Quantum Mechanics
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Lecture – 02
Introduction to Quantum Mechanics - II

Just to recap what is wavefunction which you have already seen. I have put it as a plot here.

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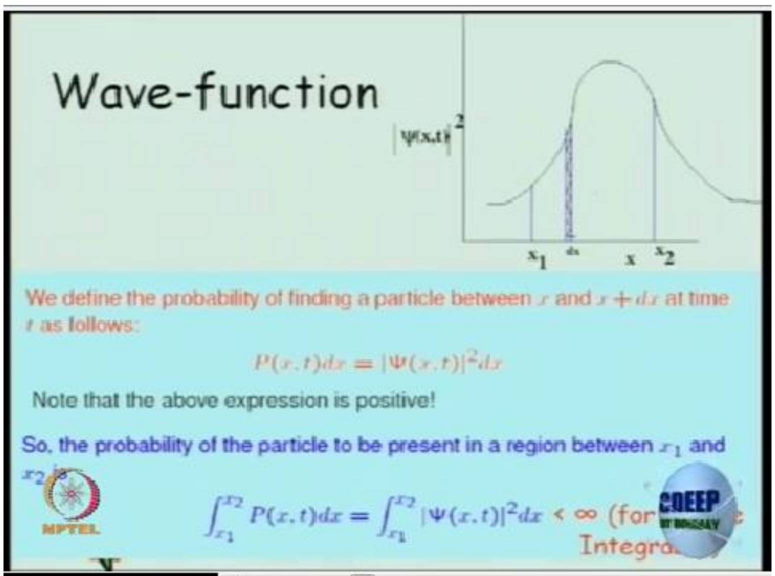

The mod of the complex wavefunction, mod squared of it, is going to be positive definite and there is a plot as a function of x and looking at the plot, you can try and define formally probability of finding a particle between x and x+dx at a specific time t, will be$|\psi(x,t)|^2 dx$. It is nothing but it is just area which is shown here. I put a shaded area here and that gives you the probability of finding the particle between x and x+dx.

If you want to find the probability of finding the particle between x_1 and x_2, what do you have to do? You have to integrate between x_1 and x_2 and that will give you the shaded area under this curve. So the probability of finding in the region x_1 and x_2, that is going to be the $\int_{x_1}^{x_2} |\psi|^2 \, dx$. So that will be the total are shaded under this curve. So one is to have some kind of a pictorial view not to mechanically do integrations, differentiation.

But you should all know that, both the math part as well as the graphical part and experimental data. All these things should be in your mind, then you understand quantum mechanics, okay. This also you have kind of being imposed when you did all the potential step function, well, barrier. In no region, you want your wavefunction to blow up, right. Did you allow anywhere the wavefunction to blow up?

If you had an exponentially growing function, if the region goes to $-\infty$, $+\infty$, then you put that coefficient to be 0, okay. So you will make sure that the probability is always a finite quantity. It is not infinite, okay. So p which we find for x lying between x_1 and x_2. This has to be

$$\int_{x_1}^{x_2} |\psi|^2 \, dx$$

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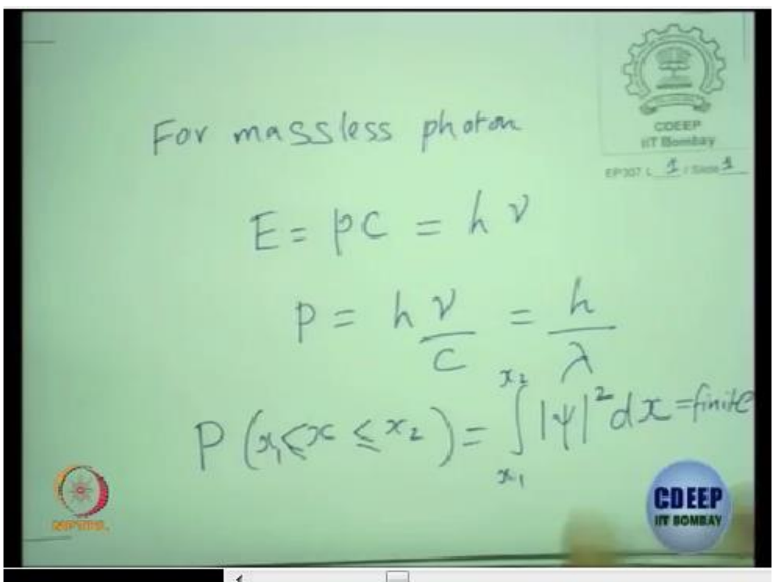

And this has to be finite. Here the mod squared, we will do a box normalisation. From that, okay, yes. So the question is that if suppose you have a wavefunction which is $e^{i\,k\,x}$.

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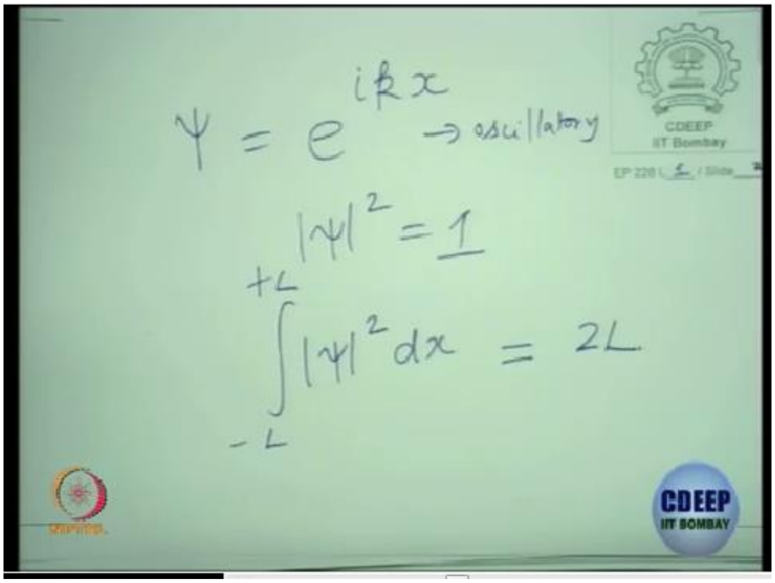

The claim is that when I do the probability $|\psi|^2$, that is 1 and $\int_{x_1}^{x_2} |\psi|^2 \, dx$, if you go from -infinity to +infinity, it will be infinity. Because this is 1, $|\psi|^2 = 1$. But what you will do is you will put it from -L to +L or something, okay. What will that be? It will be 2L, right. So we will keep it as 2L and do all your work, observable calculations which are averages and then this L will get cancelled.

So it is, even though it is not a, it looks like from this expression that it is infinity, you can regularize it in this way for the oscillatory function. These are called oscillatory functions. And you keep this L and later on you put L tending to infinity and all your calculations will all be finite, okay. So this is one of the important requirement which is called as squared integrable condition.

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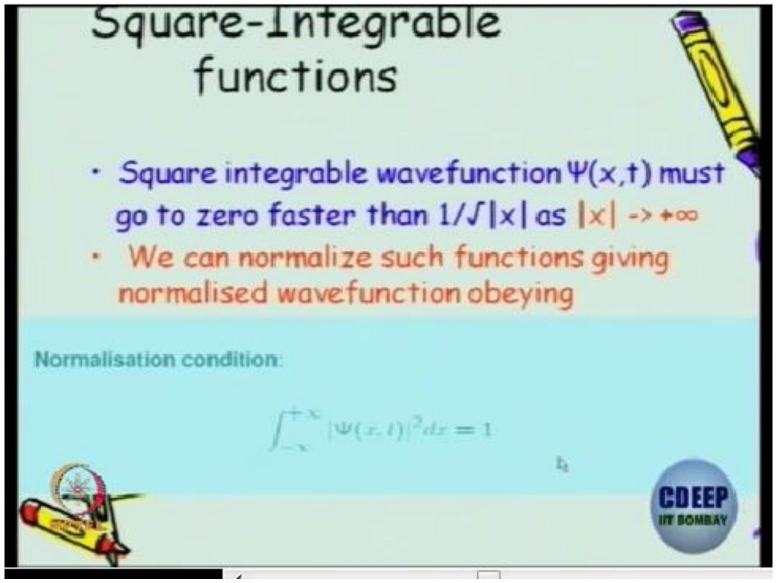

And square integrable functions, is for formal definition. If you have ψ(x,t), you have to make sure that it goes to 0 faster than $1/\sqrt{x}$ as x tends to +∞. I am looking at the positive x axis, $|x| \rightarrow \infty$ and for such functions, you can normalise them and normalisation condition is that the |ψ|^2 dx in the entire regime, the range depends on the situation but if you are looking at a region which goes from -∞ to +∞, this integral has to be equal to +1. Most of the time your wavefunction may not be normalised.

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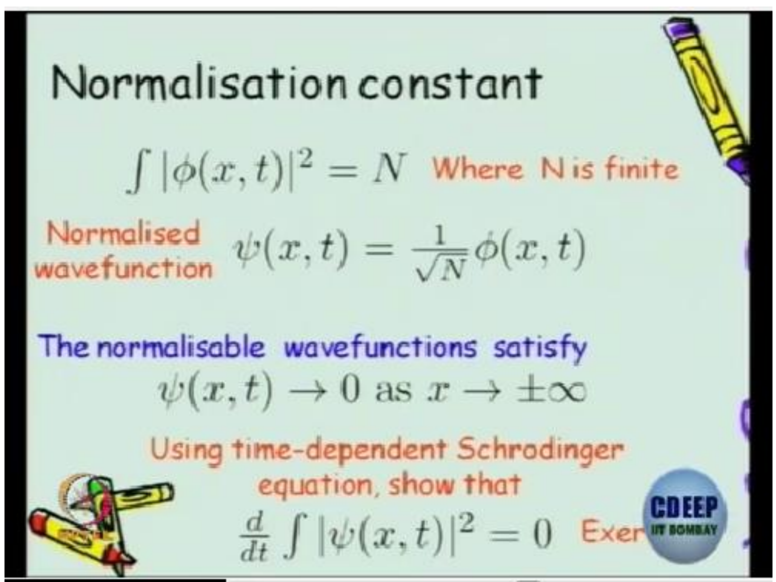

But you can normalise it. Like for example if ψ(x,t) is another wavefunction whose integral over the whole region is N, N is called as a normalisation constant and it should be finite. And how do you write the normalised wavefunction? You try to put $1/\sqrt{N}$ on the unnormalized wavefunction.

And if you try to do mod psi squared integral, it will be, that will be normalised and you also want your normalised wavefunction to go to 0 as x tends to $\pm\infty$. So these are the formal definitions of the squared integrable functions. And for you to call it as a normalizable wave function, okay. So this is one exercise which I want you to do. Use the time dependent Schrodinger equation which I showed.

The slides will also be there. I will try to put them on Moodle also for you. Show that the rate of change of probability, this is the total probability. You have seen that the total probability is normalised, it is a constant. Use the Schrodinger equation and show that it is 0, okay. That is the question?

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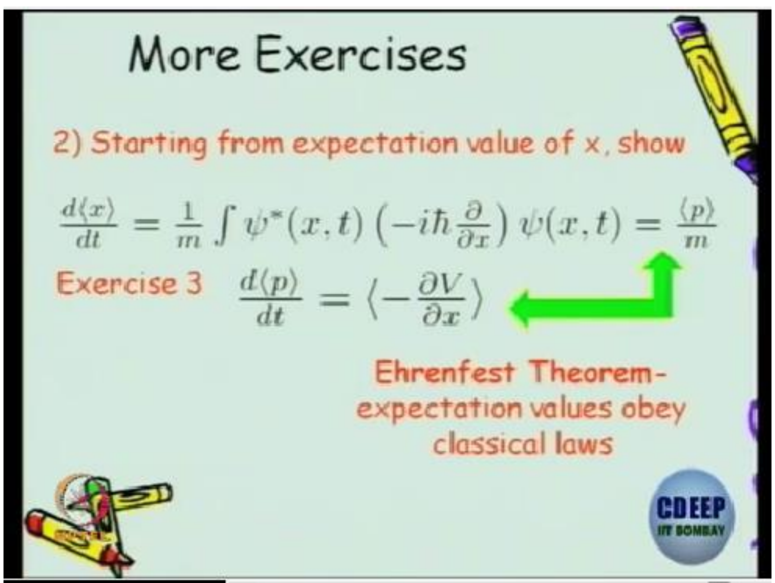

More exercises. Starting from expectation value of x, how do you write the expectation value of x? How do we write expectation value of x?

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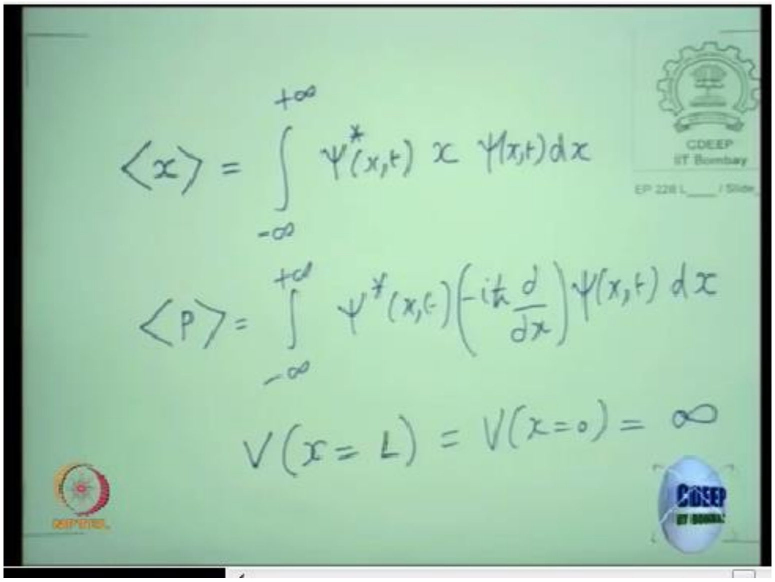

If I assume ψ to be a normalised wave function, this is the way we will write the expectation value of x, right. Just recalling what you have learnt in your first few course. So you start from the expectation value of x, show that d/dt of that expectation value, we do the algebra and show that it is expectation value of momentum. Momentum, you all know. Momentum expectation value is $-i\hbar d/dx$; so that is the momentum expectation value.

So what is this equation tell you? Classical mechanics when you do, right hand side, extreme right hand side, is actually velocity, okay. You can write this as mv, then it is expectation value of velocity. Expectation of velocity, please derive this, okay. So this is an exercise. Expectation value of velocity is rate of change of expectation value of position. Classical mechanics you did not have expectation value.

But you would have done d/dt of x to give you V, okay. If you want to match with classical laws, it is the expectation value which satisfies the classical laws. Quantum ideas, momentum is -ih d/dx, does not give you any matching with classical laws. But if you want to understand classical laws, find out the expectation value and see what equation the expectation value satisfies, okay.

So this explicitly when I do it, you see that d/dt of expectation value of x is $1/m*\langle p \rangle$which is what we expect for a classical law where we do not do expectation value. Exercise 3, is also familiar to you. If you are in the presence of a potential energy, the force law will be the -

gradient, conservative potentials if you have, the force will be proportional to $-\nabla V$, everybody knows that, right, classical.

But now, in quantum physics, your expectation values have to satisfy the equation. So please verify these things using this formal definition of how one writes the expectation value, given an indication. Please verify this and we could have a discussion on the tutorial session on Monday, okay, if you are not able to do it. But please try to do it, okay. So these classical laws satisfied by expectation value in quantum physics.

This comes under the title as Ehrenfest Theorem, expectation values obey classical laws, okay. The couple of things which you have done in the previous course, one is when we have a particle in a box. This is something which you have used.

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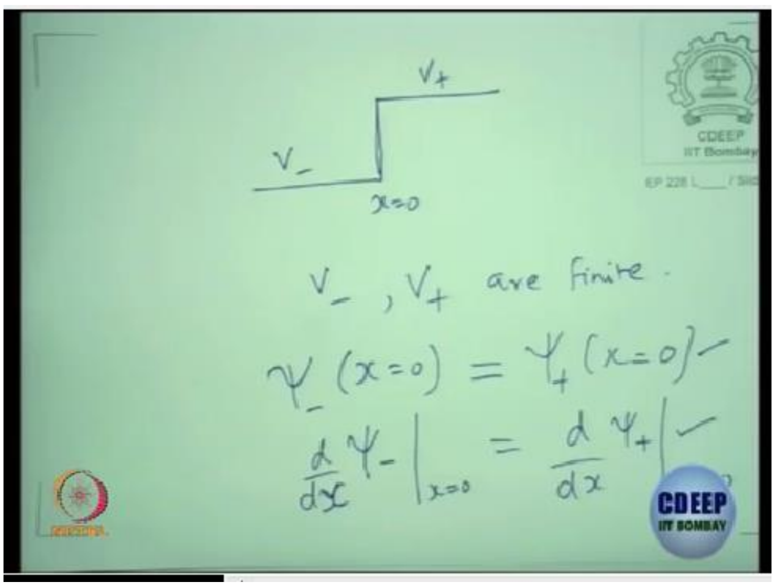

And you have also done potentials which are V_-, V_+ at x=0. So these finite, V_- and V_+ are finite. When you did this finite potentials, okay, you made sure that ψ_- the region at x=0 should be equal to ψ_+ at x=0. What else? d/dx of ψ, so this is ψ_-evaluated at x=0 should be same as or ψ_+ at x=0. So this is continuity of wavefunction, this one and this one was continuity of derivative of wavefunction or finite potential.

Once I do a particle in a box, which is removed? The second one is removed. Why? You know the reason. **“Professor - student conversation starts”** This will be finite term. So suppose you make it infinite, then you expect that? (()) (14:57). This is one way of saying it and we would like to see for other kind of potentials. What are the other kind of potentials? **“Professor - student conversation ends.”** You have all learnt about Dirac delta function in your math course? Yes? So what is that property?

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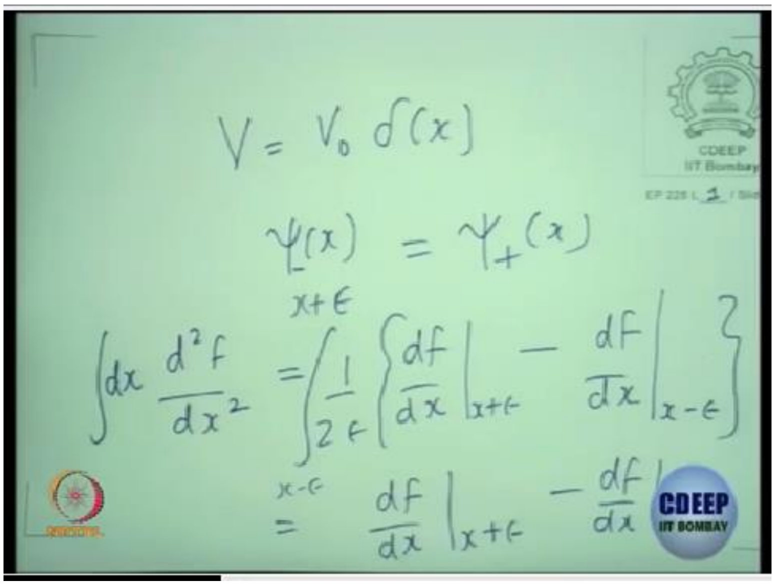

Suppose I have V as $V_0\delta(x)$. This is a delta, Dirac delta function. We expect what? We expect ψ_- of x to be same as ψ_+ of x. Continuity of wavefunction, there is no problem. Even for a particle in a box, your wavefunction should vanish that x=0 and at x=L and there is a continuity. Once there is infinite potential, wavefunction is 0 in the outside region of the box. Wavefunction is continuous.

The derivative of wavefunction cannot be checked for infinite potentials, right. So the derivative of wavefunction in general, only for finite potentials, will be continuous when you go from region 1 to region 2. This is the statement we make and as he has already pointed out, if you go and stand at the Schrodinger equation, you can actually prove these things, okay. So that is what I am going to show now, okay, just to take you on the tour of seeing it from, okay.

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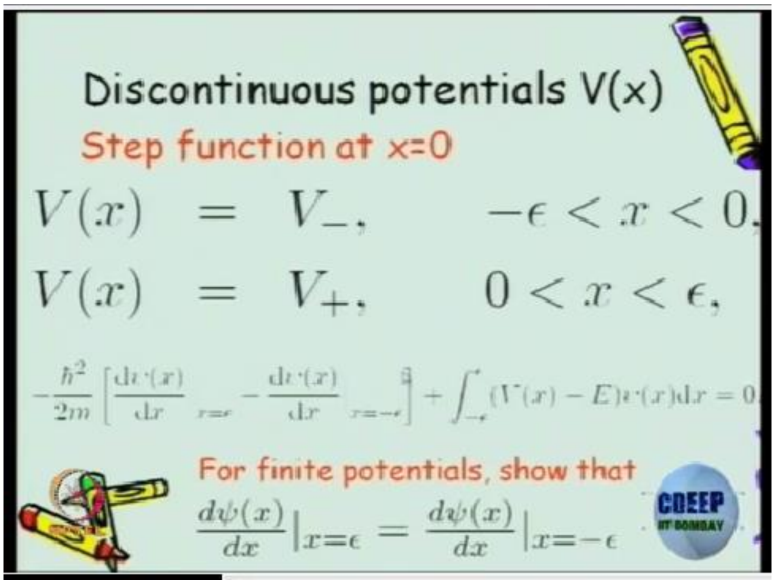

So take V of x below x=0 to be V_- and V of x to be V_+ for above x=0, x>0. If you take the Schrodinger equation and write the double derivative as difference between the single derivatives divided by epsilon and integrate over dx, so $\frac{d^2f}{dx^2}$ if you want to write, how will you write this? $\frac{df}{dx}$ evaluated at x=+ε, $\frac{df}{dx}$ evaluated at x=-ε then divided by 2ε, right.

You want to integrate this over dx. You can also integrate this over dx. You can remove this, okay. So this will give you, okay. So let us do this. So take that double derivative of the wavefunction and rewrite it as the difference between 2 single derivatives, integrate it over dx so that 1/2 ε cancels and you will have the other term, d of x-C. So this is just the Schrodinger equation which is rewritten here, an independent Schrodinger.

Now you can play around putting V of x from –ε to 0+another V of x between 0 to ε and substitute V- and V+ and take their limit epsilon tending to 0 limit, okay. We are looking flows at the boundary between the 2 regions. Is that right? So if you do that, there will be an epsilon factor multiplying. You also use the fact that psi of x is continuous. So you can pull out psi of x as psi of 0 out of the integral.

Ψ of x is continuous, so you can pull out ψ of x as ψ of 0 outside the integral and this V(x) will become V_+ +V-, okay. And you will have an epsilon because of this integral over dx. Similarly, E of ψ of 0*another ε run, okay, 2 ε. When you take the limit ε→0, what happens to the second term? Second term as long as V+ and V- are finite, epsilon*a finite quantity when ε tends to 0 is 0.

That is why the second term will become 0. The second term becomes 0, this is what he pointed it out already, you will have your first derivative of your wavefunction at $+\varepsilon$ and first derivative of the wavefunction at $-\varepsilon$ will be continuous across the boundary. Very clear from the Schrodinger equation. Will you do this intermediate step? Please do this intermediate step explicitly putting in V of x in these appropriate region, take the $\psi(x)$ out as $\psi(0)$.

Because ψ is continuous and check that you get continuity of the first derivative. Please check it?

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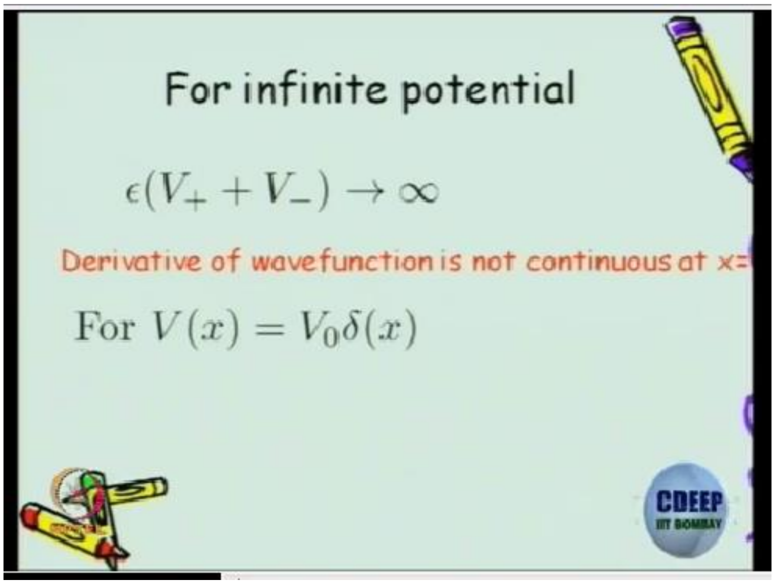

For infinite potential, suppose some region you make it infinite, okay, even if V- is 0, sorry if $V_+$is 0 and you make V- to be infinity, even then there is a problem. Because there will be an infinity multiplying a 0 and you have to be careful when you have 0 multiplying infinities, okay. When you have such problems with some potential in some regions where potential becomes infinite, you cannot assume the first derivative of the wavefunction to be continuous.

So that is why the derivative of wavefunction is not continuous for such potentials. Is that right? So what have we said?

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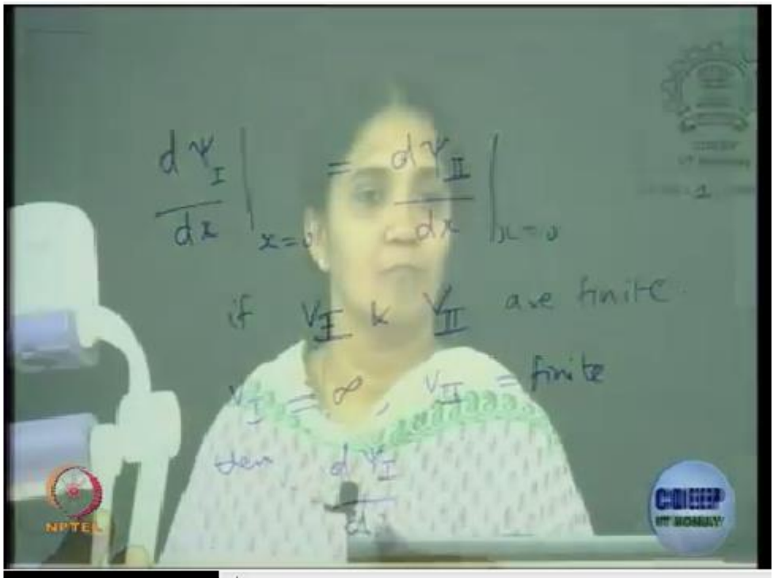

We say that $\frac{d\Psi}{dx}$ in region 1 at x=0 should be d psi in region 2 at x=0 if x=0 is the interface, if V+ or $V_1$and $V_2$are finite. If $V_1$is infinity, $V_2$is finite, then we do not have this.

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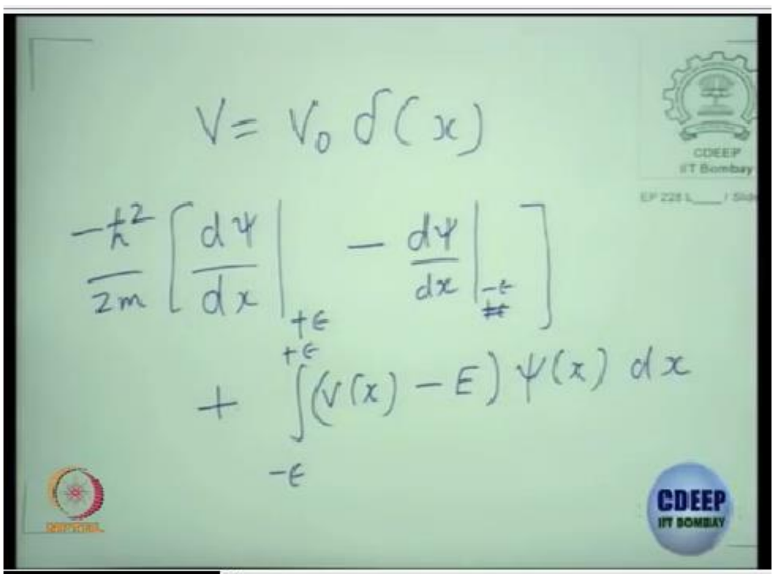

So the immediate problem which we can try to solve as V=$V_0\delta(x)$, okay. So how do we do this. We will have a $-\frac{\hbar^2}{2m}\frac{d\psi}{dx}$ at ε_+, right, minus $-\frac{\hbar^2}{2m}\frac{d\psi}{dx}$ at ε_-. Let us center it around x=0, - $\frac{d\psi}{dx}$ at $+\varepsilon$, or is the other way around, $+\varepsilon$ and this one will be $\int_{-\varepsilon}^{+\varepsilon}.(V(x)-E)\psi(x)dx$. Is that right? And we are going to substitute for V as V_0, V_0 as a constant and delta of x.

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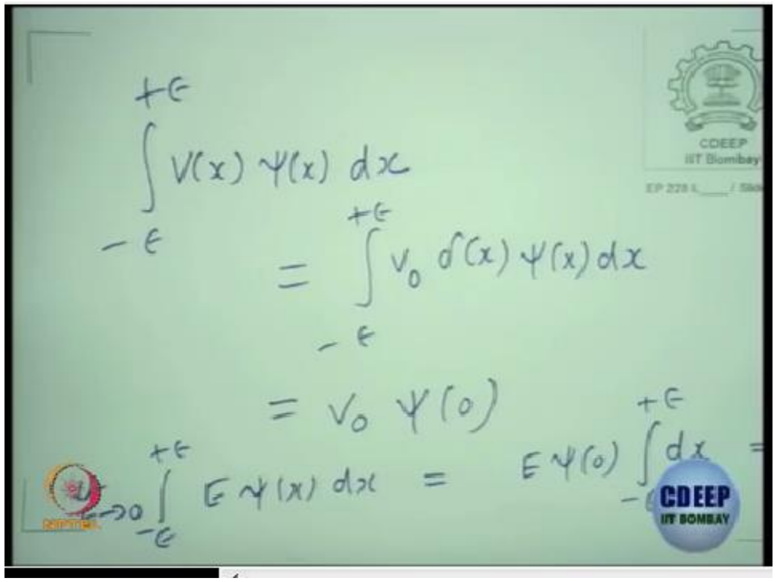

So let us substitute that, $V(x)\psi(x)\,dx$, so it will be; what is this? $V_0\,\psi(0), \lim_{\varepsilon\to 0}\int_{-\varepsilon}^{+\varepsilon} E\psi(x)\,dx = E\psi(0)\int_{-\varepsilon}^{+\varepsilon} dx,$ and in the limit, you have to take limit epsilon tending to 0. That will be? That is going to be? So this term is 0, V(x) $\psi(x)$ as $V_0\,\psi(0)$ which is finite.

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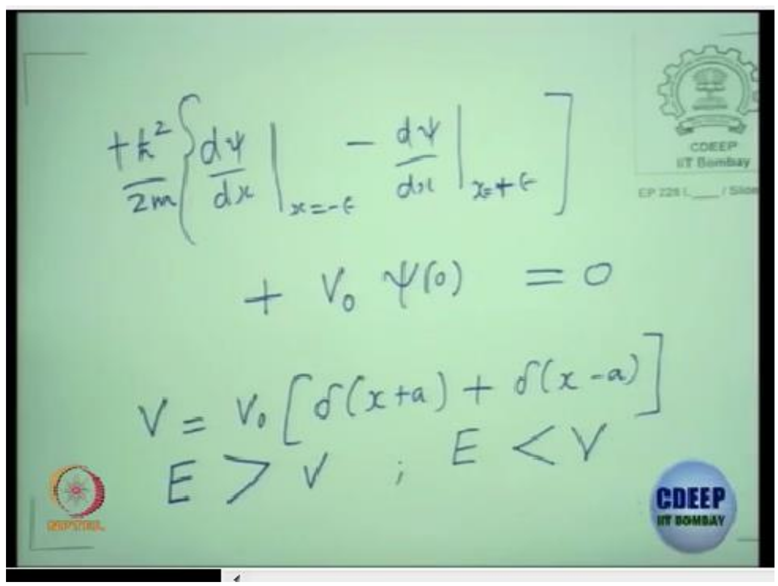

So in the context of delta function potentials, we can try and tell $\frac{\hbar^2}{2m}\left\{\frac{d\psi}{dx}\Big|_{x=-\varepsilon}\frac{d\psi}{dx}\Big|_{x=+\varepsilon}\right\}$ or the other way around, so you can remove the -sign and make it +sign here, okay, will be $+V_0\psi(0) = 0$. So what have we achieved? In the context of particle in a box, we cannot find the amount of discontinuity, right. You need not even worry about it.

Here even though it is an infinite Dirac delta function potential, I can tell the difference what should be the discontinuity element to go from the x- region to x+ region by this specific, if you know the wavefunction at 0 and V_0 is the factor multiplying the delta function potential, I know exactly the amount by which there is a discontinuity in the derivative of the wavefunction.

Suppose I give V to be $V_0\delta(x-a)+\delta(x-a)$, these are the double delta functions, so these are the various potentials where you need to get a feel of what is the solution and when can you get bounce states. You know what is the condition for a bounce state? Why do you call it as a bounce state? Particle, harmonic oscillator, what is the requirement? With a bounce state, do you know?

When is the scattering state you can get? All the free particles are scattering, right. So there are 2 regimes. If energy of the particle is greater than V, you have the scattering states possible. You have the states which are transmitted. And there is another regime which is energy of the particle<V, okay. So these are the 2 regimes which you might have, this is what you would call it as a condition for getting bounces, right.

So now what we would like to do is, let us formally, in the next lecture, we formally put in the conditions for the bounce states. Just how the way we should look at bounce states. And then we could try and do some of these delta function problems, potential, double delta function, when will it be a bounce state, when will it be a scattering state. That will depend on the sign of V_0 okay.

So these are things which we will start exploring purely from the wavefunction formalism. It is just a 1-week, we will have a warm up doing these things and we will reproduce all these things from the linear vector space notation. That is the idea. So you need to know these things. You cannot say I will forget this. You need to know the wavefunction formalism. You should also know how these can be reproduced from the Dirac notation of the vector space and Dirac Bra-ket notation, okay. So I will stop here.