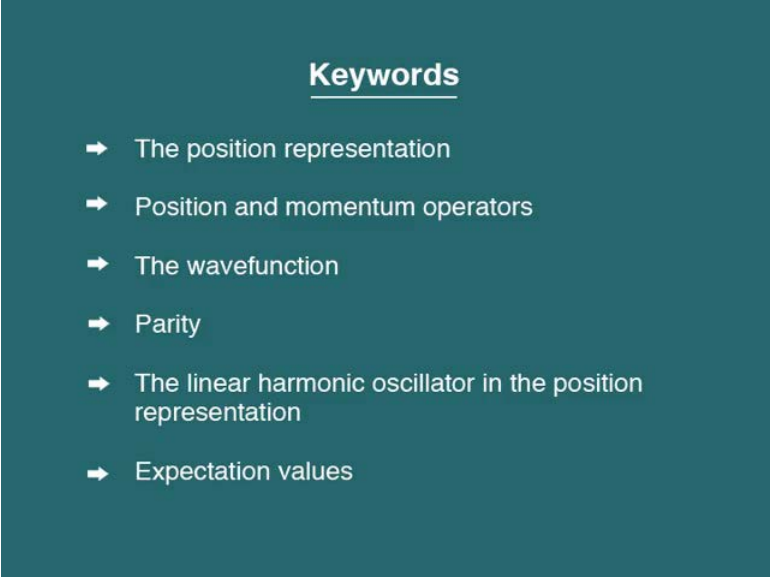


**Quantum Mechanics - I**  
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**Indian Institute of Technology, Madras**

**Lecture - 22**  
**Ingredients of Wave Mechanics**

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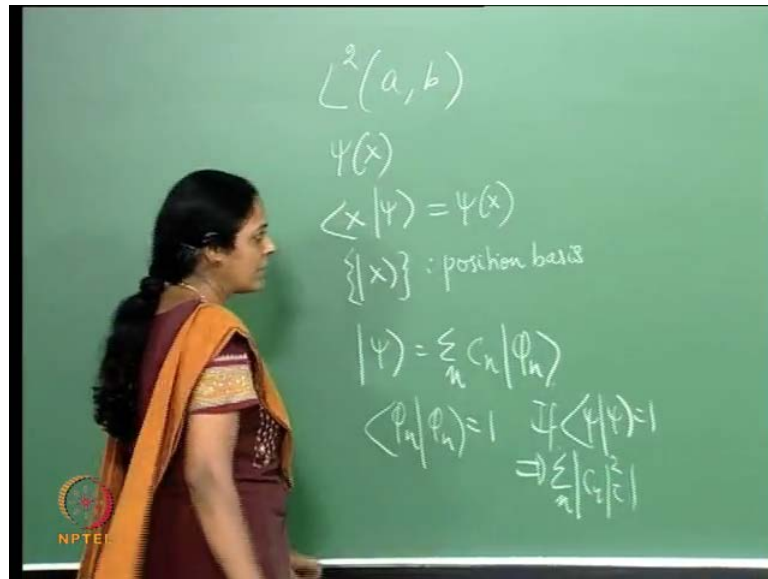


**Keywords**

- ➔ The position representation
- ➔ Position and momentum operators
- ➔ The wavefunction
- ➔ Parity
- ➔ The linear harmonic oscillator in the position representation
- ➔ Expectation values

In the last lecture, I discussed some salient features of  $L^2$ , the space of square integrable functions.

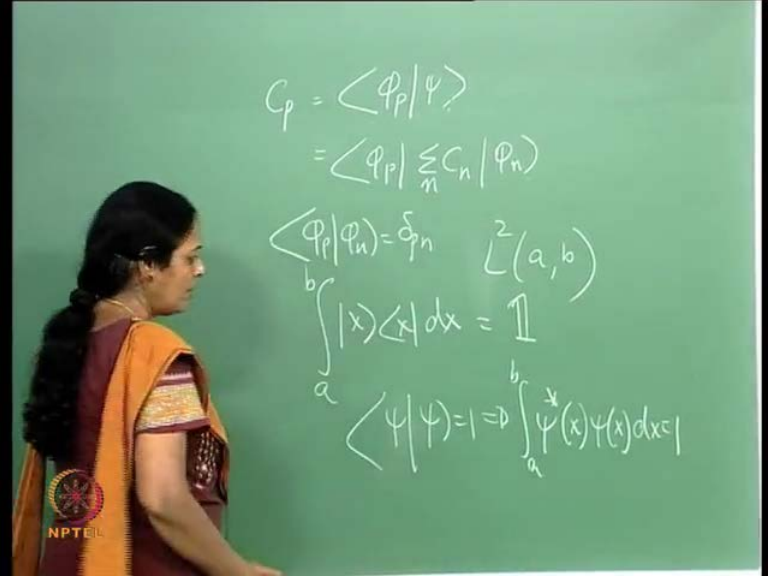
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So, that is  $L^2$  of  $a$  to  $b$  and this could be minus infinity and  $b$  could be infinity. Today, I will continue to look at square integrable functions and I will describe the concept, of the wave function. The wave function,  $\psi$  of  $X$ , introduced it last time as the state  $\psi$ , which is a ket residing in an abstract Hilbert space and  $X$  is a continuous basis set, could be the position basis. I use  $X$  for position and this object is  $\psi$  of  $X$ . So, let me quickly recapitulate how we got this.

You will recall that any ket  $\psi$  can be expanded, in terms of the basis states  $\phi_n$ , normalized basis states,  $\phi_n$ , with expansion coefficients  $c_n$ . And, if I normalize  $\psi$ , it automatically follows; that summation over  $n$  mod  $c_n$  squared is 1.

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$$C_p = \langle \phi_p | \psi \rangle$$

$$= \langle \phi_p | \sum_n C_n | \phi_n \rangle$$

$$\langle \phi_p | \phi_n \rangle = \delta_{pn} \quad L^2(a, b)$$

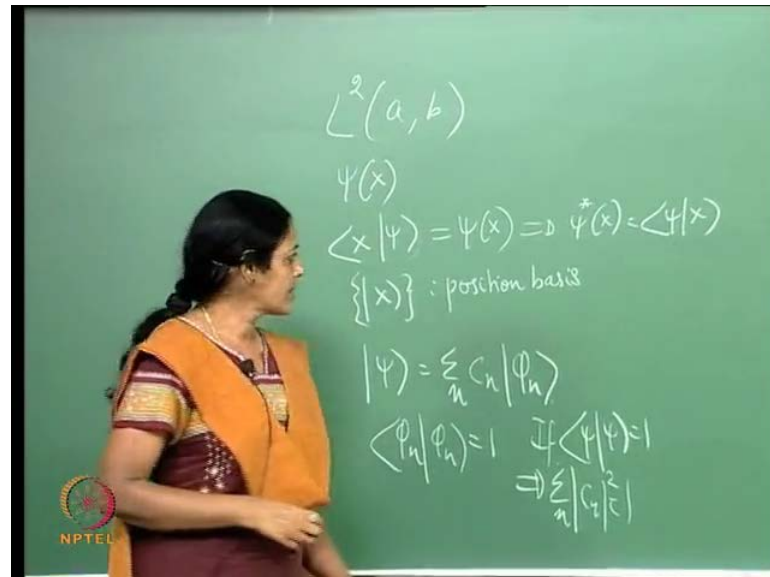
$$\int_a^b |x\rangle \langle x| dx = \mathbb{1}$$

$$\langle \psi | \psi \rangle = 1 \Rightarrow \int_a^b \psi^*(x) \psi(x) dx = 1$$

Equally true, that I get a particular coefficient  $C_p$ , as  $\phi_p$   $\psi$  inner product, because, this is like  $\phi_p$  summation over  $n$   $C_n \phi_n$ . If, I use the fact that,  $\phi_p$   $\phi_n$  inner product is  $\delta_{pn}$  and therefore, I get  $C_p$ . So, the coefficients along a certain basis are got by doing this. Take that ket which is being expanded in terms of the basis and the bra is really, that particular basis state, along which you need the coefficient. So, in that sense suppose,  $X$  is the basis set (Refer Slide Time: 00:17)  $X$  is the basis set and  $\psi$  is expanded in the position basis, this object inner product  $X$   $\psi$ , which is  $\psi$  of  $x$  which is a scalar and the analogue of  $C_{sub p}$ .

And therefore, this is simply an extension, of the definition that we had there, to a continuous basis and that is how we got  $\psi$  of  $x$  and because, the basis is a complete basis and a continuous basis. We have this over the range  $a$   $b$ . Remember we are talking of  $L^2$ , in the range  $a$   $b$  and therefore, this is the identity operator, can always introduce it wherever I want, in that sense I did this. Suppose, I have a state  $\psi$ , which is normalized to 1, I can well introduce this complete basis there, and that would amount to saying integral  $a$  to  $b$ ,  $\psi^*$  of  $x$ ,  $\psi$  of  $x$   $dx$  is 1, because, I have introduced a complete set of states.

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If psi of x is this it implies, that psi star of x is this object. The inner product of bra psi with ket x and therefore, I got that. Now, operators themselves have to be written in this basis, even as we did earlier for the two level atom. Where we had basis states and the operators were formed out of those basis states.

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Here 2 operators have to be written in this basis and therefore, the simplest operator that one can think of, is the identity operator times  $x$ .

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The image shows a green chalkboard with handwritten mathematical derivations. At the top, it states  $\hat{X} = 1x$ . Below this, it shows the identity operator as an integral:  $\int_{-\infty}^{\infty} dx' |x'\rangle \langle x'|$ . Then, it applies the operator  $\hat{X}$  to a position basis state  $|x\rangle$ :  $\hat{X}|x\rangle = x \int_{-\infty}^{\infty} dx' |x'\rangle \langle x'|x\rangle$ . The inner product  $\langle x'|x\rangle$  is identified as the Dirac delta function  $\delta(x'-x)$ . Finally, the result is simplified to  $x|x\rangle$ . An NPTEL logo is visible in the bottom left corner of the chalkboard image.

$$\hat{X} = 1x$$

$$\int_{-\infty}^{\infty} dx' |x'\rangle \langle x'|$$

$$\hat{X}|x\rangle = x \int_{-\infty}^{\infty} dx' |x'\rangle \langle x'|x\rangle$$


$$= x|x\rangle$$

$\delta(x'-x)$

So, let us see how this operator  $X$ , acts on the position basis. So, I am going to write this, as integral  $d x$  prime. Let me work in the range minus infinity infinity, this is the identity and then  $x$  is a variable, I can just pull that out. So, what happens, when, let us call this all the same, it is  $x$ . So, what happens when the operator acts on the position basis? There is this variable  $x$ ,  $d x$  prime and then I have, this object and that is a delta  $x$  prime minus  $x$ . So, the integration goes and I just have an  $x x$ . So, this is what I have. The operator  $X$  acts on the position basis, to pull out the number  $x$ .

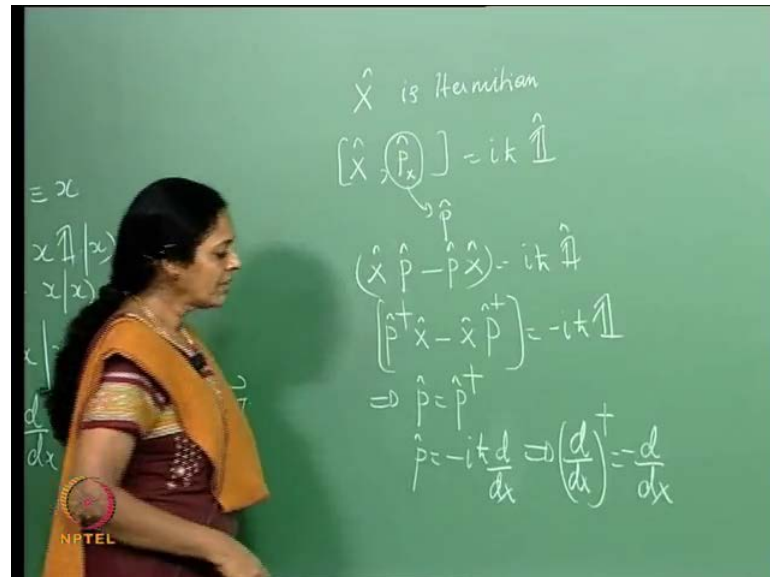
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Simplest op  
 $\hat{X} \rightarrow \hat{X} \equiv x$   
 $\hat{X}|x\rangle = x|1|x\rangle = x|x\rangle$   
 $\hat{X}|x\rangle = x|x\rangle$   
 $\hat{p} = -i\hbar \frac{d}{dx}$  In gen  $\hat{p} = -i\hbar \vec{\nabla}$



And what does it do? Because, it is the identity operator, when it acts on the basis set  $x$ , it simply pulls out the number  $x$  and that is the same as  $x x$ . So, this object is my position operator, I would simply say that the position operator is represented by  $x$ . So, I have  $x x$ , pulls out the Eigen value  $x$  and this is your Eigen value equation. Of course, the momentum operator  $p$ , was minus  $i \hbar$  cross  $d$  by  $d x$ , we are looking at one dimensions, the  $x$  axis. And in general, the operator  $p$  which is also a vector under, rotations in space is minus  $i \hbar$  cross  $\text{del}$ . And this is where we, this is a point we got up to last time.

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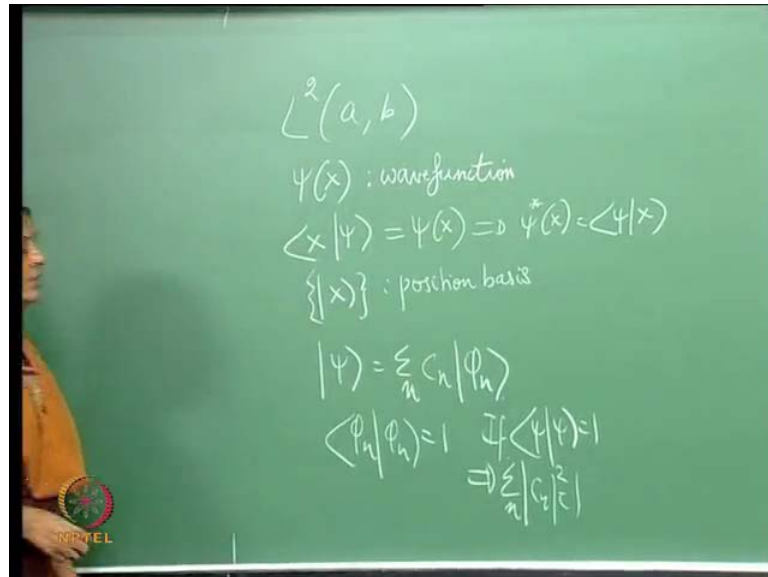
Now, let us look at the commutator. Now,  $\hat{X}$  is Hermitian. Because, it is essentially the identity operator and I have the commutator  $\hat{X} \hat{P}_x$ , I am going to just denote this by  $p$  for the moment. Is  $i \hbar$  cross identity operator and that is Hermitian, the identity operator is Hermitian. So, if we now expand, you have  $x$  to be simply replaced by the (Refer Slide Time: 06:07) number  $x$ . I am suppressing the fact that there is an identity operator there. So, if you wish, we will keep it that way,  $\hat{X} \hat{P}_x$  minus  $\hat{P}_x \hat{X}$ , is  $i \hbar$  cross identity. Take the Hermitian conjugate. So, that is  $\hat{P}_x^\dagger \hat{X}^\dagger$  which is  $\hat{X}$ , minus  $\hat{X}^\dagger \hat{P}_x^\dagger$ .

And when I take the transpose conjugate, in the case of the matrix, all elements get complex conjugated and therefore, I have minus  $i \hbar$  cross identity. Now we can compare the two of them, this implies that  $p$  is Hermitian, which is the way we want it. We want  $p$  to be Hermitian it is a Hermitian operator. Because, I would like to look at Eigen states of momentum and the Eigen values must be real. But,  $p$  is minus  $i \hbar$  cross  $\frac{d}{dx}$ , in general. We have got  $\hat{P}_x$  and therefore, it is  $d$  by  $d x$  and this is Hermitian, that implies that  $d$  by  $d x$  is not self adjoint. By self adjoint, in this context I mean Hermitian.

So, this is a simple way of seeing that,  $d$  by  $d x$ , in the case of one dimensions and  $\frac{d}{dx}$  in general. The Hermitian conjugate is minus of the operator and therefore, it is not a self

adjoint operator. Now in the case of, infinite dimensional spaces, as we will be considering, separable Hilbert spaces. So, you have a denumerable infinity of basis states, which are orthogonal to each other and normalized to 1. There will be many operators we will come across which are unbounded operators, the position operator is an example.

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But, before going into the properties of an operator, in an infinite dimensional Hilbert space, I would like to look at the state  $\psi$  of  $x$ .  $\psi$  of  $x$  it is called the wave function and the Schrodinger formulation of wave mechanics, was about  $\psi$  of  $x$ .



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In 1-dim.

$$\int_a^b \underbrace{\psi^*(x)}_{| \psi |^2} \underbrace{\psi(x)}_{| \psi |^2} \underbrace{dx}_{L} = 1$$

$\Rightarrow | \psi(x) |^2$  has dimensions  $\rightarrow \text{dim } \frac{1}{L}$

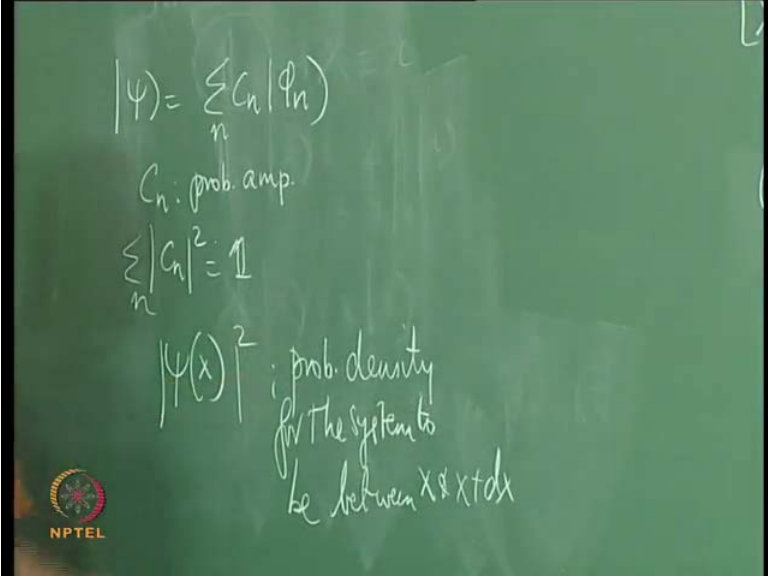
$$[ \psi(x) ] = \frac{1}{\sqrt{L}}$$

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In one dimension the facts that, integral  $\psi^*$  of  $x$   $\psi$  of  $x$ , perhaps the range is  $a$  to  $b$   $dx$ , is equal to 1. Implies, that this object  $\psi^* \psi$  has dimensions that has dimensions 1 by length, this is dimensions length. And therefore,  $\psi^* \psi$  has dimensions 1 by length and therefore,  $\psi$  of  $x$ , has dimension 1 by root  $L$ . This is in 1 dimension. Now, suppose we were doing 2 dimensions that would have been a  $d^2x$ . And therefore,  $\psi^* \psi$  would have dimensions 1 by  $L^2$  and  $\psi$  of  $x$  would have dimensions 1 by  $L$ , physical dimensions 1 by  $L$ .

And if you were working in 3 dimensional space, that would have been a  $d^3v$  of an elementary volume  $d^3v$ , which is  $dx dy dz$ , in Cartesian's and that has dimensions  $L^3$ . And therefore,  $\psi^* \psi$  would have dimensions 1 by  $L^3$  and the wave function in 3 dimensions, would have dimensions 1 by physical dimensions 1 by  $L^{3/2}$  the 3 by 2 and so on. So, this is the way we look at the dimensions of the wave function. Needless, to say that a very reasonable physical interpretation, can be given to  $\psi$  of  $x$ . We will augment and support our interpretation a little later, but, as it stands.

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The image shows a green chalkboard with handwritten mathematical expressions and text. At the top, the equation  $|\psi\rangle = \sum_n C_n |\phi_n\rangle$  is written. Below it,  $C_n$  is labeled as 'prob. amp.'. The next line shows the normalization condition  $\sum_n |C_n|^2 = 1$ . The final line shows  $|\psi(x)|^2$  followed by a colon and the text 'prob. density for the system to be between  $x$  &  $x+dx$ '. In the bottom left corner, there is a small circular logo with a star and the text 'NPTEL' below it.

$$|\psi\rangle = \sum_n C_n |\phi_n\rangle$$

$C_n$ : prob. amp.

$$\sum_n |C_n|^2 = 1$$

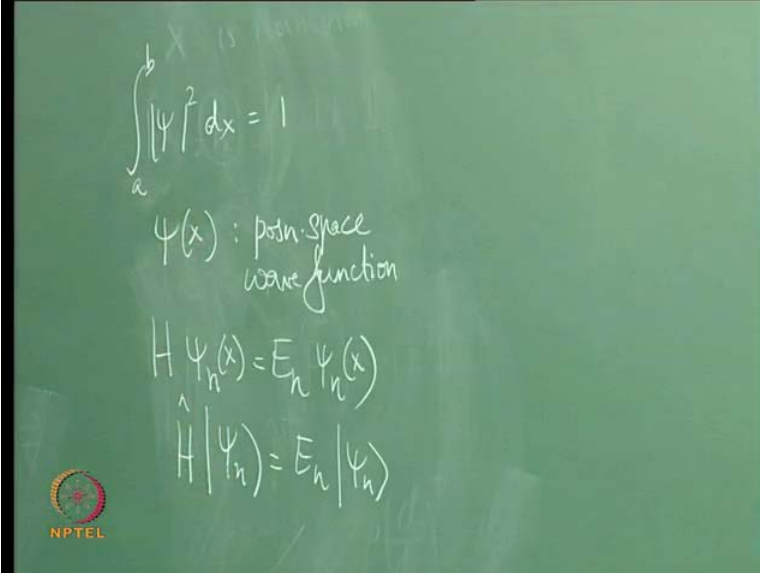
$|\psi(x)|^2$ : prob. density  
for the system to  
be between  $x$  &  $x+dx$

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Recall that in the abstract notation, where we expanded  $\psi$  in terms of the basis states  $\phi_n$ ,  $C_n$  is where the probability amplitudes and  $|C_n|^2$  was the probability density and this summation was 1, to tell you that the total probability that that particular physical system, represented by the state  $\psi$  actually exists. And therefore, the probability of its existence is 1.

Remember this is number 1 and not the identity operator. In that sense, when we write it in terms of the wave function  $\psi$  of  $x$ ,  $|\psi(x)|^2$  the whole squared, is the probability density, for the system to be between  $x$  and  $x + dx$ . And once an integration is done,  $\psi$  of  $x$  itself would be the probability amplitude and once the integration is done.

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$$\int_a^b |\psi|^2 dx = 1$$

$\psi(x)$  : position space wave function

$$H \psi_n(x) = E_n \psi_n(x)$$
$$\hat{H} |\psi_n\rangle = E_n |\psi_n\rangle$$

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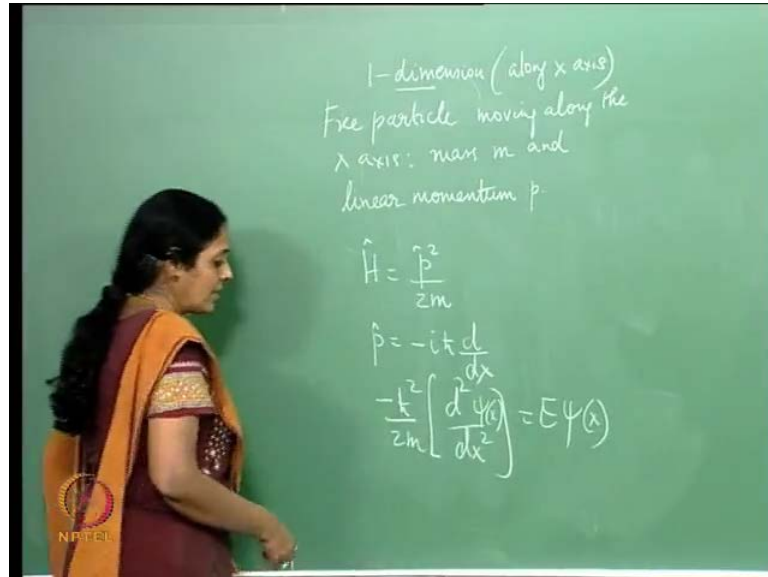
It is clear that the total probability is 1. You would expect this, because, this is the total probability that the system actually exists. Anywhere between  $a$  and  $b$  and if we are talking about a free particle travelling along 1 dimensions,  $x$  going from minus infinity to infinity. The probability that the particle exists, is given by 1. So, this is the probabilistic interpretation of quantum mechanics, which we already knew. In terms of the abstract kets, in the Hilbert space and now, we are merely working with a basis, a continuous basis in the space  $L^2$  and  $\psi$  of  $x$  is the wave function.

It is a state written in that basis, expanded in the position basis, in this case. Could have expanded it in the momentum basis, but, this is an example, of how we write a wave function. This is the position space wave function. Where  $x$  is position. Now, let us see, how exactly Eigen value equations look, when we write the equation in terms of  $\psi$  of  $x$  and in terms of operators that are expanded, or written in the position basis. So, we have the energy Eigen states,  $H \psi_n$  of  $x$  is  $E_n \psi_n$  of  $x$ .

In my earlier lectures, where I was not working with the position representation, I have the Hamiltonian acting on  $\psi_n$ , giving me  $E_n \psi_n$ . Now,  $H$  is to be written in the position representation and these should be made functions of  $x$ , because, we are working in the position basis. The reason why I have used a discrete index  $n$  is because; I

am assuming that the Hilbert space in which I am working out this problem, is a separable Hilbert space. And that indeed there is an infinite set of Eigen states and it is a denumerable infinity and that is why I use a discrete index  $n$  here.

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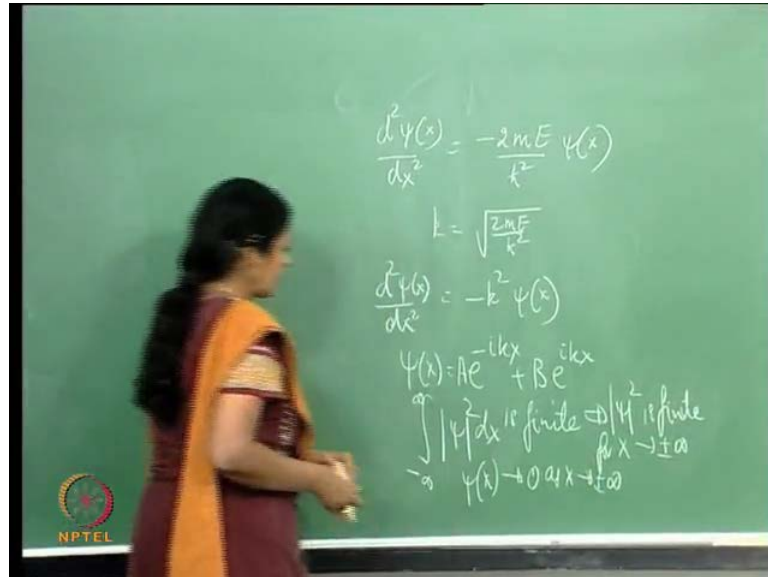
So, let us look at the simplest example. Let us look at a free particle. There is no potential and therefore, the Hamiltonian gets its contribution purely from the kinetic energy. So, I consider a free particle, this is 1 dimension; we can always generalize it, along the  $X$  axis. So, free particle moving along the  $X$  axis. The mass is  $m$  and the linear momentum is  $p$ . It is clear that the energy operator is  $p$  squared by  $2m$ . There is no potential term otherwise, I would have written a  $V$  of  $x$ .

$H$  is an operator and  $p$  is an operator and because, we are in the position representation. We are working this in the position representation and it is a 1 dimensional problem,  $p$  is minus  $i\hbar$  cross  $d$  by  $dx$ . So, we have the equation.  $\frac{1}{2m}$ , or minus  $\hbar$  cross squared by  $2m$ ,  $d^2 \psi$  by  $dx^2$  is  $E \psi$ . Where  $\psi$  is a function of  $x$ , this is the Eigen value equation that one needs to solve in order to find the energy Eigen states.

I would start off by saying  $d^2 \psi$  by  $dx^2$  and then in the case of specific problems, we will be able to see that the energy is quantized and automatically the

quantum number  $n$  would appear  $E_n$  and corresponding to each of those energies, there is a wave function  $\psi_n$  and these would be the energy Eigen states. Except that we are now writing them, in the position representation, or in the position basis.

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So, this tells me that  $\frac{d^2 \psi(x)}{dx^2}$  is minus  $\frac{2mE}{\hbar^2}$  times  $\psi(x)$  and this is a constant. So, I define  $k$  as square root of  $\frac{2mE}{\hbar^2}$  and therefore, I have  $\frac{d^2 \psi(x)}{dx^2}$  is minus  $k^2$  times  $\psi(x)$ . I can solve for this. It is clear that  $\psi(x)$  is  $e^{-ikx}$ . That is one solution, there is also another solution, which is  $e^{ikx}$  and therefore, in general,  $\psi(x)$  is  $Ae^{-ikx} + Be^{ikx}$ ,  $k$  is simply a number and as  $x$  changes  $\psi$  also changes.  $A$  and  $B$  are constants and they are to be determined from boundary conditions on  $\psi$ .

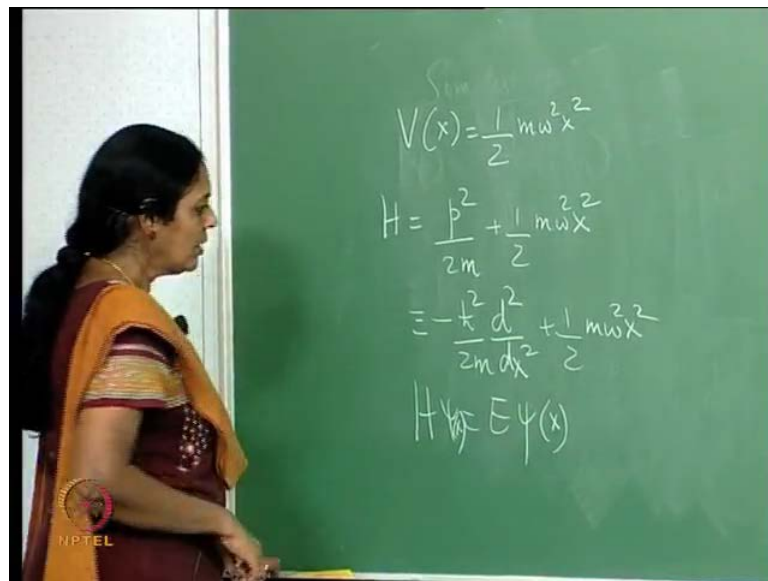
One thing is pretty obvious, that the solution is essentially a harmonic wave. This is simply a fallout of the de Broglie hypothesis. That matter has harmonic waves associated with it. The momentum  $p$  would be  $\hbar k$  and in general  $E$  would be  $\hbar \omega$ , where  $\omega$  is the angular frequency. So, this is the solution to the Eigen value problem, for a free particle moving along the  $x$  axis. I have not put in time dependence yet. I have simply written, the Eigen value problem  $\hat{H} \psi = E \psi$ , in the position representation

and got and hold of this solution for  $\psi$  of  $x$ , with  $A$  and  $B$  to be determined from boundary conditions.

It is a free particle, so, I should be able to use boundary conditions. What happens at  $\psi$  minus infinity and  $\psi$  plus infinity? That is for  $x$  going to plus or minus infinity. What is the value of  $\psi$ ? Now, there is a probabilistic interpretation to all this and since, I do require. That modulus of  $\psi$  squared  $dx$ , is finite, otherwise  $\psi$  is not even normalizable. I am working in the space  $L^2$ , which is the space of square integrable functions.

This automatically implies therefore, that  $\text{mod } \psi$  squared, is finite. As  $x$  goes to plus minus infinity and the boundary condition that we use, is that  $\psi$  of  $x$  goes to 0, as  $x$  goes to plus minus infinity. So those would be the boundary conditions, for this problem. Clearly, if there is a potential, I will not have a solution of that form,  $\psi$  of  $x$  would not be of the form  $A e^{-ikx} + B e^{ikx}$ .

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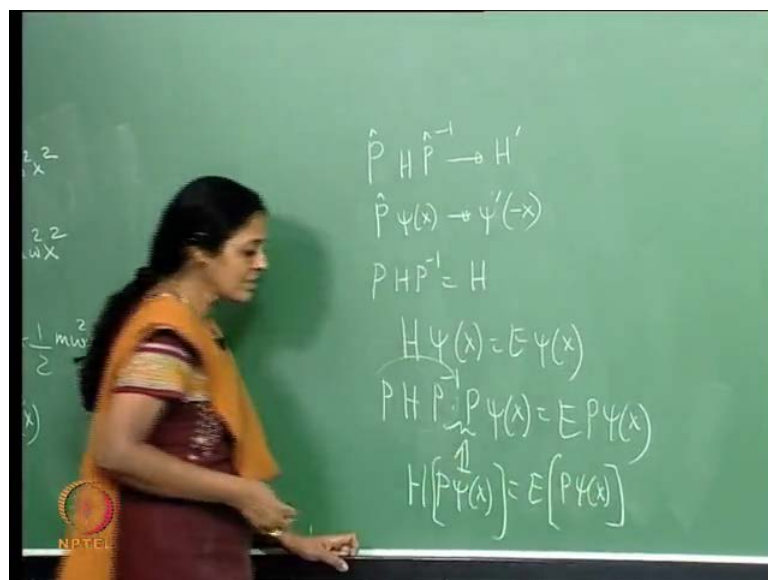
So, let us take a simple example, let us take the harmonic oscillator problem, which we have already worked out in terms of abstract kets. So, there the potential  $V$  of  $x$ , is half  $m$  omega squared  $x$  squared and therefore, the Hamiltonian of an oscillator, the momentum is  $p$  the mass is  $m$  and the angular frequency is  $\omega$ . It is  $p$  square by  $2m$ , plus half

$\omega^2 x^2$ . And therefore, in the position basis this is identical, to minus  $\hbar^2$  cross squared by  $2m$ ,  $\frac{d^2}{dx^2}$  plus half  $m\omega^2 x^2$ .

Where I have substituted  $p$  is minus  $i\hbar$  cross  $d$  by  $dx$ . It is therefore, I am pretty clear, that this formalism of quantum mechanics. Where  $\psi$  is written in the position basis, where you talk of  $\psi$  as a wave function in the position representation and so on. Would involve solutions of differential equations and in particular 2nd order differential equations, because the kinetic energy term is  $p^2$  by  $2m$ . So, this is an equivalent formalism. Whatever I had done in the past, for the linear harmonic oscillator, using  $H\psi = E\psi$  writing  $H$  in terms of  $a$ 's and  $a^\dagger$ 's.

Where,  $a$  and  $a^\dagger$  was where linear combinations of  $x$  and  $p$ , abstract operators. I could give infinite dimensional matrix representations for  $a$  and  $a^\dagger$ , upper triangular and lower triangular matrices. But, having said that did not solve it in the position basis. And therefore, solved it as a matrix  $a^\dagger a$  acting on a column vector, gives me a number, multiplying that same column vector. Instead I could use this equivalent formalism and solve for the differential equation. We shall not attempt to solve the differential equation in detail now, the equation itself is  $H\psi = E\psi$  where  $H$  is given by this and  $\psi$  is a function of  $x$ .

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But, on the other hand certain points are notable. The potential itself  $V$  of  $x$  versus  $x$  is a parabola. It is a symmetric potential, symmetric about  $x$  is equal to 0. And therefore, going back to my definition of the parity operator, this is an operator, which takes  $x$  to minus  $x$ , it is a 1 dimensional problem. It is a reflection operator which takes  $x$  to minus  $x$  and like all operators,  $P H P^{-1}$ , takes it to  $H'$ , which is a new operator and  $P \psi$  of  $x$  takes it to  $\psi$  of  $\psi'$  of minus  $x$ , which is the new state, or the new wave function. However, here is a situation, (Refer Slide Time: 22:18) where  $P$  leaves  $H$  invariant. Because, when  $x$  goes to minus  $x$   $x^2$  is unchanged  $d x^2$ , squared and similarly, here  $x^2$  is unchanged and therefore,  $P H P^{-1}$  equals  $H$ .

Now, in a context like this, where I have  $H \psi$  of  $x$  is  $E \psi$  of  $x$ . I can write  $P H P^{-1} P$ . It is clear that  $P^{-1} P$  is the identity operator, because,  $P$  takes  $x$  to minus  $x$  and therefore all operators, which are functions of  $x$ , to the same operators. Where  $x$  is substituted by minus  $x$  and the wave function  $\psi$  of  $x$  goes to  $\psi$  of minus  $x$ . Now, if I did  $P$  once more, you see,  $P^{-1}$  would simply take  $\psi$  of minus  $x$  back to  $\psi$  of  $x$ . And therefore,  $P H P^{-1} P$ , where I have introduced  $P^{-1} P$  as identity here,  $\psi$  of  $x$ ,  $E$  is a number  $P \psi$  of  $x$ . And therefore, I have but,  $P H P^{-1}$  is simply  $H$ . So,  $H P \psi$  of  $x$  is  $E P \psi$  of  $x$ .


I see that if  $\psi$  of  $x$  is an Eigen state of  $H$  with Eigen value  $E$ .  $P \psi$  of  $x$  is also an Eigen state of  $H$ , with the same Eigen value  $E$ . Now, if the Eigen value  $E$  is not degenerate, then it is clear that  $P \psi$  of  $x$  is either plus  $\psi$  of  $x$ , or minus  $\psi$  of  $x$ .



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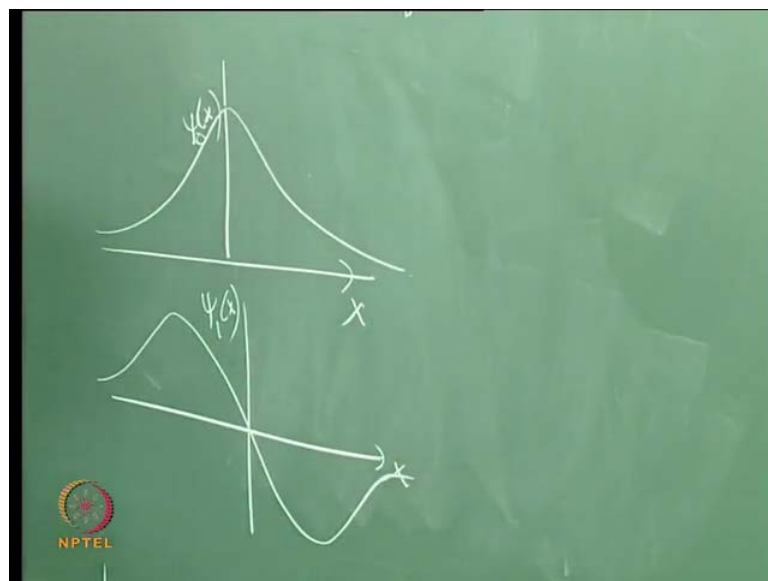
$$P\psi(x) = \psi(-x) = \pm \psi(x)$$

$E$ : non-degenerate



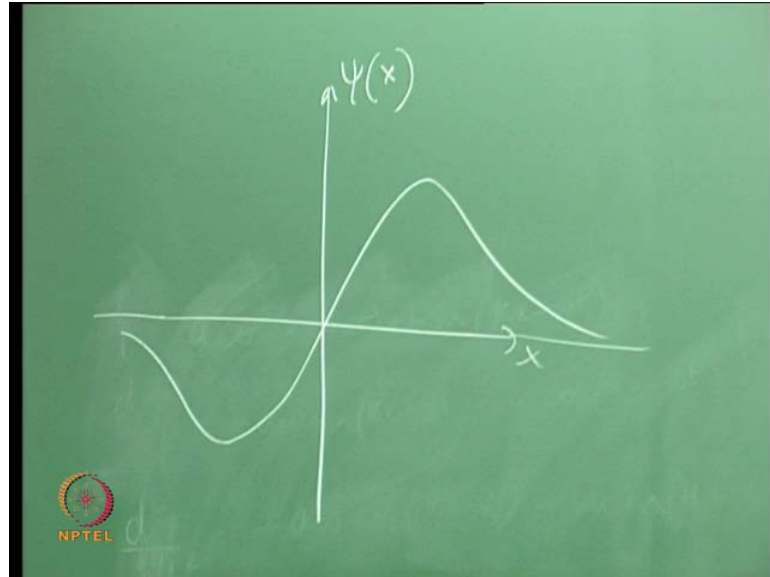
So for a non degenerate situation, as happens in the case of these single simple Harmonic oscillator  $p\psi$  of  $x$  is  $\psi$  of minus  $x$ . But, that is plus or minus  $\psi$  of  $x$ ; only then this equation is satisfied. Where  $E$  is non degenerate and therefore, the Eigen states the energy Eigen states, will have definite symmetry properties, they will either be odd functions of  $x$  or even functions of  $x$ .

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If you will recall that in the ground state, we showed that  $\psi$  of  $x$  was a Gaussian. A Gaussian function of  $x$  and therefore, it is an even function of  $x$ , going to 0 as  $x$  goes to plus minus infinity, which I would require for my probabilistic interpretation, here is an odd function of  $X$ . As  $X$  goes to plus minus infinity  $\psi$  of  $X$  goes to 0 like that.

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Look at this; this is another odd function of  $X$ . So,  $X$  goes between, its range minus infinity to infinity. So, that is an odd function of  $X$  and in fact this happens to be the wave function,  $\psi$  of  $x$  for the 1st excited state, with the simple harmonic oscillator. The 2nd excited state is an even function of  $X$ . So,  $\psi$  of minus  $X$  is plus  $\psi$  of  $X$ , as far as a 2nd excited state is concerned. 3rd excited state is an odd function of  $x$  and so on, it alternates and these are states with definite parity.

You will also recall, that I mentioned in the context of the basis states in  $L^2$ , mentioned the hermit polynomials as the basis set, essentially the basis set, for the harmonic oscillator problem, the linear harmonic oscillator problem and in that context, we did remark that, there was a definite parity, there were a set of definite parity states. The basis states were a set of definite parity states. So states which were either odd functions of  $X$  or even functions of  $X$ .

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Handwritten derivation on a green chalkboard:

$$\langle \psi | \hat{X} | \psi \rangle$$

$$\stackrel{\uparrow}{1x}$$

$$\int_{-\infty}^{\infty} dx'' \int_{-\infty}^{\infty} dx' \langle \psi | x' \rangle \langle x' | \hat{X} | x'' \rangle \langle x'' | \psi \rangle$$

$$\hat{X} | x'' \rangle = x'' | x'' \rangle$$

$$\langle x' | x'' \rangle = \delta(x' - x'')$$

$$= i \int_{-\infty}^{\infty} dx' \psi^*(x') x' \psi(x')$$

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Handwritten derivation on a green chalkboard, continuing from the previous slide:

$$\langle \psi | \hat{X} | \psi \rangle$$

$$\stackrel{\uparrow}{1x}$$

$$\int_{-\infty}^{\infty} dx'' \int_{-\infty}^{\infty} dx' \langle \psi | x' \rangle \langle x' | \hat{X} | x'' \rangle \langle x'' | \psi \rangle$$

$$\hat{X} | x'' \rangle = x'' | x'' \rangle$$

$$\langle x' | x'' \rangle = \delta(x' - x'')$$

$$= i \int_{-\infty}^{\infty} dx' \psi^*(x') x' \psi(x') \Rightarrow \int_{-\infty}^{\infty} dx \psi^*(x) x \psi(x) = \langle X \rangle$$

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Now let us look at the harmonic oscillator operators. So, what is the mean value of  $X$ , in any state  $\psi$ ? I would normally have written  $\psi^\dagger X \psi$ . In the case of the oscillator you will recall that I wrote  $X$  as a plus a dagger by root 2 and worked out the calculation by finding out the effect of  $a$  on ket  $\psi$  and so on and  $a^\dagger$  on ket  $\psi$  and so on. But, instead I could now write the whole thing as functions of  $x$ . This as we said was simply

the identity operator. Apart from  $x$  and this object, I can always introduce a complete set of states.

So, I can write it as,  $\int dx' \psi(x') x'$ . Now, that is a complete set of states that I have introduced.  $X$  and then, once more here I can introduce, another complete set of states,  $\int dx'' X \psi(x'')$ . It is clear that these are the position Eigen states and therefore, I have the Eigen value equation as follows. I also therefore, know that because of orthonormality. This is how I replace the orthonormality condition. Because, it is a continuous basis and therefore, substituting things in.

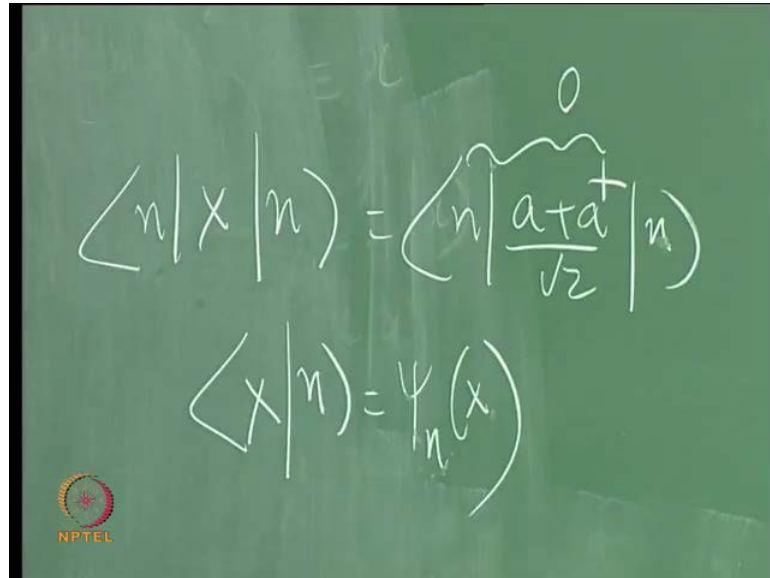
I find that one of the integrals goes, I replace all  $X$  double prime by  $X$  prime and I have minus infinity to infinity  $\int dx' \psi^*(X') \psi(X')$ . This is  $\psi^*$  of  $X'$  in our notation. This gave me the delta function and one of the integrals went and I have  $\psi(X')$ . There was a small matter of  $X$  double prime being the Eigen value and I could have put it here, the  $X$  double prime was replaced by  $x'$ . So, I could have put it here, or I could have pulled it out and put it there. This is just a variable. So I could have written it as  $\int dx' \psi^*(X') \psi(X')$ , or I could have put it there, could have put it anywhere.

And, because the integral is over  $X'$ , I can just write this as,  $\int_{-\infty}^{\infty} dx' \psi^*(X') \psi(X')$ ; this is the expectation value of  $X$ , in this state  $\psi$  of  $X$ . Now, let us look at the harmonic oscillator states. The state  $\psi$  of  $X$  has a definite parity. Perhaps we are looking at the ground state of the oscillator. Then  $\psi$  of  $X$  is an even function of  $X$  and so is  $\psi^*$  of  $X$ . In general it is clear even from the free particle case, that  $\psi$  could be a complex function of  $X$ .

Because, it could be  $A e^{ikx} + B e^{-ikx}$ . But,  $\psi^*$  of  $X \psi$  of  $X$  is an even function of  $X$ . This is odd in  $X$  and therefore, between limits minus infinity to infinity this integral vanishes. Now, let us look at the 1st excited state of the oscillator, again  $\psi$  of  $X$  is an odd function of  $X$  and so is  $\psi^*$  of  $X$ . And therefore, between them  $\psi^* \psi$ , is an even function of  $X$  and there is an  $X$  here and therefore, the whole

thing vanishes. So, it is clear that expectation value of  $X$  vanishes in every state of the oscillator.

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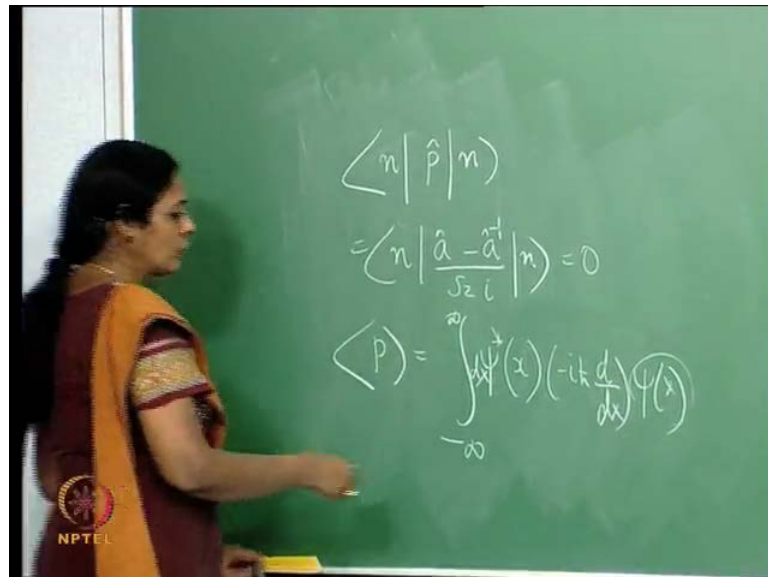
$$\langle n | X | n \rangle = \langle n | \frac{a + a^\dagger}{\sqrt{2}} | n \rangle$$

$$\langle X | n \rangle = \psi_n(x)$$

If you recall, this result was established earlier, in the abstract ket notation. Where we wrote  $X$  as  $a + a^\dagger$  by  $\sqrt{2}$  and discovered that in the energy basis, energy Eigen basis, which I referred to as ket  $n$ . My notation now, would be  $X$   $n$  is  $\psi_n$  of  $X$ . So, this is the notation now, ket  $n$  earlier written in the position basis, is  $\psi_n$  of  $X$ . This is the  $n$ -th Eigen state of the oscillator. If you wish it is the  $n$  photon state in the scenario of quantum optics, it is the  $n$  photon state written in the position representation. It is a wave function for an  $n$  photon state.

Whatever, it is an equation like expectation value of  $X$ , is  $n$   $a + a^\dagger$  by  $\sqrt{2}$   $n$ . This turned out to be 0, because,  $a^\dagger$  was a raising operator and took  $n$  to  $n + 1$  and I had the fact that all the kets are orthogonal to each other. This got it vanishing and I see it also shown here, (Refer Slide Time: 32:42) using the wave function. So, that is exactly the result that I got there in abstract notation. That we had here in abstract notation.

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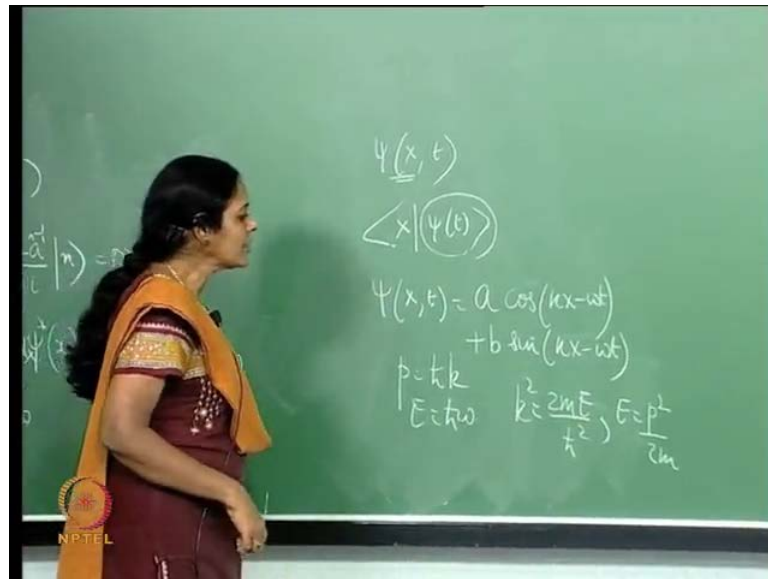
So, now let us look at expectation value of P. So, once more in the abstract notation I had  $\langle n | \hat{p} | n \rangle$ , was  $\langle n | \frac{\hat{a} - \hat{a}^\dagger}{\sqrt{2}i} | n \rangle$ . And once more the fact, that  $\hat{a}$  lowers  $n$  to  $n - 1$  and  $\hat{a}^\dagger$  raises  $n$  to  $n + 1$  and the states are orthogonal to each other. In any state any energy Eigen state of the harmonic oscillator, this was 0. In the notation that we use now, that is when we talk of wave functions, expectation value of P. In the state  $\psi$  is integral  $\psi^* \psi$ . I am working out in the position representation and P is minus  $i\hbar$  cross d by d x.

I have to be careful where I put it, because, it is a differential operator and it acts on anything that comes after it. So, there is a  $\frac{d}{dx}$  here, minus  $i\hbar$  cross are constants. The fact is, if  $\psi(x)$  is an even function of  $x$ , as is the case for the ground state. The 2nd excited state before the 4th excited state of the oscillator and so on,  $\frac{d}{dx} \psi(x)$  it is an odd function of  $x$ . This was an even function of  $x$  and therefore, this is an odd function of  $x$  and that is an even function of  $x$  and totally it vanishes between symmetric limits minus infinity to infinity.

On the other hand if  $\psi(x)$  is an odd function of  $x$ ,  $\frac{d}{dx} \psi(x)$  is an even function of  $x$ . this is an odd function, that is an even function and the answer follows. So, expectation value of  $p$  is also 0, in all these states of the harmonic oscillator. So, whatever was established in terms of abstract kets, is now being established in the position representation. We worked with  $l^2$  when we worked with abstract kets.

Where in the case of the harmonic oscillator problem, the operators  $a$  and  $a^\dagger$  etcetera: were infinite dimensional matrices and the kets, ket  $n$  for instance was an infinite component column vector with 1 as one of the entries and all other entries being 0. This is an equivalent formalism and I am explicitly trying to work out those results in this formalism.

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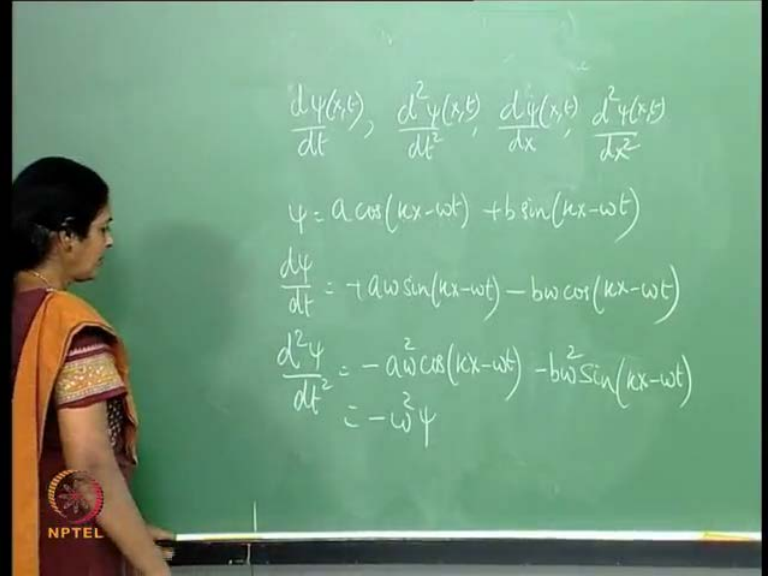


Although, we will really be taking up dynamics, somewhat later, it is still worth remembering. That the system could move in time and time is only a parameter in quantum mechanics. And therefore, I should really be writing,  $\psi$  of  $X$   $t$ , in the 1 dimensional case. So, that is the same as  $X$   $\psi$  of  $t$ . This is in the position representation. Otherwise in the abstract, I would just have had  $\psi$  of  $t$  or  $n$  of  $t$  ket and in the position representation I simply take this expansion, this inner product. Now, in general therefore, I would like to attempt to write an equation for  $\psi$  of  $X$  comma  $t$ , turns out that this is the Schrodinger equation.

I used the fact, that in general  $\psi$  of  $x$   $t$ , going back to the free particle, is a harmonic wave and therefore,  $\psi$  of  $X$   $t$  would be  $a \cos k x$  minus  $\omega t$  plus  $b \sin k x$  minus  $\omega t$ . This is if I put in time and  $\omega$  is the angular frequency the momentum  $p$  is  $\hbar$  cross  $k$  and  $E$  is  $\hbar$  cross  $\omega$ . And  $k$  squared as I have shown earlier, is  $2 m E$  by  $\hbar$  cross squared because,  $E$  is  $p$  squared by  $2 m$ . So, if I have this solution for  $\psi$  of  $X$   $t$ . It's worth finding out what the differential equation is which is obeyed. What is the differential equation which is obeyed by the wave function?



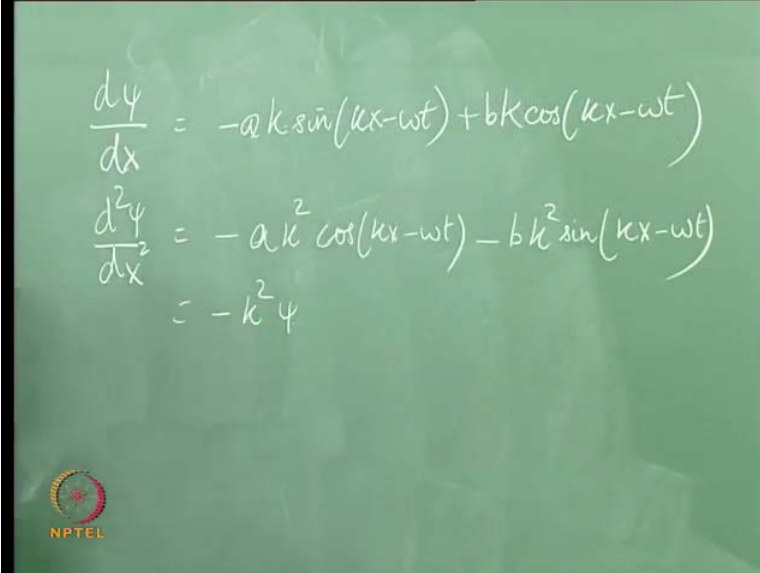
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$$\frac{d\psi(x,t)}{dt}, \frac{d^2\psi(x,t)}{dt^2}, \frac{d\psi(x,t)}{dx}, \frac{d^2\psi(x,t)}{dx^2}$$
$$\psi = a \cos(kx - \omega t) + b \sin(kx - \omega t)$$
$$\frac{d\psi}{dt} = -a\omega \sin(kx - \omega t) - b\omega \cos(kx - \omega t)$$
$$\frac{d^2\psi}{dt^2} = -a\omega^2 \cos(kx - \omega t) - b\omega^2 \sin(kx - \omega t)$$
$$= -\omega^2 \psi$$

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Now, a differential equation can be got, by trying to find out  $\frac{d\psi}{dt}$  of  $\psi$  by  $dt$ ,  $\frac{d^2\psi}{dt^2}$  of  $\psi$  by  $dt^2$ ,  $\frac{d\psi}{dx}$  of  $\psi$  by  $dx$  and  $\frac{d^2\psi}{dx^2}$  of  $\psi$  by  $dx^2$ . We look at the 1st and 2nd derivatives, of space and time and try to come up with an equation. So, I have  $\psi$  is  $a \cos kx - \omega t$ , plus  $b \sin kx - \omega t$  and therefore,  $\frac{d\psi}{dt}$  is plus  $a\omega \sin kx - \omega t$ , minus  $b\omega \cos kx - \omega t$ . So,  $\frac{d^2\psi}{dt^2}$  is minus  $a\omega^2 \cos kx - \omega t$ , plus  $b\omega^2 \sin kx - \omega t$ , minus  $b\omega^2 \sin kx - \omega t$ . So, this object is the same as minus  $\omega^2 \psi$ , this is  $\frac{d^2\psi}{dt^2}$  by  $dt^2$ .

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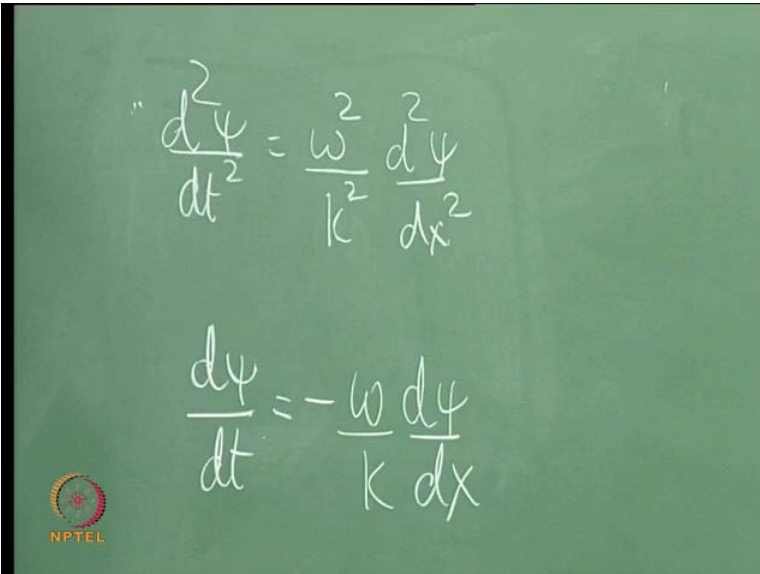


The image shows a green chalkboard with handwritten mathematical derivations. The first equation is the first derivative of  $\psi$  with respect to  $x$ , which is  $\frac{d\psi}{dx} = -ak \sin(kx - \omega t) + bk \cos(kx - \omega t)$ . The second equation is the second derivative of  $\psi$  with respect to  $x$ , which is  $\frac{d^2\psi}{dx^2} = -ak^2 \cos(kx - \omega t) - bk^2 \sin(kx - \omega t)$ . The third equation shows that this second derivative is equal to  $-k^2\psi$ . In the bottom left corner, there is a small circular logo with a red and yellow design and the text "NPTEL" below it.

$$\frac{d\psi}{dx} = -ak \sin(kx - \omega t) + bk \cos(kx - \omega t)$$
$$\frac{d^2\psi}{dx^2} = -ak^2 \cos(kx - \omega t) - bk^2 \sin(kx - \omega t)$$
$$= -k^2\psi$$

Similarly, I can find  $d\psi$  by  $dx$  and  $d^2\psi$  by  $dx^2$ , minus  $ak \sin kx$  minus  $\omega t$ , plus  $bk \cos kx$  minus  $\omega t$  and  $d^2\psi$  by  $dx^2$ , is minus  $ak^2 \sin \cos kx$  minus  $\omega t$ , minus  $bk^2 \sin kx$  minus  $\omega t$ , or that is the same as minus  $k^2\psi$ .

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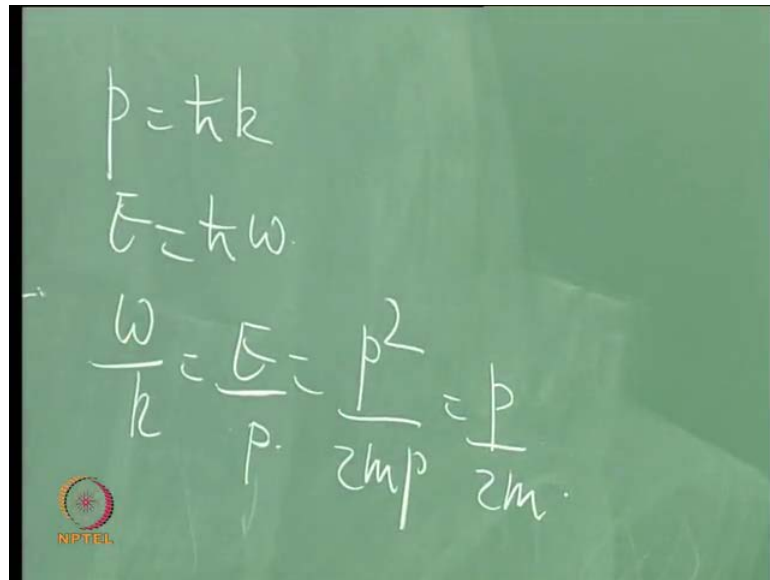


The image shows a green chalkboard with handwritten mathematical derivations. The first equation is the wave equation, which is  $\frac{d^2\psi}{dt^2} = \frac{\omega^2}{k^2} \frac{d^2\psi}{dx^2}$ . The second equation is the relationship between the first derivatives of  $\psi$  with respect to  $t$  and  $x$ , which is  $\frac{d\psi}{dt} = -\frac{\omega}{k} \frac{d\psi}{dx}$ . In the bottom left corner, there is a small circular logo with a red and yellow design and the text "NPTEL" below it.

$$\frac{d^2\psi}{dt^2} = \frac{\omega^2}{k^2} \frac{d^2\psi}{dx^2}$$
$$\frac{d\psi}{dt} = -\frac{\omega}{k} \frac{d\psi}{dx}$$

So,  $\frac{d^2 \psi}{dt^2}$  is  $\omega^2 \psi$ ,  $\frac{d^2 \psi}{dx^2}$  is  $-k^2 \psi$ . Similarly, I can equate the 1st derivatives with respect to space and time and I have  $\frac{d\psi}{dt}$  is  $-\omega \psi$  and  $\frac{d\psi}{dx}$  is  $ik \psi$ . Perhaps this is a possible equation. But, in all these cases, there is a problem. The problem is this, that if you compare,  $p$  is  $\hbar k$  and  $E$  is  $\hbar \omega$ .

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$$p = \hbar k$$

$$E = \hbar \omega$$

$$\Rightarrow \frac{\omega}{k} = \frac{E}{p} = \frac{p^2}{2m p} = \frac{p}{2m}$$

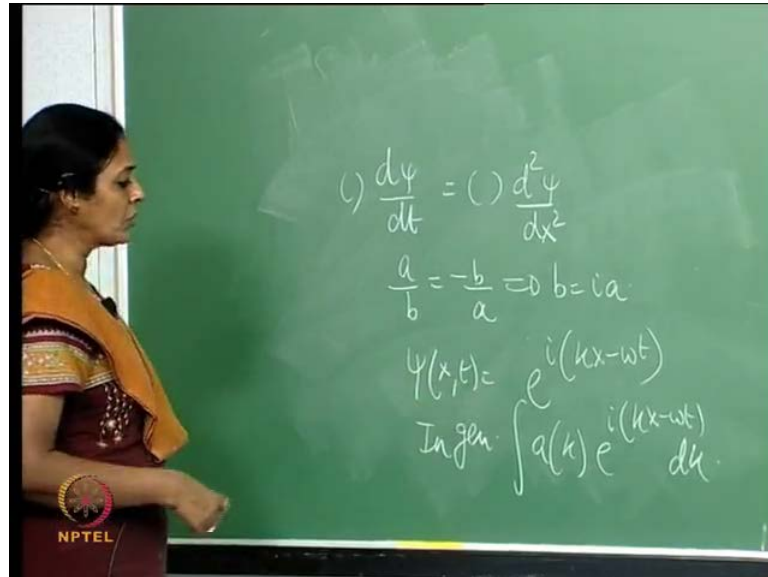
So, if you look at the ratio  $\omega/k$  for instance, that is  $E/p$  and that is  $p^2 / (2m p)$ , which is  $p / (2m)$ . That is like saying that this equation depends upon the value of the momentum, depending upon what the momentum value is the equation keeps changing.

Now we would like an equation which does not involve specific values of  $p$  (Refer Slide Time: 43:21) obviously, we need an equation which is all encompassing and therefore, you do not want to see, an explicit  $p$  dependence in the equation. And indeed you can get an equation like that, provided you equate the 1st derivative with respect to time of the wave function with the 2nd derivative with respect to space of the wave function.

If you look at  $\frac{d\psi}{dt}$  (Refer Slide Time: 41:00) I have  $-\omega \sin kx - \omega \cos kx$ ,  $\frac{d\psi}{dx}$  I have  $ik \sin kx - ik \cos kx$ . And, if this has to be equated to that, it is

pretty clear that  $a$  and  $b$ , will have to have a certain specific ratio with respect to each other. This is (Refer Slide Time: 42:36)  $-\hbar^2 k^2 \psi = E \psi$ , is  $-\hbar^2 k^2 \psi$ .

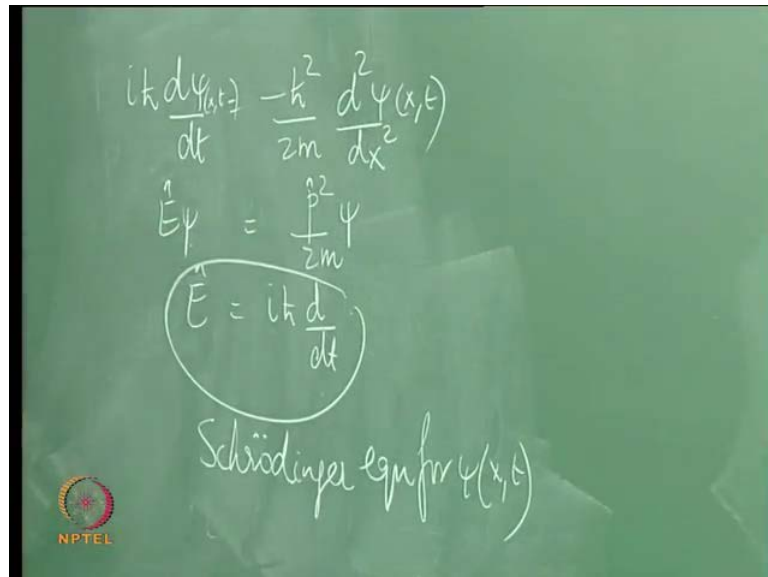
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And therefore, from this I get, if I have to equate  $\frac{d^2\psi}{dx^2}$  times some coefficient, as  $\frac{d\psi}{dt}$  times some other coefficient. Then I get  $\frac{a}{b} = -\frac{b}{a}$ , which implies that  $b = ia$  and then it follows, that  $\psi(x,t)$  is  $e^{i(kx - \omega t)}$ , apart from a phase. That is not to say that this is the only solution  $k$  is a specified number. Given the momentum  $p$  I have  $k = \frac{p}{\hbar}$ . On the other hand  $\psi$  is a function of  $x$ , given  $\omega$  these are the constants and  $\psi$  varies with  $x$  and varies with time, I in general can have super positions of this as solutions.

In general the solution is  $\int a(k) e^{i(kx - \omega t)} dk$  for all values of  $k$ . So, that is the general super position which is a solution of that equation. That is because the Schrodinger equation is a linear equation, the equation itself which I have not written down if you put in these values.

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$$i\hbar \frac{d\psi(x,t)}{dt} = -\frac{\hbar^2}{2m} \frac{d^2\psi(x,t)}{dx^2}$$
$$\hat{E}\psi = \frac{\hat{p}^2}{2m}\psi$$
$$\hat{E} = i\hbar \frac{d}{dt}$$

Schrodinger eqn for  $\psi(x,t)$

You will get,  $i\hbar$  cross  $d\psi$  by  $dt$ , is minus  $\hbar$  cross squared by  $2m$ ,  $d^2\psi$  by  $dx^2$ . That is like saying,  $p^2$  by  $2m$   $\psi$  is  $E\psi$ . Because,  $E$  is  $p^2$  by  $2m$  or  $H\psi$  if you wish and that tells you that the energy operator,  $E\psi$  and therefore, the energy operator, is  $i\hbar$  cross  $d$  by  $dt$ . This identification is possible from the Schrodinger equation, because, I know that energy is  $p^2$  by  $2m$  for the free particle. These are all functions of  $x$  and time, this is the Schrodinger equation for  $\psi$  of  $x$  and  $t$ .

Of course, if you choose not to (Refer Slide Time: 45:43) put in time, which is what we will do for the moment we will take up dynamics later. It is clear that  $\psi$  is of the form  $e^{ikx}$  or a general super position, a sum of  $k$   $e^{ikx}$ , which is what we saw earlier, when we looked at the energy equation  $H\psi = E\psi$ , without worrying about the dynamics. These are the plane wave solutions  $e^{ikx}$ . So, you have a component which is cosine and another which is sine and that is the most general solution. Boundary conditions  $\psi$  goes to 0 as  $x$  goes to plus minus infinity.

In the set of lectures to follow, we will not worry about the time development at all we will merely use the fact, that the plane wave solution is  $e^{ikx}$ , a  $e^{ikx}$  plus  $b e^{-ikx}$ . In the case of the free particle, we will work out specific problems like the harmonic oscillator, or a particle subjected to other types of potentials, like a

square well potential, or a particle penetrating a barrier; potential barrier and so on. So, these are all problems which we will study, without worrying about time at all. And then, later on, in a series of lectures, we will talk about the dynamics of a system the manner in which the system evolves with time.