Solid State Physics
Lecture 25
Introduction to Sommerfeld Theory - I

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After analyzing and finding out these things from our Drude model, now let us move on to an improved model. So, how do we improve the model? We follow the suggestions by Sommerfeld and move on to the Sommerfeld theory for metals. (Refer Slide Time: 00:48)

So, at Drude's time and also, a lot more, a lot later, it was considered to be quite acceptable that you apply kinetic theory of gases for electrons; that means, you treat the electrons using Maxwell Boltzmann statistics. But Maxwell Boltzmann statistics is not really valid for electrons because electrons are identical particles and in the context of quantum statistics, you have learnt that identical particles are like when their wave functions overlap and then, they can separate again in such a way that they cannot retain their identity; you would not be able to distinguish them at all, no matter how well you can resolve it. So, electrons are identical particles; that means, indistinguishable particles, they obey from a Dirac statistics and Maxwell Boltzmann statistics is not applicable on them in a strict sense, also you have Pauli exclusion principle that is obeyed by every fermion and electrons of fermions. So, that principle is obeyed. So, you have to consider these things, while treating electrons in a metal. Drude did not consider that because these things these theory did not exist at his time. Now, if we consider all these things, then if we consider Maxwell Boltzmann statistics, then the velocity distribution coming from the Boltzmann distribution that is given as this is the book Boltzmann velocity function. This $f_B(v) = n(\frac{m}{2\pi K_B T})^{\frac{3}{2}} e^{\frac{-mv^2}{2K_B T}}$, n is the number density times mass over twice by K_B is the Boltzmann constant times temperature. This is the Maxwell Boltzmann velocity distribution function. But this function is not applicable because we need to apply fermi Dirac statistics on this. Sommerfeld also applied Pauli Exclusion Principle and if now we consider these two things, we can find the ground state properties of the electronic gas; electron gas. So, after considering the Fermi Dirac statistics and Pauli Exclusion Principle, we assume that the electrons do not interact with one another. Why do we consider that? Well, electrons do not interact with one another that is a requirement for free electron; but that is not actually true, this is something we assume because that makes our work much simpler and let us start with something simple. Later on, we will try to move on towards more complicated stuff. So, this is called the independent electron approximation. A single electron can be described by its wave function $\psi(\overrightarrow{r})$ which is a function of its position. Now, if the electron has no interaction with the other electrons in the system, the time independent Schrodinger equation for that electron that can be written as $-\frac{\hbar^2}{2m} \bigtriangledown^2 \psi(\overrightarrow{r})$. It has no interaction with other electrons as well as the nucleus as was considered in Drude's approximations and that is also here. So, the Hamiltonian is just the kinetic energy. So, Hamiltonian operator, kinetic energy operator is $-\frac{\hbar^2}{2m}\bigtriangledown^2$ and that acts on the $\psi(\overrightarrow{r})$, the wave function of the electron to give us $\epsilon\psi(\overrightarrow{r})$, where ϵ is the energy eigen value. Now, we shall represent the confinement of the electrons to the volume by some boundary condition, for solving this Schrodinger equation. What kind of boundary conditions should we consider? We can consider that the solid is of a shape of a cube. Why cube? Because this is the simplest kind of a shape that we can work with. Anything away from cube would make situations a bit more complicated and that means, it has each side L and $L = V^{\frac{1}{3}}$ of this cube and now, we need a boundary condition. Shall we consider that outside this cube there is no electron; that means, there is no wave function, the wave function on the surface of the cube goes to 0? If we consider that kind of a boundary condition, then you can readily see that the electronic wave functions within the material, within the cube that is going to be stationary waves, subject to this boundary condition. But we are interested in transport properties; electrical transport as well as thermal transport and transport properties that means, electrons are moving that would be better represented by non stationary that is running waves. So, the wave function going to 0 at the boundary is not really suitable, then what

kind of boundary condition do we take, do we assume here? Well, periodic boundary conditions may be better. What does periodic boundary condition mean? Let us assume we have this kind of a box, its a cube, not a square. If we have this kind of a situation, then if an electron goes out from this surface; at the same time, we assume that it enters from this other kind of a surface. So, its a periodic arrangement of this box everywhere in the space that kind of a boundary condition we would impose. How do we impose this boundary condition in terms of mathematics on the wave function? (Refer Slide Time: 09:51)

So, in 1-dimension, it would mean that if you have $\psi(x + L)$; capital L is the side of the cube, it would be $= \psi(x)$. This is the boundary condition and if we go for 3-dimension, it would be $\psi(x, y, z+L) = \psi(x, y, z)$; $\psi(x, y+L, z) = \psi(x, y, z)$, $\psi(x+L, y, z) = \psi(x, y, z)$. This is also called Born-von Karman boundary condition or simply periodic boundary condition ok. After learning this periodic boundary condition, we now solve the Schrodinger equation subject to the boundary condition. The trial solution would be $\psi_k(\overrightarrow{r})$, where k is the index is given as $\psi_k(\overrightarrow{r}) = \frac{1}{\sqrt{V}} e^{i\overrightarrow{k}\cdot\overrightarrow{r}}$ V is the normalization condition within this box, and $e^{i\overrightarrow{k}\cdot\overrightarrow{r}}$ is a plane wave solution. And it will have an energy $\epsilon(\overrightarrow{k}) = \frac{\hbar^2 k^2}{2m}$. So, here $\overrightarrow{k}$ is the position independent vector, it is the wave vector. And now, let us try to see the significance of this k. If we have this kind, this form of the wave function, then this form that is the plane waveform of this wave function, it is also an eigenstate of the momentum operator. It is of course, an eigenstate of the Hamiltonian, also an eigenstate of the momentum operator and if it is an eigenstate of the momentum operator, the momentum operator can be written as $\overrightarrow{p} = \frac{\hbar}{i}\frac{\partial}{\partial\overrightarrow{r}} = \frac{\hbar}{i}\overrightarrow{\bigtriangledown}$ and when this kind of a momentum operator acts on the wave function; that means, the plane waveform, we get the eigenvalue that is $\hbar\overrightarrow{k}$. This is the eigenvalue of the momentum operator; that means, $\frac{\hbar}{i}\overrightarrow{\bigtriangledown} e^{i\overrightarrow{k}\cdot\overrightarrow{r}}$ is nothing but $\hbar\overrightarrow{k}\, e^{i\overrightarrow{k}\cdot\overrightarrow{r}}$. (Refer Slide Time: 14:37)

So, we can now interpret k as a wave vector and the corresponding the Broglie wavelength $\lambda = \frac{2\pi}{k}$ for the electron. If we now invoke the periodic boundary condition, then this allows only certain discrete values of k that would satisfy the condition and what discrete values? If we have $e^{ik_x L} = e^{ik_y L} = e^{ik_z L} = 1$, only then the boundary condition would be satisfied; not otherwise that means, we do not have the continuous values of k accessible anymore only certain discrete values are allowed. If we have $e^{ik_z L} = 1$ that means, $z = 2\pi i n$, where n is an integer. The components of k, then must take the form $k_x = \frac{2\pi n_x}{L}$;$k_y = \frac{2\pi n_y}{L}$; $k_z = \frac{2\pi n_z}{L}$; where, $n_x,\ n_y,\ n_z$ these are integers. Now, if we consider a region of the k-space and if it has a volume Ω, then this volume will contain $\frac{\Omega}{\frac{2\pi}{L^3}}$, this number of k points. So, this simplifies to $\frac{\Omega V}{8\pi^3}$. So, this is the number of k values. Other values are not allowed anymore subject to the periodic boundary condition that we have considered. In other words, the number of allowed k values per unit volume of the k space.