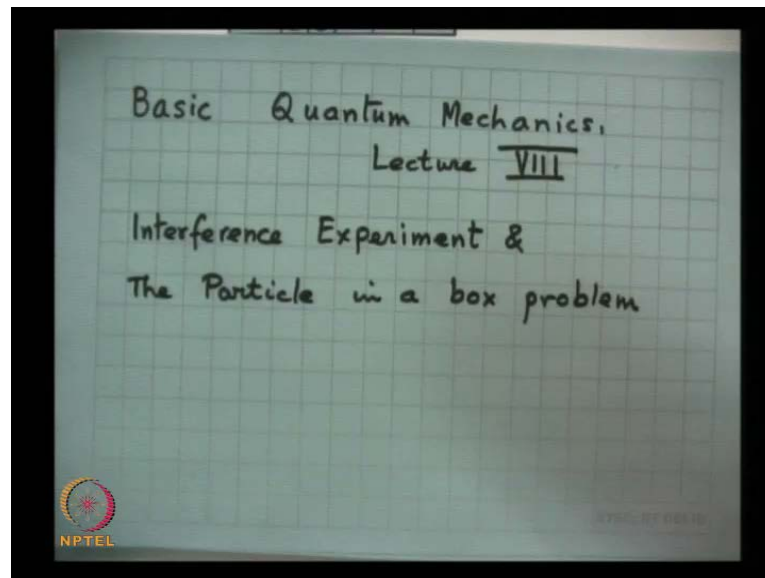


Basic Quantum Mechanics
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Module No. # 02
Simple Solutions of the One Dimensional Schrodinger Equation
Lecture No. # 05
Interference Experiment and The Particle in a Box Problem

We continue our discussion of the free particle problem. And then after that, we will discuss an eigenvalue problem in quantum mechanics and that is the particle in a one dimensional box.

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We will first discuss the interference experiment. In our last lecture, we considered the single slit diffraction experiment.

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$$\psi_b(y) = \frac{1}{\sqrt{b}} \quad |y| < \frac{b}{2}$$

$$= 0 \quad \text{elsewhere}$$

$$a(k_y) = \frac{1}{\sqrt{2\pi k}} \int_{-\infty}^{+\infty} \psi_b(y) e^{\frac{i k_y y}{h}} dy$$

$$= \dots \frac{\sin \beta}{\beta} \quad \beta = \frac{\pi b \sin \theta}{\lambda}$$

$$|a(k_y)|^2 dk_y = \dots \frac{\sin^2 \beta}{\beta^2} \quad \Delta y \sim b$$

Now in that experiment, what we did was, that we assumed that there was a slit of width b and so the electron was described by a wave function, which was constant here in this region, this is my y axis and 0 everywhere else. So, therefore, we assumed $\psi_b(y)$ as equal to $1/\sqrt{b}$ for $|y| < b/2$ and 0 everywhere else.

If I assume such a wave function, then the corresponding fourier transform that is a of p_y will be equal to $1/\sqrt{2\pi\hbar}$ cross from minus infinity to plus infinity $\psi_b(y) e^{i p_y y / \hbar}$ and this we had integrated; and we had shown that, this was equal to some constant times $\sin \beta / \beta$, where β was equal to $\pi b \sin \theta / \lambda$.

And so $|a(p_y)|^2 dp_y$, $|a(p_y)|^2 dp_y$, this is the probability for the electron or the proton to have the y component of the momentum between p_y and $p_y + dp_y$, that was would be proportional to $\sin^2 \beta / \beta^2$. And this as we all know is the single slit diffraction pattern. So, therefore, by confining the electron or the proton to pass through a slit of width b , this slit itself imparts a momentum in the y direction; and the probability distribution of that momentum is given by this expression (Refer Slide Time: 03:42).

So, therefore, where will an individual electron or proton land up on the screen I do not know, but I can tell I can predict a probability distribution. And therefore, if we were to conduct this experiment with a very large number of electrons or protons or neutrons, we

will roughly know the diffraction pattern. And from this equation it is obvious that, smaller the width greater will be the momentum that is (Δp_y) in the y direction; and greater will be the diffraction, so this is my uncertainty principle that, Δy is of the order of b .

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$$\Delta p_y \Delta y \sim h$$

$\Delta y = b$

$$p_y \sim \Delta p_y \sim \frac{h}{b}$$

$$p \sin \theta \sim \frac{h}{b}$$

$$\sin \theta \sim \frac{h}{p \cdot b} \sim \frac{\lambda}{b}$$

$p_y = p \sin \theta$

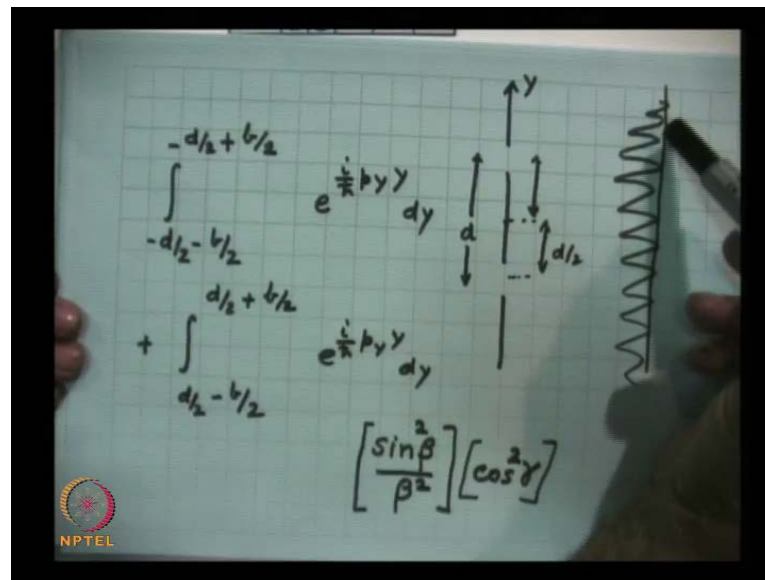
So, therefore, **you have** we have the uncertainty principle that, $\Delta p_y \Delta y$ is of the order of say h or h it does not matter, it is an order of magnitude relation. So, Δy is of the order of b . So, Δp_y is of the order of h by b , now before it entered the slit the electron was coming in this direction, so the y component of the momentum was 0. And so, therefore, this slit imparts a momentum in the y direction, since the average momentum in the y direction was 0, so p_y is of the order of Δp_y ; so, this is of the order of h by b from the uncertainty relation (Refer Slide Time: 05:43).

So, what is p_y as I mentioned that, if this is the particles momentum and if this is the angle of diffraction, p_y will be equal to $p \sin \theta$. So, this will be $p \sin \theta$ will be of the order of h by b . So, $\sin \theta$ will be of the order of h by p into b h by p is the de broglie wavelength, so λ by b .

So, smaller the value of b greater will be diffraction and so, therefore, that is consistent, smaller the value of b greater will be the momentum imparted in the y direction so, all our results are consistent with the uncertainty relation; smaller the value of Δy greater will be the value of Δp_y and greater will be the diffraction. And once again **the** on the screen you will observe this intensity distribution something like sin square

beta by beta square, you have a probability distribution, where it will land up I cannot say I can only predict a probability distribution. So, physics has ceased to be deterministic you can only predict the probability of the arrival of the electron or the proton in a certain region of space.

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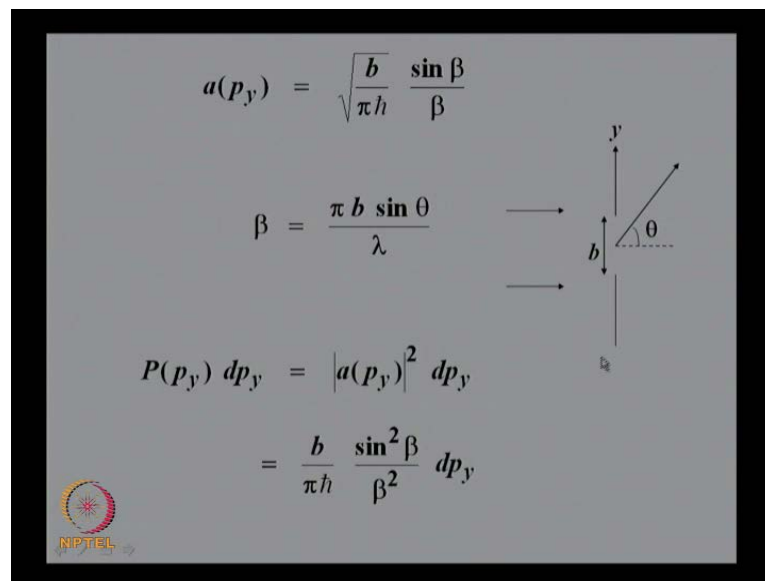
So, let me consider another simple problem related problem that instead of a single slit I have two slits. So, let us suppose each slit is of width b and then this is $d/2$ and this is minus $d/2$ and the width is width is b . So, I am sorry. So, the distance between the slit is d let me let me do this again let me do this again I have two slits, one here and one here (Refer Slide Time: 08:26), the distance between the two slits is d , so this distance is minus $d/2$ by this is $d/2$, this is $d/2$ and this is also $d/2$.

So, this is my y axis and if I assume the origin to be here, so for the first slit the integral will be from minus $d/2$ minus $b/2$ to minus $d/2$ plus $b/2$; and for this slit, it will be plus $d/2$ minus $b/2$ and then $d/2$ plus $b/2$; and we have this integral e to the power of i by h cross $p_y y$ and e to the power of i by h cross $p_y y$ multiplied by dy multiplied by dy .

If I carry out this integration and do a little bit of simplification then you will obtain $\sin \beta$ by β multiplied by $\cos \gamma$, where this is the square of this \sin square β by β square is the diffraction pattern and \cos square γ it is a very simple integration just very similar to what we had done for this single slit diffraction pattern.

So, this term is proportional to is this describe this single slit diffraction pattern and this is the two point interference pattern. So, the probability distribution on this will be something like this (Refer Slide Time: 10:33), this is the two slit interference pattern that you will observe, where will be electron land up you cannot predict you can predict a probability distribution. And so, therefore, if the experiment was carried out with a large number of electrons you will observe the two slit interference pattern.

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$$a(p_y) = \sqrt{\frac{b}{\pi \hbar}} \frac{\sin \beta}{\beta}$$

$$\beta = \frac{\pi b \sin \theta}{\lambda}$$

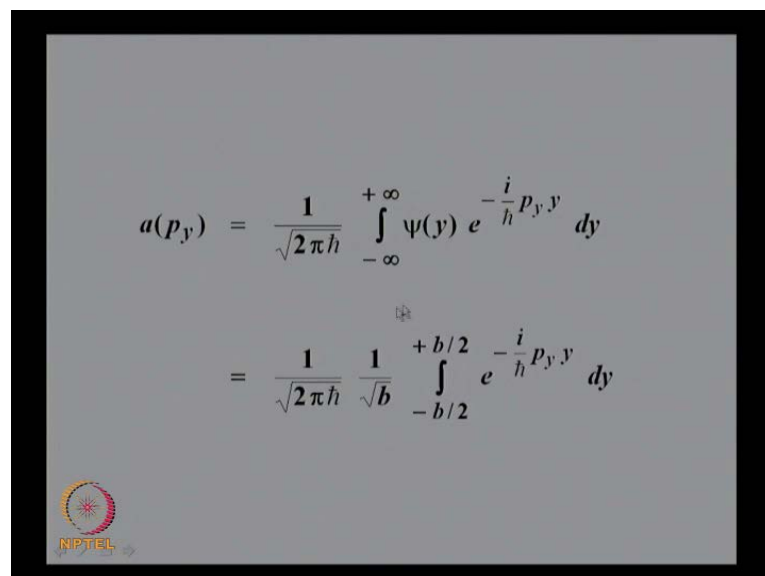
$$P(p_y) dp_y = |a(p_y)|^2 dp_y$$

$$= \frac{b}{\pi \hbar} \frac{\sin^2 \beta}{\beta^2} dp_y$$

The diagram shows a vertical slit of width b on a coordinate system with a vertical y -axis. A ray is shown passing through the slit at an angle θ to the horizontal.

So, let me go back to the slides.

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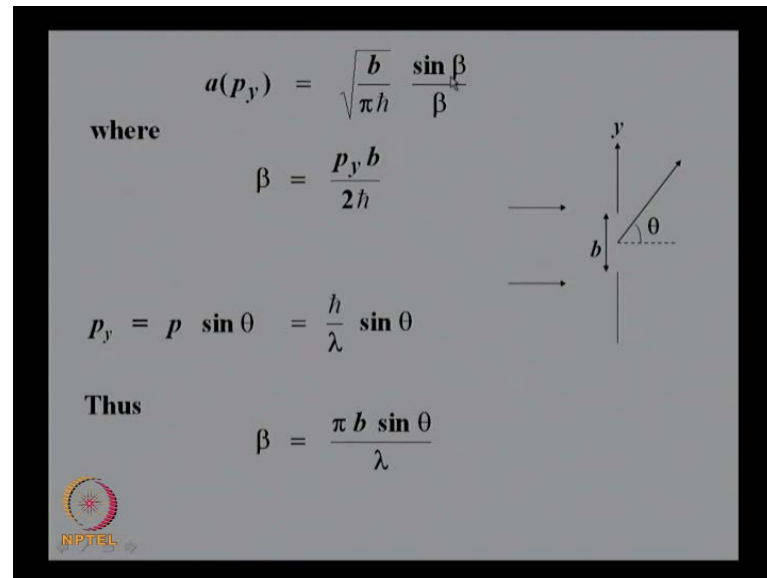
$$a(p_y) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \psi(y) e^{-\frac{i}{\hbar} p_y y} dy$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{\sqrt{b}} \int_{-b/2}^{+b/2} e^{-\frac{i}{\hbar} p_y y} dy$$

The diagram shows a coordinate system with a vertical y -axis and a horizontal axis. A slit of width b is indicated between $-b/2$ and $+b/2$ on the y -axis.

So, I first consider the single slit diffraction pattern and psi of y was non 0 from y equal to minus b by 2 to plus b by 2, where its value is 1 over root b. So, I integrate this and which I did that in detail.

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where

$$a(p_y) = \sqrt{\frac{b}{\pi h}} \frac{\sin \beta}{\beta}$$

$$\beta = \frac{p_y b}{2h}$$

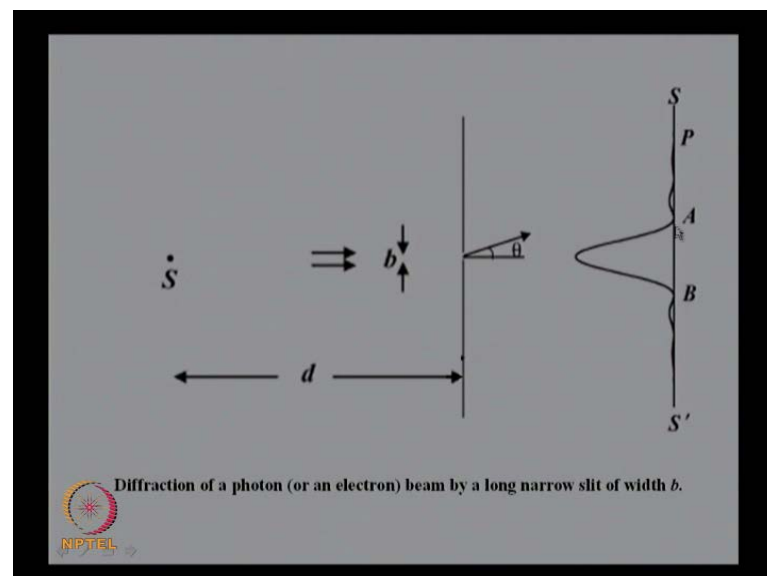
$$p_y = p \sin \theta = \frac{h}{\lambda} \sin \theta$$

Thus

$$\beta = \frac{\pi b \sin \theta}{\lambda}$$

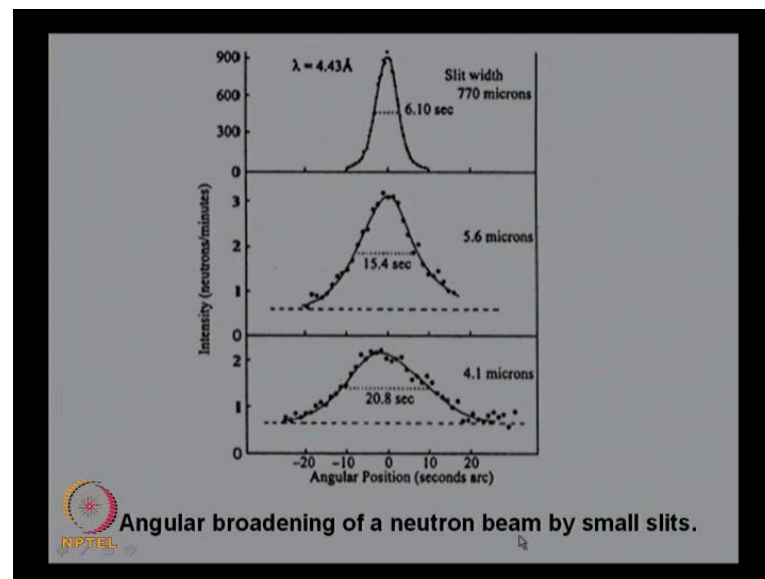
And I obtain sin beta by beta, where beta is equal to p y b by 2 h cross, h cross is equal to h by pi, so you will obtain pi b sin theta by lambda. So, this results therefore, the probability of the momentum lying between p y and p y plus d p y will be equal to a p y square d p y, which is equal to sin square beta by beta square.

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So, this is the diffraction of the electron and this is the probability distribution.

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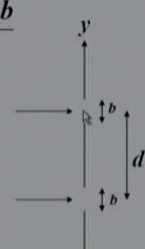



And this is the angular broadening of a neutron. So, as I mentioned that, if whether you have any neutron or proton or electrons, it will exhibit the same diffraction pattern. And each particle has a very well as I had mentioned in the very first lecture has a very well defined charge, very well defined magnetic moment, very well defined mass.

So, on the back of your mind you think that, it is a particle, but then each **it it it** it demonstrates the give rise to the diffraction pattern and I will just now I mention to the interference pattern. So, therefore, this is the diffraction pattern angular broadening of a neutron beam by small slits, that smaller the width of the slit greater will be the diffraction pattern and that is consistent with the uncertainty principle (Refer Slide Time: 12:51).

(Refer Slide time: 13:07)

Example 3 Double Slit Diffraction Pattern

$$\Psi_b(y) = \begin{cases} \sqrt{\frac{1}{2b}} & \frac{d-b}{2} < |y| < \frac{d+b}{2} \\ 0 & \text{elsewhere} \end{cases}$$



$$a(p_y) = \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{\sqrt{2b}} \left[\int_{-\frac{d}{2} - \frac{b}{2}}^{-\frac{d}{2} + \frac{b}{2}} + \int_{\frac{d}{2} - \frac{b}{2}}^{\frac{d}{2} + \frac{b}{2}} \right] e^{\frac{i}{\hbar} p_y y} dy$$


So then, we consider the double slit diffraction pattern. So, you have each slit is of width b and the distance between the center of the slit here and the center of the slit here is d . So, I assume Ψ_b of y is equal to $1/\sqrt{2b}$ under root, which is equal to from in this region and in this region (Refer Slide Time: 13:36). So then, the corresponding momentum distribution function will be the fourier transform of this (Refer Slide Time: 13:48). So, $1/\sqrt{2b}$ I take outside, so this region this integration is from in this region minus $d/2$ minus $b/2$ to minus $d/2$ to plus $d/2$ and then from here to here. It is a very straightforward integration.

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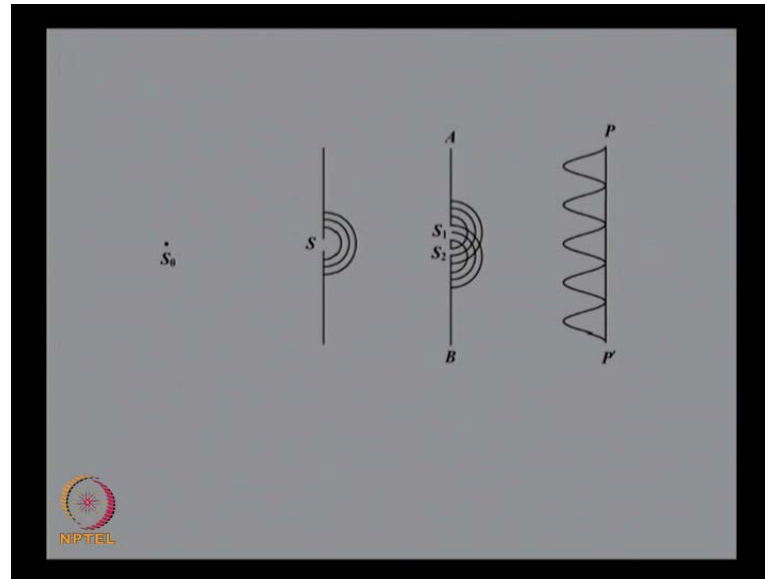
$$|a(p_y)|^2 dp_y = \underbrace{\left[\frac{b}{\pi\hbar} \frac{\sin^2 \beta}{\beta^2} \right]}_{\text{Single Slit Diffraction Pattern}} \underbrace{\left[4 \cos^2 \gamma \right]}_{\text{2 point interference pattern}} dp_y$$

$$\beta = \frac{p_y b}{2\hbar} = \frac{\pi b \sin \theta}{\lambda}$$

$$\gamma = \frac{p_y d}{2\hbar} = \frac{\pi d \sin \theta}{\lambda}$$


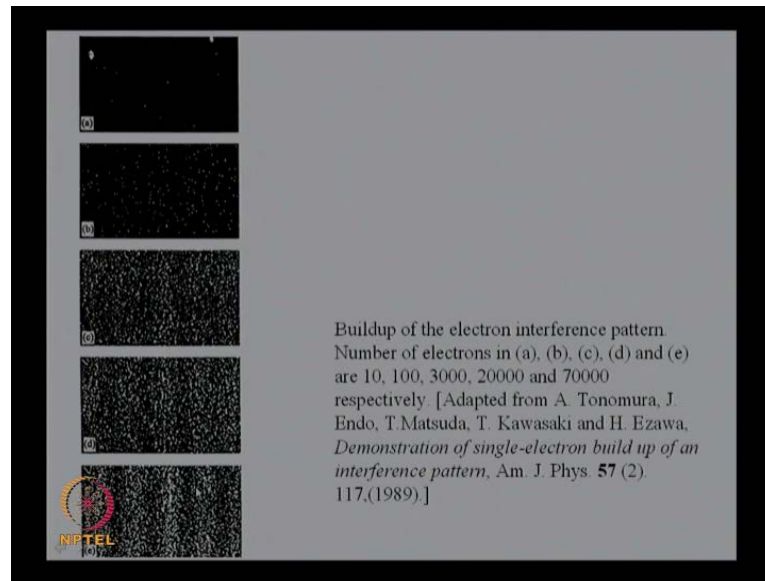
If you carry that out you will get and **and** square that the probability of the y component in the momentum lying between p_y and $p_y + dp_y$ is the product of the single slit diffraction pattern and 2 point interference pattern, where β is equal to $\pi b \sin \theta$ by λ and this is the interference pattern produced by 2 point sources separated by a distance d .

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So, therefore, the electron or the proton or the neutron is described by a wave function which is here and as well as here, it passes through both the slits simultaneously does it go through hole number 1 or hole number 2 it goes through both the holes and it interferes with itself. So, it is described by a wave function which is present here and here and it produces an interference pattern a probability distribution, which looks like this (Refer Slide Time: 15:14). And it is this probability distribution **that the quantum** that quantum mechanics predicts.

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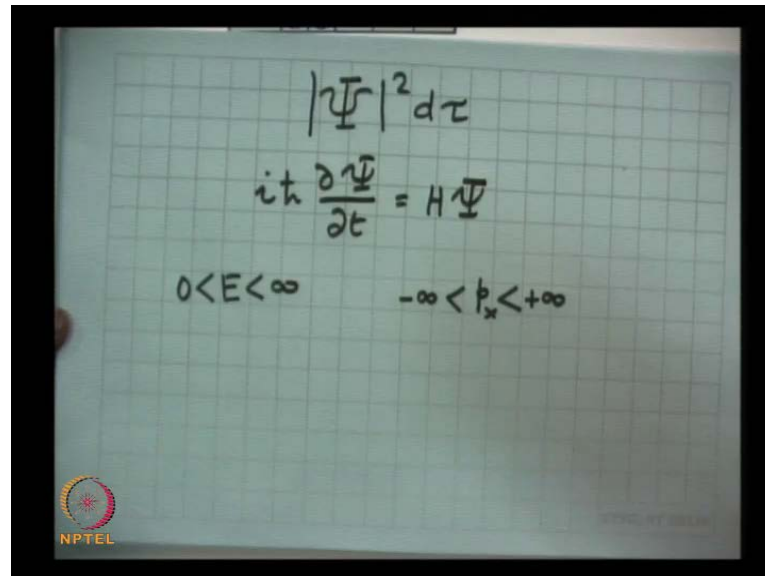
So, here is one of the very beautiful experiment that I had discussed some time back that, if you do the double slit interference pattern in a experiment with 10 electron then, where will the individual electron will land up? You cannot predict, you can only predict a probability distribution.

And, so they will have appear at random on the screen. The last photograph corresponds to 70000 electrons and then, slowly the interference pattern the fringes appear. So, each as you can see from each of the figure, the photograph electron is detected only as a total electron never half of an electron, so you detect either 1 full electron or nothing. So, each spot here corresponds to the detection of a single electron which has a certain amount of charge certain amount of mass and so on. Where will it land up is given by a probability distribution and **when they** when you have a large number of electrons, then slowly the interference pattern.

So, in the classical interference experiment, the intensity will become fainter and fainter, but the interference pattern will appear in the form of dark and bright fringes, but the **grain the** graininess of the arrival of the electron is demonstrated in this slide and which is a very important aspect of quantum mechanics, that you always detect the whole electron or the whole proton or the whole neutron never a fraction of that; but, there is a probability where will it land up one cannot predict, but one can predict accurately the

probability distribution. And therefore, the electron or the proton or the neutron is described.

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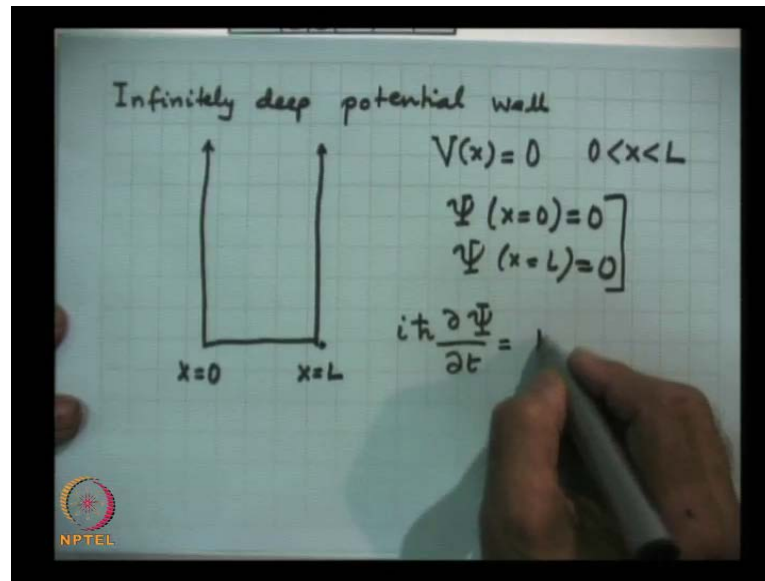
The image shows a piece of graph paper with handwritten mathematical expressions. At the top, the expression $|\Psi|^2 d\tau$ is written. Below it is the Schrödinger equation $i\hbar \frac{\partial \Psi}{\partial t} = H\Psi$. At the bottom, two inequalities are written: $0 < E < \infty$ on the left and $-\infty < p_x < +\infty$ on the right. In the bottom left corner, there is a small circular logo with the text 'NPTEL' underneath it.

So, what is an electron, what is a proton I do not know, but I can only say that, it is described by the wave function ψ , so that $\text{mod } \psi^2 d\tau$ represents the probability of the finding in the volume element $d\tau$. And what is ψ ? ψ is the solution of the schrodinger equation. So, **the** what is ψ , ψ is the solution of the schrodinger equation $H\psi$. So, that completes the free particle problem.

Now, in the free particle problem we had found that, the energy takes the energy of the particle takes a continuum of values from 0 to infinity the x component of the momentum takes a continuum of values from minus infinity to plus infinity; and e is equal to p^2 by $2m$. So, p takes all possible values from minus infinity to plus infinity and the energy of the particle can take any value between 0 and infinity.

Now, what I would like to do next is, consider all the schrodinger equation when the particle is confined in a box in a one dimensional box; and we say that, it is in an infinitely deep potential well.

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So, I have an infinitely deep potential well. So, which I described this that as if the particle is inside in the very deep potential well and **let** let me choose this as the point origin x is equal to 0 and this as x is equal to 1 and the particle is localized somewhere here and between x is equal to 0 and x is equal to 1, the particle is free.

So that, V of x is equal to 0 for x less than 0 less than 1, x lying between; and at the boundary, there is an infinite jump in the potential. And so, therefore, the electron or the proton cannot go outside the well. So, therefore, the wave function for all points greater than 1 and less than 0 should be 0. So, my boundary conditions are that the wave function should be 0 at x is equal to 0 must be 0, at x is equal to 1 must be 0, so these are known as the boundary conditions of the problem (Refer Slide Time: 21:10).

So, the particle I consider the particle in a one dimensional box of length l . So, once again I start with the time dependant one dimensional schrodinger equation, $i \hbar \frac{\partial \psi}{\partial t}$ is equal to $H \psi$ where H is equal to. So, let me write it again. So, $i \hbar \frac{\partial \psi}{\partial t}$ is equal to $H \psi$, where H is equal to. So, let me write it again.

(Refer Slide time: 21:48)

The image shows a handwritten derivation on a grid background. The equations are as follows:

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi = \left[-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi \right]$$

$$\Psi(x, t) = \psi(x) T(t)$$

$$i\hbar \psi(x) \frac{dT}{dt} = T(t) \left[-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V(x)\psi(x) \right]$$

$$\div \psi T$$

$$\underbrace{\frac{i\hbar}{T(t)} \frac{dT}{dt}} = \underbrace{\frac{1}{\psi} \left[-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V(x)\psi(x) \right]} = E$$

An NPTEL logo is visible in the bottom left corner of the slide.

So, $i\hbar \frac{\partial \Psi}{\partial t}$ is equal to $H\Psi$ and H is equal to $-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi$. So, I want to solve this equation. I have just completed the solution of the equation, when $V(x)$ is 0 everywhere that is known as the free particle solution and I obtained the most general solution describing a wave packet.

Now, whenever the potential energy function is time independent I can write the solution as $\Psi(x, t) = \psi(x) T(t)$ just as we did in the free particle case. So, this term will become $i\hbar \psi(x) \frac{dT}{dt}$, because this function depends, this is known as the method of separation of variables. And this term becomes $\psi(x) \left[-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V(x)\psi(x) \right]$, so $T(t)$ I take outside $T(t)$ and becomes $-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V(x)\psi(x) = E$.

Next the variables have still not separated out, because the left hand side contains x and time and the right hand side **time** also contains time and x . What I do is, I divide by ψT , so I get $i\hbar \frac{1}{T(t)} \frac{dT}{dt} = \frac{1}{\psi} \left[-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V(x)\psi(x) \right] = E$. Now, the variables have separated out, the left hand side is a function of time only. The right hand side is a function of space only.

So, therefore, both sides must be equal to a constant, it cannot be a function of x , it cannot be a function of time, it has to be a constant because, the left hand side is a function of time, the right hand side is a function of x . Hence, both sides must be equal to a constant. We say that, the method of separation of variables has worked and so, therefore, each side is set equal to a constant. Now, the integration is trivial.

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$$\frac{i\hbar}{T(t)} \frac{dT}{dt} = E \Rightarrow \frac{1}{T} \frac{dT}{dt} = \frac{iE}{\hbar}$$

$$\ln T(t) = -\frac{iEt}{\hbar} + \dots$$

$$T(t) = e^{-\frac{iEt}{\hbar}}$$

$$+\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x) \psi(x) = E \psi(x)$$

$$\boxed{\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)] \psi(x) = 0} \quad \text{TISE}$$

So, let me write down the the time dependant part. So, I get $i\hbar$ cross T of t dT by dt is equal to E , so this gives me that $1/T$ dT by dt is equal to e to the power of $-iEt/\hbar$ minus iEt/\hbar plus a constant. So, therefore, the integral of this equation is T of t , this is $\ln T$, so if I integrate this you get $\ln T$ is equal to $-iEt/\hbar$ plus a constant. So, T of t is equal to constant times e to the power of $-iEt/\hbar$. So, this is the solution of the time independent part time dependant part.

And the solution of the time space dependant part will be this is very simple you can write down if I take ψ on this side, so you get $-\hbar^2/2m$ $d^2\psi$ by dx^2 plus $V(x) \psi(x)$ is equal to $E \psi(x)$. And therefore, if I take if I put a plus sign here and a minus sign here and minus sign here and bring this to this side, so you get $d^2\psi$ by dx^2 plus $2m/\hbar^2$ $[E - V(x)] \psi(x)$ is equal to 0, this is known as the time independent schrodinger equation (Refer Slide Time: 27:50).

The time dependant part is so much (Refer Slide Time: 27:59). So, therefore, the total solution, so we must solve this equation for a given form of V of x we must solve this equation and for the next 2 3 lectures we will assume different forms of V of x and we will solve this time independent schrodinger equation and the time dependant part will be given by this.

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$$\Psi(x,t) = \psi(x) e^{-iEt/\hbar}$$

$$\frac{d^2 \psi}{dx^2} + \frac{2\mu}{\hbar^2} [E - V(x)] \psi(x) = 0$$

Ex 2 $V(x) = 0$ everywhere

Ex 2

$\psi(0) = 0 ; \psi(x=L) = 0$

$0 < x < L$ $\frac{d^2 \psi}{dx^2} + k^2 \psi = 0$

$k^2 = \frac{2\mu E}{\hbar^2}$

So, that **the total solution** the total solution ψ of x comma t will be equal to ψ of x e to the power of minus $i E t$ by \hbar cross. First, we will find out ψ of x and also try to find out what are the allowed values of V , allowed values of E and then, try to obtain the general solution the most general solution of the schrodinger equation.

So, till now our analysis is valid that is we, what is ψ of x ? ψ of x is satisfies this equation, $d^2 \psi$ by $d x$ square plus 2 let me replace m by μ , because for reasons that will become clear in a moment. So, the mass of a particle is represented by μ 2 μ h cross square E minus V of x ψ of x is equal to 0, this is a general equation. The only assumption is that, the potential energy function is independent of time.

So, let me solve the first example actually this is the second example. The first example was the free particle problem the first example that we had solved was V of x equal to 0 everywhere, this was the free particle problem that we had solved in great detail. The second problem that we are going to solve is **sorry sorry**, so the second problem is that we will solve is the particle in a one dimensional box.

So, we have we consider a box like this, which is 0 here and 1 here and so the wave function psi the wave function has to vanish here, because the particle cannot escape. So, psi at x is equal to 0 is equal to 0 and psi at x is equal to 1 is also 0.

So, let me try to solve this equation between 0 less than x less than 1, V of x is 0, so the schrodinger equation becomes $\frac{d^2 \psi}{dx^2} + k^2 \psi = 0$, where k^2 is defined to be equal to $2 \mu E$, μ is the mass of the particle, E is the energy of the particle and h cross is of course, the planck's constant divided by 2π .

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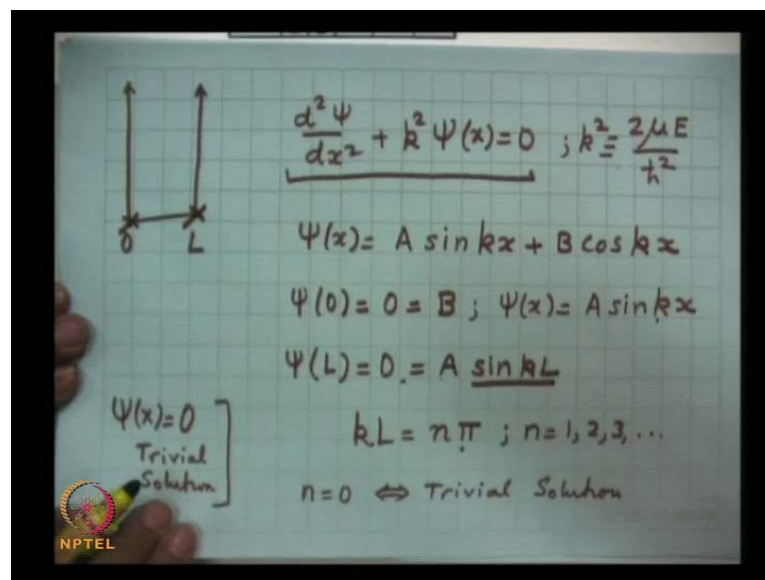


Diagram of a box from 0 to L.

$$\frac{d^2 \psi}{dx^2} + k^2 \psi(x) = 0 ; k^2 = \frac{2 \mu E}{\hbar^2}$$

$$\psi(x) = A \sin kx + B \cos kx$$

$$\psi(0) = 0 = B ; \psi(x) = A \sin kx$$

$$\psi(L) = 0 = A \sin kL$$

$$kL = n\pi ; n = 1, 2, 3, \dots$$

$$n = 0 \Leftrightarrow \text{Trivial Solution}$$

$\psi(x) = 0$ Trivial Solution

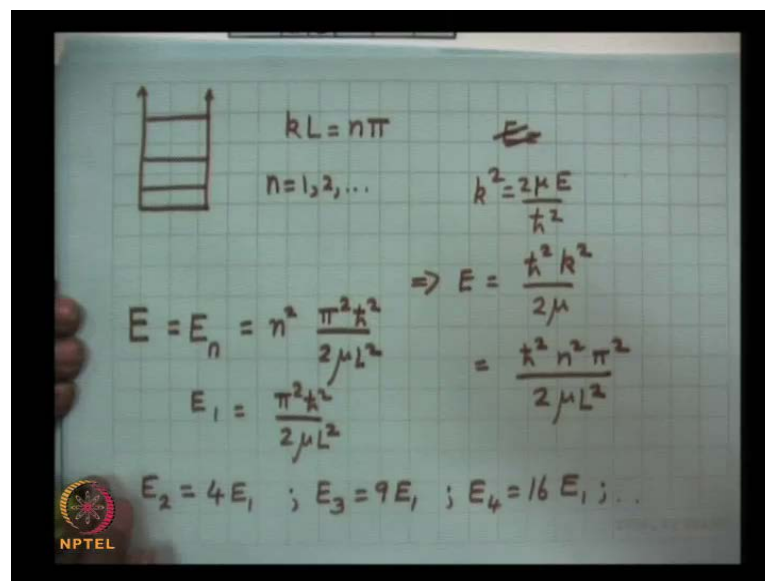
So, I write down this equation that in the region I have this particle in a one dimensional box particle in a one dimensional box between 0 and 1, the the schrodinger equation becomes $\frac{d^2 \psi}{dx^2} + k^2 \psi = 0$, where k^2 is defined to be equal to $2 \mu E$ when I write 3 signs here; that means, defined to be equal to 2μ by h cross square (Refer Slide Time: 32:10).

The solution of this equation is very simple as you all know that, psi of x is equal to $A \sin kx + B \cos kx$. Now, the wave function has to vanish at x is equal to 0, because the particle cannot tunnel can cannot go outside the well. So, psi of 0 at x is equal to 0, sin of 0 is 0, cos of 0 is 1, so psi of 0 is 0 and that must be equal to B, so B is 0. So, the the quantity B is 0, so this solution of my schrodinger equation is equal to $A \sin kx$.

Then I apply the second boundary condition, that ψ at x is equal to L is equal to 0. So, B is already 0. So, this will be $A \sin kL$. Now it has two possible solution, either A is 0 if A is 0 then, ψ of x is 0 everywhere that is known as the trivial solution, it does not correspond to any physical situation **the wave function**, if the wave function ψ of x is 0 everywhere any value of E is possible. So, there is no particle anywhere. So, that solution ψ of x equal to 0 everywhere, this is known as the trivial solution and which we will neglect.

The other thing that can happen is $\sin kL$ is equal to 0 that is kL is equal to $n\pi$, where n is equal to 1 2 3 4 I have excluded the value n equal to 0, because if k is 0 then again then **then** if k is 0 then ψ of x is 0. So, that is again the trivial solution. So, n equal to 0 corresponds to again to the trivial solution. So, we obtain that, **the** if the wave function has to vanish at x is equal to 0 and at x is equal to L , then kL must be equal to $n\pi$.

(Refer Slide time: 35:27)



Handwritten notes on a grid background showing the derivation of energy levels for a particle in a 1D infinite potential well. The notes include a diagram of the well, the boundary condition $kL = n\pi$, and the derivation of the energy formula $E_n = \frac{n^2 \pi^2 \hbar^2}{2\mu L^2}$. It also shows the first few energy levels: E_1 , $E_2 = 4E_1$, $E_3 = 9E_1$, $E_4 = 16E_1$.

So, we have found that for the wave function to vanish at x is equal to 0 and at x is equal to L , kL must be a multiple of π , where n is 1 2 3 and **since E is equal to E is equal to I am sorry** since k^2 is equal to $2\mu E$ by \hbar^2 cross square. So, therefore, E is equal to \hbar^2 cross square k^2 by 2μ , k is equal to $n\pi$ by L . So, this is equal to \hbar^2 cross square $n^2 \pi^2$ by $2\mu L^2$.

So, this becomes where n can take only discrete values n is equal to 1 2 3. So, therefore, the energy E of the particle can take only discrete values and that is E can take only a set

of values E_n , which is equal to n^2 times this constant, $\pi^2 \hbar^2 / 2mL^2$. When n is 1, so this becomes E_1 is equal to $\pi^2 \hbar^2 / 2mL^2$. So, you will have E_2 is equal to 4 times E_1 , E_3 is 9 times E_1 , E_4 is equal to 16 times E_1 and so on. So, the particle can take discrete energy levels, this is a quite a difference from classical mechanics, where a particle can take a continuum of energy values. So, you have a particle in a box can take only a set of discrete energy levels.

(Refer Slide time: 38:16)

$$kL = n\pi \Rightarrow k = k_n = \frac{n\pi}{L}$$

$$\Psi(x) = A \sin kx = A \sin\left(\frac{n\pi}{L}x\right)$$

$\sin \frac{\pi}{L}x$
 $\sin \frac{2\pi}{L}x$

$4E_1$
 E_1

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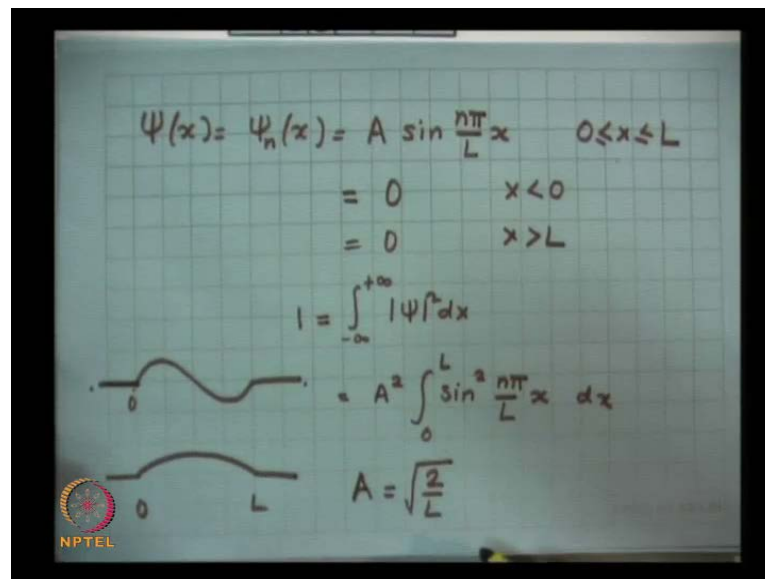
And we had shown that, the kL must be equal to $n\pi$, where n is 1 2 3 therefore, this tells us that k also can take discrete it has to take discrete values is equal to $n\pi$ by L ; so, these are the discrete values the values that k can take. The wave function ψ of x we had shown that this was equal to $A \sin kx$.

So, this will be equal to $A \sin$ of $n\pi$ by L into x . So, **you will have** you will have let us suppose this is my box in which the particle is confined and you have the ground state, this is ground state which has the value of E_1 and it has a wave function n is 1, so this will be sine of π by L into x . So, at x is equal to 0, it becomes like this and x become like this and beyond this it is 0 and beyond this it is 0, this is known as the ground state wave function (Refer Slide Time 39:45).

The second state is 4 times E_1 , so this will be sine of **2π by L** by 2π by L x . So, at x is equal to L by 2, it becomes 0, so it will be something like this (Refer Slide Time: 40:07).

And the third wave function will be something. So, it is the first wave function is symmetric about the point x is equal to L by 2, the second wave function is anti symmetric with respect to at x is equal to L by 2, the third function is symmetric; they will be since the potential as I will tell you later that, since the potential energy function is symmetric about the point x is equal to L by 2 x is equal to L by 2. So, therefore, therefore the wave functions are either symmetric or anti symmetric with respect to the point x is equal to L by 2.

(Refer Slide time: 41:10)



$$\psi(x) = \psi_n(x) = A \sin \frac{n\pi}{L} x \quad 0 \leq x \leq L$$

$$= 0 \quad x < 0$$

$$= 0 \quad x > L$$

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

$$= A^2 \int_0^L \sin^2 \frac{n\pi}{L} x dx$$

$$A = \sqrt{\frac{2}{L}}$$

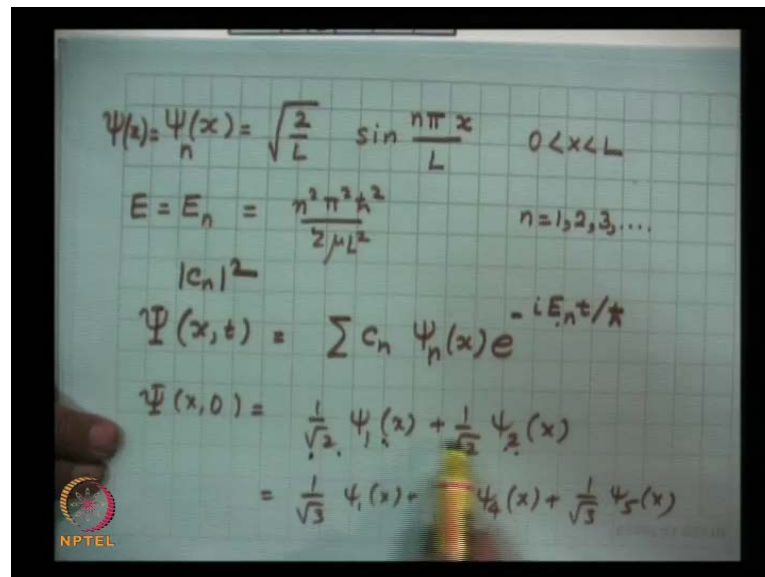
So, my wave function is something like this. So, I will have I will have the wave function, which is ψ of x I write this as, ψ_n of x which is equal to $A \sin$ of n of n pi by L into x between 0 less than equal to x less than equal to L . Let us suppose, I normalize this wave and 0 everywhere else, 0 for x less than 0 and 0 for x greater than L .

So, you will have for example, for the second state it will start from 0, this is the x equal to 0 part and then you will have like this (Refer Slide Time: 41:50), and then it will go like this (Refer Slide Time: 41:52), the first wave function will be something like this (Refer Slide Time: 41:59). So, this 0 and this is the point x is equal to L , this is the point x is equal to 0 and so on for the higher order wave functions I will so, therefore, we have solved the problem completely.

And, if I now normalize this wave function that is minus infinity to plus infinity mod ψ square dx , if I put equal to 1 then, the wave function is 0 for x greater than L and less

than 0. So, therefore, this will be equal to A square from 0 to L sin square n pi by L into x d x, you can easily integrate this equation. And if you work this out I leave this as a very small exercise, it come out to be 2 by L. So, this is known as the normalization constant.

(Refer Slide time: 43:23)



Handwritten equations on a grid background:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \quad 0 < x < L$$

$$E = E_n = \frac{n^2 \pi^2 \hbar^2}{2\mu L^2} \quad n=1, 2, 3, \dots$$

$$|c_n|^2$$

$$\Psi(x, t) = \sum c_n \psi_n(x) e^{-iE_n t / \hbar}$$

$$\Psi(x, 0) = \frac{1}{\sqrt{2}} \psi_1(x) + \frac{1}{\sqrt{2}} \psi_2(x)$$

$$= \frac{1}{\sqrt{3}} \psi_1(x) + \frac{1}{\sqrt{4}} \psi_4(x) + \frac{1}{\sqrt{5}} \psi_5(x)$$

NPTEL logo is visible in the bottom left corner of the grid.

And so, therefore, for the particle in a box problem, psi of x is equal to under root of 2 by L sin of n pi x by L, actually you should write this as **you should write this as** psi of x is equal to psi n of x, these are the discrete wave functions **these are the discrete wave functions** corresponding to the particle in a box problem for 0 less than x less than L; and the corresponding eigen values are E is equal to E n is equal to n square pi square h cross square by 2 mu L square and in both cases n takes the value 1 2 3 etcetera.

You must remember that, the wave function was psi n of x the the total wave function was equal to psi n of x e to the power of minus i E n t by h cross. Now, the most general solution of the time dependent schrodinger equation will be a sum of this, will be the linear combination C n, psi n of x e to the power of, where E n is given by this (Refer Slide Time: 45:03), and psi n is given by this (Refer Slide Time: 45:05).


This superposition of different states is a characteristic of quantum mechanics particle therefore, let us suppose you superpose only two states. So, at t equal to 0 let us suppose at t equal to 0 you can have 1 one over root 2 psi 1 x plus 1 over root 2 psi 2 of x that means, there is a half probability of finding it in the first state and the half probability of

finding in the second state you can also have something like this $\frac{1}{\sqrt{3}}$ ψ_1 plus $\frac{1}{\sqrt{3}}$ ψ_4 plus $\frac{1}{\sqrt{3}}$ ψ_5 of x , they need not be all equal, mod C 1 square as I will explain as I will try to show tell you we will represent the probability of finding the particle in the n -th state.

So, therefore, if you make a measurement will you obtain E_1 or E_2 , if this if the particle is in this state, there is a half probability of obtaining E_1 and half probability of obtaining E_2 . So, the energy is not known exactly, it is in a superposed state. So, let me show you a slide.

(Refer Slide time: 47:08)

Example 4: Particle in a 1-dimensional box




$$V(x) = 0 \quad \text{for } 0 < x < a$$

$$= \infty \quad \text{for } x < 0 \text{ and for } x > a$$

$$\Rightarrow \psi(0) = \psi(a) = 0$$


$$0 < x < a: \quad \frac{d^2\psi}{dx^2} + k^2\psi(x) = 0; \quad k = \sqrt{\frac{2\mu E}{\hbar^2}}$$

$$\psi(x) = A \sin kx + B \cos kx$$


And so we consider actually this is example number 2, particle in a one dimensional box here, unfortunately instead of capital L I have done it as small a just $((a))$ with me. So, the potential energy function is 0 between x equal to 0 and x is equal to a and it has an infinite jump at x is equal to 0 and at x is equal to a , so that the probability of finding the particle outside the well is 0. And so, therefore, the wave function must vanish at x is equal to 0 and at x is equal to a .

So, in between this region the solution the schrodinger equation is given by $\frac{d^2\psi}{dx^2} + k^2\psi = 0$, because V of x is 0, so k^2 is equal to $\frac{2\mu E}{\hbar^2}$, where μ is the mass of the particle. So, the solution of this equation is ψ of x is equal to $A \sin kx + B \cos kx$. Now, I apply the condition that ψ of 0 is equal to 0.

(Refer Slide time: 48:33)

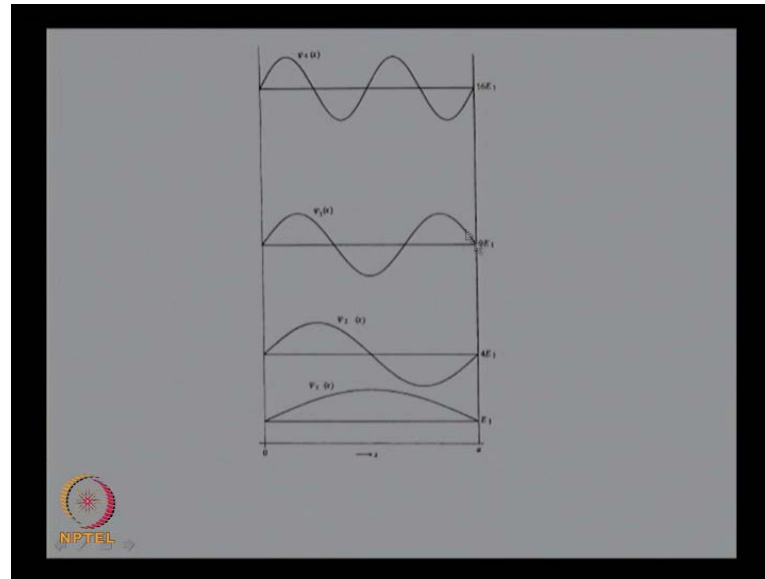
$$\begin{aligned}\psi(x) &= A \sin kx + B \cos kx; \quad k^2 = \frac{2\mu E}{\hbar^2} \\ \psi(0) &= 0 \Rightarrow 0 = B \\ \psi(x=a) &= 0 \Rightarrow A \sin ka = 0 \Rightarrow ka = n\pi \\ k^2 a^2 &= n^2 \pi^2 \Rightarrow E = E_n = \frac{n^2 \pi^2 \hbar^2}{2\mu a^2}; \quad n=1,2,\dots \\ \psi(x) &= \psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi}{a} x \quad 0 < x < a; \quad n=1,2,\dots \\ \int_0^a \psi_m^*(x) \psi_n(x) dx &= \delta_{mn}\end{aligned}$$


So, **if I** if I write x is equal to 0 then, that is 0, this quantity is 0, this is 1, so 0 is equal to B. So, therefore, **the this** this term goes out, because B is 0, so psi of x is equal to A sin kx. For the wave function to vanish at x is equal to a we will have A sin ka equal to 0 and therefore, ka must be equal to n pi, where n will take only the values 1 2 3 4 and 5 and 6 and so on, but not 0, because 0 will correspond to a trivial solution.

So, if I square this you get k square a square is equal to n square pi square. So, therefore, E is equal to h cross square k square by 2 mu, so the discrete energy levels of the problem will be equal to n square pi square h cross square by 2 mu a square; and the corresponding normalized wave functions are $\sqrt{\frac{2}{a}} \sin \frac{n\pi}{a} x$ **sorry** this should be x, n pi x by a, there has to be an x here (Refer Slide Time: 50:03), $\sin \frac{n\pi}{a} x$ by a. These wave functions are orthogonal to each other I am **sorry** there should be also a dx here (Refer Slide Time :50:18).

So, **the so** they are normalized and they are orthogonal to the any other function, where delta mn is the kronecker delta function, where delta mn is 0, when m is not equal to n and is 1 when m is equal to n.

(Refer Slide time: 50:44)



So, these are the wave functions, this is the ground state energy for which you have the wave function psi 1 of x, this is the first excited state energy, this is the second excited state and this is the third excited state (Refer Slide Time: 50:46).

(Refer Slide time: 51:00)

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi(x,t) \quad (1)$$

For the particle in a box problem $\Psi(x,t) = \psi(x) \exp\left[-\frac{iEt}{\hbar}\right]$

The solution of the eigenvalue equation $H\psi(x) = E\psi(x)$ gives:

$$\psi(x) = \psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}; \quad E = E_n = \frac{n^2 \pi^2 \hbar^2}{2\mu a^2}; \quad n = 1, 2, 3, \dots$$

These the most general solution of Eq. (1) is

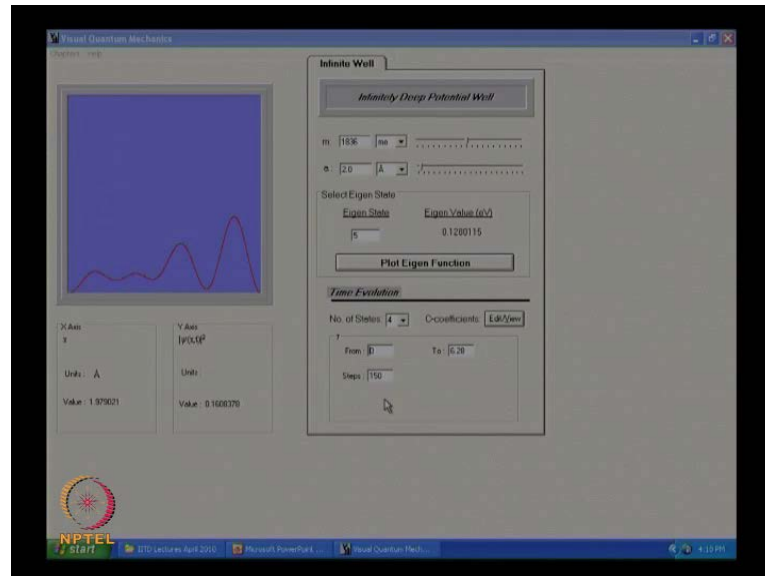
$$\Psi(x,t) = \sum_{n=1,2,3,\dots} c_n \psi_n(x) \exp\left[-\frac{iE_n t}{\hbar}\right]$$

$|c_n|^2$: represents the probability of finding the n^{th} state

So, we had started off by solving this equation this time dependant schrodinger equation and for the particle in a box problem we wrote down psi of x t is equal to psi of x e to the power of minus i E t by h cross. We obtain these are the eigen functions normalized eigen functions (Refer Slide Time: 51:24), and these are the energy eigen values (Refer

Slide Time: 51:30). So, therefore, the most general solution is **is** superposition of this and \sin^2 will represent the probability of finding the particle in the n -th state.

(Refer Slide time: 52:14)



So, let me let me show you the corresponding. So, let me consider the infinitely deep potential well problem and these are the eigen function. So, this is the x is equal to 0 and this is x is equal to L , in this particular program I have taken m is equal to 1836 times the mass of the electron that means it is a proton and A is 2 angstroms. So, this is the first eigen value, so much e V. The second eigen function I put here 2 it will have 1.0. If I put 3 then, it will have 2.0, this is symmetric about this about the point x is equal to A by 2 and then you take 4 in each wave function and this is anti symmetric.

So, about this, this is the mirror image (Refer Slide Time: 53:13), you may see that all the wave functions go to 0 at the boundaries, x is equal to 0 and at x is equal to L and then similarly, for **for** x is for 5 for the 5th it is they are alternately symmetric and anti symmetric.

Now, I superpose time wave, so let us suppose that the first **let me** let me take a simpler thing. So, let me take C_1 is equal to 1 and this I put 0 and C_2 is equal to 1 let me ok that, the coefficients are not normalized do you want the program to normalize them, the wave function has to remain normalized, so let say yes. So, I am superposing two wave functions and then, how will it evolve with time, this is the probability distribution function as it evolves with time (Refer Slide Time: 54:24).

Let me again repeat this let me write down C_1 is equal to 1 and C_2 is equal to 0. So, that only the first state is getting excited. How will it evolve with time? It does not change with time and therefore, each eigen state is known as a stationary state. If the particle is in a particular eigen state then, it will remain in that state for all times to come.

Let me superpose first 4 states, so it says C_1 is equal to 1, C_2 let me put C_1 is equal to 0 and then C_3 equal to 1. So, I have excited **I am** I am considering only the third state, the particle is in only in the third state, so ok it and then evolve. So, this is also a stationary state, it does not change with time. Finally, let me put just superpose the third and the fourth state. So, let me make this as 0.707 that is $1/\sqrt{2}$ and this also as $1/\sqrt{2}$ ok this and then evolve and this is the, this is how the probability distribution is changing with time (Refer Slide Time: 56:12).

So, initially it was like this and then it evolves like this from certain time to certain time. So, with today I have solved two problems two very important problems in quantum mechanics; the first problem is the free particle problem in which V of x is 0 everywhere, the energy forms a continuous values and so, therefore, the general solution was an integral and we studied the evolution of a wave packet.

The second problem that we studied just now was the particle in a box problem, in which the particle is confined within a box and we obtain discrete energy states and then, we studied the evolution of the wave function with time.