Solid State Physics
Lecture 44
Dynamical Aspects of Electrons in Band Theory

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Now, let us consider some Dynamical Aspects of Electrons in Band Theory. It is useful to introduce the concept of velocity, quasi-momentum, and effective mass for an electron in a band within a semi-classical picture. If we consider free electrons, then the wave function is given as $W(k, x) = \frac{1}{\sqrt{L}} e^{ikx}$ in one-dimension, with energy $E_K = \frac{\hbar^2}{2m}$. The plane waves are eigen functions of the momentum operator. The momentum operator $p = -i\hbar \frac{d}{dx}$, and these wave functions are eigen functions of this operator with eigen values $\hbar k$, that you can readily see. If we now consider an electron in a periodic potential, then its wave function is going to be a Bloch function. So, let us write down a Bloch function $\psi(k, x) = e^{ikx}u(k, x)$. But this in general is not an eigen function of the momentum operator. If we operate the momentum operator on this, we get $p\psi(k, x) = -i\hbar \frac{d}{dx}(e^{ikx}u(k, x))$. Now, this quantity from by performing the differentiation, we get $\hbar\psi(k, x) + e^{ikx}(-i)\hbar \frac{d}{dx}u(k, x)$. Now, depending on the nature of this quantity $u(k, x)$ if its derivative goes to 0, this would be an eigen function of the momentum operator, otherwise it is not. So, in general Bloch functions are not eigen functions of the momentum. But we have already discussed that the Bloch function can be represented as a linear combination of the plane waves. So, the only possible outcome of measuring the momentum on a Bloch function would be one of the eigen values of the elements in the linear combination. That means, we can have $\hbar k$ plane wave with this momentum, we can have $\hbar(k \pm \frac{2\pi}{a})$, we can have $\hbar(k \pm \frac{4\pi}{a})$ and so on. Any of these could be the outcome of the measurement of momentum because we can represent a Bloch function as a linear combination of plane waves with this momentum. Therefore, we can call $\hbar k$ as the quasi-momentum or the crystal momentum because this is one of the possible outcomes of the measure measurement of p, measurement of momentum. So, all these are also the possible crystal momentums, crystal momenta. (Refer Slide Time: 05:51)

Now, let us consider the expectation value of the momentum operator in a Bloch state. The expectation value of the momentum operator would be given as $\langle\psi(k, x)|p|\psi(k, x)\rangle$. Now, if we divide the $\langle\psi(k, x)|p/m|\psi(k, x)\rangle$, we are getting the velocity and this kind of a representation gives us the average velocity which we can calculate to find out $\frac{1}{\hbar}\frac{dE(k)}{dk}$. Therefore, the velocity vanishes at the band extrema. (Refer Slide Time: 06:40)

If we go back to the band picture here, then the extremum is here, here, here, and so on, and at the here and so on. And looking at this picture, you can clearly see that $\frac{dE(k)}{dk} = 0$, that is these are points of maxima or minima. And in that situation, the velocity of an electron would be 0 at these points, that is what we find from this expression of the average velocity.