Introduction to Solid States Physics

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Lecture – 16
Density of states Part – I

We came across the concept of a Fermi energy and we calculated this Fermi energy and it turns out that this Fermi energy is because of quantum mechanics. These Fermi energies are really high. They are not determined by the temperature of the solid, but they are rather determined by the density of electrons; the number density of electrons which are present inside the material. The Fermi energies and the Fermi velocities turn out to be very high inside the solid.

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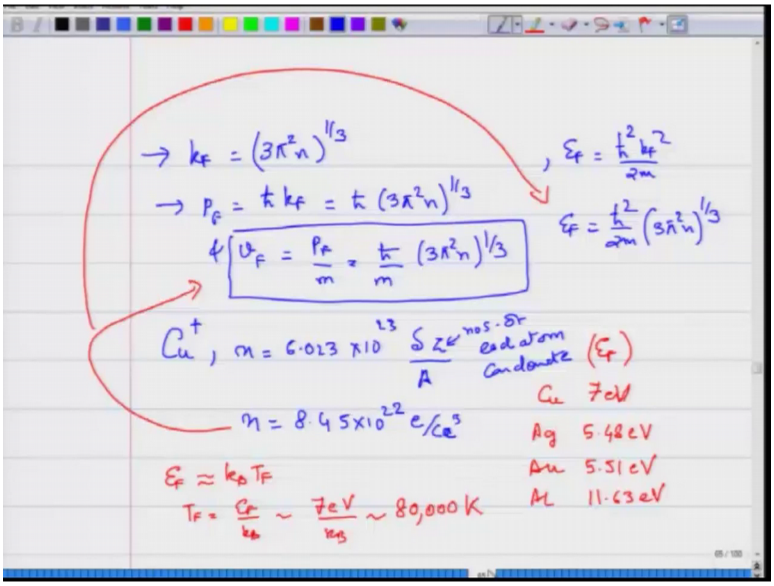

$\rightarrow k_F = (3\pi^2 n)^{1/3}$, $\varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$

$\rightarrow p_F = \hbar k_F = \hbar (3\pi^2 n)^{1/3}$

$\varepsilon_F = \frac{\hbar^2}{2m}(3\pi^2 n)^{1/3}$

$\boxed{v_F = \frac{p_F}{m} = \frac{\hbar}{m}(3\pi^2 n)^{1/3}}$

Cu^+, $n = 6.023 \times 10^{23} \frac{\delta Z}{A}$ ← nos. of each atom conducte

$n = 8.45 \times 10^{22}\ e/cc^3$

	(ε_F)
Cu	7eV
Ag	5.48 eV
Au	5.51 eV
Al	11.63 eV

$\varepsilon_F \approx k_B T_F$

$T_F = \frac{\varepsilon_F}{k_B} \sim \frac{7eV}{k_B} \sim 80,000\,K$

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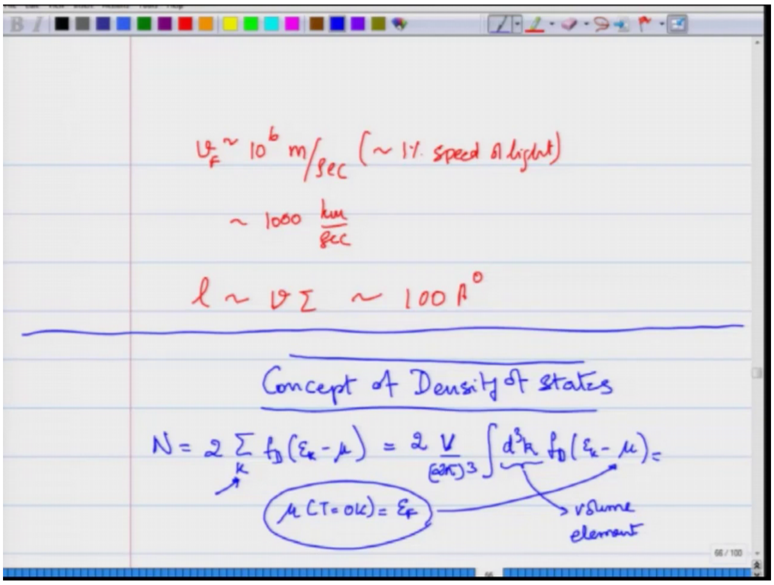

$v_F \sim 10^6\ m/sec$ (~1% speed of light)

$\sim 1000\ \frac{km}{sec}$

$l \sim v\tau \sim 100\ A^{\circ}$

Concept of Density of states

$$N = 2\sum_{k} f_D(\varepsilon_k - \mu) = 2\frac{V}{(2\pi)^3}\int \underbrace{d^3k}_{\text{volume element}} f_D(\varepsilon_k - \mu) =$$

$$\boxed{\mu(T=0K) = \varepsilon_F}$$

Next we come across a concept which is the density of states. It is a related concept which will be useful as we go along in this course. So, I will like to introduce it right here itself. If you recall how did we count the total number of particles in the solid; the total number of particles is 2 which comes from each state in the system being occupied by two electrons, k is the state the individual states and f D is the Fermi Dirac distribution which is equal to 1, for energies which are less than the Fermi energy and it is equal to 0 at energies which are greater than the Fermi energy rather chemical potential is at 0 temperature is equal to the Fermi energy.

And, the summation if we write it as an integral then d cube k is the volume element in this momentum space. So, d cube k is the volume element. So, let us relocate this expression a little closely.

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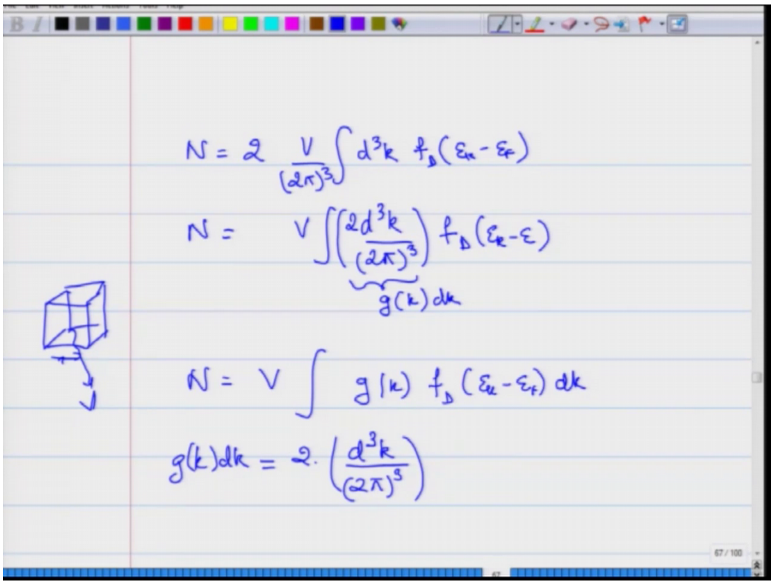

$$N = 2\frac{V}{(2\pi)^3}\int d^3k\, f_D(\varepsilon_k - \varepsilon_F)$$

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

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

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

So, N is equal to 2 into V by 2 pi cube integral d cube k integral over the volume element inside the system inside the in the momentum space and f D is the Fermi Dirac distribution minus E F, ok; for energies less than E F it is 1, for energies greater than E F it is 0. And, this we can rewrite it as then for a sample of given volume; this is the volume of the sample the for a volume of the sample of size V the integral is this quantity into the occupancy of the state the what which is governed by the Fermi Dirac distribution or the total number of particles for a sample or for a material of volume V and let me call this as g k, ok.

If I write it as g k dk, then for a material of volume V, the total number of particles is V into integral g k into f D E k minus E F dk. I will rewrite it slightly as we go along ok, but now we are defining something which is this 2 into the volume element over 2 pi cube. So, this is g k dk is 2 into this volume element in the momentum space divided by 2 pi cube.

Let us look at this a little bit more closely to give it an interpretation, what is this thing which is g k dk which is coming into the picture.

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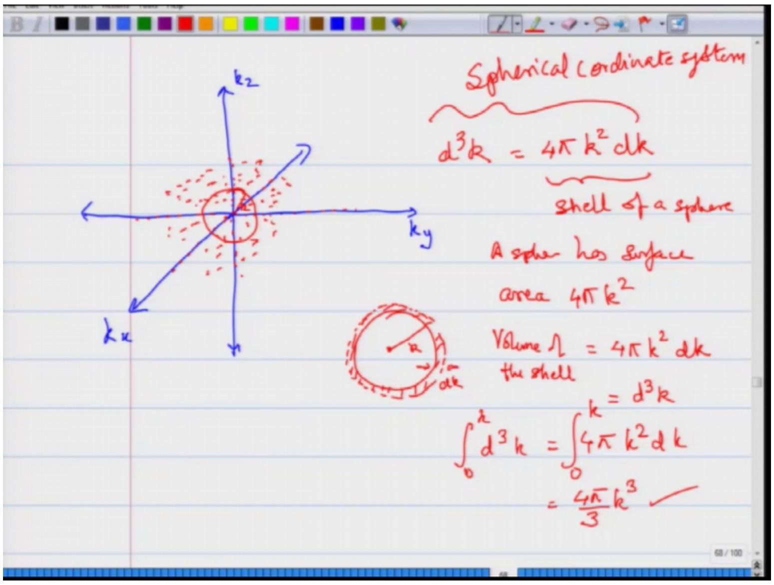

Spherical coordinate system

$$\underbrace{d^3k = 4\pi k^2 dk}$$

shell of a sphere

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

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

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

So, as I had said that for a metal in your momentum space, you can define a volume element, ok, there are integral states which are available. There are integral set of states which are available in your momentum space all over the momentum space they are distributed. There are states which are available in this momentum space and d cube k is the volume element that you are looking at in the moment space.

So, we define the volume element as 4 pi k square dk, namely it is a shell of a sphere. A sphere has surface area 4 pi square, in the momentum space a sphere has a surface area 4 pi k square if you consider from the origin a sphere, then the sphere will have a surface area of 4 pi k square and if you consider a thin shell of width dk, then the volume of this shell the volume of the shell is 4 pi k square dk which is basically your volume element.

The volume element we are considering is spherically symmetric and we are considering what is this volume element in this spherical shell around the origin; origin has the 0 momentum state and we are looking at a volume element. So, it does not depend on the theta and neither does it depend on phi. The volume element is just depends on the k vector. We are considering it as a spherically symmetric shell, ok.

So, there is no theta dependence of this volume element as well as we have integrated out of phi dependence and that is why you will have 4 pi k square dk and it is very easy to see that if you integrate this d cube k which is equal to integral of 4 pi k square dk, 0 to k integrated over 0 to k there is no theta of phi dependence. So, we have gone into the spherical coordinate system and we are defining the volume element there is no phi or theta dependence and this will give you a volume element which is 4 pi k square dk if you just integrate this is nothing else, but 4 pi by 3 k cube, which is the total volume of the sphere, ok.

So, you are allowed to write a volume element provided there is no theta and phi dependence and there is no reason to believe that in a metal you will have some angular theta and phi; namely there is some asymmetry in the momentums along x, y and z direction, we remove those complications and we consider an isotropic momentum distribution. And for this isotropic momentum distribution, we consider this spherically symmetric shell whose volume is 4 pi k square dk.

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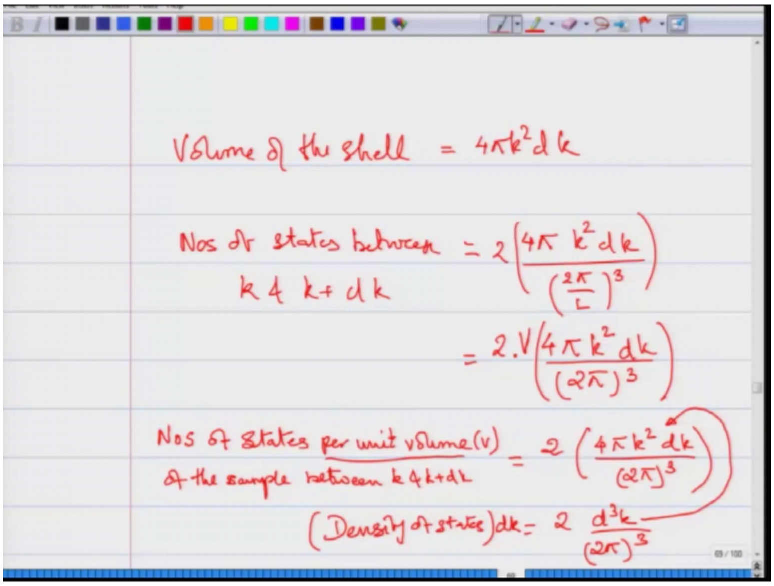

Volume of the shell $= 4\pi k^2 dk$

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 $= 2\,\frac{d^3k}{(2\pi)^3}$

The volume of the shell is 4 pi k square dk. The number of states between k and k plus dk whose volume is k 4 pi k square dk is 4 pi k square dk divided by the smallest volume element which each state can occupy, which is 2 pi by L and 2 is the number of states which are available for occupying plus minus h. So, you have this factor 2. So, you will get 2 into V 4 pi k square dk divided by 2 pi the whole cube or the number of states per unit volume; number of states per unit volume V of the metal or the sample between k and k plus dk is nothing else, but 2 into 4 pi k square dk divided by 2 pi the whole cube which is our term d cube k by 2 pi the whole cube.

The volume element we have just replaced it with a spherically symmetrical volume element because there is no momentum distribution along the x, y and z directions. There is no asymmetry in the momentum distributions in the x, y and z direction. So, the simplest case to consider is a uniform momentum distribution along the x, y and z direction. So, we consider the volume element d cube a k as is basically a volume of a spherically symmetric shell.

So, the number of states which are available between k and momentum k plus dk is the volume of the shell which is 4 pi k square dk divided by the minimum volume that you have. So, the number of states per unit volume of the sample between k and k plus dk is this and this is called the density of states into dk, ok; the number of states per unit volume between k and k plus dk.

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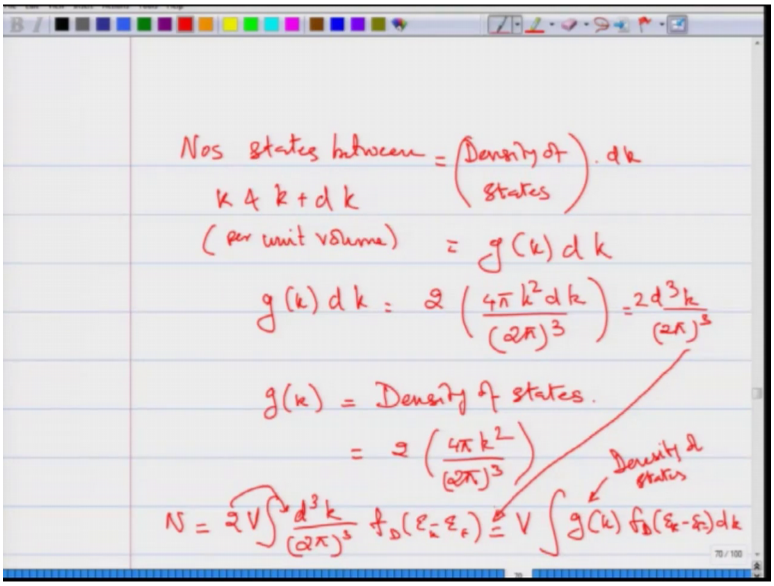

Nos states between k 4 k + d k (per unit volume) $= \begin{pmatrix}\text{Density of} \\ \text{states}\end{pmatrix} . dk$

$= g(k)\, dk$

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

g(k) = Density of states.

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

Density of states

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

So, the number of states between k and k plus dk is written as density of states into dk this is g of k dk. So, g of k dk is 2 into the number of states this is all per unit volume, g k dk is 4 pi k square dk divided by 2 pi the whole cube, ok. And, so, the density of states this is the density of states which measures what is the density of states that are available in the system that density per unit volume that we are calculating is this which is 2 into 4 pi k square by 2 pi cube.

This is nothing else but, if you recall d cube k by 2 pi the whole cube and N which was written as integral of d cube k divided by 2 pi the whole cube into f of D E minus E k minus E F; this term with the 2 inside if you take the 2 inside here this term is nothing else, but volume integral g k f D E k minus E F dk, ok. This is the density of states.

So, the density of states which are available between k and k plus dk; the number of states which are available for occupying between k and k plus dk per unit volume of the sample into the occupancy of the state which is given by the Fermi Dirac distribution that gives you the total number of particles in the system. So, this just comes out from here that this is nothing else , but this.

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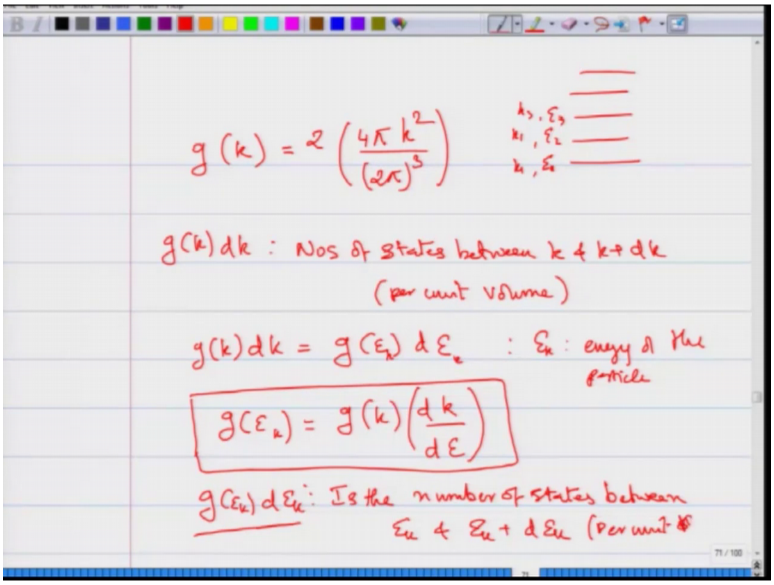

$$g(k) = 2\left(\frac{4\pi k^2}{(2\pi)^3}\right)$$

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

$g(k)\,dk = g(\mathcal{E}_k)\,d\mathcal{E}_k$: $\mathcal{E}_k$: energy of the particle

$$\boxed{g(\mathcal{E}_k) = g(k)\left(\frac{dk}{d\mathcal{E}}\right)}$$

$g(\mathcal{E}_k)\,d\mathcal{E}_k$: Is the number of states between $\mathcal{E}_k$ & $\mathcal{E}_k + d\mathcal{E}_k$ (per unit

So, g k which is the density of states per unit volume is 2 into 4 pi k square by 2 pi the whole cube and g k dk is the number of states between k and k plus dk per unit volume of the sample.

Now, the number of states as you know cannot change if the total number of states is always constant so, whether I write it in terms of momentum or if I write it in terms of energy g k dk will be equal to g of E dE where E is the energy of the particle, E k is the energy of the particle. Whether I am counting states in terms of momentum or if I am counting states in terms of energy.

So, I have states which I can label as E 1, E 2, E 3 or I can label with them as k 1, k 2, k 3, the density of such states or the total number of states between k and k plus dk is going to be the same; whether I look at it in count it in terms of energy or if I count it in terms of momentum, so, I can equivalently write my density of states in terms of energy as g of k dk by dE. And, this is the density of states which I can write in terms of energy of the particle. This is an alternative way to write the density of states instead of writing the density of states between k and k plus dk g of E k into d of E k is the number of states between E k and E k plus dE k and this is of course, per unit volume of the sample.

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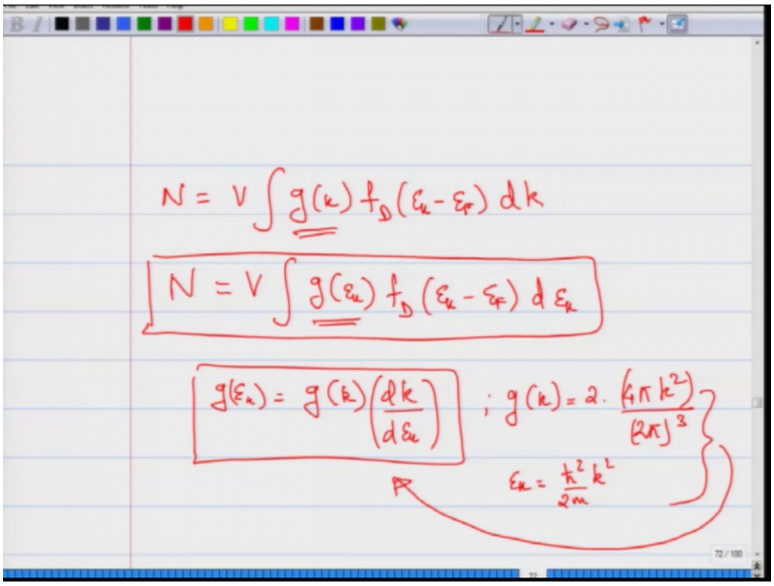

$$N = V \int \underline{\underline{g(k)}}\, f_D(\varepsilon_k - \varepsilon_F)\, dk$$

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

$$\boxed{g(\varepsilon_k) = g(k)\left(\frac{dk}{d\varepsilon_k}\right)} \; ; \; g(k) = 2 \cdot \frac{(4\pi k^2)}{(2\pi)^3}$$

$$\varepsilon_k = \frac{\hbar^2}{2m} k^2$$

So, if I want to write down the total number of particles again I can write it in terms of V into integral of g k f D E k minus E F dk and I can also write it as V into g E k; E k minus E F dE k. So, the total number of particles can now be expressed in terms of the density of states, whether you write it in terms of energy or you write it in terms of momentum the total number of particles is equal to the volume into the density of states which are available times the occupancy of those states, integrated over the entire energy states.

This will be 0, for energies which are greater than E F and it will be 1, for energies which are less than E F and g of E k is related to the density of states in momentum states by this relation. And, now, we will calculate what is the expression for g E k because, this we know is 2 into 4 pi k square divided by 2 pi the whole cube and E k is h cross square by 2m k square. So, using these two expressions we will calculate g E k which is the density of states of at energy E k.