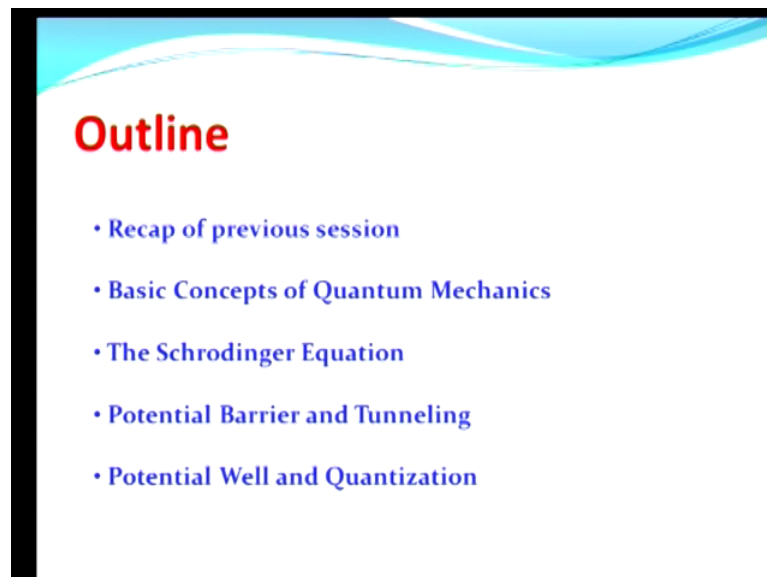


**Nanoelectronics: Devices and Materials**  
**Prof. S. A. Shivashankar**  
**Centre for Nano Science and Engineering**  
**Indian Institute of Science, Bangalore**

**Lecture - 33**  
**Basic Principles of Quantum Mechanics Contd.**

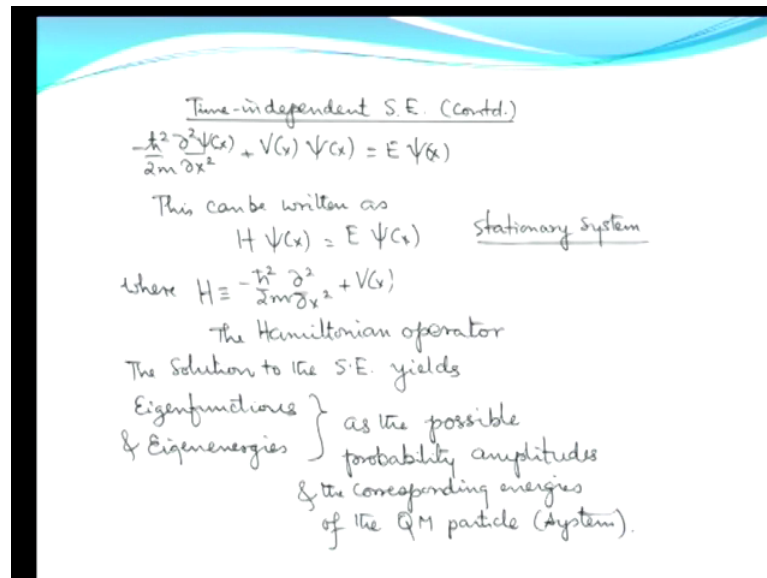
Hello. This is lecture three in this segment of a course on Nanoelectronic Device Fabrication and Characterization. And to recall this part recourse deals with nanomaterials and nanosystems and tries to understand how to deal with them.

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Now in the last session we were introduced to basic concepts of quantum mechanics, the Schrodinger equation and the concept of a potential barrier and we began to work with tunneling concepts and we will continue with that, and then we go and gone on through so called potential well and quantization of energies, that will be the agenda of today.

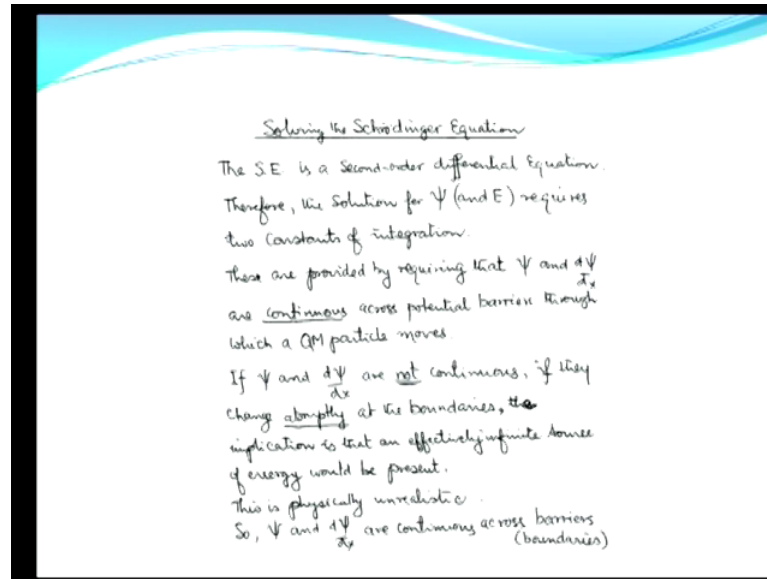
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Now, to come back to the basic precept of quantum mechanics namely the time independent Schrodinger equation, as we said yesterday it is a second order differential equation where psi represents the probability amplitude of the so called wave function that describes the motion of a particle in a quantum mechanical system.

The Schrodinger equation can be written as an operating equation as we said yesterday, where H is the Hamiltonian operator which is given by minus H square by 2 m delta square by delta x square plus V x where V is the potential that is a time independent potential and the solution of the Schrodinger equation yields the so called Eigen function, which are solutions to the equation and the corresponding values of energy which are Eigen values of energy. These are the possible probability amplitudes and the corresponding energies and therefore, the probability of finding a particle at a position x, then would be given by the probability integral namely is  $\int_0^\infty \psi^* \psi dx$  integrated over space that should give you unity and the probability itself is given by the product  $\psi^* \psi$  square modulus.

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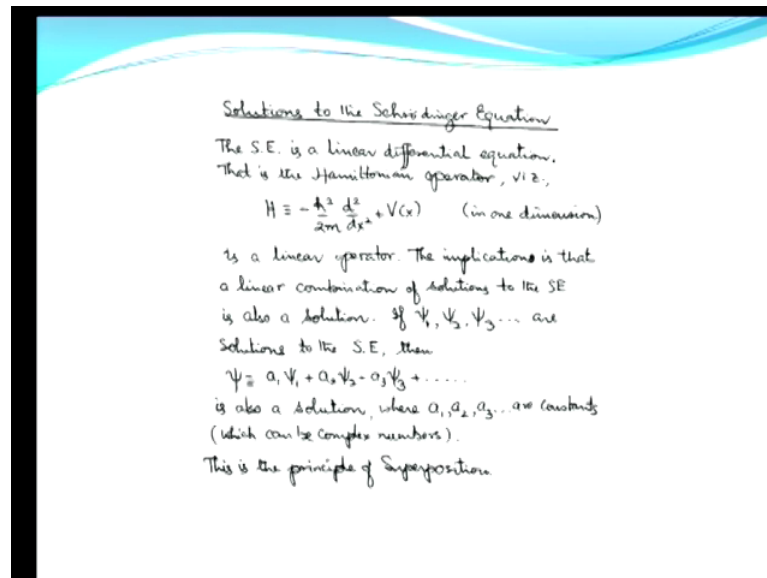


Now to repeat the Schrodinger equation is the second order differential equation therefore, a solution for psi requires 2 constants of integration and these are provided by requiring that both psi and the first derivative of psi or continuous across of any potential barrier through which a particle might be moving.

Now again to repeat what I have said yesterday psi and d psi by d x that is the first derivative, if they are not continuous if they change abruptly at a boundary, then the implication is that effectively infinite sources of energy might be required and this is of course, physically unrealistic. Therefore, the requirement for solution uses the boundary conditions that psi is continuously across a boundary as well as the first derivative of psi is continuous that gives us 2 constants of integration which allow us to solve for psi exactly.

So, this is the basic principle of solving the Schrodinger equation in the time independent case.

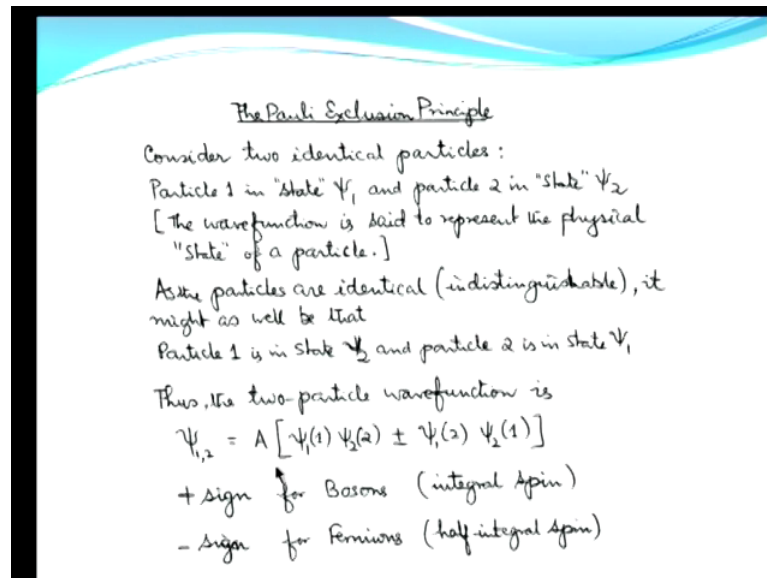
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Now let us look at it further, the Schrodinger equation is a linear differential that is the Hamiltonian operator which we have just shown here in one dimension is a linear operator. The implication is that suppose you have solutions  $\psi_1, \psi_2, \psi_3$  which satisfy this second order differential equation, then a linear combination of  $\psi_1, \psi_2, \psi_3$  such as  $a_1 \psi_1 + a_2 \psi_2 + a_3 \psi_3$  would also be a solution of the second order differential equation. Where these constants  $a_1, a_2, a_3$  etcetera can actually be even complex numbers, because what is really physically meaningful is only the square of the probability amplitude. And therefore, you can have the quantities like  $a_1$  to be complex.

Now, this is called the principle of superposition and that is applicable to all kinds of wave motion and so on. So, essentially is characteristic of a second order differential equation that is a linear differential equation. So, the principle of superposition allows us to construct various possible solutions out of the linear combination of the solutions that we might find to the Schrodinger equation.

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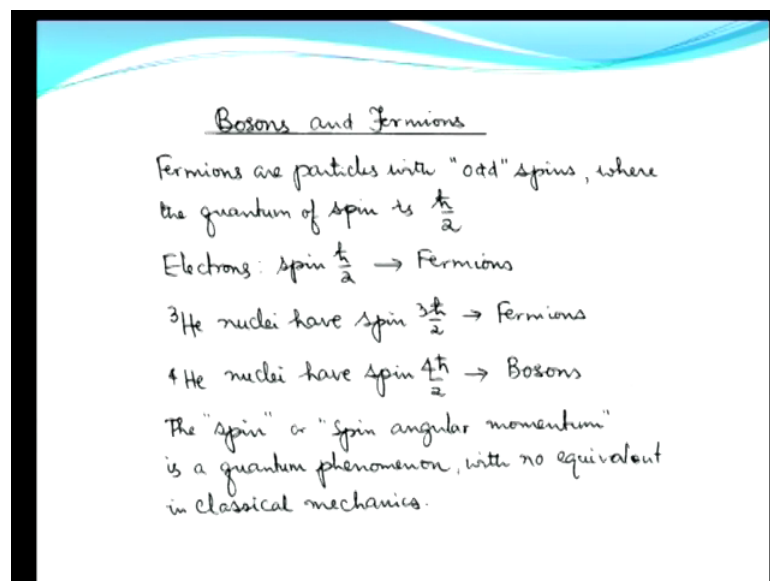
Now having dealt yesterday with some of the basics of the quantum mechanical principles, now we come to another very important quantum mechanical principle that you would have heard of namely the Pauli Exclusion Principle. Yesterday we dealt with the Heisenberg's uncertainty principle and the Pauli exclusion principle is another very important part of quantum mechanics. Now consider 2 identical particles let us say 2 electrons, particle one is in state  $\psi_1$  that is this is a particular jargon of quantum mechanics  $\psi_1$  for example, depends on the position of the particle in one dimension. So, in a particular for a particular value of the position then you call the particle as be in a state  $\psi_1$  where  $x$  for example, has a particular value.

So, we call particle one to be state  $\psi_1$  and particle 2 to be state  $\psi_2$ , now as these 2 particles are identical and they are indistinguishable, it might as well be that particle one is in say state  $\psi_2$  and particle 2 is in state  $\psi_1$  you cannot tell between those 2 particular possibilities. Thus the 2 particle wave function if you had one particle the wave function is  $\psi_1$  if you have 2 particles then you have a product of those 2 functions  $\psi_1$  and  $\psi_2$ . So, the 2 particle wave function in this case can be written either as  $\psi_1 \psi_2$  plus that is  $\psi_1$  particle one in that state  $\psi_2$  with particle 2 in that state and  $\psi_1$  with particle 2 in that state and  $\psi_2$  with particle one in that state as shown here.

Now, this is a linear combination as we have just said linear combinations are valid wave functions, but you can either have a plus sign for the linear combination here or a minus sign for the linear combination. It comes out that whether there is a plus sign or a minus sign in such a case where we are considering identical particles describing the states of an identical particle or set of identical particles it makes the big difference whether there is a some of this and are a differences of these two; these two terms the plus sign corresponds to.

So, called bosons and the negative sign correspond to so called fermions. Bosons have integral spin this spin quantum number is a very special quantum mechanical property of particles. So, if this spin is integral then it is a boson, if this spin is half integral then it is a fermion you would have learned about in your earlier classes.

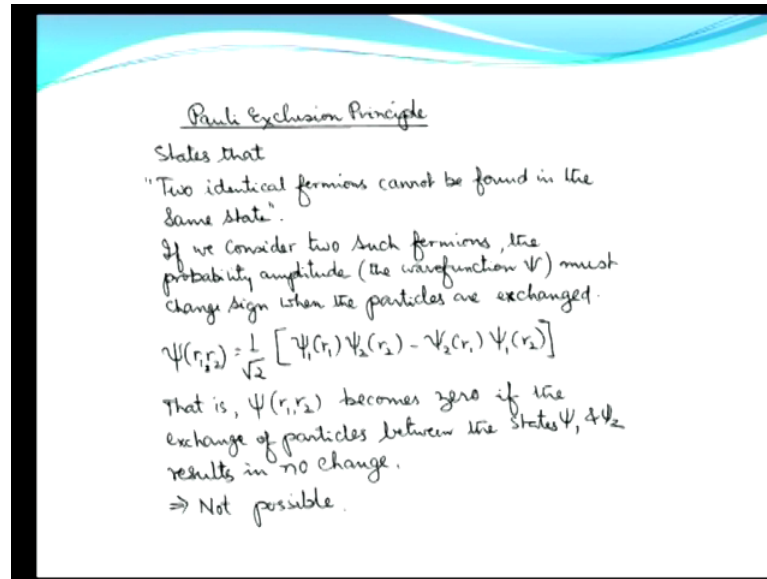
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So, we have bosons and fermions particle particles therefore, with odd spins where the where is quantum of spin is equal to  $\frac{h}{2}$ . So, if there is an odd multiple of  $\frac{h}{2}$  for a particle that is if the spin angular momentum of a particle is an odd multiple of  $\frac{h}{2}$  then it is a Fermion.

An example is electron of course, a famous example whose spin is equal to  $\frac{h}{2}$  electrons are fermions helium 3 nuclei are also fermions this spin there is  $\frac{3h}{2}$ , whereas helium 4 helium 3 is an isotope of helium the normal isotope is  ${}^4\text{He}$  I mean helium four. So, this nucleus is a spin of  $2h$  and therefore, it is a boson.

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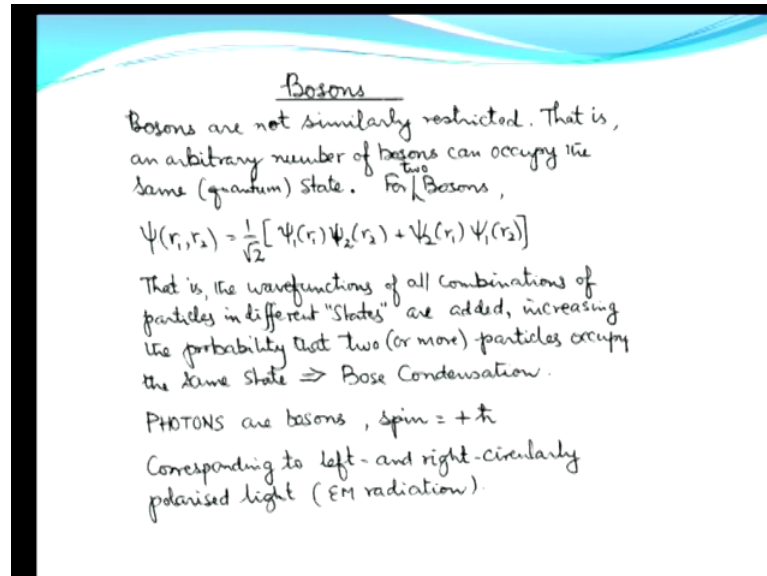
Now, as I said momentum ago this spin or spin angular momentum is a quantum mechanical phenomenon property, quantum mechanical property with no equivalent in classical mechanics. Now the Pauli exclusion principle states that 2 identical fermions cannot be found in the same state, that is the broad general statement of the Pauli exclusion principle. If we consider 2 such fermions with the probability amplitude then the probability amplitude must change sign when the particles are exchanged that is we have written here, the wave function for this 2 particle system as we have said in previous slide.

So, if you have this negative sign between these 2 terms these 2 product terms of wave functions, then you have fermions as you have said. Now you can see by the form of this particular wave function that if you exchange these 2 that is if  $\psi_1 r_1$  is same thing as  $\psi_2 r_1$  then the product becomes 0 rather the factor become 0 the 2 factors in the sum they can cancel each other therefore, the wave function becomes identically 0.

So, if there is an exchange of particles between  $\psi_1$  between the states  $\psi_1 \psi_2$  then you have a 0 wave function and therefore, this is not possible and that means, that the Pauli exclusion principle statement that 2 identical particles 2 identical fermions cannot be found in the same state reduces to mathematically this statement that the wave function should be of this kind of this particular form and if you exchange those particles then you would if they are in the same state then the wave function  $\psi_1 r_1 r_2$  is 0 and

that is not possible. So, that is the mathematical statement of the Pauli Exclusion Principle.

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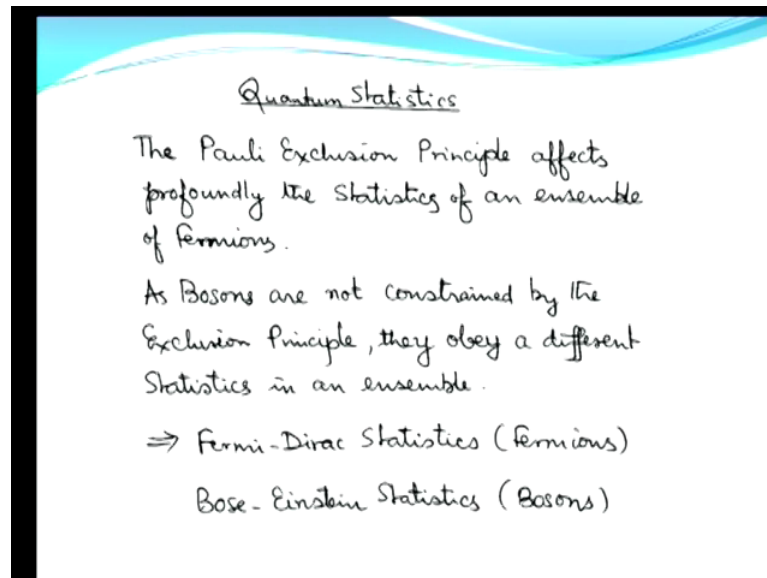


Bosons on the other hand those that have integral off spins are not similarly restricted; that is an arbitrary number of bosons can occupy the same quantum state for 2 bosons the wave function is the sum of these 2 terms as we have discussed earlier and of course, there is no way this is going to be 0 under these conditions. Therefore, wave functions of all combination of particles in different states are added which means that there is an increasing the probability of 2 or more particles occupying the same state and this is the phenomenon of Bose condensation, which is observed at very low temperatures among other conditions.

Now, it is important to remember that apart from helium 4 which is an example of a boson as we just mentioned, bosons the most important class of particles which are bosons or photons we do not think of photons as having spin, but this spin for photons is actually plus or minus  $\hbar$  sorry there is a slight error here is plus or minus  $\hbar$  corresponding to the left and right circularly polarized light, we know of polarized light, but that is the equivalent of a spin for the photon.



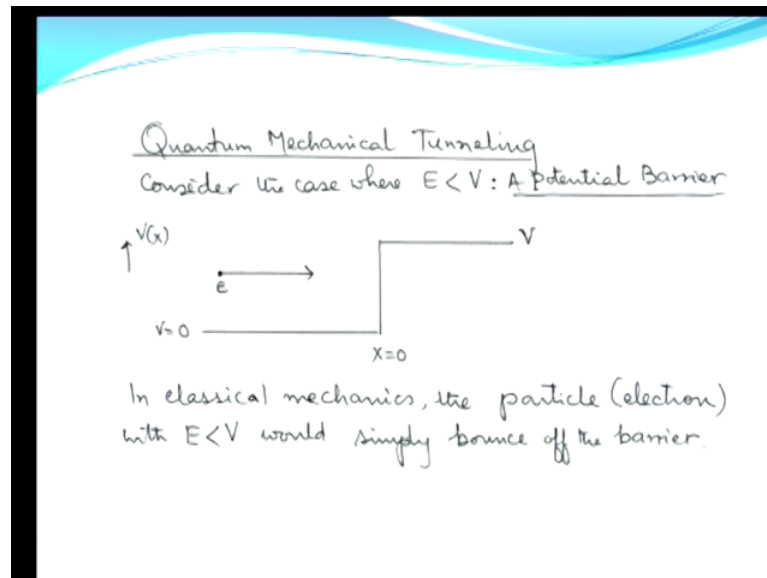
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Now, one aspect that I mention in very first lecture is the statistics of nano systems. Now when you are dealing with quantum particles then one has to formulate quantum statistics to deal with such particles on some of such particles. From the statement of the Pauli exclusion principle that we just went through it is clear, that the Pauli exclusion principle affects profoundly the statistics of an ensemble of fermions because after all no 2 fermions occupy the same state, whereas such as restriction or a constraint does not apply to bosons therefore, one can see from here although elaboration is necessary and we will try to attempt that later on, the statistics for ensemble of bosons and fermions have to be different because of this fundamental difference between the bosons and fermions namely the fermions have to obey the Pauli exclusion principle.

As a result quantum statistics is divided into 2 parts, namely Fermi-Dirac statistics which describes fermions, Bose Einstein statistics that describes bosons we will return to that in a later part of this segment.

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That is come back to what we are dealing with yesterday in the previous class that is namely quantum mechanic tunneling where we have said that we have particle with an energy  $e$  which is less than a potential barrier  $v$  that it encounters in its motion.

So on the left of this diagram for  $x$  less than 0 we have a particle moving with the energy  $e$  and to the right is a potential barrier of height  $v$  which is greater than  $v$ . As we said yesterday under these conditions the particle of the electron let us say in this case with energy  $e$  less than  $v$  would simply bounce off the barrier, it will come back that is going forward this way and then it will just bounce back and go back along the negative  $x$  direction because it cannot among the barrier.

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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)  $\psi$  is continuous across the barrier

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

To the right of the barrier,

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

where  $\kappa$  is positive

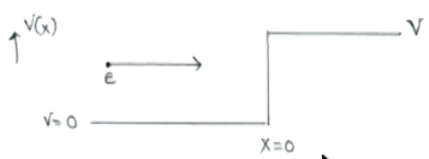
$\Rightarrow$  exponential decay of  $\psi$ .

Now what we did yesterday was to consider this as a quantum mechanical problem and in the solution to the Schrodinger equation, we found that the solutions are in the form of  $e^{-ikx}$ , but in this case  $k$  which is defined as square root of  $2m(E-V)$  or  $\hbar^2$  this becomes a complex number imaginary number.

Therefore the wave function  $e^{-ikx}$  really becomes now a real function because  $k$  itself is complex and therefore, what we have is  $A e^{-\kappa x}$  where  $\kappa$  is a real number therefore, what you have is an exponential decay of the function on the other side of the barrier that is.

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Quantum Mechanical Tunneling  
Consider the case where  $E < V$ : A Potential Barrier



In classical mechanics, the particle (electron) with  $E < V$  would simply bounce off the barrier.

You have here a sinusoidal function as the wave function over here  $e$  to the minus  $ikx$  where as on this side what you have is an exponential decay, but still a real solution to the Schrodinger a wave equation.

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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

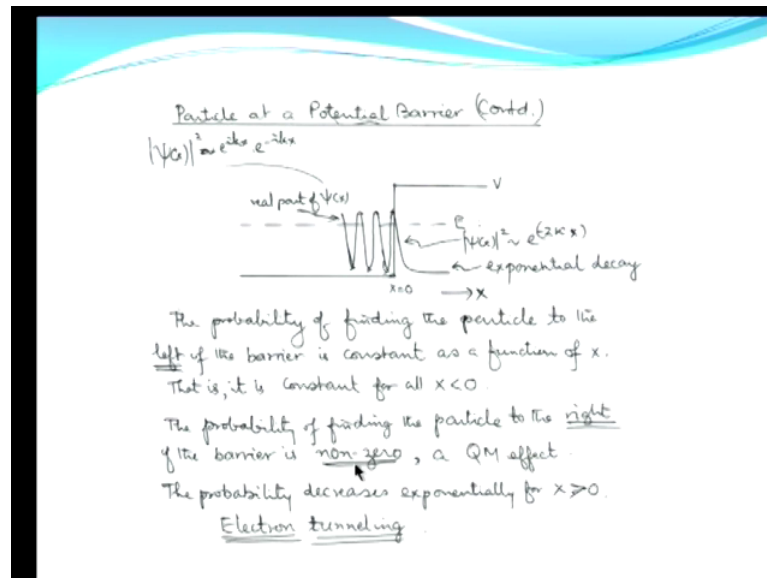
- (a)  $\psi$  is continuous across the barrier
- (b)  $\frac{\partial \psi}{\partial x}$  is continuous across the barrier.

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  $\psi$ .

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We can depict the solution to the problem of a potential barrier in the following manner namely on the left side the probability of finding the particle namely the psi square over here is just  $e^{ikx} + e^{-ikx}$ , which really is a constant therefore, the probability of finding the particle to the left of  $x = 0$  is constant as shown here.

Whereas, on other side psi now exponentially decaying function therefore, in quantum mechanics unlike in classical mechanics, this particle has its finite probability of being found in other side of barrier, but the probability of finding it goes down exponentially as the function of distance on the other side of the barrier. This phenomenon where by a particle with energy less than a potential barrier that encounters goes to other side with a finite probability is called tunneling.

In this case we are dealing with electrons we have electron tunneling and many phenomenon in quantum mechanics with practical applications depend on such tunneling phenomenon.

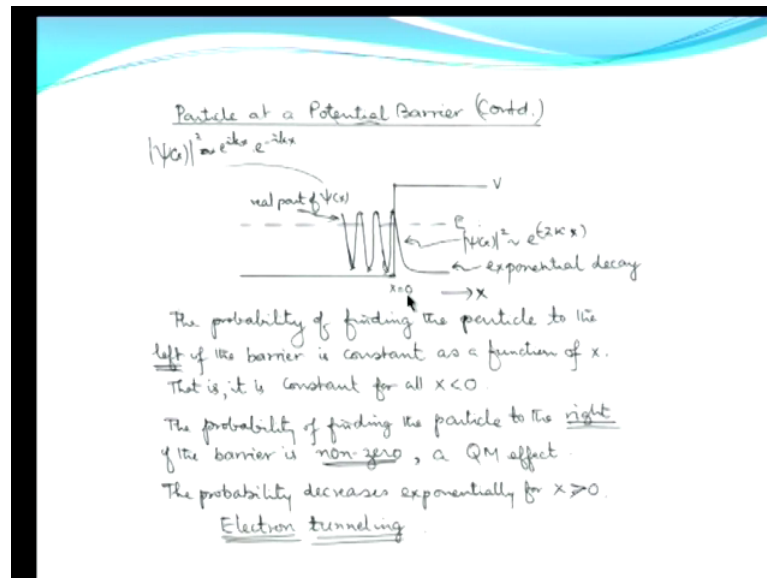
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Tunneling: An estimate  
To the right of the barrier,  $|\psi(x)|^2 = A^2 e^{-2\kappa x}$   
 $\therefore |\psi(0)|^2 = A^2$  &  $|\psi(\frac{1}{2\kappa})|^2 = A^2/e$   
 $\therefore$  The distance over which the probability falls to  $1/e$  of its value at the boundary is  $(\frac{1}{2\kappa})$ .  
Consider the work function of a metal, typically 5 eV.  
i.e.,  $V-E = 5$  eV  
 $\kappa = \sqrt{\frac{2m(V-E)}{\hbar^2}}$   
By substituting the numbers, we get  $\kappa = 1.14 \text{ \AA}^{-1}$   
i.e.,  $\frac{1}{2\kappa} = 0.45 \text{ \AA}$ .  
This gives an order of magnitude feeling for the electron tunneling process.

Can we have a estimate of the distance or which tunneling takes place. Now as we said to the right side of the barrier the probability is the square of the wave function namely a square e to the minus 2 kappa k a 2 kappa x, for x equal to 0 then therefore, this probability is a squared on the other side let us take a value of x equal to 1 or 2 kappa.

So, we are just want to equate x equal to 1 or 2 kappa, when we do that the probability for that distance is equal to A square divided by e that is at x equal to 0 the probability is a square and that x is equal to 1 over 2 kappa then the probability is A square divided by e. So, the distance over which the probability falls to one over e of its value at the boundary is one over 2 kappa.

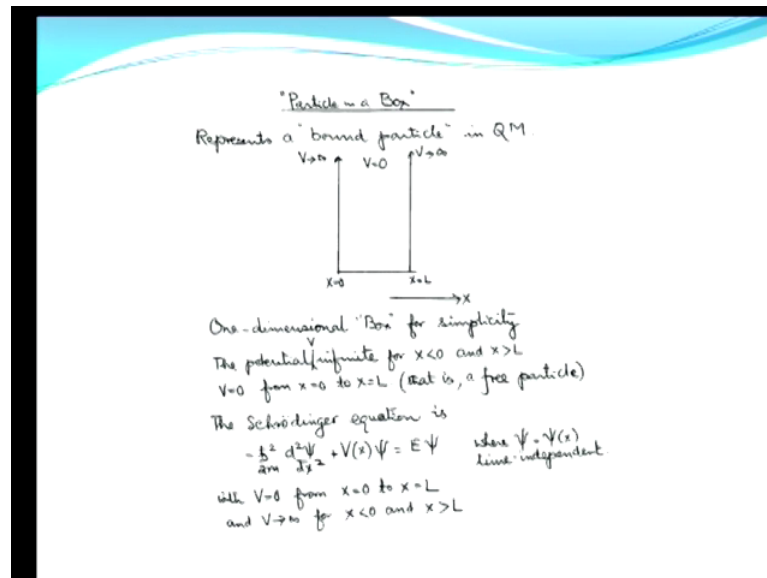
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Now, actually the problem of the potential barrier is a very important problem for example, a very common problem 2, you have electrons in metals so called free electrons. The electrons are bound to the metal and they cannot come out because there is something on is something you would have learned about it as the work function you have to provide so much energy for the electron to come out of the metal, but even if you do not provide that kind of energy, there is a finite probability for the electron to tunnel out of the metal and this estimate over here suppose you take a metal of work function 5 electron volts, then using these numbers here using these equations where kappa is given by this equation and substituting the value for the mass of the electron and so forth and  $V$  minus  $E$  is equal to 5 electron volts, then you can find that  $1/2\kappa$  is 0.25, 4 5 angstroms.

That gives an a feeling for order of magnitude of the distance on which electron tunneling can take place in such a common case of free electrons in a metal. So, it is generally negligible although as we show later, this tunneling of electrons out of a metal is actually the basis of development of the scanning tunneling microscope we will return return to that later.

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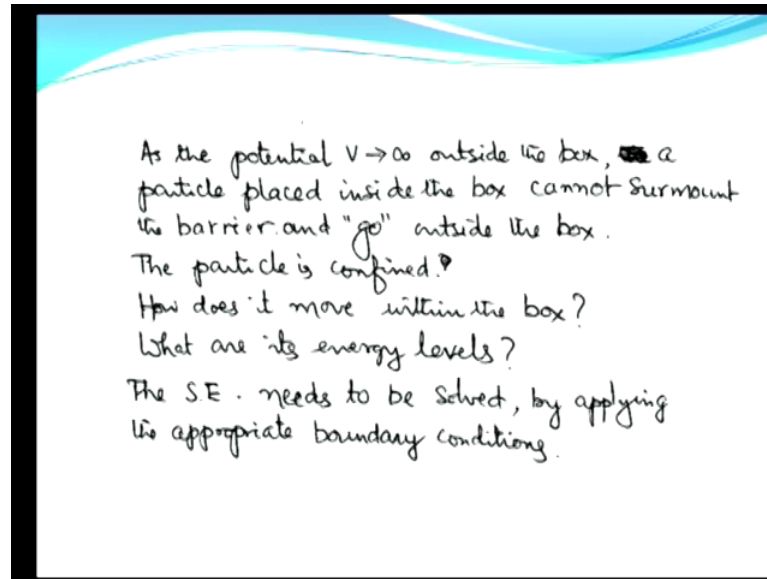


Let us now come to a problem a very well known basic problem called the particle in a box problem in a quantum mechanics. It is a colloquial way of representing a problem whereby you have a particle that is boxed what is meant by that? It is there is no potential within the box, but the box has walls of course, and those walls are infinitely high. So, we can think of the infinitely high barrier or an infinitely deep potential well in which the particle is situated. So, this diagram represents the is a schematic diagram of where you have particle in a box the potential is 0 inside the box.

Now, Schrodinger equation then is becomes simple because  $V$  is equal to 0 from  $x$  equal to 0 to  $x$  equal to  $L$ , and  $v$  is infinite outside these boundaries. So, we have to solve the Schrodinger equation to find the solutions for the problem namely what are the energy levels that the electron would assume if it is an electron that is confine to this potential well.



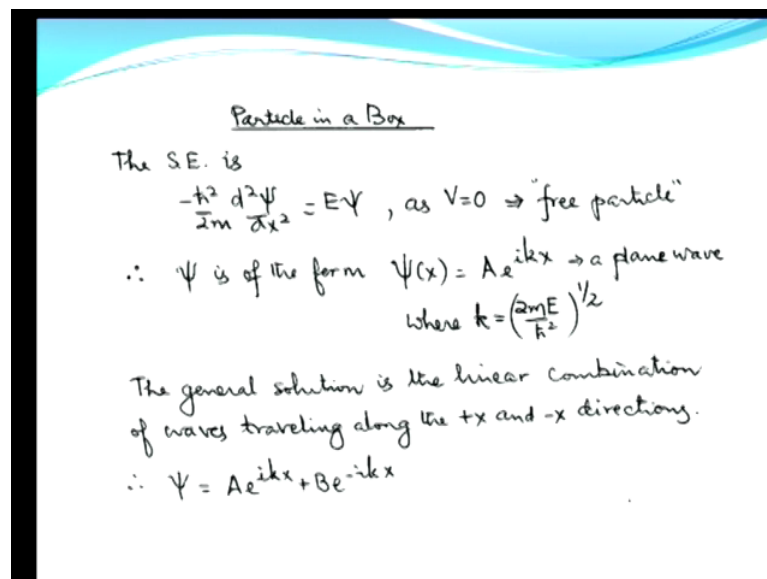
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Now, the barrier is infinitely high and therefore, the electron cannot go outside the box. So, the particle is confined how does it move within the box what are the energy levels of the particle within the box.

To do this of course, to know this the Schrodinger equation is resolved by applying the appropriate boundary conditions.

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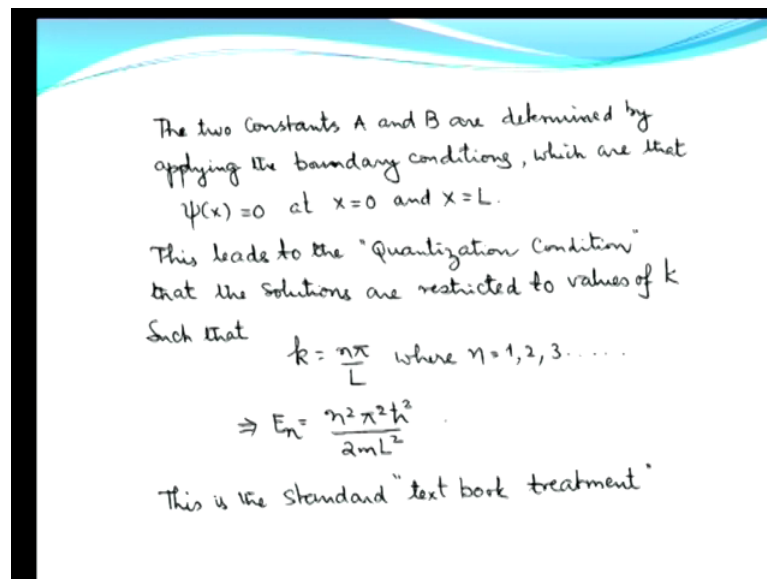


The Schrodinger equation for the particle in the box is simplified because  $v$  is equal to 0 and that equation is shown here, this is the simple equation for which we have already is

obtained the solution because it this so called free particle. In the previous session we showed that this solutions are of this form  $\psi(x) = A e^{ikx}$  which is a plane wave and  $k$  is given by this equation is related to the mass and the Planck's constant, this is really just a re statement of  $E = \hbar^2 k^2 / 2m$ . So, that is the equation from which this one comes.

So, now that is recall what is I said while ago, namely the general solution is a linear combination of waves travelling in the positive and negative  $x$  directions  $e^{ikx}$  is a solution  $e^{-ikx}$  is also a solution therefore, that general solution is a linear combination of  $e^{ikx}$  and  $e^{-ikx}$  and there are 2 constants  $A$  and  $B$ . Now remember this is a second order differential equation therefore, there are 2 constants and as we said earlier you can solve for these things by using the boundary conditions of where  $\psi$  is continuous and  $d\psi/dx$  is also continuous at the boundaries. So, this is the sort of the text book problem for solving the Schrodinger equation.

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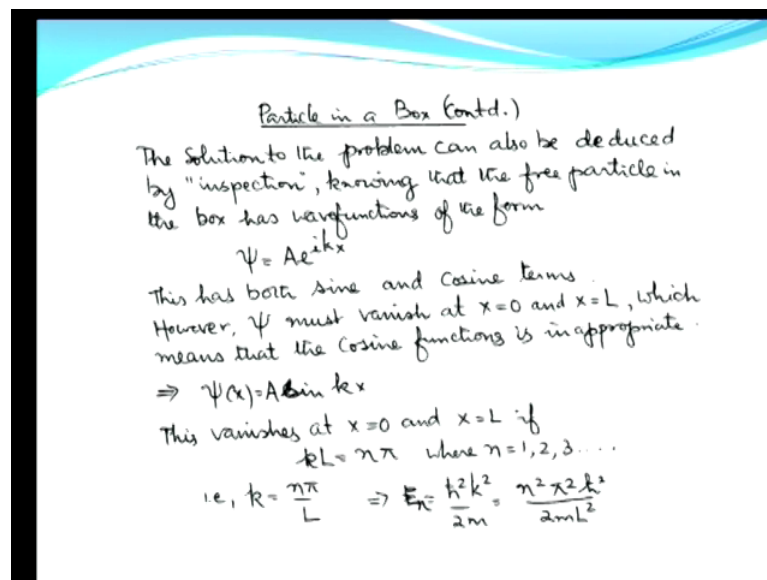


Now, one can go through the algebra of determining the constants and so on and as I said this is a text book problem, what the solutions comes out to be is that there is quantization that determines a solution, there is a quantization condition that is a solution are restricted to values of  $k$  such that  $k$  is equal to an integral multiple of  $\pi$  divided by  $L$  or  $k$  is equal to  $n\pi$  divided by  $L$  where  $n$  is equal to 1 2 3 etcetera integral numbers

positive integral numbers. Now let us note that  $k$  is inverse length over here one over the length and therefore, it is a so called reciprocal length or reciprocal wave vector.

Now, from the equation  $e$  is equal to  $\hbar^2 k^2 / 2m$  we get therefore, that the energy of the particle can have in this box is equal to  $E_n$  is equal to  $n^2 \pi^2 \hbar^2 / 2mL^2$ . So, as I said this is the standard text book treatment of the particle in the box, where one solves the Schrodinger equation and systematically obtains the solution.

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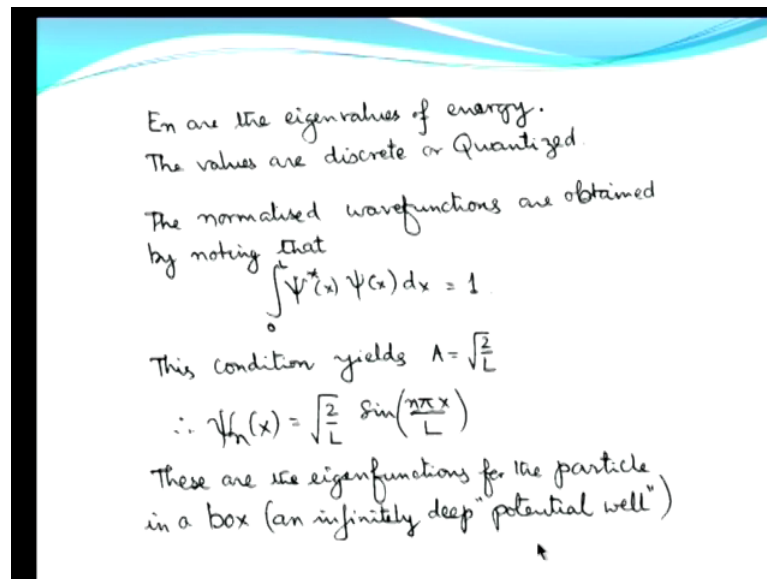


There is actually a simpler so called inspection method for knowing the solution let us say this is instructive. So, we can deduce the solution by inspection.

Knowing the free particle in the box has wave functions of the form  $\psi$  is equal to  $e^{ikx}$  as we already said. Now  $e^{ikx}$  has both sine and cosine terms, but remember that  $\psi$  must vanish at  $x$  equal to 0 and  $x$  equal to  $L$  which are the boundaries of the box. Now the cosine function is not appropriate here because the cosine function does not vanish at  $x$  equal to 0 therefore, we can limit our consideration to the function. So, we can write  $\psi(x)$  is equal to  $A \sin kx$ , where  $A$  actually is determined by the so called normalization condition that is, you integrate  $\psi(x)$  and multiplied by  $\psi^*(x)$  the complex conjugate over all of its domain from 0 to  $L$  and that gives you the condition that determines the value of  $A$  which is the normalization factor.

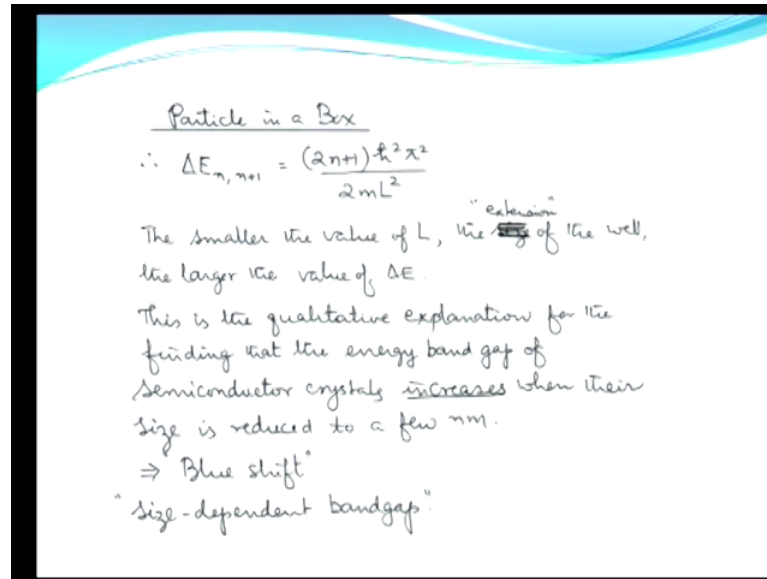
Now, coming back as you said only sinusoidal functions are valid solutions for this and you see that  $kL$  for example, this has to vanish at  $x$  equal to  $L$  therefore,  $kL$  must be equal to  $n\pi$  because this is sinusoidal function therefore, the quantization condition becomes  $kL$  is equal to  $n\pi$  where  $n$  is equal to 1 2 3 etcetera. So, we get the same answer  $k$  is equal to  $n\pi$  divided by  $L$  that can be obtained by a more elaborate treatment and of course, the Eigen values of energy are once again  $n^2 \times \pi^2$  over  $2mL^2$  square.

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So, these are the Eigen values of energy and see that these are discrete or quantized. The normalized wave functions as I said can be obtained by going through these integral where we integrate between 0 and  $L$  which is a domain of this particle and the quantization this normalization condition yields the constant to  $A$  the square root of 2 divided by  $L$  therefore, the wave functions or the Eigen functions of the particle in a box particle in a infinitely deep well are given by  $\psi_n(x)$  equal to square root of 2 by  $L$  sin  $n\pi x$  by  $L$  where  $n$  is integral.

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Particle in a Box  
 $\therefore \Delta E_{n, n+1} = \frac{(2n+1)^2 \pi^2 \hbar^2}{2mL^2}$   
The smaller the value of  $L$ , the <sup>"extension"</sup> ~~size~~ of the well, the larger the value of  $\Delta E$ .  
This is the qualitative explanation for the finding that the energy band gap of semiconductor crystals increases when their size is reduced to a few nm.  
 $\Rightarrow$  Blue shift  
"size-dependent bandgap"

Now, suppose you consider the difference in energy for such a particle in a box between 2 consecutive levels, as we are said here the energy levels are given by  $\hbar^2 \pi^2 n^2 / 2mL^2$ .

So, the value of  $e$  increases quadratically as the quantum number  $L$  as it is called this quantum number is gradually increased from 1 to 2 to 3 etcetera. So, if you take difference in energy between 2 consecutive levels namely  $n$  and  $n+1$  then that is given by  $(2n+1)^2 \hbar^2 \pi^2 / 2mL^2$ . Now notice that  $L$  is in the denominator therefore, the smaller the value of  $L$  that is the smaller the box the narrower the box then this you get a larger value for the  $\Delta E$  that is a difference between 2 consecutive levels is greater when the box is narrower. This is a sort of a qualitative I would not say explanation although I have put it down that way is a qualitative indication for the finding that the energy gap that in the semiconductors which you all heard of course, you have learnt in the earlier part of the course this course the energy gap of a semiconductors increases when the size of the crystal is reduced to a few nanometers.

So, if you take  $L$  to be a few nanometer then you can see that the difference in the energy levels of consecutive states is larger when  $L$  is smaller. So, this is. So, called blue shift in the band gap of semiconductors which are reduced in dimensions to nanometer levels we will come back to this in a more systematic fashion at a later time in this.

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**Examples:**

Consider an electron in different-sized “boxes”

1.  $L = 1 \text{ nm}$  ; then,  $E_n \approx (0.05)n^2 \text{ eV} \rightarrow E_5 = 1.25 \text{ eV} \ \& \ E_4 = 0.8 \text{ eV}$   
So, a transition from  $E_5$  to  $E_4$  will produce radiation in the infrared.
2.  $L = 1 \text{ cm}$ ; then  $E_n \approx (10^{-15})n^2 \text{ eV}$

That is, at macroscopic sizes of “confinement”, the energy levels , though “quantized”, are extremely low and very closely spaced UNLESS the quantum numbers (n) are large.

Note that, for  $E_n$  to approach one eV, n has to be of the order of  $10^7$ .

Now, let us consider some examples an electron in different sized boxes that is to illustrate the points I have just made.

Suppose L the size of the box is 1 nanometer, then you can do the arithmetic to find that  $E_n$  is given by  $0.05 n^2$  in electron volt units. If n is equal to 5 the energy Eigen energy is 1.25 eV approximately. If n is equal to 4 it is 0.8 eV. Now one point I want to once again note for you here which I forgot to mention is that the difference between successive energy levels of a particle in a box increases as n increases that is as the quantum number increases successive energy levels are separated by larger and larger differences of energy.

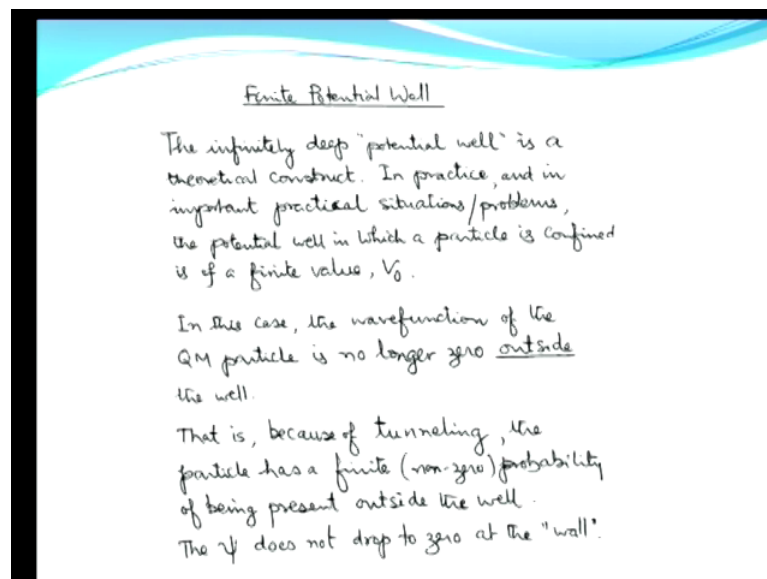
So, coming back to this particle in a box of one nanometer electron in a box one nanometer, the transmission from the level  $E_5$  level to level 4 produces radiation in the infrared because the difference in wavelength is about 0.65 eV which is in infrared. But suppose you have go to a macroscopic box one centimeter sized box which is really of physical experience, we have we have familiar with these sizes.

Then the same formula gives you that  $E_n$  is given by  $10^{-15} n^2$  in electron volt units, that is at macroscopic sizes of confinement so called confinement, the energy levels though they are quantized are extremely low and very closely spaced unless the quantum numbers are very large that is suppose n is a small number 1 or 2 or 3 or 10 something like that a small number, then you can see that  $E_n$  is

really very small in magnitude almost immeasurably small, but if the quantum number is large let us say order of 10 to the power of 7 then you begin to approach electron volt kind of differences in the energy.

Now, coming back to such a case where the energy levels are spaced very closely, but are still quantized as in the case of macroscopic object what you have here is quantization, but really extremely small differences between successive energy levels, this is the so called quazi continuous state of quazi continuous distribution of energies, where even though there is quantization is essentially impossible experimentally to learn that and that is really how Newtonian mechanics comes into play for large size object or macroscopic objects. We say in Newtonian mechanics that energy levels are continuous, but really what it is that these energy levels are quazi continuous they were so close to one another for microscopic objects that they in practice they are continuous.

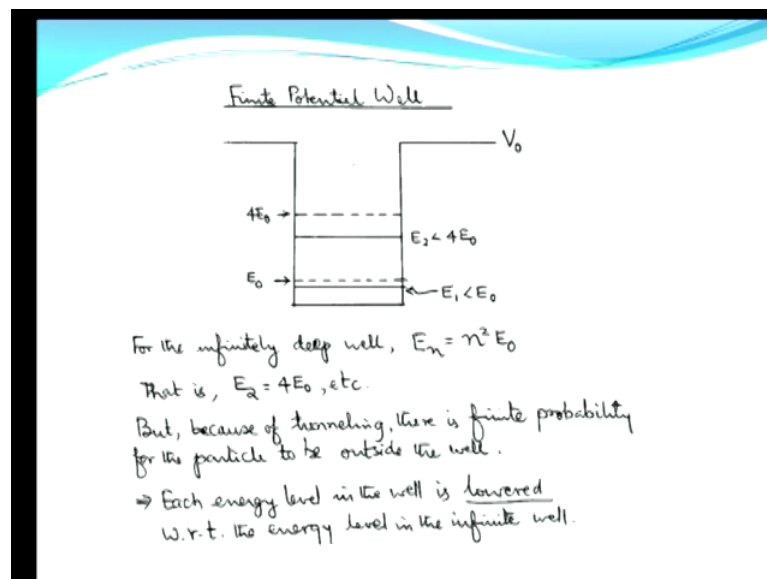
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Now so far we have dealt with the infinite potential well, the barrier is very large or infinite the particles simply cannot escape, but there is really a theoretical construct in practice and in practical situations and problems the potential well to which a particle is confined is of a finite height that is the potential well or the potential barrier has a height of  $V_0$ , which is not infinite its finite a few volts for example, as in the case of the work function of a metal.

Now what we learned earlier if you go back to the treatment of the potential barrier, we saw that in such a case you can have tunneling that spreads the wave function outside the barrier even though the barrier height is less than the energy of the particle. So, you can see that immediately when you have a finite potential well you can possibly have the wave function spread outside the barrier outside the well. And therefore, a finite potential well would be different from an infinite potential well because of the tunneling that makes the wave function outside the box finite.

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So, if actually one goes through such a finite barrier of height  $V$  knot.

Then the energy level diagram for such a case is altered slightly what is shown here is the dotted lines show the energy levels of the infinite potential well  $E$  naught the ground so called ground state to  $E$  4  $E$  naught because that is a next excited states because remember the energies are proportional to  $n$  square. So, if  $n$  is equal to 2 the energy is 4 times as much as that of the ground state.

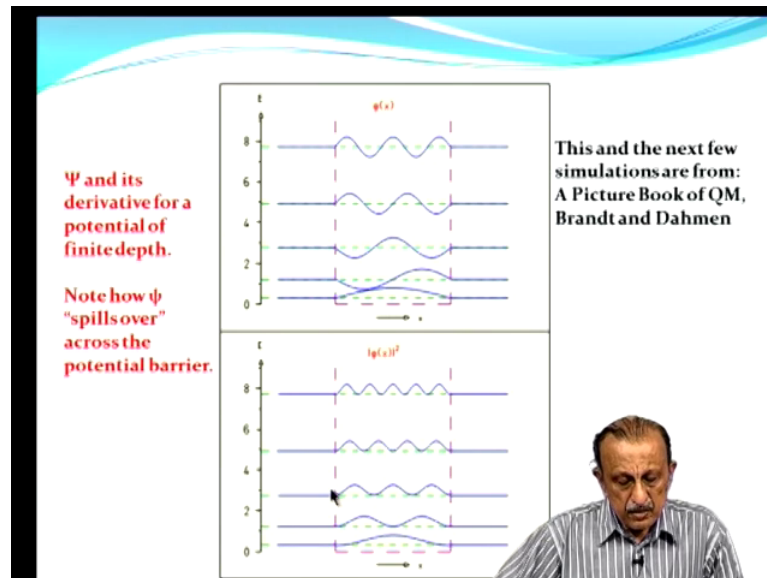
So, these dotted lines represent the energy levels of the infinite potential well when the potential is finite what I want to denote is that the resulting energy levels which one can compute through simulations is lower than the energy for the infinite well. Every energy level is diminished with respect to the infinite potential well the physical reason for that is that the wave functions spreads outside the barrier on both sides therefore, some of the



energy is dissipated outside and therefore, the energy of the particle inside the box is smaller than the energy would be for an infinite well.

So, each energy level is lowered with respect to the infinite well.

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Now, there is a very nice book called a picture book of quantum mechanics, in which the problems of the potential well and so forth are simulated through illustrate the basic and important aspects of quantum mechanics. What is shown here is the simulation of a potential well finite potential well sorry this one is simulation of infinite potential well where the wave functions for different values of the quantum number  $n$  equal to 1,  $n$  equal to 2,  $n$  equal to 3, 4 and 5 are all shown as you can see these are all sinusoidal functions.

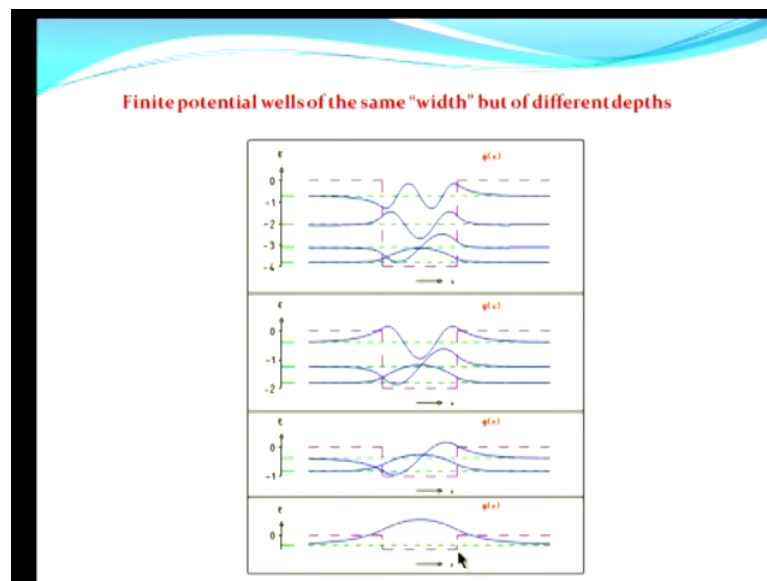
The first wave function is just a half sine wave; the second one is a full sine wave and then 3 halves 2 and 2 and half and so on. So, all of these are sinusoidal functions, these are the wave functions of the particle in an infinite box infinitely deep potential well. The bottom part of the simulation shows the variation in the probability of finding the particle at different part positions within the box remember that the probability is a square of the wave function.

So, this is the probability amplitude the wave function is the probability amplitude and this is the probability itself the modulus or the square of the wave function. So, what I

wanted to see here is that the probability for  $n$  equal to 1 varies considerably over this spreads from  $x$  equal to 0 to  $x$  equal to  $L$ . As you increase as you increase the value of  $n$  as you go to higher and higher values of  $n$  what I want to denote is that the variation in the probability of finding the particle within the box from  $x$  equal to 0 to  $x$  equal to  $L$ , that variation becomes smaller and smaller in amplitude.

So, this as I said is the case for  $n$  equal to 5, you can imagine that as you go to higher and higher values of  $n$  much larger values of  $n$  let us say 100 1000 or something this variation is smeared out essentially to become effectively constant across the potential barrier within the potential barrier. So, as the wave as the quantum number increases as the energy level of the particle increases, because the quantum number automatically needs higher energy level, as the energy of the particle increases within the box then the probability of finding the particle within the box is essentially constant throughout the box that is what the simulation show now.

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Let us go to the case of the potential well of the same width, but different depths. So, what I have shown here are 4 cases of a potential well each one deeper than the next one. So, here you have a very shallow potential well deeper, deeper and deeper, but all of them have the same width  $L$  is the same. So, what this is showing is that if the potential well is finite also very shallow then it can only accommodate one energy level as shown here only one energy level is possible within this shallow potential well.

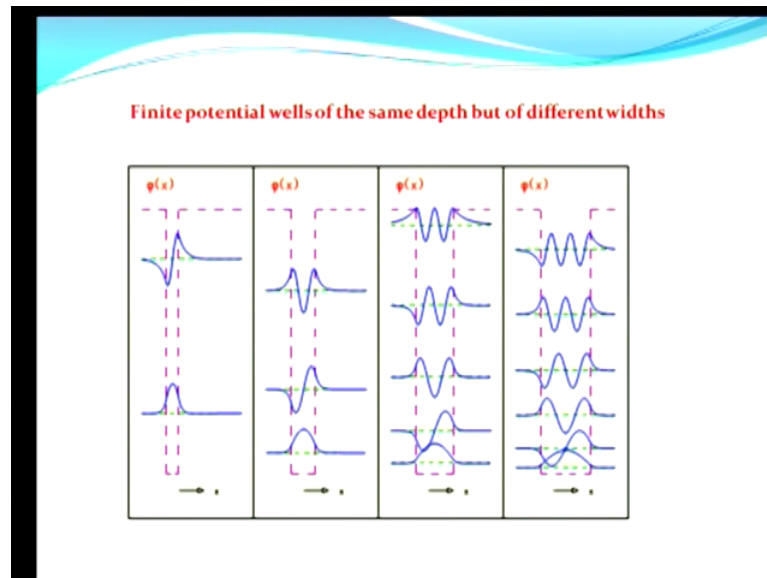
But what is really important note here is that this wave function  $\psi(x)$  over here the wave function over here, because the potential barrier is very short pseudo peak means that the particle is not really very much confined the wave function spreads outside the box considerably has a significant amplitude outside the box and also a significant extent outside the box. When  $n$  equal to 2, you can see that 3 levels or rather when the potential well is less shallow when it is deeper than the first case then 2 levels can be accommodated and the wave functions still spread outside.

But that spread is now that amplitude of the waves outside the box is now reduced compare to the previous case and so on. If you come to a case where the depth is greater, now 4 levels are accommodated in this one and you can see that the spilling over of the wave functions outside the potential boxes potential well is now reduced, but I want to also point out is that for the ground for example, the wave function is confined to the potential well than the wave function of the higher energy levels that is they tunnel out more outside the box.

Then the ones that corresponds to the ground state of a low quantum number what I want to point out is that, such wells are finite depth are really practically very important let us consider a well where are 2 energy levels that are given over here just to. One can imagine a transition from a particle or an electronic particular at the upper level to the lower level to the ground state. If the value of the  $L$  that is the extent of the potential well and the depth of the well if they are all appropriate, then this transition between the upper level and lower level in this 2 level box could then become the basis of a laser for example.

So, light emitting devices can be therefore, fashioned out of potential wells of the sort which can actually they realized in material structures of a special kind and if pump pan permits we will illustrate some examples of such potential wells and their applications.

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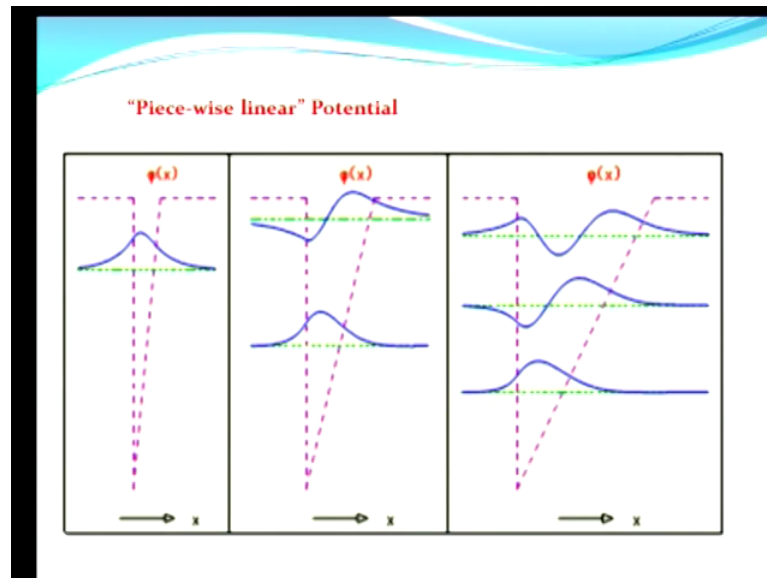


Now, let us consider a different case where you have potential wells and the same depth, but different widths. In previous case they all had the same width, but different depths. So, this alternative case is where they have different widths, but the same height or the same depths you can see that when the well is narrow when is the well is narrow then there are only this particular case there are only two possible energy levels in this narrow well has the width of the well is increased what I want to note is that the ground state energy is steadily reduced.

The ground state energy is high over here compare to the bottom of the well it is now lower over here even lower even lower and so on that is the minimum energy of the particle is greater when the confinement is greater confinement greater meaning the well is narrower. This is a direct result of the uncertainty principle when the confinement of the that even  $\Delta x$  is small  $\Delta p$  is large as we show yesterday and therefore,  $\Delta p$  corresponds to the momentum of the particle and  $\Delta p$  large means the energy is greater, that is these are direct illustration of the Heisenberg's uncertainty principle where when you squeeze the box. So, to speak when you confine the particle to a greater degree than you rise the energy levels of the particle.

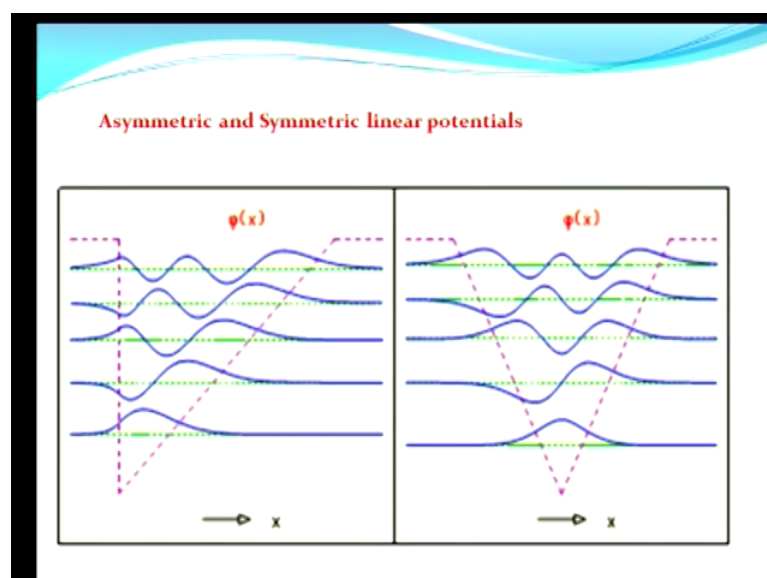
One can also deal with Rhomber these are simple functions where  $v$  equal to 0 within the box and  $v$  is  $f$  constant value outside the box.

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But it is possible to simulate cases where you have a linear variation of the potential across a length  $x$ . So, you can see that you know this is a sort of a saw tooth potential where the potential is increasing along  $x$  within the box. So, it is not constant within the box. So, in such cases one can obtain simulated solutions and you know this have a functional form that is difference slightly different from the simple case of a where the potential is constant within the box, but all these are possible through numerical solutions of the Schrodinger equation applying the right boundary conditions in any case like this.

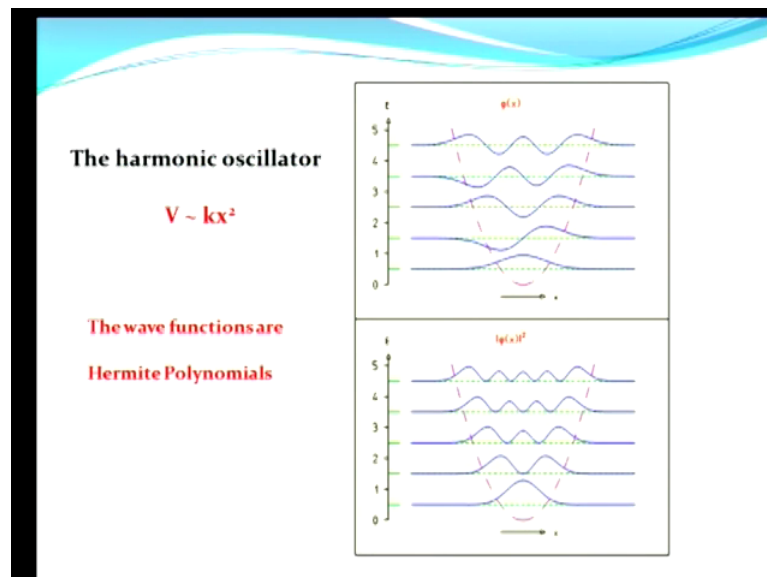
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We have here an asymmetric linear potentials this case and a symmetric linear potentials in this case over here. So, here it is you can see that there is a difference in the nature of the solutions functional forms are slightly different, but they are largely sinusoidal.

So, and then once again there are energy levels that are different and what I want to note is in this case the separation between the energy levels, successive energy levels decreases with the quantum number. Remember in the case of the infinite potential well the energy difference increases as  $n$  square here it is diminishing with  $n$ . So, the case physical case is quite different.

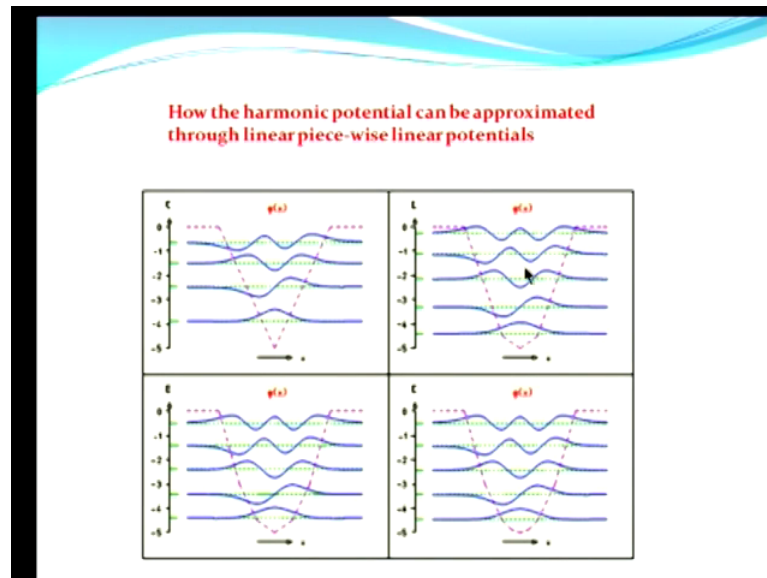
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This is a linear harmonic oscillator the  $V$  equal to  $kx^2$  function and the solutions are as you probably know or  $E_n = (n + \frac{1}{2})h\nu$  where  $n$  is an integer positive integer and therefore, the energy levels are equidistant over one another that is  $E_{n+1} - E_n = h\nu$ .

So, if you compare this case what you can see is that this is coming close to the case of the linear harmonic oscillator where this is actually constant in this case it is not constant, but it is becoming so. So, what you can imagine is that one can think of this linear harmonic potential  $kx^2$  potential has a kind of a sum.

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As a kind of a sum of this rectangular potentials and then you would have actually see that the harmonic potential can be approximated through linear piecewise potentials.

So, what we have illustrated is that one can simulate different potentials and learn about differences between how the particle in a box in different shaped boxes that is you can have a simple box of the infinite height you can have a finite height potential, where you have really squared wells vertical wells. So, to speak on the other hand you can have a v shaped saw tooth shaped to potential and such potentials can be use to stimulate an actual quadratic potential of the simple harmonic oscillator, where the solutions are well known the energy levels are quantized and equally spaced with respect to one another.

So, what you have shown today is that the Schrodinger equation can be solved for simple cases exactly analytically, but in the case more complicated case cases such as this saw tooth potential and piecewise linear potential and so on the solutions sometimes have to be approximate and they can be stimulated, but the solutions for the linear harmonic oscillator I must point out is actually exact. So, these are exact solutions involving so called Hermite polynomials as the wave functions for the simple harmonic oscillator. So, what we have done today is recapitulate the work that was discussed in the previous section.

Then we have gone on to discuss the Pauli exclusion principle and how that as the bearing on the statistics that are applicable to fermions and bosons different kinds of

statistics of this ensembles of bosons and fermions then we have return to the case of the potential barrier and illustrated the case of tunneling across a barrier and how tunneling across a barrier becomes practical and practically important when you have a particle in a finite potential well as suppose to in a infinite potential well.

So, what you will come back to next time is how such simulations can be used to build periodic potentials, that is a particle moving in periodic potential how does it behave when it is subjected to periodic potential. We will come to that in a next section.

Thank you.