Quantum Mechanics – I
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Lecture - 23
The Schrodinger Equation

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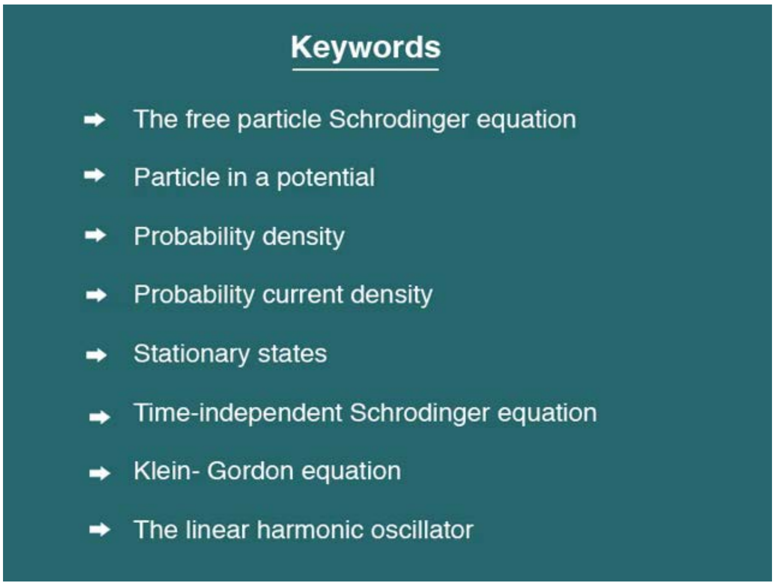

In the last couple of lectures, I spoke about, position representation, where we dealt with function spaces.

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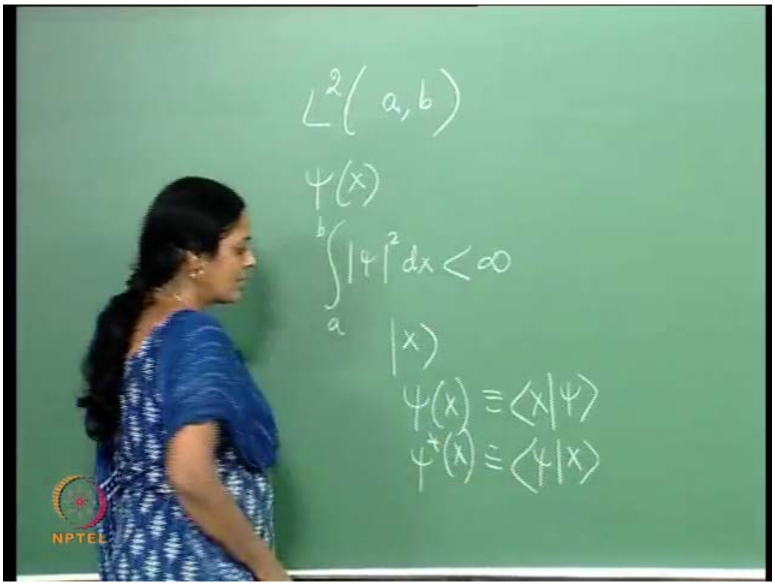

In particular, we spoke about L 2 of a b and functions in the space, or functions of a real variable x. And they satisfy, the condition of square integrability, d cube x d x, whatever, within that region of integration, is less than infinity. So, this is the function space that we are interested in and we introduce the position basis. It is a continuous basis and functions psi of x in the Dirac notation, are represented in this manner. There is a very logical reason why function psi of x is really this in a product. And therefore, psi star of x is represented in this manner.

Now, in this function space, wave mechanics is structured and the Schrodinger equation, really pertains to the behavior of the wave function psi of x, which describes the state of the system and abstract ket psi, represented in the position basis and that is called the wave function. So, basically in this lecture, I wish to continue with, the Schrodinger equation and the concept of stationary states.

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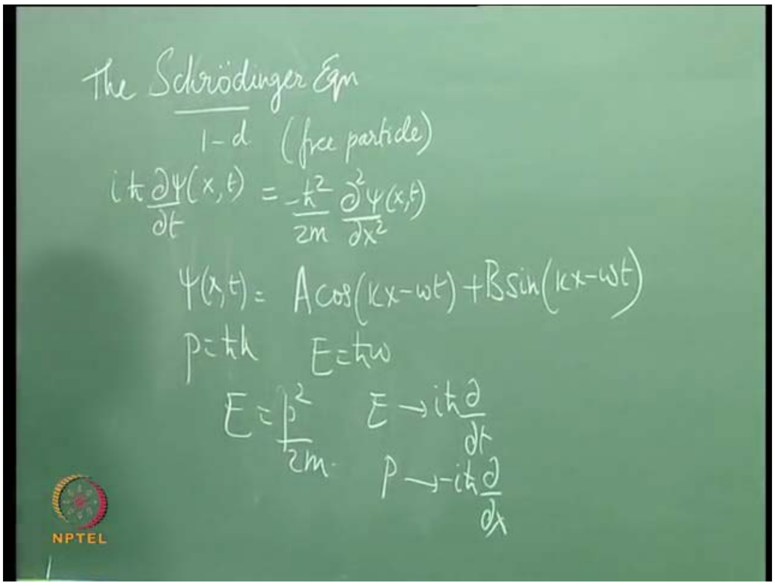

So, the Schrodinger equation, so, there we are and we stopped at a point where we said that. If, psi were a function, of x and time and this is in 1 dimension, 1 space dimension. For a free particle moving in 1 dimension, a free particle of mass m. We had this equation and this allowed for plain wave solutions. So, basically psi of x t, was of the form A cos k x minus omega t, plus B sin k x minus omega t. But, the momentum p was h cross k. There was an energy E of the particle, given by h cross omega.

And since, in classical physics for a free particle, we would have started with this equation. The analog in quantum mechanics, is to replace E by the operator i h cross delta by delta t and p by the operator minus i h cross delta by delta x, in 1 dimension. And therefore, when I put hats on these 2 objects and write E as i h cross delta by delta t and p as minus i h cross delta by delta x. I get this equation. This is called the classical quantum correspondence, at the level of replacing energy and momentum, by their respective operators; it is 1st order differential operators.

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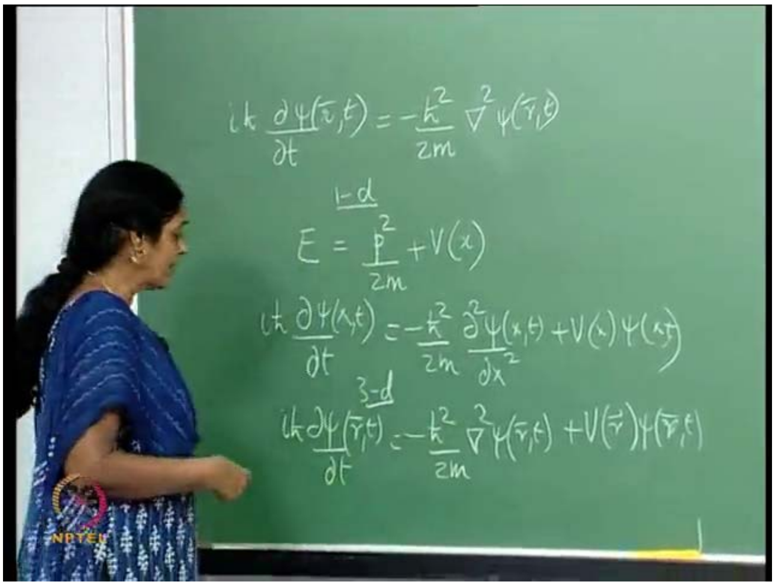

Now, suppose I have to generalize this equation. The Schrodinger equation to 3 dimensions, I will now, have psi as a function of r. Where r has three components, x y and z in Cartesian's and since p itself is minus i h cross del. The differential operator here is replaced by del squared. Where you have delta by delta x, you now have del squared. So, this is the equation for a free particle of mass m, moving in 3 dimensions. It is free therefore, there is no potential term. Now, suppose there were a potential term, let us go back and look at how we got this. In classical physics, the total energy would be the kinetic energy, plus the potential energy. This is in the position representation.

So, the potential is going to be a function of x, in 1 dimension for instance. And therefore, if I now put in this potential and write the Schrodinger equation, for a particle of mass m and momentum p, subject to a potential V of x. I have the following, now in 1 dimension, psi of x t and that is all there is to it. Of course, if I have to write the

Schrodinger equation, for a particle in 3 dimensions, subject to a potential straight forward, del square now. So, that is what we have. So, this is the Schrodinger equation for a particle subject to a potential V, is a function of r.

For the moment and for quite considerable part of the course, I would assume that, this potential is a real function of space. Because, if the potential had a complex part, that would correspond to the presence of sources and sinks. And that class of problems is not what I wish to consider now. The given this equation, I can see quite a bit happening from here.

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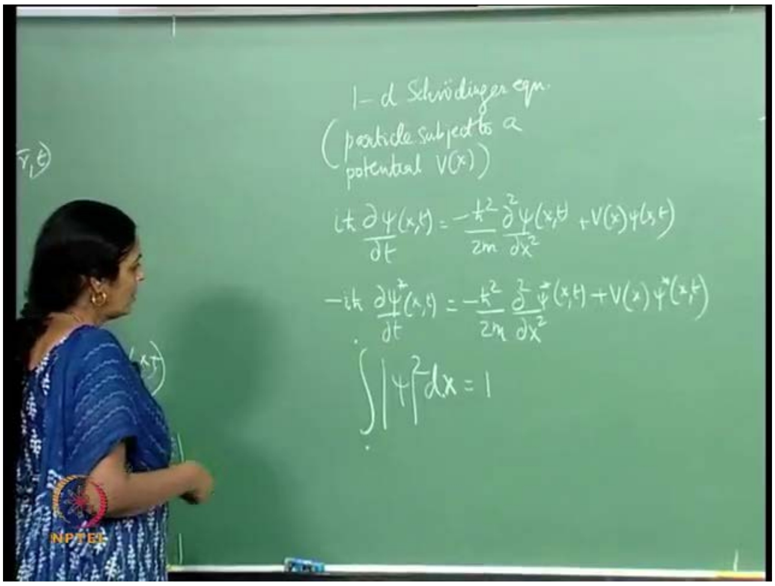

First of all psi is complex. Let us, go back to the 1 dimensional case. Schrodinger equation, particle subject to potential V of x, psi is complex in general. So, I have the following equation and then, I have an equation for the complex conjugate, which reads minus i h cross delta psi star by delta t, is minus h cross squared by 2 m, delta 2 by delta x squared psi star of x t. V is real? And therefore, I have this equation. Explicitly there is an, i that is occurring and in that sense it differs from the diffusion equation. Otherwise, there is a correspondence between Schrodinger equation and the diffusion equation.

But, there is this i, that is present there and that is the specialty of the Schrodinger equation. In general, all solutions psi or psi star cannot represent the state of the system. The instantaneous position being given by the value of x, at a given time taken on by the time parameter t. Psi has to satisfy certain boundary conditions a nd it is clear that since, we are looking at systems where, the probability of existence of the system is 1. And mod psi squared, is the probability density and we require this between the limits of d x to be 1. That is the total probability to be 1. It is clear that, the wave function psi and therefore, psi star have to belong to L 2 to the space, to the linear vector space L 2, the space of square integrable functions. Now, here I can do the following. I can pre multiply this by psi star and this by psi.

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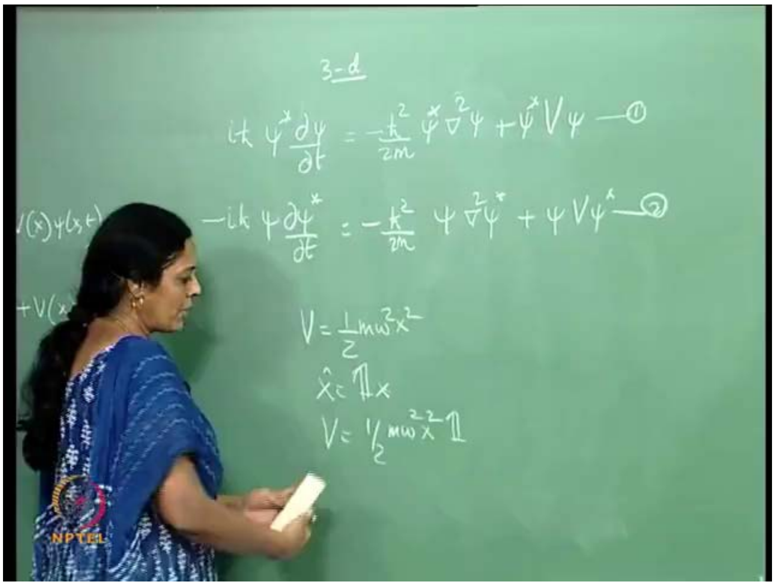

Then the 1st equation becomes, i h cross psi star, delta psi by delta t. I could do it in 3 dimensions if you wish. And therefore, let me just do it in 3 dimensions. I would not write the argument r of t, minus h cross squared by 2 m psi star, delta 2 psi by, or del squared psi now, because we are in 3 dimensions; plus psi star V psi. That is my 1st equation. The 2nd equation (Refer Slide Time: 07:36) I can just multiply this by psi and I have minus i h cross, psi delta psi star by delta t, is minus h cross squared by 2 m, psi del squared psi star now, plus psi V psi star. That is my 2nd equation.

Dough, remember that psi is a function of x, scalar function of x and so, as V, in the position representation. For instance, if you looked at a potential, which is quadratic like in the case of the oscillator. V is half m omega squared x squared and therefore, V of x. V would normally have been an operator, but, since this operator X is merely identity times x. V is half m omega squared, the number x, x squared times identity if you wish. When I am going to suppress that and I just write V as half m omega squared x squared.

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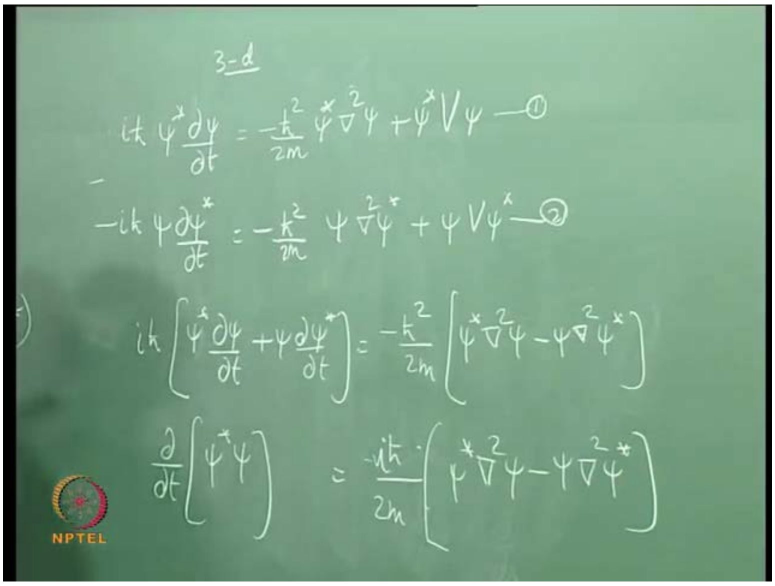

The point is that, these objects commute, in general and therefore, if I subtract 2 from 1. I have i h cross, psi star delta psi by delta t, plus psi delta psi star by delta t. Is minus h cross squared by 2 m, psi star del squared psi, minus psi del squared psi star and these 2 terms, the potential term cancels out. I can always write this as, delta by delta t of psi star psi. That takes care of these 2 terms. Is minus h cross squared by 2 m i h cross and that just gives me a minus h cross by 2 m I, which gives me an i h cross by 2 m. So, I have an i h cross by 2 m, psi star del squared psi minus psi del squared psi star. This is what I have. Now, this looks like a continuity equation, because, I can bring this, to the other side.

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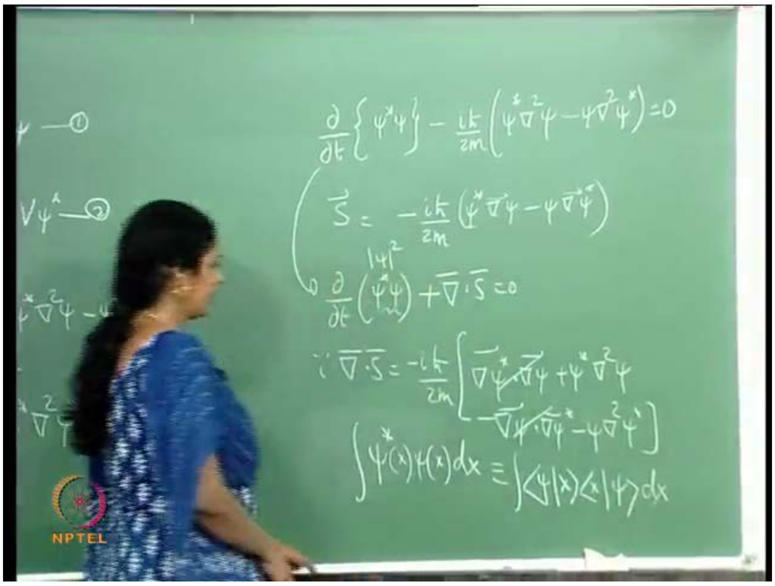

And I have, delta by delta t of psi star psi, minus i h cross by 2 m, psi star del squared psi, minus psi del squared psi star, equals 0. Define the quantity S, which is a vector. As minus i h cross by 2 m, psi star del psi, minus psi del psi star. It is a 3 dimensional vector; it is a vector on the rotations in the 3 dimensions, because, the gradient operator has a vector sign on top of it and then this equation simply becomes, plus del dot S equal 0. Because, del dot S, is minus i h cross by 2 m.

If you expand this, it is grad psi star dot grad psi, plus psi star del squared psi, minus grad psi dot grad psi star, minus psi del squared psi star. And then, these 2 terms cancel out. Giving me what I want there and therefore, with this definition of S. I have a continuity equation delta by delta t star psi star psi, plus del dot S equal 0. This object is strictly positive. Its modulus of psi, the whole squared. In 1 dimension integral, psi star of x, psi of x d x. In Dirac notation that is identical to integral, bra psi a complete set of states, ket x bra x. That integral gives me identity ket psi d x.

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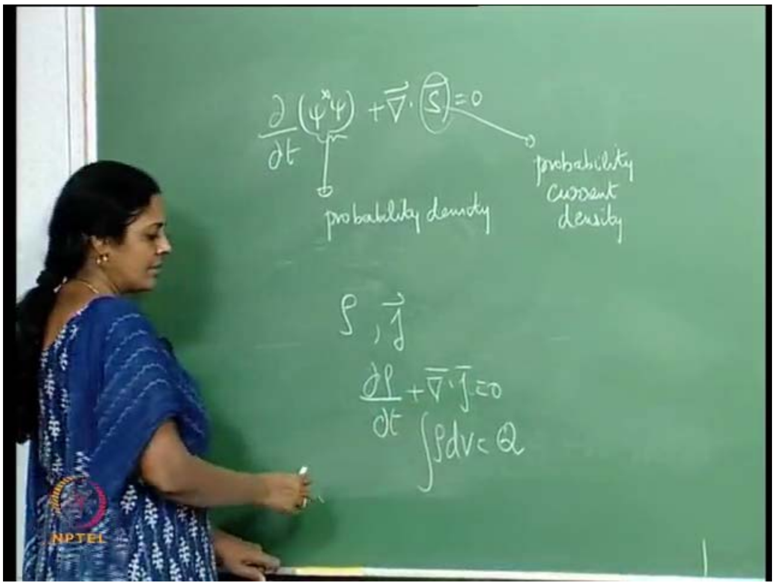

Returning to the continuity equation, I have delta by delta t, psi star psi, plus del dot S equals 0. This object is called the probability density, for very good reasons, because when you integrate over it. You get the total probability integral psi star psi d x, psi of star of x psi of x d x integral. That is the total probability and that is 1. And this object here is called the probability current density, because, it is a vector. This is analogous to the equation that you might have seen when; you did a course on electromagnetic theory. Where, given a static distribution of a given distribution of a charges.

Which, charge density rho and current density j, delta rho by delta t, plus del dot j was equal to 0 and that was, a continuity equation that you had there. This is analogous to that, except that the interpretation here is that this object psi star psi is a probability density and this is a probability current density. You might recall that, few did an integration over a space here, integral rho d v was a total charge and you showed that, the total charge was conserved. You would have shown in electromagnetic theory, that the total charge was conserved, provided certain boundary conditions were met.

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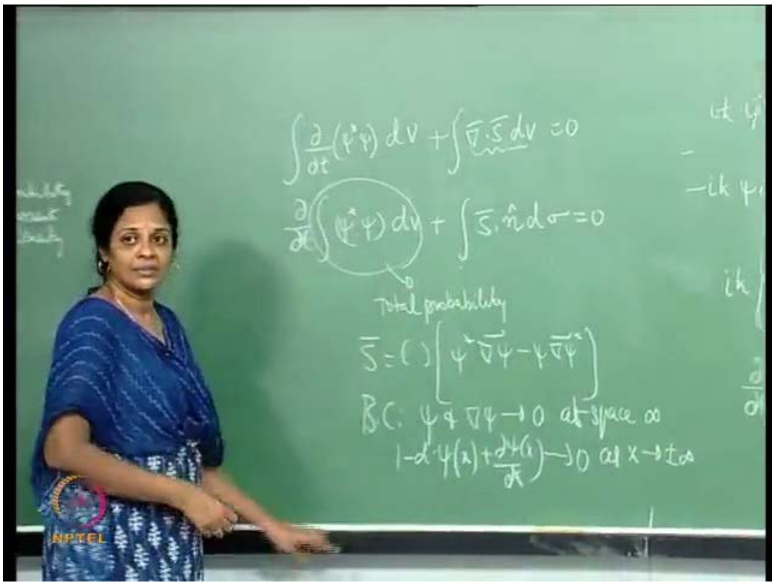

Let us precisely, what we are going to do in this context as well, because, if you look at the continuity equation in this case and do an integration over x, or over the volume, because, we are now, doing it as a 3 dimensional problem. Integral d v that is the volume, plus integral del dot S d v, that is the elementary volume. That quantity is equal to 0. I can always pull this outside and I have since, the integral is over the space. This, I can use Gauss's theorem and I can write this as a surface integral. Where d sigma is an elementary surface area, n is the unit normal and S dot n is a component of S along the direction n, perpendicular to the surface.

So, this quantity is equal to 0. The fact that the total probability. That is interpretation in quantum mechanics, the fact that the total probability does not change in time. That if you normalize the wave function, such that the probability. The total probability is 1 at a given time. The total probability that the system exists, does not change in time. That implies that delta by delta t of this quantity is 0, which means, that the surface integral should vanish and indeed does, because, of the boundary conditions. Because, S is essentially psi star grad psi, minus psi grad psi star and since, this is a surface boundary. This is the entire volume, the surface boundary is again at infinity.

So, the requirement is that, the wave function and the derivative. The 1st derivative of the wave function vanishes at infinity, space infinity. That will see to it, that S vanishes sufficiently fast. So, that this term drops out and I have delta by delta t of the total probability is equal to 0, which means the probability is conserved. The statement that probability, total probability is conserved holds for all instance of time. So, that is what we see here and therefore, this automatically takes care of the boundary conditions, for solving the Schrodinger equation. The boundary conditions are the following: the wave function and the derivative go to 0, sufficiently fast, as at space infinity.

So, in 1 dimension, psi of x and delta psi by delta x, in 1 dimension they go to 0 sufficiently fast, as x goes to plus minus infinity and so on. So, these are the boundary conditions. So, when we work with the Schrodinger equation, it is really the fact, that probability should be conserved, the total probability should be conserved, which gives rise to this boundary condition. That the wave function vanishes at plus minus infinity space infinity, we are talking about 1 dimension at x, plus minus infinity. And as x goes to plus minus infinity the 1st derivative also vanishes, goes to 0 sufficiently fast.

So, given these boundary conditions, the Schrodinger equation can be solved. Because, it involves a 2nd derivative with respect to x. And I have 2 boundary conditions. So, we can treat in the case of the time independent Schrodinger equation. We can treat this as an Eigen value problem. I will show you how to do that shortly. Impose these 2 boundary conditions. Find the Eigen values and Eigen functions. We understand, that if the potentials time is independent, as is the case here. The case that, I have been considering.

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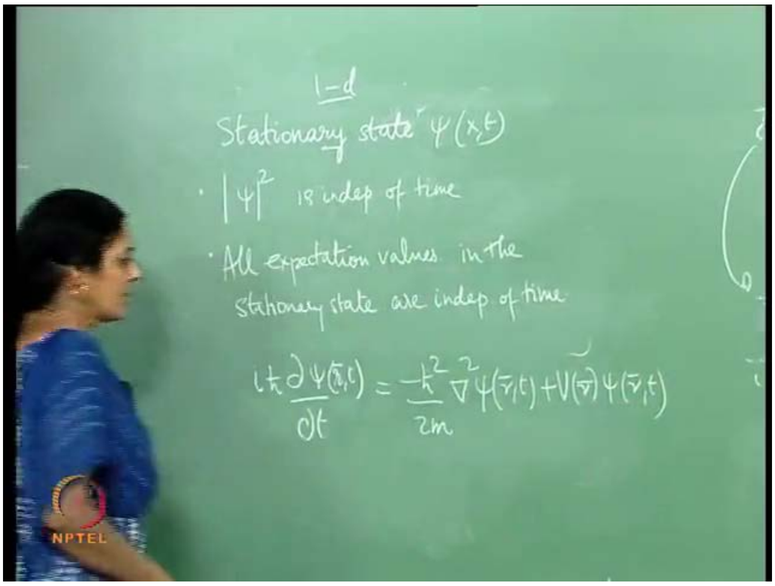

There are some, very interesting states called, stationary states. Stationary states, or wave functions, which behave like stationary states of the system, which represents stationary states of the system, satisfy the following property. First of all mod psi squared, stationary state psi for instance, in 1 dimension, can always generalize it to 3 dimensions, mod psi squared is independent of time.

All expectation values, of observables, relevant observables. In the state psi, are independent of time. They conserved in time and in general, if you have a stationary state of the system, if the system is in stationary state. You will find that the energy levels are essentially partially discrete at least. It would not be a continuous set of energy levels. The energy spectrum will at least have, some of the levels being discrete. Now, given this, I want to find out. How exactly I get stationary states of the system, when the potential is time independent? So, let us look at the equation, i h cross delta psi by delta t, let us start with 3 dimensions, is minus h cross squared by 2 m, del squared psi of r t, plus V of r psi of r t.

Let us see, if it is possible to consistently separate psi, into a space dependent part and the time dependent part.

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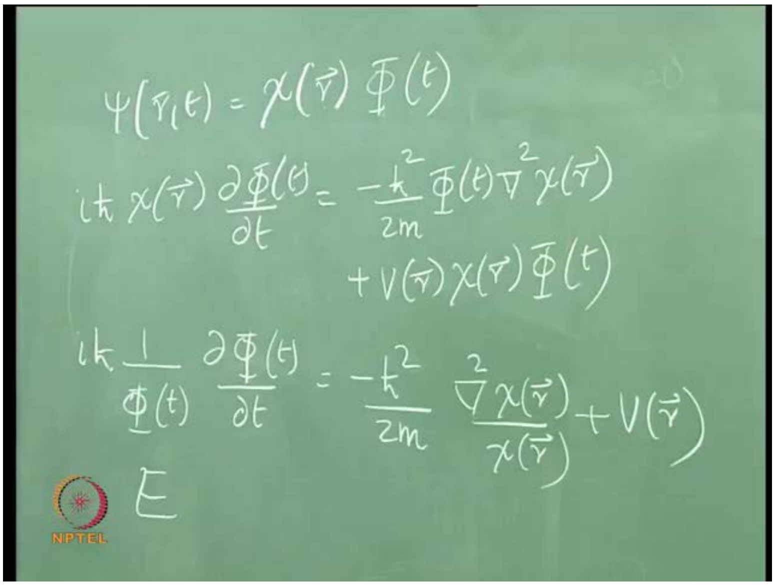

So, we write the wave function, psi of r t at some chi of r, phi of t. If I do this and feed this back into that equation. I have i h cross, the time dependence does not act on chi that is my left hand side. This space derivative does not act on phi and of course, I have plus

V of r chi of r phi of t. Can divide throughout, by chi of r phi of t and if I did that. The 1st term, the left hand side is just this, does not depend upon the space coordinate at all, this is only dependent upon time and as through, on the right hand side, plus V of r. Look at the right hand side, does not depend on time at all.

Now, if the left hand side does not depend upon the space coordinate r and the right hand side does not depend upon the time coordinate, time at all, time parameter at all and these 2 are equal. It is clear that, this is equal to a constant and that, is equal to the same constant. I call that constant E, then I have two equations.

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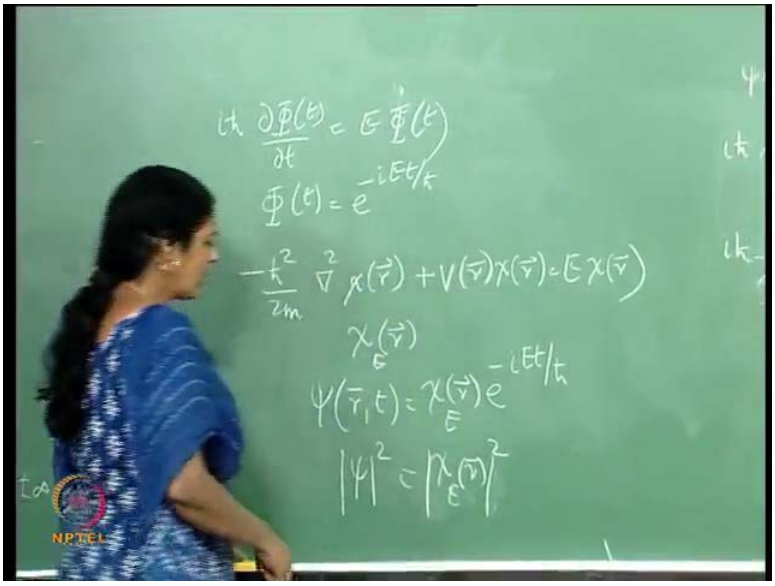

The 1st equation simply says, i h cross delta phi of t, by delta t, is E phi of t. The solution to this equation is very simple, phi of t is simply e to the minus i E t by h cross. So, that is all that I have, because, the 1st derivative pulls out a minus i E by h cross. The h cross cancels and with this I just get a plus. So, I have an E phi of t, that is all that there is to it. Now, as to that, the right hand side I have minus h cross squared by 2 m, del squared chi of r. Multiply throughout by chi of r, plus V of r chi of r, is E chi of r. So, depending upon the value of E here, depending upon the value of the constant, I am going to have a solution.

So, I should really be talking in terms a chi of r, for a given value of E. And that is what we will have to solve for, given this equation. Therefore, the total wave function of psi of r t is some chi of r, which really depends upon the value of the energy that we have, e to the minus i E t by h cross. The up short of whole thing is this. That if I now, find modulus of psi the whole squared. It is clear that, this term cancels out and I just have modulus of chi E of r, which is just chi E of r, whole squared and even if it were, in general complex, I could write it like this.

So, this is what I have. So, that is certainly 1 property of the stationary state. Equally true that if I take expectation value of any operator in the states psi of r t.

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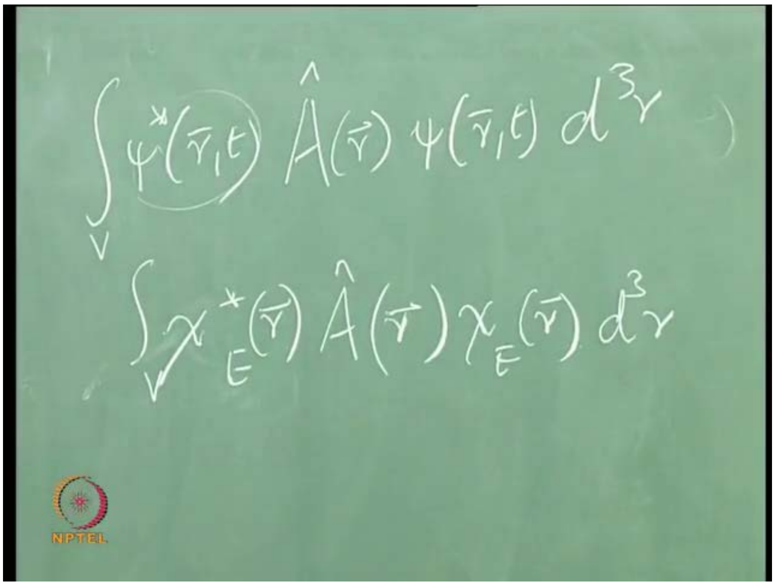

That is like, saying psi star of r t, expectation value of some operator. Let me say A, which is of course, written as a function of r. We will have to write in the position basis, psi of r t, d cubed r that is over the entire volume of integration. It is clear that, this part has (Refer Slide Time: 26:29) e to the i E t by h cross and the psi here has e to the minus i E by h cross, which cancel out. And therefore, it is really like doing chi E star of r, A of r, chi of r d cubed r and therefore, expectation values do not depend upon time. For all times I have the same expectation value.

So, in a stationary state of the system (Refer Slide Time: 26:29) the time dependent goes as e to the minus i E t by h cross.

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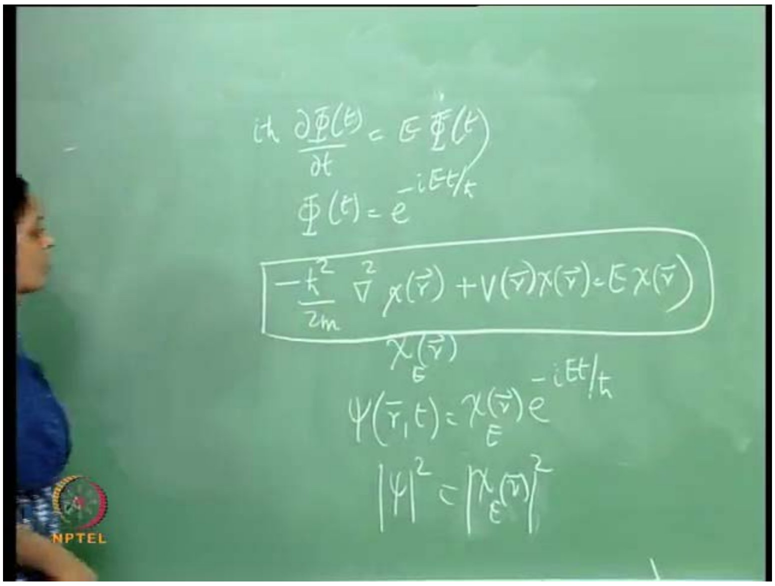

And this equation here, which one solves to find chi of r clearly has no time dependence and this is the time independent Schrodinger equation.

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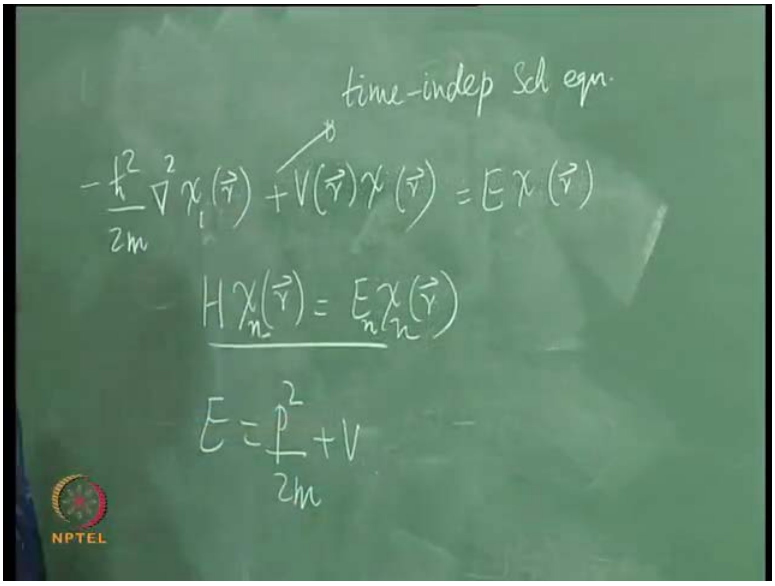

So, the time independent Schrodinger equation can be written this way, minus h cross squared by 2 m, del squared chi E of r. That came from the potential. That came from the kinetic energy. It came by p squared by 2 m, plus V of r, chi of r, is E chi of r. I could drop the E, simply remember at the back of your mind. That corresponding to, this is an Eigen value equation and corresponding to a given value of E. You have, a wave function chi of r and since this whole thing here, minus h cross squared by 2 m del squared plus V of r is a Hamiltonian. There is a potential energy part here and there is a kinetic energy part here.

So, this is merely the statement H chi is E chi, so, it is an Eigen value equation. These are the energy Eigen states, written in the position representation, it is chi of r and corresponding to the energy value here, the actual value of E you have a chi. So, if you have set of energy levels, could call them e sub n, they are discrete. You have chi sub n of r, where n takes values 0 1 2 3 etcetera. So, corresponding to the energy value E 0, there is an energy Eigen state chi naught of r, corresponding to the energy Eigen value E 1 chi 1 of r and so on.

So, this is the Eigen value equation that one likes to solve. And this is really the time independent Schrodinger equation, which is what we use, when we deal with stationery state states, of course, if you put the time dependence, then you have an i h cross delta by delta t already coming in and this kind of analysis does not go through. So, in a stationary state, if the system is in a stationary state. The time development is very simple and straight forward. Simply moves us e to the minus i E t by h cross and then the part of the wave function that depends upon the position coordinates alone.

Now, the reason why I would be interested in energy Eigen states is obvious. As, I have stated earlier even when I did things in the abstract, using matrices and column vectors. We are looking at conservative systems. Systems were; the energy is conserved during the motion of the system. So, energy is a constant of the motion and therefore, the Hamiltonian becomes, a very respectable operator. You would really like to choose as your Eigen basis, or the basis states in the linear vector space. States which are the complete set of common Eigen states, of all the constants of the motion, corresponding to that situation.

Energy is certainly a constant of the motion, because, we are looking at the conservative systems and therefore, we will look at Eigen states of the Hamiltonian and any other observable, which commutes with the Hamiltonian. In other words which is also a constant of the motion. So, in general we are looking at energy Eigen states for this reason. Now, in wave mechanics, the energy Eigen states, are written in the position representation and even if we look at separable Hilbert’s space. There are a denumerable infinity of energy Eigen values, Eigen states chi naught, chi 1 and chi 2 etcetera. Each one of them being written as a function of r, corresponding to which there is an energy Eigen value e sub n. So, you will recall that the whole problem started by saying, that in classical physics, I have this and then replacing E by i h cross delta by delta t and P by minus i h cross del.

We could do the same thing in relativistic physics. So, let me digress and comment about what happens, in relativistic physics. Take the expression for e, in terms of the momentum of the particle and so on. Replace e by i h cross delta by delta t and p by minus i h cross del.

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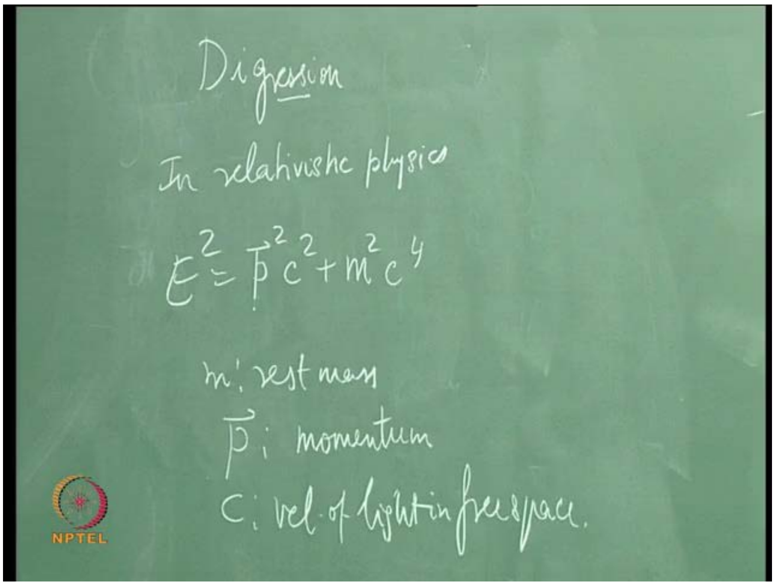

So, this is a digression, worth doing at the stage. In relativistic physics, I know that E squared, is p squared c squared plus m squared c to the 4. Where m is the rest mass of the particle and I consider the particle with momentum p, linear momentum. C is the velocity of light in vacuum and this is the expression for energy. E square is p squared c squared plus n squared c to the 4. From given this I simply have to if I want to do the quantum mechanics, of an object which is travelling relativistically, then I take this expression and I write i h cross delta by delta t for E and minus i h cross del for p. So, that gives me the following.

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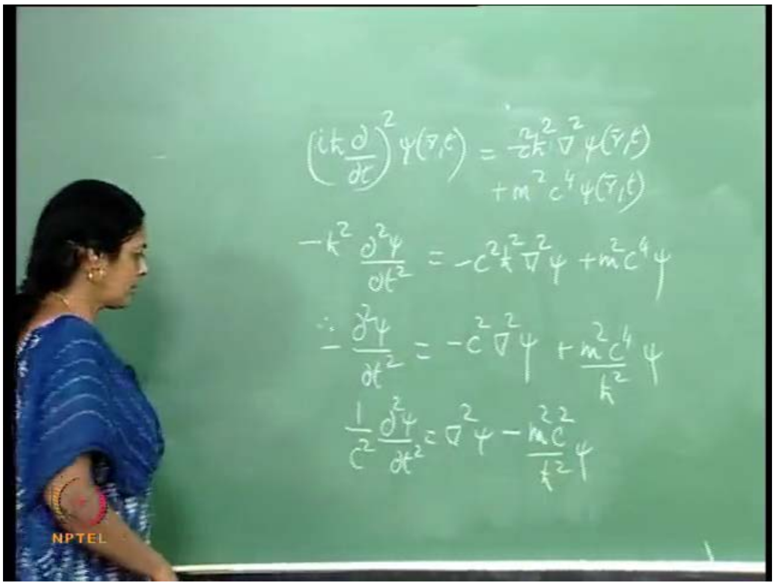

So, that is E squared and it supposed to act on psi of r t, because it is now, become an operator in quantum mechanics, is p squared there is a c squared. So, that is the constant, which can be pulled out, plus m squared c to the power of 4, psi of r t. So, that gives me minus h cross squared, delta 2 psi by delta t squared. That is E squared psi, is equal to p squared c squared, plus m squared c to the 4 psi. Therefore, I have delta 2 psi by delta t squared, minus delta 2 psi by delta t squared. I divide by h cross squared, or I can certainly divide by c squared now, or a minus c squared if you wish.

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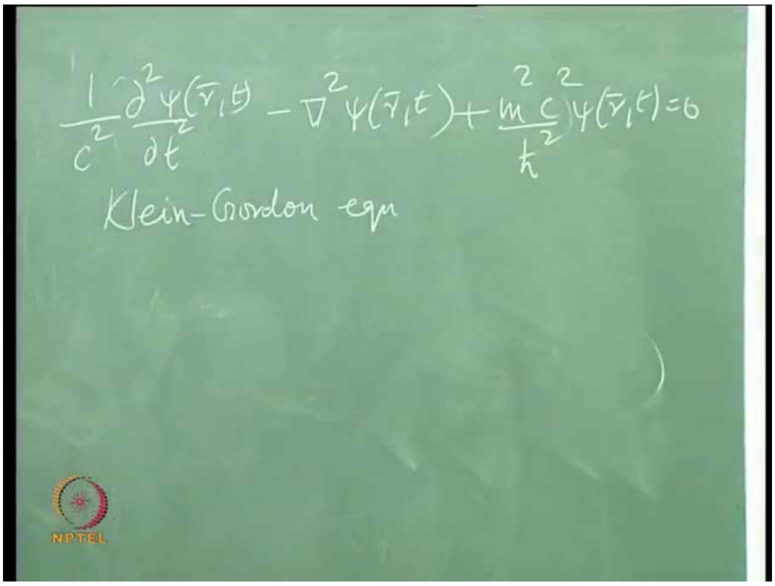

So, if I bring the del squared to this side. I just have 1 by c squared delta 2 psi of r t by delta t squared, minus del squared psi of r t, is equal to, or plus m squared c squared plus h cross squared psi of r t equal 0. That is the Klein Gordon equation. That is a relativistic wave equation. For an object, with rest mass m, moving with the momentum p and the p has been suppressed, because, I have got (Refer Slide Time: 35:39) an i h cross del replacing the operator p. So, this is what I have.

The reason why I brought this in, it is a digression. To tell you that, in all these context simply take the classical expression, for energy in terms of momentum mass of the particle potential and so on. Replace the energy by i h cross delta by delta t and the momentum the linear momentum, by minus i h cross del. If you are looking at 3 dimensional space, or minus i h cross delta by delta x in 1 dimension along the x axis. And then you get the corresponding equation. The quantum mechanical equation; which one is supposed to solve for the wave function, psi of r t. That is my way of a digression.

Now, returning to the non-relativistic case, which is all that we will be looking at. I have the following.

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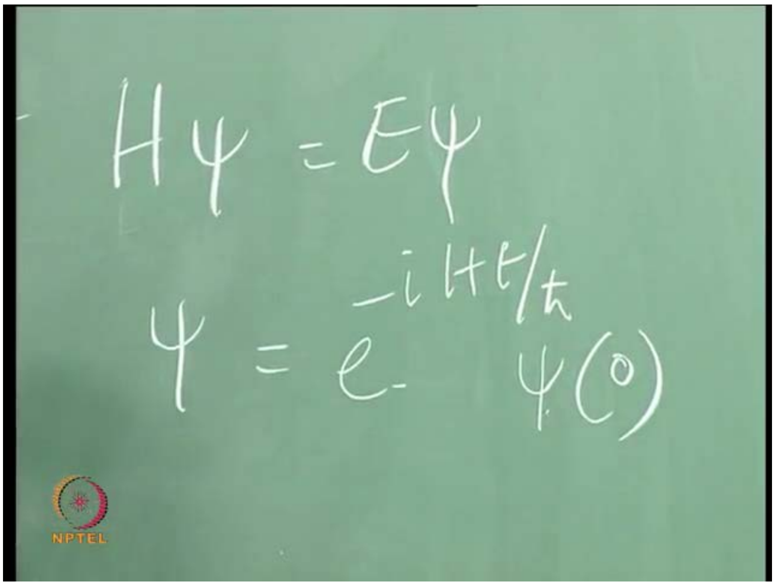

In general, I seem to have a situation; H psi is equals E psi. Look at this (Refer Slide Time: 30:08) minus h cross squared by 2 m del squared plus V is the Hamiltonian, acting on the wave function. In this case I called it chi, is E chi. So, the formal solution for psi, is e to the minus i H t by h cross, psi of 0. So, this is what I have.

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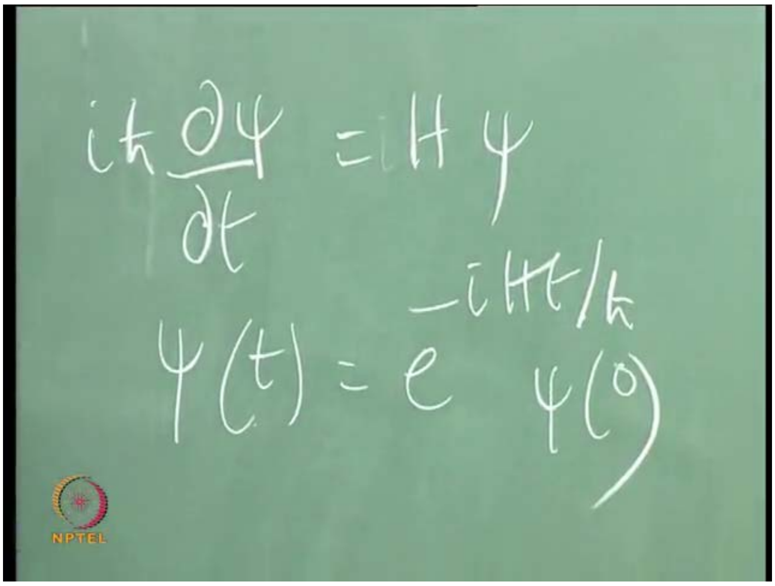

So, let me look at the Schrodinger equation itself, i h cross delta by delta t psi, is H psi. And therefore, the solution is psi of t, is e to the minus i H t by h cross, psi of 0. Now, one thing is clear that, if I give you psi at the initial time, whatever, may be the initial reference time. I can find psi at any other later time. Without knowing the value of, without knowing what psi was, at any time between 0 and t. All I need to know is the initial values psi of 0 and I can give you psi at any instant of time, later time. Do not need to know the value of psi, at any time between 0 and the time of interest to me.

So, in that sense, this is a mark of process. There is no memory of the path, that is taken. The manner in which psi changed, with time but, merely the initial value. Value of psi at time t equal 0. That is the point where bearing in mind and now; we will look at specific examples, to see how we can solve the time independent Schrodinger equation. We are looking out for a stationary states and that is precisely why we got there. So, we will substitute various values, for V of r. Start with the 1 dimensional problem first. Substitute for V of x and then get the Eigen value equation set up.

And solve for the Eigen function and the Eigen values, energy Eigen values and the Eigen functions. The Eigen functions are functions of position, we are working in the position representation. Clearly we should be able to match, with what we did earlier for these systems. For instance, we have already worked out. The Eigen value problem, for a 1 dimensional harmonic oscillator and there we saw, that the energy Eigen values were of the form, n plus half h cross omega, where omega is the angular frequency of the oscillator and n takes the values 0 1 2 3 and so on.

Now, here we would for instance, work out the harmonic oscillator problem. In the frame work of wave mechanics, which means we solve for an equation. Like, (Refer Slide Time: 30:08) this in the position representation. So, we will substitute, V of x in 1 dimensions, V of x is half m omega squared x squared. We should be able to retrieve the same form for the Eigen value. We should be able to get hold of the Eigen functions. And as we have seen earlier, in other ways, the ground state for instant for instance is a Gaussian function, of position. We should be able to retrieve all those results.

So, the Schrodinger formalism is an equivalent formalism to what I have already done, using abstract operators.

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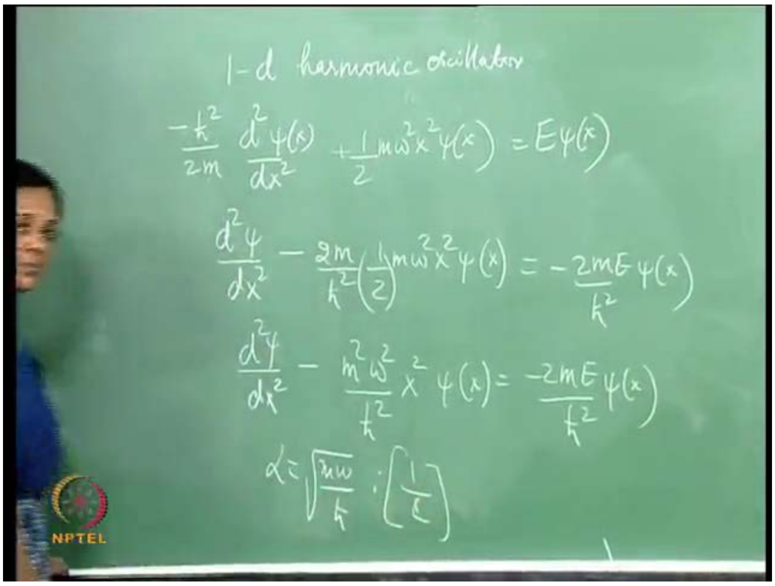

And now, I will illustrate the whole thing for the harmonic oscillator, in wave mechanics, that is using the Schrodinger formalism. So, 1 dimensional harmonic oscillator, so, starting with the time independent equation, we have minus h cross squared by 2 m. Looking at stationary states of the oscillator. So, the time development is simply e to the minus i e t by h cross. So, I have minus h cross squared by 2 m, d 2 psi of x by d x squared, where psi is the wave function, plus half m omega squared x squared psi of x, is equal to E psi of x.

So, we just have d 2 psi by d x squared. So, I can take this there and I just have minus 2 m by h cross squared, times half m omega squared x squared psi of x, is minus 2 m by h cross squared E psi of x. So, that just gives me, d 2 psi by d x squared, minus m squared omega squared by h cross squared, x squared psi of x, is minus 2 m E by h cross squared psi of x. When you solve these equations, it is always good to find out, what is the length scale, the natural length scale in the problem. You will recall that when I did this, using the abstract operator method. I defined a and a dagger, the raising and lowering operators for the harmonic oscillator and then we had x and p. In terms of a and a dagger and we realize then.

That root of m omega by h cross, has dimensions of inverse length and that is why we define x in terms of a and a dagger, which were dimensionless quantities. As a plus a dagger x was a plus a dagger by root 2, multiplied by an overall root of h cross by m omega. The similarly, for p. Because, root of m omega h cross came out as a coefficient, to take care of the dimensions of linear momentum, now, to solve these differential equations. It is good to scale out such dimension quantities. Find out the natural scale in the problem, in this case it is a length scale. Find out the natural length scale and scale out.

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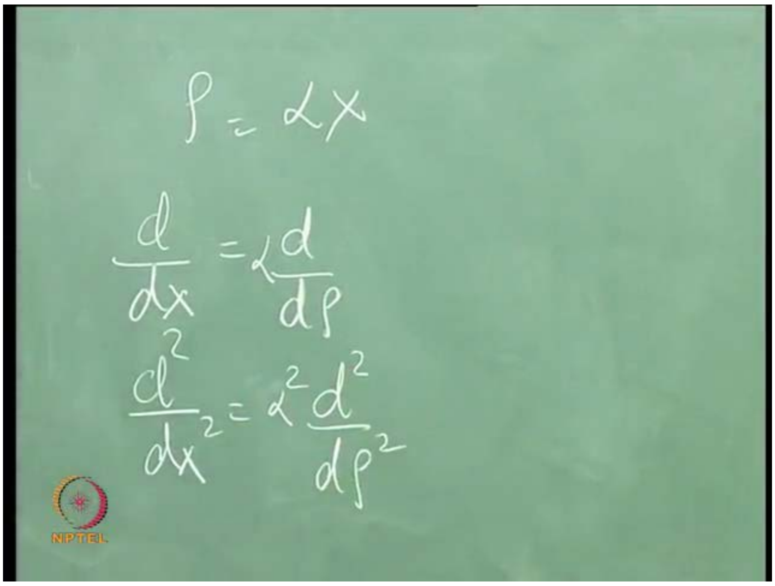

So, you define an object rho, which is alpha X and clearly rho is dimensionless. Because, X has dimensions of length and this object (Refer Slide Time: 42:40) has dimensions 1 by length. Then, d by d x is simply, d by d rho, times d rho by d x, which is alpha and d 2 by d x squared is again alpha squared d 2 by d rho squared.

So, we can now write this equation, recast this equation. In terms of a dimensionless variable rho and that is the good way of doing the problem. And do not have to keep track of m's omegas and so on. They will appear naturally, in the final solution of the problem and a lot of things can be read of very easily by using dimensionless quantities, when we solve the differential equation. This would be a general technique that we will use.

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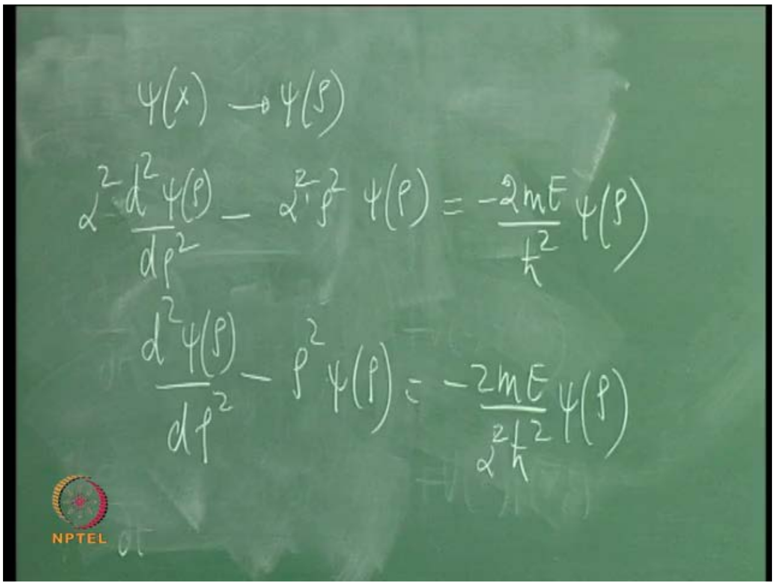

We now have therefore, psi of r psi of x, has now become psi of rho and we have d 2 psi of rho by d rho squared. That is the 1st term (Refer Slide Time: 42:40) but, then there is an alpha squared multiplying it, minus the 2nd term, this is an alpha to the 4 x squared. Keep it as x squared, we will take care of this later. Psi of x, which becomes psi of rho, I have to write this also in terms of rho which I will because rho is alpha x.

So, x squared is rho squared by alpha squared, so, I have that. Is equal to minus 2 m E by h cross squared, psi of rho that is what we have. So, divide throughout by alpha squared and you have d 2 psi of rho by d rho squared, minus rho squared psi of rho, equals minus 2 m E by h cross squared alpha squared psi of rho.

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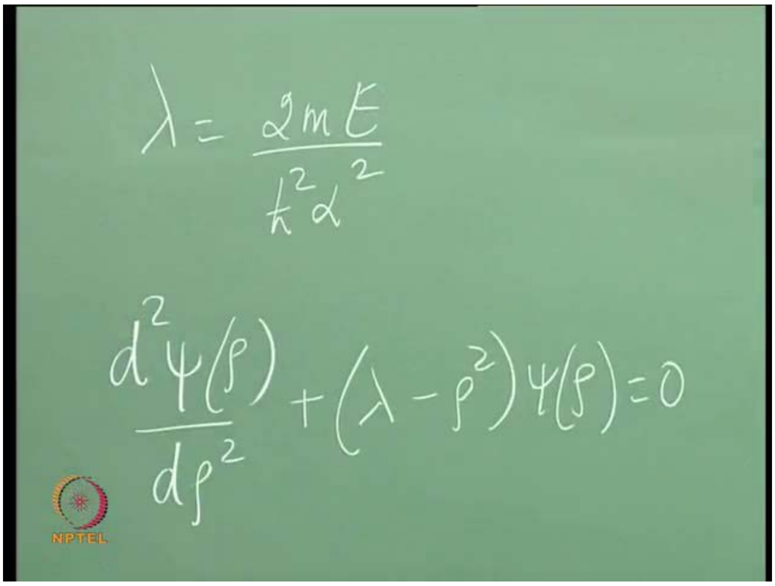

So, I define lambda, which is 2 m E by h cross squared alpha squared. Now, you can check that lambda is a dimensionless quantity and then the equation itself becomes d 2 psi of rho by d rho squared, plus lambda minus rho squared psi of rho equals 0. So, this is the equation that I have to solve and the idea is to find out the value of lambda. The values that lambda can take and the possible admissible solutions psi of rho. This is the manner, in which we will approach the problem and is a good place to stop. We will take it out from here in the next class.