Quantum Physics
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Lecture No. # 08

The first order of business is to compute this number, the inner product x with p.

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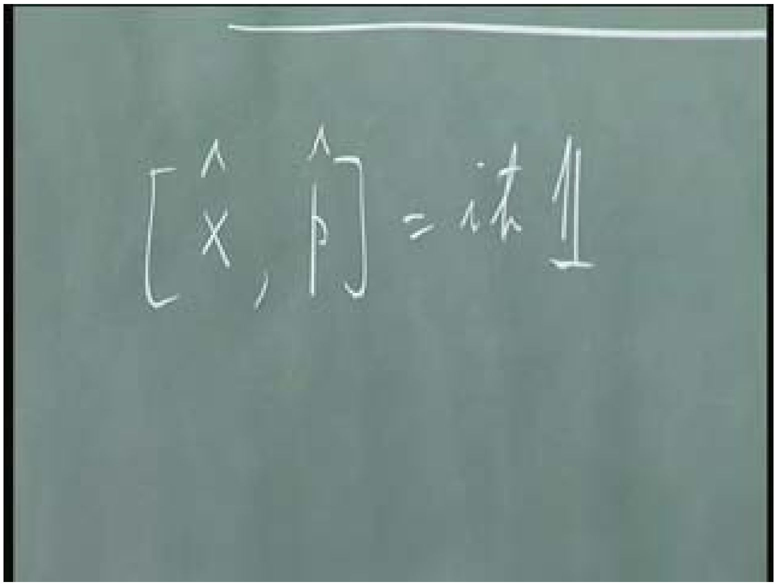

You recall that p ket vector stands for a momentum Eigen state of a particle moving on a line and x ket vector stands for a position eigen state. What we would like to find out is, given the commutation relation, x commutator p is ih cross times the unit operator, what's the overlap between a position Eigen state and a momentum eigen state. We know already that when two operators don't commute with each other, you can't find a complete set of common eigenstates for these two operators. So the question is, given the commutational relation which is an input information borrowed from classical mechanics from the Poisson bracket, what would be this quantity (Refer Slide Time: 01:30 min).

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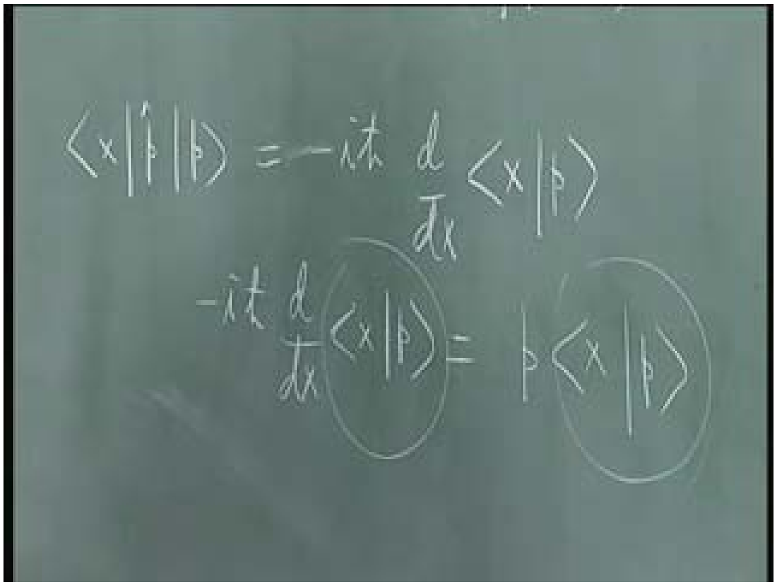

$$\langle x|\hat{p}|p\rangle = -i\hbar \frac{d}{dx}\langle x|p\rangle$$

$$-i\hbar \frac{d}{dx}\boxed{\langle x|p\rangle} = p\boxed{\langle x|p\rangle}$$

But we already saw last time that momentum operator in the position basis is nothing but - ih cross d over dx of the representative of the state psi in the position basis. So we established this relationship last time that followed from this commutational relation. So it says in the position basis, the momentum operator acts as if its - ih cross the derivate operator with respect to x. we will use that information to compute what this quantity itself is here (Refer Slide Time: 03:30). Instead of psi, you replace it with the momentum eigenstate in this equation and that's going to immediately tell us what the answer is. So we have x p on p = - ih cross d over dx x with p. but of course the momentum operator acting on a momentum Eigen state just produces the momentum eigen value.

So this p is a number you call it p_0 if you like. so this says - ih cross d over dx of x with p = p times x with p because this is a number that comes out when this operator acts on it, it produces the eigen value which comes right out of the matrix element and its equal to this(Refer Slide Time: 04:27). So this is some function of x labeled by p. that function, call it f of x if you like, and satisfies an ordinary differential equation in the x variable.

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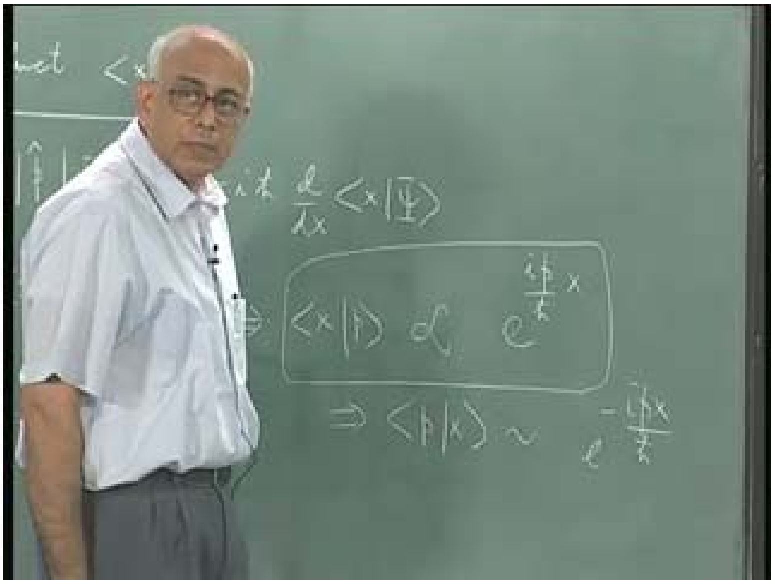

The solution implies that x with p is proportional to e to the power. So this is just a constant ip over h cross x. that's true for every p. we could have changed the value of this p to some other eigen value. Whatever be the eigen value, you get this equation here with that eigen value present and this (Refer Slide Time: 05:19) x sitting here. This (Refer Slide Time: 05:22) is a function of x because it's a position space representative of a certain ket vector. That ket vector is labeled by this p here (Refer Slide Time: 05:30). So this gives us a fundamental result which says x with p apart from some normalization constant is essentially a phase factor.

Notice that in that exponent there is no question of putting operators or anything like that both x and p are numbers actual numbers they are eigen values actually. So corresponding to the bra x, we have an eigen value x that's a number sitting on the right and corresponding to ket p, you have an eigen value p that's on the right again. This immediately implies that p with x is proportional to e to the power - ipx over h cross. Now the labels x and p are interchanged in this case. This is the p space representative of a position eigen state x.

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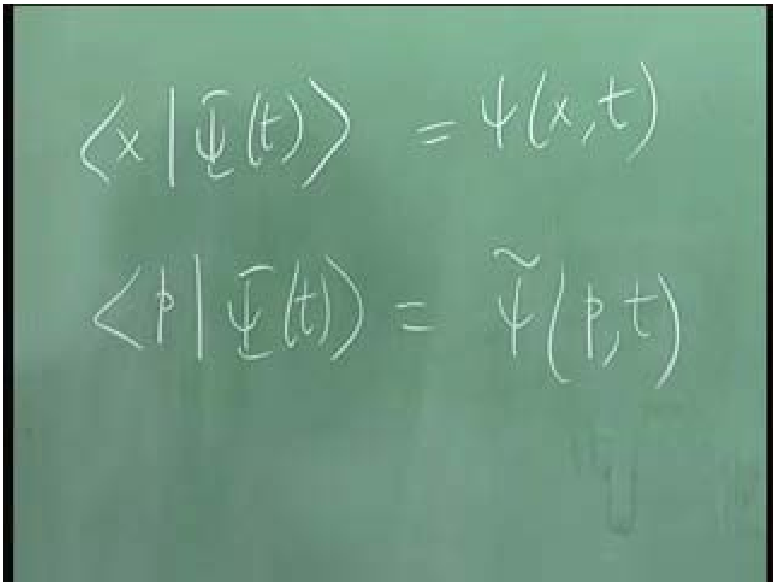

$$\langle x | \Psi(t) \rangle = \psi(x,t)$$

$$\langle p | \Psi(t) \rangle = \tilde{\psi}(p,t)$$

We already proved remember that if you took a state vector psi of t and you asked what is its position space representative, this was equal to psi of x ,t and similarly in the momentum basis it was equal to psi tilda of p, t.

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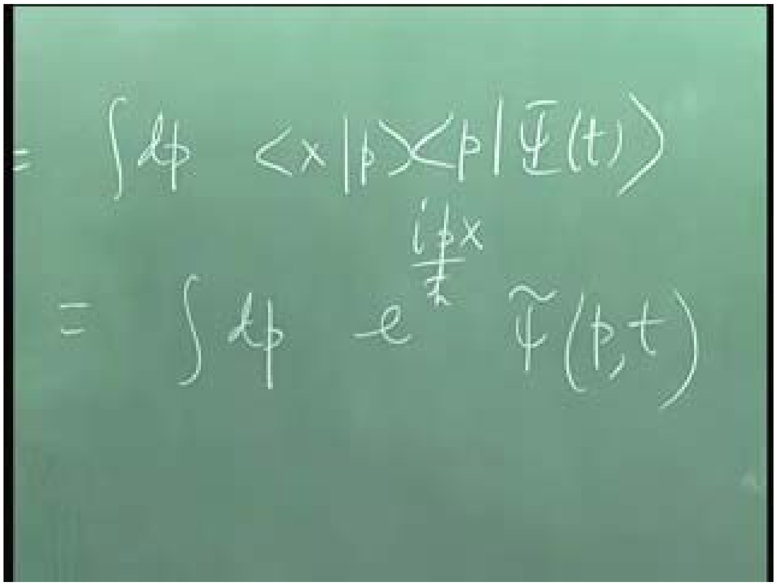

$$= \int dp \, \langle x | p \rangle \langle p | \Psi(t) \rangle$$

$$= \int dp \, e^{\frac{ipx}{\hbar}} \, \tilde{\psi}(p,t)$$

And that is psi tilda of p , t was related to integral dp x p p psi of t. I insert a complete set of states there (Refer Slide Time: 07:26) and this is equal to integral dp, e to the ipx over h cross and psi tilda of phi p, t. So it says that psi of x t is the Fourier transform of psi tilda of p and t and vice versa. And you can fix the constants by adjusting by having a Fourier transform normalization convention.

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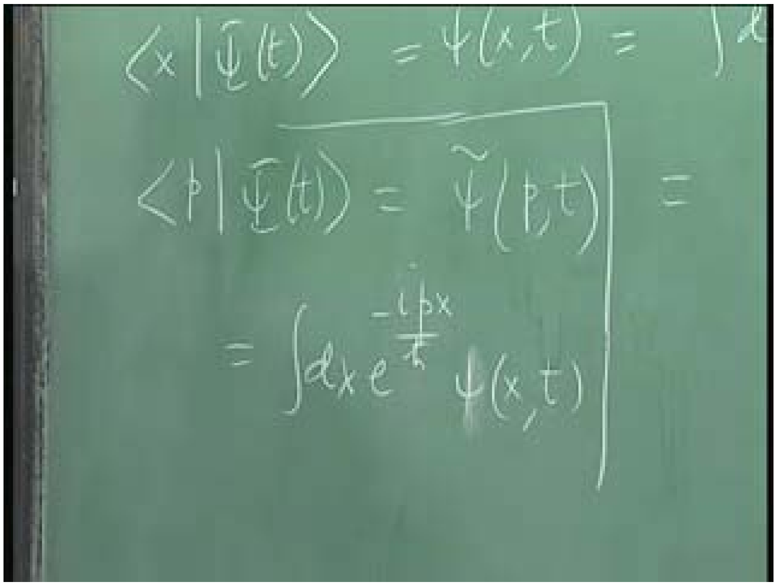

$$\langle x | \Psi(t) \rangle = \psi(x,t) = \int d$$

$$\langle p | \Psi(t) \rangle = \tilde{\psi}(p,t) =$$

$$= \int dx\, e^{-\frac{ipx}{\hbar}}\, \psi(x,t)$$

And of course psi tilda of p and t is integral dx e to the power - ipx over h cross psi of x, t. so that establish is my assertion made earlier that the position space and momentum space wave functions of a quantum mechanical particle are Fourier transforms of each other. That immediately tells us that if one of them is square integrable, so is the other square integrable. Because you know by the Parseval's theorem, mod psi squared of x, t integrated over dx is equal to the same thing for mod psi tilde. So that’s just a consideration of probability statement and both of them belong to L_2. This incidentally is also one way of looking at the statement that the space L_2 is self-dual. So the Fourier transform of a square integrable function is also square integrable. So much for this overlap x , p, one can generalize this to three dimensions.

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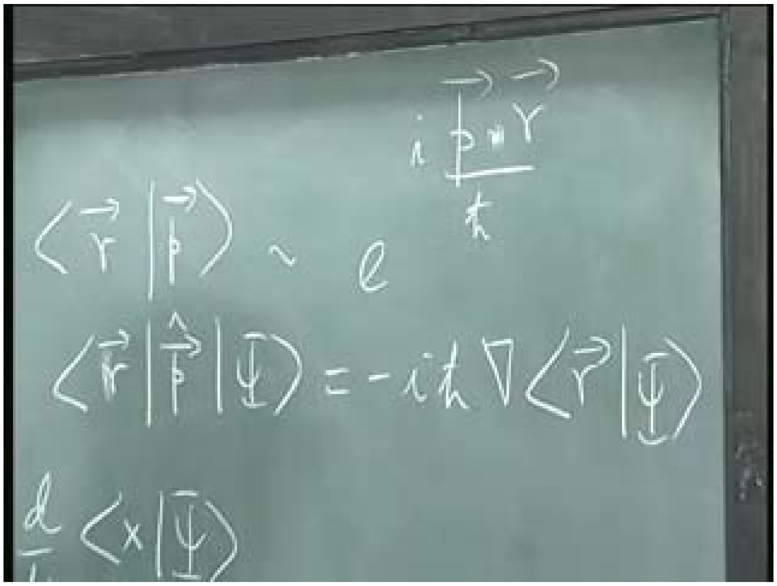

$$\langle \vec{r} | \vec{p} \rangle \sim e^{\frac{i \vec{p} \cdot \vec{r}}{\hbar}}$$

$$\langle \vec{r} | \hat{\vec{p}} | \Psi \rangle = -i\hbar \nabla \langle \vec{r} | \Psi \rangle$$

$$\frac{d}{\,} \langle x | \Psi \rangle$$

So if you have in three dimensions, the momentum eigen state p labeled by the moment of vector p and you ask what's its position space representative, this is proportional to e to the power i p dot r over h cross in three dimensions. And similarly the other quantity is e to the power -ip dot r. and in that case, this relation here (Refer Slide Time: 09:34) becomes r p operator acting on psi = - ih cross the gradient operator acting on r, psi. The gradient is with respect to r.

So we have this very important statement that in L_2 -infinity, infinity the representation of with momentum operator is in fact - ih cross the gradient operator. So that's the basic reason why differential operators appear so naturally in quantum mechanics because automatically starting with the original canonical commutational relation between a coordinate and its conjugate momentum, the derivative operator appears naturally. So this is why the Schrodinger equation for it turns out to be a differential equation. We can now write down the Schrodinger equation for a particle moving in space. Let's do this in three dimensions.

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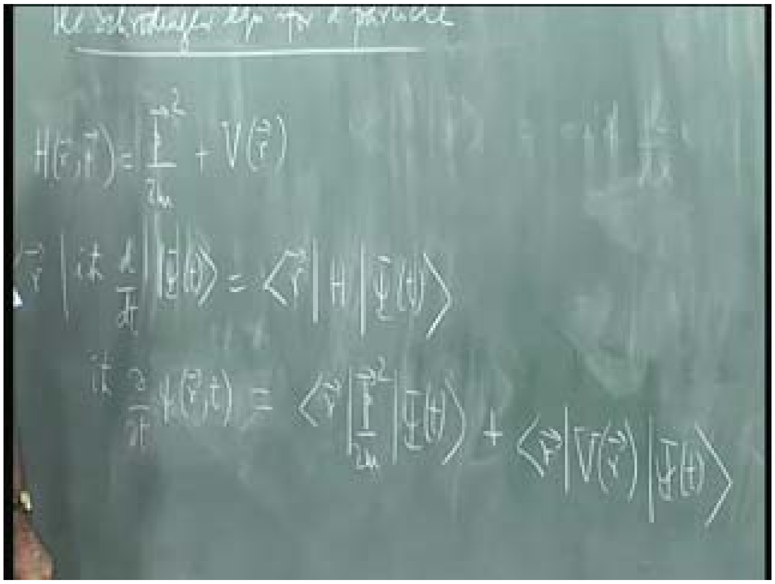

$$H(\vec{r},\vec{p}) = \frac{\vec{p}^2}{2m} + V(\vec{r})$$

$$\langle \vec{r} | i\hbar \frac{d}{dt} | \Psi(t) \rangle = \langle \vec{r} | H | \Psi(t) \rangle$$

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r},t) = \langle \vec{r} | \frac{\vec{p}^2}{2m} | \Psi(t) \rangle + \langle \vec{r} | V(\vec{r}) | \Psi(t) \rangle$$

We are now talking about non-relativistic physics. So the Hamiltonian of this particle is p squared over 2 m + some potential which is a function of the coordinates alone. The Schrodinger equation is ih cross d over dt psi of t equal to the Hamiltonian operator acting on psi of t. that's the abstract equation. The question is what does it look like in the position basis. And to do that all you have to do is to take the position basis, some particular labeled position Eigenstate r and take scalar products on both sides with respect to this. So out here I put r H psi of t (Refer Slide Time: 12:11).

I want you to note particularly the fact that this psi of t, the abstract state vector that is not burden by labels like r p and so on and so forth. That's just the state of the system. It's a vector in some Hilbert space. The variables that describe a physical system are in this case r and p and you talk about eigen states of those variables. But this (Refer Slide Time: 12:43) is some abstract state. It doesn't have any labels except it changes with time. So I could pull this out and write ih cross d over dt r with psi of t but this is the wave function of the particle in the position basis and I have got a name for this. So this is equal to psi of r and t. just the wave function and the position basis. But now this looks like a function of 2 variables and I must be careful to note that the time derivative acts on the explicit time dependence here.

Therefore this should really be written as ih cross delta over delta t. you make it completely unambiguous that this (Refer Slide Time: 13:48) t derivative is going to act on that t dependence, which came from the t dependence of the state vector. And this (Refer Slide Time: 14:00) is equal to on this side you have an r and then you have a p squared, which is an operator over 2 m acting on psi of t + r, a v of r and then a psi of t once again. We can now simplify both these terms. The matrix element of p in the position basis is - ih cross the gradient acting on r on psi. Therefore p squared is - ih cross gradient dot - ih cross gradient because p square is just p dot p.

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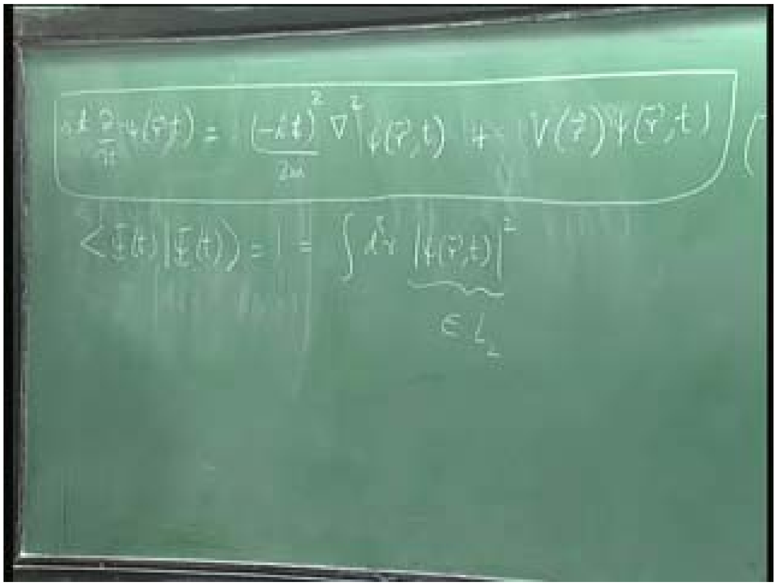

$$\boxed{i\hbar \frac{\partial}{\partial t}\psi(\vec{r},t) = \frac{(-i\hbar)^2}{2m}\nabla^2\psi(\vec{r},t) + V(\vec{r})\psi(\vec{r},t)}$$

$$\langle\Psi(t)|\Psi(t)\rangle = 1 = \int d^3r\, \underbrace{|\psi(\vec{r},t)|^2}_{\in L_2}$$

So it says ih cross delta over delta t psi of r , t = - ih cross squared del squared because del dot del is del squared when acting on scalars, over 2 m psi of r, t + a certain quantity. The psi acting on V(r) is unknown but I know about r operator acting on r bra vector as it just pulls out the real eigen value r. Therefore any function is an eigen state of a function of r as well and it pulls out just the corresponding function of r that v of r is. suppose thisV of r = r squared + e to the power - r as an operator, then it acts on this bra vector it pulls out r squared + e to the power - r as an eigen value. Therefore we could write this as V of r and now this is an ordinary function multiplying bra r with psi which is psi over r, t.

It's acting on a bra, so it should really be V star of r star. But now I am talking about Hermitian Hamiltonian. Since I would like its eigen values to be real, I have assumed this function V to be real. If its complex, then we should have to interpret what the imaginary part means. There are problems where there is need for complex potential. When you have a beam of particles impinging on a quantum mechanical target, part of it would be scattered and part of it would be absorbed. Then one uses a complex V in order to take into account absorption because then probability needn't be conserved. The Hamiltonian need not be Hermitian. So it is necessary to take into account those situations but right now I have in mind a particle in a real potential here.

So this is the position space wave function for particle and this is what you would have seen in the hydrogen atom problem. This is precisely what you have to seen in the hydrogen atom problem where V of r is Coulomb potential that an electron sees in a hydrogen atom. It's minus some constant over r. of course some simplification occurs in this partial differential equation when you have spherical symmetry. if V of r is spherically symmetric and depends only on the distance r without a vector sign, then it's convenient to take this del squared and write it out in spherical polar coordinates and solve the problem by separation of variables by assuming that this wave function psi of r vector, t is a product of functions of r, theta and phi. It's a complicated equation. It's not a trivial equation even for a single particle. Its first order in time and second order in the space variables here. Now it's a complicated partial differential equation. you need to specify initial values, boundary conditions and so on.

What boundary condition would you specify for a physical particle moving in three dimensional space? You would say that total probability of the existence of the particle is 1. Therefore you would normalize your psi of t by saying that at all instance of time this probability amplitude shall remain equal to one but that written out in the position basis is nothing but d 3 r psi of r, t whole squared. By d 3 r, I mean the volume element in real space. And that's true for all time. That condition is called the normalization condition. It implies therefore that this wave function psi of r, t, the position space wave function is a member of L_2 but L_2 with 3 independent variables x, y and z or r, theta and phi. It follows that this can only be true if as the radial distance goes to infinity, mod psi goes to 0. That's necessary but not a sufficient condition. It should go to 0 sufficiently fast that this number remains finite and bounded.

Now you can ask what sort of problems can I solve with this. Well, by separation of variables, you can solve all those problems where this partial differential equation splits in to equations for each of the independent variables. The separation into time is not very hard. But the separation of the space variables depends on the form of V of r. it's not very clear what would happen in general. In the equation for a free particle, there would be no V of r. then you can't normalize it because the free particle moves all the way from -infinity to infinity. And if it's in a momentum eigen state, it goes like e to the ip dot r whose mod is 1 and therefore cannot be normalized. Then you would pretend that you would put it inside a box of some size l and let l go to infinity. This is called box normalization. We will come back to this when we do the particle in a box problem.

But you could also ask in what coordinate systems does del squared separate in three dimensions. That's the problem purely in calculus and in turns out there are 11different orthogonal coordinate systems which are Cartesian, spherical polar, cylindrical polar coordinates, oblates spheroidal, prolate spheroidal, parabolic cylinder, elliptic coordinates and so on. There is a mathematical condition on what's called the Stackel determinant which specifies this. But this is not of too great interest because unless the potential has that kind of symmetry, you won't choose that particular given coordinate system. All spherically symmetric potentials is what you choose. If its Cartesian symmetry you choose Cartesian coordinates and so on, we will solve a few such problems. But this equation is what I would like you to examine and appreciate. Well, the first thing one could do is actually get rid of the time dependence. That brings us to the idea of eigen states of the Hamiltonian stationary states. A stationary state of a quantum mechanical system by definition is an eigen state of the total Hamiltonian of the system. Any stationary state is an eigen state of the Hamiltonian of the system. In general, the Hamiltonian operator may have very large number of eigen states. in general, an infinite number of eigen states. Anyone of them is called a stationary state.

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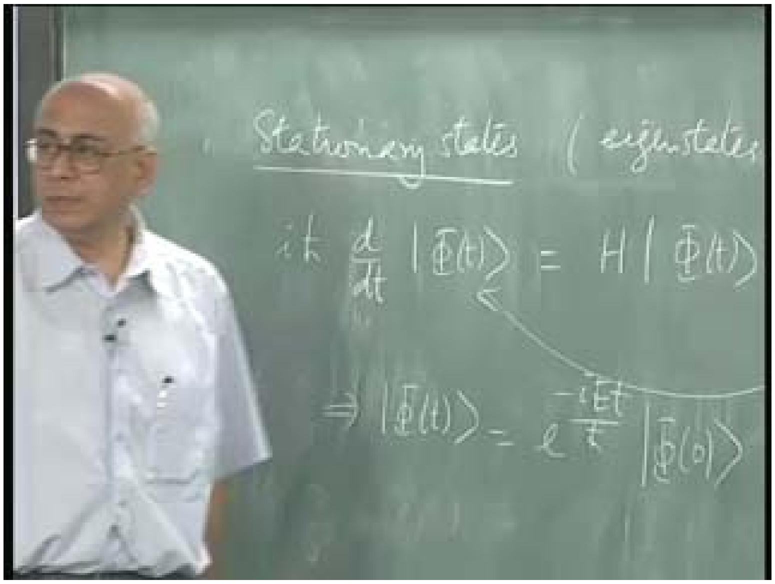

So eigen states of H itself says ih cross d over dt psi of t must be equal to H psi of t for any state. But if it’s an eigen state of the Hamiltonian, then H on psi reproduces the same state. Lets’ use phi for an eigen state of the Hamiltonian for the moment.

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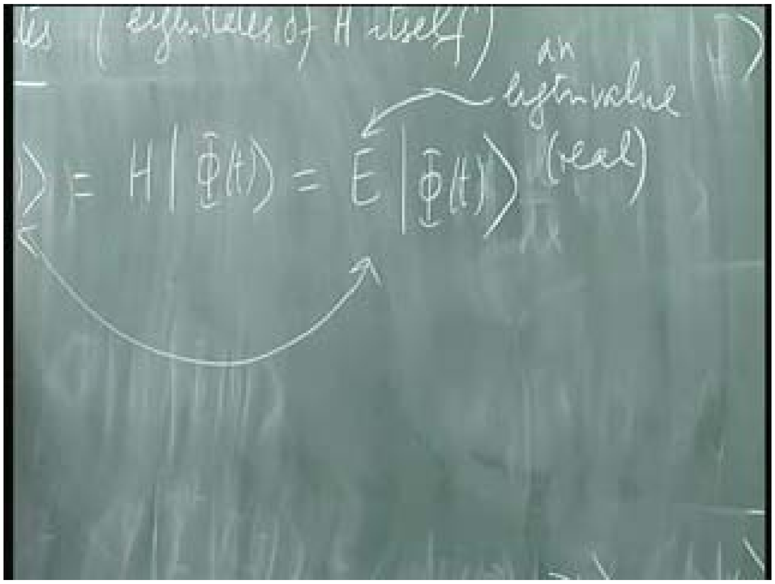

So this (Refer Slide Time: 24:01) is equal to phi (t) but this is equal to Eigen value times phi (t). since I know that the Hamiltonian classically in conservative systems really represents the total energy of a system, the value of the Hamiltonian gives you the total energy. I borrow that language and go over to quantum mechanics and I say the eigen of the Hamiltonian. let me call it E. as yet we don’t know whether this E is continuous or a discrete positive or negative we don’t care we do know its real and the reason is I insist that the Hamiltonian be made up of observables and therefore its eigen values are guaranteed to be real for the systems we are looking at.

So skip this (Refer Slide Time: 24:53) line and use this fact here so this guy is the eigen value and eigen value and its real and phi (t) is the corresponding eigen state. Of course there is no guarantee that phi (t) is unique for a given E. there maybe more than one such eigen state. And after all when you diagonalize matrices you know that an eigen maybe repeated in which case you have two or more eigen vectors for the same eigen value. If you have finite dimensional matrices, the eigen values are all discrete. n by n matrix can at best have n distinct eigen values but that’s not true when you have other more complicated operators. In general, the eigen value spectrum could be partly discrete, partly continuous and so on. To start with, it’s a real number.

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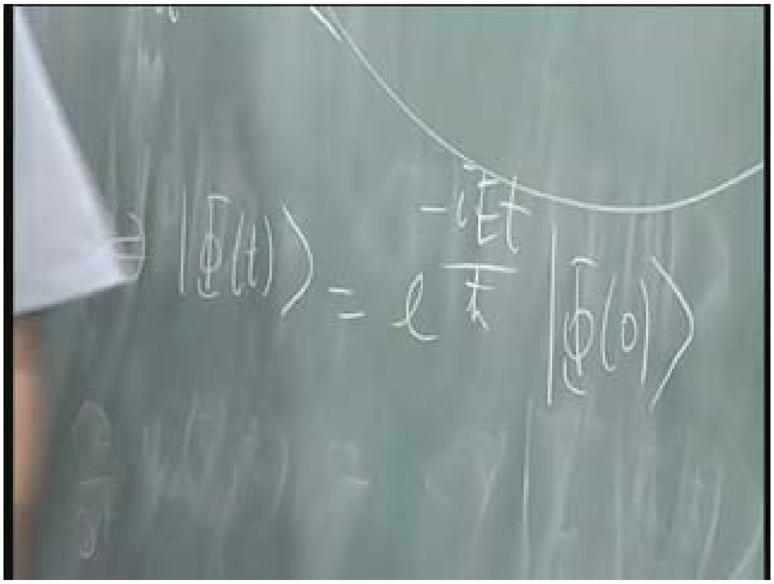

$$|\Phi(t)\rangle = e^{-\frac{iEt}{\hbar}} |\Phi(0)\rangle$$

Then it immediately follows that phi (t) is e to the power – i E t over h cross, phi of 0. In other words, the Schrodinger equation is solved trivially for an eigen state of the Hamiltonian. Moreover, the time dependence of the Hamiltonian of the state vector is just the initial state multiplied by a phase vector. A factor whose modulus =1. Whereas, that’s not true in general it is certainly true when you have an eigen state of the Hamiltonian that the time dependence of the state is utterly trivial.

Any factor of the form e to the i theta is called a phase factor or the modulus one complex number. Apart from a phase factor, the initial state persists. So if you have a quantum system in an eigen system of its Hamiltonian, it remains so. Apart from a phase factor which is unimportant in some sense because it doesn’t change the normalization; phi (t), phi (t) remains equal to phi of zero, phi of zero, a single exponent oscillating with a frequency which is equal to E over h cross. The reason it’s not true in general is because we can use this now to ask if I can use this to write down the Schrodinger equation solution in general.

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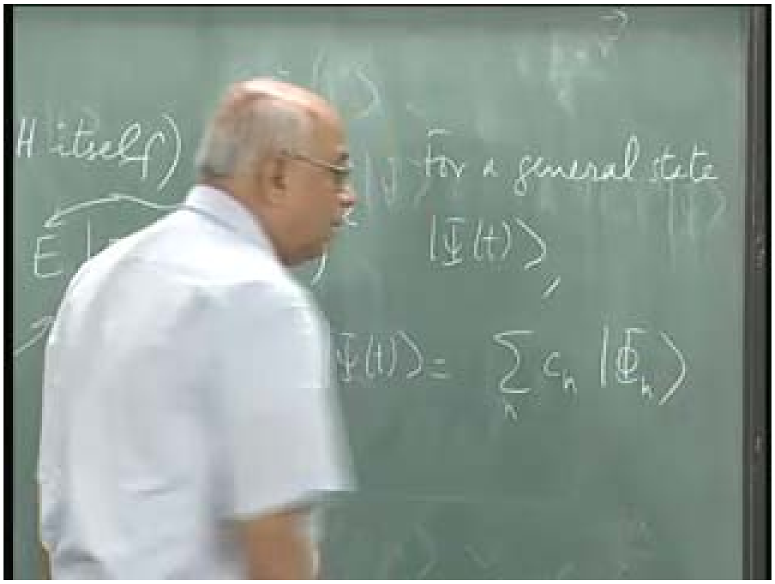

Well, for a general state psi of t, we could do the following. we could write psi of t = a summation over the eigen states of the Hamiltonian and lets pretend for a minute that the eigen states are labeled by some quantum number n. just a set of quantum numbers. Let me use the index n for it. We will see later that this n could be a continuous variable. But symbolically if it's written in this form C_n phi n where these (Refer Slide Time: 28:41) are eigen states of the Hamiltonian .Then its easy to say that I have two ways of looking at this.

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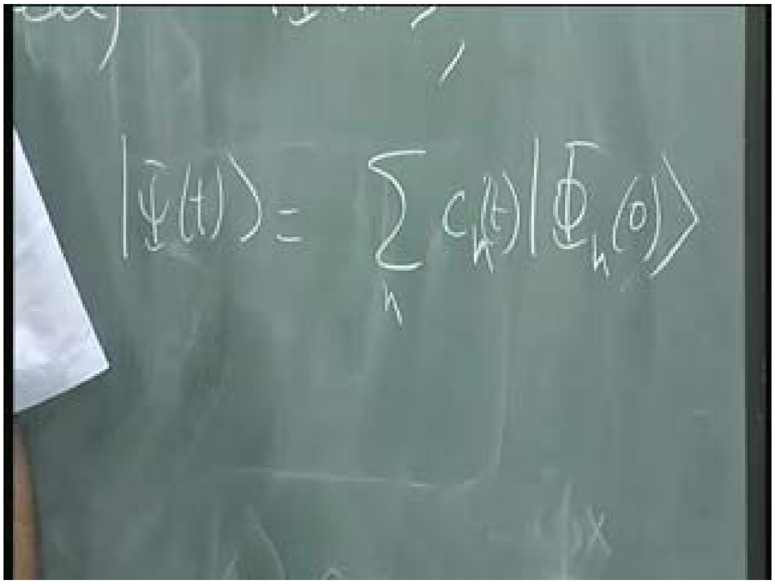

One of them is to say I will choose as my basis set phi $_n$ (0) at t = 0 in which case the time dependence of this gets thrown into Cn (t).

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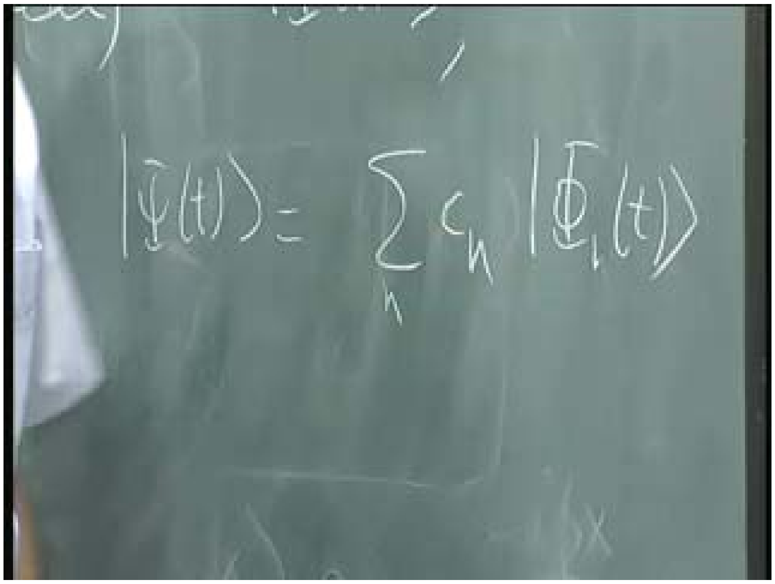

The other way of doing it is to choose my coefficients once and for all, in which case the time dependence gets thrown into this (Refer Slide Time: 29:11).

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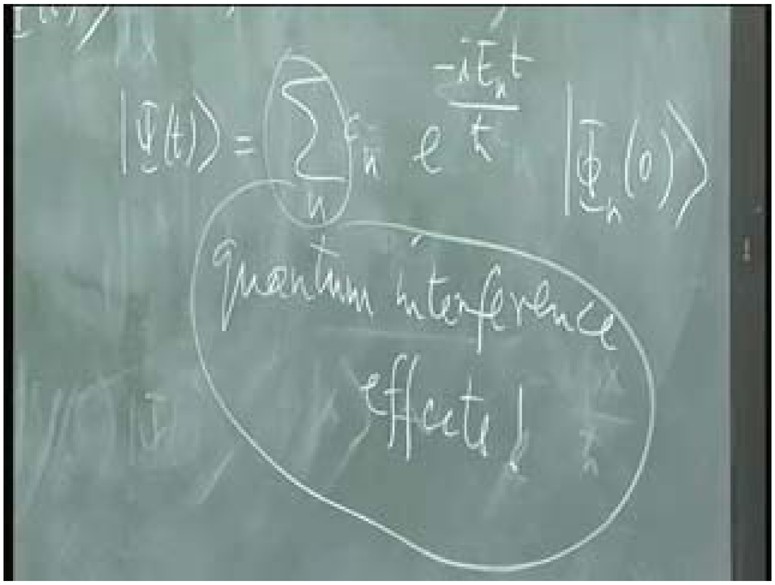

Now psi of t = summation over n C_n e to the power – i E_n t over h cross, phi n of 0. I will frequently use this without the 0 here but without any time argument. By that you must understand that I have chosen a basis set once and for all which is time independent. How do I notice it's a basis? There is a theorem which tells me that if I choose an appropriate set of mutually commuting observables pertaining to a system, then these are all adjoint operators. Then the common set of Eigen state is can be made orthonormal, is linearly independent and spans the space; in other words it forms a basis.

In suspicious cases, I should check whether I have covered everything. But right now take it as an assertion that the Hamiltonian in general, will provide such a basis set. You could ask what happens about degeneracy. Take again the hydrogen atom problem. The basis set is provided by the stationary states of the system which are labeled by 3 quantum numbers n, l and m. the energy happens to depend only on n but in the more general case, it would depend on n, l and m as well.

So I have used a single symbol to take into account all possible quantum numbers. In general, there will be more than one quantum numbers. In general, there would be as many quantum numbers as there are degrees of freedom in the system. And for a particle moving in space, there are three degree of freedom. That is why in potential problems in three dimensions there would be at least three quantum numbers.

There maybe more if there are internal quantum numbers in the system like spin, hypercharge, and strangeness and so on and so forth for elementary particles but there are at least three quantum numbers. The coefficients (Refer Slide Time: 32:07) are the overlap at t = 0 of phi n with psi and they are time independent. Now what is different about this as opposed to this in the time dependence? (Refer Slide Time: 32:13). There is a superposition of states here. There is a single state here and it's multiplied by a oscillating phase factor. Here you have time oscillating phase factors but there are different phase factors for different states. Notice carefully that as the state changes, they even change the energy eigen value to show that they are different for different states.

By the way e to the i E t is the sin and cosine. So think of it in terms of sins and cosines. You have got sin, a single frequency. That's just a sinusoidal wave but you add more and more frequencies. You add sinusoidal waves with different frequencies and then what happens is you could have interference. You could have beats, groups formed, modulation etc. so all the effects that you could have when you superpose more than one frequency would start appearing here (refer Slide Time: 33:29). In fact in general, if this spectrum goes up to infinity, then all kinds of wild possibilities happen. These different frequencies are in general not multiples of each other. So when you add up different time frequencies which are not even commensurate with each other, you could even have an aperiodic function. The function could become aperiodic which goes right up to infinity. It's not a Fourier series because that would happen if the E_n was just n. then you will have cos nt and sin nt. But they are some complicated functions of n. they may have n squared n cube and all sorts of dependences. So it can become horrendously complicated. in fact all quantum interference phenomenon happen because of this superposition implied here. (Refer Slide Time: 34:19). x and y coordinates are orthogonal to each other. A general vector in two dimensions is a superposition of something along x and something along y. they are orthogonal to each other. That’s the whole point so that the coefficients will uniquely determine this vector, psi of t. if they were not orthogonal, that’s not true. Then you have oblique coordinates. So I have assumed these have been orthogonalized by the Gram Schmidt procedure and there is a superposition and the time dependence is exceedingly complicated. It need not even be periodic. It could be almost periodic or quasi periodic. It could be very complicated in general. So it need not even have periodicity. They are highly irregular functions. So it’s not a Fourier series at all. In principle it’s written down very easily. But in practice this is a very intricate function. So this summation here (Refer Slide Time: 35:39) leads to quantum interference effects. Let’s see what happens in the position basis in a similar situation.

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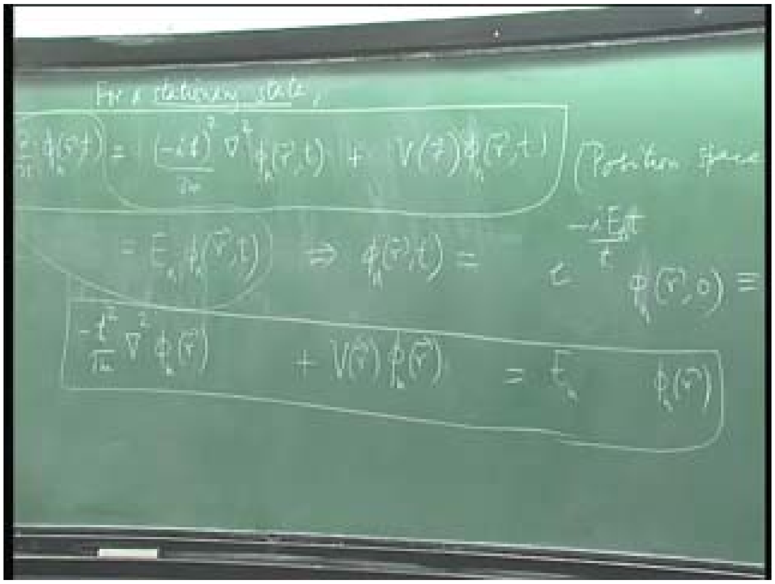

Well, all we have to do is to plug this whole thing here (Refer Slide Time: 35:55) and write this as equal to E psi r and t because I know ih cross of r and t is E psi of r and t. you have to solve this equation. Now what does ih cross delta over delta t psi equal to E psi imply? This immediately implies that psi of r, t is proportional to e to the power - iEt over h cross. Only then if you differentiate with respect to t, you end up with this quantity here (Refer Slide Time: 36:42). What does the constant of proportionality depend on? It can depend on r. so I shouldn’t call it a constant. I should immediately say this is equal to a function of r times this (Refer Slide Time: 37:00).

What notation shall I use for that function of r? It’s the value of psi of r, t at t = 0 because if I put t = 0, the exponent goes to one. So without any loss of generality I could really write this as psi of r, 0. Let’s change the state vectors as phi with a subscript n. Again that this little n which is labeling the eigenstates of the Hamiltonian, it may actually be more than one label. It could be a set of quantum numbers. So this is what a given position space wave function would do for a stationary state.

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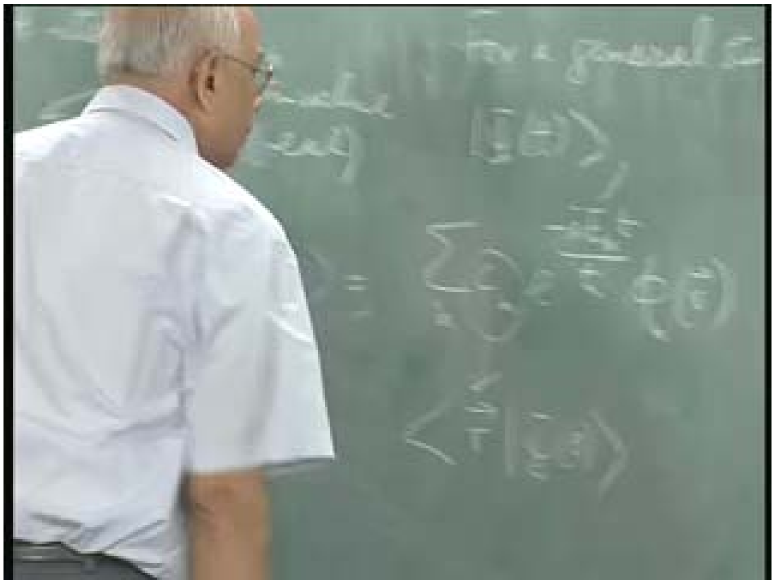

And of course this expansion that I have written down here, if I now work in the position basis and I write a r here, that goes right across and hits this (Refer Slide Time: 39:40). This becomes phi n of r. and what is c_n? It was the overlap in the position basis between r and the state of the system at t = 0. So it says that general state at time t in the position basis, the wave function is just given by the superposition. The crucial thing here is to find out what are these functions and how do I solve them? Well that I solve by putting it back in here (Refer Slide Time: 40:40). I use that fact that H psi = ih d over dt psi, but I use the fact that this phi is a stationary state by saying H psi = E psi and I solve it and the solution looks like that for each of these eigen states (Refer Slide Time: 40:55)

Now I put that back in this (Refer Slide Time: 41:02) portion out here. it says - h cross squared over 2 m del squared phi n of r times e to the power - i E_nt by h cross + V (r) phi n of r e to the – iE_nt by h cross = En times phi e to the - iEnt by h cross phi n of r. that's what the Schrodinger equation becomes for a stationary state. But there is no derivative with respect to t. I have removed it. I have in fact solved the t dependence here. And this (Refer Slide Time: 41:58) factor of course cancels out. That's exactly what happens when you separate variables and I am left with this equation here. For each Eigen state, the position space representative of that eigen state satisfies this partial differential equation (refer Slide Time: 42:24). It's still a partial differential equation but at least you have got rid of the t. and of course if you work in one dimension, it's an ordinary differential equation. This is called the time independent Schrodinger equation. What's the difference between the time dependent Schrodinger equation and the time independent Schrodinger equation as a differential equation? The second one is an Eigen value equation.

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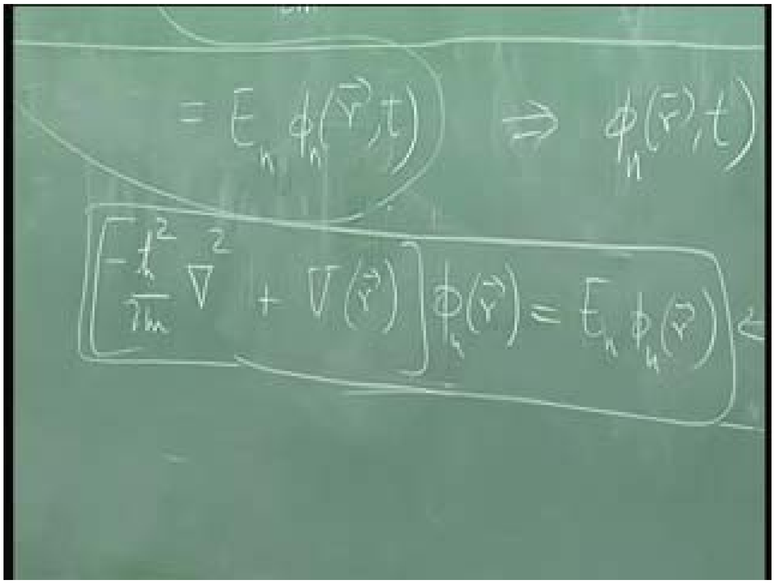

This (Refer Slide Time: 44:00) quantity here says take this differential operator del squared + V of r, act on phi n of r and you are guaranteed to get a real number times phi n of r. this is an eigen value equation. It’s a homogeneous equation. So is the other one because if you multiply phi by a constant. Then of course you solve this, subject to boundary conditions now, there is no time here, so impose normalization if you like and then outcome the eigen values.

Now what we are going to do is to take the time independent Schrodinger equation or the eigen value equation, and the statement is if you give me a general state of the system, no matter what it is and you tell me the initial state, I will tell you the future state by actually computing these eigen functions, substituting in this equation here (Refer Slide Time: 45:26). This (Refer Slide Time: 45:31) is a constant which tells me at t = 0 and that gives me the solution at anytime. So that’s the strategy. You have to find the Eigen values of the Hamiltonian and after that the general time dependence of the state is obvious. It’s just a superposition of these Eigen functions with suitable phase factors. So this is the way you would solve in principle, the Schrodinger equation.

So we exploit the fact that the Hamiltonian plays a very special role it’s the generator of time translations for the system. So it’s not surprising that the time dependence of its eigen states is particularly simple and that is used to put in the time dependence of a general state of that. But the price you pay is you have to solve an eigen value equation. And now it turns out that very interesting things happen when you have an eigen value equation because you are familiar with the vibrations of a string clamped at both ends. You have a secondary wave operator, its eigen values and eigen functions would depend not only on the operator but also on the boundary conditions. If you have a string which is clamped at both ends or left one end loose and the other end free, the normal modes change completely. So not only is this differential operator important but its boundary conditions are also important in determining the spectrum.

We will see in a minute that if you put the particle in a box, the energy levels get quantized. Immediately as opposed to a free particle, this could have any energy from 0 to infinity. As soon as you put it inside a box, even if it’s free inside the box, the boundary conditions will ensure that only a certain set of energy is allowed. So that’s going to emerge as a consequence here. So let me make this general statement that any confinement of a quantum system tends to quantize something. So you have put a particle in a box, it quantizes the energy levels. You put in a potential which is a confining potential again, the energy levels get quantized under suitable conditions. You take angular momentum and you know angular momentum is quantized in units of Planck's constant, and the reason is the corresponding dynamical variables, the angles really don’t run from - infinity to infinity but run from 0 to 2 pi for the Azimuthal angle and 0 to pi for the polar angle. That is enough to produce quantization.

So when Schrodinger first solved the wave equation and he wanted to reproduce the hydrogen atom spectrum, he wasn’t sure how he was going to produce a discrete spectrum. Because you put hydrogen atom you put an electron in the Coulomb potential of proton, there is no box. There is no confinement. The potential extends all the way to infinity. So where is the confinement? when he consulted David Hilbert at Gottingen, the greatest mathematician of the time, pointed out to him that the requirement of square integrability of the wave function which was needed for total probability =1 is sufficient to say the requirement of special case of square integrability, meaning that the wave function has to belong to a L_2. That boundary condition is enough to make the spectrum discrete. In the hydrogen atom, that was certainly the case. So even a condition like without a physical box, just the fact that the whole wave function mod squared must be finite, when you integrate, that is sufficient to produce a discrete spectrum.

So an important lesson, in eigen value equations the eigen value is determined not just by the operator for differential operators but also by the boundary conditions. That specifies the class of solutions. So the spectrum itself is determined by the operator plus the boundary conditions always. So let’s take that problem and simplify it enormously to do our one dimensional particle in a box problem. We will complete this tomorrow but let me set it up now.

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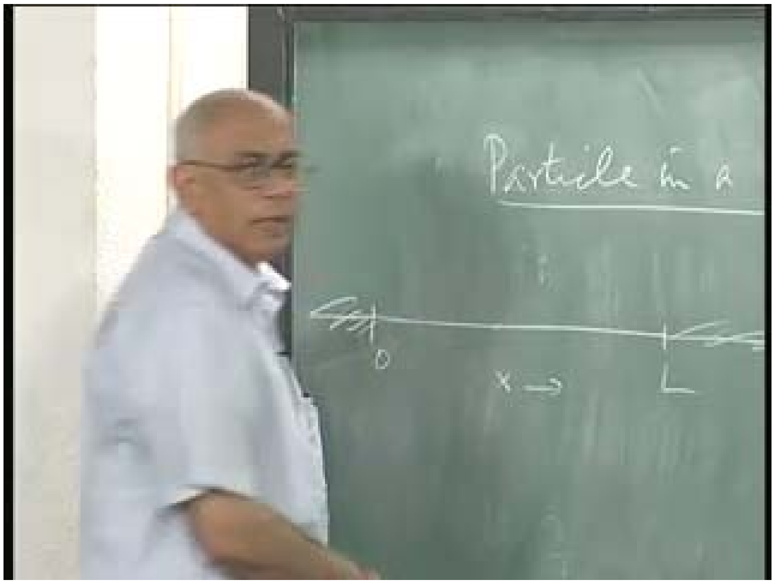

Sometimes it’s called free particle in a one D box but I will point out to you that is not as free as all that. So now I have the x axis and on the x axis, from 0 up to l on the x axis I have a box and there is a quantum particle put inside it. The outside of the box is not accessible to the particle. And I assume that the walls of the box are perfect reflectors. No absorption at the end. Classically this is a very simple problem to solve. So let’s do this completely classically, figure out what happens and then come back to the quantum problem. We will write down the Schrodinger equation and solve it. Because a fairly surprisingly large part of quantum phenomenon can actually be understood by this trivial list of problems. So let me use this as a kind of exercise which we can do very easily in order to explain all these phenomena one by one.

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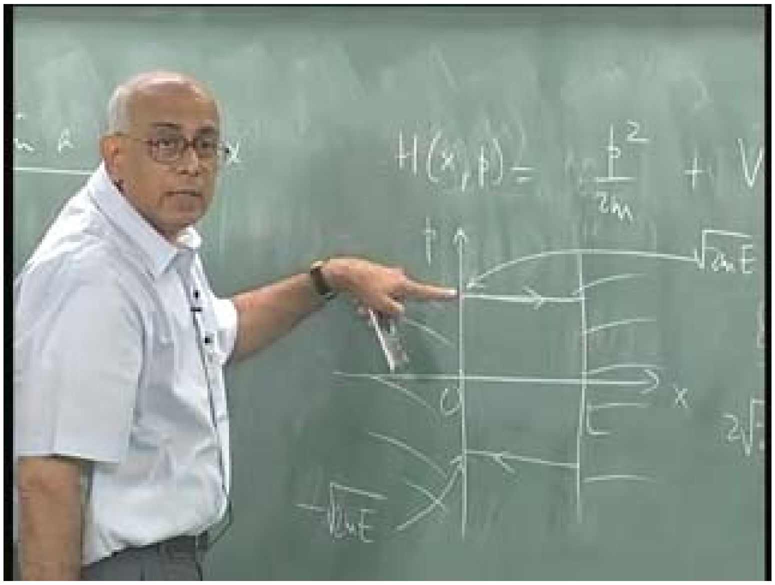

The first thing we have to ask is what the Hamiltonian of the particle is. Classically the Hamiltonian of the particle is just p squared over 2 m. just the kinetic energy + a potential. So let's write that potential as a function of x alone. This potential is zero inside the box and I don't want the particle outside. So it's infinite outside rigid walls. What does the phase diagram look like?

There is x, (Refer Slide Time: 52:50) here is p, this particle can only exist between zero and l. so this is a forbidden region and that's a forbidden region and then depending on what you do inside, what the initial conditions are, the particle will start moving. so classically if you start at some point here and its moving with a velocity, with a momentum p, let's say it goes up here (Refer Slide Time: 53:07) it slams against the wall momentum reverses comes back here and keeps doing this. So it's quite clear that this is going to just be straight line trajectories. so if it starts here (Refer Slide Time: 53:20) it goes up there, it hits the wall, it reverses momentum, comes back here, hits this wall, jumps up, reverses and keeps following this trajectory. And you have to specify for me the number p which is equivalent to specifying the total energy.

So this (Refer Slide Time: 53:41) intercept is square root of 2 m and this (Refer Slide Time: 53:43) intercept is - square root of 2 m. that's the phase trajectory. It's discontinuous at the two ends because this particle instantaneously reverses momentum. There is nothing more. That's it for any p. it is just going to back and forth in this fashion. Let's do for Bohr-Somerfield quantization.

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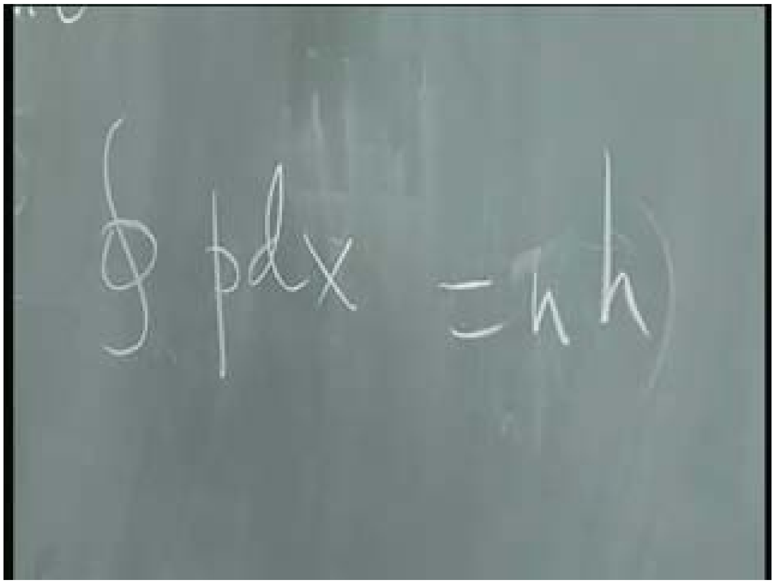

$$\oint p\,dx = nh$$

The old rule set integral for a periodic orbit pdx was equal to Planck's constant times an integer. That’s the Bohr quantization rule. This was postulated Niels Bohr. Of course after the Schrödinger equation came in, this got thrown out but its actually back and this is the semi-classical result. I will come back and explain why this is a very profound result. Suppose we apply that to this problem. The integral pdx over a closed period is the area of this thing here (Refer Slide Time: 54:57).

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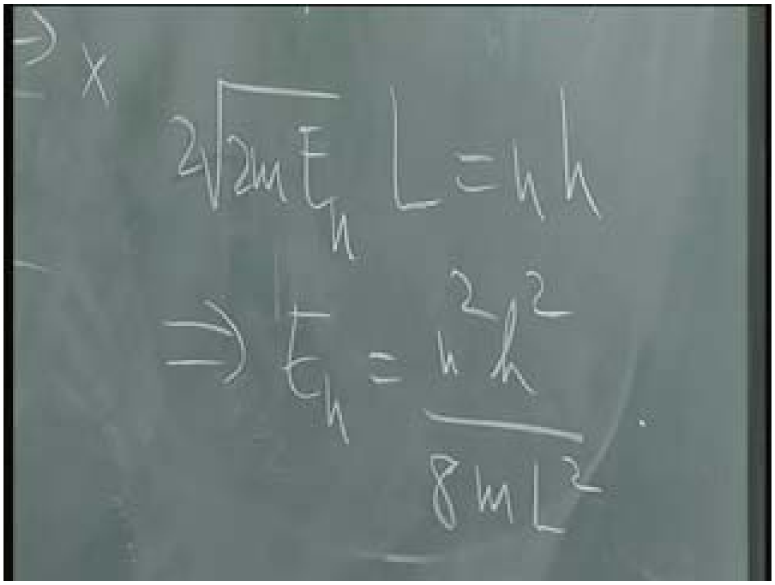

$$2\sqrt{2mE_n}\,L = nh$$

$$\Rightarrow E_n = \frac{n^2h^2}{8mL^2}.$$

That area is the area of the rectangle which is twice square root of 2mE this length multiplied by the length L times is equal to nh. That must be true for n = 1, 2, 3, etc. So let’s label the E writing E_n and this immediately implies that E_n = n squared h squared over 8 mL squared. So it immediately predicts quantization of the energy. It says these are the only allowed values for the energy.

What we have to see is whether the exact Schrodinger equation which we are going to solve, imposing correct boundary conditions, reproduces that. And in this case this was believed to be true only for sufficiently large n but it will turn out here that in this case, this is in fact true as an exact result. If you solve the Schrodinger equation, this is exactly what you get and we will try to understand why this is true. So that will be our starting point tomorrow. We will start with the time independent Schrodinger equation in one dimension for the simple potential problem and try to solve this. Meanwhile think a little bit about whether the energy Eigen states are also position Eigen states are not for this particle. Thank you!