Introduction to Solid States Physics

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Lecture – 17
Density of states Part – II

In the last lecture, we had come across the concept of the Density of states.

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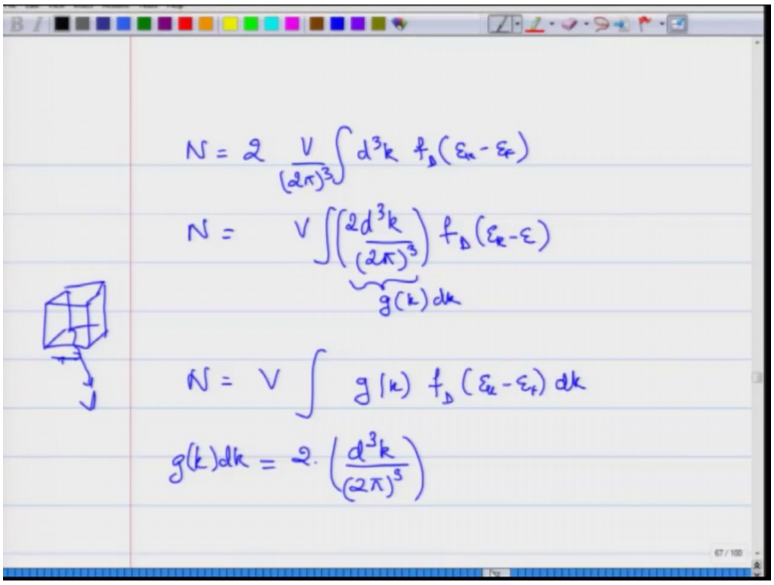

$$N = 2\frac{V}{(2\pi)^3}\int d^3k\, f_D(\varepsilon_k - \varepsilon_F)$$

$$N = V\int \underbrace{\left(\frac{2d^3k}{(2\pi)^3}\right)}_{g(k)\,dk} f_D(\varepsilon_k - \varepsilon)$$

$$N = V\int g(k)\, f_D(\varepsilon_k - \varepsilon_F)\, dk$$

$$g(k)dk = 2\cdot\left(\frac{d^3k}{(2\pi)^3}\right)$$

Basically, if you do a counting of the total number of particles then the total number of particles we had seen you can write it as 2, which is each state has two electrons spin up and spin down. 2 pi cube by V is nothing else, but the smallest volume in the phase space, integrated over the entire phase space or entire momentum space, you integrated over the entire momentum space and the occupancy of every state is given by this E K minus E F and so, we can rewrite this N as equal to integral of 2 into d cube k by 2 pi cube into the Fermi Dirac distribution and this quantity is 2 into d cube by 2 pi cube.

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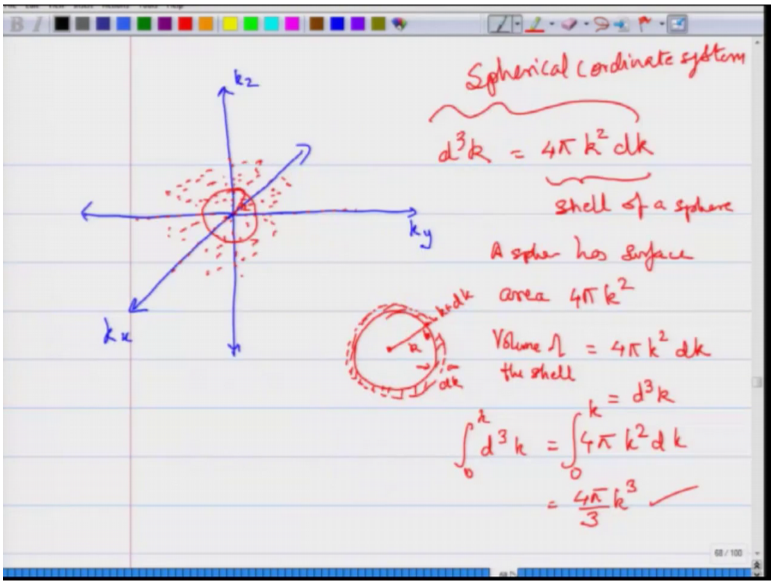

Spherical coordinate system

$$\underbrace{d^3k = 4\pi k^2 dk}_{\text{shell of a sphere}}$$

A sphere has surface area $4\pi k^2$

Volume of the shell $= 4\pi k^2 dk = d^3k$

$$\int_0^k d^3k = \int_0^k 4\pi k^2 dk = \frac{4\pi}{3}k^3 ✓$$

This is the total number of states which are present between k and k plus dk which is what we had calculated that assuming that there is no asymmetry in the momentum distribution of the electrons and it is completely spherically symmetric. To find out how many states are present between k and k plus dk we consider it as a spherical shell whose volume is 4 pi k square dk. This is the volume of the spherical shell between k and k plus dk; you divide it by the smallest volume which is available.

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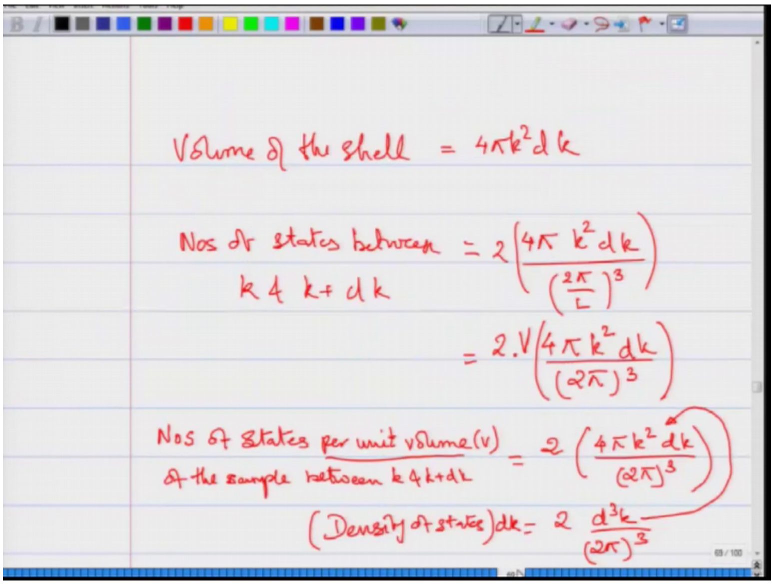

Volume of the shell $= 4\pi k^2 dk$

Nos of states between k & k+dk $= 2\left(\frac{4\pi k^2 dk}{\left(\frac{2\pi}{L}\right)^3}\right)$

$$= 2.V\left(\frac{4\pi k^2 dk}{(2\pi)^3}\right)$$

Nos of states per unit volume (V) of the sample between k & k+dk $= 2\left(\frac{4\pi k^2 dk}{(2\pi)^3}\right)$

(Density of states)dk $= 2\,\frac{d^3k}{(2\pi)^3}$

And, then you will have a measure of the density of states.

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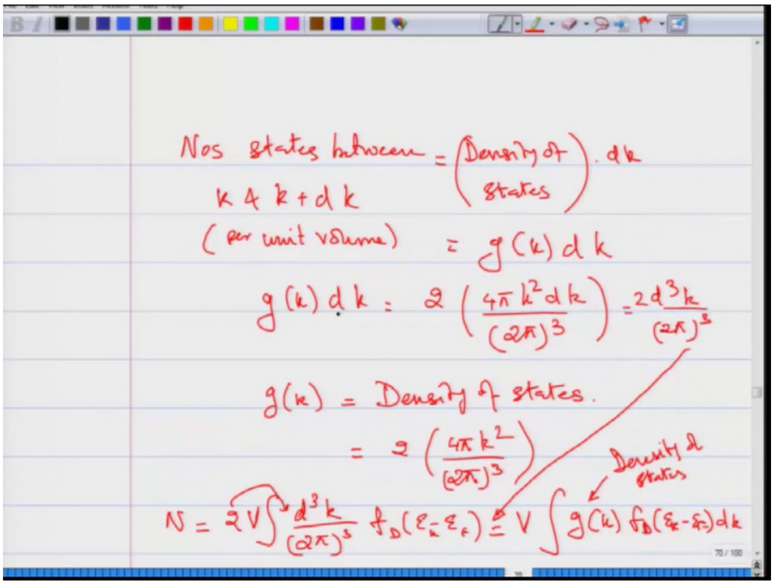

Nos states between k & k + dk (per unit volume) $= \left(\text{Density of states}\right) . dk$

$= g(k)\, dk$

$g(k)\, dk = 2\left(\frac{4\pi k^2 dk}{(2\pi)^3}\right) = \frac{2 d^3k}{(2\pi)^3}$

$g(k)$ = Density of states.

$= 2\left(\frac{4\pi k^2}{(2\pi)^3}\right)$

$N = 2V \int \frac{d^3k}{(2\pi)^3} f_D(\varepsilon_k - \varepsilon_F) = V \int g(k) f_D(\varepsilon_k - \varepsilon_F)\, dk$

Density of states

Where, g k is the density of states and g k dk is the total number of states per unit volume which are present between that momentum interval of k and k plus dk. So, we had looked at all of this and so, you can write down your total number as V into g k f D E minus E k dk, ok. So, the total number you can write a total number of particles, you can rewrite it in terms of density of states, ok.

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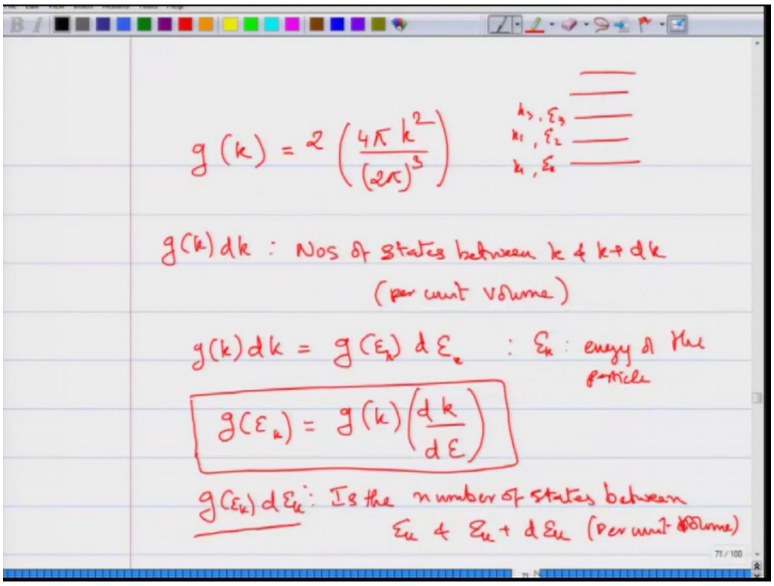

$g(k) = 2\left(\frac{4\pi k^2}{(2\pi)^3}\right)$

k_3, ε_3

k_2, ε_2

k_1, ε_1

$g(k)\, dk$: Nos of states between k & k + dk (per unit volume)

$g(k)\, dk = g(\varepsilon_k)\, d\varepsilon_k$: ε_k : energy of the particle

$$\boxed{g(\varepsilon_k) = g(k)\left(\frac{dk}{d\varepsilon}\right)}$$

$g(\varepsilon_k)\, d\varepsilon_k$: Is the number of states between ε_k & $\varepsilon_k + d\varepsilon_k$ (per unit volume)

And, since g k dk is the total number of quantum states that are present between k and k plus dk in the solid therefore, since the total number of states is going to remain constant whether you are going to look at it in the momentum in terms of momentum or whether you are going to look at it in terms of energies the total number is always constant. So, g k dk is equal to g E d E.

Whether you do a counting of the total number of states with respect to energy, each state is labeled either with the energy or with the momentum and the two are related to each other. So, the total number of this is always the same g k dk the total number between k and k plus dk is equal to g of E dE, where g of E dE is the total number of states which are available between energies E and E plus dE. So, you can rewrite this g E the density of states in terms of energy as g k dE by dk.

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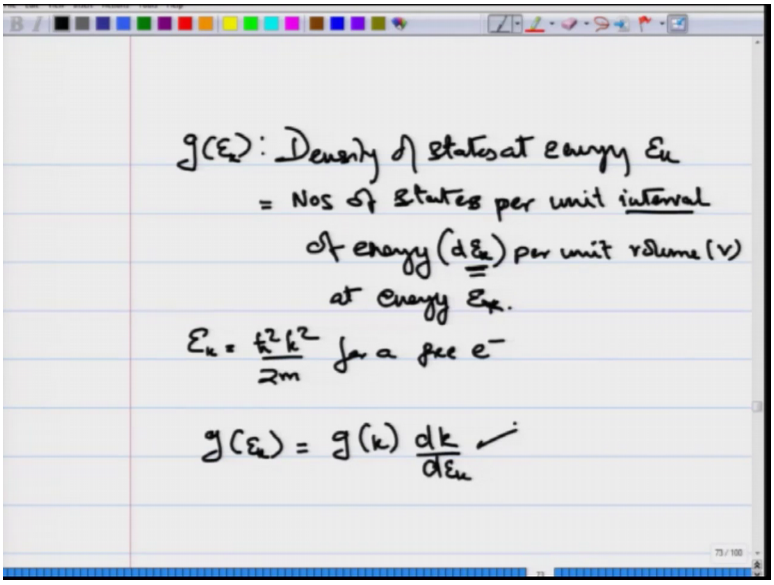

$g(\mathcal{E}_k)$: Density of states at energy $\mathcal{E}_k$

= Nos of states per unit interval of energy ($d\mathcal{E}_k$) per unit volume (V) at energy $\mathcal{E}_k$.

$\mathcal{E}_k = \frac{\hbar^2 k^2}{2m}$ for a free e^-

$g(\mathcal{E}_k) = g(k)\frac{dk}{d\mathcal{E}_k}$ ✓

So, we can write g E which is the density of states at energy E k, this is the density of states at energy E k is the number of states per unit interval of energy the interval of energy is d E k. So, this is the number of states per unit interval of energy per unit volume of the sample V at energy E where, k is the momentum this is E k. It is given a subscript E k because the energy is related to the momentum E k is nothing else, but h cross square k square by 2m for a free electron. So, this is the density of states.

And, g of E k is g k dk by d E k, this we have already seen. So, let us now go ahead and calculate this.

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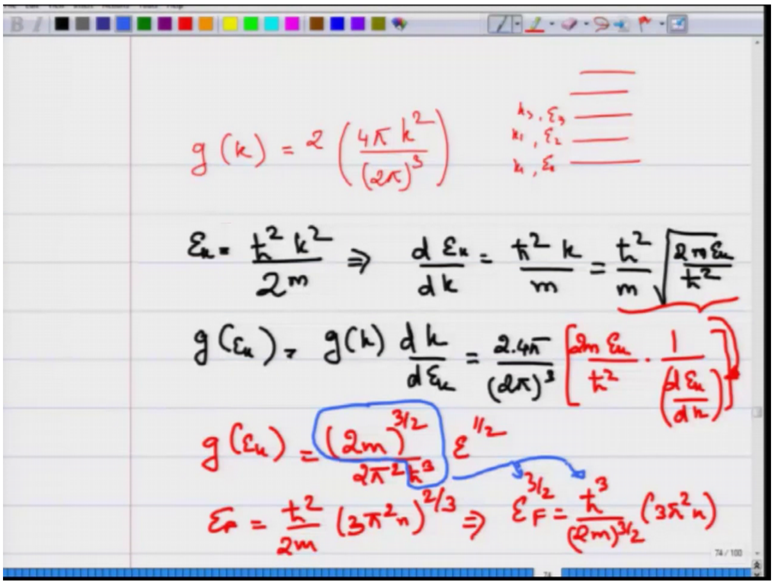

$$g(k) = 2\left(\frac{4\pi k^2}{(2\pi)^3}\right)$$

$k_3, \mathcal{E}_3$

$k_2, \mathcal{E}_2$

$k_1, \mathcal{E}_1$

$$\mathcal{E}_k = \frac{\hbar^2 k^2}{2m} \Rightarrow \frac{d\mathcal{E}_k}{dk} = \frac{\hbar^2 k}{m} = \frac{\hbar^2}{m}\underbrace{\sqrt{\frac{2m\mathcal{E}_k}{\hbar^2}}}$$

$$g(\mathcal{E}_k) = g(k)\frac{dk}{d\mathcal{E}_k} = \frac{2.4\pi}{(2\pi)^3}\left[\frac{2m\mathcal{E}_k}{\hbar^2}\cdot\frac{1}{\left(\frac{d\mathcal{E}_k}{dk}\right)}\right]$$

$$g(\mathcal{E}_k) = \boxed{\frac{(2m)^{3/2}}{2\pi^2\hbar^3}}\,\mathcal{E}^{1/2}$$

$$\mathcal{E}_F = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3} \Rightarrow \mathcal{E}_F^{3/2} = \frac{\hbar^3}{(2m)^{3/2}}(3\pi^2 n)$$

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So, if you recall that g k is equal to 2 into 4 pi k square dk divided by 2 pi cube and E k is h cross square k square by 2m which implies that dE by dk is h cross square k by m or h cross square by m. So, therefore, dE by dk and this k I can rewrite again in terms of 2m E k by h cross square. So, g E which is g k dk by dE k can be rewritten as you put in this 2 into 4 pi divided by 2 pi the whole cube for k square you can use k square is equal to 2m E by h cross square from this expression you can put it here.

So, 2m E k by h cross square into 1 over dE k by which you can get it from here and if you put all of these here you will get the following expression that this is equal to 2m by 2 pi square 2m raised to 3 by 2 h cross cube E raise to half. This is the density of states that you get if you put all of this into this expression if all of these you get it here where for this you will put in you will get the density of states as this.

And now recall that E F is equal to h cross square by 2m 3 pi square n raised to 2 by 3. So now, you can also write down your constants all of these constants you can write it in terms of this ok, you can write it in terms of E F. So, if you put in this in terms of E F, then you can get these expressions 2m raised to 3 by 2 over h cross cube, you will get it from here itself you can see that if you raise it to the power of 3 by 2, E F if you raise it to the power of 3 by 2 you will get h cross cube divided by 2m raised to 3 by 2 3 pi square n which is nothing else, but related to this term. You see that this is present in this term.

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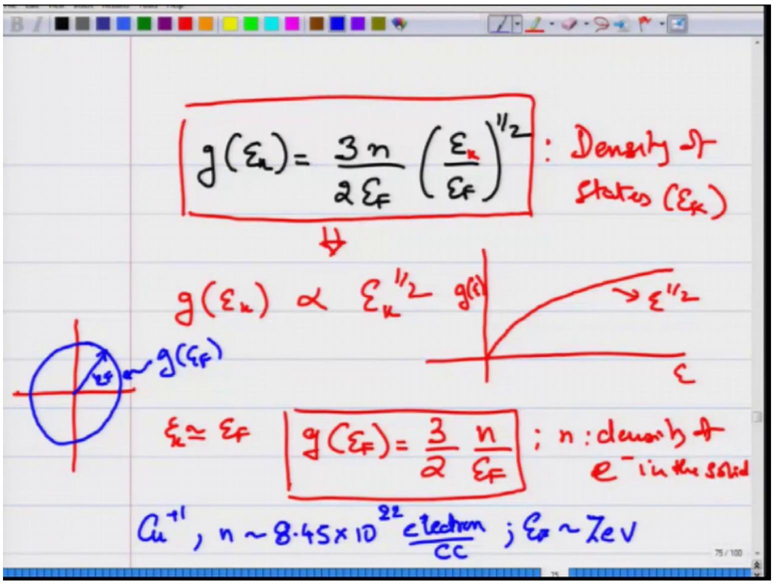

$$\boxed{g(\varepsilon_k) = \frac{3n}{2\varepsilon_F}\left(\frac{\varepsilon_k}{\varepsilon_F}\right)^{1/2}}$$: Density of states (ε_k)

$\Downarrow$

$g(\varepsilon_k) \propto \varepsilon_k^{1/2}$

$\varepsilon_k \simeq \varepsilon_F$ $\boxed{g(\varepsilon_F) = \frac{3}{2}\frac{n}{\varepsilon_F}}$; n : density of e^- in the solid

Cu^{+1}, $n \sim 8.45 \times 10^{22} \frac{\text{electron}}{\text{CC}}$; $\varepsilon_F \sim 7eV$

So, you can rewrite this and you can get an expression for g E k equal to 3 n by 2 E F E by E F raised to half this is the expression for the density of states as a function of energy. You can see this is the density of states at any energy E k. What is important to note from here is that the density of states E k is proportional to E k raised to half which means that the density of states g E as a function of E will be going as E raise to half. In a 3-dimensional metal the density of states changes as the square root of the energy.

So, if your energy is E k is close to E F then the density of states at E F is 3 by 2 n by E F where n is the density of electrons in the solid and E F is the Fermi energy. So, at the Fermi energy the density of states is proportional to the number of electrons that you have inside the solid the density of electrons that you have inside the solid. That determines: what is the density of states that you get at the Fermi level.

So, if you have a Fermi level then the density of states that are available on the Fermi level the g at E F; that means, per unit interval of energy per unit interval of energy the number of states that you have per unit volume is actually proportional to the total number of particles. And so, for example, for copper the number density of electrons inside copper we have seen is roughly 8.45 into 10 to the power of 22 electrons per CC.

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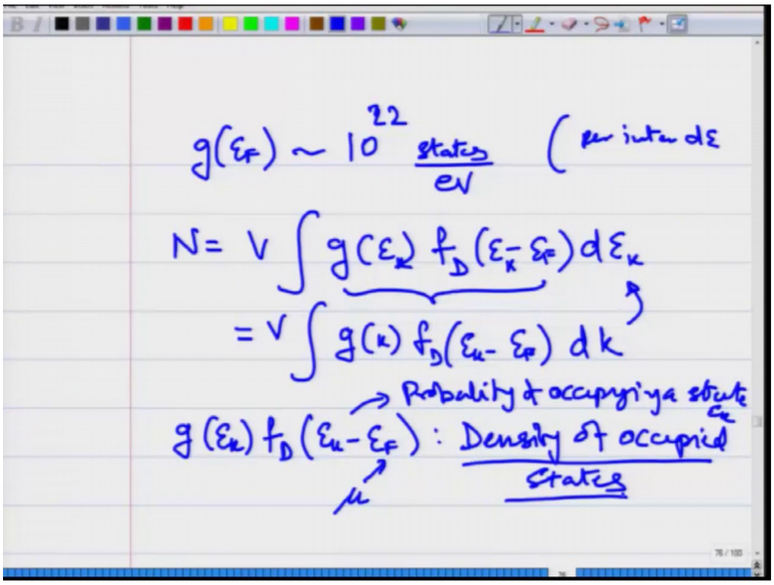

$$g(\varepsilon_F) \sim 10^{22}\ \frac{\text{states}}{\text{eV}} \quad (\text{per interval } d\varepsilon$$

$$N = V \int \underbrace{g(\varepsilon_k)\, f_D(\varepsilon_k - \varepsilon_F)}\, d\varepsilon_k$$

$$= V \int g(k)\, f_D(\varepsilon_k - \varepsilon_F)\, dk$$

Probability of occupying a state ε_k

$$g(\varepsilon_k)\, f_D(\varepsilon_k - \varepsilon_F) : \underline{\text{Density of occupied states}}$$

μ

And, your E F is about 7 electron volts which gives you a density of states at the Fermi energy of the order of 22 states per electron volt; that means, this many number of states are present such a large number of states are present per interval dE per interval dE at E F. This is the number of states of 10 raised to 22 states per electron volt. For example, this is typically in copper per electron volt you have this many number of states which are available.

Now, if you go back and look at the total number of particles then the total number of particles can be written as g of E Fermi Dirac E minus E F dE which is the same as writing it as g of k Fermi Dirac E k minus E F dk, but g k dk is equal to g of E dE and so, you can rewrite this expression also equivalently like this. And, here there is a product of the density of states at energy E k into the Fermi Dirac distribution E k minus E F or you can also replace it by the chemical potential mu, so, g k the density of states into the Fermi Dirac distribution.

And, this is the density of occupied states because this factor f D gives the probability of occupying a given state this gives the probability of occupying a state E k and g E k is the number of states or the density of states per unit interval which is available at E k. So, this gives the density of occupied states.

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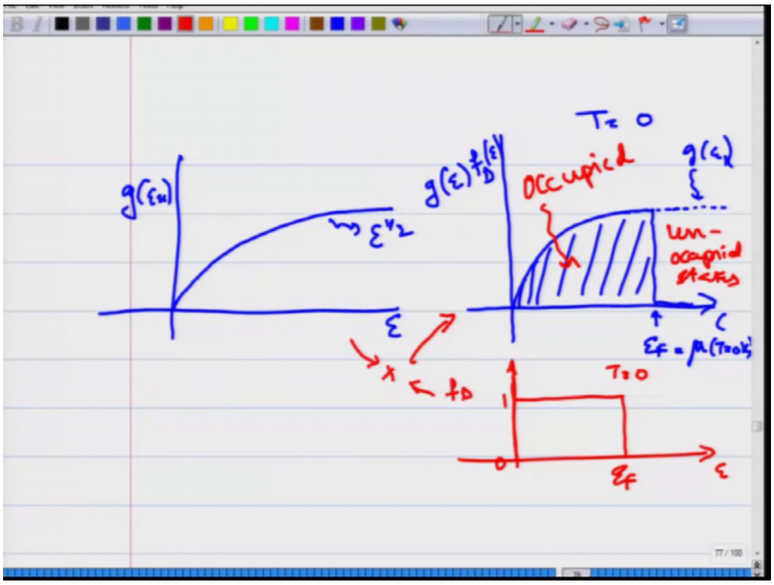

So, if I plot g E k vs E k it goes as E raised to half, but a more important quantity is that how many even if it goes as E raised to half how many of these states are actually occupied. So, at temperature T equal to 0 g E k into f D as a function of E will look like this which is equal to the chemical potential at temperature T equal to 0 Kelvin and these are the occupied states this is the density of the occupied states these are all occupied. And although this is g of E k although it continues as a raise to half above the Fermi energy these are unoccupied states.

And, the reason why this happens is because if you recall you are taking a product of this function which is proportional to E raised to half with the Fermi Dirac distribution as a function of energy at T equal to 0, this goes from a value 1 to 0 at E F at T equal to 0. So, if you take the product of this these two if you take a product of these two functions you will end up with this function which gives you the density of occupied states.

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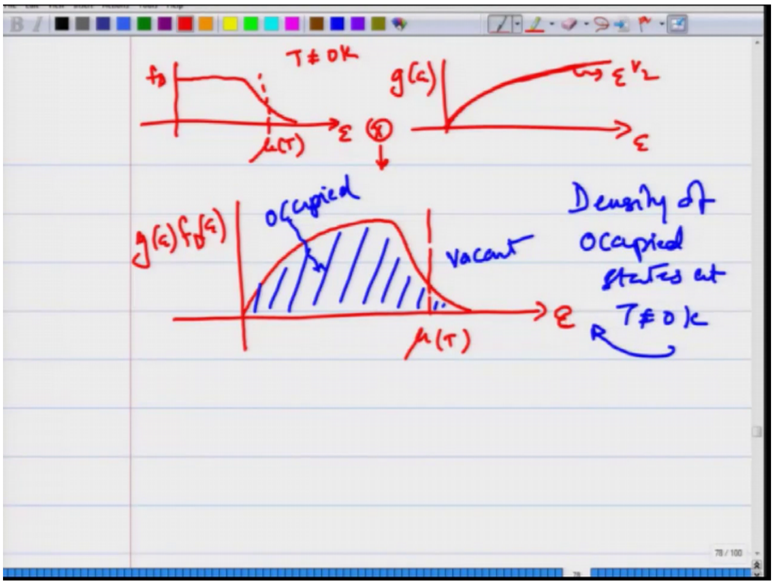

At finite temperature your Fermi Dirac distribution changes slightly at finite temperature your Fermi Dirac distribution chemical potential at temperature T this is the chemical potential T naught equal to 0 Kelvin and g of E as a function of E is still E raised to half it goes as E raised to half, ok. So, if you take the product of these two functions then the density of occupied states g of E f of D E as a function of E will look slightly different from what I had shown you for temperature T equal to 0, where this is the chemical potential mu at T this is the chemical potential and all of this is occupied and these are vacant.

The reason for this is that the probability distribution at finite temperature increases slightly above the chemical potential because particles from lower energy state around the Fermi energy are getting excited to the higher energy state and so, around and above the chemical potential you have some occupancy. So, the density of occupied states this is the density of occupied states at T naught equal to 0 Kelvin that is this and this is the energy. So, this is energy E. This is the behavior and a temperature T equal to 0, this is roughly similar, ok.

So, with this we come to these important concepts which will be used throughout this course; one is the density of states, the density of occupied states, what is their behavior as a function of energy. These are certain common themes that we will use from now on quite regularly while describing various properties of the solid.