Solid State Physics
Lecture 27

Electronic States at Finite Temperature

Hello, we have already discussed how Sommerfeld changed the Drude model, modified the Drude model to make it to improve it something further by considering the concept of identical that is indistinguishable particles. We have so far worked out the consequences of the modifications of Sommerfeld for absolute zero temperature. If we have finite temperature that is non zero temperature what is going to happen as a consequence of that. Let us discuss that part now. So, we want to first discuss the electronic states at a finite temperature, and then we will see what are the consequences of that in case of transport properties of electron be it electrical transport or thermal transport. (Refer Slide Time: 01:39)

So, first let us understand the single electron states and many electron states. This understanding is important for proceeding further. Single electron state means a state that can accommodate only one electron. And many electron state means an array of states, an array it may not be a physical array, a conceptual array of states in each state one electron may be there that state may also be empty something like that. In a number representation say you have 3 electron states, 3 electron state. And your 3 electron state may be represented as $|001\rangle$ that means the first and the second single particle states are empty, the last one is filled or maybe as $|010\rangle$ or as $|100\rangle$ – this is for one electron being filled. If we have two electrons filled, it may be like $|011\rangle$ or $|101\rangle$ or $|110\rangle$. And if all single particle states are filled, then the three particle state would look like $|111\rangle$ that is the only possibility for that. So, each part in this is the single electron state. And in entire situation, its a many electron state. And these are some states that I have shown. There may be other states for example linear combination of these states. Like with some complex coefficient, this kind of states is also possible, $C_1|001\rangle + C_2|010\rangle + C_3|100\rangle$ this kind of linear combination of these states is also possible. So, these are our many particle states. Now, when the temperature is not 0, it is necessary to examine the excited state of the n electron system that we have at hand and its ground state as well. According to the basic principles of statistical mechanics, if we have an n particle system in the thermal equilibrium at a temperature T say, then its properties should be calculated by averaging over all n particle stationary states assigning appropriate weight to each state. So, the weight, if we call it P_N particle system and E is the energy of that system, then $P_N(E) \propto e^{-E/K_BT}$. You know this from statistical mechanics and this was due to Boltzmann. Now, if we want to write this weight that is probability $P_N(E) \propto e^{-E/K_BT}$ in its explicit form.. And if we divide it by the partition function, we will get the probability of this. So, $P_N(E) \propto \frac{e^{-E/K_BT}}{\Sigma e^{-E_\alpha{}^N/K_BT}}$, two indices that we are using here – I will explain that soon. So, what is this? This entire thing $\Sigma e^{-E_\alpha{}^N/K_BT}$ is the partition function as you have already learnt in your statistical mechanics course whatever statistical mechanics course you have done so far. And this $E_\alpha{}^N$, this is the energy of the $alpha^{th}$ stationary state of the N electron system. So, here you have seen that for three particle system, you can have many different ways of constructing the system, constructing the state. For N particle system, you will have many more ways of constructing the state. And out of those ways, this is the $alpha^{th}$ state that we are talking about. And this $alpha^{th}$ state contains N particle. So, this is the energy of that state. $\Sigma e^{-E_\alpha{}^N/K_BT}$ this is the partition function. When we divide this quantity by the partition function, we get the probability. (Refer Slide Time: 08:18)

And if we want to calculate the free energy Helmoltz free energy that would be given as $F = U - TS$. Where U is the internal energy, T is the temperature, and S is the entropy of the system. Now, the quantity that we have used earlier $\Sigma e^{-E_\alpha{}^N/K_BT}$, this quantity is transformed as e^{-F/K_BT} after performing the sum. And if we have this, then in terms of F that is the free energy, we can write $P_N(E) = e^{-(E-F_N)/K_BT}$. Once we have this, now because of the exclusion principle, if we want to construct an N electron state we must fill n different one electron levels, we cannot accommodate two or more electrons into one level that is no longer allowed by the Pauli Exclusion Principle. Therefore, each N electron stationary state can be specified by listing which of the one electron state levels are filled in the state and which are empty just like what we have done in the number representation.