Solid State Physics
Lecture 42

Plane-Wave Basis for Nearly Free Electrons

Hello, after discussing the tight binding method, we are going to discuss the Nearly Free Electron system and we are going to represent that system with plane wave basis. (Refer Slide Time: 00:41)

So, how are we going to deal with it? We wish to obtain the eigenvalues and eigenvectors of the Hamiltonian given as $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(X)$. Now, we will start from an empty lattice eigenvalues and eigenfunctions. At a given k value, the crystal wave function can be represented as $\psi_k(x)$, this quantity can be expanded as a linear combination of the plane waves. So, the plane waves are given by $W_{k_n} = \frac{1}{\sqrt{L}}e^{i(k+h_n)x}$ where L is the length of the crystal, one-dimensional crystal and h_n, this quantity is given by $n\frac{2\pi}{a}$, a is the lattice constant. Now, if we want to find out the Hamiltonian matrix element between the basis functions, then we can write $\langle W_{k_m}|H|W_{k_n}\rangle$, this gives us the matrix element which is represented as $\langle W_{k_m}|H|W_{k_n}\rangle = \frac{\hbar^2}{2m}(k+h_n)^2\delta_{mn}$. If m and n are different, then this quantity is going to be 0, it only contributes if m and n are equal $\langle W_{k_m}|H|W_{k_n}\rangle = \frac{\hbar^2}{2m}(k+h_n)^2\delta_{mn} + \frac{1}{L}\int_0^L e^{-i(h_m-h_n)x}V(x)\,dx$ which may be given as $\langle W_{k_m}|H|W_{k_n}\rangle = \frac{\hbar^2}{2m}(k+h_n)^2\delta_{mn} + V(h_m-h_n)$. So, this is a new quantity that we have introduced which is nothing but this quantity and so, what does it mean? $V(h)$ denotes the Fourier transform of V(x) that is what it means. (Refer Slide Time: 06:14)

So, if we now write a matrix of the Hamiltonian and if we try to diagonalize it on the basis set of plane waves, we will get a secular equation for the energy eigenvalues and that secular equation may be represented as $\|[\frac{\hbar^2}{2m}(k+h_n)^2 - E]\delta_{mn} + V(h_m-h_n)\| = 0$.