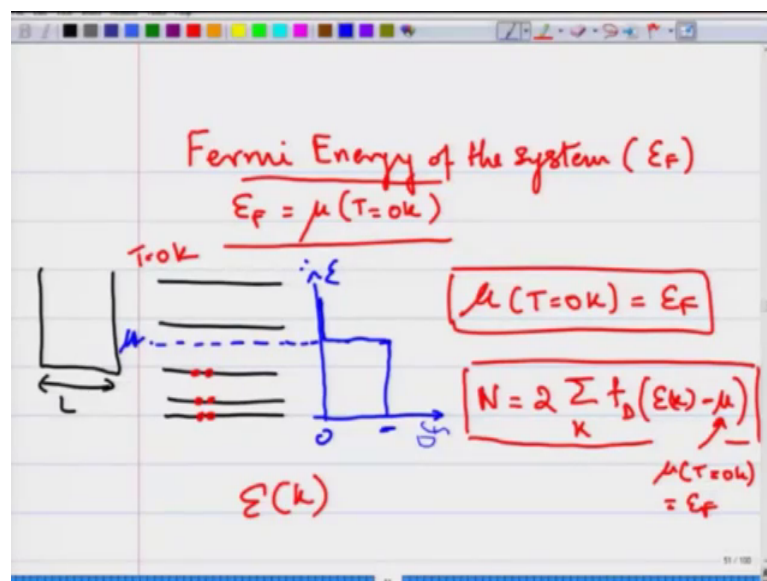


Introduction to Solid State Physics
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Lecture – 13
Introduction to Sommerfeld's Theory of electrons in a metal Part – III

We had begun looking at the Sommerfeld's picture of how an electron moves through the solid and the important thing with Sommerfeld's realized was that the electron does not really follow the kinetic theory of gases. Its distribution is not like a Maxwell Boltzmann distribution, but the distribution follows quantum statistics. Inside the solid you have states energy states which are available and the electron fills up these energy states and the way they these states are filled up is governed by the Fermi Dirac distribution.

(Refer Slide Time: 00:53)



So, there is a chemical potential μ up to which the states are occupied with our occupancy or with a probability of 1, and above it becomes 0. The 0 temperature chemical potential is an energy level which is close to the maximum energy which the particles have at 0 temperature and that is what we call as the Fermi energy. And the general way to determine your chemical potential is that, if you count all the number of states which are occupied, then these are all the states which are occupied up to the chemical potential multiplied by two particles per state, then the total number of particles

you will get the total number of particles. So, if you solve this equation you will get your chemical potential.

(Refer Slide Time: 01:43)

e^- free electron in this solid? Quantum particle.

$-\frac{\hbar^2}{2m} \nabla^2 \psi_k = E_k \psi_k$

Schrodinger's eqn for a free particle

$E_k = \frac{\hbar^2 k^2}{2m}$ → Energy of free particle

$\vec{p} = \hbar \vec{k}$

$\psi_k(x, y, z)$ = wave function of the particle enclosed in this cube.

So, we consider that the solid is a cube of sides of length L we had seen this already and you write down the Schrodinger's equation for the free electron, whose energy is given by this E_k is equal to $\hbar^2 k^2 / 2m$ and ψ_k is the wave function of the electron.

(Refer Slide Time: 02:07)

① e^- is confined inside the solid with volume $V = L^3$

$\psi_k(x, y, z) = \psi_0 e^{i\vec{k} \cdot \vec{r}}$ Plane wave

$\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$ plane wave solution of free e^-

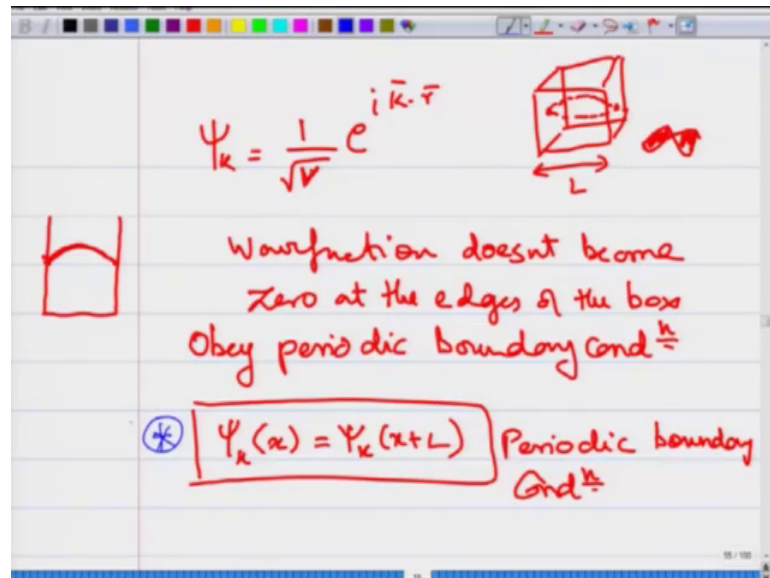
Volume of the metal $\rightarrow V$

$\int_V \psi_k^* \psi_k d^3r = 1 \Rightarrow |\psi_0|^2 V = 1$

$\Rightarrow |\psi_0| = \frac{1}{\sqrt{V}}$

Being free electron we consider it like a plane wave. So, this is your plane wave solution for the free electron, which is moving through the solid. And you consider the solid has a finite volume, you normalize it and you get the constant the amplitude which is $1/\sqrt{V}$ by square root of V for this wave function and then you have to put some boundary conditions on this wave function.

(Refer Slide Time: 02:29)



Now, is it that all momentum states because you want to generate the energy states which are available inside the solid, using the plane wave, you want to generate what are the energy states available are there a continuum of states or are there some finite discrete set of states which are available. And for that some of will used the periodic boundary conditions.

So, in your problem of just a single electron inside a box you consider that the wave function becomes 0 at the two edges, but this has a problem because it gives rise to standing waves inside the solid which you want a propagating mode, you want electrons to actually propagate through the solid you do not want them to be static and you do not want them to be standing wave type solutions.

(Refer Slide Time: 03:39)

Waves with nodes at edges. Not allowed.

$\Psi_k(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$

1D case $i k_x x$

$\Psi_k(x) = \frac{1}{\sqrt{V}} e^{i k_x x}$

$\Psi_k(x) = \Psi_k(x+L)$

$e^{i k_x x} = e^{i (k_x)(x+L)} \Rightarrow e^{i k_x L} = 1$

$\Psi_k(x) = \Psi_k(x+L)$

So, what Sommerfeld considered was this very important periodic boundary condition. That the wave function at x is equal to the wave function at x plus L and this leads to solutions which are of the travelling wave form where this is not a solution where you have nodes, but instead this is a solution, so you do not have nodes at the edges of the sample. And if you use this sort of a periodic boundary condition in one dimension then you will get a condition on your wave function which is e raised to $i k$ into L is equal to 1 which gives you a condition on your momentum, that the momenta is going to be integral multiples of 2π by L .

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$k_x = \frac{2\pi n}{L} \Rightarrow e^{i k_x L} = 1$

$n: \text{integer}$
 $n = 0, 1, 2, \dots$

$\Psi_k = \frac{1}{\sqrt{V}} e^{i k_x x}$

$k_x = \frac{2\pi n}{L}$

$\Psi_k(x) = \Psi_k(x+L)$

$\Psi_k(x, y, z) = \Psi_{k_x}(x) \Psi_{k_y}(y) \Psi_{k_z}(z)$

$\Psi(x+L, y+L, z+L) = \Psi(x, y, z)$

The net wave function $\psi(x, y, z) = \psi(x) \psi(y) \psi(z)$. So, these are the momenta in the x, y and z direction, ok. So, we write the net wave function as the product of these wave functions and then you can show that you can write down the periodic boundary condition as $\psi(x+L, y, z) = \psi(x, y, z)$ and $\psi(x, y+L, z) = \psi(x, y, z)$ and $\psi(x, y, z+L) = \psi(x, y, z)$. Namely, there is a periodic boundary condition along the x direction along the y direction as well as along the z direction. And all of this leads to the condition on k_x , k_y and k_z . So, let us write down the conditions on k .

(Refer Slide Time: 05:11)

Handwritten notes on a whiteboard:

$$e^{ik_x L} = 1, \quad e^{ik_y L} = 1, \quad e^{ik_z L} = 1$$

$$k_x = \frac{2\pi n_x}{L}, \quad k_y = \frac{2\pi n_y}{L}, \quad k_z = \frac{2\pi n_z}{L}$$

$n_x = 0, 1, 2, \dots$
 $n_y = 0, 1, 2, \dots$
 $n_z = 0, 1, 2, \dots$

Momentum or energy states inside the solid

$N = 2 \sum_{\mathbf{k}} f_D(\epsilon_{\mathbf{k}} - \mu)$
 $T=0\text{K}; \quad N = 2 \sum_{\mathbf{k}} f_D(\epsilon_{\mathbf{k}} - \epsilon_F); \quad \mu = \epsilon_F \text{ at } T=0\text{K}$

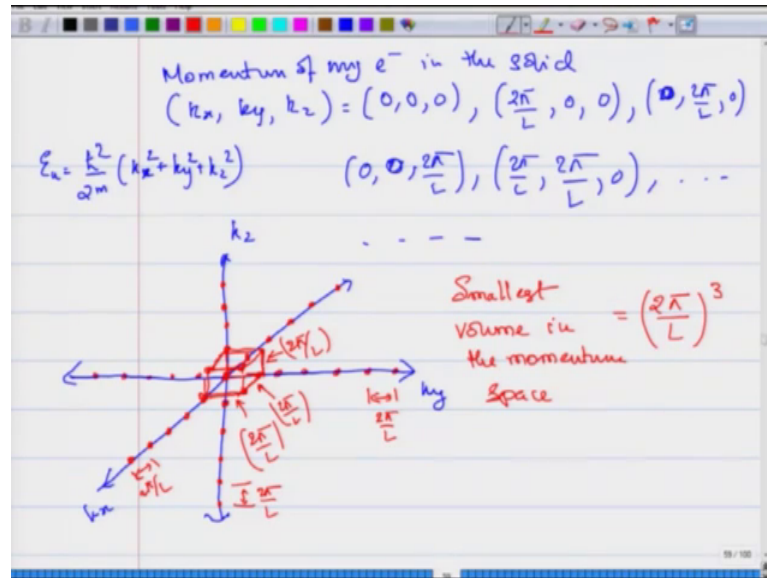
A small 3D cube diagram with side length L is drawn next to the text.

So, you will have $e^{ik_x L} = 1$ we consider that the cube is symmetric it has a side of length L, length, width and height are all of length L, and so if you use the periodic boundary conditions you will have this $e^{ik_y L} = 1$ and $e^{ik_z L} = 1$. And this will put conditions on k_x , these will give you your momentum states or the energy states, k_y is equal to $2\pi n_y / L$ and k_z is equal to $2\pi n_z / L$. These are your different momentum states, where n_x is 0, 1, 2 and so on; n_y is 0, 1, 2; n_z is equal to 0, 1, 2 and so on. So, these are your different momentum states.

So, you generate your momentum or energy states inside the solid which is a cube with sides of length L. And now the states that you generate you will have to start filling up. So, can we use this expression, N is equal to summation of all the momentum states this is the Fermi Dirac distribution $e^{k - \mu}$, which at 0 temperature at $T = 0$

Kelvin this expression N is equal to twice of summation of all momentum states f D, E k minus E F as mu is equal to E F at 0 Kelvin. So, can we use this expression to evaluate what is the fermi energy of the system for this solid?

(Refer Slide Time: 07:19)



If I look at the momentum of my electron in the solid it has momentous k_x , k_y and k_z . And these will be typically for $n \times n \times n$ you know you will have $0, 0, 0$; you will have 2π by $L, 0, 0$; $0, 2\pi$ by $L, 0, 0$; $0, 0, 2\pi$ by $L, 2\pi$ by $L, 2\pi$ by $L, 0$. And like this you will have a discrete set of states you will have a discrete set of momentum states inside the solid, each of them have their own kinetic energy which is given by E_k is equal to $\frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2)$. So, from these discrete momenta states you will get discrete energy states which will then be filled up based on Fermi Dirac distribution.

So, now, let us look at this momentum space k_x , k_y and k_z , this is the 0 momentum state which is the $0, 0, 0$ and every subsequent state either in the k_y direction or in the k_z direction or in the k_x direction all the momentum states are spaced by a distance of 2π by L . These are the discrete momentum states or the energy states in the momentums. These are the discrete momentum states that we have we are drawing here which we have obtained just now and the spacing between any two points in either direction is either 2π by L .

And you can draw what is the smallest. So, there is a point in the k_x, k_y plane which will have $2\pi/L$, this is this point which is in the k_x, k_y plane which will be this similarly there will be another point here, and you will have another point here, and you will have another point here. So, you will have one such cube like this there are no momentum states which are available. So, the smallest volume in the momentum space is equal to $2\pi/L$ the whole cube. This is the smallest volume because this distance has $2\pi/L$ this is $2\pi/L$ and similarly this length is $2\pi/L$, ok.

You can show for yourself that this is the smallest volume. Below this volume there is no states which are available.