Solid State Physics
Lecture 43
Nearly Free Electron Approximation

Lecture - 43

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Now, we consider some important particular cases to understand exactly what this kind of problem lead to. Let us consider the nearly free electron approximation and within that approximation let us try to find out the band dispersion relation energy momentum dispersion relation. If we consider a one dimensional momentum space, then the momentum axis may be represented like this. This is our k-axis let us say this is zero momentum let us draw that with green this line corresponds to 0, this is $\frac{\pi}{a}$, on this side here this is $-\frac{\pi}{a}$, then here it is $\frac{2\pi}{a}$, here it is $-\frac{2\pi}{a}$, this is $\frac{3\pi}{a}$, this is $\frac{3\pi}{a}$ and so on. So, this is the momentum space that we have drawn and if we now want to represent the free electron energy momentum dispersion, that would look somewhat like let me draw a bit steeper that would look somewhat like on this side its a parabola that is what it will look like. Maybe this one represents a better parabola. So, I will erase the first part which looked more like a straight line. So, if we have this kind of a picture energy momentum dispersion relation for free electron, let us see what we will get for nearly free electron system. Now if we consider $k = \pm\frac{\pi}{a}$; that means, this point or this point here. Then the energy the corresponding energy would be represented as $E_0 = \frac{\hbar^2}{2m}\frac{\pi^2}{a^2}$ this is the free electron energy here and here this is E_0 the drawing is not perfect. So, these two energies look not to be the same, but in principle they are the same the reason that they look to be different is the mistake in drawing. Now if we consider $k = \pm\frac{3\pi}{a}$, then we will see that the energy equals thrice of sorry it would be $E = 9E_0$, $3^2 = 9E_0$ and it will go it will move on it will be. So, many energies that we can calculate for different values of k. Now one interesting thing to mention is that the green vertical lines that we have drawn here those are the boundaries of the Brillouin zone. If we consider small strength of a periodic potential for this system then we can consider two elements in the basis. (Refer Slide Time: 05:41)

The basis elements in that case may be represented as at $k = \pm\frac{\pi}{a}$, the basis elements that we are interested in would be $\psi_1(x)$ which is a plane wave with $k = \frac{\pi}{a}$. So, the wave function is $\psi_1(x) = \frac{1}{\sqrt{L}}\exp i\frac{\pi}{a}x$ and $\psi_2(x) = \frac{1}{\sqrt{L}}\exp -i\frac{\pi}{a}x$. So, this wave function is $\frac{1}{\sqrt{L}}\exp i\frac{\pi}{a}x$. Now if we diagonalize the crystal Hamiltonian and want to find out the energy eigen values, then we will get something like this a secular determinant like this $\begin{vmatrix} E_0 - E & V_1 \\ V_1 & E_0 - E \end{vmatrix}$ = 0 This is the secular equation that we will have where V_1 is the potential at $\frac{2\pi}{a}$. This is the Fourier transform of the crystal potential corresponding to the lowest reciprocal lattice wave number. Now we see that the two-fold degenerate empty lattice states of energy E_0 are now split. The corresponding energy eigen values would be $E = E_0 \pm |V_1|$ absolute value. And the same reasoning holds for the other empty lattice degenerate states at the point $k = 0$ and $k = \pm\frac{\pi}{a}$. So, if we now try to draw that here what would we draw? We would draw it draw the new band somewhat like this and here it would be a bit higher. So, the next place it is crossing is somewhere here, it will come here and then it will approach this place say here. So, we can draw another band like this this kind of a band can be expected. So, we can understand qualitatively in the nearly free electron approximation that the origin of the energy gaps of the one dimensional crystal that we have come that we have calculated in the context of chronic penny model, this comes due to the splitting of the twofold degeneracy of the empty lattice that is produced by periodic potential. So, you can see that there is a little gap opened here. So, this is the kind of gap that we discussed in the context of chronic penny model. We can also determine the analytically the behaviour of the energy bands near the boundary of the first Brillouin zone. So, what we have calculated here is just these two points these two points we did not really calculate this part of the band I

have just drawn it because intuitively you cannot imagine something else but let us calculate it. Let us suppose that the wave number k is very near to the boundary, but not exactly at $\pm\frac{\pi}{a}$ its somewhere a bit away. (Refer Slide Time: 10:44)

So, the basis function that we have considered earlier that would change now. We will have $\psi_1(x) = \frac{1}{\sqrt{L}}\exp\left(i(\frac{\pi}{a} - \Delta k)x\right)$ and the energy corresponding energy of this plane wave $E_1 = \frac{\hbar^2}{2m}(\frac{\pi}{a} - \Delta k)^2$. And the other basis function $\psi_2(x) = \frac{1}{\sqrt{L}}\exp\left(i(-\frac{\pi}{a} - \Delta k)x\right)$ and this has the energy $E_1 = \frac{\hbar^2}{2m}(\frac{\pi}{a} + \Delta k)^2$. So, the secular equation would be obtained by the determinant $\begin{vmatrix} E_1 - E & V_1 \\ V_1^* & E_2 - E \end{vmatrix}$=0. If we have this then the eigenvalues that can be calculated $E = \frac{1}{2}(E_1 + E_2 \pm \sqrt{(E_1 + E_2)^2 + 4|V_1|^2})$. Now if we insert in this expression the values of E_1 and E_2 that we have calculated here we will be able to write $E(\Delta k) = E_0 + \frac{\hbar^2(\Delta k)^2}{2m} \pm \frac{1}{2}\sqrt{16E_0\frac{\hbar^2(\Delta k)^2}{2m} + 4|V_1|^2}$ and this is given with $E_0 = \frac{\hbar^2}{2m}\frac{\pi}{a^2}$. (Refer Slide Time: 15:06)

Now if we have Δk small within this approximation we can expand this energy as a function of $E(\Delta k) = E_0 + \frac{\hbar^2(\Delta k)^2}{2m} \pm |V_1|[1 + \frac{2E_0}{|V_1|^2}\frac{\hbar^2(\Delta k)^2}{2m}] + ...$ if we ignore the other terms then we can write the effective mass of an electron for the upper and lower energy bands as. If we consider m^*, then $\frac{1}{m^*} = \frac{1}{m}(1 \pm \frac{2E_0}{|V_1|})$. You are familiar with the term effective mass effective mass means if we ignore the potential and consider that there are quasi-particles that are free with a mass m star, then they can be subject to this potential weak potential that we have in place they can be considered free particles with this mass the quasi particles with this mass they are moving in the crystal without in the influence of any potentials. For weak potentials small potentials and for small values of Δk we can perform this kind of an analysis to arrive at this kind of an expression for the effective mass of the system of the quasi particles in case of small energy gap. So, V_1, $2V_1 = \ energy\ gap$, if this one is $|V_1|E_0$, then the effective mass is also expected to be small ok. Now, let us see this picture. So, you will see that this picture that we have drawn with black is consistent with what we have obtained and if we now draw the next band, the next band would look somewhat like somewhat like this and so, on will go on here in the first Brillouin zone. So, this can be put in the other Brillouin zones as well, but repeating them in the first Brillouin zone gives you the entire picture of the band structure with the gaps that you can clearly see here. If you put it in the other zones that is also fine there is no problem in terms of physics, but this is customary. This is this way within the first Brillouin zone the band structure is often plotted that captures every information from every other Brillouin zone. Now if we consider semiconductors with small energy gaps, then we also find that the effective mass in that semiconductor for electrons is small giving rise to very high mobility of the carriers.