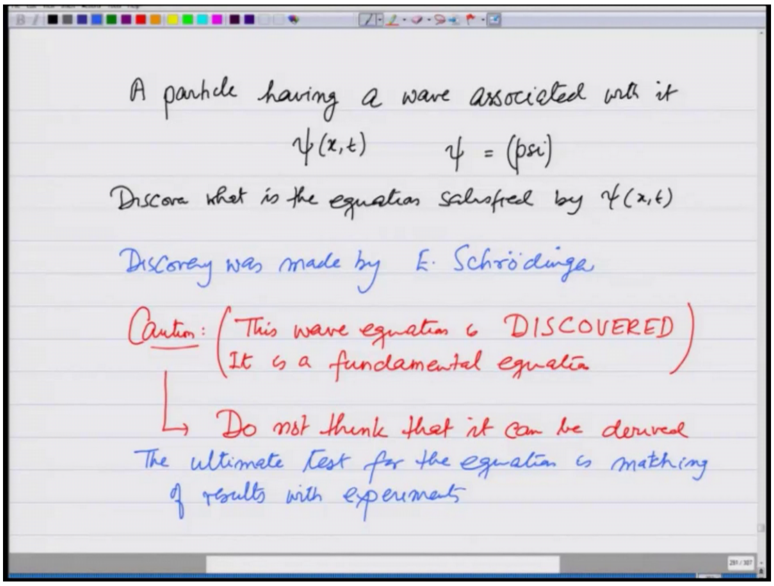
Introduction to Quantum Mechanics
Prof. Manoj Kumar Harbola
Department of Physics
Indian Institute of Technology, Kanpur

Lecture - 05
The stationary-state Schroedinger equation and it is solution for particle in a box

(Refer Slide Time: 00:17)

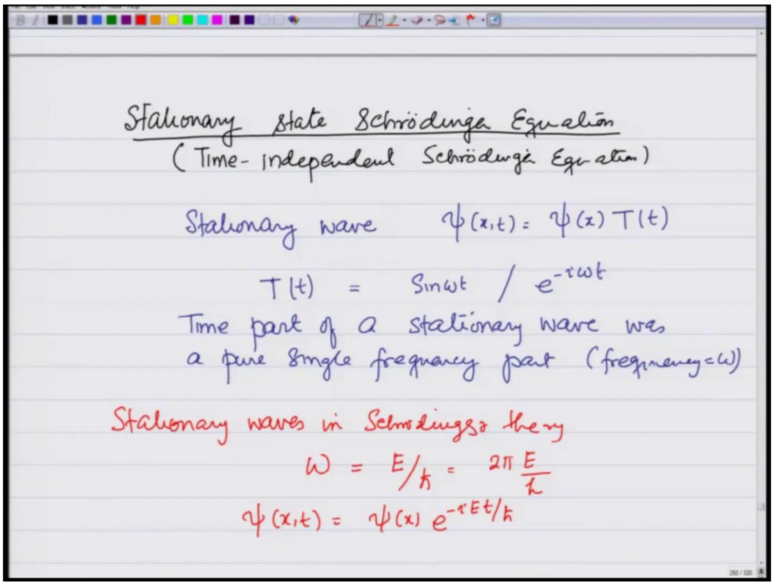


So, I am introduced you to the idea of particle having a wave associated with it. And the previous lecture I gave it a notation psi x t. This is pronounced psi it is pronounce as psi, it is Greek letter. And we want to now discover what is the equation satisfied by psi x t. So, there is a wave associated. We do not know what that amplitude means how can we say what we still want to discover what is the equation satisfied by. And this discovery who was made by Erwin Schroedinger.

Who proposed an equation for psi and right now I will focus on time independent psi, now stationary psi. Right now I will focus on stationery psi x t, but a discovery of e Schroedinger was made for psi x t both stationery as well as time independent. Now this I want to give a word of caution, and the caution is that this equation is discovered, it exists somewhere and is discovered. And therefore, it is a fundamental equation. So, this is what I am telling you and the caution is do not think that it can be derived. It can be discovered by looking added from different means it can be justified the ultimate test is experiment. The ultimate test for the equation is matching of results with experiments.

So, he propose this equation I discovered this now we say discovered because once it is discovered it all the reserves that he found from this to matching with experiments, but it is a fundamental equation it can be discovered by different means, but it is a fundamental equation it cannot be derived from anything else. So, please be aware of that lot of people say derived Schroedinger equation that is a wrong statement to make. So, we will want to now kind of arrive at this equation and discover whether it is right or what. So, having given this background what I want to focus on now is this stationary state Schroedinger equation.

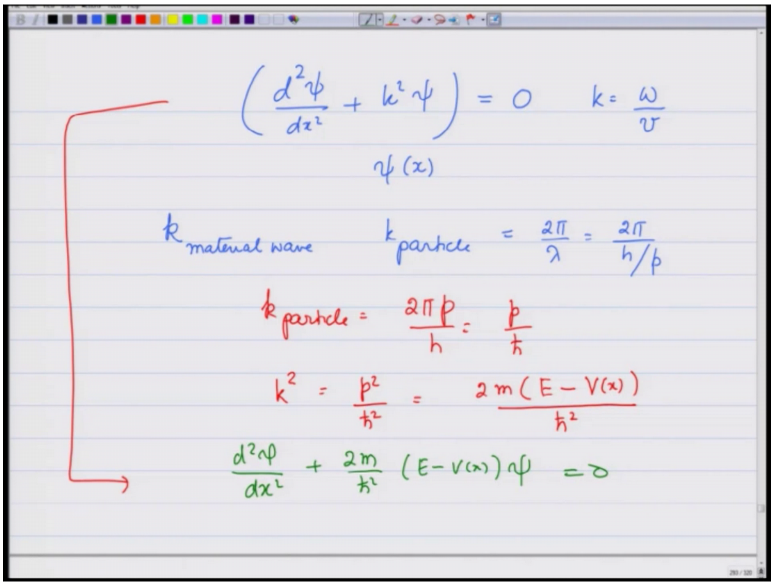
(Refer Slide Time: 04:01)



Or what is also known as time independent Schroedinger equation. Let me this give you a little background if you recall from our discussion on the waves a stationary wave was something that had now I will talk in terms of psi x t. Space part, let us write this as psi x and a time part and they were separated. And time part for a stationary wave was of the form sin omega t or e raise to minus I omega t and take it is real or imaginary part. So, time part of a stationary wave was a pure single frequency part right. And that was frequency or angular frequency was omega in the same manner the stationary waves in Schroedinger's theory will have a pure omega which will be given as E over h cross which is same as 2 pi E over h ok.

So, psi x t again is going to be written as some psi of x e raise to minus I e t over h cross. And we are looking for the equation for this psi x part.

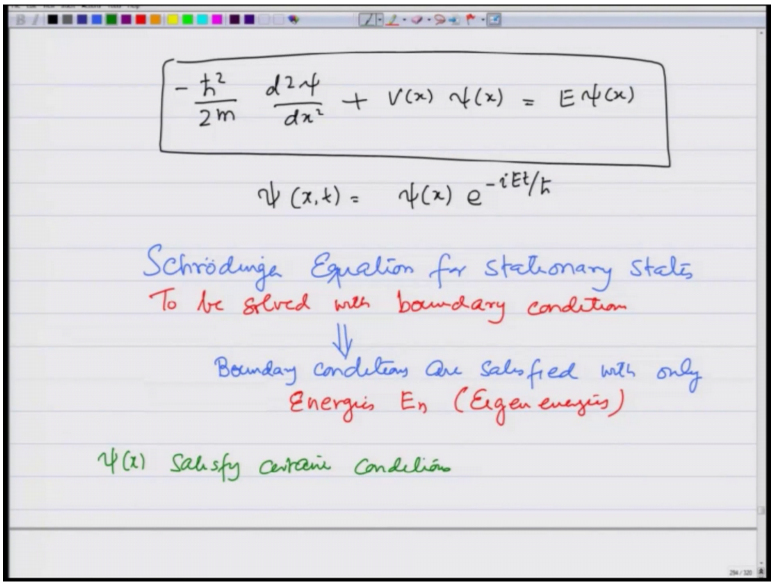
(Refer Slide Time: 06:37)



Recall from the stationary waves and I am focusing on one dimension. D psi by d x square plus k square psi was 0 when psi depends only on x and there is a pure wave. And k was nothing but omega over v. Let us go back to that (Refer Time: 07:04). So, can I argue from here that a similar equation access for material waves. So, let us see what is k for material wave. Or k for a particle, it is given as 2 pi over lambda. Which is nothing but 2 pi over lambda is h divided by p. So, I can write k particle is 2 pi p over h or p over h cross. And therefore, k square is going to be p square over h cross square, and for a particle of energy E p square is nothing but 2 m energy E minus the potential energy v x divided by h cross square, that is p square.

Let us substitute this here. When I substitute this here I am going to get d 2 psi over d x square, plus 2 m over h cross square e minus v x psi is equal to 0. Can this be equation for the particle waves?

(Refer Slide Time: 08:37)

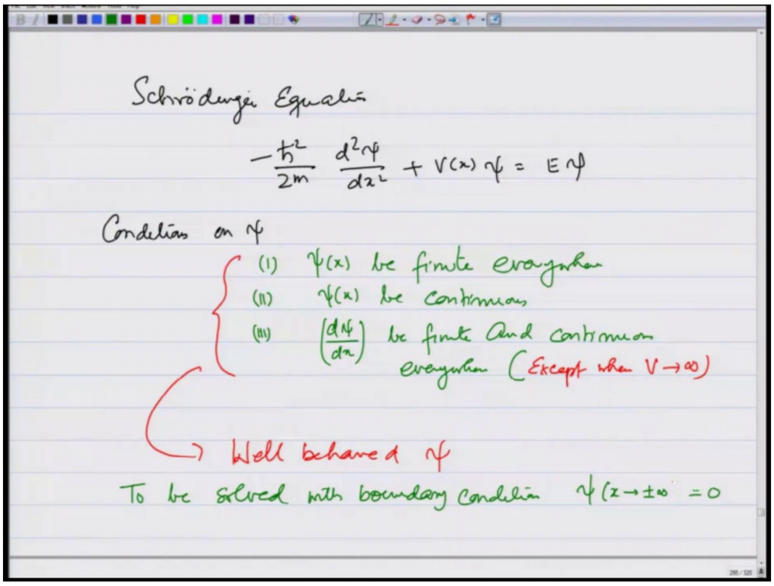


So, this by manipulation gives you minus h cross square over 2 m d 2 psi over d x square plus v x psi x equals E psi x. This is what Schroedinger proposed and the time dependence of this psi x t would be equal to psi x that will be calculated from the equation above times e raised to minus I e t over h cross. So, this is a stationary wave oscillating with frequency e by h cross. Can this be the equation for the waves test? As I said earlier is the solution of this and comparison with the experiments or earlier known results.

So, we will solve this and try to see if this gives the results that were known earlier. And if the match with the experiments. So now, this equation is to be solved. So, this is known as the Schroedinger equation, for stationary states. And as I said earlier this is to be solved with boundary conditions. And when you solve a problem with boundary conditions if you recall again from the example of string in my lecture on waves, boundary conditions means that the boundary conditions are satisfied with only certain energies E n and these will be known as Eigen energies. And these will represent the stationary state energy of the system for example, in hydrogen atom they will give you the energy is determined earlier.

So, we have to check that, and we also demand that psi x satisfy certain conditions.

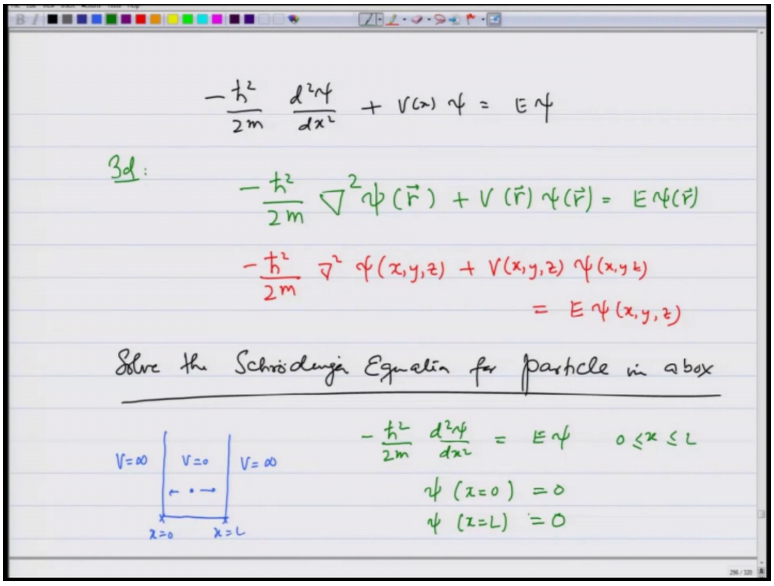
(Refer Slide Time: 11:12)



So, the equation we are saying the Schroedinger equation is minus h cross square over 2 m, d 2 psi over d x square plus v x psi equals E psi. And conditions on psi are number 1, psi x be finite everywhere number 2 psi x be continuous. Number 3 d psi by d x be finite and continuous everywhere. Let me write a warning here except when v goes to infinity or v is not well behaved. So, all these 3 things I would say are the well behaved psi. So, we are going to demand that the solutions be finite everywhere psi be continuous everywhere and d psi by d x be continuous and finite everywhere. So, that the second derivative can be also taken.

So, this is and this is to be solved with boundary conditions. And the boundary condition is going to be as we said earlier that wave function wherever it is finite there is a particle is to be found there. So, wherever particle is not to be found and; that means, generally x tend into plus or minus infinity will demanded psi be 0 or looking at the physical situation psi should vanish wherever the particle is not to be found at all, otherwise is finite continuous and is derivative finite in continuous. It is 3 dimensional generalization can also be written.

(Refer Slide Time: 13:32)

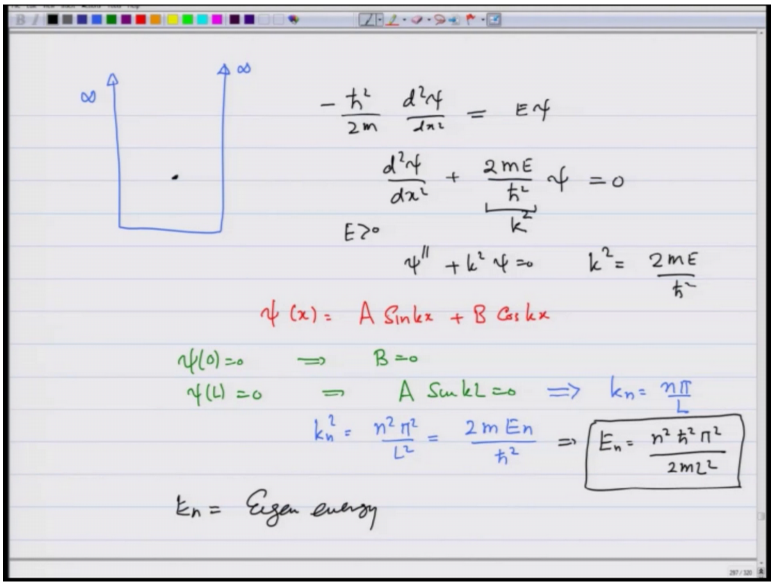


So, the one dimensional equation is minus h cross square over 2 m d 2 psi over d x square plus v x psi equals E psi the 3 dimensional in generalization is going to be minus h cross square over 2 m laplacian would replace, the second derivative there is square psi and it is going to be a function of r; that means, x y and z plus v r psi r equals E psi r.

Let me write it in terms of x y and z also minus h cross square over 2 m del squared psi of x y and z that is what that r vector means plus v as the function of x y and z psi x y and z is equal to E psi x y and z, this is going to be the equation. Now let us solve this for a simple system. Solve the Schroedinger equation for particle in a box. And this solution we have already obtain earlier from Wilson Summerfield quantization condition now we are going to solve it is Schroedinger equation and see what answer it gives. In this case what we are going to have is a box in which the potential is infinite outside the box, and potential is 0 inside let us say this is x equal 0 x equals L and the particle is moving around here.

So, the Schroedinger equation is that minus h cross square over 2 m d 2 psi over d x square plus v is 0 is equal to E psi for x between 0 and l. And psi x equals 0 is 0 that is the boundary condition because beyond x equals 0 a particle cannot exist potential is infinity and therefore, any finite energy particle cannot be there and psi at x equals L is 0. So, these are the boundary conditions, let us see what the solution is lie.

(Refer Slide Time: 15:57)

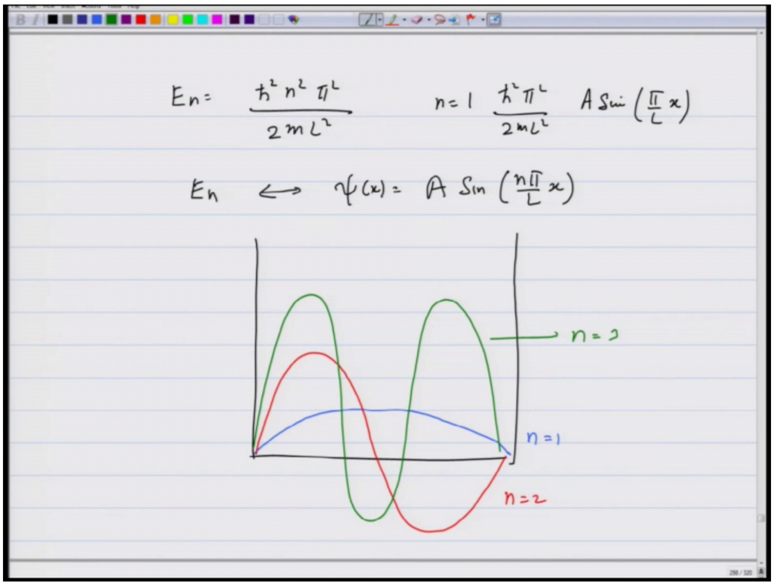


So, I am solving for particle in a box v tend into infinity outside, particle is inside and the equation is minus h cross square over 2 m d 2 psi over d x square is equal to E psi. And therefore, d 2 psi over d x square plus 2 m E over h cross square psi is equal to 0. And for e greater than 0 this is very simple to solve call this k square. So, this equation becomes psi double prime plus k square psi is equal to 0, where k square is 2 m E over h cross square and this solution we have already know from the string solution.

Psi x is going to be A sin of k x plus B cosine of k x. And psi 0 is equal to 0 implies B equals 0. Psi at L equal 0 implies A sin k L is equal to 0. And therefore, this boundary condition is satisfied only for k n equals n pi over L. And therefore, k n square which is n square pi square over L square is equal to 2 m E for n divided by h cross square and this immediately tells me that E n is equal to n square h cross square pi square over 2 m L square. Which is the same answer as obtained earlier by Wilson Summerfield quantization conditions. So, you see Schroedinger equation gives me the same answer except, now that I have solved it now I have obtained that answer through the solution of a wave equation. And the energies that I stationary energies appear as Eigen energy.

So, E n is an Eigen energy, it is only for these energies that the boundary conditions is satisfied properly. So, in the wave picture it is the boundary condition that gives you those discrete Eigen energies. Because only for those energy is the boundary condition is satisfied. What about the wave function?

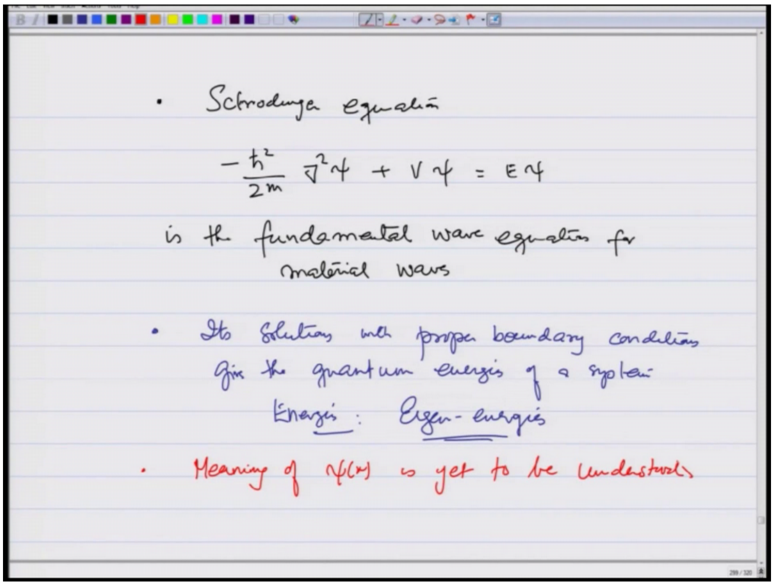
(Refer Slide Time: 18:28)



So, if I look at E n which is h cross square n square pi square over 2 m L square it is going to be n equal to 1 is going to give me h cross square pi square over 2 m L square energy. And the wave function is going to be sin pi over L x times a constant a which we have not determined so far. For higher ns is going to be sin n pi over x l. So, E n and the corresponding wave function psi x is some constant A sin n pi over L x, how do these wave functions look so?

Let me plot this here. For n equal to 1 it looks exactly the same as a string wave function. This is n equal to 1, for n equal to 2 is wave function looks like this. This is n equal to 2. For n equals 3 this wave function looks like this. So, you see as we go to higher and higher energies, wave function bends more and more and that make sense, because lambda becomes smaller and smaller, So it gains more kinetic energy. So, you can see right away that more wiggles more turning off the wave function around means higher kinetic energy. And the solutions exactly like the wave solution for a string. So, one should not feel really scared about you know solving the Schroedinger equation it is a wave equation like equation on a string. And eigenvalues are now related to the stationary state energies of a quantum system. With that introduction and simple example I conclude this lecture by stating that number 1.

(Refer Slide Time: 20:19)



Schroedinger equation minus h cross square over 2 m del square psi plus v psi equals E psi is the fundamental wave equation for material. Waves number 2; it is solutions with proper boundary conditions give the quantum energies of a system.

These energies are known as the Eigen energies. I have introduced the idea of eigenvalues earlier in the wave lecture. And meaning of psi is yet to be understood.