is a very nice little sinusoid and that is time. And now, if somebody asked us the same two questions, if somebody asked us is to vend it the signal occur we find that this is a very bad question or we find that is a very weird question because it is a sinusoidal signal and there is no particular moment when the signal occurred the signal has been present in all points in time.

On the other hand if somebody asked us as to what is the wavelength of the signal this question seems to be a very nice clear question it is a very clear answer because we can now, point to the exact wavelength of the signal and therefore, we know the exact frequency of the signal. So, if you were to take the Fourier transform of this signal, you would find that it is got a very unique frequency component that corresponds to the frequency of the sinusoidal signal.

So, this is the key idea behind you know it is a key concept or the key puzzle behind the Heisenberg's uncertainty principle, which is if the location in time or in space is very clear then the message on the frequency or the wavelength is very very unclear. And on the other hand if the idea of the frequency or the wavelength is very very clear, then the location in time or in space is very very unclear, and it is this parent it is this balance between these two errors or the uncertainty that are addressed by the Heisenberg's uncertainty principle.

So, in one form what the Heisenberg's uncertainty principle says is that if you have if you were to perform an experiment say with the electron, and you were to be measuring the position of the electron and you were to be measuring the momentum of the electron simultaneously, ok. And if you were to have an error in the estimate of the position of the electron and an error and the estimate of the momentum of the electron then the product of these two errors have got a bound and that bound is defined by  $\hbar$  by 2. And what this inequality says is that one cannot estimate the position of an electron and the momentum of an electron to the, to an accuracy which wherein the errors or the product of the errors lie below  $\hbar$  by 2.

Or other words if I were to define the position of the momentum define the position of the electron to the infinite accuracy, I define the position absolutely accurately such that  $\Delta x$  is 0. Then I will have a very large inaccuracy in the position or in the error in the momentum I cannot define the error in the momentum at all there will be an infinite error possibility and vice versa. So, this is the definition of the Heisenberg's uncertainty principle, ok. And I have given you a very interesting you know reasoning behind you know our experiment on the electron gun over here we will not discuss it here, but if you have any questions just let me know. It is uses the Heisenberg's uncertainty principle to talk about the events of the experiment.

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Quantum Mechanics

The Wave function

$\psi$

Contains information on all measurable parameters of the particle

If we consider 1D (say x direction), the wavefunction is  $\psi(x,t)$

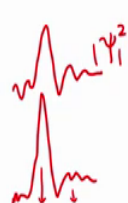
$\psi\psi^*$  = Probability density of finding the particle between x and x+dx

If  $\psi(x,t)$  is real,  
Probability of finding the particle between x and x+dx =  $|\psi(x,t)|^2 dx$

Probability of finding the particle between x=a and x=b is  $\int_a^b |\psi|^2 dx$

*"Wave-fun"*

$\psi$





So, now, we have a particle that is also called a wavelike behaviour and I want to now, start modelling it. So, I can associate a momentum to it, I can associate energy to it, I can wavelength to it and I want to model this aspect of this wave particle, ok. So, there is everything is this wave particle and I want to start modelling this entity, ok.

And a convenient way to do it is through something called as the wave function, which is usually denoted by the symbol  $\psi$ . Now, what is this wave function? Ok, it is for all practical purposes it is a mathematical function it is a function of space and time and it contains all the measurable parameters of the particle, ok. And by operating on this wave function I can extract all the parameters that I would like about this particle and we will sort of look into this in greater detail.

So, if you say that you are only talking about a 1D x dimensional case you can say the wave function is a function of  $x$  and  $t$  which is time, ok. Now, it could be a complex function. So, this product which is the wave function times its conjugate, is the probability density function of finding the particle, ok. So, it is basically the it is its related to the expectation of a particle existing between 2 different between 2 regions, and that is a very strong point, ok, which means if I know the wave function I can estimate I can get an estimate of what the probability is of finding a particle between two regions between two points let us say between  $x$  and  $x$  plus  $d x$ .

If  $\psi$  is a real number then this is simply  $\psi$  square and therefore, the probability of finding the particle between  $x$  and  $x$  plus  $d x$  is  $\psi$  square  $d x$ , because this is my probability density and that is  $\psi$  square  $d x$  is the total probability of finding the particle between  $x$  and  $x$  plus  $d x$ . So, what is this saying? It saying that if I have a wave function that looks like this, for example if this is my  $\psi$  of  $x$ .

Then I can take the magnitude of  $\psi$  and I can take the square of it, ok. So, let us say that does something like this. So, what this is it is the probability density of finding the particle which means that according to this wave function the probability of finding the particle in this region is the largest. And the probability of finding the particle here is not 0, but it is not as large as finding the probability finding the particle in this region, ok. So, that is the implication of this and just going by these arguments if I need to find what is the probability of finding the particle between say two locations  $x$  equal to  $a$  and  $x$

equal to b, then it is simply the summation of these probabilities, which is an integral of from a to b of psi square dx, ok. So, that is the probability of finding a particle.

Now, let us look at some more properties of this wave function. It is a very important concept.

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### Quantum Mechanics

#### Operators

Contains information on all measurable parameters of the particle.

Some useful operators:

Momentum Operator: $\hat{p}_x = \frac{\hbar}{i} \frac{\partial}{\partial x}$	Thus, $\frac{\hbar}{i} \frac{\partial \psi}{\partial x} = p_x \psi$
Energy Operator: $\hat{E} = -\frac{\hbar}{i} \frac{\partial}{\partial t}$	Thus, $-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = E \psi$

$\psi = e^{i(kx - \omega t)}$   
 $\frac{2\pi}{\lambda} \quad 2\pi\nu$   
 $\downarrow \quad \downarrow$   
 $i(kx - \omega t)$

Kinetic Energy:  $\frac{p_x^2}{2m} = \frac{1}{2m} \frac{\hbar}{i} \frac{\partial}{\partial x} \left( \frac{\hbar}{i} \frac{\partial \psi}{\partial x} \right) = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}$

$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\frac{\hbar}{i} (-i\omega) \psi = \hbar\omega = \frac{\hbar}{2\pi} 2\pi\nu = \hbar\nu$

So, we said that the wave function contains all measurable parameters of the wave particle and we said that these measurable parameters could be obtained or extracted from the wave function by operating on it. So, what are some of the useful operators? Ok, so we now, look at the momentum operator and the energy operator and therefore, using these to define something called as the kinetic energy operator. So, let us say I need to find the momentum of the particle in the x direction, ok. So, this happens to be the momentum operator and I will give you an argument as to why this is the momentum operator, ok.

If I need to find the energy of the particle or the wave particle, then this is my energy operator. So, what this means is if I take this operator and use it to operate on this wave function psi then I will get the momentum of the particle in x direction times psi. And similarly this is the energy the particle time psi. And if I want to find out what is the kinetic energy its p square by 2 m, which is 1 by 2 m into the momentum operator operating it on itself and then the wave function which is basically your 1 by 2 m h bar

square by  $\hbar$  square into  $\frac{d^2 \psi}{dx^2}$ , which is  $-\frac{1}{2m} \hbar^2 \frac{d^2 \psi}{dx^2}$ .

So, this is my kinetic energy operator. So, you could imagine this particular element here to be my kinetic energy operator, when it is operated on the wave function I get the kinetic energy. So, you have these operators and they tell you what the momentum is the energy is and the kinetic energies etcetera.

So, just to give you a quick feel for why this is the momentum operator, ok. So, let us say for the sake of argument let us say my  $\psi$  is a plane wave, ok. So, let us say it is  $e^{i(kx - \omega t)}$ , where  $\omega$  is the angular frequency,  $k$  is my wave vector. So, this is  $\frac{2\pi}{\lambda}$ , this is  $2\pi \nu$  where  $\nu$  is the frequency in hertz,  $t$  is time and  $x$  is the distance and  $i$  is basically the square root of minus 1. So, wherever you see  $i$  it is simply your complex number, ok. So, let us say let us assume this my wave function, ok.

Now, let us use the momentum operator on this. So, what is the momentum operator? Momentum operator is  $\hbar$  by  $i \frac{d}{dx}$ , since it is all in one dimension you can just write it as  $\frac{d}{dx}$ , but nevertheless. So, this is nothing, but  $\hbar$  by  $i$  and taking the derivative with respect to  $x$  you have  $i$  into  $k$  into  $e^{i(kx - \omega t)}$ . Now, this term here is nothing but your  $\psi$  itself and therefore, what this is  $\hbar$  by  $i$  into  $i$  into  $k \psi$ , which is  $\hbar k$  you can cancel the  $i$  here and  $k$  is nothing but  $\frac{2\pi}{\lambda}$ .

So, it is  $\frac{2\pi \hbar}{\lambda}$  which is equal to  $\frac{h}{\lambda}$  which is nothing, but the momentum of the particle. So, therefore, we could agree we have checked for ourselves that, this seems to be yielding the momentum of the particle in the  $x$  direction. So, now, let us look at the energy operator, ok. So, let us use the same kind of argument with this particular wave function and let us look at the energy.

So, if I were to use this operator, which is  $-\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$  on the wave function what do I get? Now, taking the time derivative of the wave function I should end up with  $-\hbar \omega$  into  $\psi$  itself, which is the exponential term. And this is nothing but  $\hbar \omega$  which is  $\hbar \cdot 2\pi \nu$ , which is  $h \nu$  which is my energy, ok. So, that is why this is an energy operator and it seems like it is all fine. And the momentum operator just derived from the moment the sorry the kinetic

energy operators just derived in the momentum operator and therefore, this is the kinetic energy operator.

So, the essential message of these two slides was basically you can use the wave function to define the, what you say the measurable properties or model the measurable properties of the wave particle. And you can use all these operators on this wave function to extract information about the position the momentum the energy etcetera.

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Quantum Mechanics

Properties of The Wave function ψ ← Normalization

Contains information on all measurable parameters of the particle

ψ must be a solution of Schrodinger's Equation (Energy Balance)

ψ must be continuous

dψ/dx must be continuous

ψ must be normalizable - i.e. it cannot for eg. blow up.

This condition is realized by noting that the particle must exist somewhere in all allowed regions and that the Probability of finding the particle somewhere is 1

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1$$

$\psi = e^{xp(x)}$   
 $x \rightarrow \infty$   
 $x \rightarrow -\infty$

The wave function as we have described now, is a purely mathematical entity, and before it can be applied to explain the laws of physics it must be constrained and it must be made to follow a certain set of rules. So, what are these rules? So, these rules are basically the conditions or constraints it is imposed by the physical laws. And the very first rule is that the wave function must be a solution to something called as the Schrodinger's equation.

The Schrodinger's equation is nothing but energy balance equation or an energy conservation equation, which says the kinetic energy plus the potential energy is equal to the total energy. The second condition is that the wave function must be continuous you cannot have discontinuities in the probability of finding a particle in one region to now. The third is that the first derivative of the wave function with respect with in space must also be continuous because this is connected to the momentum of the particle of the wave particle.

And the final condition states that the wave function must be normalizable, ok. And what that essentially means is that is two things the first is since the wave particle or the does exist in some point at some point in space say between minus infinity and infinite. And since this is the probability of finding that wave particle in the space that probability must be equal to 1, ok. And this limitation will imply that the wave function cannot take a nature that will result in it blowing up.

So, for example, and what we mean by blowing up is for example, let us say that the wave function has got a nature that looks like this which is an e exponential of x, and let us say x goes from 0 to infinite we are looking at this region of space. So, we see that as x heads towards infinite the wave function the amplitude of the wave function also heads towards infinite this cannot be allowed to happen, ok. So, the wave function is limited or the value or the only possible solutions of the wave function must be limited by these criteria by this integral.

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## Quantum Mechanics

### The Schrodinger's Equation

$$\text{Kinetic Energy} + \text{Potential Energy} = \text{Total Energy}$$

Potential Energy: Depends on the potential terrain the particle is placed in= $V\psi$

$$\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi = -i\hbar \frac{\partial \psi}{\partial t}$$

*Handwritten notes: K.E. under the first term, P.E. under the second term, Total Energy under the right-hand side.*

Time independent Schrodinger Equation

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi = E\psi$$

*Handwritten notes: K.E. under the first term, P.E. under the second term, Total Energy under the right-hand side.*

So, let us look at what is the Schrodinger's equation. So, as we mentioned the Schrodinger's equation is an energy conservation equation, which equates the kinetic energy to the, which says the kinetic energy plus the potential energy is equal to the total energy. Now, you have already seen the kinetic energy operator and we found that this operator operating on the wave function yields the term for the kinetic energy the potential energy is dependent on the potential terrain or the potential profile in which this

wave particle sets and based on the different experiments or the different models that we study this potential terrain needs to be identified and defined correctly. And the total energy which is the summation of the potential and kinetic energy is given by the total energy operator operating on the wave function. So, this is the total energy.

Now, in this definition we find that the total this is a time dependent Schrodinger's equation, because the total energy has got a derivative of the wave function with respect to time but it is also possible to study the time independent Schrodinger's equation. So, for example, if we want wave functions or solutions that describe the stationary states, ok. You can solve something called as the time independent Schrodinger's equation in which case the total energy is simply treated as a constant, ok.

So, we lose the time derivative and we write Schrodinger's equation as the kinetic energy plus the potential energy is equal to the total energy. And from this point on we will try to use the Schrodinger's equation to try and describe some simple models, which will help us understand the nature of the wave particle and different potential profiles better.