Solid State Physics
Lecture 40
The Tight-Binding Approximation

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Hello. We are going to discuss the Tight-Binding Method now. The tight-binding method is essentially the linear combination of atomic orbitals in within periodic boundary condition, in case of solids. Since, it is the linear combination of atomic orbitals for solids, we must have the Bloch condition satisfied. Otherwise, it is very similar to what we have done for a linear chain of hydrogen atoms. So, here also in the context of tight-binding method, we are going to first analyze what happens in one-dimension, and then we will discuss something about more like two or three-dimensions. So, if we consider this formalism the tight-binding formalism, we can imagine construction of a crystal from a hypothetical periodic one-dimensional sequence of n atoms that are equivalent, like hydrogen atoms. So, we can draw the atoms like this and so on. Let us say this atom is at position 0, and this is the potential axis, this is the x axis, the position axis. The potential would look somewhat like, at the atomic site the potential goes sharply down and in between the potential is up. So, the potential looks somewhat like this, and this is repeated because we are considering an infinite solid, with we are treating that with periodic boundary condition. And if we say that the electron under consideration has this much energy which we call E_a, it has this much energy. This site we call t_0, this is t_1, t_2, t_3, t_4 and so on. In this direction, it is t_{-1}, t_{-2}, t_{-3} and so on. For each atom we focus our attention on a given local orbital let us say the local orbital is denoted as phi_a and the corresponding energy is E_a which is less than the barrier height as we have drawn here. And phi_a is similar to the s orbitals in case of hydrogen atom chain that we have considered, but this in this generic picture we call it phi_a. Now, it is convenient to represent the crystal Hamiltonian, in the basis of these localized functions. So, the basis set can be given as phi_a. We write its argument as the, its the position argument $phi_a(x - t_n)$. If we have the n^{th} site, then when $x = t_n$ the argument would be 0. So, the that represents the orbital corresponding to that particular site. And we form a set of such orbitals such states for varying n, that gives us a basis step state for expanding the electronic state single particle state for this solid under consideration. We need not be very specific about the Hamiltonian at this stage, but we need to use the translational symmetry of the lattice, in order to be able to get something useful, understand the useful properties of the wave function and the eigen states. So, here we define the onsite and the hopping terms of the Hamiltonian. We first defined the onsite terms $\langle \phi_a(x-t_n)|H|\phi_a(x-t_n)\rangle = E_0$, and $\langle \phi_a(x-t_n)|H|\phi_a(x-t_{n\pm1})\rangle = \gamma$. This kind of states that should represent hopping to the nearest neighbor, we call it γ. And the rest are 0, if it is ± 2, ± 3 and so on, then we consider no hopping there. So, no hopping beyond nearest neighbors. This is something we assume. Now, for simplicity due to the localized nature of the atomic orbitals, the hopping integrals involved for second and third and subsequent neighbors we have treated them, we have considered them as 0. So, the value of the interaction energy γ, this has to be negative, in order to form a solid form a crystal, otherwise it will disintegrate. (Refer Slide Time: 09:32)

So, the localized functions ϕ_a, they do not satisfy the Bloch theorem because they do not satisfy the Bloch theorem and we need a single particle state of the electron in this solid to satisfy the Bloch theorem, we have to construct the single particle state like capital $\Phi(k, x)$. It can be represented as the normalization constant $\frac{1}{\sqrt{N}}\Sigma_n e^{ikt_n}\phi_a(x - t_n)$. If we construct the single particle state in the solid, this way, if we expand it this way then what happens? Where n is the number of unit cells in the crystal, the this we can show that this satisfies the Bloch theorem, the Bloch condition, therefore, this can be called the Bloch sum. How does it satisfy the Bloch condition? Let us check that. If we try to evaluate this quantity $\Phi(k, x + t_m)$ let us say because we want a different index not the same index everywhere. If we want to calculate this, where t_m is m times the lattice constant, this would be equal to $\Phi(k, x + t_m) = \frac{1}{\sqrt{N}}\Sigma_n e^{ikt_n}\phi_a(x + t_m - t_n)$. Just from this definition here, we can write it this way. And this quantity can be expressed as $e^{ikt_m}\frac{1}{\sqrt{N}}\Sigma_n e^{ik(t_n - t_m)}\phi_a(x - t_n + t_m)$. This quantity here is nothing but capital $\Phi(k, x)$, according to this definition. In place of t_n we have put $t_n - t_m$. So, that does not change anything essentially; that means, we obtained that this quantity is equal to the Bloch sum of with argument $(k, x + t_m)$, the capital $\Phi(k, x + t_m) = e^{ikt_m}\Phi(k, x)$. This is the Bloch condition. So, this kind of construction satisfies the Bloch condition, therefore, this sum is a Bloch sum we have established that. Now, for simplicity we assume orthonormality of the orbitals centered on different atoms. If n is different, then these orbitals are orthonormal that is what we assume. If that happens then the Bloch sum is also orthonormal. So, the N, capital N number of itinerant Bloch itinerant, Bloch sums, that can span the Hilbert space just like the localized function ϕ is. But the Bloch sums for different k values, they cannot mix under the influence of a periodic potential. (Refer Slide Time: 14:40)

With these understanding the energy dispersion of the band originating from the atomic orbitals. Let us say we consider the atomic orbitals $\phi_a(x - t_n)$, set of these for different values of n, the energy dispersion of the bands originating from these atomic orbitals can be given as $E(k) = \langle \Phi(k, x)|H|\Phi(k, x)\rangle$. So, this is the onsite kind of matrix elements. And in the particular case of the matrix element of the Hamiltonian between atomic orbitals, we know that this is for the same kind of orbital it is E_0 and for different kind of orbitals that is nearest neighbor it is γ. So, just like we have derived it earlier in the context of linear chain of hydrogen atoms, we can find the energy dispersion relation here, exactly that $E = E_0 + 2\gamma \cos ka$. Now, this expression clearly shows us that the most elementary level that the enfold degenerate states of the non-interacting atoms are smeared, and they lead to a bandwidth of 2γ, sorry 4γ, 2γ here and for cosine value being $+1$ its 2γ, being -1 its -2γ. So, the bandwidth would be 4γ, $4|\gamma|$. Now, we can expand the cosine in terms of powers of k. If we have small k, we can retain up to second order term not beyond that, and we can then write $E(k) = E_0 + 2\gamma - \gamma a^2 k^2$, this way. The quadratic term that is this term here can be written in the form $\frac{\hbar^2 k^2}{2m^*}$. It is similar to the free electron case, while m^* is the effective mass; that means, we are considering electrons as quasi particles with certain effective mass that represents the free electron like picture ignoring the potential that it is subjected to. So, m^* can be given as $\frac{\hbar^2}{2\gamma a^2}$. The effective mass is small if the hopping parameter gamma is large, and if the hopping parameter is small, then the effective mass is large which is obvious. If the mass is, if the quasi particle is very heavy it cannot hop easily, if it is light it can easily hop. That is all it says.