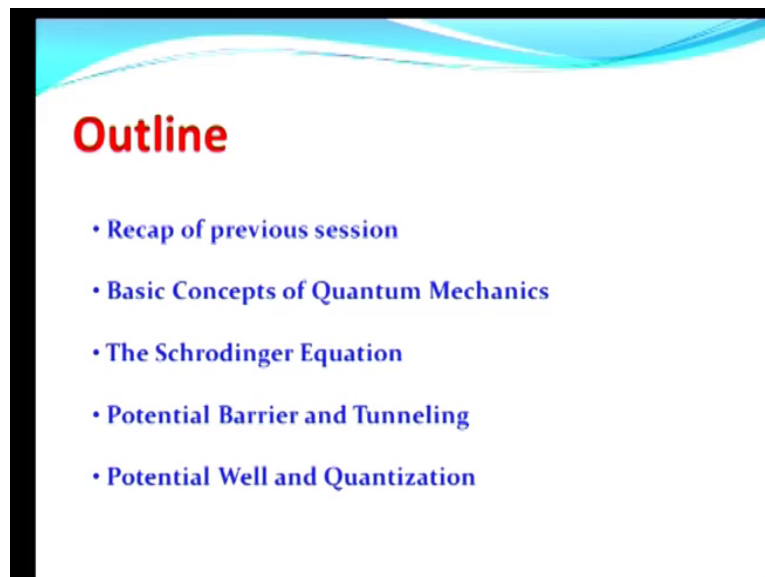


Nanoelectronics: Devices and Materials
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Lecture - 32
Basic Principles of Quantum Mechanics

Hello. This is the next session of this third segment of the course on Nanoelectronics Device Fabrication and Characterization. And as I outlined last time, this segment is concerned about nano material systems and making an attempt on to understand what concepts are necessary to deal with nano systems. Now, what I will do this time is to recap what we did in the previous session.

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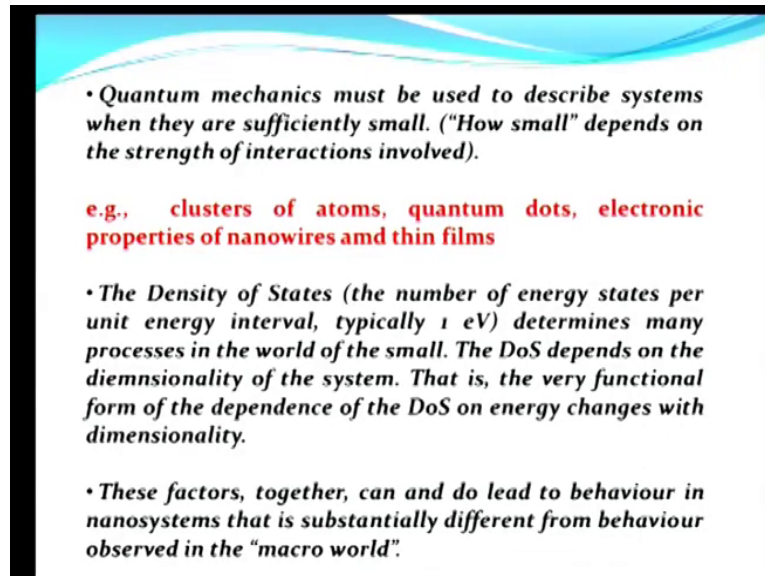


And then go on to the basic concepts of quantum mechanics because it is necessary; as I mentioned last time to use quantum mechanics to deal with small scale systems. And within the quantum mechanical aspects of this segment, we will deal with the Schrodinger equation, the potential barrier and tunneling concepts and also deal with what happens when a particle is in potential well and quantization of energy that takes place under these circumstances.

Now, what we get in the last class is really to try to first define nano systems and then we went on to point out that quantum mechanics is necessary to deal with such systems. And actually also statistical mechanics because while quantum mechanics is necessary to deal

with a nano particle or let us say a quantum particle like an electron, a nano system typically consists of thousands, hundreds and thousands of these nano particles. So, therefore, it is necessary to deal with statistical mechanics aspects of such systems.

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- *Quantum mechanics must be used to describe systems when they are sufficiently small. ("How small" depends on the strength of interactions involved).*
- *e.g., clusters of atoms, quantum dots, electronic properties of nanowires and thin films*
- *The Density of States (the number of energy states per unit energy interval, typically 1 eV) determines many processes in the world of the small. The DoS depends on the dimensionality of the system. That is, the very functional form of the dependence of the DoS on energy changes with dimensionality.*
- *These factors, together, can and do lead to behaviour in nanosystems that is substantially different from behaviour observed in the "macro world".*

Therefore what we did last time was to point out that quantum mechanics must be used to describe systems when they are sufficiently small and how small these should be depends on the strength of the interactions involved among these particles. So, you can have clusters of atoms, quantum dots, electronic properties of nano wires and thin films and so on; all dealt with as quantum systems.


There is a concept that I mentioned last time; I will repeat it although we will deal with that in the next class namely the density of states; that is the number of energy states per unit energy interval typically in electron volts, that determines how many processes in the world of this small are determined or how these process are determined.

So, the density of states is an important aspect of dealing with nano systems. So, the very functional form of the dependence of the density of states on energy changes with the dimensionality. As I have mentioned last time, you can have nano systems with the 0 dimensions, 1 dimensions, 2 dimensions and 3 dimensions therefore, the density of the state depends on the dimensionality of these systems.

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Quantum Mechanics dominates (dictates) the behaviour of atoms , whereas Statistical Mechanics is pertinent to understanding the behaviour of ensembles of atoms and molecules.

The science and technology of Nanosystems is where atomic (quantum) behaviour of matter intersects the behaviour of complex systems:

Quantum Mechanics  **Statistical Mechanics**

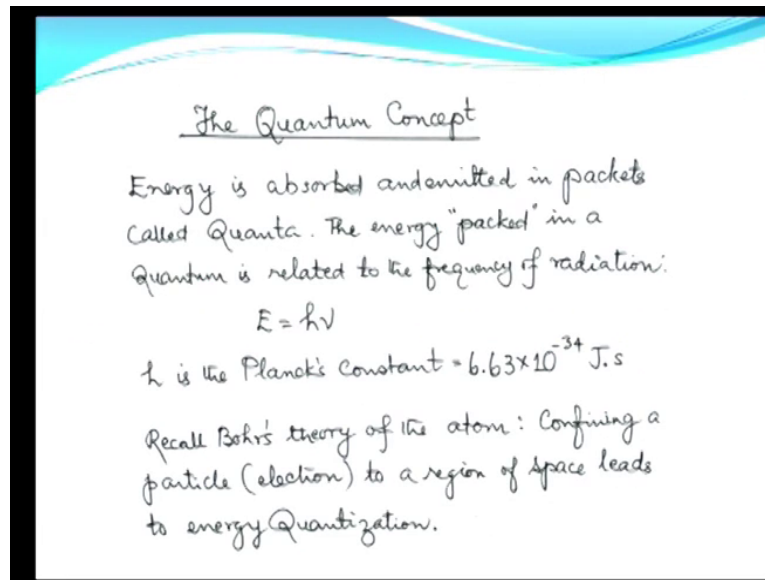
As nanosystems may contain up to tens of thousands of atoms, their behaviour is not necessarily quantum mechanical

**How "quantum mechanical" (microscopic) is a system?
--- depends on the strength of interactions involved**

Now, as I said one has to deal with also this part systems where you might have hundreds or thousands of these quantum particles together in a nano system. While quantum mechanics dominates the behavior of atoms, statistical mechanics is necessary and its pertinent to understanding the behavior of ensembles of these atoms and molecules. Therefore, the science and technology have nano systems is where there is an intersection of the behavior or complex systems with that of quantum behavior.

Therefore quantum mechanics and statistical mechanics have to be used together to deal with these systems. As I said a nano systems they consist of tens of, thousands of atoms and each of them is a quantum mechanical system and how quantum mechanical a system, how microscopic a system depends on the strength of interactions as I already mentioned.

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So, what you should do this time is to understand some basic concepts of quantum mechanics. All of you would be familiar right from much earlier classes that you have taken; that energy is absorbed and emitted in packets called quanta or a quantum.

Now, this was the basic discovery of Planck's more than 100 years ago and what he said was energy is packed in a quantum and the energy in such a quantum is given by E is equal to $h\nu$, where h is the Planck's constant whose value is 6.63 into 10 to the power minus 34 joule second and ν is the frequency of the radiation involved. Now again early in your learning you have found or you learned about the Bohr's theory of atom and you have learned how by confining a particle; in this case an electron into a region of space in this case around the nucleus of the hydrogen atom; such confinement leads to energy quantization that is the electron in such a system, such a an environment can only take discrete values.

Unlike what would happen in Newtonian mechanics, where there is no such restriction and energy supposed to be continuously variable for a particle; moving in under any force field. So, that is the distinction between the quantum concept and the classical concept which is dealt with in the Newtonian mechanics.

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Wave-particle Dualism

de Broglie: Consider a freely propagating particle.
Its position can be predicted by associating
with it a wave of wavelength

$$\lambda = \frac{h}{mv}$$

where v is its speed (magnitude of velocity).

λ is related to the question: "When is a
system quantum mechanical and when is it
classical?"

Now, a primary aspect of the development of quantum theory was the postulate of de Broglie; who said that if you consider a freely propagating particle then its position can be predicted by associating with it a wave of wavelength λ given by h/mv , where v is the speed of the particle, m is its mass and h of course, is the Planck's constant. So, what you have here is a relationship between a particle in the Newtonian sense with the mass m and wave motion because λ the wavelength is associated with a wave.

So, these two are earlier considered to be incompatible that is particle motion and a wave motion and de Broglie's concept brings them together. So, λ the value of λ is related to the question when this system to be considered quantum mechanical? And when is it classical?

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The Electron as an example:
 $m_e = 9.1 \times 10^{-31} \text{ kg}$; charge $q = 1.6 \times 10^{-19} \text{ C}$
The energy gained by an electron moving through a potential difference of 50 kV (as in a TEM) is
 $E = \frac{1}{2} m v^2 = qV = 1.6 \times 10^{-19} \cdot 5 \times 10^4 = 8 \times 10^{-15} \text{ J}$
 $\therefore v = \sqrt{\frac{2E}{m}} = 1.3 \times 10^8 \text{ m/s}$
 $p = mv = 9.1 \times 10^{-31} \times 1.3 \times 10^8 = 1.2 \times 10^{-22} \text{ m} \cdot \text{kg} \cdot \text{s}^{-1}$
 $\lambda = \frac{h}{p} = \frac{6.63 \times 10^{-34}}{1.2 \times 10^{-22}} \approx 5.5 \times 10^{-12} \text{ m} = 5.5 \text{ pm}$

So, this can be illustrated actually by considering an electron as an example of a quantum particle or by applying the de Broglie rule to the electron whose mass is 9.1 into 10 to the minus 31 kg and a charge of 1.6 into 10 to the minus 19 coulombs.

And if you subject it to a potential of 50 kilo volts as typically happens in an electron microscope example, then it gains energy and that energy is given by E is equal to half mv square and that is equal to q into v , where q is the charge of the electron and v is the potential across which it has been taken; namely 50 kilo volts. So, if you do the arithmetic you find that the velocity of the electron under these conditions would be about 1.3 into 10 to the power 8 meters per second.

And therefore, the momentum which is m into v turns out to be 1.2 into 10 to the power minus 22 meter kg per second. Since λ the de Broglie wavelength of the electron is the ratio of the Planck's constant of the momentum then, arithmetic tells us that λ is of the order of 5 into 10 to the power of 12 meters or about 5 pico meters. Now, it is important to keep in mind; when we look at these numbers, it is a very small distance very small length; 5 into 10 to the power minus 12 meters is a very small length and therefore, a very small sizes for a particle.

But the size of the electron, there are different ways to estimate it; the size of the electron is of the order 10 to the minus 16 meters. Therefore, what you have see is that the wavelength of the wave associated with the electron that has just gone through a potential

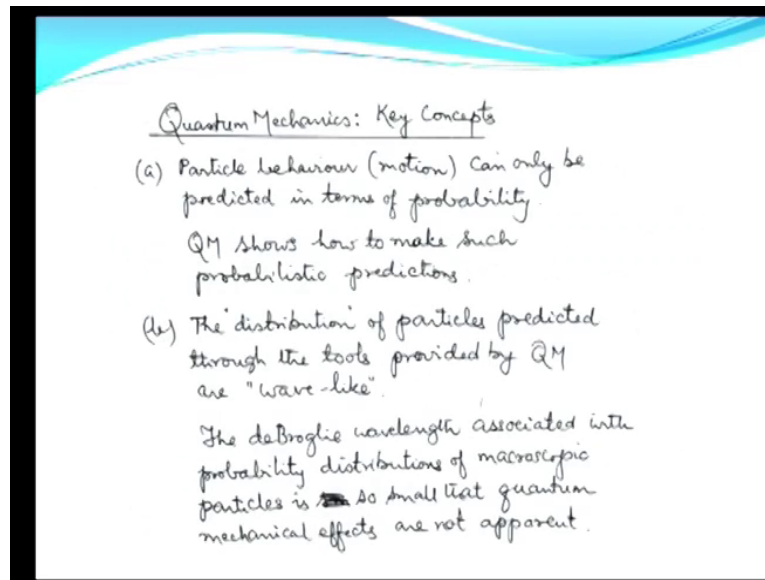
difference of 50 kilo volts is much larger than the size of the electron itself; the physical size of the electron itself.

In other words the de Broglie wavelength associated with an electron of this energy is significantly greater than the size of the electron itself. Therefore, you can see that the application of quantum mechanics in this case; probably should be significant or it must be necessary because the de Broglie wavelength associated with the electron is; so, much larger than the size of the electron itself. Again by extending the argument, suppose you think of a nano particle and think of its size or rather the mass of that to be of the order of let us say a pico gram; 10 to the power of minus 12 gram.

Now, if you try to calculate the wavelength of the de Broglie wave that is associated with that, you will see that it is a much smaller number than the de broglie wavelength of the electron because the mass is in the denominator. Therefore, when the mass is greater λ becomes much smaller therefore, if you have a pico gram of material with about the same energy, then you will find that the wavelength of that is orders of magnitude smaller than the size of the particle itself.

Therefore, what it illustrates is that when the wavelength associated with a particle or a physical object is much smaller than its dimension, then quantum mechanics does not apply and in such a case; it is valid to treat the particle using Newton's laws of motion. So, that is a kind of an order of magnitude argument for where one has to deal with quantum mechanics.

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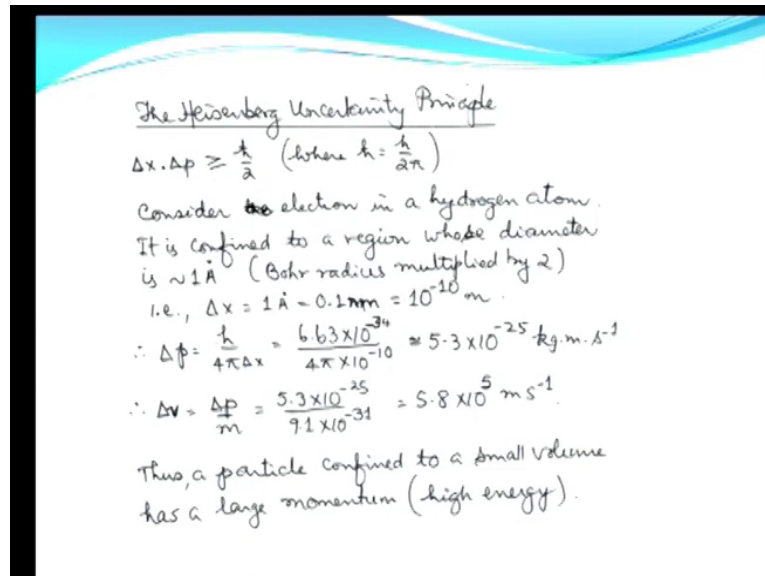
Now, what are the key concepts? Some of the key concepts I should say because I will deal with some of them today and some of them tomorrow. What are the key concepts of quantum mechanics? One is that the particle behavior or motion can only be predicted in terms of a probability; that is quantum mechanics shows how to make such probability predictions of the motion of a particle; that is subject to quantum mechanical laws.

This is the contrast with Newton's laws where, it is not a question of probability it is a question of certainty, you can predict where for example, the moon will be in the orbit around the earth on a given day that is how you are able to predict the precised time and date of an eclipse for example. Therefore, that kind of certainty is possible because quantum mechanical considerations do not apply to large objects, where the de Broglie wavelength is very much smaller than the size of the object.

Now, further the distribution of the particles predicted through the tools of quantum mechanics; as I said you know we really talk about probabilities and therefore, we have to talk about distribution of these probabilities. So, therefore the distribution of this particles is wave like, so there is a concept which we will have no time to go through in this short segment of the course. The concept is a particle is to be associated or described as a wave packet. So, it is a wave like distribution that represents a particle in quantum mechanics. Now as I already said the de Broglie wavelength associated with the probability distribution of macroscopic particles large objects is so, small that the quantum mechanical effects are not a parent and certainly not observable with any tool that we

have today.

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The Heisenberg Uncertainty Principle

$$\Delta x \cdot \Delta p \geq \frac{h}{2} \quad (\text{where } h = \frac{h}{2\pi})$$

Consider ~~the~~ electron in a hydrogen atom.
It is confined to a region whose diameter is $\sim 1 \text{ \AA}$ (Bohr radius multiplied by 2)
i.e., $\Delta x = 1 \text{ \AA} = 0.1 \text{ nm} = 10^{-10} \text{ m}$.

$$\therefore \Delta p = \frac{h}{4\pi \Delta x} = \frac{6.63 \times 10^{-34}}{4\pi \times 10^{-10}} \approx 5.3 \times 10^{-25} \text{ kg} \cdot \text{m} \cdot \text{s}^{-1}$$
$$\therefore \Delta v = \frac{\Delta p}{m} = \frac{5.3 \times 10^{-25}}{9.1 \times 10^{-31}} = 5.8 \times 10^5 \text{ m s}^{-1}$$

Thus, a particle confined to a small volume has a large momentum (high energy).

Another important aspect of quantum mechanics is the Heisenberg uncertainty principle; again something that you would have come across earlier in your schooling. One statement of the Heisenberg uncertainty principle; which is actually in inequality is Δx into Δp is greater than or equal to $\frac{h}{2}$.

Now, $\frac{h}{2\pi}$ which is really the Planck's constant divided by 2π has a special significance in quantum mechanics therefore, we shall generally use $\frac{h}{2\pi}$ instead of h . So, what this equation is saying is that; there is a limit to the precision with which one can simultaneously determine Δx and Δp ; that is the uncertainties in momentum and the position of a particle. That is you cannot have 0 for both, you cannot have 0 for Δx and 0 for Δp at the same time, there is a minimum uncertainty associated with both.

And if you increase the uncertainty in; rather if you try to make the measurement of the position precise then the uncertainty in the momentum goes up correspondingly in such a way as to keep the inequality intact. So, this is a direct result of what you said earlier namely that in quantum mechanics, one describes particle motions through probabilities and not certainties. Therefore, the Heisenberg uncertainty principle is an integral part of the foundation of quantum mechanics.

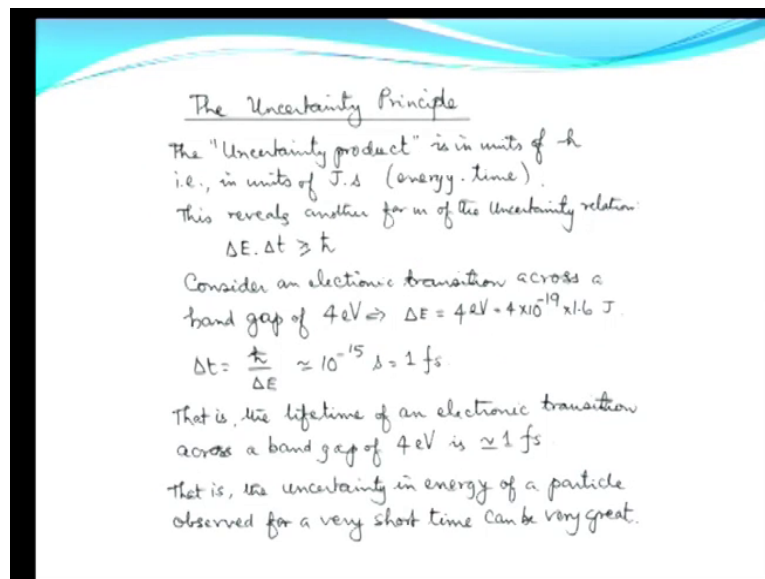
Now, again to illustrate this consider an electron in hydrogen atom which is confined to a region let us first consider the first Bohr orbit, the size of that orbit is 1 angstrom

approximately that is a bohr radius multiplied by 2. Therefore, there is an uncertainty in the position of the electron around the nucleus of the order of 1 angstrom; therefore, Δx is of the order of 1 angstrom.

Using the uncertainty principle then we see that the minimum Δp is h divided by $4\pi\Delta x$; using the above inequality and that transferred to be 5.3×10^{-25} kilogram meter per second. And therefore, the uncertainty in the velocity which is Δp divided by m is of the order of 5.8×10^5 meter per second; that actually gives us an order of magnitude of the velocity of the electron as it moves around the nucleus under its electrostatic force. So, what is actually says is that a particle that is confined to a small volume has a large momentum. Now what we have shown here is Δp , we have calculated Δp here as about 10^{-25} kilogram meter per second.

If we use that momentum to calculate the energy of the electron through the formula $E = p^2 / 2m$; to get an order of magnitude what you will find is that the only the arithmetic view what you will find is that, the energy of the electron in such a circumstance where it is confined is easily find to be of the order of several electron volts which we know to be true from our Bohr theory. Therefore, what this shows is that using the uncertainty principle, it is possible to calculate the order of magnitude of energies that quantum mechanical particles would have under certain known circumstances.

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Now, recall that the uncertainty principle is really the product of Δx and Δp and

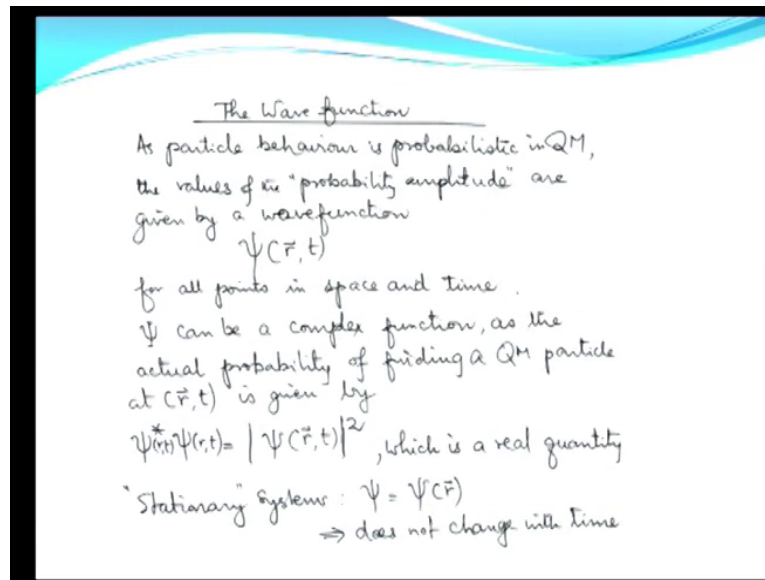
the product is greater than or equal to the Planck's constant. Recall that the units of the Planck's constant is energy multiplied by time; joule second; therefore, this suggests I have used the wrong word here, I said this reveals; I should say this suggests. Another form of the uncertainty relationship which we could write as $\Delta E \Delta t \geq h$, ΔE representing joules and Δt representing second together forming the units for the Planck's constant.

Now, consider an electron that undergoes a transition across a band gap of 4 electron volts in some semiconductor. You know semiconductors have band gaps, we will written though that later. Consider an electron that undergoes an electronic transition across the band gap of a semiconductor whose band gap is 4 electron volts. Therefore, ΔE in this case can be taken to be 4 electron volts. So, if you do not know for example, whether the electron is in the upper band or the lower band; therefore, ΔE is equal to 4 electron volts.

Using the uncertainty relationship we can see that therefore, Δt which is h divided by ΔE according to the uncertainty relationship; turns out to be of the order of 10^{-15} seconds or one femto second. Therefore, what this says is that the lifetime of an electronic transition across a band gap of 4 electron volts is of the order of 1 femtosecond. That is the uncertainty in the energy of a particle observed for a very short time; 1 femtosecond is very great.

Therefore, what another formula the uncertainty relationship is that if you try to measure the energy of a quantum particle within a very short period of time. If you try to make an observation if its energy make a measurement of its energy over a very short period of time then the result that you get of the energy is uncertain by a large proportion. Again; that means, that you cannot determine the energy of a quantum particle precisely; unless you make the measurement over very long periods of time; that is what it means.

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Now, coming back to the probabilistic behaviour of quantum particles that is the probabilistic behaviour that quantum mechanics asserts for particles in the quantum mechanical regime. The values of the probability amplitude are now postulated to be given by a wave function; represented typically by the Greek letter psi which is a function of the position r and time t . So, this is analogous to the Newtonian concept of how you can define a particle by its position as a function of time. So, you follow the motion of a particle by saying where it is going to be as a function of time.

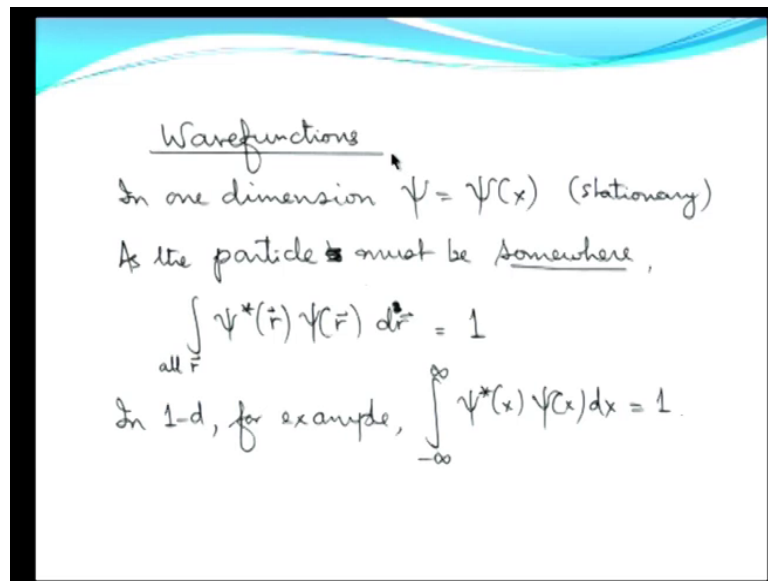
So, this is an analogous concept where we have a probability amplitude; we will come back to why it is called the amplitude momentarily; that is given by psi of r and t . And r and t define where the quantum mechanical particle is in time and space. An important aspect of quantum mechanics; again as a departure from classical mechanics is that psi can be a complex function. Because what you have said earlier is that psi is the probability amplitude, again by a certain interpretation of quantum mechanics due to max born. the meaning of the meaning of psi lies in the probabilistic interpretation of quantum mechanics which means that the modulus of psi squared, the wave function squared is the quantity that represents a probability of finding the particle at a position r ; at a time t .

Now as I said, the wave function is a complex quantity; it can be complex therefore, psi square modulus of psi square is really the product of the complex conjugate of psi and the real psi. Therefore, what you have here is the real quantity; so, the even though the probability amplitude can be complex psi square, the probability of finding the particle at a

given position, at a given time is a real quantity.

Now, it is possible that this $\psi(r, t)$ is actually just $\psi(r)$; where it is independent of t that is the probability of finding the particle is independent of the time for a given position r . In that case what you have is a stationary system. In that case what you get is $\psi(r, t)$ equal to $\psi(r)$. That is the probability of finding the particle at a position r is independent of time; such a system is a stationary system.

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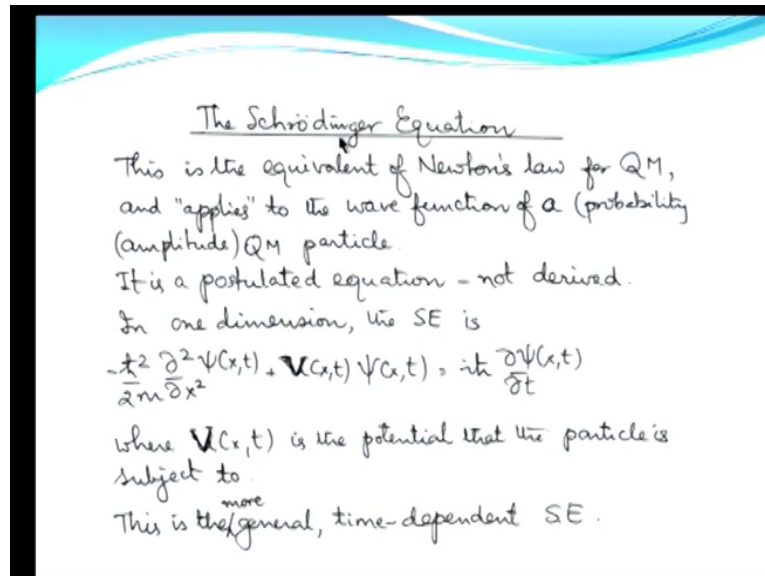
Now, continuing the concept of the wave function what I wrote in the previous slide is the wave function where it is a function of r which is a three dimensional position vector with you know Cartesian coordinates x , y and z , but to simplify things we can consider the wave function as a function of x only; in one dimension.

And if you write ψ is equal to $\psi(x)$ without the t there; then you have a stationary wave function. It is a simple fact that such a particle has to be found somewhere; that is you would have the particle somewhere in the universe. Therefore, if x for example, or varies all over the place that is you go from minus infinity to plus plus infinity for example, and you integrate this probability function ψ^* into ψ if we integrate this, then the integral should be equal to unity because that says the probability of finding the particle somewhere is exactly equal to 1.

In one dimensions, this becomes minus infinity to plus infinity integral of $\psi^* \psi$ is equal to 1. So, this is how one defines the certainty of finding the particle somewhere within the

domain of interest.

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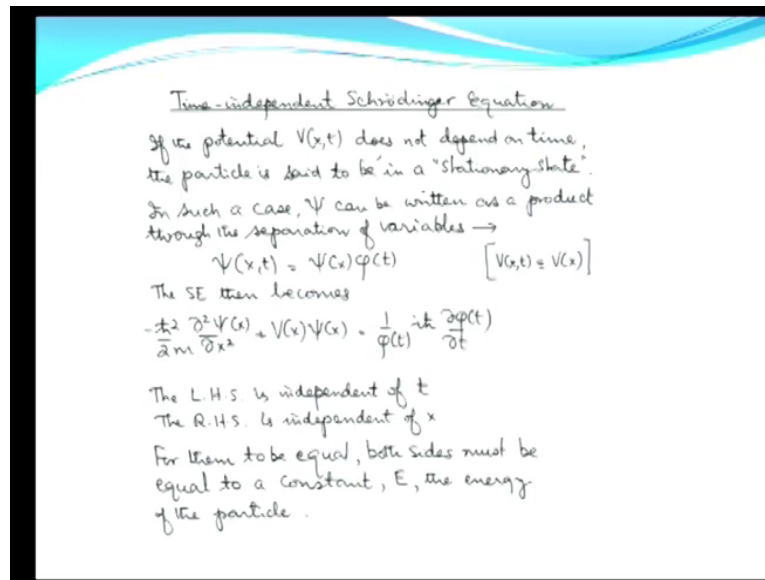


Another basic aspect of quantum mechanics is the Schrodinger equation. The Schrodinger equation is the equivalent of the Newton's law of quantum mechanics and it applies to wave functions or the probability amplitude of a quantum particle. Now just like Newton's laws, the Schrodinger equation is a postulate. So, you one cannot derive Schrodinger equation. Although, how it takes on the forum it does has its roots in the development of classical mechanics in the later stages.

Now in one dimension this Schrodinger equation has this form, where the first term is a second derivative in space. So, minus h bar square by 2 m; delta square psi delta x square and at the second function or the second term has the potential function V x t is the time dependent potential to which this particle is subject. So, it is moving under this potential and the right hand side has the time derivative of the wave function multiplied by i and h bar. So, this itself the presence of i the square root of minus 1, once again asserts that this is a quantum mechanical system where you can have complex functions.

Now this is so called time dependent Schrodinger equation because on the left hand side you have a derivative with respect to space and the right hand side you have a derivative with respect to time therefore, it is the time dependent Schrodinger equation.

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However, it is possible to deal with and actually more common to deal with the time independent Schrodinger equation. If the potential $V(x,t)$ does not depend on time, then as I said you would have a particle in a stationary state. If the potential is independent of time then the solution to Schrodinger equation which describes the motion of the particle, they are time independent therefore, you have a stationary state. In such a case one can write $\psi(x,t)$ as the product of a time independent part and a time dependent part. So, we write $\psi(x,t)$ as $\psi(x)$ into $\phi(t)$ because now the potential function $V(x,t)$ is just $V(x)$ independent of a time; then the Schrodinger equation becomes.

If we go back to how the Schrodinger equation was in the previous slide and we substitute $\psi(x,t)$ as $\psi(x)$ into $\phi(t)$, then it is the Schrodinger equation then becomes; as shown here you get a separation of the spatial part on the left hand side and the time dependent part on the right hand side. So, the left hand side is independent of time and the right hand side is independent of x . Now they are equal, if they are to be equal then they both must be a constant.

So, on the left hand side you have a time independent part; on the right hand side you have a time dependent part both of them are being equal, then they are equal to a constant with respect to time and space. So, this is the energy of the system; why it is called the energy and so, on? Is a part as I said of Hamiltonian mechanics and so on; we have no time to go into that, but this turns out to be the energy of the system.

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Time-independent S.E. (Contd.)

$$i\hbar \frac{\partial \varphi(t)}{\partial t} = E \varphi(t)$$
$$\Rightarrow i\hbar \frac{\partial \varphi(t)}{\partial t} = E \varphi(t) \Rightarrow \varphi(t) = \exp\left(-i \frac{E}{\hbar} t\right)$$
$$\Rightarrow \Psi(x,t) = \psi(x) \exp\left(-i \frac{E}{\hbar} t\right); E = \hbar \omega$$
$$\therefore \Psi^*(x,t) = \psi^*(x) \exp\left(+i \frac{E}{\hbar} t\right)$$
$$\Rightarrow \Psi^*(x,t) \Psi(x,t) = |\Psi(x,t)|^2 = |\psi(x)|^2$$

This is the probability of finding the particle at x .

This is independent of time \Rightarrow Stationary state.

So, we take the right hand side and therefore, we write we can write the time dependent part equal to e ; the constant that is the energy of the system. So, this is a simple first order time dependent differential equation and the solution is such that therefore, ψ if you solve this is simple equation; ψ then becomes ψ of x into e to the minus i into e by \hbar bar into t , where e because we have a quantum system e is equal to \hbar bar ω .

Because this is what Planck postulated earlier, so e is equal to \hbar bar ω . Therefore, one has a simple sinusoidal function for the wave function more here. Now ψ x t therefore, is the product of ψ x ; the space dependent part multiplied by exponential that is the time dependent part; notice that this is a complex function.

Therefore the complex conjugate gives us a change of sign in the exponent therefore, the product of ψ and ψ star, the complex conjugate becomes a real function ψ x squared actually ψ x squared. So, what you see here is that this probability is there for independent of time; that is what we have now is the stationary state, the probability of finding a particle in a given position is independent of time, we have a stationary state. So, this is the simple consequence of being able to separate the variables because the potential is independent of time.

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Time-independent S.E. (Contd.)

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) \psi(x) = E \psi(x)$$

This can be written as

$$H \psi(x) = E \psi(x) \quad \text{Stationary System}$$

where $H \equiv -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$

The Hamiltonian operator

The solution to the S.E. yields

Eigenfunctions & Eigenenergies } as the possible probability amplitudes & the corresponding energies of the QM particle (System).

Now, again we equate the left hand side in the Schrodinger equation which was the space dependent part to E and when you do that what you get this equation; is the equation at on this line the time independent Schrodinger equation minus \hbar bar square divided by $2m$ second derivative of ψ plus V into ψ is equal to E into ψ . So, this is the famous time independent Schrodinger equation.

This can be written for shorthand as $H \psi = E \psi$, where H which is the. So, called Hamiltonian operator is the second derivative differential operator represented by minus \hbar bar square over $2m$, second derivative of with respect to space plus $V(x)$. So, this Hamiltonian is therefore, set to operate on the wave function and the result of that operation of this second derivative operator on the wave function is for us to get the wave function back with the energy as its factor.

So, the solution to the Schrodinger equation therefore, yields what are known as Eigen functions that is; functions that give us exact solutions to the Hamiltonian operator and Eigen energies that is the exact energies that such a quantum mechanical system would have. So, what one typically does in quantum mechanics is to solve the time independent Schrodinger equation for a known potential. For example, you may have a constant potential, you may have a potential such as; the hydrogen atom where it is the central potential, you could have a simple harmonic oscillator where you have a corresponding potential for V and so, on.

Therefore the primary object of quantum mechanics is to solve the Schrodinger equation for a given potential. And sometimes of course, you actually approximate a potential in order to be able to solve a physical problem as often happens.

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Particle in a Constant Potential

$V(x) = V$. The S.E. becomes

$$\Rightarrow -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V \psi(x) = E \psi(x)$$

$$\Rightarrow -\frac{\partial^2 \psi(x)}{\partial x^2} = \frac{2m(E-V)}{\hbar^2} \psi(x)$$

Solution: $\psi(x) = A e^{ikx}$ with $k^2 = \frac{2m(E-V)}{\hbar^2}$

Note: k is real or imaginary (complex) depending on whether $E > V$ or $E < V$.

Now, let us consider a particle in a constant potential that is V is equal to V , it is not space dependent, then the Schrodinger equation is simplified you have minus \hbar square about $2m$, $\Delta^2 \psi(x) + V \psi(x) = E \psi(x)$. It is rearranged this way, where you have the second derivative that is equal to the wave function multiplied by a constant; E is a constant to be found, V is the potential and these are m and \hbar are constants for a given particle.

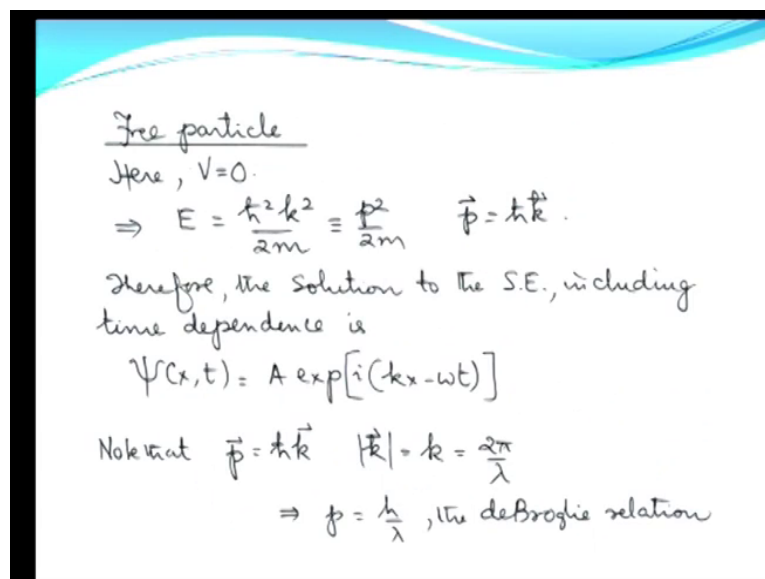
The solution for this is straight forward as long as for example, in this case the solution is $A e^{ikx}$; where k is given by $k^2 = 2m(E-V)/\hbar^2$; so this is a simple sinusoidal function. So, what we have a solution for the motion of the particle is through the wave function $\psi(x)$, which is the sinusoidal function. That is the motion of a quantum mechanical particle in a constant potential that is time independent, position independent is just a sinusoidal wave.

Now k as you see here is related to the potential and the mass of the particle. Now k into x because it is in the exponent kx is dimensionless; therefore, k must have a dimension that is the inverse of the dimension of x and its position. Therefore, this is the; so called reciprocal vector; x is the real vector real space. So, this k belongs to the reciprocal space

which you would have come across for example, in x ray diffraction.

Now, looking at the form of the equation for k square; k is real or imaginary, depending on whether E is greater than equal to V or is greater than V or E is less than V. So, the motion of the particle therefore, depends on the relative value of the energy that the particle may have with respect to the constant potential in which it is moving. A simple case of the constant potential is where V is equal to 0; in that case E is you can see here from this equation; if v is equal to 0, then e is equal to h bar square k square over 2 m.

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The image shows a slide with handwritten text and equations. The title is "Free particle". Below it, it says "Here, $V=0$ ". Then it shows the equation $E = \frac{\hbar^2 k^2}{2m} \equiv \frac{p^2}{2m}$ and $\vec{p} = \hbar \vec{k}$. Next, it says "Therefore, the solution to the S.E., including time dependence is" followed by the wave function $\Psi(x,t) = A \exp[i(kx - \omega t)]$. Finally, it states "Note that $\vec{p} = \hbar \vec{k}$ $|\vec{k}| = k = \frac{2\pi}{\lambda}$ " and " $\Rightarrow p = \frac{h}{\lambda}$, the deBroglie relation".

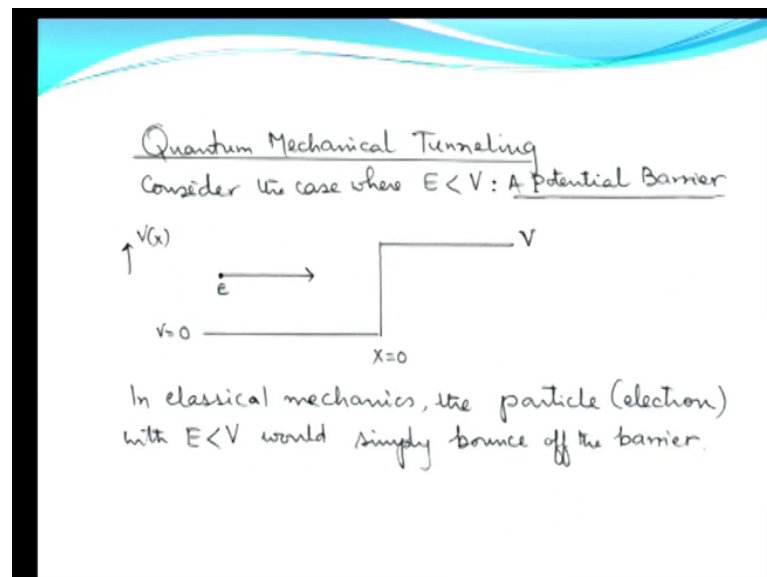
So, in such a case you have a simple expression for energy and if energy is also written as p square over 2 m, where p is the momentum; we can then see that p the momentum can be written as h bar k. So, there is a direct relationship between the momentum of the particle and the wave vector of the particle or the reciprocal vector of the particle.

Now recall that in the earlier case, where we have a time independent Schrodinger equation $\psi \times t$ is ψ into exponential E to the power of minus i into E by h bar t; e by h bar is just omega. So, what we have is $\psi \times$ into t x t is equal to $\psi \times$ into E to the power of minus i omega t. So, we bring that over here to write the general solution for the Schrodinger equation for a particle with moving under zero potentials; so called free particle.

So, you have the space dependent part which is A e to the i k x; a sinusoidal function with respect to space and the time dependent part is also sinusoidal. Therefore, the wave

function of a free particle has the form of a wave both in time and space. Now note that p is equal to $\hbar k$ and k is equal to actually $2\pi/\lambda$ and therefore, what you get is p is equal to $\hbar h/\lambda$ which is the de broglie relationship; so, everything is consistent.

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We can proceed next to dealing with the very important concept of quantum mechanical tunneling, which is an illustration of the solution of the problem of a particle with energy E ; that is trying to surmount a barrier of potential V ; V being greater than E . So, that is represented in this diagram; so, a particle is moving towards a potential barrier whose height. So, to speak is greater than the energy that the particle processes.

The barrier is erected at x equal to 0; now in classical mechanics this particle let us say an electron with energy E that faces a potential barrier of V greater than E ; would simply bounce of the barrier that is think of this is a projectile, it comes here finds the barrier cannot surmount the barrier. So, it just gets back; goes back considering that you have an elastic collision. Now what this quantum mechanics tell us about what happens in such a case.

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The Potential Barrier

But QM imposes boundary conditions that lead to a solution different from the "classical" one.

The Boundary conditions are

(a) ψ is continuous across the barrier

(b) $\frac{\partial \psi}{\partial x}$ is continuous across the barrier.

To the right of the barrier,

$$k = \sqrt{\frac{2m(E-V)}{\hbar^2}} = i \sqrt{\frac{2m(V-E)}{\hbar^2}} \Rightarrow \psi = e^{-Kx} = \psi(x)$$

where K is positive

\Rightarrow exponential decay of ψ .

Now, quantum mechanics imposes boundary conditions that lead to solutions different from the classical one. Now, what are the boundary conditions? That is remember what you are dealing with in quantum mechanics are solutions in the form of the probability amplitude namely the wave function. In such a case, what should really happen with respect to the solution? What are the conditions that the solutions should satisfy?

The boundary conditions are ψ is continuous across the barrier; that is if you take the barrier, if you take the wave function just to the left of the barrier and a wave function just to the right of the barrier, they should be continuity. In other words you are thinking about continuous function as in the case of mathematical analysis. So, I want analytical continuity for the wave function for values of x just less than 0 and just greater than 0.

And also the derivative of the wave function should also be continuous across the barrier; that is once again the derivative of ψ with respect to x to the left of the barrier should be the same as a derivative just to the right of the barrier. So, we are talking amount continuous ψ as well as continuity in this first derivative of ψ . So, these are the conditions that a quantum mechanical solution should satisfy.

Now, why these conditions? Why these conditions is that; suppose the wave function was discontinuous at the barrier at x equal to 0. Suppose the first derivative of the wave function was discontinuous at x equal to 0; that is there is sudden jump in ψ across this barrier and there is a sudden jump in the derivative of ψ across this barrier. What that implies is that, you would have to provide; since the derivative for example, can be infinite

across the barrier because that is the second derivative becomes infinite if the first derivative discontinuous and the first derivative becomes infinite if the wave function is discontinuous at this boundary.

Now such discontinuities are singularities really mean that there must be some large amount of energy infinite amount of energy that would be responsible for such discontinuities. In real physical situations, that are not the case therefore, the boundary conditions for the solution of the problem would be typically that ψ is continuous across the barrier and the first derivative of ψ is continuous across the barrier.

Now, one thing I forgot to say along the way is that the Schrodinger equation as we have written here is a second order differential equation. Now because it is a second order differential equation, the solution to that or the integration of the equation to get solutions would involve two constants. So, you have to determine two constants to have complete solution for the second order differential equation. And those two constants would then be determined by these boundary conditions that we just defined.

That is our two boundary conditions that the solution must satisfy and there are two constants should be determined. Therefore, it is possible using these conditions to determine the solutions to the Schrodinger equation uniquely. Now, let us look at the case of the barrier height being greater than E ; then k is equal to square root of $2m(E - V)$ divided by \hbar square. Now E is less than V therefore, what we now have is an imaginary quantity. So, k is now an imaginary quantity; i into square root of all this.

Therefore, the solution to the Schrodinger equation which if you remember this spatial part of it is just E to the $i k x$ that solution now has A into ψe to the $i k x$; now you have a an imaginary quantity multiplied by i , so that becomes a real quantity. Therefore, what you have is the solution for x as A into ψE to the minus; κx where κ is the quantity in the square root; it is a real quantity.

So, what you have is not a sinusoidal wave function for the solution, but you have an exponentially declining because k is positive, what you have is an exponentially decaying function. So, when you have a particle going across a barrier of this art then what you have is a case where; over here where E is less than V , you have sinusoidal variation for the solution.

But across the barrier because of continuity conditions, it falls exponentially down on the

other side. So, you have an exponential decay of the wave function on the other side of the barrier that is; x greater than 0. Now remember that in classical mechanics, the chance of this particle being on the side of the barrier is 0. The fact that the wave function is non zero on this side, even if it is exponentially declining; it means that there is a finite probability, the wave function is essentially square root of probability as we said because probability is given by ψ^2 .

Therefore, a non zero value of the wave function on this side of the barrier means that there is a non zero probability of the particle being here. So, this phenomenon where in quantum mechanics a particle with what would be an insufficient energy in classical mechanics is able to surmount a barrier that is larger than its energy; this is called tunneling, which is a very very important part of quantum mechanics.

There are actually devices that operate on the concept of tunneling and there are very important measurement instruments, you would have heard about the scanning tunneling microscope the STM, which actually opened the era of nano sciences, nano technology, so that depends on the concept of tunneling.

So, this arises from the Schrodinger equation and the boundary conditions that are necessary to be imposed on realistic physical systems that obey quantum mechanics. So, we will stop here and we will continue next time after reviewing these concepts, but before we leave for the day; what I would like to say is that we have tried to over here introduce the basic concepts of quantum mechanics. Some of the basic concepts I should say because we are not come to a couple of others. And use that to tell us how the motion of a particle in a quantum mechanical system is to be calculated; the Schrodinger equation. And a simple example of the Schrodinger equation almost to the first example that gives us a; an unusual result, a characteristic result of tunneling which is a very important part of quantum mechanics.

Thank you.