Solid State Physics
Lecture 45
Semiconductor Crystals

Hello. So, far we have been discussing the electronic structures in different materials; we have discussed the linear combination of atomic orbitals, we have also discussed the nearly free electron approximation and we have seen how band gaps are there and the energy at the band edge gets modified from the free electron model. Now, we will discuss the electronic structure of one particular class of interesting materials that is Semiconductors. (Refer Slide Time: 00:56)

So, what are semiconductors? We know that metals are the materials that have no band gap, therefore there are free electrons; insulators are where there are large band gaps. So, say the here we have the valence band and this one is the conduction band; there is a huge band gap here that we can see this much, this is a band insulator. And semiconductor is something like this and the other band comes here. So, there is a band gap, but that gap is much smaller than that of a band insulator. So, this kind of a material is called semiconductor, because it is a bad conductor at a high temperature that is the reason it is called semiconductor; but not because of its bad conducting nature, rather it can become active element in the circuit upon doping of course that, these materials are so important. So, what are the kind of semiconductors that we have? First we need to understand the band gap this kind of band gap that I have drawn here is energy versus momentum picture. So, momentum is the k vector the. So, we need to plot it in Brillouin zone it, the Brillouin zone or a k vector is the three dimensional quantity; it has three components, we can call it $k_x, k_y and k_z$. There are three components of the vector and E(k_x, k_y, k_z) is a function of these three components of the vector. So, if we want to plot the full band dispersion, energy momentum dispersion relation; we would require a four dimensional plot, which is not possible. We do not have any four dimensional system four dimensional image that we can analyze with our eyes. Therefore, what we do? We consider a Brillouin zone; if we have the Brillouin zone something like this. Say this point is X point, this point is M point, this point is Γ point and so on. So, these are the high symmetry points and we draw lines between the high symmetry points; for example, from X to Γ, from Γ to M like that and X $\rightarrow$ Γ $\rightarrow$ M this kind of a direction can be called a high symmetry direction. In different shape of Brillouin zone these points are different and accordingly the band is drawn along different high symmetry lines. Now, if we consider a semiconductor with this kind of a band gap that is drawn here. So, the valence band maximum and the conduction band minimum that correspond to the same k point. So, the gap is at a given k point; in that kind of a situation, this kind of a gap is called direct band gap. Obviously, the other one is indirect band gap; that means if we have a valence band somewhat like this and the conduction band is say somewhat like this, there is a gap certainly. If I draw a line here and a line here, there is a this much amount is the gap; but this gap is indirect gap, because you can see that this gap is not at one given k point, this is one k point what where the conduction band minimum occurs and this is another k point where the valence band maximum occurs, this is the valence band maximum and this is the conduction band minimum. In case of direct band gap, we can write the gap $\epsilon = \hbar\omega_g$, where for example, if a photon comes in with ω_g frequency, angular frequency; it hits an electron, it can excite that electron to the bottom of the conduction band, minimum of the conduction band. But in case of an indirect band gap what happens; we would require $\hbar\omega = \epsilon_g + \omega_g$. What do we mean by that? So, we would have this much is the band gap ϵ_g here in case of indirect band gap material; we would excite this one first to here, this much energy and then it will non-radiatively decay here, this is a non radiative decay and that loses some energy as well as shifts the momentum, that is what we need here. And this extra amount of energy is this, this extra amount of energy is this much. So, when it moves to another momentum, it releases some energy in the form of a phonon and this is this ω is the phonon frequency. (Refer Slide Time: 08:37)

Now, let us consider motion of electrons under the influence of an electric field in the bands of a semiconductor. If we look at the motion of a wave packet when an electric field is applied, suppose that the wave packet is made up of wave functions assembled near a particular wave vector; if we have a wave vector k, the wave packet we assume it to be assembled near this, then the group velocity, as the quantity group velocity is defined, it is denoted as v_g, which is given as $\hbar^{-1}\frac{d\epsilon}{dk}$, this is the group velocity. And in three dimension we can write the $\overrightarrow{v} = \hbar^{-1}\overrightarrow{\bigtriangledown_k}\epsilon(\overrightarrow{k})$ in k space the energy. If we consider work done, that is $\delta\epsilon$ on the electron by the electric field. So, we call the electric field E here; energy is epsilon and electric field is capital E. If we consider a time interval δt; then we can write the work done $\delta\epsilon = eEv_g\delta t$, that is force times the displacement. Here we observe that, $\delta\epsilon = \frac{d\epsilon}{dk}\delta k$ and $\delta\epsilon = \hbar v_g$ from the expression of group velocity here. If we compare the above equations; then we can write $\delta k = -\frac{eE}{\hbar}\delta t$. $\hbar\frac{d\overrightarrow{k}}{dt}$ this is the force, that is $\hbar\frac{d\overrightarrow{k}}{dt} = -eE$. Now, we may write this in terms of external force. So, this quantity can be called the force vector, external force vector. With this kind of a notation, the force term also includes the electric field and the Lorentz force on an electron under a magnetic field; if we apply an apply a magnetic field on the system, then the Lorentz force also comes in the force, external force term. So, what is the Lorentz force? In cgs unit we can write the Lorenz force as $\hbar\frac{d\overrightarrow{k}}{dt} = -\frac{e}{c}(\overrightarrow{v} \times B)$ and if we move on to SI unit, that is $\hbar\frac{d\overrightarrow{k}}{dt} = -e(\overrightarrow{v} \times B)$. (Refer Slide Time: 13:56)

Now that the group velocity is given by, we just recall from the previous; the group velocity is $\overrightarrow{v} = \hbar^{-1}\overrightarrow{\bigtriangledown_k}\epsilon$, $\frac{d\overrightarrow{k}}{dt}$ this quantity can be written as from our previous expression $\frac{d\overrightarrow{k}}{dt} = \frac{e}{\hbar^2 c}\overrightarrow{\bigtriangledown_k}\epsilon \times \overrightarrow{B}$. This is in CGS unit, if we write in SI unit, we will not have the c anymore; $\frac{d\overrightarrow{k}}{dt} = \frac{e}{\hbar^2}\overrightarrow{\bigtriangledown_k}\epsilon \times \overrightarrow{B}$, this is the expression. So, we see from the vector cross product that, in a magnetic field an electron moves in a direction perpendicular to the gradient of energy; the change in momentum is perpendicular to the gradient of energy, because we are taking a cross product of it with another vector, no matter what the vector is, it would be perpendicular to this quantity. Therefore, the electron moves on a constant energy surface, this is an important thing to note. Let me explain this a bit more; we know that magnetic field does not do any work. So, the magnetic field is applied here with the electron is moving under the influence of magnetic field, that is what we are assuming here. And in this kind of a situation, the electron cannot have its energy changed; because then the magnetic field would end up doing some work. So, we have the gradient as we find from this expression, we have the gradient of energy and the electron moves perpendicular to the gradient of the energy; therefore it has to move on a constant energy surface in the momentum space, we are not talking about the real space here. Now, let us introduce the concept of hole. What is a hole? The properties of vacant orbitals in otherwise filled band; that means we have a band, that has for example one vacant site, otherwise the band is completely filled, that kind of a vacant position is called a hole and its properties are very important in semiconductor physics. If we consider under the influence of electric and magnetic field; the behaviour of a hole it behaves like +e charge and it has a momentum, that is the crystal momentum $\epsilon(\overrightarrow{k}_h) = -\overrightarrow{k}_e$ and $\overrightarrow{k}_h = -\epsilon(\overrightarrow{k}_e)$, its velocity is the same, the group velocity $\overrightarrow{v}_h = \overrightarrow{v}_e$. And its effective mass $m_h = -m_e$; electron is a real particle, it has some mass and hole has negative of that mass. Mass cannot be negative for a real particle; which means hole is not a real particle, hole is a quasi particle. We often represent electrons also as quasi particles when we talk about band structure, when we talk about the electron actually under a weak potential; but we try to represent it as if it was a free particle. And when that kind of a situation arises; we consider the electron to have an effective mass, so that we can apply the theory of free electron on that with that effective mass. So, that electron that we talk about at that time is not a real particle, it is also a quasi particle. So, that brings us to the concept of effective mass.