

Quantum Mechanics
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Lecture – 06
Tutorial 1 - Part II

So in the last tutorial, we have already seen problems based on particle in a box and we have calculated the probability, density and we have also seen the bound state energy problems. So now let us get start doing the problems based on probability current density and few more problems which will give you more flavour of the first part of the tutorial.

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3. Let $P_{ab}(t)$ be the probability of finding a particle in the range $(a < x < b)$ at time t .


(a) Show that

$$\frac{d}{dt}P_{ab}(t) = J(a, t) - J(b, t)$$

where $J(x, t) = \frac{i\hbar}{2m} \left(\psi(x, t) \frac{\partial \psi^*(x, t)}{\partial x} - \psi^*(x, t) \frac{\partial \psi(x, t)}{\partial x} \right)$

is called the probability current density.

(b) Suppose the particle is unstable and has a lifetime τ , then we require the violation of conservation of probability. That is, $P(t) \equiv P_{(a=-\infty, b=\infty)}(t) = e^{-t/\tau}$ (time-dependent). This form can be achieved by taking a complex potential $V(x) = V_0 - i\Gamma$ where V_0 and Γ are real. Find $\frac{dP(t)}{dt}$ and determine in terms of Γ .



And here problem 3 is about the finding, so let P_{ab} be the probability of finding the particle between a range that is a and b at a particular time. So the problem is to show that the derivative of the probability density is equivalent to or equal to the current density at a at time t, - the current density at that be the time t where this is the definition of current density $J(x, t)$. So $J(x, t)$ is nothing but the probability current density.

So this is the first part and the second part is then your, so in the first part, we have a problem wherein we are finding the probability of the particle in a box. So we will take the potential to be real. In the second part, the potential is replaced by complex potential $V_0 - i\Gamma$. So where V_0 and Γ are real quantities and this potential is complex. So how the probability will get modified and

what will be the rate of probability and what it will be in terms of this Γ . So let us get started.

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③ The probability of finding a particle in the range $a \leq x \leq b$ ①

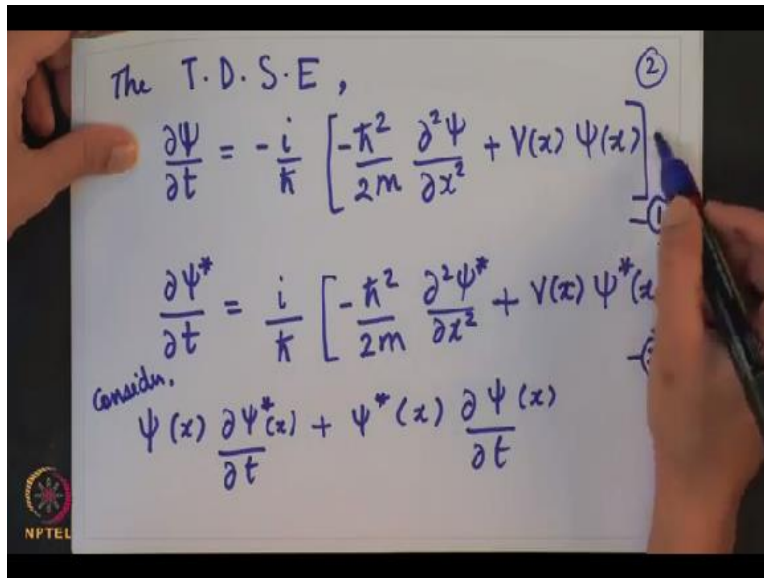
$$P_{ab} = \int_a^b \psi^*(x,t) \psi(x,t) dx$$
$$\frac{dP_{ab}(t)}{dt} = \int_a^b \left(\frac{\partial \psi^*}{\partial t} \psi + \psi^* \frac{\partial \psi}{\partial t} \right) dx$$

So third problem of the first tutorial, so we write the probability of finding a particle in the range between $a \leq x \leq b$ is given by, let me call that as P_{ab} . P_{ab} will denote the probability between the range a and b , will be given by $\int_a^b \psi^*(x,t) \psi(x,t) dx$. So this is the general expression and since we have to find out between the 2 limits, I will write it as integral from a to b . Now we have to evaluate this quantity, okay at some t , okay.

So the probability, you take the derivative of probability with respect to time and since t is independent of x , I can simply take the derivative inside the integral, simple mathematics. So I can write this as ψ^* and I will use the shorthand notation, I will drop the parenthesis. This will be, I will have 2 terms, ψ^* derivative with respect to t and ψ and the other term would be ψ^* derivative with respect to ψ and this entire thing, $*dx$.

So this is what we have. Now we have to rewrite it in the form given to us in the question which is we have to write this as the probability current density.

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So now the next step would be, we write the time-dependent Schrodinger equation. So the time-dependent Schrodinger equation is given by, so I am using a short form here, time-dependent Schrodinger equation will be what? $\frac{\partial \psi}{\partial t}$ this is the energy operator which will come with $i\hbar$ which I will take on the right. So this is my $i\hbar$. This will come on this side. You have a minus sign.

This will be nothing but $\frac{\hbar^2}{2m}$, then I have a momentum operator, $\frac{d^2}{dx^2}$ is written like this, $+V(x) \psi(x)$. So this is my time-dependent Schrodinger equation. What I do here is I just take the *, that is I take the complex conjugate. So when I take this *, this - will become +, so I have \hbar^2 , sorry $-\frac{i}{\hbar} \left(-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} \right) + V(x) \psi(x)$. Now this wavefunction will become ψ^* . And here in this problem in part A, the potential is real. So $V(x) = V(x)^*$, so it to remain as $V(x)$ and we have a $\psi^*(x)$, okay.

Now what we have to do is you have to write this in the form of the current density. So what was the expression for the current density? It was of this form, $\psi(x) \frac{\partial \psi^*(x)}{\partial t} + \psi^*(x) \frac{\partial \psi(x)}{\partial t}$. You have to evaluate this. So you consider this part, okay. So when you use these 2 equations, that is you multiply the first equation by a ψ and the second equation by ψ^* , what you obtain is that ψ and ψ^* term for the potential will get cancelled, okay.

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$$\begin{aligned}
 &= \frac{-i\hbar}{2m} \left[\frac{\partial^2 \psi^*}{\partial x^2} \psi(x) - \frac{\partial^2 \psi}{\partial x^2} \psi^*(x) \right] \\
 &\text{I.P.} \\
 \frac{dP_{ab}}{dt} &= \frac{-i\hbar}{2m} \left[\frac{\partial^2 \psi^*(x,t)}{\partial x} \psi(x,t) - \psi^*(x,t) \frac{\partial \psi(x,t)}{\partial x} \right] \Bigg|_a^b \\
 &= -J(x,b) + J(x,a) \\
 \frac{dP_{ab}}{dt} &= [J(x,a) - J(x,b)]
 \end{aligned}$$

So what I will get is I can simplify this as $\frac{-i\hbar}{2m}$, then I have $\frac{d^2\psi^*}{dx^2}$, okay. So first term will be with a * and I have a $\psi(x)$, -, I have $\frac{d^2\psi(x)}{dx^2}\psi^*(x)$, okay. This is what I have. So now what I have to do is, I have to do integration by parts and then after doing integration by parts, what I obtain is just a simple form that is let me get back to our expression which is this expression, dP/dt is this.

So I have substituted for these 2 quantities and I have multiplied the first equation by ψ^* and the second equation by ψ and I have just added those 2 equations. So this would give me simply this expression there was a integral dx. So when you do integration by parts, what you obtain $d\psi^*/dx$, okay.

So I am missing the parenthesis everywhere. You write it everywhere or you can just use the shorthand notation, x, okay. So this is the form you get when you perform or rather even before doing integration by parts, you have this form, okay. And then what you do is, you can actually rewrite this as, you have to put the limits of integration. So the first part, when you put $x=b$, you obtain a, so there is a -sign already.

So the first part when $x=b$, you obtain $J(x,b)$, - the lower limit that is I will have a minus and minus plus, so that will be x, a. So in the end, what I get here is, in the end, I have $dP_{ab}/dt = -$, okay. So here these steps, this to this requires integration by parts. So here I have done integration by parts

remember, okay. Once you do the integration by part, you will obtain this expression and then you put the limit and obtain the a part of problem 3, okay.

Then what do we do in the next part is, okay. In the B part, you are having the potential which is not real, it is imaginary. So the entire exercise you will repeat from 1 to what we did now, okay. And then what we do is we will have an additional term or an additional contribution coming from the imaginary part.

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$$P(t) = P_{-a,a}(t) = e^{-t/\tau}; V = V_0 - iV \quad (4)$$

$$\frac{dP_{a,b}}{dt} = \int_a^b \frac{\partial \psi^*}{\partial t} \cdot \psi dx + \int_a^b \psi^* \frac{\partial \psi}{\partial t} dx$$

$$= J(a,t) - J(b,t) - \frac{2\Gamma}{\hbar^2} \int_a^b \psi \psi^* dx$$

$$a, b \Rightarrow -\infty, \infty$$

So the imaginary part, so let me write what is given to us? It is given that P of t at P, now a and b are replaced by $-\infty$ and $+\infty$. Final expression what we obtain in terms of P(t) will be of some form in which we have to compare with this expression, okay. So now the probability is given by, probability density which we calculated in the previous example was given by, let me write a shorthand notation again, $t=a$ to b , then I have $\psi^* \psi$, I mean the same expression I will write for $\psi^* V$.

So I will just rewrite here, $\psi^* \psi$ and I have a dx and then I take the derivative. So I will have 1 term, + the second term will be, okay, same way. Again I will repeat the same procedure. I will substitute for the time-dependent wavefunction, using the time-dependent wavefunction, I will substitute for these terms and what I obtain is I will again obtain the same expression, first part of the expression will remain the same because we have the, remaining part of the wavefunction is

the same expression is the same. Only we have the additional term of the additional contribution coming from the potential. Now the potential here is remember V is nothing but $V_0 - i\Gamma$. So the additional contribution will come from $i\Gamma$. So this V_0 and $i\Gamma$ are real. So I will have an additional term. What is that additional term? Will be, so this step you have to work out. So in between ψ^* dx , okay and between the limits a to b .

Let me correct this also, a to b , okay. So here what we will do is we have obtained the same result + additional contribution coming from the potential. This you can simply work out. This because of the complex part, there will be 2 contributions. So I have a $2\Gamma\hbar$ not \hbar . Now what we will do is? We will replace a and b by $-\infty$ and ∞ , okay. So when we replace this by ∞ and $-\infty$, what do I obtain.

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$$\frac{dP_{-\infty, \infty}}{dt} = -\frac{2\Gamma}{\hbar} \int_a^b \psi^* \psi dx$$

$P(t)$

$$P(t) = e^{-\frac{2\Gamma t}{\hbar}} \equiv e^{-t/\tau}$$

$$\Gamma = \frac{\hbar}{2\tau} \quad \text{or} \quad \tau = \frac{\hbar}{2\Gamma}$$

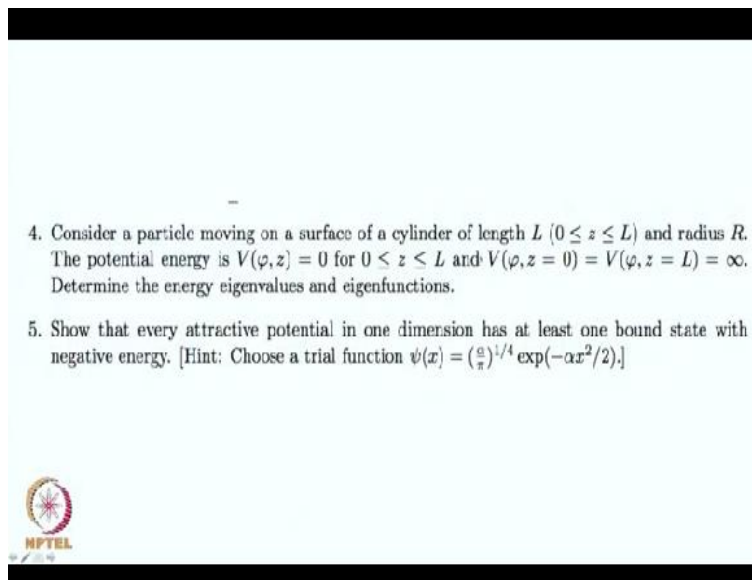
dP/dt at $-\infty$ and $+\infty$ will be 0. So as you all know that at $-\infty$ and $+\infty$, the current density will be 0 because the wavefunction at $x=0$ is 0. So you will be left with $\frac{-2\Gamma}{\hbar} \int_a^b \psi^* \psi dx$ or $\psi^* \psi dx$, does not matter. So now after doing this, you can easily write this as, this is dP/dt and you have an integral. So you can just integrate throughout and obtain \hbar cross t , okay.

It is very simple and it can be shown, okay. Because this you know is nothing but $P(t)$, okay. So you have $dP/dt - 2\Gamma\hbar P(t)$. So what we obtain is this expression. So now you compare this with what is given to us. What is given to us is $e^{-it/\tau}$, okay. So now the time dependent wavefunction,

the probability at time $t = \text{some } T$, will be given by this or $-\infty$ to $+\infty$ and so you can actually write the relation between $\gamma(\Gamma)$.

So what will be γ ? γ will be just in terms of τ if you want to write, what we can do is 2τ or τ is nothing but $\frac{\hbar}{2I}$, okay. So this is what we obtain, okay. Then we go to the next problem which says that in the next problem, it says that you have a particle which is moving on the surface of a cylinder, okay.

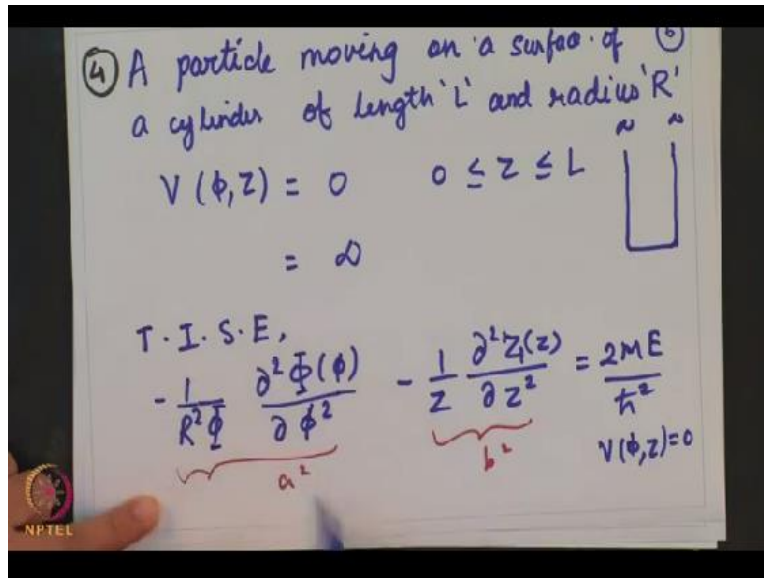
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A particle is moving on the surface of a cylinder of length L . So along the z direction, so z is between 0 and L and r is the radius of the cylinder. Potential energy is given by this. So for the region between 0 and L , potential is 0 and at the boundaries, V is infinity. So you can imagine this or consider this as a particle in a potential well with an infinite potential. Same as you have seen, 1-dimensional potential well problem.

So it is very simple to determine the energy eigen values and energy eigen values and eigen functions. So the trick will be the same. You start, okay, so here it will be very convenient to use cylindrical coordinates. So I will be using that. You can use Cartesian coordinates also.

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For a particle moving on a surface of a cylinder of length L , okay and a radius r , okay. So we are given this potential well problem where in V of ϕ , Z is 0 for $0 < z < L$. So inside the potential well, the potential is 0 and it is infinity elsewhere. V is 0, V is infinity. So at these points, V is infinity, okay. And this is the radius, this is the length of the cylinder. Now let us get started. So we use Cartesian coordinates to write the time-independent Schrodinger equation.

So using Cartesian coordinates, you can solve this but I will use cylindrical coordinates. So we have write the time-independent Schrodinger equation in terms of the cylindrical coordinates in this form, okay, $-\frac{1}{R^2 \phi} \frac{\partial^2 \Phi(\phi)}{\partial \phi^2} - \frac{1}{z} \frac{\partial^2 Z(z)}{\partial z^2} = \frac{2mE}{\hbar^2}$, okay. This is the standard form. Now we are talking about the particle inside the potential. So V is ϕ , Z is 0, okay.

So we do not have the potential term. And this you can write as some a square and this you can write as some b square. This is an equation with 2 variables. Let me call this as capital $\Phi(\Phi)$. Now I have confusion.

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$$-\frac{1}{R^2} \Phi = a^2$$

$$\Phi(\phi) = e^{ia\phi R}$$
 Apply the b.c

$$\Phi(\phi + 2\pi) = \Phi(\phi)$$

$$\Rightarrow a = \frac{l}{R} \quad l = 1, 2, \dots$$

$1/R$ square capital Φ , okay. Let me come back here to; so here this was nothing but this is equal to a square, okay. I am just rewriting this part quickly. $\frac{\partial^2 \Phi(\phi)}{\partial \phi^2}$, okay. This is equal to a square. Now you can easily calculate $\Phi(\phi)$. It is very simple, okay. So now this can be written as ψ is $e^{ia\phi}$, okay. And you have a factor of r which is coming from here. So you have a R also. Let me write it here, okay. So this will be the solution.

So now the next step would be to apply the continuity or boundary condition. So at the boundary, is equal to ϕ , this we know, right at the boundary. That is at after 2π rotation, ϕ will be equal to capital ϕ , okay. Which would give us the relation between a and R . So a will be some $l \cdot R$, okay. This again you can just substitute here and you get this expression. So where l can take any value from 1 to n , okay. So this is the relation between l and R , okay.

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Along the length of the cylinder

$$\psi(z) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi z}{L}\right)$$

$$b = \frac{n\pi}{L}$$

$$\frac{\hbar^2}{2m} [a^2 + b^2] = E$$

$$\frac{\hbar^2}{2m} \left[\frac{l^2}{R^2} + \frac{n^2\pi^2}{L^2} \right] = E$$

So the next step would involve to calculate the second part, that is B part along the length of the cylinder, particle in 1-dimensional box, I can write the solution simply as $2/L$, okay. Now this is the Z component, there is a length of the cylinder, is like a 1-dimensional particle in a box. So this can be written as $n\pi z/\text{the width}$, that is L , okay. Here I have used L , okay. This is the standard way of representing the particle in a box, solution for the wavefunction for a particle in 1-dimensional box, okay.

So now it can be inferred from here that b is nothing but $n\pi/L$, okay. So the wavefunction is given by $\sqrt{\frac{2}{L}} \sin(b \cdot z)$. So now this final expression is or the energy eigen value is $\hbar^2/2m^*$, we have a which is nothing but, so I will write this as $a^2 + b^2$ which we saw will be nothing but $E = \frac{\hbar^2}{2m} \left[\frac{l^2}{R^2} + \frac{n^2\pi^2}{L^2} \right]$, okay. Fine.

This is the capital L. This is the small l remember. This is E. So this is the energy eigen value. And the wavefunctions you have seen. And the fourth, so in the fifth problem, what we do is few steps. I will just illustrate here. So fifth problem is based on the attractive potential in 1-dimension.

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4. Consider a particle moving on a surface of a cylinder of length L ($0 \leq z \leq L$) and radius R . The potential energy is $V(\varphi, z) = 0$ for $0 < z < L$ and $V(\varphi, z = 0) = V(\varphi, z = L) = \infty$. Determine the energy eigenvalues and eigenfunctions.
5. Show that every attractive potential in one dimension has at least one bound state with negative energy. [Hint: Choose a trial function $\psi(x) = (\frac{\alpha}{\pi})^{1/4} \exp(-\alpha x^2/2)$.]



So the question is show that every attractive potential in 1-dimensional box has at least one bound state with negative energy and you can prove this using a trial wavefunction.

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(5) $V(x) < 0 \quad \forall x$
 $V(x) < 0$ for some value of x .
 $V(x) \rightarrow 0 \quad x = \pm \infty$

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - |V(x)|$$

$$\psi(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}$$

So the fifth question, you can start by taking now, so V of $x < 0$ or $<$ or $= 0$ for all x . And V of x is 0 for some x , right. So attractive potential you mean a piecewise continuous wavefunction or piecewise continuous function V of x such that V of $x <$ or $= 0$ for all x 's and it is less than 0 for some value of x , okay. So now V of x we know that at $x = \pm$ -infinity vanishes. It will go to 0 for \pm -infinity.

So now let us write down the Hamiltonian operator H is $-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$. Now we are talking about the attractive potential. So let me put here $|V(x)|$, okay. So V is negative, so I have put a mod sign. So now if I want to use the trial wavefunction, trial wavefunction is $\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{\alpha x^2}{2}}$. So now if I operate this on this trial wavefunction, what do I get? Let us work out this quickly.

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$$\hat{H}|\psi(x)\rangle = \left(\frac{\hbar^2}{2m} \alpha (1 - \alpha x^2) - |V(x)|\right) |\psi(x)\rangle$$

$$\langle \psi | \hat{H} | \psi \rangle \leq 0$$

$$\langle \psi | \hat{H} | \psi \rangle = \left(\frac{\alpha}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} \hat{x} e^{-\alpha x^2} dx$$

$$\langle \psi | \hat{H} | \psi \rangle = \frac{\hbar^2 \alpha}{2m} - \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} |V(x)| e^{-\alpha x^2} dx$$

Simply what we will do here is H on this operator, okay. So when you operate the Hamiltonian operator on this wavefunction, you can see that this wavefunction has this exponent and when you take, operate this Hamiltonian, you will have to differentiate the exponent twice. So what you obtain is, I will skip the in between steps for you to try out, $\frac{\hbar^2}{2m} \alpha (1 - \alpha x^2) - |V(x)|$ and I rewrite in terms of $\psi(x)$.

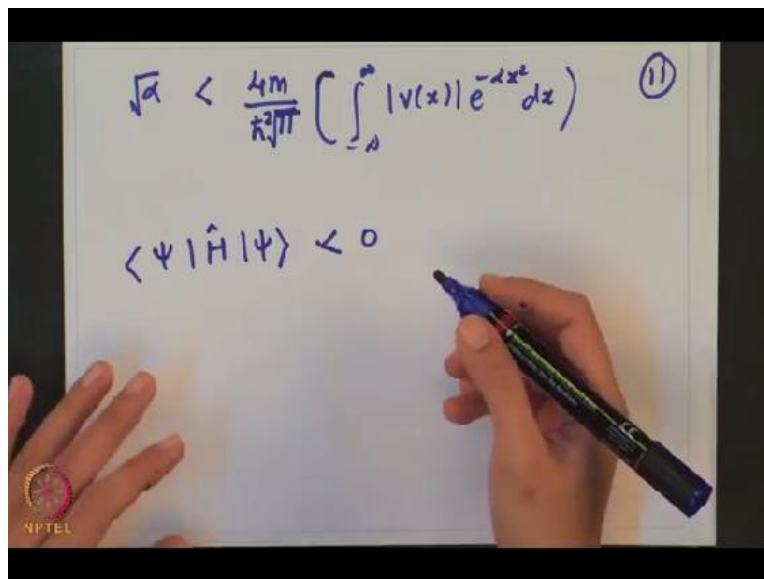
We have to argue that $\psi < 0$, okay. So what will be the condition on α such that the bound state, so when I calculate the expectation value, this should give me a bound state energy that is the negative energy. So if E is < 0 , so what will be the condition on α such that I get the bound state, negative bound state, negative energy or at least one bound state. So what I do is, I have to actually calculate, okay.

So again you apply the other end, you apply the wavefunction, okay. So the wavefunction when you apply on this, you will get, let me write one more step for you so that you know how to

proceed, okay. So from -infinity to infinity, then I have this entire block or this entire expression, okay. And I have a $\psi^*\psi$, okay. So $\psi^*\psi$ one part I have already written. So you will have e raise to; so let me call this as some x, okay.

So this is some x and then I have $e^{-\alpha x^2}$, okay. This entire thing would come here. And then you have to perform integration and once you perform the integration, what you obtain is this expression $\sqrt{\alpha}$, okay $\frac{4m}{\hbar^2\sqrt{\pi}}$ we have picked up from there, $\frac{\alpha}{\pi}$, okay and so you will have 2 parts in this integral. First part I have written the final solution. The second part is nothing but here potential part, you have $e^{-\alpha x^2} dx$, okay, from -infinity to infinity.

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So now we can see from here that it is the conditional alpha from here we can see that it is possible to have at least 1 bound state when α or rather square root of alpha is less than $\frac{4m}{\hbar^2\sqrt{\pi}}$, so square root of alpha is less than $\frac{4m}{\hbar^2\sqrt{\pi}}$, okay, *this integral, okay. So the condition on alpha is that this alpha should be less than this value. That will ensure that we have at least 1 bound state, that is this gives us a negative energy value, okay.

These were the 5 problems of the first tutorial. In this manner, we will be discussing the other tutorials also which are in the pipeline. So after every 4 lectures, you will have tutorial based on those lectures. So see you in the next tutorial.