## **Introduction to Quantum Mechanics Prof. Manoj Kumar Harbola Department of Physics Indian Institute of Technology, Kanpur**

## **Lecture – 06 Solution of the stationary-state Schrodinger equation for a simple harmonic oscillator**

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In the previous lecture, we introduced the wave equation for material waves and this the Schrodinger equation which is minus h cross square over 2 m, I am writing the 3 dimensional origin psi x, y, z plus v x, y, z psi x, y, z equals  $E$  psi x, y, z and we saw that with the boundary conditions, it gave us Eigen function, so I am going to now put, E n as a subscript. So, that it indicates that there is a Eigen function psi n corresponding to energy E n in one d. This equation was minus h cross square over 2 m d 2 psi over d x square plus v x psi x equals E psi x and again I am going to put that n to denote that there is an Eigen function.

It satisfies the boundary conditions for those Eigen values E n. So, this is equation you solve it for one dimensional particle in a box problem and found the energy Eigen values to be the same as those given by old quantum theory the equation is to be solved to be solved with boundary conditions and gives Eigen energies and Eigen functions. So, this is a completely new way of looking at the quantum problem I am solving a wave equation and through the Eigen values and Eigen energy is I am getting my answers and we yet to interpret psi, but let us solve in this lecture this equation for another one dimensional problem that we already know the answer of.



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And that is a simple harmonic oscillator for which a particle moves in a potential let us see the potential is centered around x equals 0.

So, the potential that is given for the particle of mass m is one half m omega square x square and therefore, the wave equation or the Schrodinger's equation for this becomes minus h cross square over 2 m d 2 psi over d x square plus 1 half m omega square x square psi x equals E psi x and this equation is to be solved with the boundary condition and boundary condition here is going to be because now suppose I take a particle of energy E; it can go anywhere and you will see actually wave can also penetrate through the region of finite potentials. So, psi x as x goes to plus or minus infinity should be 0 that is a boundary condition we are going to solve this equation with because far away from the origin is hardly any chance that I will find the particle and therefore, the wave function must vanish there.

Let us see; how do we go about solvency equation. So, first let us look at the behavior of psi x for extending to very large value plus or minus infinity in that case, I am going to have minus h cross square over 2 m d 2 psi over d x square plus 1 half m omega square x square psi x as x goes to plus or minus infinity the term m omega square x square

becomes very very large and d 2 psi by d x square can also become very large. So, E is going to be insignificant. So, I can approximately write this as 0 that will give me the asymptotic solutions it is not the true solution just the solution when x goes to plus or minus infinity now let us solve this.

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................  $77.1.9.948.0$  $2 \rightarrow \pm \omega$   $-\frac{\hbar^2}{2m} \frac{d^2\phi}{dx^2} + \frac{1}{2} m \omega^2 x^2 \phi(x) = 0$  $\frac{d^2\psi}{dx^2} - \frac{m^2\omega^2}{\hbar^2}x^2 \psi(x) = 0$ <br>  $\psi(x) = A e^{-\frac{m\omega}{\hbar^2}x^2}$  $\psi(x) = A e^{-\frac{m\omega}{2k}x}$ <br>  $\frac{d\psi}{dx} = A - \frac{m\omega}{k}x e^{-\frac{m\omega}{2k}x^2}$ <br>  $\frac{d^2\psi}{dx^2} = A\left(\frac{m\omega}{k}\right)^2 x^2 e^{-\frac{m\omega}{2k}x^2} - A \frac{m\omega}{\hbar}e^{\frac{m\omega}{2k}x^2}$ <br>  $\int_{\omega} dm \ x \to \infty \quad \text{or} \quad A\left(\frac{m\omega}{k}\right)^2 x^2 e^{-\frac{m\omega}{2k}x^2}$ <br>  $\psi(x \to \pm \infty) \$ 

So, I have for x tending to plus or minus infinity minus h cross square over 2 m d 2 psi over d x square plus 1 half m omega square x square psi x is equal to 0 or I can write d 2 psi over d x square minus m square omega square over h cross square x square psi x is equal to 0. Since we are only interested in the solution which is true in this limit, I am going to ignore any terms that are smaller than x square. So, I can in that limit rights psi x as some constant e raised to minus m omega over h cross. In fact, 2 h cross x square.

Let us see; how does this work out. So, if I take d psi by d x this is going to be equal to A times minus m omega over h cross x e raised to minus m omega over 2 h cross x square and if I now take the second derivative d 2 psi over d x square. They will come out to be A times m omega over h cross square x square e raised to minus m omega over 2 h cross x square minus A m omega over h cross e raised to minus m omega over 2 h cross x square.

That is why you can easily check this by doing this differentiation and which in the limit of extending to infinity, I can write approximately as A m omega over h cross square x square e raised to minus m omega over 2 h cross x square and you can see that this

cancels the other term in the equation therefore, it satisfies the equation. So, could this be the solution by itself, but right now what we have found is that psi x as x tends to plus or minus infinity goes as A e raised to minus m omega over 2 h cross x square.

Let us now substitute this in the original equation the true Schrodinger equation and see what the answer comes out to be. So, if I put this in the original Schrodinger equation.

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x.



Which is minus h cross square over 2 m let me write psi double prime for d 2 psi by d x square plus 1 half m omega square x square psi where psi double prime is nothing, but d 2 psi by d x square, then I find that this is going to be minus h cross square over 2 m and this we have found to be equal to their constant A m omega over h cross square x square psi x minus A m omega over h cross psi x plus 1 half m omega square x square times A psi x.

In fact, in some writing side even this A should not be there. So, let me; I can just cut this out, I can write that psi x is A e raised to minus m omega over 2 h cross x square. So, I get minus 1 half m omega square x square psi x plus h cross omega by 2 psi x plus 1 half m omega square x square psi x and I cancel these 2 terms. So, I get h cross omega over 2 psi x you notice therefore, that this wave function psi x equals some constant A e raised to minus m omega over 2 h cross x square goes to 0 as x tends to plus or minus infinity and satisfies the equation that when I put it in this equation gives you a constant time psi

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So, what I have shown you is that in the Schrodinger equation d 2 psi by d x square plus one half m omega square x square psi x equals E psi x the Schrodinger equation for a particle in a simple harmonic oscillator potential, if I take psi x to be A e raised to minus m omega over 2 h cross x square and substitute this in the equation. So, left hand side gives me h cross omega by 2 A e raised to minus m omega over 2 h cross x square; that means, this itself psi x equals A e raised to minus m omega over 2 h cross x square is an Eigen function because it satisfy a boundary conditions with the Eigen value E n equals h cross omega by two.

Recall that the lowest energy in the Heisenberg's formulation of quantum mechanics was also h cross omega by 2. So, this represents the lowest energy Eigen state lowest energy Eigen function and how does this function look if you plot it, it is maximum in the middle and then goes down as e raised to minus x square this is how it looks. So, this is psi x I plotted against x you can see that it has minimum number or largest possible wavelength and therefore, it is really the lowest energy system I mean this is I am just telling you know very qualitative way what about other Eigen states.

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........  $\psi(x) = f(x) e^{-\frac{mQ}{2k}x^2}$  $f(x)$  should not increase fasta that<br> $e^{m\omega_{hk}x^L}$  as  $x \rightarrow \pm \infty$  $f(x) = \sum C_n x^n$  $f(x) = x$   $\psi(x) = A x e^{-\frac{mQ}{2h}x^2}$  $\frac{d\psi}{d\tau} = \psi^{\prime}$  =  $Ae^{-\frac{m\omega}{2k}x^{x}} - A\left(\frac{m\omega}{k}\right)x^{x}e^{\frac{m\omega}{2k}x^{x}}$  $= \phi^{\prime\prime} = -3A(\frac{m\omega}{\hbar})x e^{-\frac{m\omega}{2\hbar}x^3} + A(\frac{m\omega}{\hbar})^2x^3$ 

Now, that we can also generate by writing psi x as sum f x e raised to minus m omega over 2 h cross x square where f x should not increase faster than e raised to m omega over 2 h cross x square as x tends to plus or minus infinity if it increases faster, then the wave function would not go to 0 as x goes to plus minus of infinity. So, f x should not increase faster. In fact, what I am going to do is a f x as a finite polynomial some constant C n x raised to n and see what happens. So, let us now first try f x equals x. So, that the corresponding psi x is going to be sum constant a x e raised to minus m omega over 2 h cross x square then the corresponding psi prime which is d psi by d x is equal to a e raised to minus m omega over 2 h cross x square minus A m omega over h cross x square e raised to minus m omega over 2 h cross x square.

Let us take its double derivative. So, d 2 psi by d x square which is psi double prime is going to be equal to a m omega over h cross x with a minus sign e raised to minus m omega over 2 h cross x square even I differentiate the second term that also gives me an x term and therefore, this is going to become actually 3 A m omega over h cross omega x minus this and the next term is going to give me minus minus plus a m omega over h cross square x raised to 3 times e raised to minus m omega over 2 h cross x square when I substitute all this in the Schrodinger equation what I am going to get is as follows.

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So, the Schrodinger equation is minus h cross square over 2 m psi double prime plus one half m omega square x square psi equals e psi and I am going to substitute this. So, I get minus h cross square over 2 m inside I am going to get minus 3 A m omega over h cross times x e raised to minus m omega over 2 h cross x square plus A m omega over h cross square x cube e raised to minus m omega over 2 h cross x square plus 1 half m omega square x square times A x e raised to minus m omega over 2 h cross x square if you look at it carefully you will notice that this term cancels with this term.

When you multiplied by minus h cross over 2 m and what you get is equal to plus 3 h cross omega by 2 times x e raised to minus m omega over 2 h cross x square which is nothing, but 3 h cross omega by 2 times psi x. So, again find the constant times the wave function and this is also therefore, an Eigen value and this is the corresponding wave function how does it look.

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So, if I look at this potential this new wave function is 0 at the origin goes up and comes down on the other side it comes down and goes like this. This is x e raised to minus m omega over 2 h cross x square and compare to the ground state wave function which was looking like this you can see that this has more bigger more turning its lambda is shorter. So, its kinetic energy is higher.

So, it is higher energy in fact, you can show that as you go to higher and higher energies these are going to be wave function is more and more vehicles in general therefore, I can write psi x equals sum f x e raised to minus m omega over 2 h cross x square and derive an equation for f x which I will give in the assignment and then write f x as sum C n times x raised to n finite polynomial and solve for C ns by matching the conditions in the 2 sides and when you do that what you find is fs come out to be either even or odd.

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 $\mathcal{E}_{\mathcal{G}^{\mu\nu}}$  alin for  $f_n$ Equality for form of the centrer evaluation of the function of the function of the function of the function of  $(n+\frac{1}{2})\hbar\omega$  $AC = \pm 6$ 

So, you derive an equation for f n and find fs to be either even or odd functions an energies come out be n plus one half h cross omega which is exactly the same that we found in Heisenberg formulation of quantum mechanics.

So, this is another instance where the wave equation has give me given me the results already known delta e is h cross omega, but the answer that comes is through a very different approach by solving a wave equation with appropriate boundary conditions are the 2 approaches equivalent is Heisenberg's formulation the same as Schrodinger's formulation is just that is 2 different ways of writing this will explore next week for the time being we have now found a fundamental equation known as a Schrodinger equation which gives the same answers in the cases that we have solved as other theories. So, this is the fundamental equation of quantum mechanics.