Quantum Mechanics
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Lecture – 03
Review of Particle in Box, Potential Well, Barrier, Harmonic Oscillator-I

So today what I am going to do is I am going to do a fast track on whatever you have learnt in your first year. So that you know there is some kind of a continuity and you will appreciate further, okay. So whoever has learnt already maybe a little bit you know repetition but it is good to go over this repetition once so that you are all with me, okay.

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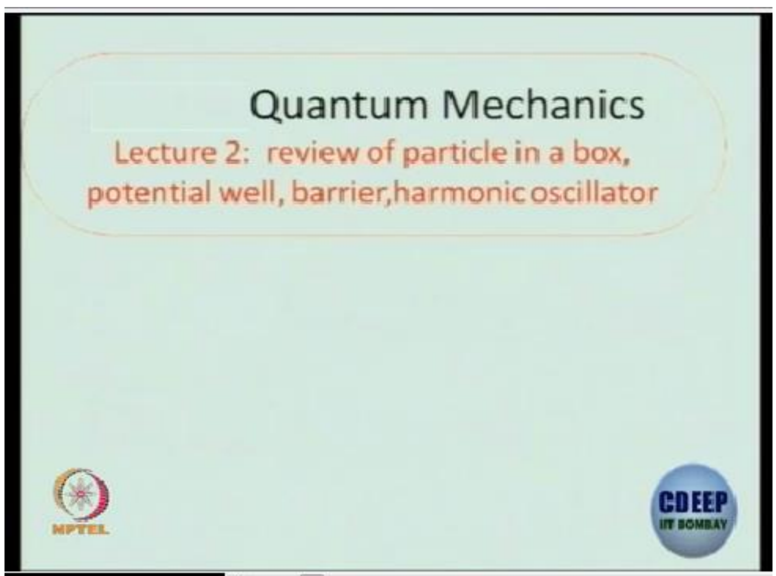

So review of particle in a box, potential well, barriers, step potential, harmonic oscillator is the theme for today. And slowly I will take you on to the delta function and some of the properties of one dimensional problems, bounce states, scattering states.

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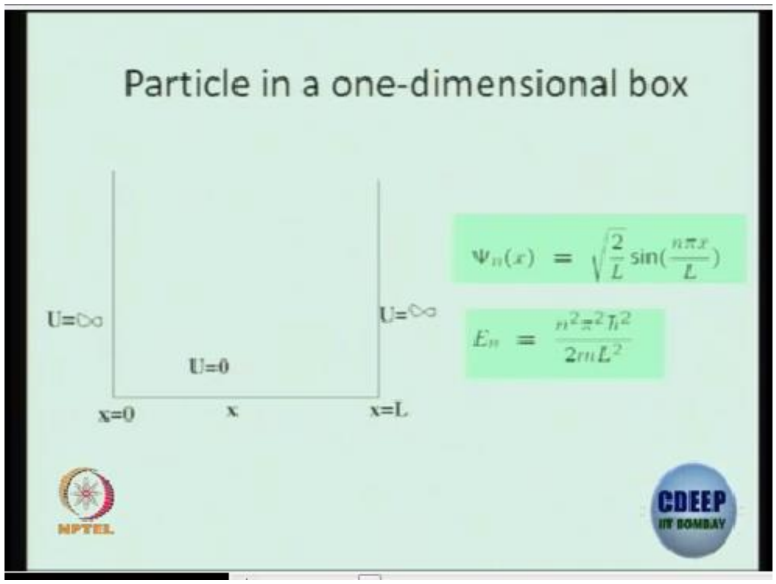

Particle in a 1-dimensional box all of you even in the middle of a sleep, I am sure all of you know now. Is that right? What is it? You put an infinite potential at 2 coordinates in 1-dimension at x=0 and x=L and inside the box, you treat like as if it is like a free particle. It is not exactly a free particle because it is bound by these kinds of potential. It is constraint. So what is the wavefunction of such a particle?

You have tried to evaluate using time independent Schrodinger equation, right. And found that the wavefunction which satisfies the time independent Schrodinger equation, the normalised wavefunction, is root of 2/L*Sin(n pi x/L). Everybody has derived this. I am sure you have done it. If you have not, if you do not remember, please go back and take a look at it, okay. And the corresponding, once I say solution to time independent Schrodinger equation, what does it mean?

You have to give both the wavefunction as well as the corresponding energy eigen values, okay. So the E_n are the corresponding energy eigen values and they are also discretized, integer multiple n squared, multiplying a common factor which is $\hbar^2\pi^2/2mL^2$, the L is the length of the box. So this is what we mean by a solution to a time independent Schrodinger equation, okay.

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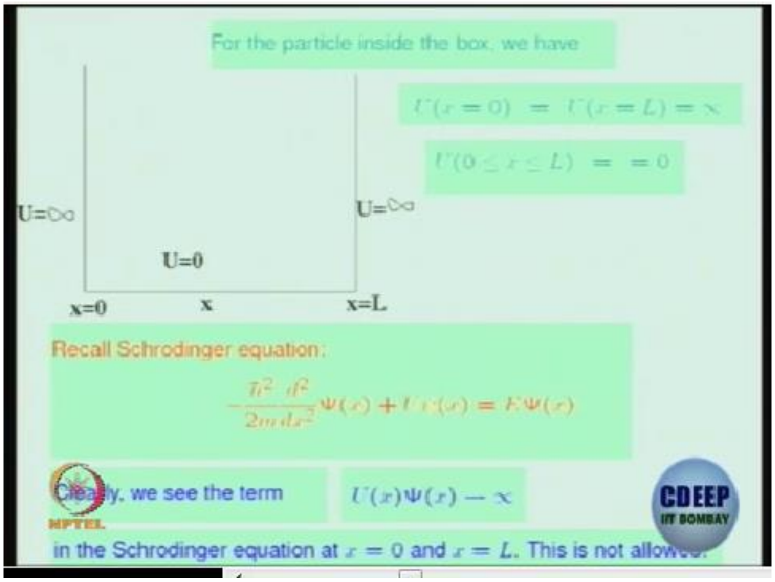

For a particle in a box, you put in these condition in the derivation and then you recall this Schrodinger equation, substitute the fact that U(x)ψ(x) is tending to infinity, right, because U is tending to infinity. So this is something you need to worry.

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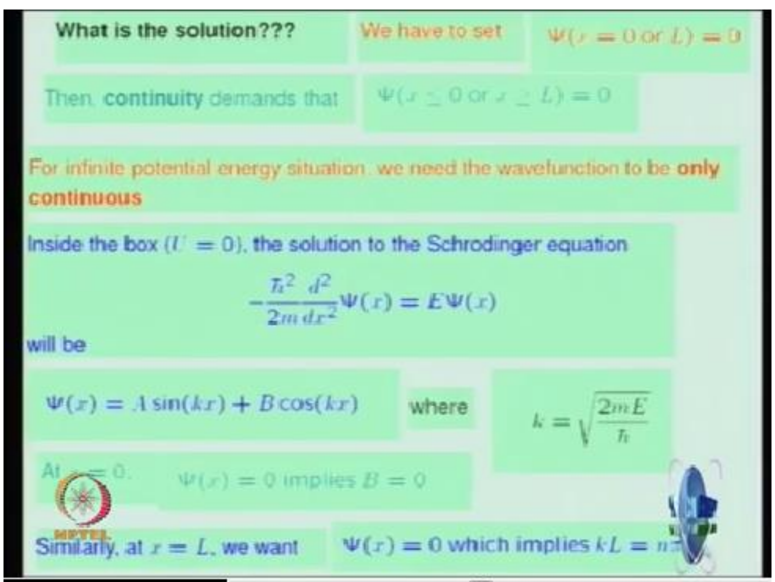

So then you find the solution by setting the wavefunction to be 0 at x=0 and x=L and wavefunction has to be continuous, right. So this is something which I said even in the last lecture that wavefunction has to be continuous even for infinite potentials but derivative of wavefunction will not be continuous. This is something which I stressed in the last lecture. Once you put this in, we need the wavefunction to be only continuous, no derivative.

And inside the box, you put U=0 in the time independent Schrodinger equation. This is what I was saying. And the most general solution is the linear combination of sin and cos. And imposing where k is proportional to square root of the energy. And at x=0, you want your wavefunction to vanish. And that forces you to make B to be 0. This is the way you went through the derivation. Similarly, at x=L, you can try and show that it will be again 0 if the k is quantized in this fashion, kL=nπ.

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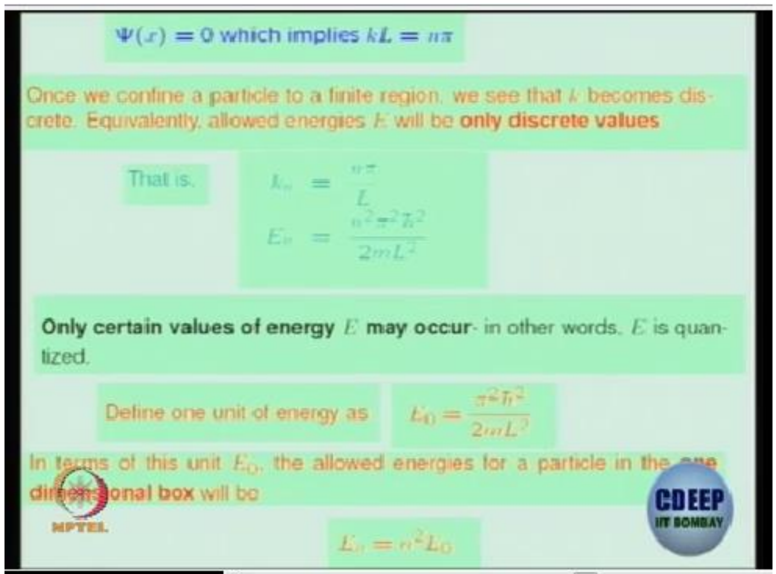

So once you use this, you see this one thing, when U is 0, the particle is like the free particle, right. But if you put the free particle with some kind of a constraint, putting a constraint as potential is infinity at x=0 and x=L, the k which would have been continuous for a free particle is no longer continuous. It becomes discrete. The k which is given here, kL=n π where k is n π/L, that discretization is happening because of the constraint which you have put in that the particle cannot move beyond x=0 and x=L, okay.

This is the first feature which you see for a particle which almost looks like a free particle but not actually. It is constraint with the potential being 0 and infinity. If it was not there, what will be the form? k can take any value from -∞ to +∞ in continuous fashion. You agree? So this k being discretized is because of putting this constraint that it cannot move beyond x=0 and x=L.

It has to move only between x=0 and x=L. Is that right? So discrete values start showing up if you start putting in such kinds of bounds, infinite potential boundaries, if you start putting in, then you start seeing that the energies are no longer continuous. It becomes discrete. So you cannot have arbitrary energies like free particle can have from -, you know, all possible energies positive values form 0 to infinity in continuous fashion.

Here you will have the energies to be discretized and only selective values. So these are quantum features which you would not have seen in classical physics. If I give you a free particle like $\frac{p^2}{2m}$ and say that p can take -∞ to +∞ in continuous fashion. Now you cannot see it, okay. So you can put in these quanta just like the Planck way of writing. You can define one unit of quanta to be this $\frac{\pi^2\hbar^2}{2mL^2}$. And then you can rewrite all the allowed energies for a particle in a 1-dimensional box as n^2E_0.

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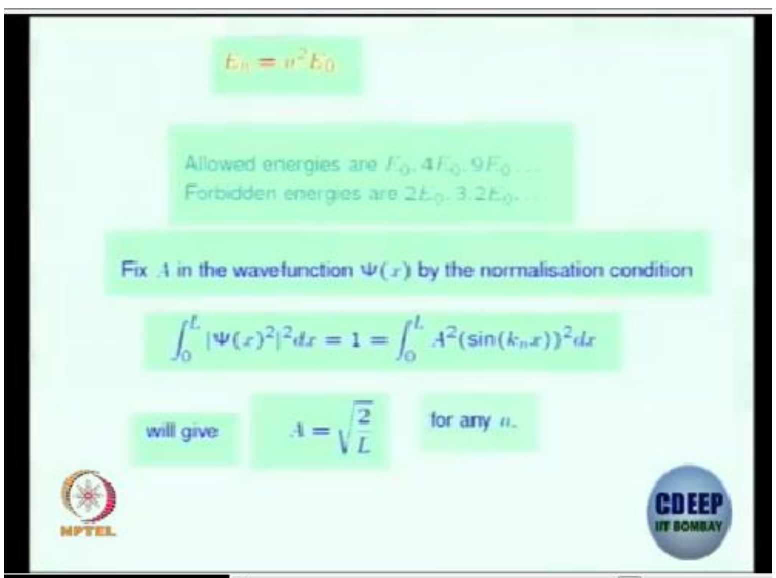

So E_n is now discretized with quanta n squared multiplying E_0. So not all energies are allowed. Energies which are allowed are in the series. Somebody ask you whether $2E_0$ can be found in the spectrum? No, 3.2 E_0, no and so on. So you can start saying forbidden energies are these. Such things you cannot see in your classical system. This is why the Bohn's orbits were very specific. You cannot go somewhere in between.

You have to be in one stationary orbit to go to the other stationary orbit and so on, okay. This normalisation fixing depends on your domain of integration. Here the wavefunction is non-0 between 0 and L. So you need to put this normalisation condition and fix the normalisation. So these things I am sure you have done it in your first year course.

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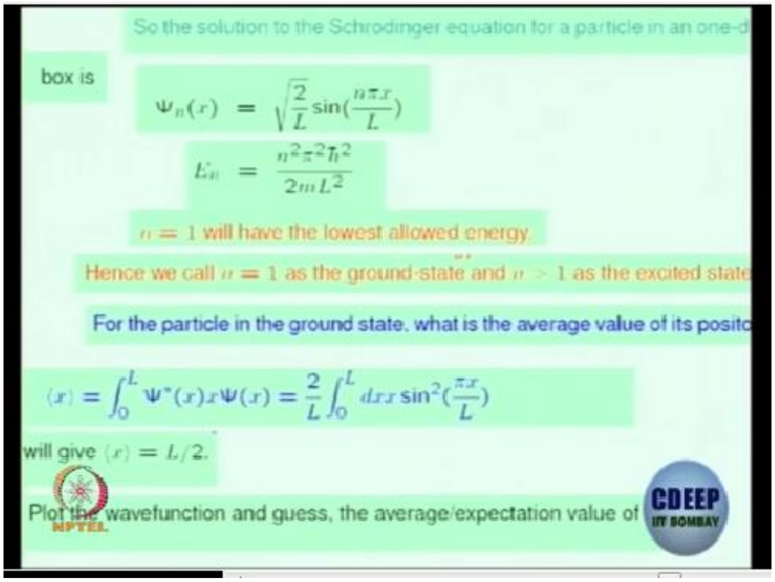

And you have that, you have the 2 final wavefunction which I had it in my first slide as this in the corresponding energies quantized as n squared E_0 and the lowest energy is n=1 and not n=0 for the wavefunction is Ψ_1, n=1 is lowest energy level, corresponding energy is E_1 which is equal to E_0 and the wavefunction is ψ_1(x). And n>1 are the excited states and what is the average value position also called expectation value?

This also we discussed last time. Formally which is $\psi^*(x)x\,\psi(x)$, the operator x, ψ evaluated. These things, these integrations you can do and verify that the average value of the position is L/2 and you can also plot wavefunctions. It is the sin function, you can plot what is the expectation value of x and so on, okay.

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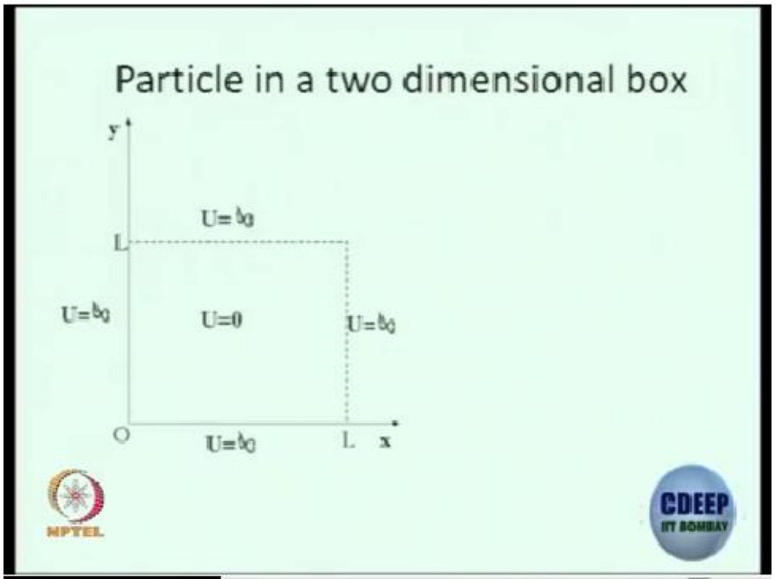

So far we did 1-dimensional box. You can make it into a 2-dimensional box, what is the modification? You have x and y axis, okay. And the particle, you are taking a square box. We could take a rectangular box also if you want but just for simplicity, let us take a square box. So the diagram explains where the potential is infinity and inside the square box, it is 0.

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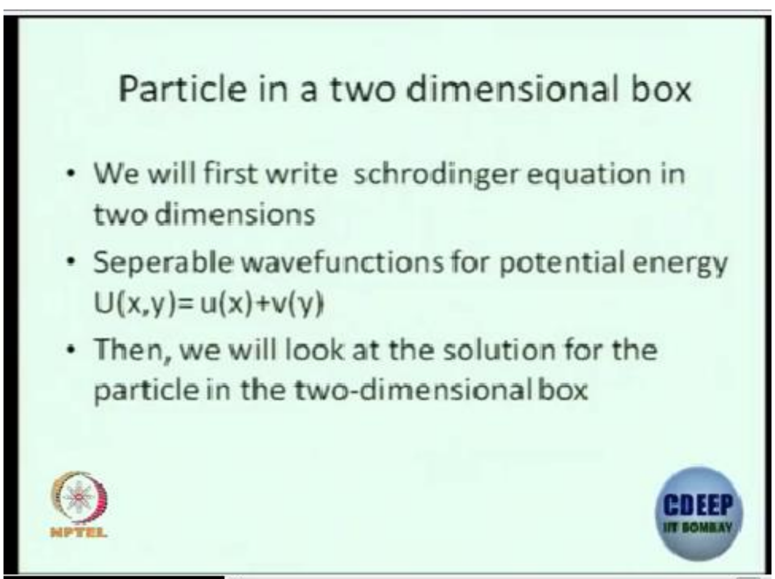

So what do we have to do? You have to first write the Schrodinger equation in 2-dimension. Then separate wavefunctions for potential energy, separable wavefunctions. If your potential energy cannot be written as sum of a potential energy for x+ sum of potential energy for y, then separable wavefunctions is not applicable. I am sure you know of this, right.

So separable wavefunctions, at least this particle in a 2-dimensional box falls into this class where U (x,y) is 0 for all x and y which is less than L, right, between 0 and L if x and y are taking values, U(x,y) is 0 and you can treat this condition being satisfied. So you can do separable wavefunction. And then we look at the solution of particle in the 2-dimensional box.

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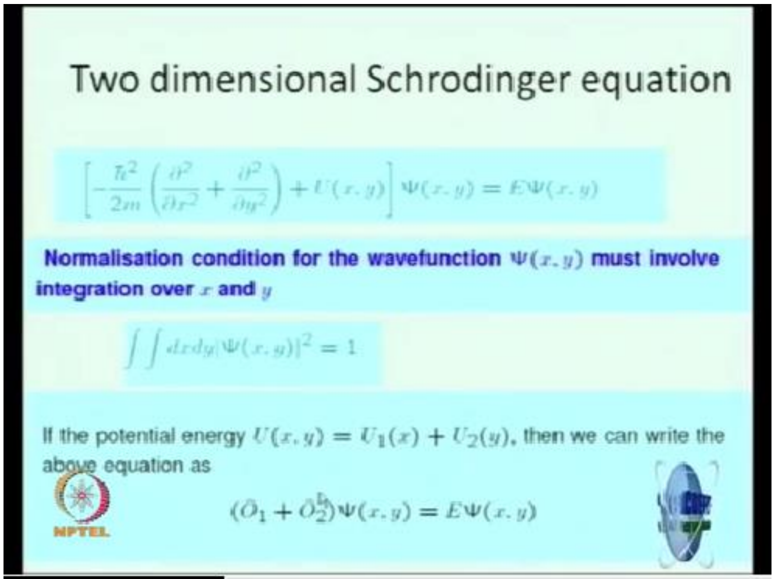

So 2-dimensional Schrodinger equation is again time independent. You earlier had on a $\frac{\partial^2}{\partial x^2}$ in particle in a 1-dimensional box. You will also have a $\frac{\partial^2}{\partial y^2}$ term. So that is the first step and $\Psi(x,y)$ will be a function of both x and y. And normalisation condition will involve not just integration over x, should also do an integration over y, right.

It is not 2-dimensional problem, straightforward extension. This is what is it? So you can put the limits as 0 to L and 0 to L for the particle in a 2-dimensional box. If the potential energy is $U_2(x) + U_2(y)$, then I can write the above equation, the top equation as an operator O which depends only on x and another operator which depends only on y and acted on $\psi(x,y)$. So this is the main theme in your differential equations.

If you can split the differential operators which depends only on x and another differential operator which depends only on y, then what is possible? $\psi(x,y)$ can be written as ψ of some kind of a $f(x)$ another, some other function of y, right. So that possibility exists only if you can write your differential operator into linear sum of 2 differential operators where one is dependent on x and another one is dependent on y.

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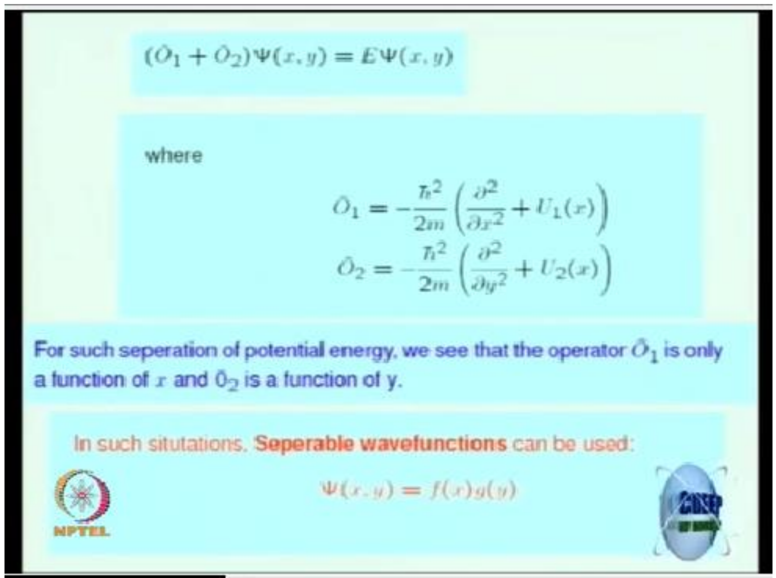

So the 2 differential operators are these. One, O_1 which is dependent on only x and O_2which is dependent on only y, differential operators, sorry this one has to be, there is a typo here, U_2 should be y, just correct it. U_2 should be y, okay. For such separation of potential energy, you can write separable functions, I am calling it as f(x) g(y).

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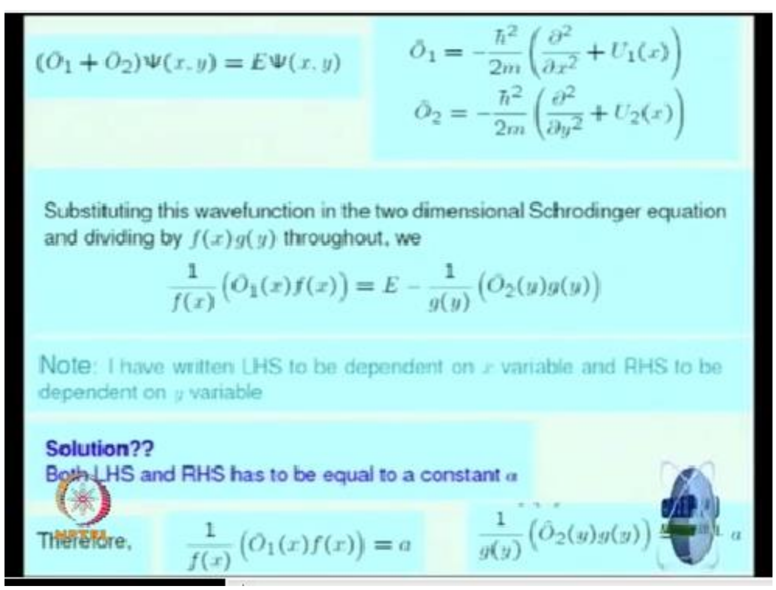

Even though I am stressing on particle in a box, this is applicable for other situations also. This is a formal 2-dimensional Schrodinger equation, how you can separate. If your potential energy is a sum of, you know, different coordinates potential energies. So now you substitute it into a 2-dimensional differential equation, Schrodinger equation and divide by f(x) g(y) and you will get the p which is x dependent.

Put it on the left hand side. p which is y dependent, put it on the right hand side and they will be related up to a factor of V. So this is the exact expression or equivalently this+this will be equal to E. Because we have divided by psi, okay. Please check it. So this is just for convenience. LHS is only dependent on x and RHS is dependent on y. And you can equate both of them to be equal to some constant A and solve for the constant which will again become a differential 1-dimensional differential equation.

Solve for f(x), okay. And similarly, you can solve for g(y) which will be the second 1-dimensional differential equation. So we will now solve for the wavefunction for particle in a 2-dimensional box.

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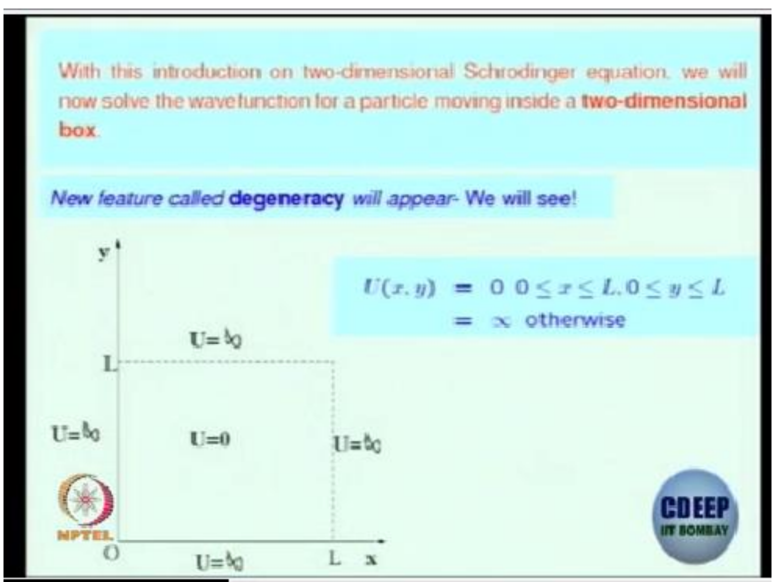

What are the things which you see here? First thing which you will observe compared to particle in a 1-dimensional box is that, there can be 2 different wavefunctions which can have the same energy. So that is what is called as a degeneracy. Degeneracy will not show up in a 1-dimensional particle in a box, okay. 1-dimensional particle in a box can also be felt as it is a bound state. It is bound inside x=0 and x=L, okay. So this is the first thing which you will observe.

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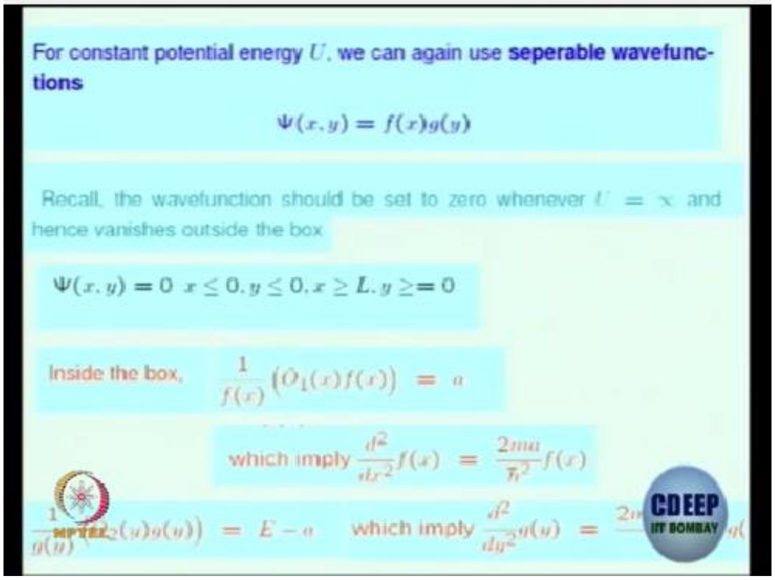

So let us solve this solution, $\psi(x, y)$ we are justified now that we can write f(x) g(y) even for particle in a 2-dimensional box. And recall the wavefunction should vanish at x=L or y=L, that you know and similarly x=0 and y=0. So put in those conditions on your wavefunction. What is the form you will get? Inside the box, you have to solve this differential equation. This equation is nothing.

But your a is similar to your k which we did, k^2, no different in 1-dimensional problems, okay. So $\frac{d^2f}{dx^2}$ is $\frac{2ma}{\hbar^2}$, call this as your k^2. Here just for simplicity, we will call it as k_x^2 if you want, okay. And similarly, you have the other equation, it is not equal to a but it is E-a. Is that fine? All of you are with me?

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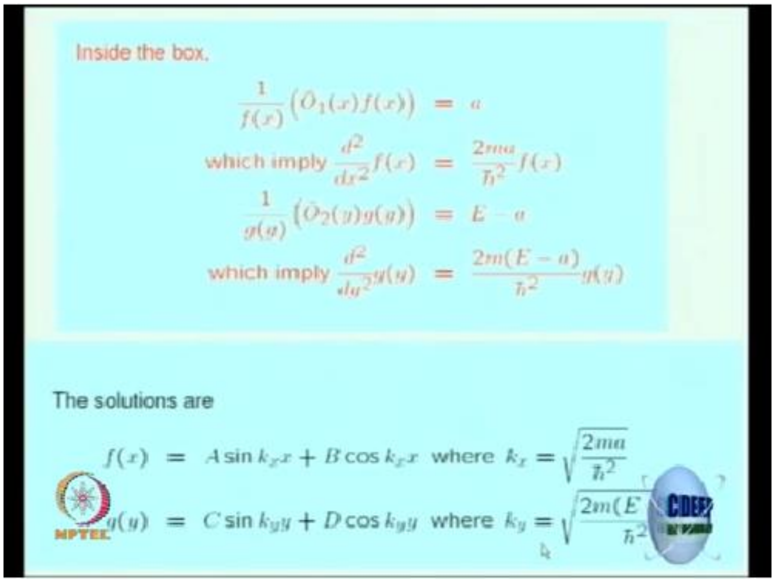

Okay, just to summarize, so these are the set of equations, formal operator equation is written. The explicit form is given in the second line and then you have a formal operated equation for the y dependence and explicit differential operator is given in the second line. What is the solution? Very simple. I am sure all of you know the solution. You can write the first one as f(x) as A sin(k_x x)+B cos (k_x x).

Similarly, g(y), so you put a subscript x for the k just to keep track that is $\sqrt{\frac{2ma}{\hbar^2}}$ and k_y is $\sqrt{\frac{2m(E-a)}{\hbar^2}}$. So what is the condition? k_x is this and k_y is this.

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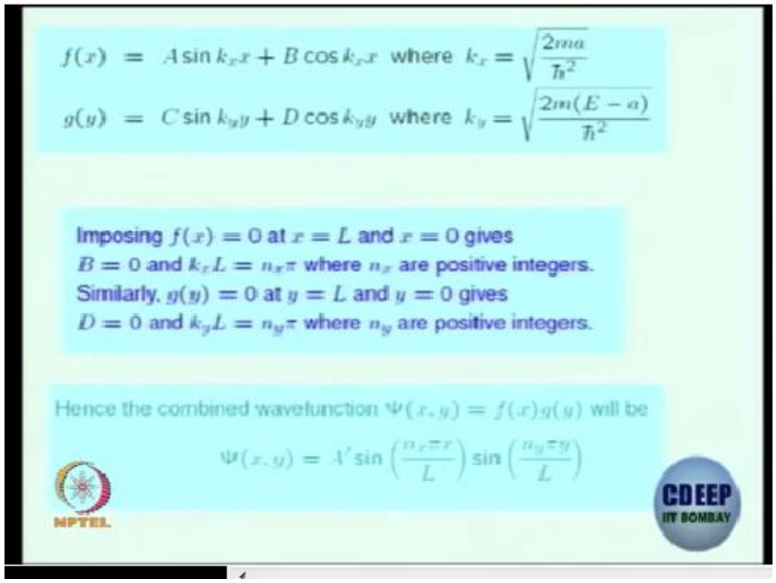

And you impose the condition f of x=0 at x=0 and x=L which will make B=0 and $k_y$will be quantized. Similarly, $k_y$will be quantized and D will be 0. So the combined solution for a 2-dimensional particle in a box up to a normalisation is a product of 2 sin functions exactly similar with one with n_x as the integer quantum number and n_y as another integer quantum number, okay.

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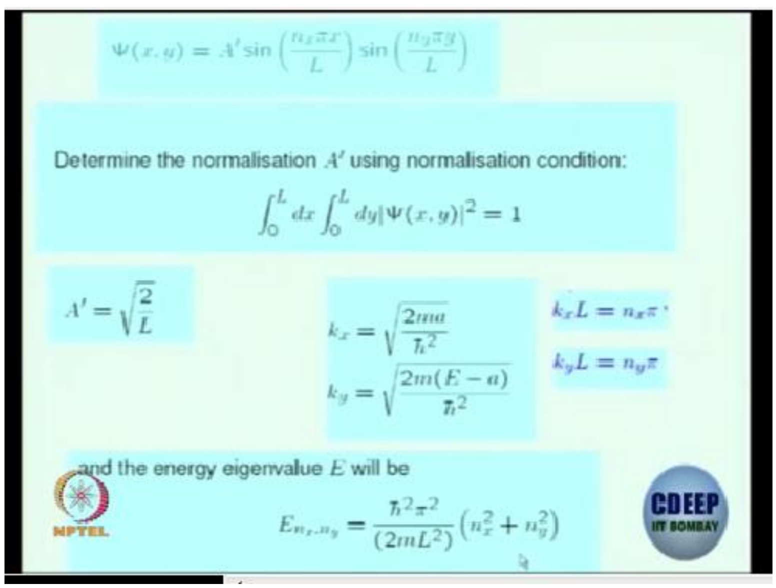
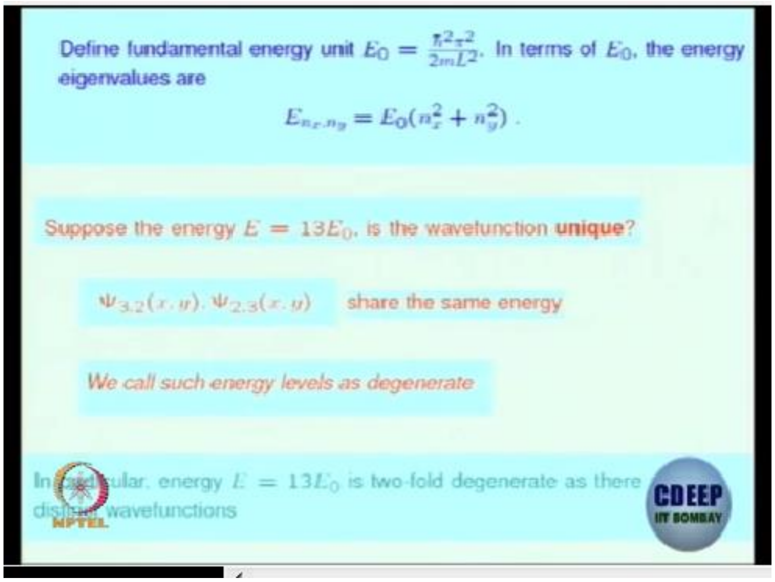


And how do you fix the normalisation? You integrate over dx as well as dy because it is a 2-dimensional problem and you can fix the normalisation. Is this correct? A prime is $\sqrt{\frac{2}{L}}$ or it is going to be just 2/L, has to be 2/L. For each integration, that will be a $\sqrt{\frac{2}{L}}$. So this also you should correct.

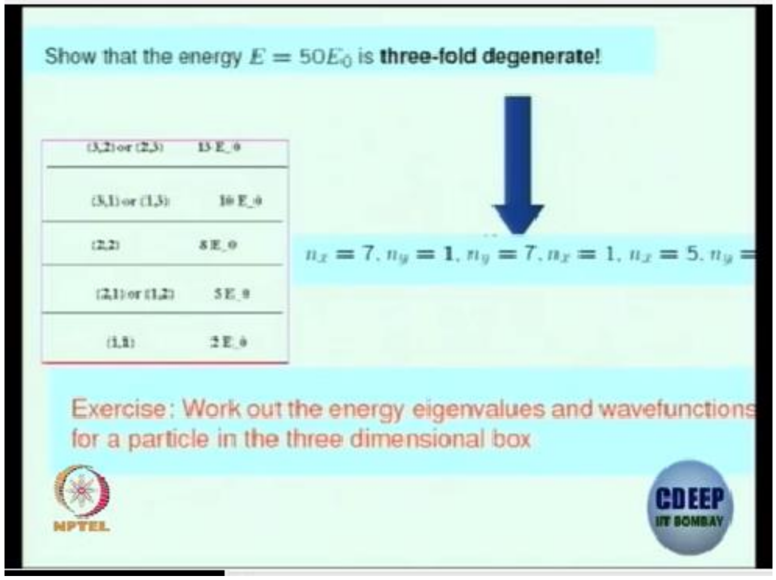
And the corresponding energy for a specific wavefunction, the wavefunction here I should put an n_x, n_y subscript.

For that wavefunction, the corresponding energy will be $n_x^2 + n_y^2$. **(Refer Slide Time: 20:00)**



Again you can define a fundamental energy unit and rewrite the particle energies in a 2-dimensional box as $E_0(n_x^2 + n_y^2)$. This is an exercise for you. If I tell you that the energy of a particle in a 2-dimensional box is $13E_0$, is the wavefunction unique? What are the possibilities? (2, 3) and (3, 2), so the wavefunction has n_x as 3 and n_y as 2.

There can also be another wavefunction but n_x as 2 and n_y as 3. Both will share the same energy eigen value, so that is why these 2 wavefunctions are degenerate at that level that energy level you will say is 2 fold degenerate. Symmetry of the 2, yes. So I will give you one more thing where you will see an accidental symmetry, one more, okay. So it happens because of the symmetry of the square but that could also be accidental symmetry, okay. So let me try and give you that example. **(Refer Slide Time: 21:21)**



$50E_0$, what are the possibilities? There is no symmetry there. So that could also be accidental degeneracy because the number adding as nx squared+ny squared to be some specific value, can have so many possibilities. Case of $13E_0$, the symmetry of the square tells you, you can interchange n_x and n_y, that is what you were saying. But when you do it for 50E0, not only that symmetry but you also have accidental things that you will have nx as 7, ny as 1, that gives you 50E0, ny as 7, nx as 1.

You also have nx=phi and ny=phi. So it is a 3 fold degeneracy. Such possibilities also exists. So case by case you have to find the degeneracy. It is not always 2 fold degenerate. It can be more than that. That is all I am trying to say. So I have given you a flavour of doing it for 2-dimensional box. It is not difficult to do a 3-dimensional box. You first put there y is a dependence on the right hand side, x dependence on the left hand side.

Put it to be a constant. And then the y is that you separate it as y and z, go systematically, so you will have an f of x, g of y, h of z and you can write it as a product of 3 sin functions, right. It is a very straightforward exercise. The first, if you understand 2-dimension, you can get to. What happens to degeneracy? The cubical symmetry will allow permutation of nx, ny, nz.

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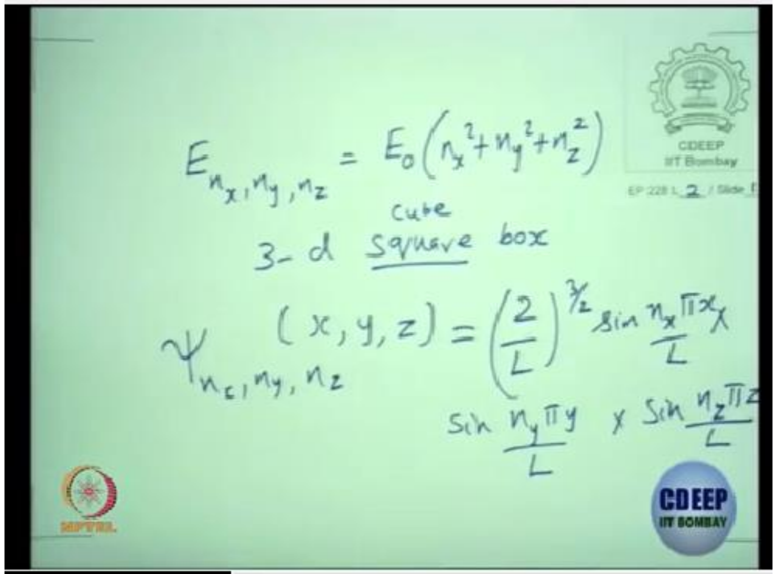

Energy will be energy Enxnynz=E0*nx squared+ny squared+nz squared, 3D box, square box or I should technically call it as cube, okay. Is that okay? So E of nx ny nz as nx squared+ny squared+nz squared, put a 3D square box. Can again workout degeneracies here and you can also write what is the wavefunction x y z to be, can write it as 2/L to the power of 3/2*sin nx pi/L*sin ny pi/L, x is there, right and then sin nz pi z/L.

Is that okay? What will be the modification if you try to put it in, kind of a cuboid with L1 L2, length, breadth, height to be L1 L2 L3. You have to accordingly modify these things. If you do the modification, this E0 is also cannot be written as couniversal E0, you have to appropriately put a by L1 squared, by L2 squared, by L3 squared. You know what is that? And there is no symmetry in that case, that can only be accidental coincidence of (()) (25:22). Is that alright, okay?

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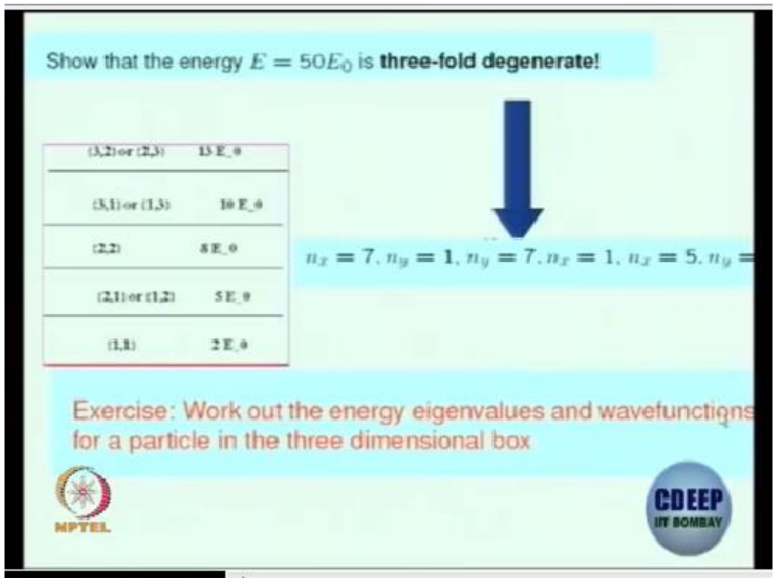

So the list which I have given is for the 2-dimensional box and then I have said for you to work it out. There will be some assignment problems on 3D box and you can try and fix it, okay.