Lecture - 05
Introduction of Quantum Mechanics in Solar Photovoltaics - III

Welcome everyone to our module five of this course. In the last few modules, we have learnt about some basic concept of quantum mechanics. We have started with Schrodinger equation as we have learnt that in the subatomic scale, we cannot use Newtonian mechanics. And we have also solved Schrodinger equation in two simple cases. In first, we have considered the particle in a box problem.

And then the second we have considered the particle in a finite potential well box. And we have applied some boundary condition to the solution of Schrodinger equation which gave us some physically admissible solution. And in terms of energy eigenvector and energy eigenfunction.

But now the question is even if we know the energy of the different state, how these electrons are occupied in the different states and what is the probability of the occupancy that will give that what is the number of the electron in different energy states. And finally, that is very important because that gives us the current conductions. So in this module, we will talk about that.

One important concept in this regard is Fermi-Dirac distribution function. It is worthwhile to mention that previously in the statistics we know there are three different types of statistics exist. One is Maxwell Boltzmann statistics another is Fermi-Dirac statistics another is Bose-Einstein statistics. But here we are talking about Fermi-Dirac distribution. What is Fermi-Dirac function?

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Fermi Distribution Function

- The kinetic energy of the electron gas increases with temperature. Therefore, some energy levels become occupied which were vacant at zero temperature, and some levels become vacant which were occupied at absolute zero.

- The distribution of electrons among the level usually described by the *distribution function, f(E)*, which is defined as the probability that the level E is occupied by an electron.

- Thus if the level is certainly empty then, $f(E) = 0$, while if it is certainly full, then $f(E) = 1$. In general $f(E)$ has a value between zero and unity

The kinetic energy of the electron gas increase with temperature. As we know that if the temperature increase, so the random thermal fluctuations of the electron about that mean position that also increase and which ultimately increase the kinetic energy. Therefore some energy level become occupied where some energy level become vacant at the temperature of absolute zero.

The distribution of the electrons among the different level is described by a distribution function. And that distribution function we call it f as a function of energy E, which is defined as the probability that the level E is occupied by an electron. So the distribution function gives us the probability of occupancy of a energy state with energy E by an electron.

Thus if the level is suddenly empty if that means if there is no electron in the state, then the probability of occupancy is zero. That is why we write that f E is equal to zero. Whereas, if the probability of occupancy is complete, if the state is certainly full, then we can write f E = 1. And since it is a probability value, all other value can run between 0 and 1. So in general, f E has a value between zero and unity.
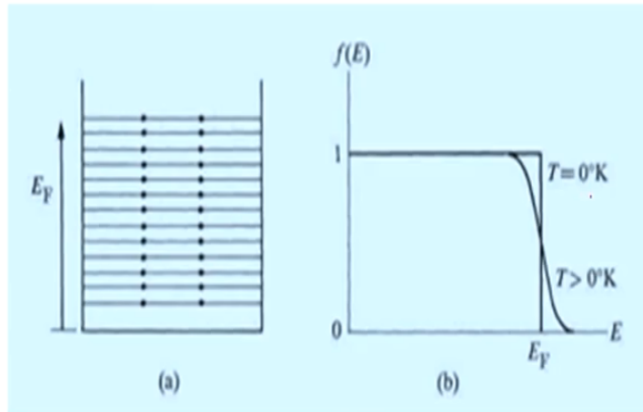
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Fermi Distribution Function

Fig:- (a) Occupation of energy levels according to the Pauli exclusion principle, (b) The distribution function $f(E)$, at $T = 0$ K and $T > 0$ K.

In this diagram, we are showing how does the Fermi-Dirac distribution function looks like. You look at in our diagram figure a, there are some energy level which we have drawn; x axis is the energy and we have drawn few energy levels which are discrete and electrons they are occupying this energy levels. But how the electrons are distributed among the different energy levels at absolute zero that probability is given by Fermi-Dirac distribution function.

And that we have plotted here in figure b where the distribution function f E at T = 0 Kelvin and T greater than 0 Kelvin is plotted.

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Fermi Distribution Function

- It follows from the preceding discussion that the distribution function for electrons at $T = 0$ K has the form

$$f(E) = \begin{cases} 1, & E < E_F \\ 0, & E > E_F \end{cases}$$

- That is, all levels below E_F are completely filled, and all those above E_F are completely empty. This function is plotted in Fig. (b), which shows the discontinuity at the Fermi energy.

The function is such that the value of this probability function f E is zero when E greater than the Fermi energy F and it is 1 where E less than F. It follows from the

preceding discussion that the distribution function for the electron at T = 0 Kelvin has the form f E = 1 when E is less than E F and f E = 0 when E greater than E F. Let us look at the previous diagram.
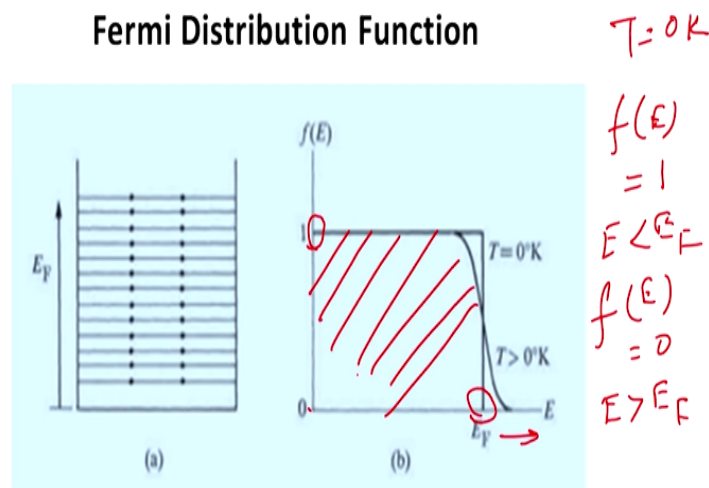
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Fig:- (a) Occupation of energy levels according to the Pauli exclusion principle, (b) The distribution function f(E), at T = 0 K and T > 0 K.

So this is the energy E = E F. When the value of E is less than E F then your y axis value is 1. So f E = 1 when E less than E F. And when the value of E is greater than E F that means in this region the function value is 0, the y axis value is 0, you see here. So f E = 0 when E greater than E F. So that means this function has an abrupt discontinuity at this particular point E F.

And all this phenomena is happening at T = 0 Kelvin. So we can say that T = 0 Kelvin there is an energy level E = E F below which all the energy states are occupied and above which the all the energy states are empty and this particular energy level is called the Fermi energy. So that is all level below f are completely filled and all those above f are completely empty.

And this function is plotted in figure b which shows the discontinuity at the Fermi energy. But again it is important to mention that we are considering here the temperature at 0 Kelvin. If we go to some other temperature the distribution function will looks different form.

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Fermi Distribution Function

- When the system is heated ($T > 0$ K), thermal energy excites the electrons. However, all the electrons do not share this energy equally, as would be the case in the classical treatment, because the electrons lying well below the Fermi level E_F cannot absorb energy. If they did so, they would move to a higher level, which would be already occupied, and hence the exclusion principle would be violated

What will happen if we increase the temperature now when the system is heated that means T greater than 0 Kelvin, thermal energy excites the electron. However, all the electrons do not share the energy equally as would be the case in the classical treatment. Because the electrons lying well below the Fermi energy or E F cannot absorb energy.

If they did so, then they would move to a higher level which could already be occupied and thus it will obviously violate the so called Pauli exclusion principle. So that means all the electrons cannot absorb the similar amount of energy. Previously, we have learnt like particle in a box problem if I have one particle in an one dimensional box, how to solve the Schrodinger equations and what are the energy eigenvalue and what are the wave function.

But here we are considering a more realistic case an electron in an atom. An atom is a three dimensional example. So now the problem statement is we need to solve the particle in a three dimensional box. Similar to one dimensional model Fermi energy for free electron gas in three dimension can be calculated.

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Free Electron Model in three Dimension

Similar to one dimension model Fermi energy for free electron gas in three dimension is calculated. From Schrödinger equation in three dimension

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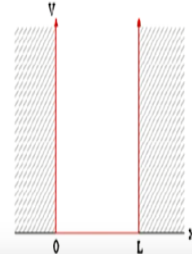$$\left[-\frac{\hbar^2}{2m}\nabla^2\right]\Psi = E\Psi \cdots\cdots(1)$$

Potential inside the three dimensional box is considered zero and infinite at the walls as shown in the Fig. then

$$\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\frac{\partial^2\Psi}{\partial z^2}+k^2\Psi = 0\cdots(2)$$

Then using the method of separation of variables we got

$$\Psi(x,y,z) = \Psi_x(x)\Psi_y(y)\Psi_z(z)\cdots\cdots(3)$$

Now we can write the Schrodinger equations in three dimension like this following equation 1, minus h bar square by 2m del square psi is equal to E psi. Here this quantity which is pronounced as a del is a Greek later. It is a three dimensional analog of del square plus del x square plus del square del y square plus del square del z square.

Potential inside the three dimensional box is considered zero and infinite at the walls. So here you take the same example of a particle in a box but this potential is a three dimensional case here. Here the potential is zero but at the two side potential blows out. But the box is now a three dimensional box. So I can write down, I can expand this operator in the three scalar form.

So I can write del square psi del x 2 plus del square psi del y 2 plus del square psi del z 2 plus kappa square psi is equal to 0. Where you already know what is the definition of the kappa that is square root of 2mE by h bar square. Then using the our favorite method of separation of variable we can write the wave function psi which is now depends on three spatial coordinates x, y, and z. So we can write it as a product of a function which depends only on x.

A product of a function which depend only on y and a function which depends only on z. And if we substitute this value of psi as a product of a function which depends on x, y and z into our equation 2 what we will get is the following.

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Free Electron Model in three Dimension

Substituting equation (3) in equation (2) and dividing by $\Psi_x \Psi_y \Psi_z$ we got

$$\frac{1}{\Psi_x(x)}\frac{\partial^2 \psi}{\partial x^2} + \frac{1}{\Psi_y(y)}\frac{\partial^2 \psi}{\partial y^2} + \frac{1}{\Psi_z(z)}\frac{\partial^2 \psi}{\partial z^2} + k^2 \psi = 0$$

This makes the equation valid for all possible x , y and z terms only if terms including $\Psi_x(x)$ $\Psi_y(y)$ and $\Psi_z(z)$ are individually equal to a constant :-

$$\frac{1}{\Psi_x(x)}\frac{\partial^2 \psi}{\partial x^2} = -k^2$$

$$\frac{1}{\Psi_y(y)}\frac{\partial^2 \psi}{\partial y^2} = -k^2$$

$$\frac{1}{\Psi_z(z)}\frac{\partial^2 \psi}{\partial z^2} = -k^2$$

Where $k^2 = k_x^2 + k_y^2 + k_z^2$.

$$\frac{1}{\Psi_x(x)}\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0$$

And if we further divide the equation by this product psi x, psi y, and psi z so we will get this equation 1 over psi x del 2 psi del x 2 plus 1 over psi y as a function of y del 2 psi del y 2 plus 1 over psi z del 2 psi del z 2 plus kappa square psi is equal to 0. You remember in the one dimensional case we have only one equation. We have only one equation 1 over phi del 2 phi del x 2 plus kappa square psi is equal to 0.

But in three dimension we have x coordinate, we have y coordinate, and we have z coordinate. That is why the wave function depends upon three different coordinates. That is why there are three partial derivative, one on x another on y, another on z and then the terms which contains the energy This makes the equation valid for all possible values of x, y, and z.

And it is possible only if the terms including psi x, psi y, and psi z are individually equal to a constant. So what we can do here we can write the first part along with this kappa square part is equal to a constant, second part is equal to a constant, and third part is equal to a constant. So we write it mathematically by the following three equation. 1 over psi x the first part into delta psi del x 2 plus kappa square psi is equal to 0.

If we take kappa in the right hand side we will get minus kappa square. So here we are doing where psi x as a function of x, del 2 psi del x 2 plus kappa square psi is equal to 0. Now it is only possible if this terms is individually equal to a constant. So

what we can write 1 over psi x del 2 psi del x 2 is equal to minus kappa square. Similarly, I can write the second terms which is dependent on y.

I can write the third term which is dependent on z and the total kappa square value is k x square plus k y square plus k z square or kappa x square plus kappa y square plus kappa z square.

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Free Electron Model in three Dimension

The solutions to the wave equation where V(x) = 0 are sine and cosine functions

$$\Psi = A Sin(k_x x) + B Cos(k_x x)$$

Since the wave function equals zero at the infinite barriers of the well, only the sine function is valid.

Thus, only the following values are possible for the wave number k :-

$$k_x = \frac{n_x \pi}{L}, k_y = \frac{n_y \pi}{L}, k_z = \frac{n_z \pi}{L}$$

Recalling from the density of states 3D derivation k-space volume of single state cube in k-space is :-

$$V = \left(\frac{\pi}{a}\right)\left(\frac{\pi}{b}\right)\left(\frac{\pi}{c}\right) = \frac{\pi^3}{V}$$

Now the solutions of this wave equation where V x is equal to zero that will you know that it depends on sine and cosine function. So the wave function solution for the x it will be psi is A sin k x x plus B cosine k x x. And similarly we will get for the y component, similarly we will get for the z component. Since the wave function equals zero at the infinite barriers of the well only the sine function is valid.

So basically if we put that, if we boundary condition that the wave function is zero at the infinite barriers of the well, that means if we put x is equal to zero the wave function psi is equal to zero and if I apply this boundary condition in this particular equation, what will happen? A sin 0, sine 0 is 0 plus B cosine 0; B cosine 0 is 1. And the left hand side is zero. So my zero is equal to 0 plus 1 into B.

So that means B is equal to zero. So these terms goes out or cancels leaving psi is equal to A sine k x x. Thus only the following possible values of the wave number are allowed where k x is equal to n pi x by L, k y is equal to n pi y by L and k z is equal to n z pi by L. And these are here n is has a individual component along x, y, and z. So

we can also write the total solution as a product of the x component, as a product of the y component and the z component.

Recalling from the density of stress 3D derivation now if we all everything is in a k-space, so the volume of the single state cube in a k-space is V is equal to pi by a into pi by b by pi by c. So here as we know that if we go from a simple space to a k-space or reciprocal space, that each of the dimension like a is replaced by its reciprocal that is vector 1 by a.

So similarly for b we have 1 over b and for c we have 1 over c. So if I multiply this thing pi over a pi over b into pi over c I will get the volume of the sphere in the k-space and that is equal to pi cube divided by a into b into c or pi cube by V where V is equal to a into b into c.
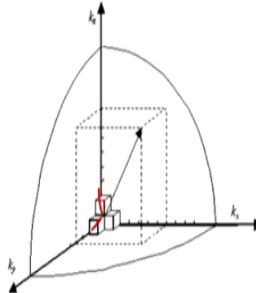
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Free Electron Model in three Dimension

k-space volume of sphere in k-space :- $V_{Sphere} = \frac{4\pi k^3}{3}$ where $k = \sqrt{\frac{2mE}{h^2}}$

Then Number of filled states in a sphere :-

$N = V_{Sphere} / V_{Single\text{-}state} \times 2 \times \left[\frac{1}{2} \times \frac{1}{2} \times \frac{1}{2}\right]$

$N = \frac{4\pi k^3}{\frac{\pi^3}{V}} \times 2 \times \left[\frac{1}{2} \times \frac{1}{2} \times \frac{1}{2}\right]$

A factor of two is added to account electron spins

Correction factor for redundancy in for the two possible identical states

k-space volume of the sphere in k-space so that we can write V sphere is 4 pi by 3 k cube where k is here root over 2mE by h bar square. Then number of filled states in a sphere N is equal to the volume of the total sphere divide by the volume of a single state into 2 that comes due to the spin degeneracy into 3 times half. And that half comes because of the correction for the redundancy of the two possible identical state.

So the N, the total number of filled state in the sphere is the volume of the sphere which is 4 pi by 3k cube that we have written in the numerator divided by volume of a single state that is pi cube by V, pi cube by a into b into c into 2 where the factor of 2

comes from the electron spins. We know that electron has two different kind of spin state, spin up and spin down.

So in every case we have to multiply with two possible combination. That is why we multiply it by this factor 2. And every time there is a possibility that we are considering the states the same states two time, along the x dimension, along the y dimension, as well as the z dimension. To get rid of that we multiply the whole things by three times half.

So the correction factor for the redundancy in the two possible identical state has been removed by multiplying half in the each dimension. If we plot this thing you can look like this. Here x axis is like cakes, this is your k x, this is your k y and this is your k z and these are the like a normal cube and these are the small cube which is occupied here.

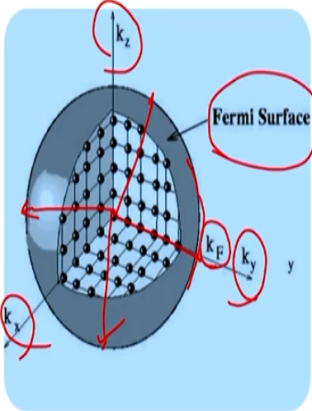**(Refer Slide Time: 15:21)**

Free Electron Model in three Dimension

$$N = \frac{k^3 L^3}{3\pi^2} = \frac{k^3 V}{3\pi^2}$$

Here k_F is the radius of Fermi sphere and known as Fermi wave vector k_F have components like k_x, k_y, k_z
So now no. of electrons N will be

$$N = \frac{k_F^3 L^3}{3\pi^2} = \frac{k_F^3 V}{3\pi^2}$$ on further modifications

in equation we got:-

So the value of N by this statement will comes out N is equal to k cube L cube by 3 pi square. Now L cube you can write it as a V. So you can write k cube V by 3 pi square where k F is the radius of Fermi sphere and known as the Fermi wave vector k V and components as k x, k y, and k z. Let us look at this sphere. The surface of this sphere is called the Fermi surface.

And the energy on the surface of the sphere is called the Fermi energy E F and I have drawn k F, k x in this way, k y in this way and k z on the vertical directions. And the k

vector which has a radius of this sphere that is the Fermi wave vector and the energy on the surface of the sphere that is called the Fermi surface. So k F is the radius of the Fermi sphere as you can see from this diagram.

You can draw it here, you can draw it here, that is also k F, that is also k F, that is also k F. This is the wave, the radius of the sphere and you call it as a Fermi wave vector k F. And since we have now three different direction so it will have three different components k x, k y, and k z. So the number of electrons the N will be k cube into L cube divide by 3 pi square or k F cube into V by 3 pi square on further modification.

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Or we can write k F is equal to 3 pi square N by V to the power whole 2 by 3.

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It follows from the previous equations, if you write N is equal to K F cube V divide by 3 pi square. So I can write here that 3 pi square N by V is equal to K F cube, right? 3 pi square N by V is equal to K F cube. So 3 pi square N by V F square is equal to k F cube. So K F will be 3 pi square N by V to the power 2 by 3. You can consider that it is a Fermi velocity or you can consider the volume as V.

So K F is equal to 3 pi square N by V two third. K F is the Fermi wave vector and it has a also a form you can write E F is equal to h bar square K square by 2m. That comes from the momentum formula. So we can write E F is equal to if we substitute the value of K from here what we will get? E F is equal to h bar square by 2m, this h bar square into 2m into 3 pi square N by V two third.

That is what we have written, 3 pi square N by V two third. And similarly the Fermi velocity V F is h bar by 2m 3 pi square N by V one third where N by V that gives the number of electron per unit volume and it is called an electron density. So you can also replace this electron density by the small letter n, small n. So we have found out like how to distribute the electrons in the different states.

But it does not mean that all the electron states are available. In this context a very important idea is the density of states.

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Density of States

❖ The **density of states (DOS)** of a system describes the number of states per interval of energy at each energy level available to be occupied. It is mathematically represented by a density distribution and it is generally an average over the space and time domains of the various states occupied by the system.

❖ A high DOS at a specific energy level means that there are many states available for occupation. A DOS of zero means that no states can be occupied at that energy level.

❖ Moreover The density of states function describes the number of states that are available in a system and is essential for determining the carrier concentrations and energy distributions of carriers within a semiconductor.

The density of states or DOS of a system describes the number of states per interval of energy at each energy level available to be occupied. It is mathematically represented

by a density distribution and is generally an average over the space and time domains of the various states occupied by the system. Let us give a good example. Let us say in a typical classroom there are hundred benches are there and there are hundred students are there.

It does not mean that all the bench has been occupied by the all the students. It is very much possible that some students are absent. Since we have hundred bench in this room, we cannot say that all the benches have been occupied by the all the students. It depends upon how many students are present there. Density of state similarly talks about how many available benches available for the electron to occupy.

Just like in a classroom bench tells it like how many benches are available for the students, density of states tells you how many energy states are available for the electron to occupy them. A high density of states at a specific energy level means that there are many states available for occupation. If a density of states is zero, that means no states can be occupied at a particular energy.

So even if the electrons are there, if the density of states value determine what will be the occupancy. Moreover, the density of state function describes the number of states that are available in a system and is essential for determining the carrier concentration and energy distribution of carriers within a semiconductor. We represent the density of states by different symbols.

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Density of States

❖ The DOS is usually represented by one of the symbols g, ρ, D, n, or N and can be calculated by :-

$$D(E) = \frac{dN}{dE}$$

❖ In semiconductors, the free motion of carriers is limited to two, one, and zero spatial dimensions. So DOS can be calculated in three, two, one and zero dimensions.

One of the symbols you can use either by g or rho or D, n or capital N. Different textbooks follows different format. Here we are using this format where we are representing the density of states by the capital letter D as a function of E and we can write it as dN dE. So physically what it means that it is the number of available energy states per unit energy between E and E + D.

So density of states tells you the number of available energy states to the electron per unit energy range. In a semiconductor the three motions of the carrier is limited by two, one, or zero or spatial dimensions. So the density of states can be calculated either for zero or for one or for two or even for three dimensions.

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Density of States in Three Dimension

Here energy from three dimensional free atomic model is

$$E_F = \frac{\hbar^2}{2m}(3\pi^2 N/V)^{\frac{2}{3}} \longrightarrow \left(\frac{2mE_F}{\hbar^2}\right)^{3/2} = 3\hbar^2\left(\frac{N}{V}\right)$$

$$N = \frac{V}{3\pi^2}\left(\frac{2mE}{\hbar^2}\right)^{3/2} \quad\checkmark \qquad \Rightarrow N = \frac{V}{3\hbar^2}\left(\frac{2mE}{\hbar^2}\right)^{3/2}$$

and density of states in three dimension will be:-

$$D(E) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2} \qquad D(E) = \frac{dN}{dE}$$

as stated initially for effective mass $m \to m^*$ density of states will be

$$D(E) = \frac{V}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2} E^{1/2}$$

Let us look at how does the density of states looks like in a three dimension because that is the more physically realistic situation. Energy from three dimension as we have learned so far in a free atomic model is E F is equal to h bar square by 2m 3 pi square N by V two third and you can pull out N from these equations and you can write N is if I rearrange this equation little bit we will get N is V by 3 pi square 2m E by h bar square to the power 3 by 2.

You can simply follow this from here. So if I multiply the left hand side by 2mE F by h bar square times 3 by 2 is equal to 3 pi square N by V. Now we need to calculate this N. So N is equal to V goes here in the top divided by 3 pi square into 2mE divide by h bar square to the power 3 by 2. That is exactly we have written here. And that is what the N capital N comes, the number of electrons.

And we have defined the density of states. Density of states D that is the number of available energy states per unit energy. So what you have to do, we have to differentiate this function as with respect to E. So that is what we have done here so and that gives that D is equal to V by 2 pi square 2m by h bar square to the power 3 by 2 into E to the power half.

So that means in three dimension density of states is proportional to the E to the power half of square root of energy. Now we know that in a periodic lattice or any crystal electron mass is represented by the effective mass. So effective mass actually comes from the idea of a complex potential distribution functions. So if you replace the effective mass as m is equal to m star, density of states will be D E is V by 2 pi square 2m star by h bar square 3 by 2 E to the power half.

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Density of States in Three Dimension

and finally effective density of states per unit volume is

$$D(E) = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}(E - E_c)^{1/2}$$

And finally, effective density of states per unit volume D is equal to 1 by 2 pi square 2m star by h bar square to the power 3 by 2 E minus E c to the power whole half where E c is the conduction band energy.

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Density of States in Two Dimension

For calculating the density of states for a 2D structure, we can use a similar approach as 3D, the previous change to the following:-

k-space volume of single state cube in k-space is :-

$$V = \left(\frac{\pi}{a}\right)\left(\frac{\pi}{b}\right) = \frac{\pi^2}{L^2}$$

k-space volume of sphere in k-space :-Vcircle $= \pi k^2$

Then Number of filled states:-

$$N = V_{circle} / V_{Single\text{-}state} \times 2 \times \left[\frac{1}{2} \times \frac{1}{2}\right]$$

$$N = \frac{k^2 L^2}{2\pi} \qquad \text{where k=} \sqrt{\frac{2mE}{h^2}}$$

Similarly, we can calculate the density of states in two dimension. For calculating the density of states for a 2D structure, we can use a similar approach as 3D, the previous change to the following. K-space volume of the single state cube in k-space. Here instead of three dimensions in two dimension we have two different dimension. So we can take either a and b or a and c or b and c.

In this particular case, we have taken a and b. So the volume is pi by a into pi by b. That is pi square divided by a into b. So you have two different dimension, so we have written pi square divided L square. K-space volume of the sphere in k-space if you write what is the volume of a sphere in a k-space? V circle that is pi k square because we are considering here two dimensional case pi r square.

Then the number of filled states will be a N is equal to V circle, the total volume of the circle divided by the volume one single state can occupy into 2 that comes from the spin degeneracy into two times half just to avoid the redundancy because we can calculate the same state twice. If we do that, we will get N is equal to k square L square by 2 pi where k is equal to root over 2mE by h bar square.

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Density of States in Two Dimension

$$N = \frac{\left(\sqrt{\frac{2mE}{\hbar^2}}\right)^2 L^2}{2\pi} = \frac{mL^2 E}{\pi\hbar^2}$$

The density per unit energy is then obtained as:-

$$\frac{dN}{dE} = \frac{mL^2}{\pi\hbar^2}$$

The density per unit energy ,per unit volume is:-

$$g(E)_{2D} = \frac{\frac{mL^2}{\pi\hbar^2}}{L^2} = m/\pi\hbar^2$$

as stated initially for effective mass $m \rightarrow m^*$ density of states will be

$$g(E)_{2D} = m^*/\pi\hbar^2$$

And N comes like square root of 2mE by h bar square whole square L square divide by 2 pi is equal to mL square E by pi h bar square. And as you know the density of states is obtained by differentiating this equation with respect to E if we do that, we will get dN dE is equal to mL square pi h bar square because if you differentiate this quantity with respect to the energy, so then this will go.

And what will left out is dN by dE is equal to mL square by pi h bar square. So the density per unit energy per unit volume that can be written as g in a two dimension is mL square by pi h bar square divided by L square. So L square and L square cancels out, this L square and this L square leaving you m divided by pi h bar square. And if you replace this m as the effective mass m star so the density of states will be g E 2D is equal to m star by pi h bar square.

Because now we have replaced the m with the effective mass m star, okay. So we have considered the three dimensional case, we have considered the two dimensional case. Now let us consider the one dimensional case.

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Density of States in One Dimension

For calculating the density of states for a 2D structure, we can use a similar approach as 3D, the previous change to the following:-

k-space volume of single state cube in k-space is :-

$$V = \left(\frac{\pi}{a}\right) = \frac{\pi}{L}$$

k-space volume of sphere in k-space :- $V_{Line} = k$

Then Number of filled states:-

$$N = V_{circle} / V_{Single\text{-}state} \times 2 \times (1/2)$$

$$N = \frac{k}{\pi/L} \times 2 \times \left[\frac{1}{2}\right]$$

(handwritten) $W = \dfrac{k}{\pi/L}$

For calculating the density of state for a 2D structure, we can use a similar approach as 3D, the previous change to the following; k-space volume here, since we are considering only one dimension, so the volume of the k-space of a single state cube will be V is equal to pi over a that is pi by L. Now k-space volume of the sphere in the k-space, that is only a line that is simply K.

So the number of filled state will be V line divided by V single state into 2 that comes from the spin degeneracy into half. That is to avoid the redundancy because there is a possibility that we can count the same state twice. So if we do that, what we will get is the following; k divide by pi by L in the first term into 2 into half. So this 2 and this 2 cancels out leaving out N is equal to k divide by pi by L. This L goes up.

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Density of States in One Dimension

$$N = \frac{kL}{\pi} \qquad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$N = \sqrt{\frac{2mE}{\hbar^2}} L/\pi = \sqrt{2mE}\, L/\hbar\pi$$

The density per unit energy is then obtained as:-

$$\frac{dN}{dE} = \frac{(2mE)^{-\frac{1}{2}} mL}{\hbar\pi}$$

The density per unit energy ,per unit volume is:-

$$g(E)_{1D} = \frac{\frac{(2mE)^{-\frac{1}{2}} mL}{\hbar\pi}}{L} = \frac{(2mE)^{-\frac{1}{2}} m}{\hbar\pi}$$

(handwritten)

$$N = \frac{(2mE)^{1/2} L}{\pi\hbar}$$

$$= \frac{(2m)^{1/2} L\, E^{1/2}}{\pi\hbar}$$

$$\frac{dN}{dE} = \frac{1}{2} E^{-1/2} \frac{(2m)^{1/2} L}{\pi\hbar}$$

So you get N is equal to kL over pi where your k or sometimes this is called kappa is equal to square root of 2mE by h bar square. So your n is equal to square root of 2mE by h bar square where I have replaced this value of k with here k. I will get this factor times L by pi. So we can also write as square root of 2mE L by h bar because h bar square if you take a square root the h bar will come outside the square root and h bar into pi.

To find out the density of states again the same protocol what you have to do. We have to differentiate the N with respect to the energy. Let us do that. And what we get is the following. dN dE is equal to 2mE to the power minus half mL divide by pi h barr. So you have N is equal to 2mE to the power whole half L by pi h bar. You can also write it as 2m to the power whole half L divide by pi h bar into E to the power half. We can write also that.

So now we have to do dN dE. So basically it will be half minus 1 that is minus half, right? And you have the same constant 2m divide by pi h bar and L. So thus you will get this quantity. So density of state per unit energy per unit volume you can write as gE one dimension is 2mE to the power minus half mL by h bar pi divide by L. So you can write it also 2mE by minus half m divide by h bar pi.

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Density of States in One Dimension

and finally $g(E)_{1D} = (1/\hbar\pi)\sqrt{m/2E}$
as stated initially for effective mass $m \rightarrow m^*$ and also kinetic energy $E \rightarrow E_c$ then density of states will be:-

$$g(E)_{1D} = (1/\hbar\pi)\sqrt{m^*/2(E - E_c)}$$

Play (k)

And finally, if I simplify it finally, we will get the density of states for a case of one dimension is one over pi h bar square root of m by 2E. As stated initially for effective mass m is equal to m star and also kinetic energy if E goes to the E c that is the

conduction energy, then the density of states will be we replace here with m with m star and you replace E with E minus E c. So what do you will get this following; g E 1D is equal to 1 over pi h bar square root of m star by 2 E minus E c. One can also calculate the density of states for zero dimension.

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Density of States in Zero Dimension

When considering density of states for a 0D structure (i.e. quantum dot),no free motion is possible. Because there is no k-space to be filled with electrons and all available state exist only at discrete energies , density of states for 0D is described by delta function.

$$g(E)_{0D} = 2\delta(E - E_c)$$

When considering density of states for zero dimensional structure that is an example is a quantum dot. What is a quantum dot? A quantum dot are a fine particle whose dimensions are between 1 to 10 nanometer. So this particle, so size dependent optical properties and sometimes science dependent electrical properties and they are very interesting for the fabrications of solar cell, light emitting diode and different optoelectronic properties.

Now to find out the number of electrons or how the electrons are distributed there, it is important to find out what is the density of states in this zero dimensional quantum dot structure. So here the motion is confined, so no free motion is possible. Because there is no k-space to be filled with electrons. And all available state exist only at a discrete energies.

Density of state for zero dimension is described usually by a delta function where g E gE 0D is equal to 2 into delta function E – E c. So we have leaned like you know what does or how the density of states to be calculated in the case of a three dimension, two dimension, one dimension as well as zero dimension.

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Density of States

Degrees of freedom	Dispersion (kinetic energy)	Density of states	Effective density of states
3 (bulk)	$E = \dfrac{\hbar^2}{2m^*}(k_x^2 + k_y^2 + k_z^2)$	$\rho_{DOS}^{3D} = \dfrac{1}{2\pi^2}\left(\dfrac{2m^*}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{E - E_C}$	$N_c^{3D} = \dfrac{1}{\sqrt{2}}\left(\dfrac{m^* kT}{\pi \hbar^2}\right)$
2 (slab)	$E = \dfrac{\hbar^2}{2m^*}(k_x^2 + k_y^2)$	$\rho_{DOS}^{2D} = \dfrac{m^*}{\pi \hbar^2}\sigma(E - E_C)$	$N_c^{2D} = \dfrac{m^*}{\pi \hbar^2}kT$
1 (wire)	$E = \dfrac{\hbar^2}{2m^*}(k_x^2)$	$\rho_{DOS}^{1D} = \dfrac{m^*}{\pi \hbar}\sqrt{\dfrac{m^*}{2(E - E_C)}}$	$N_c^{1D} = \sqrt{\dfrac{m^* kT}{2\pi \hbar^2}}$
0 (box)	–	$\rho_{DOS}^{0D} = 2\delta(E - E_C)$	$N_c^{0D} = 2$

Now if we plot this thing, how does it will look like, that is also interesting to see. But before that, let us tabulate our whole calculation. In the case the 3, 2, 1 or 0, we called as a degrees of freedom. And the example, corresponding example is given in the bracket. If a three dimensional system for an example a bulk system anything like bulk chalk. Second system is a slab, is a two dimensional system.
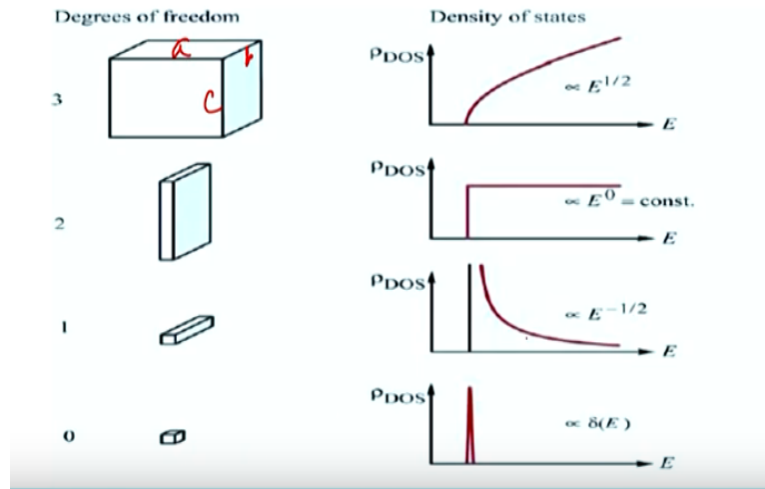
Third system is a one dimensional system, like a wire. And the last systems is a zero dimensional system. In the case of a three dimensional system energy h bar square by 2m star , k x square plus k y square plus k z square. We have all three different components k x, k y, and k z. In the case of a two dimensional we have two component, k x and k y. In the case of a one dimensional case, it has only k x square.

Now the density of states in the case of the three dimensional row density of state is 3D, that is one over 2 pi square 2m star by h bar square to the power 3 by 2 square root of E – E c. So it depends on square root of E – E c. In a case of a two dimensional case it is m star by pi h bar square sigma E – E c. In the case of a one dimension case it is m star by pi h bar square root of m star by 2 into E – E c.

Whereas in the case of a zero dimensional case it is a delta function, 2 delta E – E c. In the extreme right hand column we are showing the effective density of states.

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Density of States

Degrees of freedom

Density of states

3

ρ_{DOS} $\propto E^{1/2}$ E

2

ρ_{DOS} $\propto E^0 = $ const. E

1

ρ_{DOS} $\propto E^{-1/2}$ E

0

ρ_{DOS} $\propto \delta(E)$ E

In this diagram we are plotting the density of states for the different degrees of freedom and how does it look like.In the case of a three dimension an example is a cube here. You see you have three dimension; a, b, and c. So the density of states looks like this. In the case of a two dimension it looks like this. In the case of a one dimension it looks like E to the power minus of and the case of a zero dimension, it is a delta function.

It is very important to remember this diagram, because this will help us further to calculate the number of electrons in the corresponding states. Once we know the density of states, and if we know the Fermi-Dirac distribution function, the total number of electron in that state will be simply the product of the density of states and the Ferm-Dirac distribution function.

So depending on the structure, whether it is a bulk state or whether it is a three dimensional state, or whether it is a two dimensional state, if we know the density of function if we simply multiply the density of one state with the Fermi distribution function and if we integrate it over the specified energy level we will get the number of electrons.

Once we can find out the number of electrons it is also easy to find out the another type of charge carrier like number of holes. And that we will do in our next module. In our next class we will start with the basic semiconductor physics and we will show

how to calculate the number of electrons and number of holes in the systems which we will follow up with our device physics. Thank you.