Introduction to Solid State Physics
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Lecture – 55
Going beyond free electron model: Periodic crystal potential and Bloch's theorem for the wavefunction

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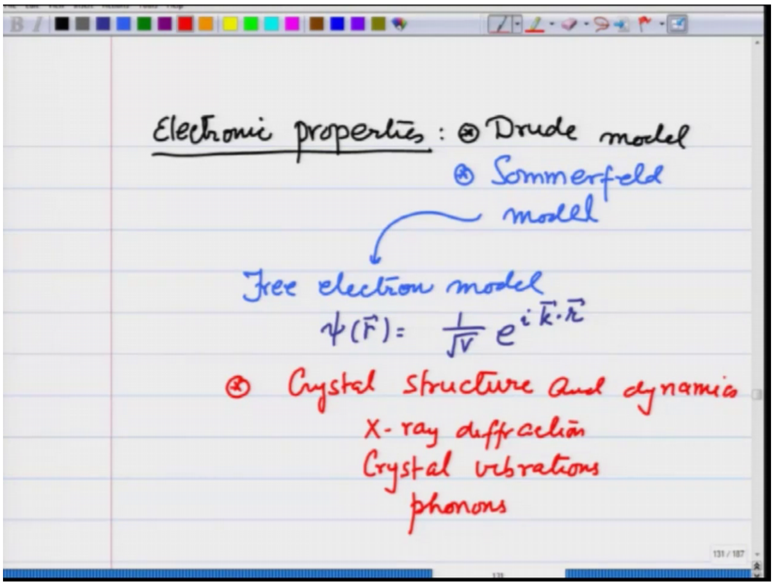

Electronic properties : ⊛ Drude model
⊛ Sommerfeld model

Free electron model

$$\psi(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$$

⊛ Crystal structure and dynamics
X-ray diffraction
Crystal vibrations
phonons

So far you have learned about electronic properties and lattice properties. In the electronic properties, you learned about Drude the model, then you learned about Sommerfeld model. This was essentially free electron model, in which the electrons are moving in a homogeneous potential in a constant potential background. And therefore, the solution the wave function for these was 1 over square root of v e raised to i k dot r with periodic boundary conditions over the volume v.

And then you went on to learn about crystal dynamics, crystal structure and dynamics, where you were told about X-ray diffraction, then crystal vibrations and their quantized form called phonons. With all these electrons and phonons, you also calculated the thermal properties, transport properties of the systems. This week we are going to start with the real crystal structure, in that we want to learn what happens, when we take into account the ionic potential of the background ions in a crystal.

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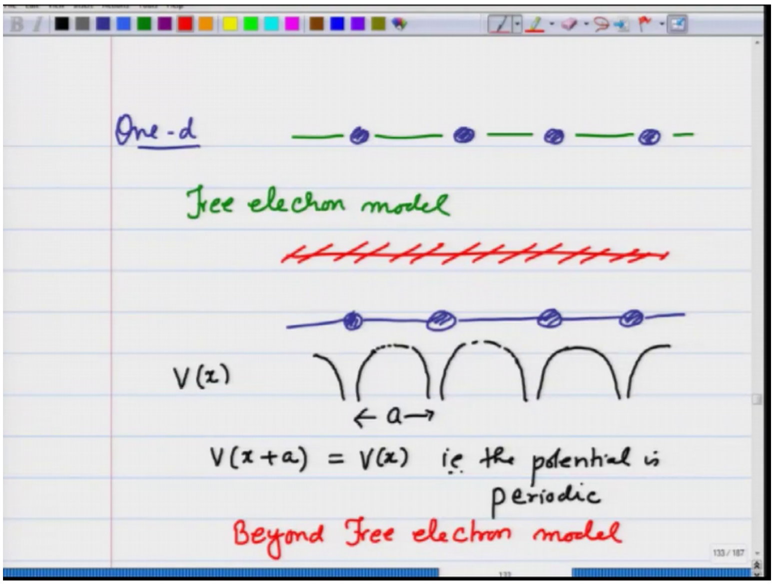

$V(x+a) = V(x)$ i.e. the potential is periodic

So, recall that in one day for simplification I have these atoms in a crystal that are connected. And in the free electron model, what we did instead of these ions sitting there we took a free constant potential of free electron moving all around. Instead when I take the ionic background into consideration, the potential is not going to be this constant. Instead if I plot it, it will go deep near the ions become flatter in between, and again go deep near the ions again become flat in between go deep and like this. So, this is the potential let me call it V x and it repeats itself over the distance between the ions, and therefore V x plus a is equal to V x that is the potential is periodic.

So, now we wish to study what happens when we have this potential in the system. So, I have to go beyond the free electron model. So, what we are really doing is we are moving towards real crystals. And going beyond free electron model, and see how it affects the energies, how it affects the wave function and so on. So, let us first look at physically what is going to happen.

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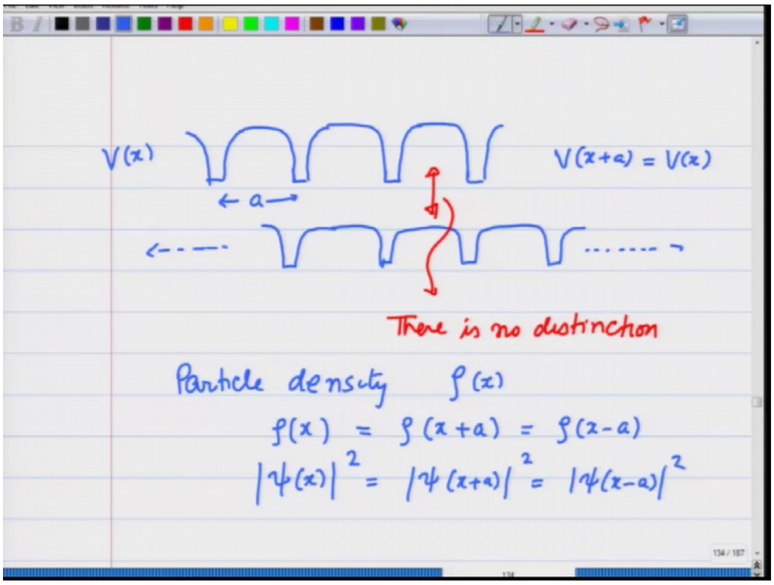

$V(x+a) = V(x)$

There is no distinction

Particle density $\rho(x)$

$$\rho(x) = \rho(x+a) = \rho(x-a)$$

$$|\psi(x)|^2 = |\psi(x+a)|^2 = |\psi(x-a)|^2$$

So, I have this potential periodic potential in which these electrons are moving. I am just making this potential symbolically let me even make it finite value. So, this is V x V x plus a is equal to V x. So, there is the translational symmetry. In that if I move these potentials, the whole system by a that means, if I bring this potential like this that means I have shifted the whole thing by one lattice constant remember this is infinitely large this way infinitely large this way nothing really changes, you cannot distinguish between curve 1 and curve 2.

So, let me show this, between these two there is no distinction. If there is no distinction, you are going to see the probability of finding an electron or the electron density the same as it was before you shifted the potential. What it means is that, if I have particle density let us call it rho x, then rho x, if I shift this system rho x plus a is going to be the same as rho x it is going to be the same as rho x minus a. That means if I have shifted the coordinate system all the lattice itself by an amount a, which is the lattice spacing the density does not change. That means if I take the wave function psi x take a mod square, this is same as psi x plus a mod square, this is the same as psi x minus a mod square, it does not change. You cannot really distinguish between the two systems. What does it mean?

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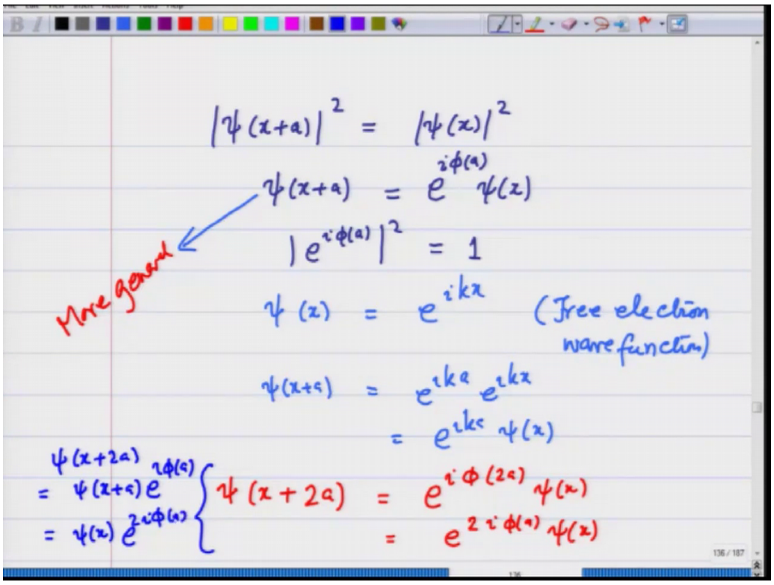

$$|\psi(x+a)|^2 = |\psi(x)|^2$$

$$\psi(x+a) = e^{i\phi(a)}\psi(x)$$

More general

$$|e^{i\phi(a)}|^2 = 1$$

$$\psi(x) = e^{ikx}$$

(Free electron wave function)

$$\psi(x+a) = e^{ika}e^{ikx}$$

$$= e^{ika}\psi(x)$$

$$\psi(x+2a) = \psi(x+a)e^{i\phi(a)} = \psi(x)e^{2i\phi(a)}$$

$$\psi(x+2a) = e^{i\phi(2a)}\psi(x) = e^{2i\phi(a)}\psi(x)$$

So, when I have psi x plus a mod square I am just now taking the plus sign is equal to mod psi x whole square, it means that psi x plus a can at most differ by psi x by a phase e raised to i phi let me call it function of a, because mod e raise to i phi a square is equal to 1. This is going to be the form of the wave function. Now, this is different from when I had psi x is equal to e raised to i k x, which is a free electron wave function. Although in this case psi x plus a is equal to e raised to i ka e raised to i k x, which is e raised to i k a psi x, this is a very limited form of the wave function.

This on the other hand the upper one, this is more generally this admits any wave function that transforms like this. And when is this possible we look into that. Now, notice one thing, we will now try to find the form for phi a. So, psi x plus 2 a will be equal to e raised to i phi 2 a psi x, I could do this psi e raise to x plus 2 a in two steps. And I could also write this as e raise to 2 i phi a psi, x, you may be wondering how did I get the second step. So, let me show this on the side I could do psi x plus 2 a is equal to psi x plus a times e raised to i phi a, and this then becomes psi x e raise to 2 i phi a.

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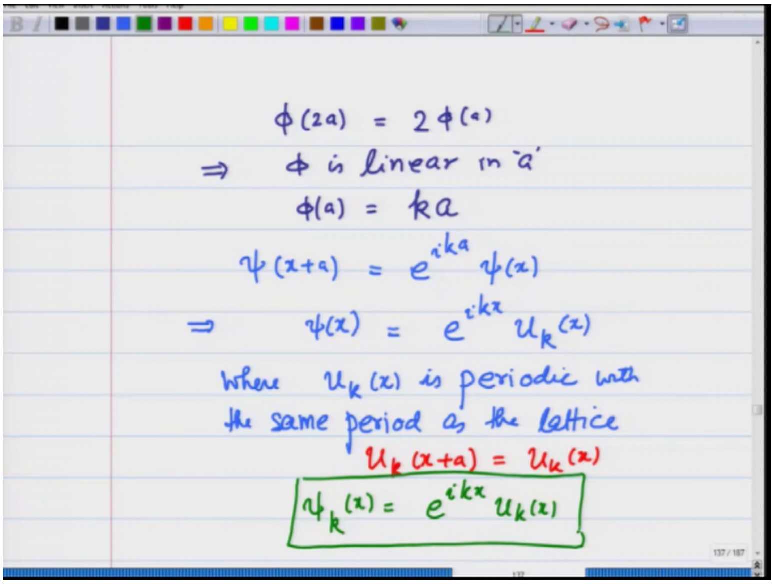

$$\phi(2a) = 2\phi(a)$$

$\Rightarrow$ ϕ is linear in 'a'

$$\phi(a) = ka$$

$$\psi(x+a) = e^{ika}\psi(x)$$

$$\Rightarrow \quad \psi(x) = e^{ikx} u_k(x)$$

where $u_k(x)$ is periodic with the same period as the lattice

$$u_k(x+a) = u_k(x)$$

$$\boxed{\psi_k(x) = e^{ikx} u_k(x)}$$

So, what we have is that the form of phi is such that phi 2 a is equal to 2 phi a implies phi is linear in a. And therefore I can write phi a is equal to some k constant a, then we conclude that psi x plus a is going to be e raise to i k a psi x. And this immediately implies that psi x is of the form e raised to i k x U k U may depend on k x were u k x is periodic with the same period as a lattice. And that means, U k x plus a is equal to U k x. And we have then concluded that the wave functions, I now label it with k x is equal to e raised to i k x U k x that is the form of the wave function. Let us spend some time on this wave function.

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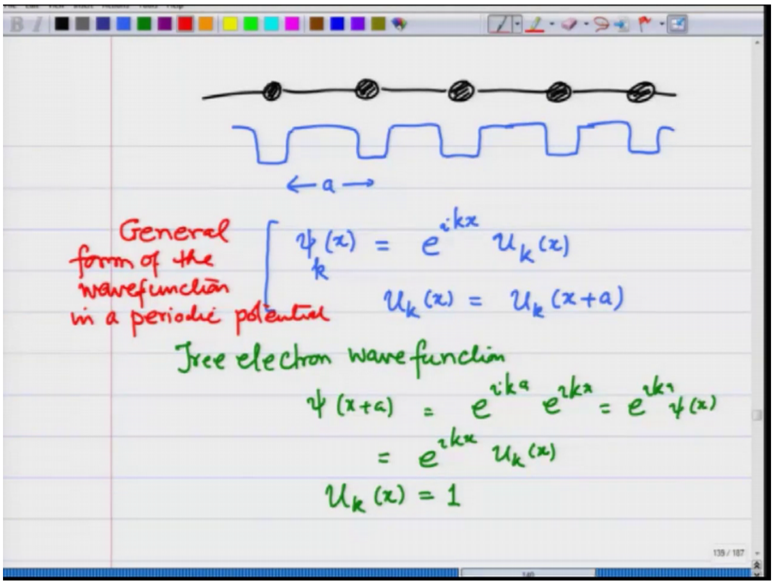

General form of the wavefunction in a periodic potential

$$\psi_k(x) = e^{ikx} u_k(x)$$

$$u_k(x) = u_k(x+a)$$

Free electron wavefunction

$$\psi(x+a) = e^{ika} e^{ikx} = e^{ika}\psi(x)$$

$$= e^{ikx} u_k(x)$$

$$u_k(x) = 1$$

So, to recap I have this one-dimensional system, where the potential is periodic with period a. In that case, the wave function psi x and I will label it with k is of the form e raised to i k x U k x, where U k x is periodic with the same period as the lattice. Notice that this property is also satisfied by the free electron wave function as we pointed out earlier, because if I take free electron wave function, then psi x plus a is going to be e raise to i k a e raised to i k x, which is e raised to i k a psi x..

And I can also write this as the form e raised to i k x U k x, but in this case U k x is equal to 1 or a constant right. So, this is a very special case of the general form of the wave function that we have written earlier. So, this form is the general form of the wave function for a single particle in wave function in a periodic potential, where the case of free electrons happens to be a very special case.

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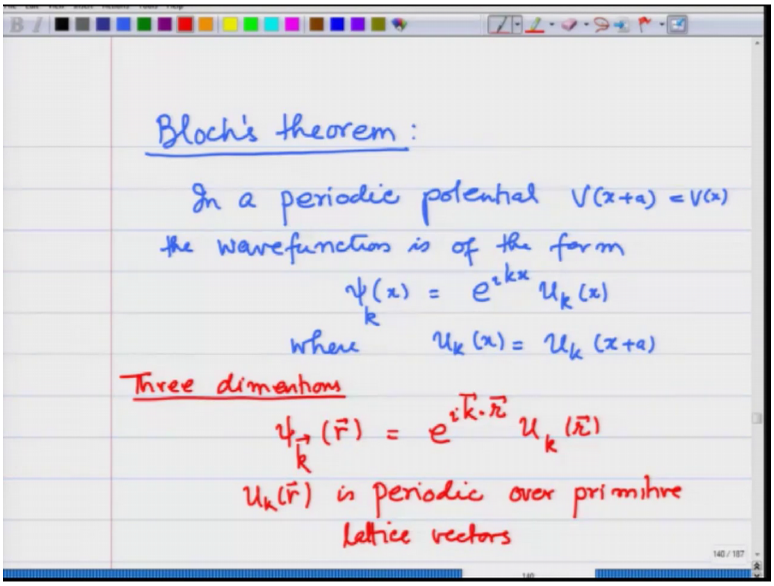

Bloch's theorem :

In a periodic potential $V(x+a) = V(x)$ the wavefunction is of the form

$$\psi_k(x) = e^{ikx} u_k(x)$$

where $u_k(x) = u_k(x+a)$

Three dimentions

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_k(\vec{r})$$

$u_k(\vec{r})$ is periodic over primitive lattice vectors

So, this is known as Bloch's theorem. What does Bloch's the state that m a periodic potential V x plus a equals V x. The wave function is of the form psi k x, where k is the label for the wave function equals e raised to i k x U k x, where u k x is periodic. This is in one dimension. In three dimensions, I would have psi k will be a three-dimensional vector r is equal to e raised to i k dot r U k r, where U k r is periodic over a primitive cell, a primitive lattice vector. So, it is periodic over primitive lattice vectors.

And therefore, any combination of those so this is the three-dimensional case. I will focus and these lectures on one-dimensional case to give you an idea what happens when you follow Bloch’s theorem, and what happens when you take this form of the wave function, and how the properties of electrons or a particle in a lattice change.