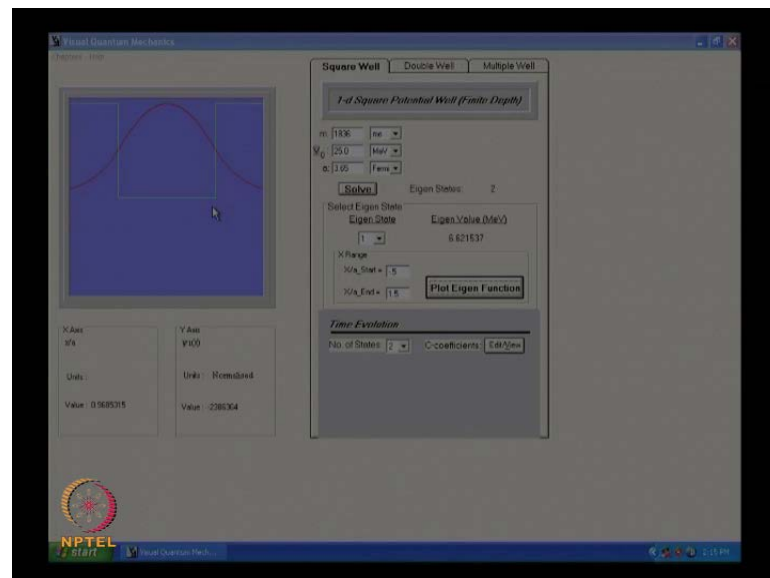


**Basic Quantum Mechanics**  
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**Indian Institute of Technology, Delhi**

**Module No. # 04**  
**Simple Applications of Schrodinger Equation**  
**Lecture No. # 03.**  
**Particle in a Box, Density of States**

Previous lecture we had started a discussion of particle in a box problem we consider the particle in a three dimensional box of volume 1 cube and obtained the energy states of that; however, before that we had discussed a the one **dimension** corresponding one dimensional problem and I thought today we will start our discussion on showing the actual wave functions corresponding to a particle in a one dimensional potential well.

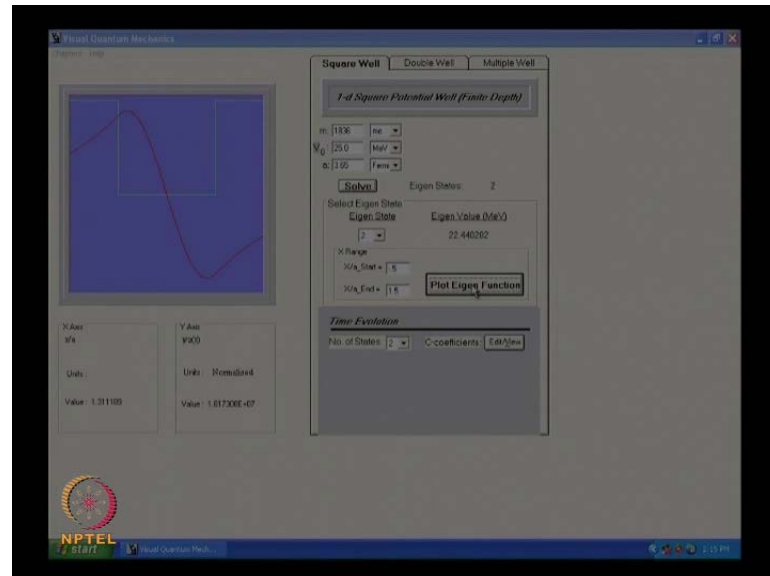
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So, this is the software that we have developed and if you could show the the laptop then we consider a proton of mass eighteen hundred thirty six the electron mass and the potential depth is 25 m e v and as we had discussed earlier we assume that the width of the potential well is 3 point 6 5 Fermi that is 3 point 6 5 into 10 to the power of minus 15 m e v for this the values of alpha we had found to be 2 point 0 and we had obtained two discrete Eigen functions. So, this is the potential well and the first Eigen function has the

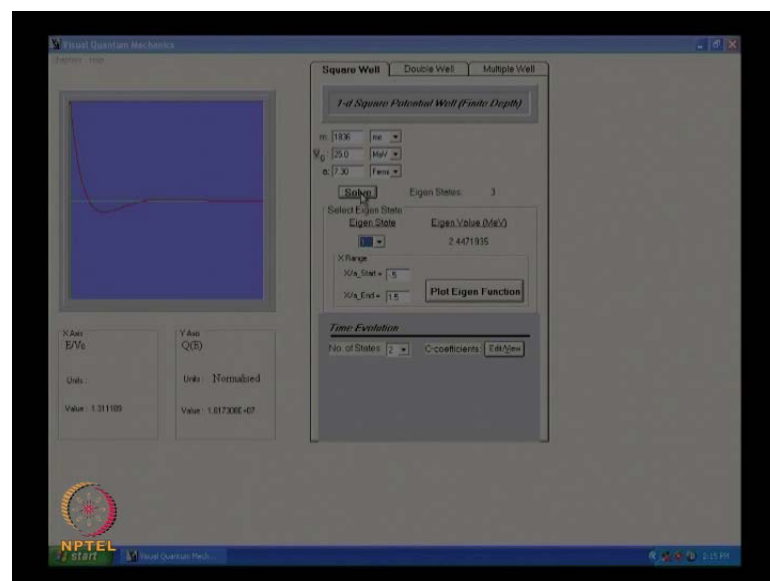
value of 6 point 2 m e v and it is a symmetric state the second Eigen function has a energy Eigen value of 22.44.

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Right at the edge of the potential well and it will be an ant symmetric Eigen function now let me make this two times the this value. So, that instead of 3 point 6 5 we write 7 point 3 0 Fermi.

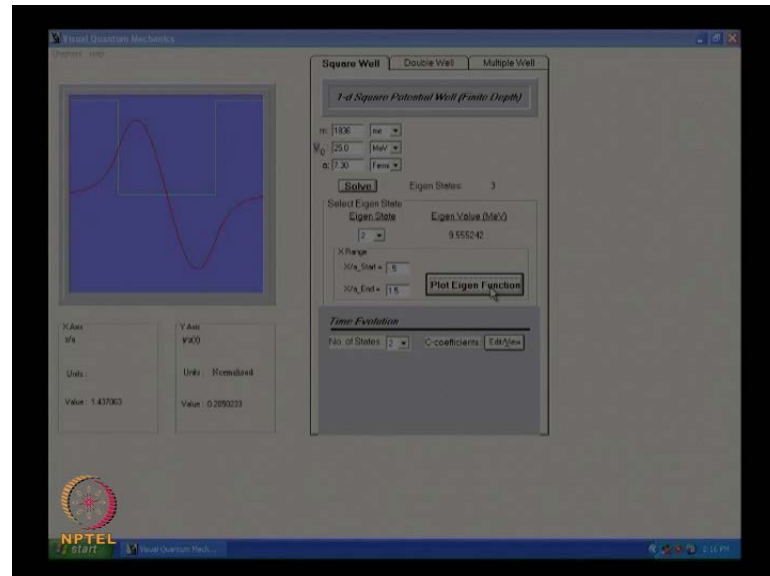
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So, that the width of the potential well has now increase now we have 3 Eigen states the same potential well with a width which is now three Fermi will have three Eigen states

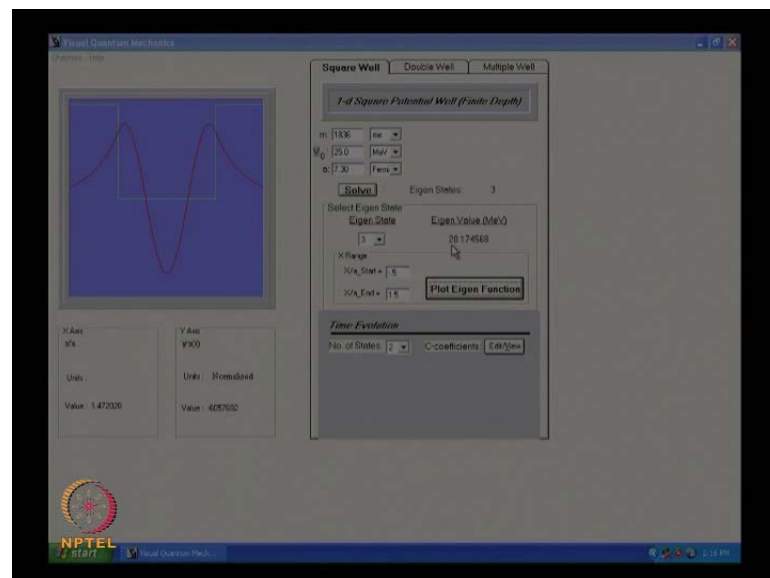
the ground state will have will be symmetric function of  $x$  which has an energy Eigen value of 2 point 4 5 and m e v and the second one will have a Eigen value of 9 point 5 5.

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which is an ant symmetric function of  $x$  and the third Eigen state will have the energy.

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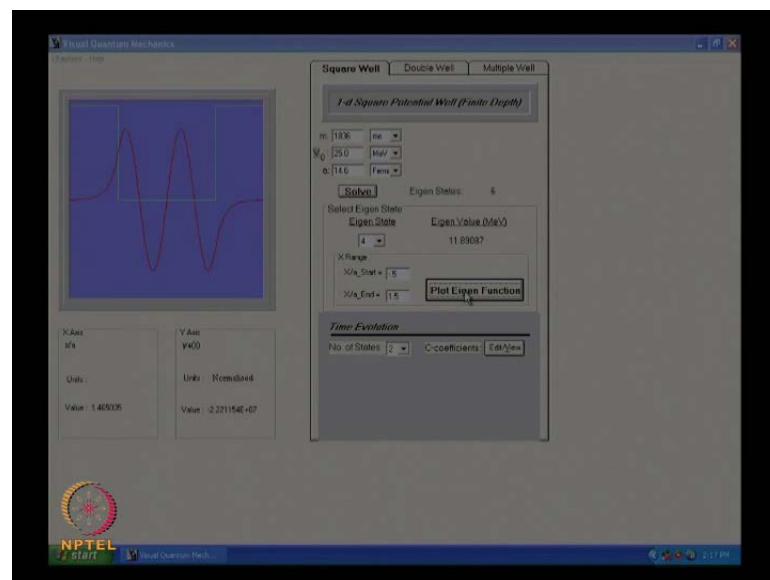


Which is twenty point one seven and again it is symmetric now if I make the value of  $a$  twice of this. So, that instead of 7 point 3 Fermi if I made fourteen point 6 Fermi. So, that the width of the potential well has been made double let us solve this.

Now, we have six discrete Eigen values and first Eigen value which is the ground state which has an Eigen value of point seven six m e v is a symmetric function of  $x$  and it is more confined within the potential well the second one will be has a Eigen value of three point zero two which is ant symmetric inside the well it is a sign function and outside the well it is an exponentially decaying function

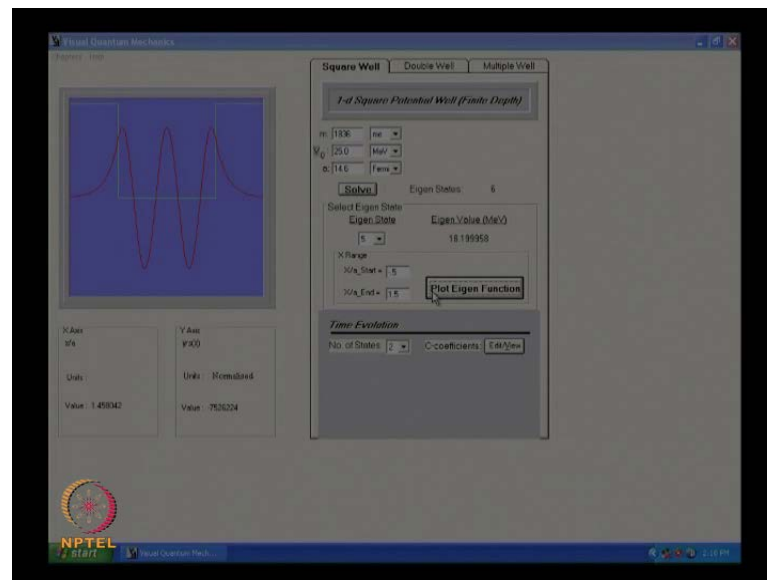
Similarly, the third Eigen state will have an energy six point seven seven and m e v which will be symmetric inside the well it is a cosine function outside is an exponential function outside its an and it is symmetric about the central point because the potential is also a symmetric function of  $x$ .

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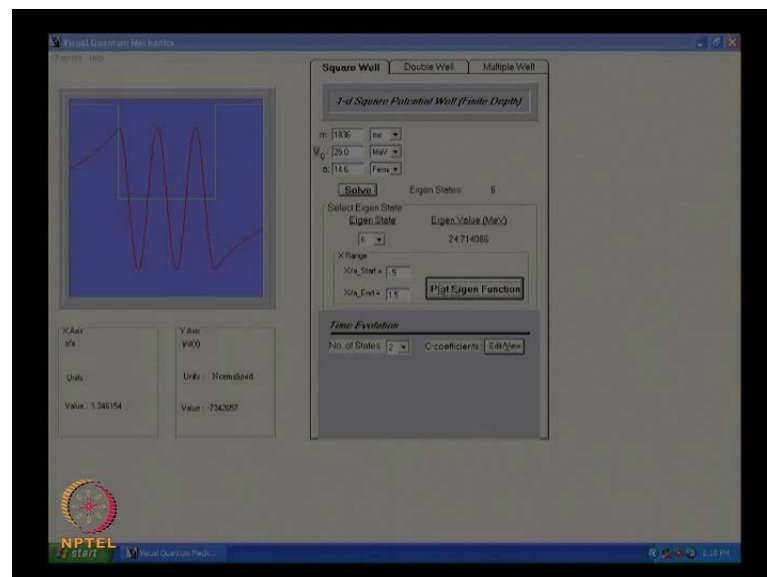
So, the fourth Eigen function the energy Eigen value is 11 point 9 m e v and it is an ant symmetric function of  $x$  that is inside the well you have a sin function and outside the well it is a an exponentially decaying function.

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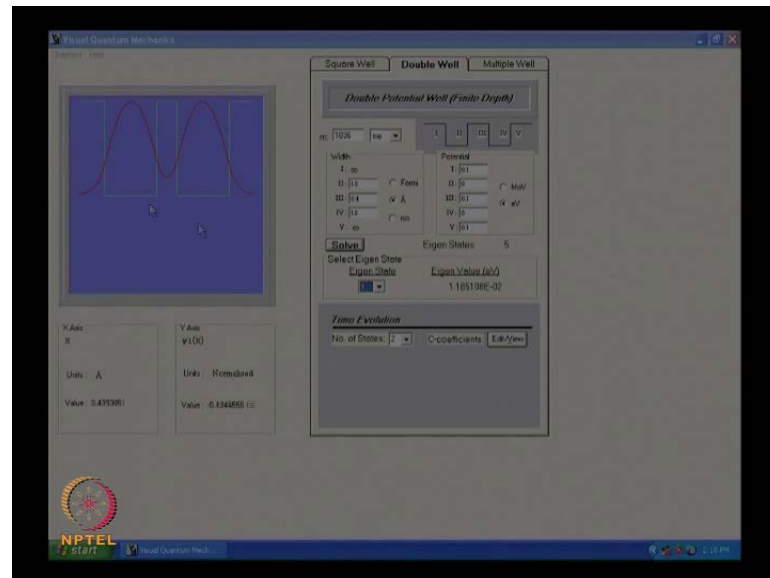
Similarly, fifth Eigen value is eighteen point two m m and it is a symmetric function and finally, the sixth Eigen function is is has is a ant symmetric function of x is exponentially decaying here and exponentially decaying here and inside the core we have sixth Eigen function.

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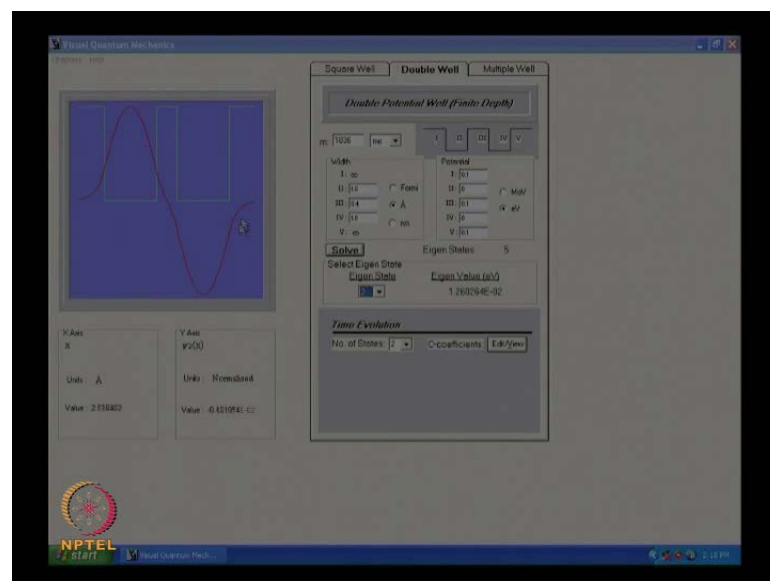
So, this is the software that we had developed I had shown you earlier this is the basic quantum mechanics book on basic quantum mechanics in which we have develop a software to understand basic simple problems in quantum mechanics.

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So, this is how a square well potential looks like if I had solve the double well problem then the wave functions will be like this this double well problem is also a symmetric function of  $x$ . So, the wave functions are either symmetric or ant symmetric.

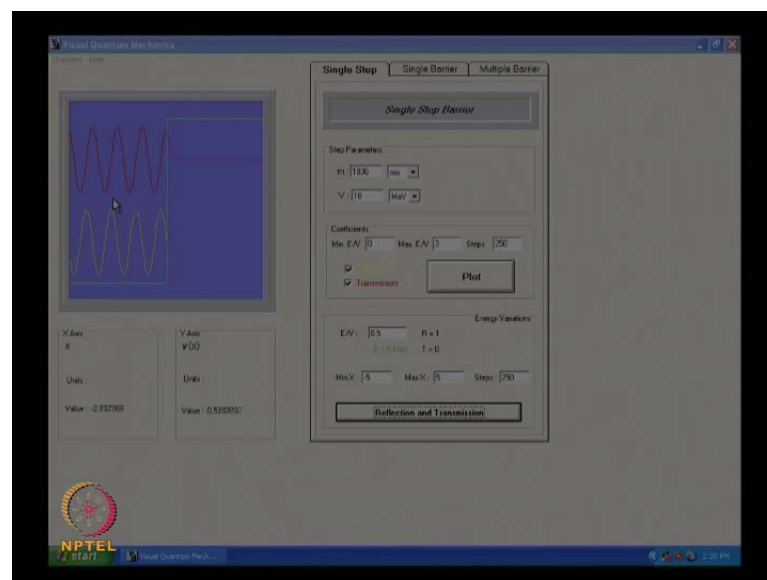
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So, the first wave function is like that and second wave function is like that and. So, on and the software allows you to calculate the Eigen value for a multiple well problem, but that is slightly complicated because we have to develop a numerical method for solving the Schrödinger equation it is possible to do that it is not very straight forward, but it is little it will take some time.

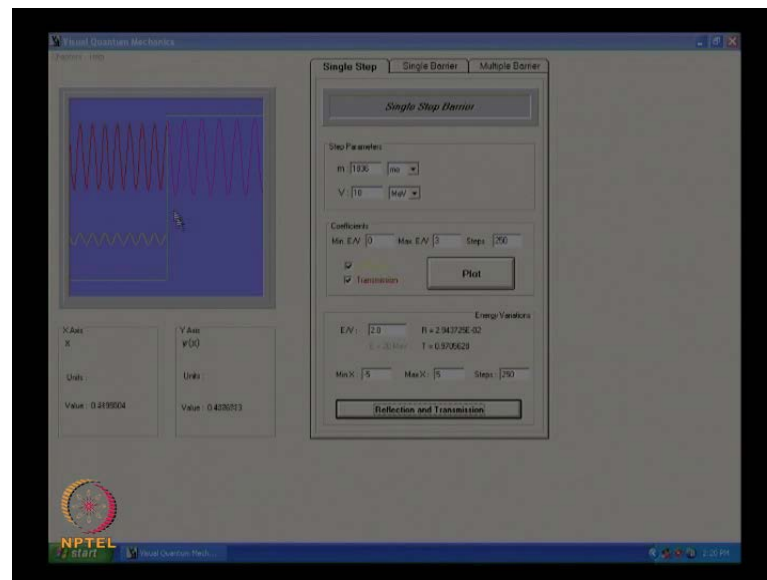
Maybe at the end of the course we can we can discuss that before we go to the particle in a box problem let me consider the **potential** the single step barrier and let me assume that this step is ten m e v the mass of the particle is 1836 times the mass of the electron which is the mass of the proton and it experiences the potential step of ten m e v. So, this is the reflection and the transmission coefficient.

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So, you have here the incident energy incident energy is point five the reflection coefficient is one there is a total reflection. So, this is the incident wave this is the reflected wave and and then there is an evanescent wave here the reflection is complete. So, this is what. So, if particle is incident from the left on a potential step which is of height ten m a b and it is a proton and that we are assuming and we consider an energy of the proton which is half of this value which is a five m e v five m e v if we make it make it more than ten m e v let us suppose a by v it becomes 2 point 0 2 point 0 then then we will find that there is an incident wave here there is a transmitted wave here then there is a reflected wave here.

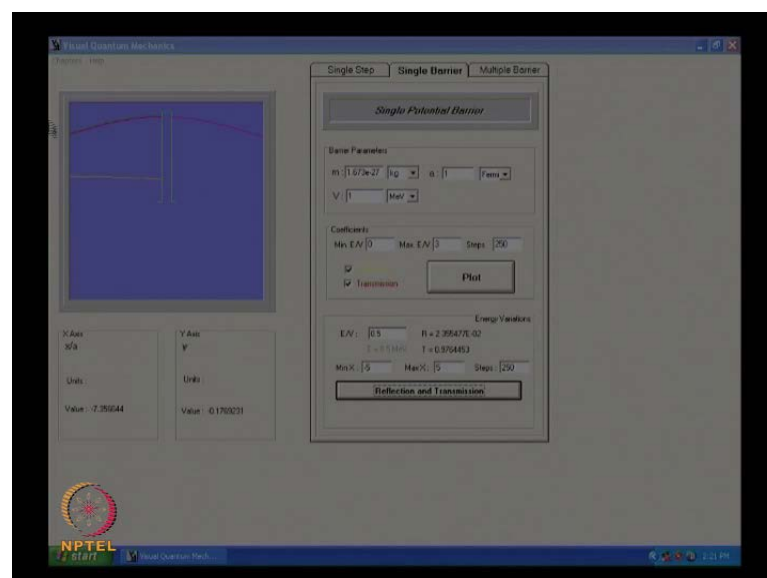
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So, so the reflection coefficient is about point 03 point 0 3 and that is about three percent reflection and the transmission coefficient is ninety seven percent the ninety seven percent.

So, you can see that that the amplitude of the wave is slightly larger here and that is the consequence of the fact that the we have to calculate we have to be careful in calculating the transmission coefficient we have to consider the currents and not just the amplitudes. So, the  $r$  plus  $t$  the reflection plus the transmission coefficient must be equal to unity.

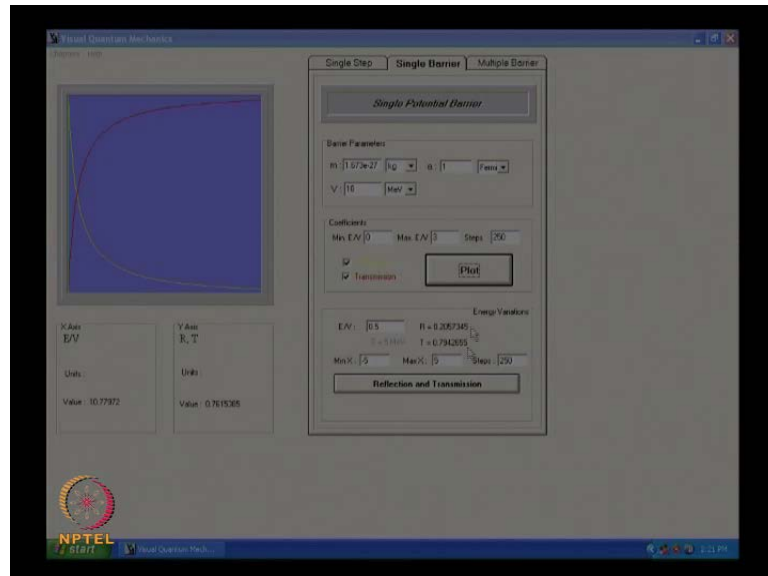
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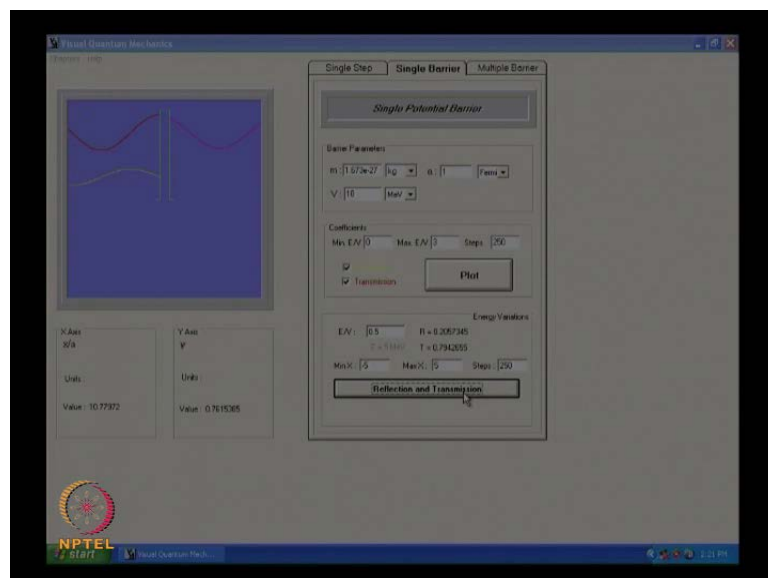
So, this is what the single step looks like then we consider single barrier and. So, you have an incident wave here and a reflected wave here and a transmitted wave here.

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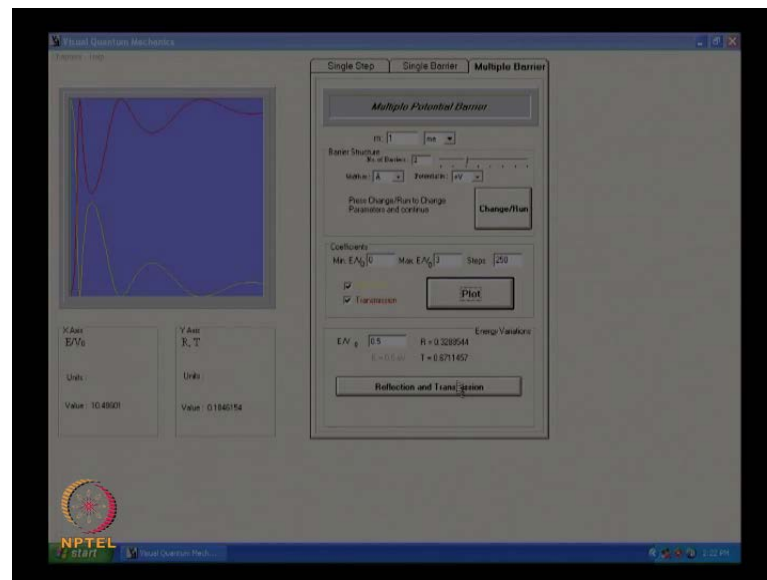
So, let me make this as ten m e v this is a proton and this is the reflection coefficient and the transmission coefficient and.

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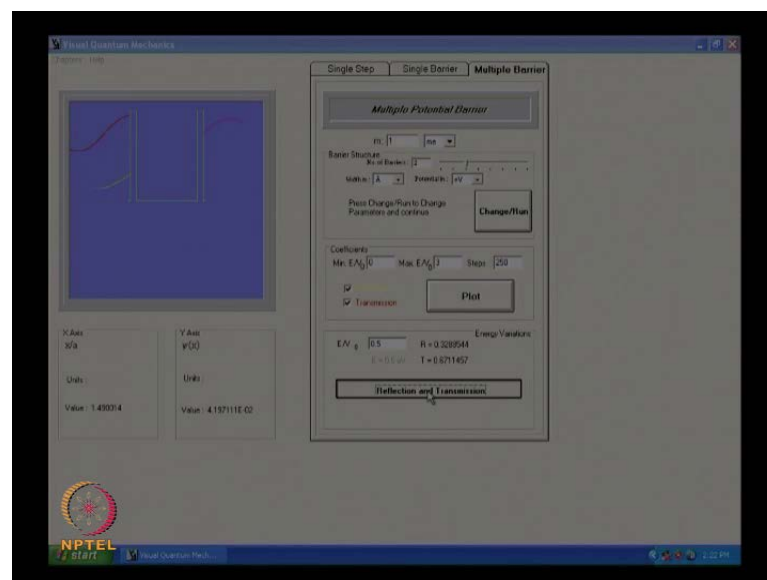
So, this is the incident wave this is the reflected wave and this is the transmitted wave.

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And you can go to multiple variant problems also very very straight forward we consider these are the reflection and transmission coefficient

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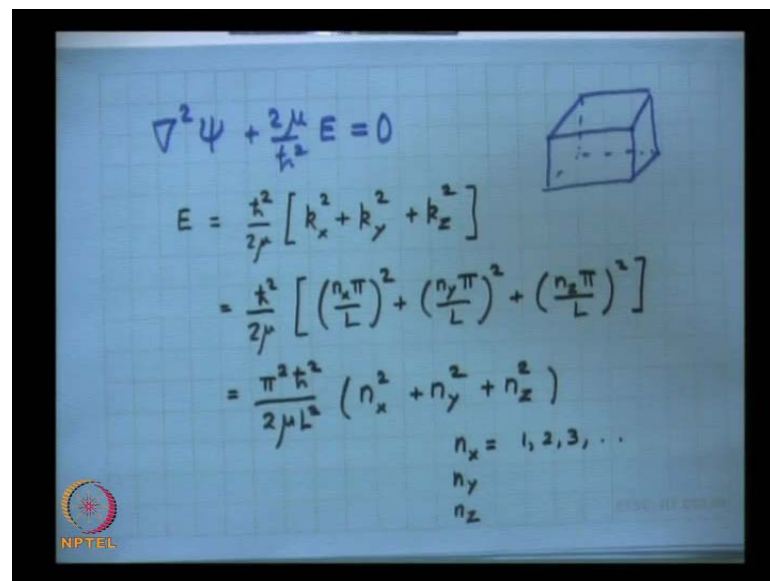


Any particular potential energy variation can be used can be put into the software to calculate the reflection and the transmission coefficient you can have here we have two potential bumps you can have three four or any number and you can use the software to calculate the you can use the software to calculate the reflection and

transmission coefficient for a for a single barrier or a multiple barrier or for any in a any potential energy distribution that one can think of.

So, we now. So, this sought of completes the the analysis of potential step and potential barrier and also the potential well problem that we had discussed in our previous lecture we continue our discussions on on for a particle in a box and we will calculate the density states for such a problem.

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$$\nabla^2 \psi + \frac{2\mu}{\hbar^2} E \psi = 0$$

$$E = \frac{\hbar^2}{2\mu} [k_x^2 + k_y^2 + k_z^2]$$

$$= \frac{\hbar^2}{2\mu} \left[ \left( \frac{n_x \pi}{L} \right)^2 + \left( \frac{n_y \pi}{L} \right)^2 + \left( \frac{n_z \pi}{L} \right)^2 \right]$$

$$= \frac{\pi^2 \hbar^2}{2\mu L^2} (n_x^2 + n_y^2 + n_z^2)$$

$n_x = 1, 2, 3, \dots$   
 $n_y$   
 $n_z$

We had in the previous lecture we had considered the solution of the Schrödinger equation  $\nabla^2 \psi + \frac{2\mu}{\hbar^2} E \psi = 0$  inside the box we consider box which is of length  $L$  height  $L$  and width  $L$

So, that this is the box that we had considered and and we this is an infinitely deep potential well. So, the wave function was vanishes at each point on the surface and we obtained the the following  $E$  was equal to the energy Eigen value was equal to  $\frac{\hbar^2}{2\mu} [k_x^2 + k_y^2 + k_z^2]$  and had obtained  $\frac{\hbar^2}{2\mu} \left[ \left( \frac{n_x \pi}{L} \right)^2 + \left( \frac{n_y \pi}{L} \right)^2 + \left( \frac{n_z \pi}{L} \right)^2 \right]$

So, these are the discrete Eigen values of the problems. So, you can take the  $\pi^2 \hbar^2 / 2\mu L^2$  inside. So, you have  $\pi^2 \hbar^2 / 2\mu L^2 (n_x^2 + n_y^2 + n_z^2)$

$n_y^2$  plus  $n_z^2$  and as we have discussed in the previous class these can take any integer  $n_x$  is equal to 1 2 3 4.

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$$\Psi(x,y,z) = \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{n_x\pi}{L}x\right) \sin\left(\frac{n_y\pi}{L}y\right) \sin\left(\frac{n_z\pi}{L}z\right)$$

$$0 < x,y,z < L$$

$$n_x, n_y, n_z = 1, 2, 3, \dots$$

$$E = \frac{\pi^2 \hbar^2}{2\mu L^2} (n_x^2 + n_y^2 + n_z^2)$$

$$n_y = -2$$

$$n_x^2 + n_y^2 + n_z^2 = \frac{2\mu L^2 E}{\pi^2 \hbar^2}$$

$$E = 10 \text{ MeV}$$

$$= 10^6$$

Similarly,  $n_y$  and similarly  $n_z$  they will not a negative value will not not lead to any state it will not lead to a wave function that is because that the corresponding wave functions are given by the normalized wave functions are given by  $x, y, z$  two by  $L$  this is the normalization factor as you know three by two then  $\sin$  of  $n_x \pi$  by  $L$   $\sin$  of  $n_y \pi$  by  $L$  times  $x$  times  $y$  times  $n_z \pi$  over  $L$  into  $z$  these are the rigorously correct wave function normalized wave function corresponds corresponds of course, zero less than  $x$  comma  $y$  comma  $z$  less than  $L$ .

Wave function is non zero only inside the box and of course, next  $n_y, n_z$  takes the values one two three four five integers if I take the value zero then of course, this whole wave function becomes zero. So, that is the trivial solution. So,  $n_x, n_y, n_z$  equal to 0 that is that corresponds to a trivial solution and also if I take say  $n_y$  equal to minus 2 then if I take plus two and minus two it will only change the sign of the wave function to which the wave function is always arbitrary. So, it will not lead to any energy state or any wave function. So, that we restrict ourselves to only positive integers value integral value of  $n_x, n_y, n_z$ .

Now, as we had mentioned in the previous slide the energy Eigen values are  $\pi^2 \hbar^2$  cross square by two  $\mu L^2$  square  $n_x^2$  plus  $n_y^2$  plus  $n_z^2$  as you know

$h$  cross is a constant for a given box  $L$  is a constant  $\mu$  is the mass of the particle that is the constant now I want to find out the total number of energy states whose energy lies is less than  $e$ . So, therefore, I rewrite the above equation like this  $n_x^2 + n_y^2 + n_z^2$  is equal to  $\frac{2\mu L^2 e}{\pi^2 h^2}$ .

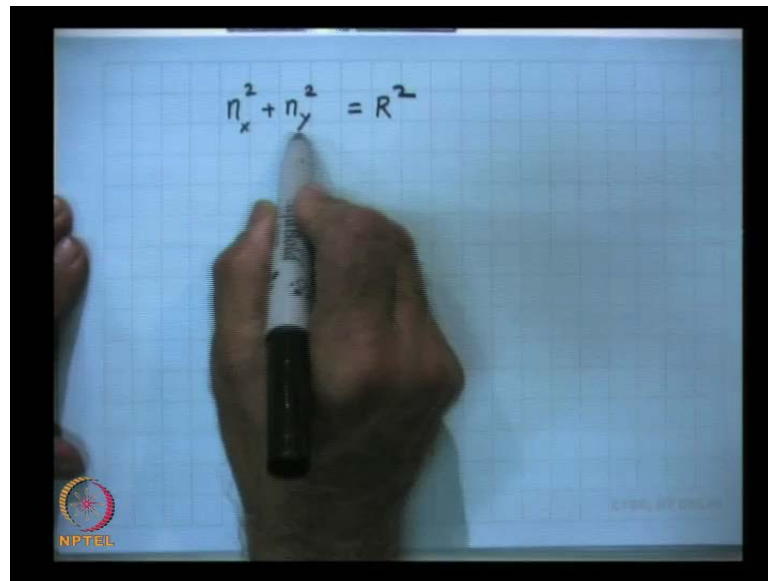
So, let us suppose I put say equal to ten  $m_e v$  then for given value of  $\mu L$   $h$  cross this right hand side is a number is a dimensionless number and. So, therefore, if I assume say  $e$  is equal to ten  $m_e v$  then the right hand side becomes a number.

Let us suppose it is a number like say ten to the power of six it is all number then had to find the sets of integers such that the sum of their squares is less than ten to the power of six. So, that is a very easy geometric method to do that. So, let me restate the problem the problem is I want to find out the total number of states whose energy is less than  $e$  i take a fixed value of  $E$  say ten  $m_e v$  and I substitute in this expression and find the right hand side.

I know the particle which in this case will be electron. So, I know the electron mass let us suppose it is one meter by one meter by one meter by or one centimeter by one centimeters by one centimeter. So, I know what is  $L$  and what is  $h$  cross and I if I specify the value of  $e$  then the right hand side is a number.

Let that number be one million let us suppose. So, I want to find the sets of integers such that the sum of their square will be less than ten to the power of six. So, you can see  $n_x$  can be one two three four six. So, on  $n_y$  can be large number of numbers and  $n_x$  will be a large number of numbers of course, none of the integers will be more than ten to the power of three that is the largest value of either  $n_x$   $n_y$  or  $n_z$  will be less than thousands because if it is thousand then that number itself is the square of that will become ten to the power of six

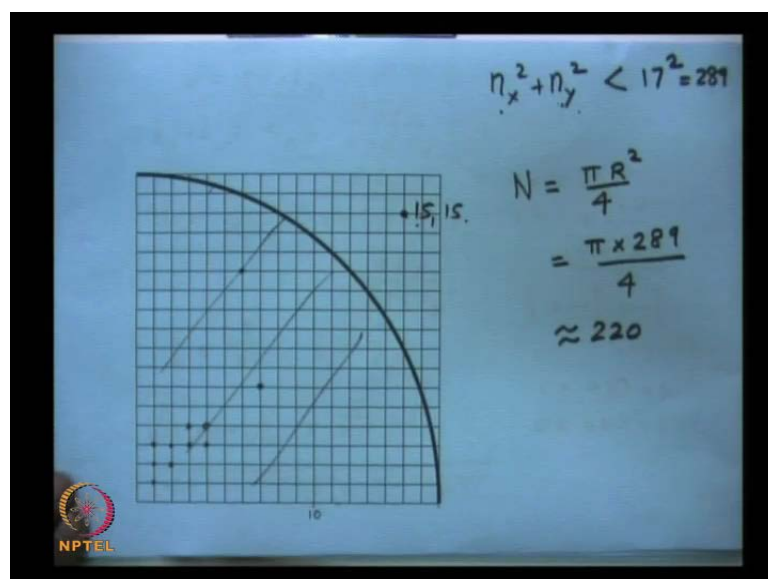
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A hand is shown writing the equation  $n_x^2 + n_y^2 = R^2$  on a grid background. The hand is holding a black marker. The equation is written in the upper left quadrant of the grid. In the bottom left corner, there is a small circular logo with the text "NPTEL" below it.

Now, let me tell you the method of calculation and before that let me do a simpler two dimensional problem and that is let me consider the total number of sets of integers such that the sum of their squares is less than  $r$  square.

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Now, in order to understand this I had drawn a graph paper and you see each corner on this is an integer this is 1 1 this is 2 2 this point is 1 2 this point is 1 3. So, I want to calculate this radius that I had drawn is of radius seventeen units.

So, 1 2 3 10 11 12 to seventeen three ten eleven twelve to seventeen. So, I want to find out the sets of integer such that  $n_x^2 + n_y^2$  is less than seventeen square and this as we all know is two eighty nine. So, I of this graph paper I draw the quantum of the circle because  $n_x$  only positive integers and each point on this graph paper is associated with a particular set of values  $n_x$  and  $n_y$  for example, here this is 5 comma 5 or 6 comma 5.

This is seven comma eight or something like that. So, any point inside this will be such that their sum of the squares will be less than because this is the radius of circle any point outside for example, here this is 15 here and 15 here. So, for this this 15 and 15. So, this the sum of the squares may see to 89

So, therefore, if I want to find out the sets of integers who sum of square is less than two eighty nine then it will be the number of points number of corners that are there with e and with each points I can associated associated the unit area.

So, that the total number of states such that the value of  $n_x^2 + n_y^2$  is less than two eighty nine will be the area of this quantum of this circle which is  $\pi R^2$  by four. So, therefore, in this particular case the the area of the circle is  $\pi R^2$  and since we are considering the fourth of then because we are restricting the ourselves  $n_x$  and  $n_y$  positive. So, in this case it will be  $\pi$  into  $R^2$  which is two eighty nine divided by four and I think the approximate value is two twenty it will come out to be not an integer, but these are approximate calculations. So, therefore, each corner

Each point on this matrix of this grid corresponds to an Eigen state corresponds to an integer integer value of  $n_x$  and  $n_y$  and. So, therefore, in with e[ach]- with each point is associated with a unit area there and. So, therefore, number of points in this quadrant will be approximately equal to the area of the quadrant when this value of  $R$  is very large and. So, therefore, the total number of states will be approximately equal to  $\pi R^2$  by four now.

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$$n_x^2 + n_y^2 = R^2$$

$$N = \frac{\pi R^2}{4}$$

$$n_x^2 + n_y^2 + n_z^2 = R^2$$

$$N(E) = \frac{1}{8} \times \frac{4\pi}{3} \times R^3$$

$$n_x^2 + n_y^2 + n_z^2 = \frac{2\mu L^2 E}{\pi^2 \hbar^2} = R^2$$

$$N(E) = 2 \times \frac{\pi}{6} \left[ \frac{2\mu E}{\pi^2 \hbar^2} \right]^{3/2} = \frac{\pi}{3} \frac{(2\mu)^{3/2}}{\pi^3 \hbar^3} E^{3/2}$$

So, this was the case. So, if I want to find out the sets of integers such that I want to find out  $n_x^2 + n_y^2$  is less than  $R^2$  then I have to draw a quadrant of a circle of radius  $R$  and the number of sets of integers will be equal to  $\pi R^2$  by four.

But our problem is slightly more complicated because now I have sets of three integers  $n_x^2 + n_y^2 + n_z^2$  is equal to  $R^2$ . So, I want to find out the sets of integers such that their sum of the squares is less than or equal to  $R^2$ .

So, I have to take the three dimensional plane. So,  $n_x$ ,  $n_y$  and  $n_z$  and each point on this we may be draw small small cubes here and each corner will be of a point will correspond to an integer value of  $n_x$ ,  $n_y$  and  $n_z$ . So, they will be total number of states for which  $n_x^2 + n_y^2 + n_z^2$  is less than  $R^2$ .

Now, it will be the volume of the cube the octant one eighth because they are only considering positive values of  $n_x$ ,  $n_y$  and  $n_z$  here we had  $\pi R^2$  by four, but it had eight octants three dimensional geometry. So, the total number of states will be equal to one eighth that is the octant multiply by the volume of the sphere that is four  $\pi$  by three into  $R^3$ .

Now, if you recollect that we had  $n_x^2 + n_y^2 + n_z^2$  this is equal to  $\frac{2\mu L^2 E}{\pi^2 \hbar^2}$ . So, this was my  $R$ . So, the total number of state. So, four this is two. So,  $N(E)$  will become  $\pi$  this is  $R^3$  this is  $R$



square. So, this will be raised to the power of 3 by 2 3 by 2 and in each state if I am considering electrons you can have spin up and spin down. So, that the number of available states for the electron will be two times this. So, this will be the total number of states whose energy is less than E. So, this becomes equal to if I simplify this pi over three two mu raised to the power of 3 by 2 divided by pi cube h cross cube times e to the power of 3 by 2

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The image shows handwritten mathematical derivations on a grid background. The equations are as follows:

$$N(E) \approx \frac{(2\mu)^{3/2}}{3\pi^2 \hbar^3} E^{3/2}$$

$$g(E)dE$$

$$g(E) = \frac{dN}{dE} = \frac{(2\mu)^{3/2}}{2\pi^2 \hbar^3} E^{1/2} \quad e^{-\infty} = 0$$

$$F(E) = \frac{1}{1 + e^{(E-E_F)/kT}} \quad E_F$$

At  $T=0$

$$F(E) = 0 \quad E > E_F$$

$$F(E) = 1 \quad E < E_F$$

NPTEL logo is visible in the bottom left corner.

So, therefore, we obtained that the total number of states whose energy is less than E is approximately one pi cancels out with pi cube and. So, you will have two mu raised to the power of 3 by 2 divided by three pi square h cross cube into E raised to the power of 3 by 2.

So, this is the total number of states whose energy would be less than E and we have taken into account the fact that each state can be occupied by two electrons by two electrons spin up and spin down. So, this is the total number of states whose energy would be less than E

Now, last time we had shown that the density of states total number of density of state is defined like this g of d E is the number of states whose energy lies between e and e plus d E and the we had shown that the density of states will be equal to d n by d E. So, that is a very straight forward differentiation.

So, that will become three by two. So, this will become three three will cancel out two pi square h cross cube multiplied by two mu raise to the power of three by two a to the power of half this is an extremely important formula for density of states which is extensively in used in solid state physics and in many other area and this density of state is such that the that g of E is proportional to a to the power of half.

Now, let me apply this say this concept to to the case of electrons as we know that in sodium we consider the sodium metal now inside that metal associated with each sodium atom there is an electron which is almost free

So, therefore, we assume that with each atom there is a free electron which is free moved inside the metal, but it cannot escape from the metal. So, it is actually inside a three dimensional box that we had we had being consider. So, let us suppose the I am sure you are familiar with what is known as the Fermi derived distribution the Fermi derived distribution which is usually represented by the symbol capital f is a function of temperature and is the probability of occupation of a of a particular state and this function is given by one plus E to the power of E minus E F by k t .

If at temperature at t absolute zero at absolute zero if e is greater than E F then this is positive. So, it is E to the power of T is extremely small. So, it is E to the power of plus infinity. So, F of E is 0 for E less than E F 0 this is known as the Fermi energy.

and the Fermi energy is a function of the temperature. So, at absolute zero I am this is e greater than E F I am So, because when E is greater than E F this quantity becomes positive. So, this E to the power of infinity E to the power of infinity is infinity. So, one over infinity is zero.

On the other hand for e less than E F 0 e less than E F 0. So, this quantity is negative. So, it is e to the power of minus infinity if it is e to the power of minus infinity and this is 0 f of E this quantity is 0 this is 1 over 1. So, f 1.

So, therefore, at absolute zero all the states below the Fermi energy are occupied and all the states above the Fermi energy are unoccupied the probability of occupation is zero and for all energy states for which the energy is less then E F 0 the probability of occupation is one.

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$$\begin{aligned}
 N &= \int_0^{\infty} F(E) g(E) dE \\
 &= \int_0^{E_F} g(E) dE \\
 &= \frac{(2\mu)^{3/2}}{2\pi^2 h^3} \int_0^{E_F} E^{1/2} dE \\
 &= \frac{(2\mu)^{3/2}}{3\pi^2 h^3} V E_F^{3/2}
 \end{aligned}$$

So, let me calculate the total number of total number of electrons inside the metal unfortunately we are using the same symbol  $n$  which is the total number of electrons inside a metal. So, this will be equal to the density of states multiplied by the probability of occupation of the state. So, this is the probability of occupation of the state multiplied by  $g$  of  $E$   $dE$  and from zero to infinity.

This is the rigorously correct expression at absolute zero we find all that states  $f$  of  $E$  is one for less than  $E_F$ . So,  $E_F$  and beyond that it is zero. So, this will become  $g$  of  $E$   $dE$  and. So, therefore, you will obtain if substitute the value of  $g$  of  $E$ . So, this will become two  $\mu$  raise to the power three by two divided by two  $\pi$  square  $h$  cross cube  $e$  to the power of half  $dE$ . So, 0 to  $E_F$  this is a very trivial integral.

The integration is two by three  $e$  to the power of three by two evaluated between zero and  $E_F$ . So, this will become two by three  $E_F$  raise to the power of 3 by 2. So, this two this two this will come here. So, this two will cancel out with this two and we will therefore, obtain that the expression that two  $\mu$  raise to the power of 3 by 2 divided by  $\pi$  square  $h$  cross cube multiplied by three  $E_F$  raise to the power of three by two.

I am for this multiplied by there is a factor which is  $L$  cube which I have missed sorry. So, even here you may correct that there is a factor which is multiplied by the volume of the box. So, I am there is an  $L$  square factor here. So, when you take the three by two

factor of that. So, there is an L cube factor here. So, L cube is the volume of the box which is present everywhere. So, this factor I have missed.

So, you have here there is a factor v where v is equal to L cube. So, I can either write L cube I can either write v. So, here you have multiplied by v. So, let me this write it down once again. So, the total number electrons inside the metal will be two mu raise to the power of 3 by 2 divided by 3 pi square h cross cube multiplied by v.

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$$n = \frac{N}{V} = \frac{(2\mu E_{F_0})^{3/2}}{3\pi^2 \hbar^3}$$

$$2\mu E_{F_0} = (3n\pi^2 \hbar^3)^{2/3}$$

$$E_{F_0} = \frac{\hbar^2}{2\mu} (3\pi^2 n)^{2/3}$$

Example Na 0.97 gm/cm<sup>3</sup>.

$$n = \frac{6.023 \times 10^{23} \times 0.97}{23} \approx 2.54 \times 10^{22} \text{ electrons/cm}^3$$

So, let me rewrite this. So, you have here n is equal to two mu E F 0 raise to the power of three by two divided by three pi square h cross cube and there is a volume here. So, I put the volume here. So, this is the total number of electrons in volume v. So, this is the electron density number of electrons per centimeter cube.

So, from this we can write down two mu E F 0 is equal to 3 n pi square h cross cube raise to the power of 2 by 3. So, this is the final result for the. So, you will get E F 0 E F 0 becomes h cross square by two mu multiplied by three pi square n raise to the power of two by three.

Now, if I consider this is the expression for the Fermi energy of the energy of electron at absolute zero now let me consider the sodium metal example let me consider sodium metal sodium it has a density of point nine seven actually I am using grams per centimeter cube and if I use the Avogadro's number then the total number of electrons if

I issue one electron per atom and then there are  $6.023 \times 10^{23}$  atoms for 23 grams this is the atomic weight multiplied by the density

Then you will get approximately  $2.54 \times 10^{23}$  electrons per centimeter cube we are using here is the c g s system of units. So, once again I consider sodium metal which has a density of 0.97 grams per centimeter cube 23 grams of sodium will have  $6.023 \times 10^{23}$  atoms.

Each atom will have one electron. So, that twenty three grams will contain twenty three grams of sodium will contain  $6.023 \times 10^{23}$  electrons and since the density of sodium is 0.97 grams per centimeter cube the number of electrons per unit volume will be equal to this number divided by 23. So, if you carry out the calculation then it comes out to be  $2.54 \times 10^{23}$  electrons per centimeter cube.

Now, if you substitute this number in this expression and you know the value of  $h$  cross you know the value of mass. So, this comes out and you transform into electron volts this will come out to be 3.2 electron volts. So, so this is the Fermi energy at absolute zero at absolute zero

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$$\langle E \rangle = \frac{\int_0^\infty E g(E) F(E) dE}{\int_0^\infty g(E) F(E) dE}$$

$$\approx \frac{3}{5} E_{F_0} \left[ 1 + \frac{5\pi^2}{12} \left( \frac{kT}{E_{F_0}} \right)^2 + \dots \right]$$

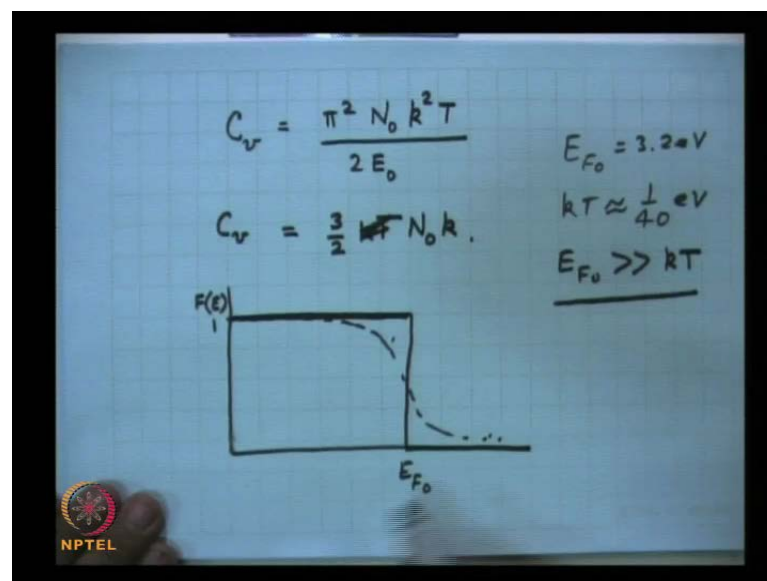
$T \approx 300^\circ\text{K}$   
 $kT \approx \frac{1}{40} \text{ eV}$   
 $E_{F_0} \approx 3.2 \text{ eV} \gg kT$

$T=0$   
 $\langle E \rangle = \frac{3}{5} E_{F_0}$

Now, the average energy the average energy is given by the zero to infinity  $\int_0^\infty E dE$  of  $E F(E)$  divided by zero to infinity  $\int_0^\infty E dE$  of  $E F(E)$  we have calculated this for for a at absolute zero if I calculate this at a particular temperature the calculation are slightly cumbersome, but the final result is average energy is  $\frac{3}{5} E_F$  not approximately equal to  $1 + \frac{5}{12} \pi^2 kT$  by  $E_F$  whole square plus. So, on.

So, usually you know at at at room temperature for example,  $T$  equal to 300 degree Kelvin 300 degree Kelvin  $kT$  is about one fortieth of an electron volt and we have just now seen that  $E_F$  for electron is about three point two electron volts. So, so  $E_F$  not is much much greater than  $kT$  and. So, therefore, although the sodium metal is at 300 degree Kelvin, but we can assume that almost all the that the the situation is somewhat similar that exist at 0 degree Kelvin and we say it is in an almost degenerate state.

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That is all the levels up to  $E_F$  are filled up and beyond  $E_F$  all the states are empty using this expression for the average energy at  $T$  equal to 0 at absolute 0 the average energy is equal to  $\frac{3}{5} E_F$  and since  $kT$  by  $E_F$  is usually a very very small number for normal temperature. So, therefore, the correction term is very very small is usually very small and using this expression we can calculate the we can calculate the electronic specific heat and we will find that electronic specific heat I leave this is an exercise will come out to be  $\frac{\pi^2}{2} N_0 k^2 T$  divided by  $2$  times  $E_F$ .

And the the the if I consider this to be a free gas then the then the then the specific heat comes out to be at constant volume  $\frac{3}{2} k_B T$   $\frac{3}{2} \frac{3}{2} n k_B$ . So, this specific heat is extremely small and this is a consequence of the fact that that you see at absolute zero at absolute zero the Fermi function is something like this this is  $E_F$  this is the Fermi function  $f$  of  $E$  and you have all the states filled up below  $E_F$  and all the states are empty above that.

At room temperature for example, in sodium it will be something like this. So, only a small number of states around this  $E_F$  we have a slightly lesser probability now only these electrons will go here when you heat it up. So, these electrons really do not contribute to this specific heat and. So, therefore, the electronic contribution to these specific heat is much less than what we would expect from the classical if we had assume that the electron behaves like a classical gas.

Even the electrons in the in in white dwarf can be approximately assume to be free and the and in a complete degenerate state and that leads to the theory of white dwarf star which is almost which is quite easy to understand once we have understood this the free electron theory from the particle in a box problem.

So, that we conclude this part this solution we consider the solution of the Schrödinger equation the solution of three dimensional Schrödinger equation for an electron confine in a box we found the energy levels and from the expression for the energy level we calculate at the density of states and then the expression for the total number of electrons inside the box and we applied it to the sodium metal and we assume that there is only one electron per atom then we calculated the Fermi energy at absolute zero.

Since the Fermi energy at absolute zero is much much greater than  $k_B T$  then we find that  $E_F$  was about three point two electron volt and at normal temperature  $k_B T$  is about one fortieth electron volt. So,  $E_F$  is much much greater than  $k_B T$  and therefore, say that at normal temperature at not too high temperature the electrons inside the metals is in an complete is in an almost completely degenerate state and what we imply is that as far as the Fermi function course.

We can assume a assume it assume the temperature to be absolute zero and we say all the states below  $E_F$  are filled up and all the states above  $E_F$  are empty. So, that concludes one one section of the course mainly the solution of the Schrödinger equation

for typical one dimensional and in the last case in three dimension also the solution of the Schrödinger equation for the particle in a box problem

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Angular Momentum Problem

$$\vec{L} = \vec{r} \times \vec{p}$$

$$L_x = y p_z - z p_y$$

$$L_y = z p_x - x p_z$$

$$L_z = x p_y - y p_x$$

$$p_x \rightarrow -i\hbar \frac{\partial}{\partial x}$$

$$p_y \rightarrow -i\hbar \frac{\partial}{\partial y}$$

$$p_z \rightarrow -i\hbar \frac{\partial}{\partial z}$$

$$L_z \psi = -i\hbar \left[ x \frac{\partial \psi}{\partial y} - y \frac{\partial \psi}{\partial x} \right]$$

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Our next topic of discussion is the angular momentum problem. So, we continue our discussion on the on the angular momentum problem now how do we start this in classical mechanics the angular momentum of a particle as you all know is defined by this following vector relation  $L$  is equal to  $R$  cross  $p$  where  $R$  is the position vector and  $p$  is the momentum vector.

So, if take as you all know  $L_x$  will be  $y p_z$  minus  $z p_y$  similarly  $L_y$  and similarly  $L_z$   $L_z$  will be  $x p_y$  minus  $y p_x$   $z p_x$  minus  $x p_z$  you have in cyclic order  $y z x$   $x y z$   $y z x$ . So, there in an  $x y z$ . So, they are all in cyclic order. So, these are the definitions of the  $x$   $y$  and  $z$  components in angular momentum of classical mechanics.

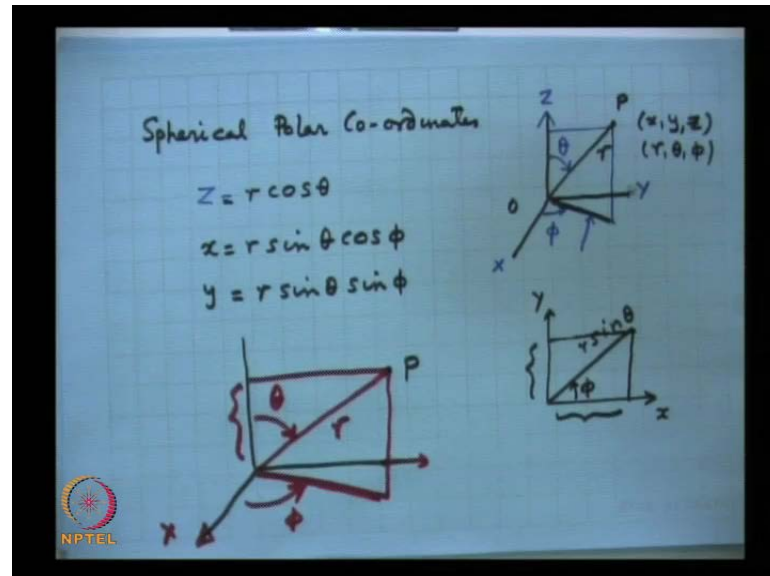
We take over the same definitions in quantum mechanics except now that we consider the operator representation of the  $p_x$   $p_y$  and  $p_z$  that is we replace  $p_x$  by minus  $i \hbar$  cross delta by delta  $x$  and  $p_y$  by minus  $i \hbar$  cross delta by delta  $y$  and  $p_z$  replaced by minus  $i \hbar$  cross delta by delta  $z$

So, they are now considered as operators for example,  $L_z$  will become equal two minus  $i \hbar$  cross  $x$ . So,  $L_z$  operating on a wave function will become  $x$  delta by delta  $y$  psi



minus  $y \delta \psi$  by  $\delta x$ . So, this is the operator representation and it will lead to very important consequences as we will just now show.

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However to discuss for the properties of the angular momentum operators it is necessary to introduce the spherical polar coordinates I am sure all of you are familiar with spherical polar coordinates and in this system of coordinates a point  $p$  as you all know is represented for example, as  $x y z$  and also as  $R \theta \phi$ .

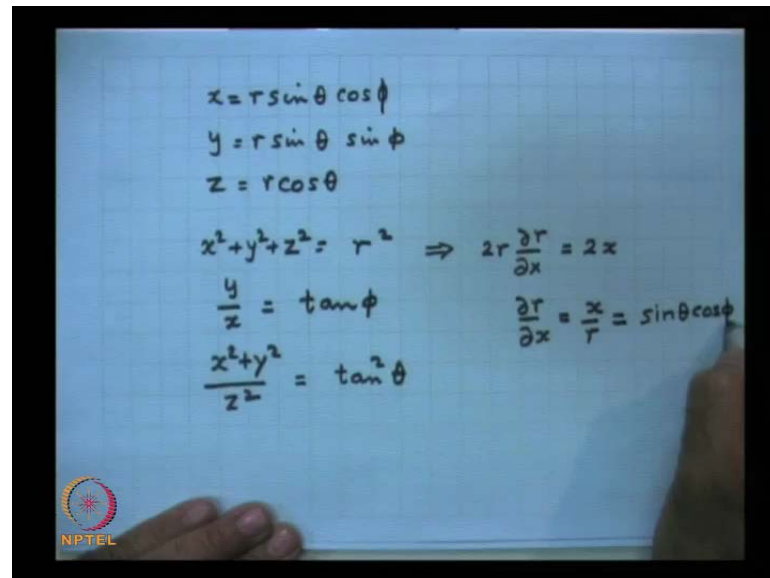
You this is the origin then this the point  $p$  this distance is  $R$  this is the  $z$  axis this angle this is known as the polar angle this is  $\theta$  and this is my  $x$  axis and this is the  $y$  axis. So, I drop a perpendicular on the  $x y$  plane and this angle is denoted by  $\phi$ . So, therefore, on the  $x y$  plane on the  $x y$  plane this length is equal to therefore, the  $z$  coordinate.

This  $z$  will be equal to the  $z$  is equal to  $R \cos \theta$  and if I drop the perpendicular here this length will be  $R \sin \theta$ . So, you have here the  $x$  and  $y$  axis  $x$  and  $y$  axis and this distance is  $R \sin \theta$  and this angle is  $\phi$  and therefore, this distance is  $R \sin \theta \cos \phi$   $x$  is equal to  $R \sin \theta \cos \phi$  and  $y$  is equal to  $R \sin \theta \sin \phi$  because you draw a perpendicular from here then this distance is equal to  $R \sin \theta \sin \phi$ .

So, once again if I have if I have any point  $p$  any point  $p$  here and therefore, if the the the distance here is  $R$  this is the azimuth angle this is  $\theta$  and. So, therefore, this distance is

$R \cos \theta$  then I drop a perpendicular on a  $x$   $y$  plane this is my  $x$  axis and this is the  $y$  axis this angle is  $\phi$  and this side is  $R \sin \theta$ . So, the  $x$  coordinate is  $r \sin \theta \cos \phi$  and the  $y$  coordinate is  $r \sin \theta \sin \phi$ .

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Handwritten mathematical derivations on a grid background:

$$x = r \sin \theta \cos \phi$$

$$y = r \sin \theta \sin \phi$$

$$z = r \cos \theta$$

$$x^2 + y^2 + z^2 = r^2 \Rightarrow 2r \frac{\partial r}{\partial x} = 2x$$

$$\frac{y}{x} = \tan \phi$$

$$\frac{x^2 + y^2}{z^2} = \tan^2 \theta$$

$$\frac{\partial r}{\partial x} = \frac{x}{r} = \sin \theta \cos \phi$$

An NPTEL logo is visible in the bottom left corner of the image.

Now, we will use the we will represent the angular momentum operators in in spherical polar coordinates. So, using this let me rewrite this. So, you have  $x$  is equal  $R \sin \theta \cos \phi$   $y$  is equal to  $R \sin \theta \sin \phi$  and  $z$  is equal to  $R \cos \theta$  if you square and add them then you will obtain  $x$  square  $y$  square plus  $z$  square you see this  $x$  square plus  $y$  square will be  $R$  square  $\sin$  square  $\theta$  because  $\cos$  square  $\phi$  plus  $\sin$  square  $\phi$  will become one. So,  $R$  square  $\sin$  square  $\theta$  plus  $R$  square  $\cos$  square that will be just  $R$  square. And the second will be that if I divide this. So, you will be having  $y$  by  $x$  will be  $\tan \phi$   $y$  by  $x$  will be  $\tan \phi$  and then  $x$  square plus  $y$  square by  $x$  square this will be  $R$  square  $\sin$  square  $\theta$  by  $R$  square  $\cos$  square  $\theta$ . So, that will be equal to  $\tan$  square  $\theta$ .

So, these are the three relations that relate the spherical these are the six relations. So, which relate the Cartesian coordinate with this spherical polar coordinates for example, here if I differentiate partially with respect to  $x$  i will get  $2 R \delta R$  by  $\delta x$  is equal to  $2 x$ . So, therefore,  $\delta R$  by  $\delta x$  will be equal to  $x$  by  $R$  and here this is  $R \sin \theta \cos \phi$ . So, this is just  $\sin \theta \cos \phi$

So, you will continue our discussions from this point onwards **thank you**.