Micro and Nanoscale Energy Transport
Dr. Arvind Pattamatta
Department of Mechanical Engineering
Indian Institute of Technology, Madras

Lecture - 08
Fundamentals of Quantum Mechanics Part 2

Good Morning. Today we will continue our discussion with respect to the Schrodinger's equation.

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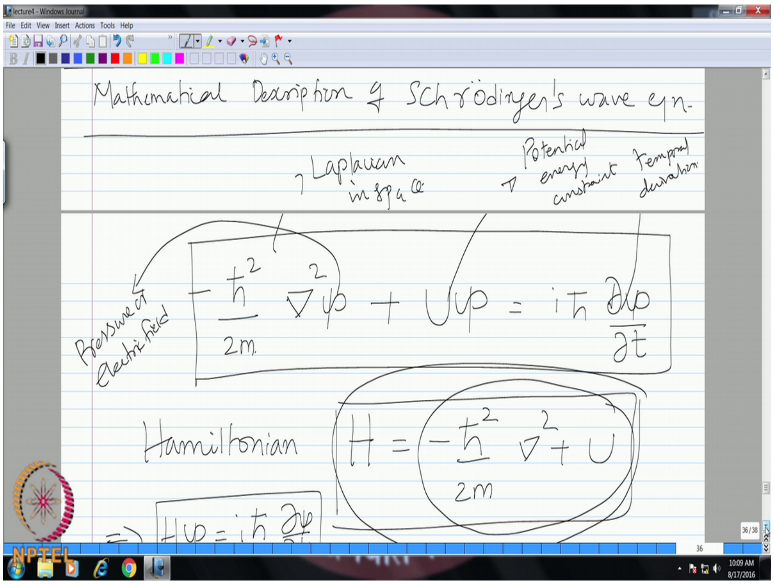

So, the Schrodinger's as equation mathematically has 3 terms, the first term on the left hand side is nothing but the Laplacian term in space, this is spatial derivative. This particular equation describes the wave function, and this wave function can be anything, that could be for electromagnetic wave or pressure wave.

The second term which is the potential energy constraint, and the term on the right hand side is the temporal derivative, describing the evaluation of this wave function in time. So, the operator that is shown here represented here is called the Energy operator or the Hamiltonian operator. So we will see that today class that expected value or the probable value of this Hamiltonians the energy, poses by the electron or whichever electromagnetic wave.

So, the Schrodinger's wave equation originally conceived by Schrodinger, and however he did not physically understand the relevance of this wave function. So, it was born who gave a physical interpretation to the wave function, he says that the wave function itself by itself does not carry much meaning.

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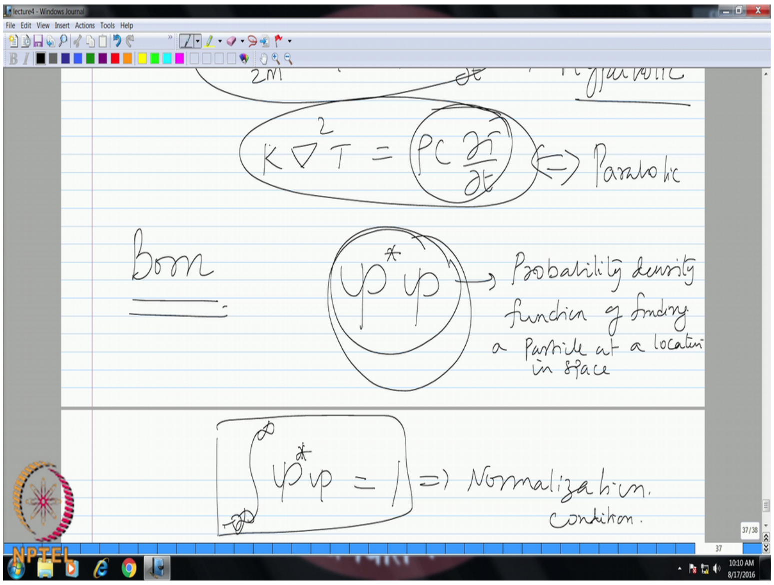

But, if you take the product of the basically psi star, which is the conjugate of this wave function and multiplied with the wave function, this will give the probability of locating a particles somewhere. Therefore, according to the normalization condition, to find the particle somewhere in the infinite space, from minus infinity to plus plus infinity the product of this psi star, psi should be equal to one and not only that, So, in order to find out the expected or the probable values of other quantities, such as the actual coordinate.

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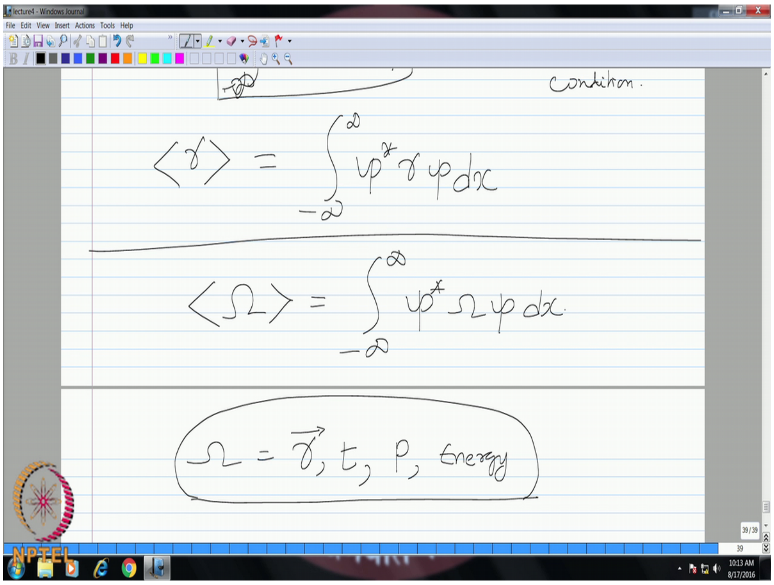

For example; the actual coordinate is a represented by r it could be x y and zee. x comma y comma zee. So, this is obtained by again, minus infinity integrating, minus infinity to infinity, psi star into r psi.

So, this if you are talking about this is your physical space, this is d x. So, if you same thing should be with respect to the integral psi star, psi, d x should be equal to one. So, the same thing can be extended to other derived quantities, we will look at the most important once today. For example, you can also have very common representation some capital omega, which is some quantity that you need to know the expected value. So, this is always obtained as, minus infinity to infinity, psi star, omega psi d x. So, where omega could be the coordinate r vector, it could be the time it could also be the momentum, and it could also be energy.

So, you need from the Schrodinger's equation finally, what you are interested is all these quantities could be, where the particle is exactly located within the infinite domain, and what is the exact time of location of this particle, what is the momentum processed by this particle and what is the energy. So, seen quantum mechanics nothing is 100 percent sure. So, there is always an uncertainty given by the Heisenberg uncertainty principle. So, we only call these as expected value or probable value. So, we know that in the real wild that also we are governed by several probabilities, but always we go through them and know for sure that the probability has become a possibility.

For example; when you take a train or a bus there is only a probability that you will which the place B so; anything can happen between places A and place B. So, according to quantum mechanics, this is only a probability that you will reach of certain place B could be 80 or 90 percent, but finally, you reach that place and you know for sure that, that is become a possible 100 percent.

Therefore, in quantum mechanics all though we know that these things are really are there, I mean there is always some uncertainty associated in estimating these quantities, so, these are therefore called as "Expected Quantities" Especially these expected quantities become more probabilistic at very very small scales. Because the values themselves are very small, so the values of energy or momentum they themselves so small that, the you cannot estimate them with you know great accuracy of the way that your estimating macro scale variables.

For example; if you take temperature at room and you have 2 or 3 different thermocouples. So, each thermocouple will be having a 0.1 or 0.2 degrees error by itself. So, one thermocouple will read for example, 25.5 with other will be 25.6, but still both are suppose to be fairly agreeing with each other, because there individual uncertainties are plus are minus 0.1 degree Celsius.

Now, in the small scales, the actual value that you are measuring is less than the uncertainty itself. When you are talking about resolution, if your resolving something less than 0.1 degrees, then there is a lot of uncertainty in that measurement and that is why the entire quantum mechanics deals with this kind of uncertainties.

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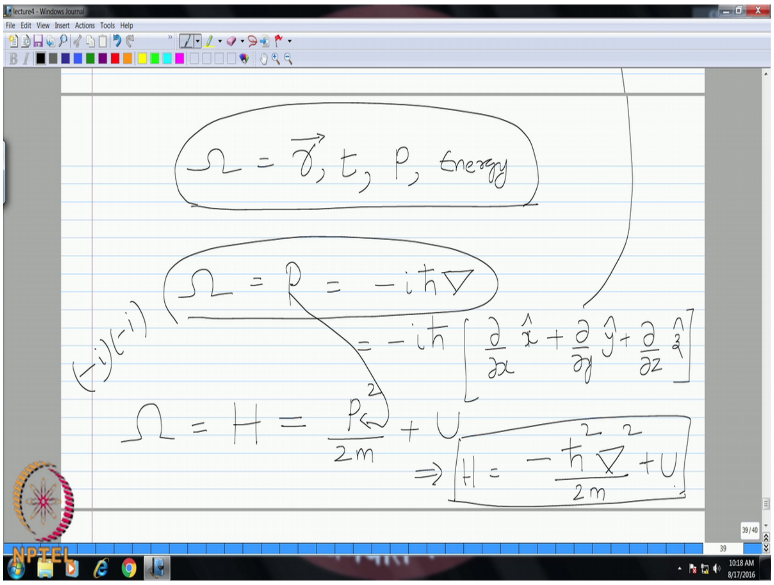

Now, what is the momentum operator that we have to u sed, if you are capital omega is your momentum operator, now these momentum operators are very specific. So, you have to exactly know how they look. So, this is given by this particular derivative here, that is nothing, but in the Cartesian coordinate system, this is d by dx, let me use unit vector as x because I all ready used the complex variable I and do not want to confuse that, d by dy this is the unit normal d by dz.

This is basically the momentum operator. So, we just put this momentum operator into this; that means you take the derivative of the wave function and you calculate this and then you multiplied with the complex conjugate and then you integrated and that should give you the expected value of the momentum. So, this is the operator, but in order to calculate the expected value of momentum. This operator has to be substituted into this particular expression here, to get the expected value. We will see that we will do some examples slowly.

Similarly, you have to understand the energy operator. The energy operator is represented by this Hamiltonians symbol H and how do you calculate the energy if you look at particle picture, it is basically the momentum square by 2 m, plus your potential energy. So, this is your kinetic energy, this is your potential energy. Now if you look at p square by two m, you can also write this from the momentum operator here, you can substitute for p into this particular expression. So, what does that give you; so, therefore, the

Hamiltonian H will be, so you have minus i h delta are the whole square. So, what do you have, minus i into minus i minus 1. Minus of modified plans constant square into, so this becomes Laplacian divided by 2 m the whole square.

Student: (Refer Time: 10:07) No. So, minus i into minus i, i square is minus 1 and then you have another minus. So, it is minus, i square is minus 1, minus of minus plus again you have another minus, you have to be careful. It is not minus i into i, it is minus i into minus a. So, you have therefore, minus h modified plans constraints square del square by 2 m, plus you have u.

So, you remember now if you go back to the Schrodinger's equation, the structure of the Schrodinger's equation on the left hand side, so if you just multiply this by the wave function. So, this is basically the operator that is on the left hand side of the wave equation. So, that is why we called that operator as the "Hamiltonian or the energy operator" because the energy operator itself is nothing but, minus x square, Del square by 2m plus u, so the Schrodinger equation.

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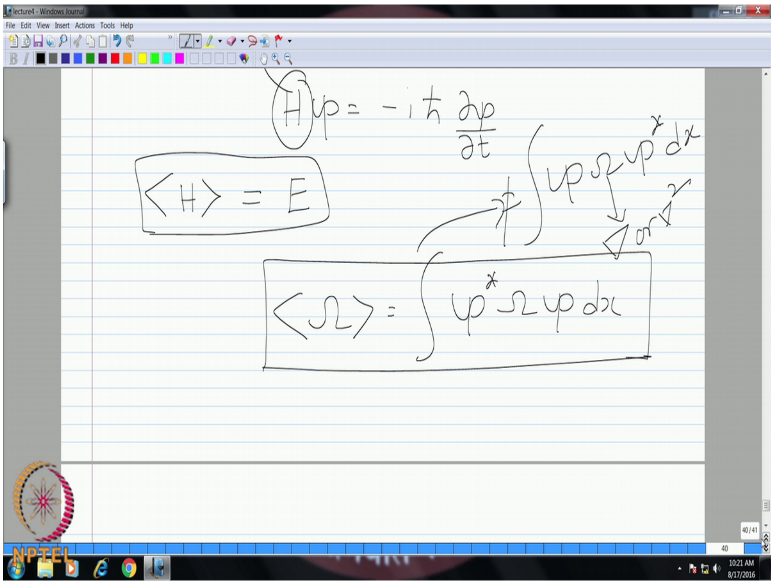

Now will be therefore, h psi will be equal to, minus i h bar, d psi by d t. So, this h is nothing but, this Hamiltonian h and now will see what is this Hamiltonian and how is it actually related to the energy. So, if you now take the expected value of this Hamiltonian operator. So, now this is just the operator, now we you need they expected value of this energy or the Hamiltonian, it turns out to be the actual energy. We will see this we will see this now in a short way, but you just understand that this is what you get.

And, now the one more caution with the respect to the use of this particular order, we have psi star omega psi d x to calculate the expected value of any quantity, we should be careful that, we cannot simply switch between psi and psi star, especially when you have these gradients and Laplacian operators. So, they will be different if you operate your psi with Del and then you multiplied with psi star that will be different from operating on psi and multiplying with psi star.

So, if for example, you cannot flip this and say this is psi omega psi star d x, especially if you are operator omega will involve gradient or del square. So, that is with the momentum and energy operators. The position operator it does not matter, you can flip between psi and psi star, but you have to be very careful, but this order is always what you have to follow.

So, the order of taking the derivative and then multiplying is very important. So, the other thing that, is also of interest in quantum mechanics is the uncertainties, right now we have found out the probability or the expected value, but what is the uncertainty in the determination of each of these quantities, because in quantum mechanics is uncertainty is are very high. So therefore, we need to also use an expression, so the operator for uncertainty. Again in uncertainty also you have what is called as expected value of uncertainty. So, the uncertainty itself cannot be certainly stated, there is an expectation of uncertainty there.

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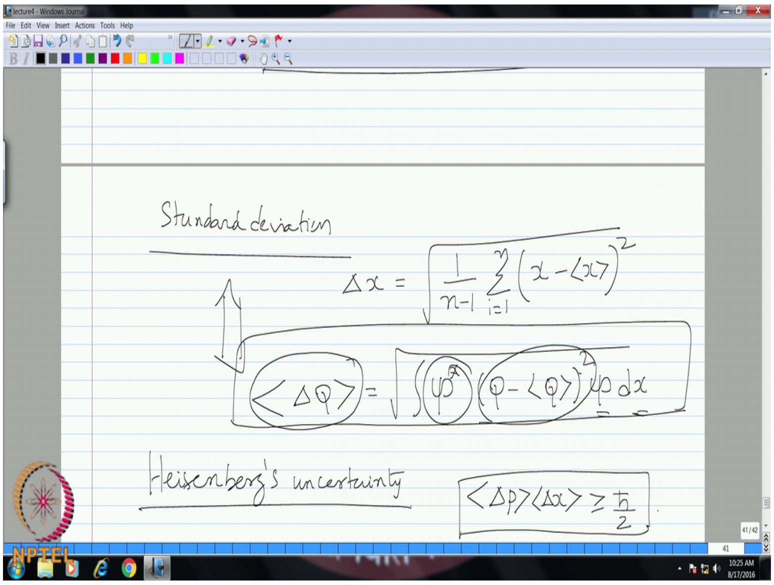

So, for example if you look at definition of standard deviation, in the real world the standard deviation is the indicator of uncertainty, how do we define it. For example standard deviation in some quantity x, how do we define? We take one our square root, if you have say n points you have n minus 1, i is equal to 1 to n, we take the difference between the actual value minus the mean value.

So, the mean value is your, use this operator here to state that this is the mean value n square of this. So, this gives you the uncertainty in the real world. Similarly in quantum mechanics, there is an analogy, but we cannot exactly translate this to that, in quantum mechanics we calculate the uncertainty in some quantity let us say Q.

So, the expected value of the uncertainty, turns out to be square root of again integral psi star and then Q minus the expected value of Q because the particular quantity, minus the expected value of that. And we take square of this, multiplied it again with psi d x, because you see this any quantity if you want to calculate the expected value you have to, always multiply psi star with that and psi d x integrated. So, that will be a common theme.

Now, if you want to calculate expected value of uncertainty, now this uncertainty itself is the value would minus the expected value the whole square, and then the square root that. So this is the quantum mechanical way, to determine the uncertainty of it could be energy, it could be momentum, it could be position, it could be time, Q could be anything. So, the expected value of uncertainties always estimated using this particular equation here. So, from this we can actually show, we can do some examples today tomorrow and the next week. We can actually prove that the Heisenberg uncertainty principle is always satisfied, if you calculate your uncertainty from this particular expression so that means, Heisenberg uncertainty principles states that, if you consider for example, the location of a particle in space. So, you cannot say for sure, that is the exactly located at a particular position.

So, there is uncertainty associated with this location or if you say that this is located exactly here that means, there is a problem with the momentum. So, therefore, in general it says that, the expected value of uncertainty in momentum multiplied with the expected value of uncertainty in position should always be greater than or equal to modified plans constant by 2.

So, this is one of the uncertainty theorems, the other is with the respect to energy and time. Instead of momentum and space you can also transform this into a space of energy, the expected value of uncertainty in energy and time, should also satisfy your uncertainty condition.

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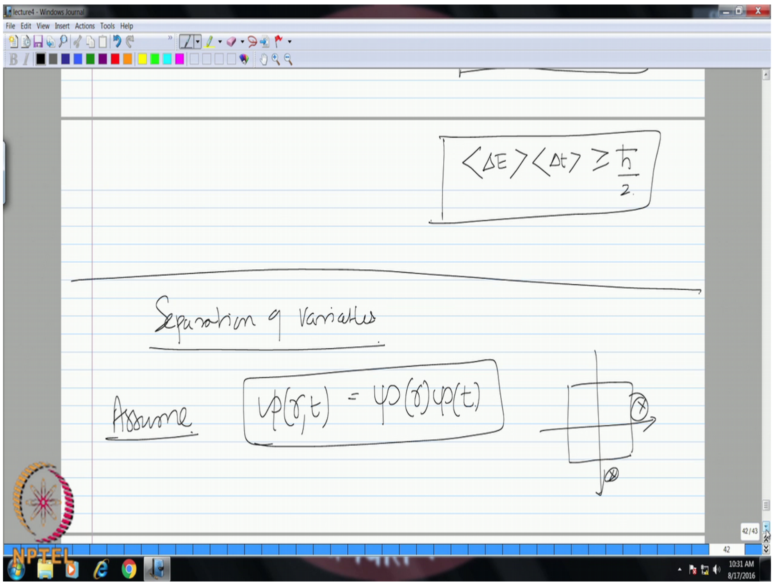

So, you have to basically know these things as facts you know. So, you do not have to worry about how they came, whether they will be satisfied. They will be satisfied if your work out simple problem and you will be able to calculate the uncertainties, multiply them and you will find out that this will always be satisfied.

Now what we will do next is to go ahead, and try to solve this Schrodinger equation. So, now our stated I have given you the Schrodinger are equation, also how do we calculate the expected values of many derived quantities such as momentum, energy and so on. So, then we have to now go ahead and solve for the wave function. Only if you know the wave function can be substitute and calculate all these expected values.

Therefore, how do we solve the Schrodinger wave equation? What we will do. So now, if you see the nature of this; this is the wave equation and not only that it is a partial differential equation and if you look at the entire equation like this, you have a special derivative on the left hand side, you have a temporal derivative on the right hand side. And we can start with the simpler case maybe where we can ignore the potential energy constraint, but if you retain the potential energy constraint, then the solution becomes little bit complex. Especially, because you should know what is the value of this potential energy constraint and usually it could be constant and certain cases, but more often it turns out to be a function of some other variable like x.

So, in that case then again partial differential equation will have non-constant coefficients, which becomes again difficult to find the direct solution, but still what we will do is, will approach the solution by separation of variables. So, this is the normal direct method of solving simple partial differential equations. So, how many of you have actually taken course there, separation variables is been covered you. So, only 2 or 3 and how about the rest, you do not know to basically solved.

So, in this particular course I cannot spend one lecture on teaching a how to, but I will just give you procedure and it is going to be similar for other equations. So, with the respect to the starting as equation, now that you have a wave function, now which is the function of 2 variables; one is the position the other is time. So, will assume that we can actually find solution, which is the product solution of 2 independent solutions, one which is the function of position, the other which is the function of only time. So, please remember that this quantity on the left hand side is the function of both r and t.

So, we are assuming that the partial differential equation is linear and the boundary conditions are also supporting the linearity such that we can use this assumption, where we can say that they are product of independent solutions, one only a function of r, the other only a function of t.

So, not only the partial differential equations (Refer Time: 22:25) there are non-linear PDS which cannot be solved like this. The other important condition for separation of variables is, you should have at least two homogeneous boundary conditions, in a particular direction. So, two homogeneous means, if you have a 2 dimensional system like this in one direction, either in this direction or this direction, you should have homogeneous boundary conditions.

So, if we have one homogeneous boundary condition here and one this side and the other 2 non homogeneous again this is not possible because we need to create ordinary differential equation called the “Eigen function problem” and this Eigen function problem can have Eigen values only in the direction where we have homogeneous boundary conditions.

So, therefore, these are some of the conditions unfortunately the Schrodinger equation, for most of the basic cases, you can find solutions using separation of variables. So, assuming this and if you substitute into the actual Schrodinger equation. Can you convert the partial differential equation into non ordinary differential equation? Using this assumption here, what we are now trying to do is, where trying to transform psi which is the function of r t. Psi which is the function only r, and we use another variable y here, capital y which is the function of t. That means we are trying to break this p d into ordinary differential equations one in space, one in time and then individually solve, that is the only way of solving a p d.

So, can you attempt that, I will give you some 5 minutes time all of you. So, when you differentiate with the respect to space, the term y will be constant and vice versa. Student (Refer Time: 25:10) for simple cases that we will be dealing now, to understand the basic energy states of free electrons, most of the basic cases, text book cases are all solvable using separation variables, we will see all those cases, particle in a box, we have hydrogen atom, we have a rotational system all these can be still solved, but only problem comes when your potential energy constraint is becoming not a constant, but a function of sum x. So, still separation variables will work, but finally, the ODE that is left out is having non constant coefficient and that cannot be simply solved. So, that has to be numerically solved. So, that will be a problem.

So, you substitute this into the p d and you also divide throughout by psi of r, y of t. So, what do you get on the left hand side.

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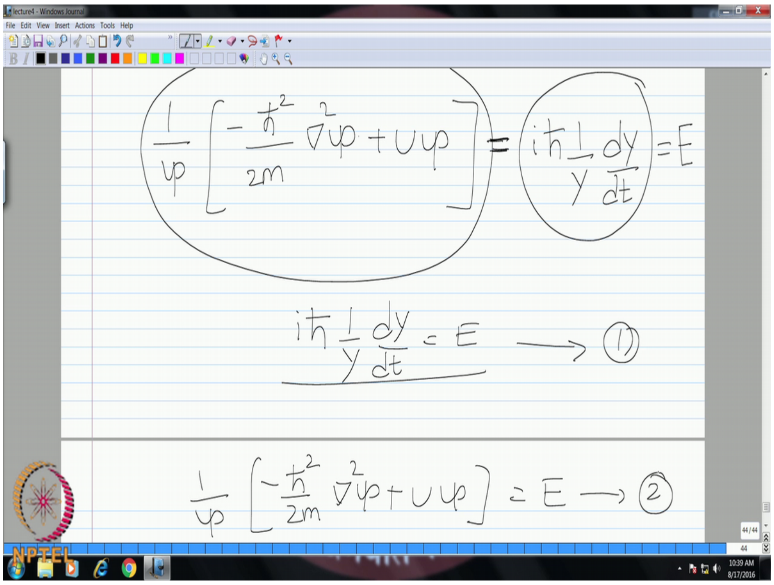

So, let me write the equation down and you please verify it, 1 by psi, minus h bar square by 2 m, Del square psi plus u psi, this is what the ODE that you get on one side. The other ODE with respect to time will be i h bar, one by y, d y by d t. So you converted such that, this is now a ODE with respect to space and this is an ODE with respect to time. Now where the ODE, now still this is is this is a single equation.

So, you have to see that to satisfy this particular equation, we have derivatives, ordinary differential equation with respect to space on the left hand side, with the respect to time on the right hand side. Therefore, these 2 terms can be equal only when there equal to some constant. Let this constant be termed as E. Now I am giving this name E here not by coincidence, because we will show that the expected value of the Hamiltonian is also nothing but the zee, what is the expected value of Hamiltonian? That is the energy and that is why I am giving this E here, I could give this lambda and then later showed that this is nothing but expected value of Hamiltonian and then therefore, that is the energy. So, not at avoid all that I am directly saying that this is nothing but E, which is the energy. So, therefore, now we have split this into 2 ODE. The first ODE will be, basically this is equal to E, and the second ODE will be this is equal to E.

So therefore, if you solve the ODE with respect to time, so that you now separated the partial differential equation into 2 ODE, the first ODE with the respect to time is this, and second ODE with the respect to space is this. So, therefore, you have 2 ODE. PDA separated into 2 ODE.

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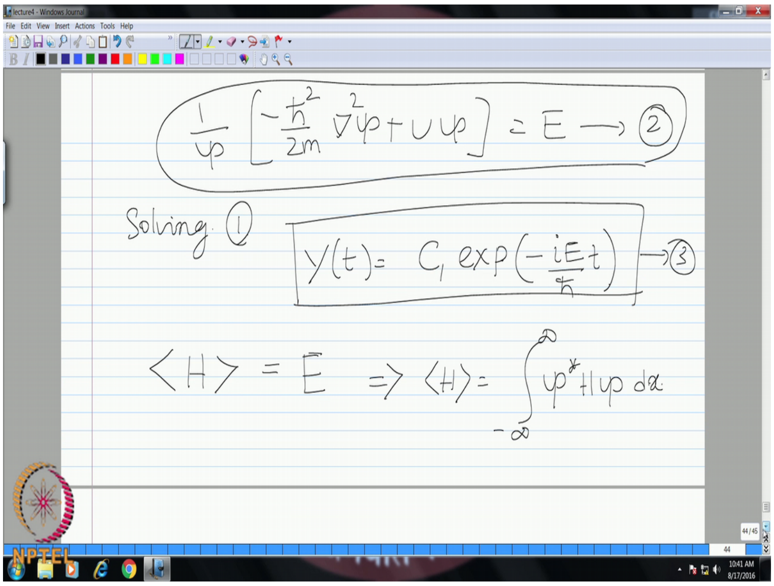

So, what is the solution to the ODE 1 that is a simple first order ODE? So, the solution should be y of t, should be some constants C1 let us say. Now this will be what exponential function. So, you can say d y by y is equal to e d t and if you integrated you have loan of y is equal to ET plus m constant. Therefore, Y will be C exponential of what. So, this entire term will go inside. So, you have therefore, minus if you take i on the other side, it becomes minus i. Minus i and you have E we have by h bar times t. So, this is your solution to the ODE in time. Let us call this is 3.

So, just keep this as it is now, because a final solution is the product of the 2 independent solutions. So, this will directly multiplied to the solution for 2. So, we will just leave it now this is a simplest solution. So, what it says the wave function is now, varying or decaying with time, in this particular manner exponential.

So, now what we had earlier discussed about showing that the expected value of Hamiltonian is nothing, but energy E, can be now prove on from using this equation 2. So, this is what we will show. So, I will just start this and I want you people to continue. So, what is the expected value of H, how do we calculated, minus infinite to infinite psi star H.

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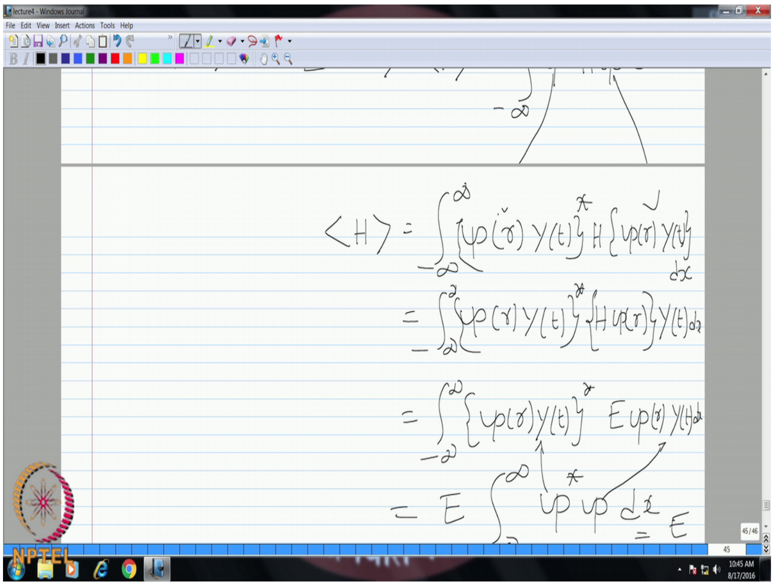

So, now let us write this operator. So, what is your operator H? So, this we will expend. So, what will do is let us not touch the H, we will only expend for psi and psi star. So, psi star is the function of r and t. So, we will use the separation of variables method; will separate into the product solution of.

So, we have psi of r and y of t and this whole star, this is the complex conjugate of that solution. Times we have H into we have psi of r, y of t, d x this is fine. So, we have just use the separation of variables for the complex conjugate and for the wave function. So now, we use the ODE 2. So, this H of psi of r this Hamiltonian is what? The Hamiltonian will be operated only because it is a function of space. So, therefore, H will operate only on psi of r. So, therefore, this can be written as H into H psi of r. So, this can be actually one more step you can write it psi of r, y of t whole star H into psi of r, into y of t, d x. So, this is the actual operation that is done. The Hamiltonian will be operating on the psi; this is the function of only position.

Therefore, now we go back to 2 and what do we see from 2. So, this is entire term here is, one by psi, H of psi is equal to E. So therefore, H psi can be replaced by E psi. So this entire term is now, E psi and since E is a constant; so we can actually take this term E out and therefore, this will be E of minus infinite to infinite.

So, we once again convert back to our regular wave function psi, which is the function of r and t. Psi star, psi, and d x. So, psi star which is the function of r and t, this is psi which is the function of r and t is a constant pulled out. So what is this one? So, therefore, this becomes equal to E. So, we have shown that, therefore the expected value of Hamiltonian is nothing, but this E which is also the energy.

So therefore, we can rewrite the equation 2, the ODE 2 in space can be rewritten has minus H square by 2 m Del square psi.

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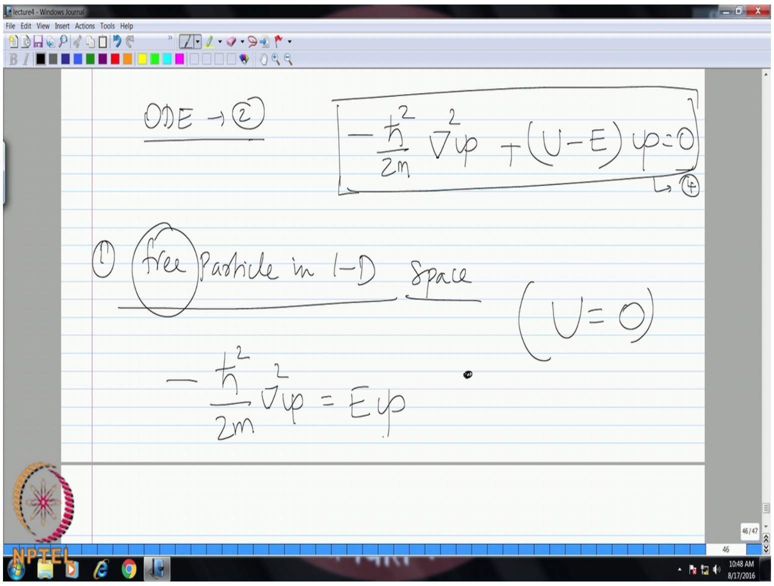

We can bring the E to the left hand side and we can write this as U minus E psi is equal to zero. So, this is becomes the second ODE to be solved, will call this as equation number four. So, and just rewriting this equation here by bringing, E side to the left hand side.

So, now depending on to solve this, what do we need to know the potential energy constraint U.? So, once we know that this ODE also can be solved for psi and also we need to boundary conditions, the how many boundary conditions do we need? Since it is a second order ODE we need to boundary conditions this specify.

Now we will go into the solution part, so the first case, simple case that we will be taking is free particle in one dimensional space; that means, you just have some particle like this just in space and you want to solve the wave nature of this particular particle. So in this case what is the potential energy constraint? Zero; because a particle is free, that is free to go anywhere in one dimensional space.

There is no constraint on the particle. Therefore, potential energy constraint is a zero; this is the simplest case that we can solve the Schrödinger equation. So, therefore, we all ready know the time solution, exponential function of time. Now the ODE becomes much simpler, we have Del square psi equal to, we have this is equal to use. So, U is equal to 0. So, this will be equal to E psi. So, since is one dimensional space we can expand the Laplacian here.

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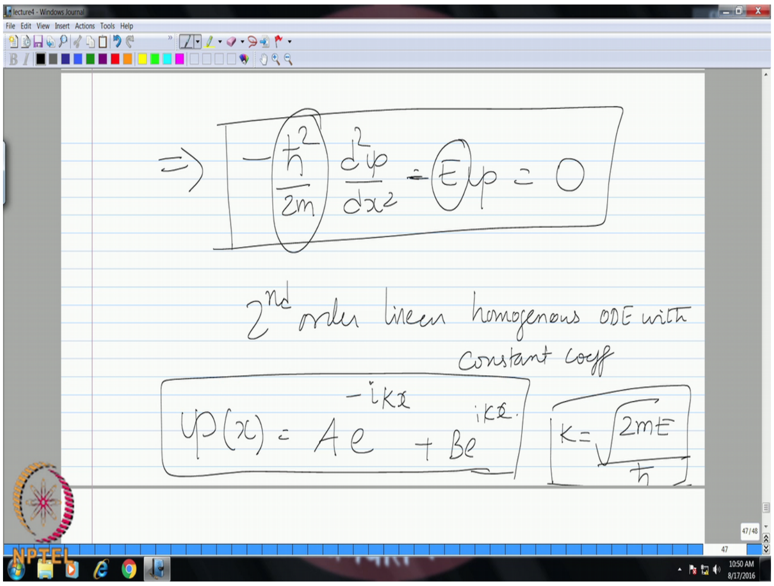

So, this is minus H square by 2m, we have d square psi by d x square minus E psi is equal to 0. So, this is the second order linear ordinary differential equation with constant coefficients, you see this coefficient is a constant, this is also a constant and this is homogeneous because the right hand side term we have equal to 0. So, second order linear homogeneous ODE with constant coefficients.

So, what is the kind of solution for this? So, we can either write this in terms of exponential functions or trigonometric functions. So, what we will like to do is, use the exponential functions here. So, therefore, we can write the solution for psi of x as A e power minus i k x plus B e power i k x or we can also write this purely in terms of A cause k x plus B sign k x.

So either in term of trigonometric functions or exponential functions; So, this they solution for this particular ODE, what is k here? So where k is related to square root of 2m t and h bar comes out side this square root. So, we absorbed all these constants into another constant k directly. So now therefore, you can relate your energy directly to this constant k here and what is the final solution psi of x comma t.

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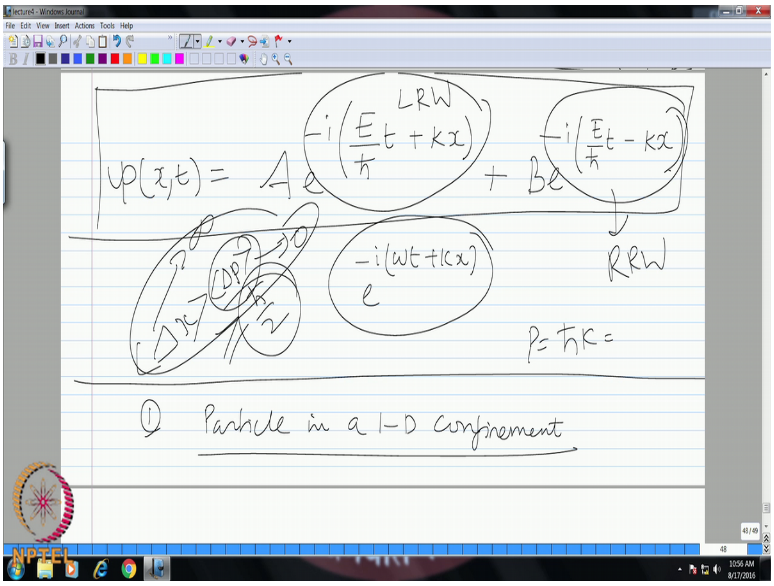

So, we multiply the time solution to the space solution and therefore, what do you get, A e power minus I, with respect to time what do you have, minus i E by h bar t. So will take minus i out, so E by h bar t plus k x; similarly we have Be minus I E by h bar t minus k x. So, this is your final solution. So, in this case we do not have any boundary conditions because the particle is not within any system, it is just free in space moving from minus infinity to plus infinity.

So, this is your final solution. So, what do you have here? So, you remember our representation of wave. So, we have used e power minus i omega t plus k x. So, this we generally use if you have waves earning on one direction and then we omega t minus k x to represent the waves running on the opposite direction.

Therefore, what this tells you is that you have waves which can run either on the right hand side or the left hand side and they have combination of waves running on right and left which are present as the solution to the wave function and there is also equal probability that you have both the waves running on the right and left because this is the free particle in space you cannot say that there are more waves running on the left, then on the rights. So, you have equal probability to find waves running on both the right and the left.

So therefore, the first term here will be corresponding to what left running wave this is your left running wave, and the second term here corresponds to your right running wave. So, final solution is super position of left running waves and right running waves a linear super position.

So, that is all it is. So, what we are now seeing is the wave nature of one particle which is free in space. So, what the Schrodinger's equation tells you is quantum mechanical picture, this particular particle is nothing, but consisting of waves which are running either on the right side towards the positive x direction, or towards the left side towards the negative x direction and therefore, the solution is super position of just these waves that is it. How do we relate this wave number to energy, is given by this particular relation here. So, this is the very very simple picture of free particle, so to start with.

So also you can observe one thing with the respect to the Heisenberg uncertainty principle. So, in this case the position cannot be exactly determined, because it is a free particle, it could be anywhere from minus infinity to infinity. And what about the momentum; the momentum of the particle can be exactly determine here because you have the wave vector k, which is related to constant e. So, all these are constants.

Therefore, your momentum p is equal to h bar k, is now exactly determined from this particular expression, but still Heisenberg uncertainty principle has to be satisfied, because now you have the uncertainties infinite in determining the position. So, finally, your delta x uncertainty and delta p uncertainty multiplied together should be greater than or equal to h bar by 2, these should be satisfied. Although now it is say that, this is approaching 0, but this approaching infinity, and therefore this product of this will be satisfying Heisenberg uncertainty principle. See for a free standing wave, you cannot exactly say the position, it is anywhere from minus infinity to infinity. So, uncertainty is infinity approaching infinity whereas, a momentum is approaching a very certain value.

So, next we will stop here today, the next case that we will take is the particle, in a 1 D confinement. So, when we started the introduction to wave, I just solve the simple wave equation, for a particle subjected to a confinement, a thin film or whatever it is, and then we got the solution in terms of sins of cosines, we found out the solution for the energy and so on.

And now we are going to do the same example in a more regress way, by solving the Schrodinger's equation. So, this we will take up tomorrow, we will first complete the one dimensional case, then we go to a 2d confinement.

So, so for in the free standing particle there is no quantization, here just continuous waves. Now we will see that, once you may put a confinement, the quantization will start appearing will start getting discreet energy levels and so on. So the real quantum mechanics will start with the confinement.

Thank you.