Solar Photovoltaics :
Fundamental Technology and Applications
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Lecture - 03
Introduction of Quantum Mechanics in Solar Photovoltaics - I

Welcome everyone. In today's lecture we will discuss about the importance of quantum mechanics in photovoltaics. In last two lecture we have discussed about different source of energy. For example, we have talked about conventional source of energies like coal, natural gas and oil. And we have also discussed about non-conventional source of energy like wind energy, tidal energy, geothermal energy and solar energy.

We also said that, based on their resources, these kind of energy can be classified into renewable and non-renewable energy. And finally, we discussed about the solar energy and we said that out of the different forms of renewable energy, solar energy is a clean and green source of energy and it is very popular. Now in this course, we are going to study about the solar cells in details.

To understand the solar cell it is very important to have a preliminary and basic concept of the quantum mechanics. In this course we are not going to learn in details about the quantum mechanics. But we will learn that much amount of quantum mechanics which is needed to understand the working principle of a solar cell.

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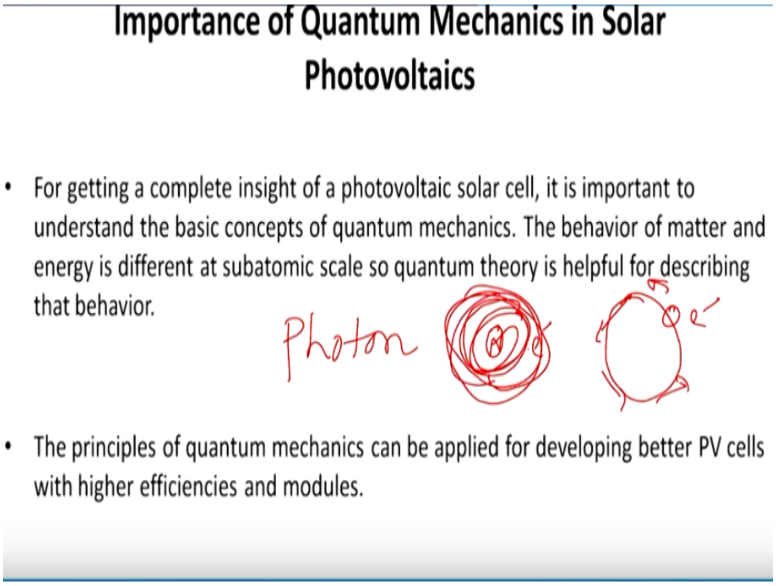

Importance of Quantum Mechanics in Solar Photovoltaics

- For getting a complete insight of a photovoltaic solar cell, it is important to understand the basic concepts of quantum mechanics. The behavior of matter and energy is different at subatomic scale so quantum theory is helpful for describing that behavior.
- The principles of quantum mechanics can be applied for developing better PV cells with higher efficiencies and modules.

So for getting a complete insight of the photovoltaic solar cell, it is important to understand the basic concept of quantum physics. The behavior of matter and energy is different at subatomic scale than the macroscale. So quantum theory is usually essential to understand the behavior at the subatomic scale. And the principle of quantum mechanics that can be applied for developing better PV cells with higher efficiencies and molecules.

So what do we mean by that? Let us give an example. Okay, let us consider this chalk. This is a bulk material. Now if I throw this chalk with some kind of force, let us say 10 Newton, so we know that this chalk will go and then it will hit somebody. If I know its initial velocity, and since we know its final velocity is zero so we can calculate how much distance it will move. Okay?

Or if we know its final velocity, if we know its distance, then we can find out its initial velocity. If I make this chalk half, let us say I crack it into two piece and if I throw each of this piece with 10 Newton force I can again calculate by using the Newton's law. But let us imagine a situation I keep on doing this cutting this chalk and comes to a dimension which is something like 10 to the power -9 meter or which is like 10 to the power -10 meter.

In that scale, when the chalk is there, we call it for example, nano chalk. The question is whether we can apply the similar amount of 10 Newton force to this nano chalk or even if we apply, whether we will be able to calculate the distance it will cover. So this is a big question. The question is not about whether Newton's law is right or wrong at the sub atomic scale, but the question is, it is the scale which prohibits the use of the Newton's law at such a small scale.

When you talk about electron or proton or neutron or any other subatomic particle, we cannot directly use Newton's law of motions. To find out the kinetics of any particle or any subatomic particle, we simply cannot directly use Newton's law. It does not means that Newton law is wrong, but it is the smallness of the scale, which prohibits us to use this Newton's law in that scale.

So how we describe the kinematics or motion of this particle? We all know that flow of the electron is the current and in a photovoltaic solar cells, we basically are going to study about this current and voltage. Now this current is coming due to the flow of electron. Now to understand this flow of electron, we really need to understand what kind of force is acting on them and if a certain kind of force is working on them, what will be their trajectory, what will be their motion.

We cannot explain this in terms of the classical physics or classical mechanics. A completely new kind of mechanics, or completely a new kind of physics is necessary to explain this. And that is what the quantum mechanics. And the quantum mechanics evolution has happened over a quite a long amount of time. J.J. Thompson first give the concept of the electron.

Later on Rutherford from his famous alpha particle scattering experiment has said that most of the space in the atom is free and there is a massive positively charged nucleus at the center of the atom and electrons which are negatively charged particle they orbit around that nucleus. Now from the classical Maxwell theory of the electromagnetism, which was there in the place for quite a long time.

So this Maxwell's theory of electromagnetism they say that any radiating or any accelerating electric charge they radiate. Now if the electron moves in a circular orbit, let us say like this is the electron and it moves in this circular orbit. So at each and every moment, its direction is going to be changed. So that means it is accelerating.

So if the electron accelerates like this way, very soon it will lose its energy and falls on the nucleus.

For example, if we consider this is the atomic structure, I have my nucleus which is at the center, this is the nucleus and electron is orbiting around this nucleus. So according to the Maxwell's theory of electromagnetism, very soon electrons will make a serpentine path and will fall on the nucleus. So there will be no atomic stability. But in the contrast we all know that atoms are stable and all the solid exist.

The second part from this Rutherford experiment, which was not able to explain in the classical physics is the origin of line spectrum in the electromagnetic spectrum. According to the Rutherford theory, we should get a band like spectrum, whereas the spectroscopic has seen a line spectrum in most of the materials. Both of these anomalies were not able to explain by the Rutherford’s theory.

And it was understood that a complete new kind of theory is required to explain this phenomena. By the time Einstein explained his photoelectric effect. So what he says that extending the Planck’s black body radiation that when any hot body emits radiation it not only emits the energy as a bundle of energy, but it also absorbs the energy in bundle of energy.

So that means if it emits the energy in bundle of energy and if it absorbs the energy in bundle of energy, when the energy is in the space there also it exist as a bundle of energy. So this bundle of energy he gave a name called photon. So the quantum of this energy he gave a name called photon and he described the light as a photon or as a particle.

Phenomena like photoelectric effect like Compton effect can be explained by this photon picture or particle picture of the light wave. At the same time Niels Bohr came and he was trying to improve upon the existing Rutherford’s theory. Combining the concept of the Einstein and the blackbody radiation theory of the Planck, Bohr has extended the idea of the Rutherford Planck’s model.

And what he said that electron cannot move arbitrarily in any of the orbits like this, but it can rotate only in those orbits where its energy is fixed. So if I fix its energy so then electron in a particular orbital has a fixed quantum of energy and this explains most of the dilemma or most of the anomaly existing in that times and that was the origin of quantum theory.

Now so far we have considered the light either as a wave or as a particle. For example, when we want to explain phenomena like polarization or deflection or scattering, we consider the light as a wave. We take an example for interference or diffraction we consider light as a wave. But when we talk about photoelectric effect, we talk about Compton effect, we consider light as a particle.

So that means, light can exist as a wave and it can also exist as a particle. So it has a dual nature. Now we are already discussing about the electrons motion in the atom by then. So the normal question which arise in the people's mind if the light can exist as a wave as well as a particle, can particle also exist as a wave and that was comes the famous de Broglie equations.

De Broglie in his PhD thesis first proposed that any particle like electron can also exist like a wave.

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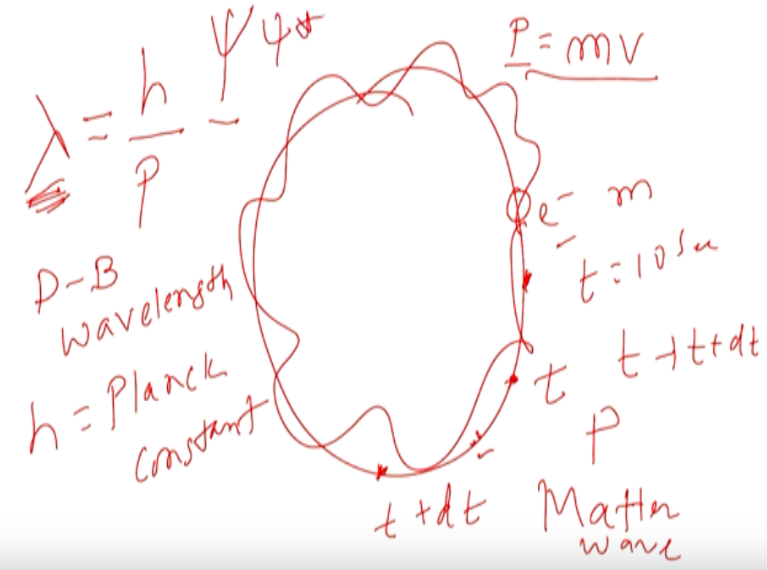

And he explained the things if this is an atomic orbital and if this is a electron, so this atomic particle electron they can exist like a wave and how does this wave will be distributed here? So this will be distributed like this. So here is the one very interesting point. When we talk about the electron as a particle, we talk about its charge, we talk about its mass.

And if we know what is its charge and what is its mass and if we know the centrifugal force, we can find out the location. But the moment we go to describe the electron as a wave, then we have distributed it over a dimension rather than restricting it at particular positions. Now if I ask you the questions at time t = 10 sec, where is this electron? So the probability of electron being here and here are same.

You can say that electron is here, somebody can say the electron is here. So the point is that we cannot definitely say that electron is either here or here. What makes more sense instead of telling if electron is here or here, the probability of getting electron between this point and between that point is maximum or probability of electron between this point and that point is maximum.

If this point is represented by time t and if this point is presented by time t + dt so in a time interval between t to t + dt the probability of finding the electron between this point and this point is maximum. So now we are talking about in terms of probability. So quantum mechanics talks in the language of the statistical mechanics. Here we talk everything in terms of the probability.

And when we represent the electron as a wave so obviously, there will be a wavelength associated with this electron and de Broglie called that wavelength as a lambda, because if there is a wave there will be a wavelength. But this is the wave properties of the electron. Now electron has a mass m. It has a velocity v. So that means it has a momentum which is m times v.

This momentum is the particle properties of the electron, whereas this wavelength is the wave like properties of the electron. How one can correlate this wave like properties with this particle like properties. That is what the de Broglie did. So what he said that the wavelength of the electron lambda is equal to the Planck's constant h divided by the momentum P.

And this wavelength we call as de Broglie wavelength. And h here is the Planck constant. Corresponding to every subatomic particle, whether it is a electron, whether it is a proton, or whether it is a neutron, we can find out the corresponding de Broglie wavelength if we know the charge and mass of that particle. So what we are telling here the electron which is a particle can also exist as a wave.

And this kind of wave is called matter wave. In quantum mechanics, the state of any particle is represented by a wave function. And a wave function is usually written by the symbol called psi. Now psi is a quantity which represents the probability of finding the particle somewhere in the space. Another important point here is that in classical Newtonian mechanics, we mainly deal with the Euclidean geometry.

But in quantum mechanics, we consider the complex space. In quantum mechanics, the probability density makes more logical sense, than the only wave function. So since psi is a complex quantity, I can find the positive quantity that the position probability density by multiplying the psi with its complex conjugate. Let us take an example.

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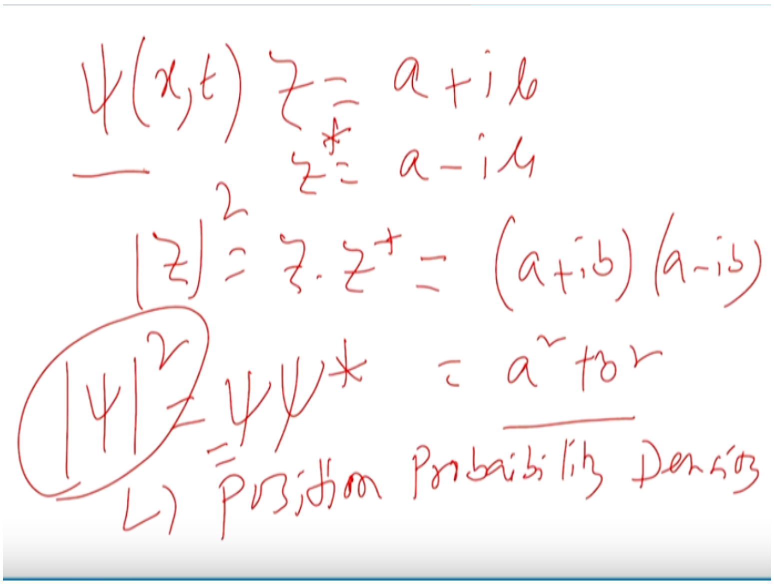

$\underline{\psi(x,t)}$ $z = a + ib$

$z^* = a - ib$

$|z|^2 = z \cdot z^+ = (a+ib)(a-ib)$

$\boxed{|\psi|^2} = \psi\psi^* = \underline{a^2 + b^2}$

↳ Position Probability Density

Let us take an arbitrary complex number, a + ib. What will be the complex conjugate of this quantity, a – ib. If I multiply z with z star, I will get mod of z square and that is equal to (a + ib) (a – ib). You get a square plus b square. And this is the really useful physically measurable quantity. Similarly, if your wave function is psi, if I multiply it with complex conjugate, which is called psi star, then you get mod psi square which is called position probability density.

And this position probability density is physically more significant than the wave function. And wave function is always a function of the positions and times. So these are the some fundamental postulates of quantum mechanics, which is important to learn in the beginning before we go to the kinematics equation which govern the quantum mechanics.

In quantum mechanics, the state of a particle is represented by the wave function psi. And the probability of any particle or finding of any particle is represented by the probability density and probability density is physically more meaningful than the only probability. Okay, let us comes back to our photovoltaic systems.

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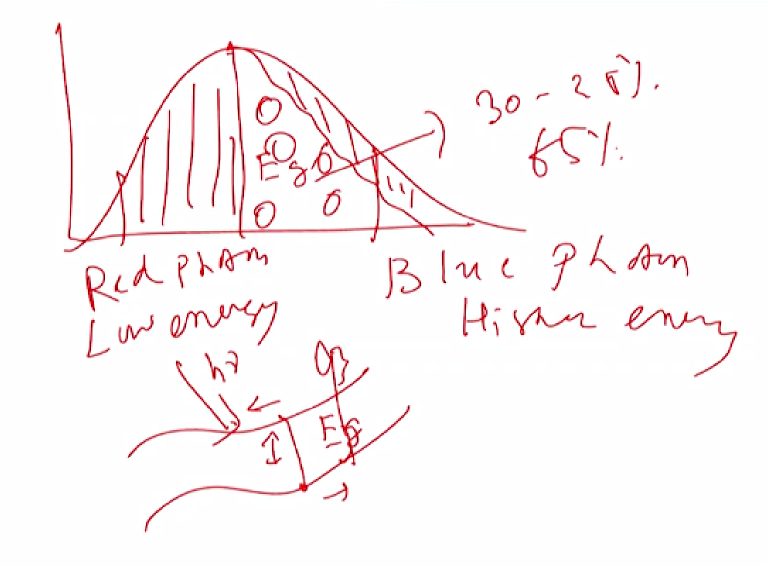

Most of the time the solar spectrum comes like the spectrum or rainbow. Now on the left hand side, I have red photon. Red photon is larger wavelength photon. That means they have low energy. And the right hand side we have blue photon and blue photon is have a lower wavelength. That means they have higher energy. For time being consider this is my solar cell and photon beams falls on the solar cells.

So what will happen? There will be an electron which will absorbs this photon beam and it will go from the ground state to the excited state and the electrons will start moving from here and the whole will move in the opposite directions. If we connect a load in the outside circuit we will get a current in the outside circuit. Now if this energy is Eg the band gap, which corresponds to Eg at the spectrum.

Now this part of the spectrum which is red photon that does not contribute to the absorptions. So that get lost. Similarly, the blue photon, they have a slightly higher energy than the band gap energy. So this part is the excess than the band gap energy. So that excess energy will get lost by the heat energy to the piston. So the only useful energy is 30 to 35%, which we can harness from the spectrum.

But our goal is to make a highly efficient solar cell. Let us say for example 65% solar cell, how can I do that things? Either we need to use the whole spectrum or we can do it by intelligently designing new materials or new interfacial layers on our electrodes so that the band gap can be tuned properly. To do this thing, we need to understand also the quantum mechanics very well.

So that is why a basic idea of quantum mechanics is very necessary. In classical physics, Newton's law describes the kinematics of a particle.

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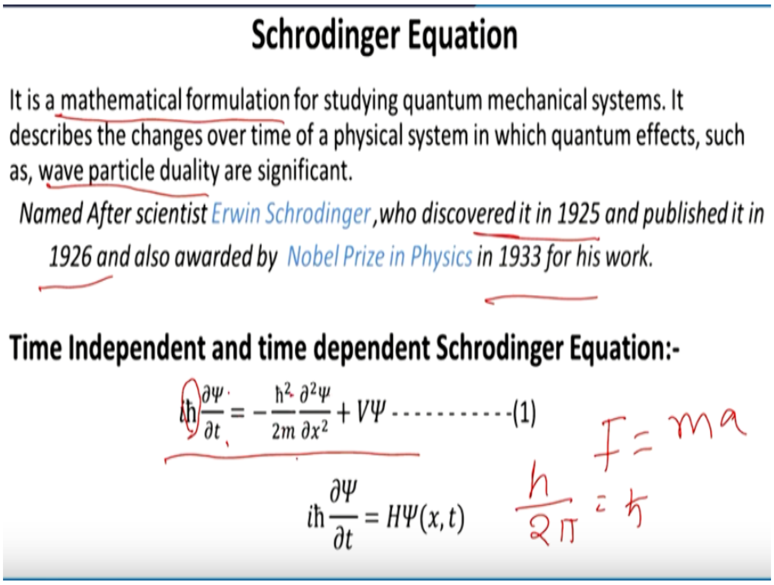

Schrodinger Equation

It is a mathematical formulation for studying quantum mechanical systems. It describes the changes over time of a physical system in which quantum effects, such as, wave particle duality are significant.

Named After scientist Erwin Schrodinger, who discovered it in 1925 and published it in 1926 and also awarded by Nobel Prize in Physics in 1933 for his work.

Time Independent and time dependent Schrodinger Equation:-

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi \text{ -----------(1)}$$

$$F = ma$$

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi(x,t)$$

$$\frac{h}{2\pi} = \hbar$$

If I apply a force f, if I know the mass of the particle m, so we can write from Newton's second law, force is equal to mass times accelerations. We can find out what is accelerations. So in classical mechanics, the position of a particle can be described as a function of force. But quantum mechanics, we just gave an example of a nano chalk, when you were talking about the electron proton, how can we find out its positions?

What equation govern the time evolutions of this wave function? So that was given by Schrodinger equation. Schrodinger equation is actually a mathematical formulation for studying quantum mechanical system. It describes the change over time of a physical system in which quantum effects such as wave particle duality are significant.

When you discussed about this de Broglie hypothesis we said that the electron can also exist as a wave. So that means electron can exist as a particle, it can also exist as a wave. So it shows a dual nature and that phenomena is called wave particle duality and that is purely quantum in nature. Schrodinger who formulated these equations, he discovered this in 1925 and published his work in 1926.

And because of his outstanding work, he was given Nobel Prize in Physics in 1933. There are different formulations of quantum mechanics like Schrodinger formulation. Similarly, there is a matrix formulations of the quantum mechanics and also there are path integral formulations of quantum mechanics. Paul Dirac, he has combined this Schrodinger formulation and matrix formulations.

Here we are not going in details about the all different formulations. We will learn about the Schrodinger equations and how we can use this Schrodinger equation to understand the dynamics of a system. The Schrodinger equation in one dimension is written like this; i which is an imaginary number times the reduced Planck's constant which is called as h bar.

If h is my Planck's constant h by 2 pi that is called the reduced Planck's constant h bar; i h bar partial derivative of psi with respect to time is equal to minus h bar square by 2m plus double partial derivative of psi with respect to position plus B psi.

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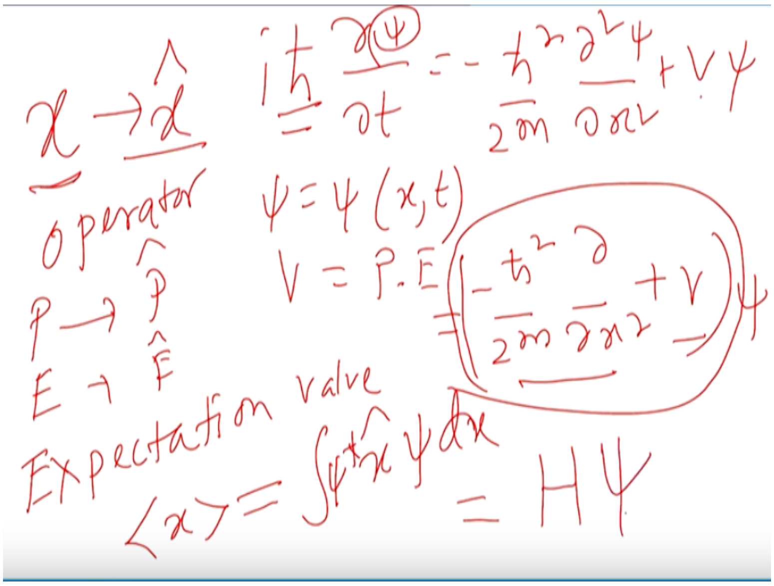

So what we just written that i h bar del psi del t is equal to minus h bar square by 2m del 2 psi del x 2 plus v psi. Here psi is my wave function which is a function of position and time. And h bar is the reduced Planck's constant. And v the potential energy, v is the potential energy. Now you look at this equation, the right hand side, we have minus h bar square by 2m del to del x 2 psi plus v psi.

So we can also write the right hand side by minus h bar square by 2m double partial derivative with respect to x plus v if we consider the v as an operator time psi. In quantum mechanics, every physically measurable quantity is represented by an operator. Let us say I want to measure the length of this chalk.

In classical mechanics or in classical physics what I should do, I will take a normal scale I will put the one end of the scaling in one side and then I will put another side in here and I will measure what is the length either in inch or in centimeter. But in quantum mechanics, we cannot measure the positions of this chalk like this way. We cannot use a scale there for the case of the electrons or protons.

So if I want to measure the positions of a this nano chalk let us consider this chalk is no longer a bulk chalk but a nano chalk and I want to measure the length of this chalk. And let us say the length of this chalk is x okay, this x. Now this x in quantum mechanics is represented by putting a hat or cap sign on top of this x and this is written as this is spelled as x hat or x cap and this is called operator.

Corresponding to every dynamical variables there is an operator in quantum mechanics. Like momentum they have a operator called momentum operator. Energy has an operator that is called energy operator. And when this operator operates on wave function I get the result of measurement. The result of measurement in quantum mechanics is called expectation value.

And another weird fact associated with quantum mechanics is that it says that every time we do a measurement the systems falls in a completely different system. So next time when we do measurement, we are not measuring on the same system. Third time when we are doing measurement, we are not measuring on the same systems. So every time we are not measuring at the same system.

So finally after doing n successive measurement, what we get is an ensemble average of all successive measurements. And we call that measurements value as an expectation value. And the expectation value of this length x that is represented by a symbol like this. And mathematically this expectation value is calculated by putting the operator on the wave function.

And to make it more physically meaningful we learnt that to multiply it by complex conjugate and integrating over the space on which the electron is confined times the integrate. So this bracketed part here that corresponds to a operator in quantum mechanics and this operator is called the Hamiltonian operator H. The first part here corresponds to the kinetic energy and the second part here corresponds to the potential energy.

So sometimes if you replace this whole part under this bracket by this letter h so then this becomes h times psi.

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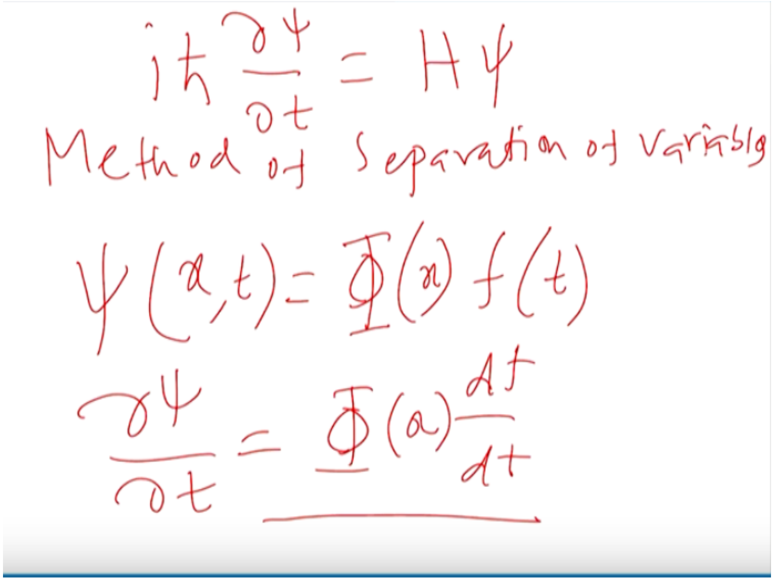

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi$$

Method of Separation of Variables

$$\psi(x,t) = \Phi(x)f(t)$$

$$\frac{\partial\psi}{\partial t} = \underline{\Phi}(x)\frac{df}{dt}$$

So basically what we have written is that i h bar del psi del t is equal to h psi. That is the one dimensional Schrodinger equations. Now this equation depend on the positions as well as the time. So this is an example of a coupled equation. We need to decouple them for practical application.

So that means, we need to make these equations in such a way, one part will contain the time part, another part will contain only the spatial part. And this is done by a method called method of separation of variables. We also mentioned it here.

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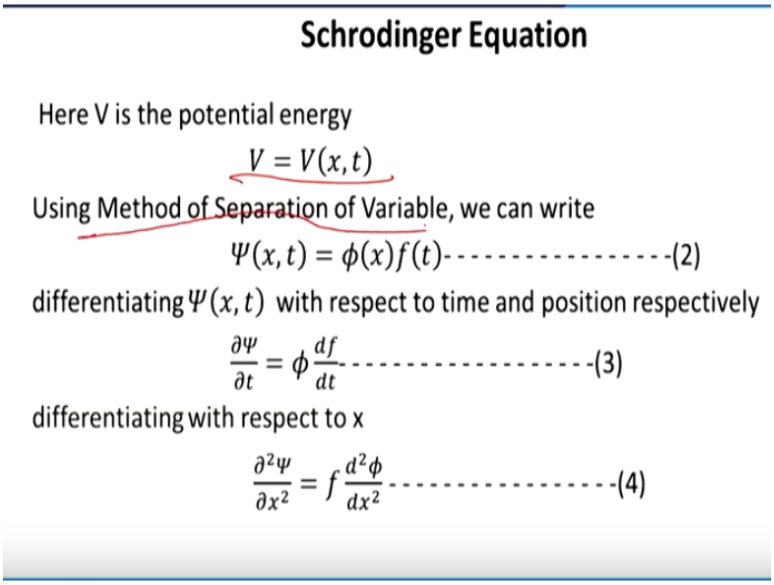

Schrodinger Equation

Here V is the potential energy

$$V = V(x,t)$$

Using Method of Separation of Variable, we can write

$$\Psi(x,t) = \phi(x)f(t)\text{-----------------(2)}$$

differentiating $\Psi(x,t)$ with respect to time and position respectively

$$\frac{\partial\Psi}{\partial t} = \phi\frac{df}{dt}\text{------------------(3)}$$

differentiating with respect to x

$$\frac{\partial^2\Psi}{\partial x^2} = f\frac{d^2\phi}{dx^2}\text{----------------(4)}$$

You can see that the potential energy is also a function of the positions and the time and the method we are going to use to decouple this equation is called method of separation of variables. So in this method, we write this wave function psi which is a function of positions and time as an independent product of two function where the first function depend only on positions and the second function depends only on time.

Now we are exposed to little bit of differential calculus and integral calculus. Assuming that fact, let us do a partial differentiation of this psi with respect to positions and with respect to time. Let us do the time part first. So if I do a derivative of this wave function with respect to time what I will get? I will get del psi del t is equal to phi x df dt because now it is a not a partial integral, it is a full integral.

If I substitute this in my Hamiltonian equation, if I substitute this in my Schrodinger equations, what I will get? So that is the time part.

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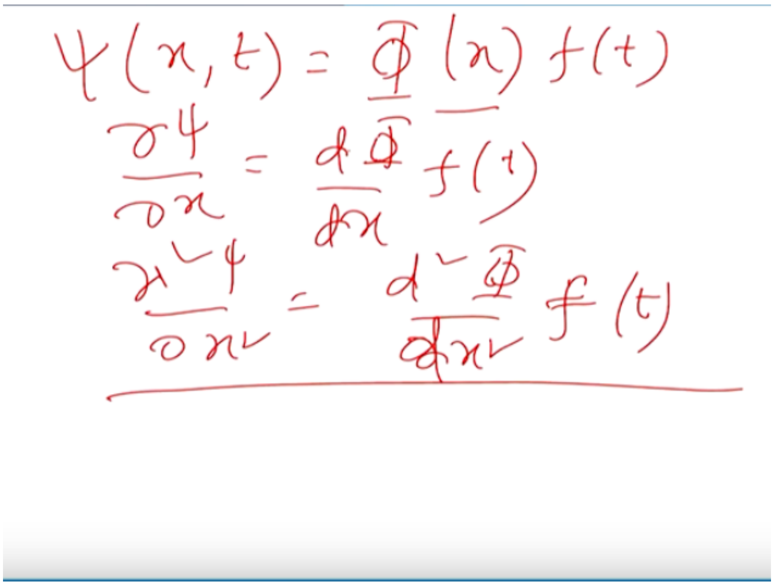

$$\psi(x,t) = \underline{\Phi}\,\underline{(x)}\, f(t)$$

$$\frac{\partial \psi}{\partial x} = \frac{d\Phi}{dx} f(t)$$

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{d^2\Phi}{dx^2} f(t)$$

And the second part of the equation was the spatial part. Now I have to deal with the spatial part. So if I differentiate the spatial part two times, then I will get if I do it one time I will get del psi del x is equal to d phi dx ft and if I do it another time I will get del 2 psi del x 2 is equal to d 2 phi dx 2 ft. Let us substitute this, the spatial derivative part and this time derivative part in the original Schrodinger equations. So what we will get here is the following.

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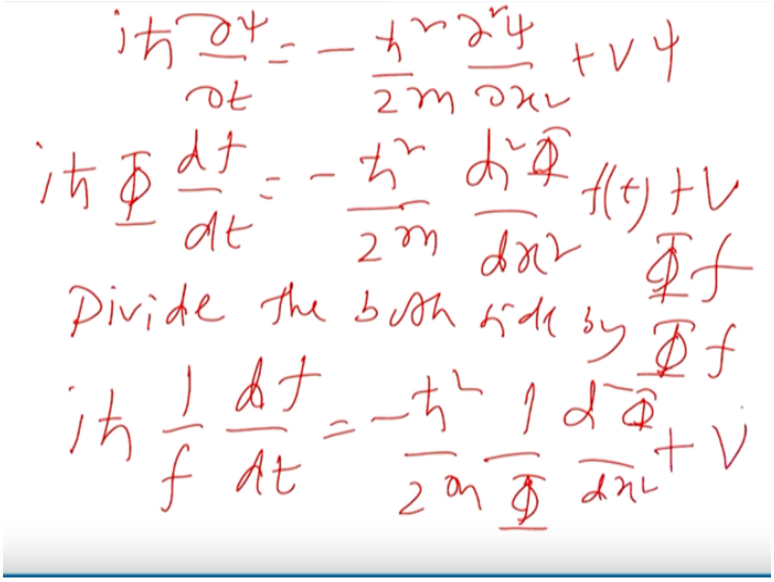

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi$$

$$i\hbar \Phi \frac{df}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\Phi}{dx^2} f(t) + V\Phi f$$

Divide the both side by Φf

$$i\hbar \frac{1}{f}\frac{df}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\Phi}\frac{d^2\Phi}{dx^2} + V$$

The first part was ih bar del psi del t is equal to minus h bar square by 2m del 2 psi del x 2 plus v psi, right. So if we plug in from the previous derivative what we will get that ih bar phi df dt is equal to minus h bar square by 2m del 2 psi del x 2 we have done it last time that is d 2 phi d x 2 ft. If we substitute this so we will get d 2 phi d x 2 ft plus v is the potential energy into the wave function psi which is the product of phi and f.

Now if we divide the both side by phi times f. You divide the left hand side and right hand side by phi times f. What you will get here on the left hand side? You will get ih bar 1 over f df dt and right hand side what you will get? Minus h bar square over 2m 1 over phi d 2 phi dx 2 plus v.

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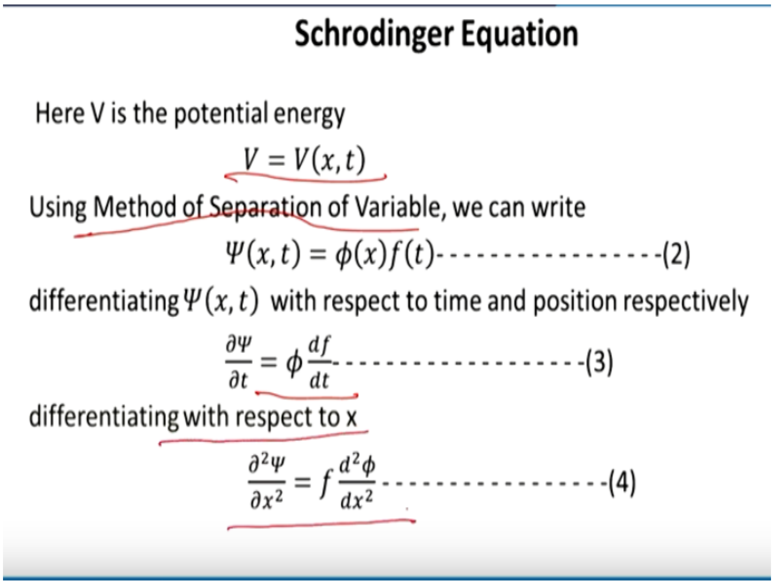

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differentiating with respect to x

$$\frac{\partial^2\Psi}{\partial x^2} = f\frac{d^2\phi}{dx^2} \text{-----------------(4)}$$

That exactly we are showing here. Differentiating psi x, t with respect to time and position, we get del psi del t which is phi into df dt and differentiating with respect to x we get del 2 psi del x 2 is equal to f d 2 phi dx 2.

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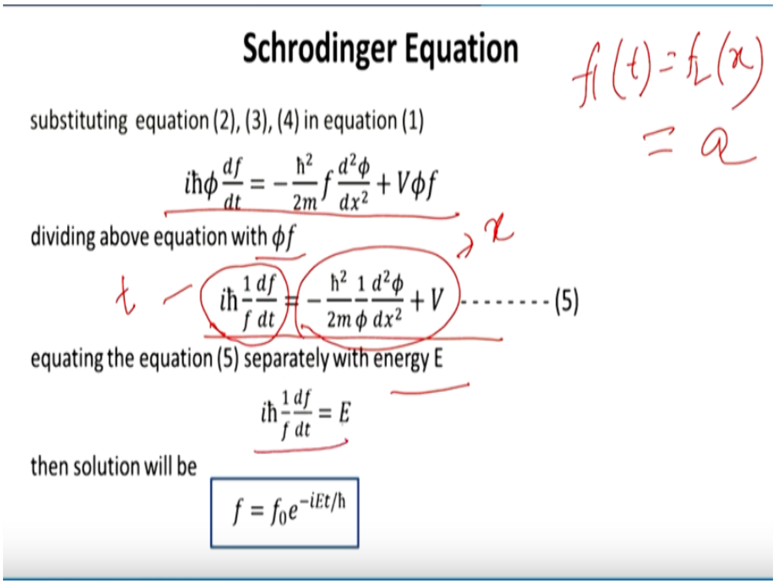

Schrodinger Equation

$f_1(t) = f_2(x)$

$= a$

substituting equation (2), (3), (4) in equation (1)

$$i\hbar\phi\frac{df}{dt} = -\frac{\hbar^2}{2m}f\frac{d^2\phi}{dx^2} + V\phi f$$

dividing above equation with ϕf

x

t

$$i\hbar\frac{1}{f}\frac{df}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\phi}\frac{d^2\phi}{dx^2} + V \text{ --------- (5)}$$

equating the equation (5) separately with energy E

$$i\hbar\frac{1}{f}\frac{df}{dt} = E$$

then solution will be

$$\boxed{f = f_0 e^{-iEt/\hbar}}$$

Now if we substitute this in the Schrodinger equation and subsequently divide by the phi into f, we get a equation which looks like that. Now you look there is an interesting fact. The left hand side here is a function of the time only. And the right hand side here is a function of positions only. This side is a function of time, this side is a function of the positions.

So I have an equation where f 1 is a function of time is equal to f 2 is a function of x. How that can be true simultaneously? If both of them is equal to a positive constant a, and let us consider that constant is the energy E. So if we consider that constant is energy E, so I can equate the left hand side ih bar 1 over f df dt is equal to E.

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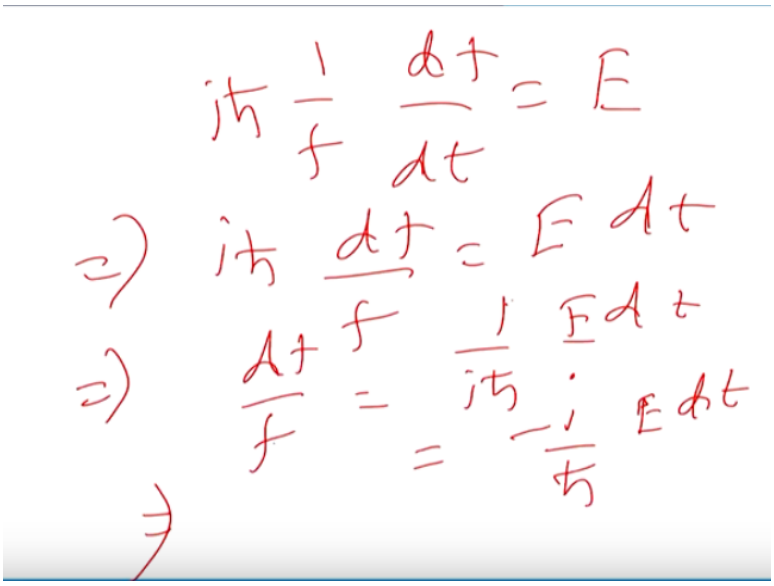

$$i\hbar \frac{1}{f}\frac{df}{dt} = E$$

$$\Rightarrow i\hbar \frac{df}{f} = E\,dt$$

$$\Rightarrow \frac{df}{f} = \frac{1}{i\hbar} E\,dt$$

$$= -\frac{i}{\hbar} E\,dt$$

$$\Rightarrow$$

And if we integrate this equation, ih bar 1 over f df dt is equal to E, what we will get; iH bar df by f is equal to E dt. If we multiply that we can also write df by f 1 over ih bar E dt, if the iH bar comes on the right hand side, right. So 1 over i is we can multiply top and bottom by i. So this is i and this will be i square and i square is -1. So that means we will get –i by H bar E dt. So if we integrate the previous equations this df by f, also this right hand side so what we will get?

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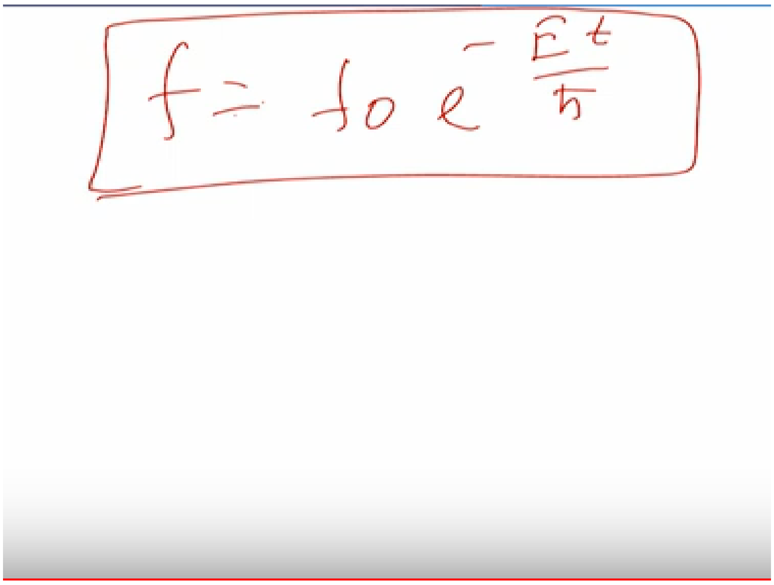

$$\boxed{f = f_0 e^{-\frac{Et}{\hbar}}}$$

We will get f is equal to f 0 e to the power minus iEt by h bar. This is the solutions of the time dependent part of the Schrodinger equations. So this is the solution for the time dependent part of the Schrodinger equation; f is equal to f 0 e to the power –iEt by h bar.

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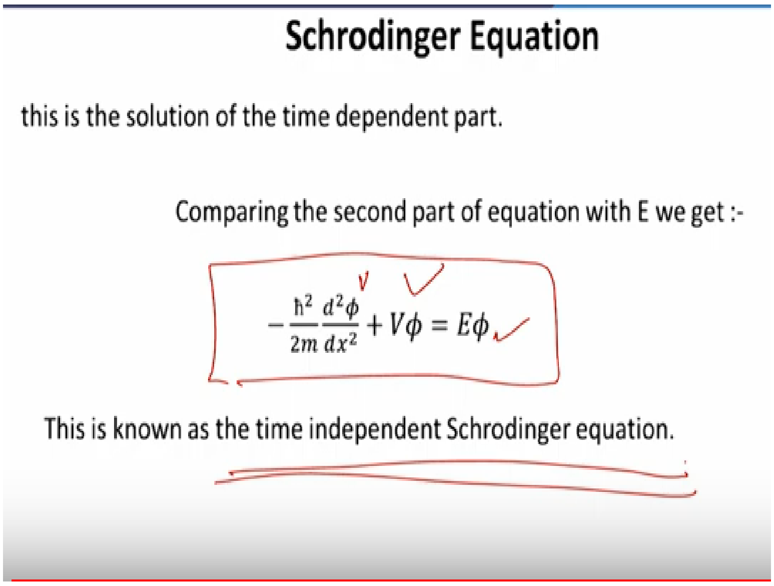

Schrodinger Equation

this is the solution of the time dependent part.

Comparing the second part of equation with E we get :-

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} + V\phi = E\phi}$$

This is known as the time independent Schrodinger equation.

We are left out with the spatial part. What was our spatial part? Our spatial part was this. Minus h bar square by 2m d 2 phi dx 2 V phi is equal to E phi where V is the potential and this is called time independent Schrodinger equation. As you can see, the d 2 phi dx 2, here phi is now a function of the positions only as we have defined it earlier. And phi is also a positions, function of positions.

So everything here is a function of positions. No time here. So that is why it is a time independent Schrodinger equation. So starting with time dependent Schrodinger equation we have now derived a time independent Schrodinger equations. And once we come across this point, rest of the quantum mechanics is solving this equation for different value of the potential.

When you are talking about the electron in a metal or electron in a semiconductor, basically we are going to solve this equation subjected to the different boundary conditions. We first start with the typical example. Electron in a metal. This is sometime represented as particle in a box problem or a particle in an infinite potential wall.

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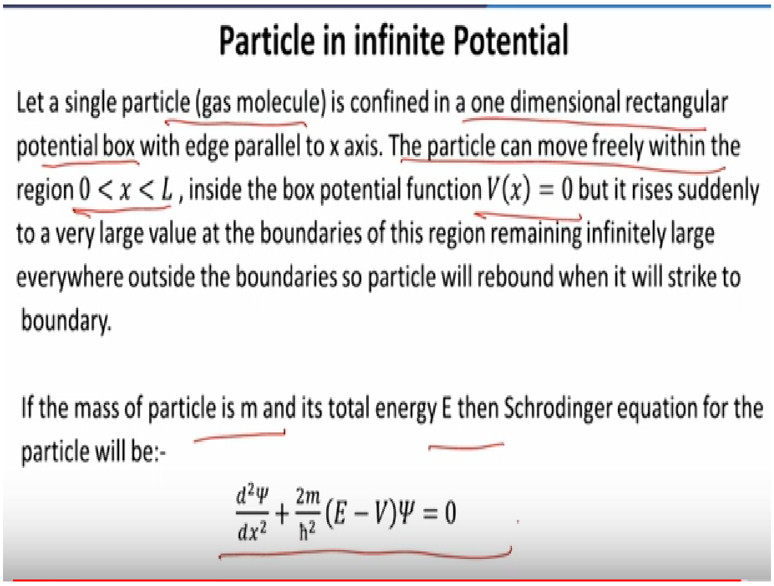

Particle in infinite Potential

Let a single particle (gas molecule) is confined in a one dimensional rectangular potential box with edge parallel to x axis. The particle can move freely within the region $0 < x < L$, inside the box potential function $V(x) = 0$ but it rises suddenly to a very large value at the boundaries of this region remaining infinitely large everywhere outside the boundaries so particle will rebound when it will strike to boundary.

If the mass of particle is m and its total energy E then Schrodinger equation for the particle will be:-

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\Psi = 0$$

Let a single particle like gas molecule is confined in a one dimensional rectangular particle box.

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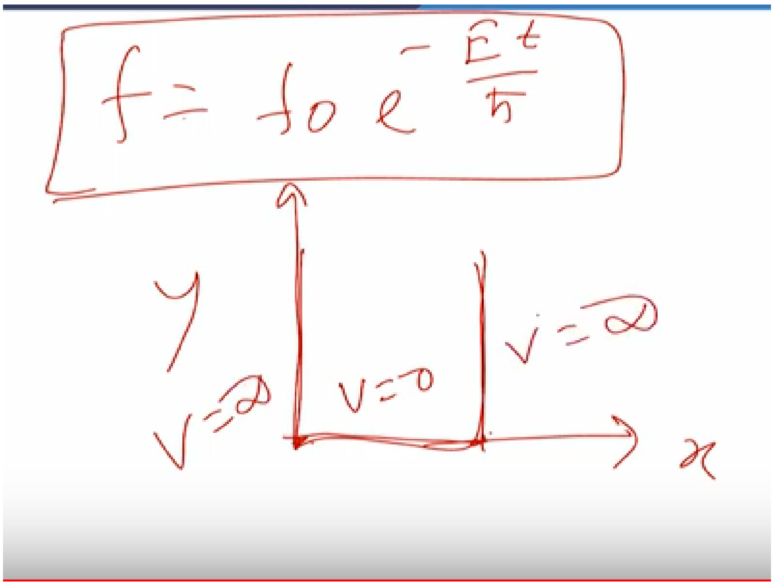

So you consider, here this is your x axis. This is your y axis. The particle is confined in a one dimensional rectangular potential box. So the potential energy between these two end is zero. And at this two boundary potential is infinite. The length of this box is L. This particle can move freely within the region between x 0 to L.

Inside the box the potential energy is zero but at the wall it suddenly goes asymptomatically and becomes infinite. So if the mass of the particle is m and its total energy is E then we can write the time independent Schrodinger equation d 2 psi dx 2 + 2m/h bar square E - V psi = 0.

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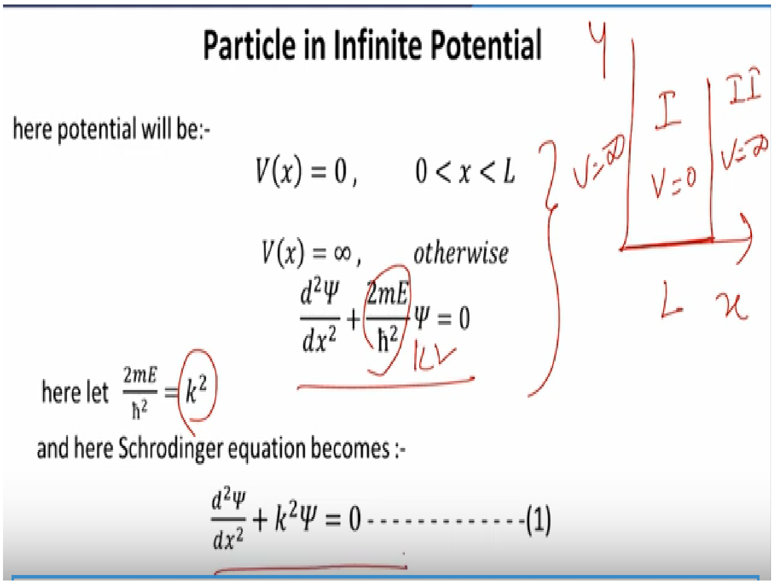

Particle in Infinite Potential

here potential will be:-

$$V(x) = 0, \qquad 0 < x < L$$

$$V(x) = \infty, \qquad otherwise$$

$$\frac{d^2\Psi}{dx^2} + \frac{2mE}{\hbar^2}\Psi = 0$$

here let $\frac{2mE}{\hbar^2} = k^2$

and here Schrodinger equation becomes :-

$$\frac{d^2\Psi}{dx^2} + k^2\Psi = 0 \text{-------------}(1)$$

So this is exactly the representation of the potential here. You can draw the diagram here also. So this is your x axis, this is your y axis, this is your potential. The length or the dimension of this potential box is L. So V x is equal to zero here. And V is equal to finite at this two boundary. We need to solve this Schrodinger equation at this region and also at this region.

Here the potential described by this function. So I have written that d 2 psi dx 2 plus 2m by h bar square psi is equal to 0 and you consider this 2mE by h bar square as a constant k square. If you replace this as a constant k square the equation will be d 2 psi dx 2 plus k square psi is equal to 0.

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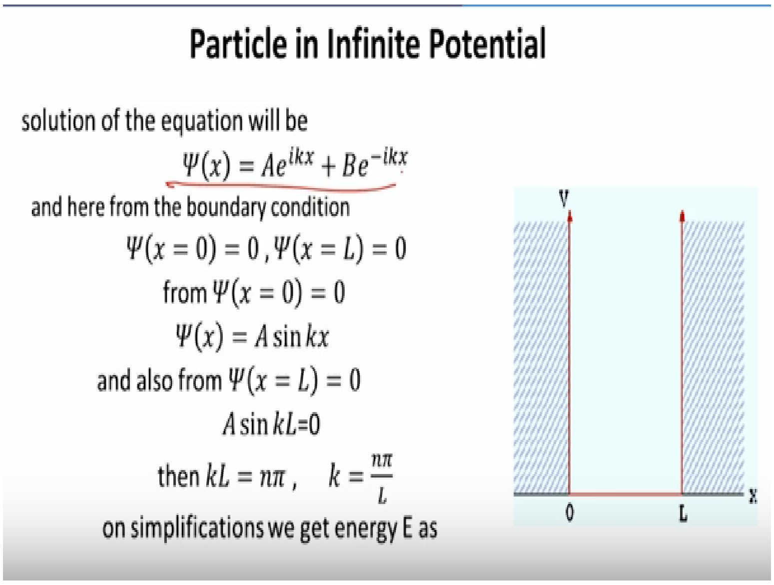

Particle in Infinite Potential

solution of the equation will be

$$\Psi(x) = Ae^{ikx} + Be^{-ikx}$$

and here from the boundary condition

$$\Psi(x=0) = 0, \Psi(x=L) = 0$$

from $\Psi(x=0) = 0$

$$\Psi(x) = A\sin kx$$

and also from $\Psi(x=L) = 0$

$$A\sin kL = 0$$

then $kL = n\pi, \quad k = \frac{n\pi}{L}$

on simplifications we get energy E as

And the solutions of these equations will be Ae to the power ikx plus B e to the power minus ikx. If we apply the proper boundary conditions, what we will get that

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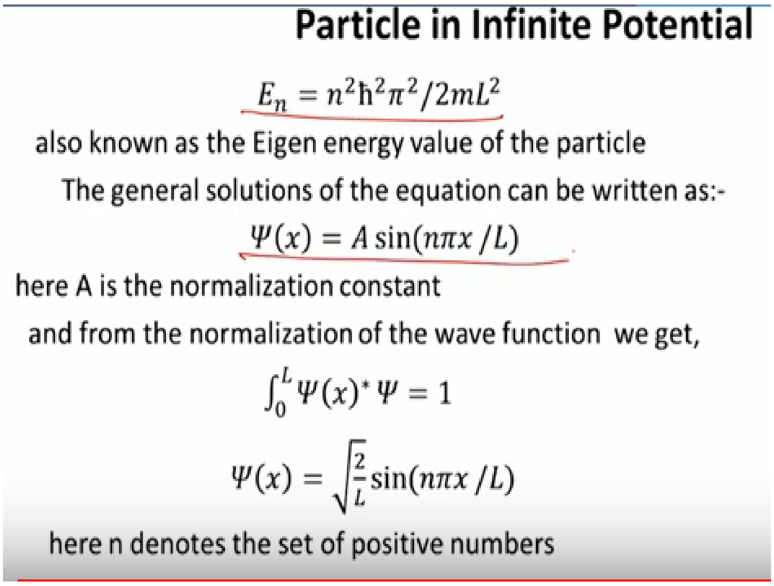

Particle in Infinite Potential

$$E_n = n^2\hbar^2\pi^2/2mL^2$$

also known as the Eigen energy value of the particle

The general solutions of the equation can be written as:-

$$\Psi(x) = A\sin(n\pi x/L)$$

here A is the normalization constant

and from the normalization of the wave function we get,

$$\int_0^L \Psi(x)^*\Psi = 1$$

$$\Psi(x) = \sqrt{\frac{2}{L}}\sin(n\pi x/L)$$

here n denotes the set of positive numbers

The energy value is n square pi square h bar square by 2mL square and the wave function is A sin n pi x by L. We will conclude this module with this and in the next class we will see that how this application of the boundary condition is going to influence our wave function as well as the energy level. Thank you.