Solid State Physics
Lecture 34

The Bloch Theorem in one Dimensional Periodicity

Hello. So far we have been discussing about free electrons, but most of the electrons in solid cannot be absolutely free. They are at least subjected to a weak periodic potential; the potential having the periodicity same as the periodicity of the lattice. So, let us try to understand what is the minimum that we can understand about the electronic states subject to a periodic potential. So, let us start with one dimensional such case, so that our mathematics and our understanding becomes easier and then we will move on to more complicated situations. So, let us start discussing a one dimensional periodic potential and electron under the influence of that kind of a potential. (Refer Slide Time: 01:23)

So, if we consider an electron in a one dimensional potential and if we express that potential as $V(x)$, then the corresponding Schrodinger equation would be $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$, $\psi(x)$ is a wave function of the electron and it is a function of x. Now, the solution for Schrodinger equation is known for free electrons for which the potential is always $V(x) = 0$, harmonic oscillators for which the potential is given as $V(x) = \frac{1}{2}kx^2$ and uniform electric field for which the potential is expressed as $V(x) = e\overrightarrow{E}x$. This is not the energy, this is the electric field E here. So, the, for these kind of systems the solution to the Schrodinger equation is known. But, here we have certainly a potential of different kind. We have a periodic potential it is not very strong, but it has the periodicity of the lattice, we do not know exactly what the potential is. The potential would be different for different kind of systems, but the exact potential we are not interested in at this stage. We are interested in what we can qualitatively understand even without knowing the exact form the form of the potential, but knowing the fact that the potential is periodic in the periodicity of the lattice. So, $V(x)$ in this context is a periodic potential, and if we have a crystal with lattice constant 'a' then the potential is also periodic in a; that means we can write $V(x) = V(x + ma)$. What is m? m is any arbitrary integer. This kind of a periodicity is there in the potential. So, the Fourier transform of a periodic potential $V(x)$, that can include only plane waves, and the wave number for the Fourier expansion can be given as $h_n = n\frac{2\pi}{a}$. (Refer Slide Time: 06:21)

Now, if we express this potential $V(x)$ in terms of a Fourier series, we can write $V(x)$ as $\Sigma_{n=-\infty}^{\infty} V_n e^{ih_n x}$. And, in general if we have $V(x)$ not to be periodic, we can still have a continuum we can still have a we can have a continuous Fourier transform, but when $V(x)$ is periodic, it is a discrete Fourier transform with discrete Fourier coefficients, otherwise we will have a continuous Fourier coefficients that can be expressed in terms of integrals. Anyway, so if we start with no potential; that means, free electron kind of a system if we start with this $V(x) = 0$, then the wave functions in the Fourier expansion $W_k(x)$, these are just plane waves normalized to arbitrary length of the lattice $W_k(x) = \frac{1}{\sqrt{L}}e^{ikx}$. The normalization condition has been chosen so that this wave function $W_k(x)$ is normalized within the lattice, within the interval $0 < x < L$. Now, the wave number k, these are real and the energy eigenvalues are given as $E = \frac{\hbar^2 k^2}{2m}$ that we have learned so far. The plane waves make a complete set of orthonormal function that can be used for expansion of any wave function. So it can be used as a basis set. Now, let us consider the eigenvalue problem when the potential is periodic, but not 0. So, we have a periodic potential can that can be expressed in Fourier series as $V(x) = \Sigma_{n=-\infty}^{\infty} V_n e^{ih_n x}$. We have let us say this kind of a periodic potential at hand. And, now if we consider the Hamiltonian operator as $= \frac{p^2}{2m} + V(x)$, if we apply this operator to the plane wave, then what do we get? (Refer Slide Time: 10:25)

$H|W_k(x)\rangle$, this quantity belongs to let us say a subspace S_k. what kind of a subspace is that? This subspace is a subspace of plane waves, they have wave numbers $k+h_n$, we have the definition of $h_n$in such a way that this subspace can be given as the set of $S_k = W_k(x), W_{k+h_1}(x), W_{k-h_1}(x), W_{k+h_2}(x), W_{k-h_2}(x)$and so on. So, please go through this idea of subspace and how, what we are doing here a few times so that you understand it properly. Now, we can see that the subspace S_k that we have chosen here it is closed under the application of the Hamiltonian operator. That means, if we apply the Hamiltonian on one of the, its elements, we will get another element within this set. We will get whatever element that is within this set. We will not get it outside this set. So, diagonalization of the Hamiltonian operator within the given subspace S_k provides rigorous eigenfunctions of the Hamiltonian operator and we can level the eigenfunctions of the Hamiltonian operator as $\psi_k(x)$. So, now if we consider another wave number k', the corresponding subspace would be $S_{k'}$. $S_{k'}$ is different from S_k, it is not related to S_k, it is it will have completely different elements, provided S_k and $S_{k'}$ these are not related by integer multiples of $\frac{2\pi}{a}$. So, S_k and $S_{k'}$ are different if $k' \neq n\frac{2\pi}{a} \pm k$. If this condition holds then these two subspaces are different. Now, on the contrary, if we consider that k is if instead of not equals to if we put equal sign here; that means, if we consider $k = k' + n\frac{2\pi}{a}$, this implies that S_k and $S_{k'}$ they coincide. You can easily see by inspecting the elements in this set. Now this allows, this fact that they coincide allows us to define a fundamental region in the k-space, which is $-\frac{\pi}{a} < k \leq \frac{\pi}{a}$. This is the fundamental region, if you go beyond this you will just repeat the properties that are found in this region. You will not get anything new outside this region; therefore, this is the fundamental region. And, this region includes all the different k levels giving independent S_k subspaces. So, this fundamental region is as you can see of length $\frac{2\pi}{a}$ and this is called the first Brillouin zone or the Brillouin zone. (Refer Slide Time: 16:56)

If we consider a generic wave function, $\psi_k(x)$ that is obtained by diagonalization of the Hamiltonian in the subspace S_k, so this wave function can be expressed as an appropriate linear combination of the plane waves. So, what kind of plane waves, what kind of linear combination can express a generic wave function in this subspace? $\Sigma_n C_n(k)$, these are the coefficients of the plane waves then the normalization constant $\frac{1}{\sqrt{L}}e^{i(k+h_n)x}$. This is the expansion for any generic wave function $\psi_k(x)$. Now, it is convenient to write introduce a new function $u_k(x)$ which gives us $\Sigma_n C_n(k)\frac{1}{\sqrt{L}}e^{ih_n x}$. So, this k part is not included in u_k, this one. $u_k(x)$ this h_n part is taken here which is nothing but can be written in a bit different form $\Sigma_n C_n(k)\frac{1}{\sqrt{L}}e^{in\frac{2\pi}{a}x}$, putting the form of h_n here. So, it is clear that this function $u_k(x)$ is a function with the same periodicity of the potential. You can see that from here, if $x = a$ or integer multiple of a, it will show you clearly what the value becomes, it will go back to the same value. So, it is a periodic function with the same periodicity of the potential that is of the lattice. Now, if we have defined this quantity then we can write this generic wave function of that electron under the influence of a periodic potential as $\psi_k(x) = e^{ikx}u_k(x)$ kind of a form we can derive out of these analysis. Now, $u_k(x)$, if we take $u_k(x + a) = u_k(x)$ because u_k is periodic in a. So, this expression here is called the Bloch theorem. This holds for the wave function of an electron subject to periodic potential. So, what is the statement? We can see that the generic wave function of an electron subject to a periodic potential can be expressed as an exponential function e^{ikx} multiplied by a function that is periodic in the lattice. It has the same periodicity of the lattice. Let us express the Bloch theorem in words, because it is very important. (Refer Slide Time: 21:34)

Let us write it down. Soon we will see how powerful this theorem is. Any physically acceptable solution of the Schrodinger equation in a periodic potential takes the form of a traveling plane wave modulated on the microscopic scale by an appropriate function with the lattice periodicity. So, what is the traveling plane wave? It is the e^{ikx}, that part that is the traveling plane wave and $u_k(x)$ is the appropriate function with the lattice periodicity. This is the Bloch theorem. We can also state it in an alternative form. We can write that $\psi_k(x + t_n) = e^{ikt_n}\psi_k(x)$, where $t_n = na$where that is any translation in the direct lattice. So, the Bloch theorem guarantees the itinerant form of a wave function.