

Introduction to Solid State Physics
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Lecture – 60
Equivalence of wave vectors k and $k+G$ and reduced zone scheme

In the previous lecture, we discussed Bloch's theorem the nature of wave function in periodic potentials and I had said that I will solve Kronig Penney model which is an exactly solvable model. But before doing that I want to spend some more time discussing the Bloch wave function and its properties and how states are counted and how this leads to an understanding of semiconductors metals and insulators and their behavior.

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In a periodic potential

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

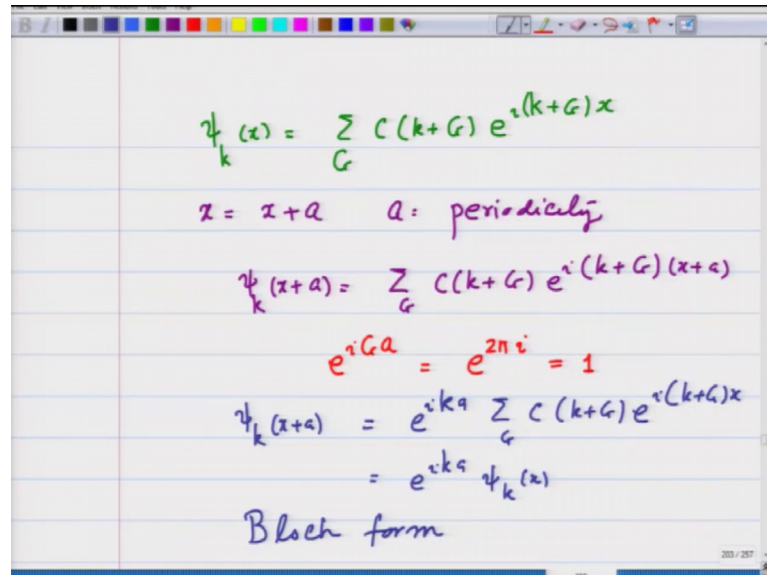
In 3d

$$\psi_{\vec{k}}(\vec{r}) = C_N e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r})$$
$$\psi_{\vec{k}}(\vec{r}) = \sum_G c(k+G) e^{i(k+G)\cdot\vec{r}}$$

So, we had discussed that in a periodic potential the wave function $\psi_k(x)$ is of the Bloch form $e^{ikx} u_k(x)$. I can put a normalization constant in front of it like C_N and confine my discussion most of the time to single dimension. However, in general also it is true that in 3d the wave function has $\psi_{\vec{k}}$ which is a vector quantity as a function of \vec{r} is of the form $C_N e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r})$, where $u_{\vec{k}}$ is periodic with the primitive lattice vector.

So, we also express this vector again I come back to 1 dimensional case $\psi_k(x)$ as equal to summation $\sum_G C_{k+G} e^{i(k+G)x}$ and I showed you that this satisfies Bloch form let us look at it again.

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$$\psi_k(x) = \sum_G C_{k+G} e^{i(k+G)x}$$

$$x = x+a \quad a: \text{periodicity}$$

$$\psi_k(x+a) = \sum_G C_{k+G} e^{i(k+G)(x+a)}$$

$$e^{iGa} = e^{2\pi i} = 1$$

$$\psi_k(x+a) = e^{ik_a} \sum_G C_{k+G} e^{i(k+G)x}$$

$$= e^{ik_a} \psi_k(x)$$

Bloch form

So, the wave function $\psi_k(x)$ is equal to summation $\sum_G C_{k+G} e^{i(k+G)x}$, if I put x equals $x+a$, where a is the periodicity then $\psi_k(x+a)$ becomes summation $\sum_G C_{k+G} e^{i(k+G)(x+a)}$. If you notice then e^{iGa} is nothing, but $e^{2\pi i}$ which is equal to 1.

Therefore, a does not really affect the G part of the wave function and I end up getting that $\psi_k(x+a)$ is equal to e^{ik_a} summation $\sum_G C_{k+G} e^{i(k+G)x}$ which is nothing, but $e^{ik_a} \psi_k(x)$ the Bloch form. So, it satisfies Bloch's equation. Now I am going to look at it from a different perspective and see, what the wave function.

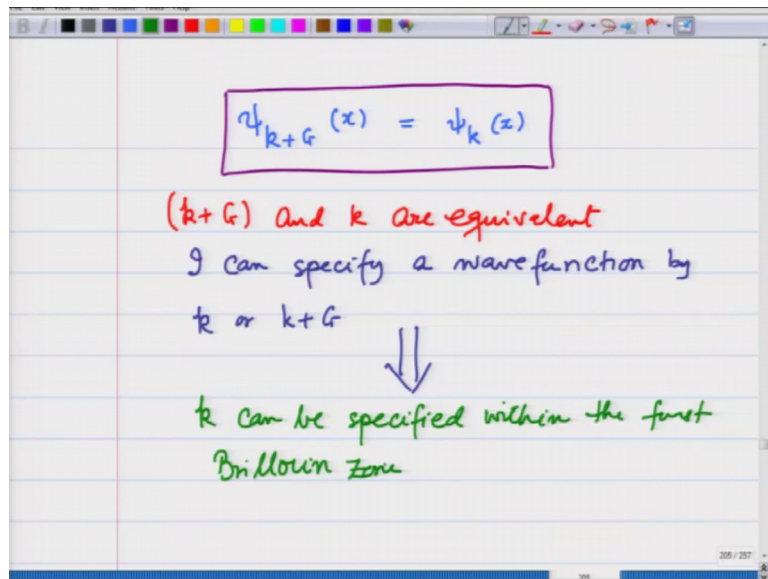
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The image shows a whiteboard with handwritten mathematical derivations. At the top, it states $\psi_k(x) \leftrightarrow \psi_{k+G'}(x)$. Below this, the wave function $\psi_{k+G'}(x)$ is expressed as a summation over G : $\psi_{k+G'}(x) = \sum_G c(k+G'+G) e^{i(k+G'+G)x}$. A red note says "Take $G+G' = G''$ ". This leads to the equation $\psi_{k+G'}(x) = \sum_{G''} c(k+G'') e^{i(k+G'')x} = \psi_k(x)$. The final conclusion is "The wavefunctions $\psi_{k+G'}(x)$ and $\psi_k(x)$ are identical".

$\psi_k(x)$ becomes if instead I consider $\psi_{k+G'}$ does it represent something else and what happens when I make this transformation and let us look at that. When I substitute k by $k+G'$ this wave function becomes $\psi_{k+G'}(x)$ which will be equal to summation G $c(k+G'+G) e^{i(k+G'+G)x}$.

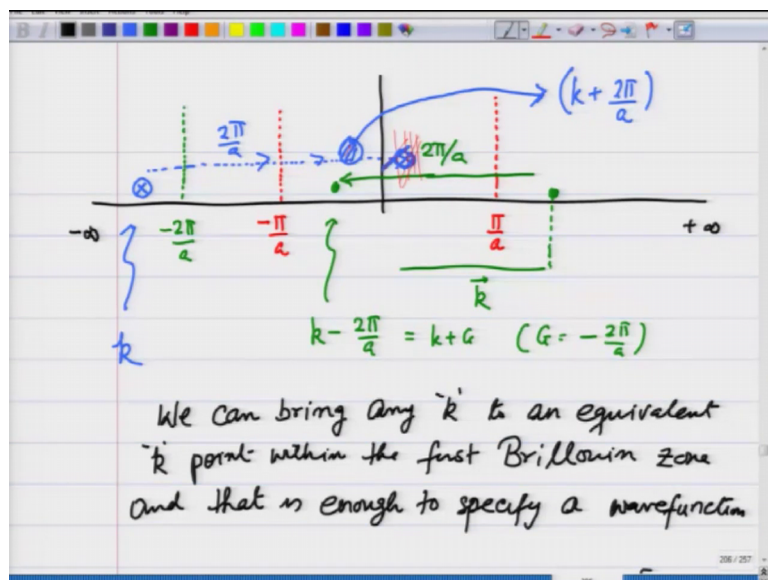
Now, take $G+G'$ to be some other reciprocal space vector G'' then I have $\psi_{k+G'}(x)$ is equal to summation instead of G now I can add over G'' and I get $c(k+G'') e^{i(k+G'')x}$. Since G'' is being added over same thing as adding over G this is precisely the same as $\psi_k(x)$. So, what do we conclude? We conclude the wave functions $\psi_{k+G'}$ and $\psi_k(x)$ are identical; I am underlying this identical they are identical what does it mean let us understand that.

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So, we have said that ψ_{k+G} if I add a reciprocal space vector G to k this is same as ψ_k . What it means is that $k+G$ and k are equivalent, I can specify a wave function by k or $k+G$ where G is any reciprocal space vector and this implies that k can be specified within the first Brillouin zone, let us reflect on that a bit.

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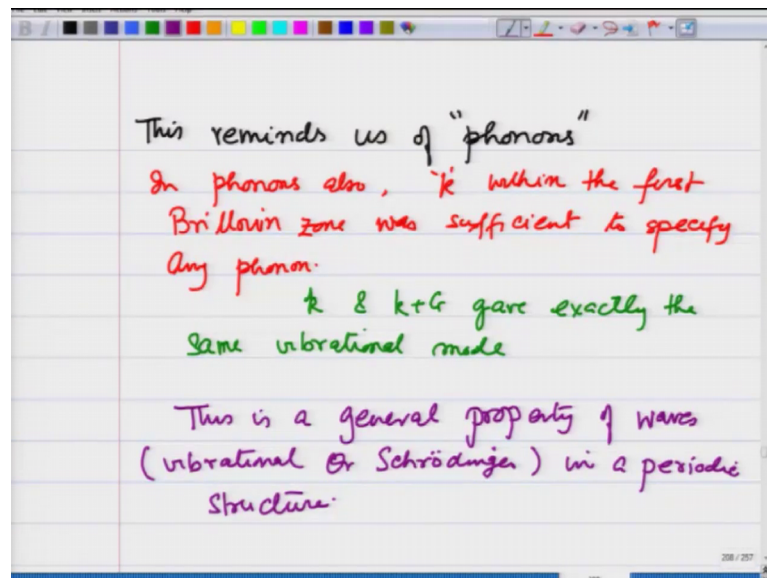
So, suppose I have this case space extending from minus infinity to plus infinity and I had this first Brillouin zone here minus π by a to π by a . If I have a wave vector let us say at this point suppose this is a wave vector k , this would give me exactly the same

wave function if I subtract it 2π by a from this and brought it here. This point is for this k , k minus 2π by a , in other words this is k plus G , where G is equal to minus 2π by a .

Let us look at another point let us say here even outside minus 2π by a let us say this point is over here. I can translate it by adding 2π by a to this and if I do that, I would have moved it somewhere here this is 2π by a this way. This point is some k and this point would have been k plus 2π by a , I made a slight mistake here this point k plus 2π by a does not come here. So, I am going to cut it with a fine pen it actually moves somewhere here. So, I am going to make it again this point moves over here.

So, it is this point which is it is this k plus 2π by a . Nonetheless the point is that by adding appropriate reciprocal space vector I can bring all the k points to the first Brillouin zone and that is enough to specify a wave function. So, let us write it again we can bring any k to an equivalent k point within the first Brillouin zone and that is enough to specify a wave function. Now, this should remind you of something, let us write that this.

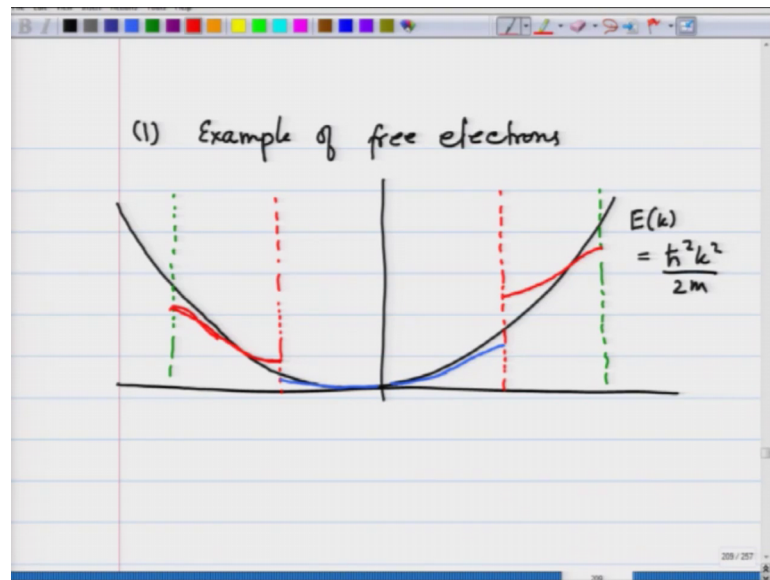
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Reminds us of phonons; what happens in phonons? In phonons also k within the first Brillouin zone was sufficient or enough to specify any phonons; any phonon. So, k and k plus G gave exactly the same vibrational mode and this happens in electrons also.

So, this is a general property of waves be it vibrational or Schrodinger wave in a periodic structure. So, if you have a periodic potential, periodic lattice constants since like those k within the first Brillouin zone is enough to specify any wave in that structure. Let us now look at some examples through this.

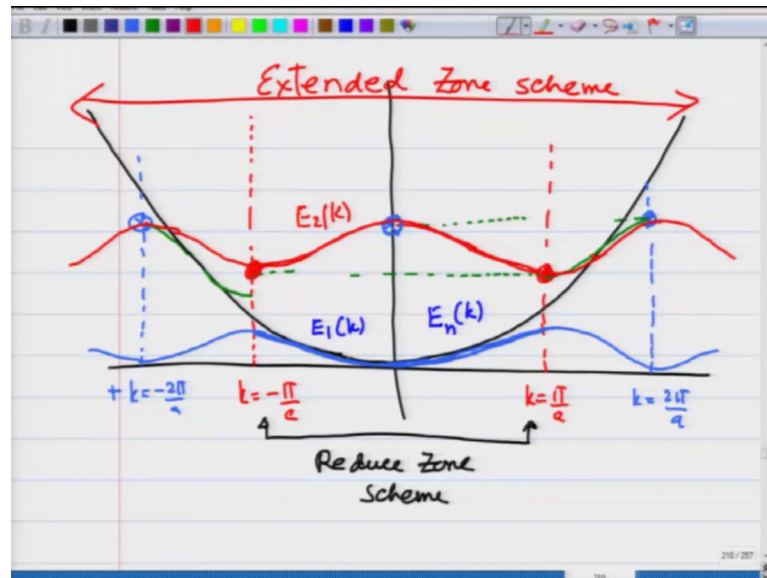
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1st example of free electrons; remember what we have done so far in discussing free electrons and after that the nearly free electron model is that if I look at the free electron $E(k)$ versus k curve and here is the boundary of the first Brillouin zone it is the second one this is how the black curve this is how the free electron curve looks. And when I apply a nearly free electron model the energy curve changes a bit near the boundary and I am making it here schematically and then in the second zone it goes like this in the second zone it will go like this and so on.

And if you recall from the lectures earlier I can translate all this into the first Brillouin zone and I had said that, I owe you an explanation for this and this is what I am explaining right now. So, let me make this figure more accurately in the next slide; we tried doing that here.

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So, here is the curve and let us make the first Brillouin zone which is right here and the second Brillouin zone which is right here and I said that the curve becomes something like this, the actual energy curve and I do nearly free electron model in the second zone it will again split here by $2v_g$ and it will become like this.

So, let us make it here will become something like this and when I translate this into the first Brillouin zone. Remember how we translate the points the point out here would be translated by two pi and it will go to this point right here. Similarly point out here will become equivalent to this point and this will also come here. So, what happens now is that this curve this point is translated here this point would be translated here by 2π , let me make it more clearly this point out here on the right side gets translated here.

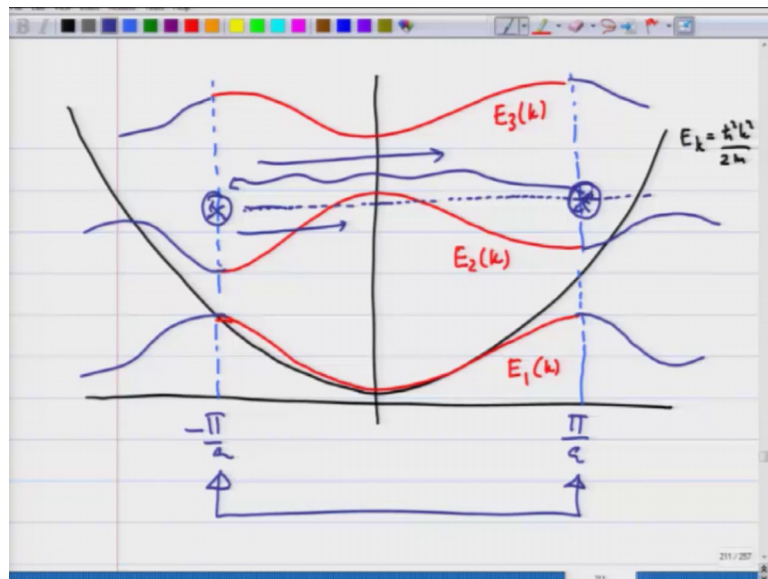
So, what you see now is that this curve will become like this and when the other part gets translated it will become like this. So, here is your band diagram or energy versus k diagram in the first Brillouin zone. And if I were to extend let us say I want to say let me also make these points this is k equals π by a this is k equals minus π by a , the blue ones is k equals 2π by a , the blue one out here on the left hand side is k equals minus 2π by a . If I were to see no let me see it in the whole k space then what I will do is k plus g is equivalent to k and therefore, this curve would start behaving like this.

Because these all these points are equivalent. The orange curve the upper band would start doing this. When I bring all the curve only within the first zone then it is called

reduced zone scheme, I am looking at all the bands in the first zone. If I plot them over the entire k space although it is not fruitful, but sometimes it goes to visualize things this is the extended zone scheme.

If I remain within the reduced zone scheme so, suppose I do not look at left and right here I would put the energy as E as a function of k, but it is as a function of k for each band then I will label the band as E_n . For example, the blue one here would be $E_1(k)$ the orange one would be $E_2(k)$ and so on and the higher bands. So, it becomes E_n as a function of k within the zone. Let me now make this diagram once more to make things clearly visible.

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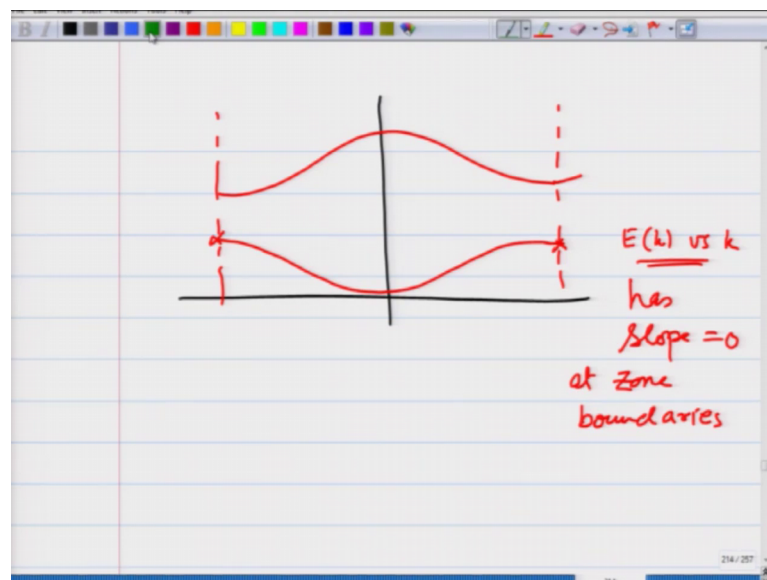
So, I had this curve for $E(k) = \frac{\hbar^2 k^2}{2m}$ and in the reduced zone scheme let me make this zone extended like this, I have these bands like this next one will be again like this and so on this will be $E_1(k)$, this will be $E_2(k)$ third one will be $E_3(k)$ and so on. And if I want to extend them further they will go like this does not teach me anything new, but nonetheless sometimes go to visualize what is happening.

So, either suppose I am going from left to right let me look at band 2. If I am going from left to right let me make this arrow I can go to the right starting from point minus pi by a to plus pi by a I can go to the right I am showing by this dashed line go to the right reach the point plus pi by a in the extended zone scheme, I will go further and increase k or in

the reduced zone scheme I will say that this point which I am showing by a cross is again equivalent to this.

So, I can come back to this point start all over again. So, I can keep repeating myself periodically within the first zone because the point π/a and $-\pi/a$ are equivalent. So, in the reduced zone scheme I go to π/a and jump back to $-\pi/a$ because that point is equivalent to π/a or in the extended zone scheme I can keep extending k , but that is exactly the same as k minus π/a ; so, I can always come back. So, this is how you look at k . If you have noticed carefully you must have seen that when I made this graph.

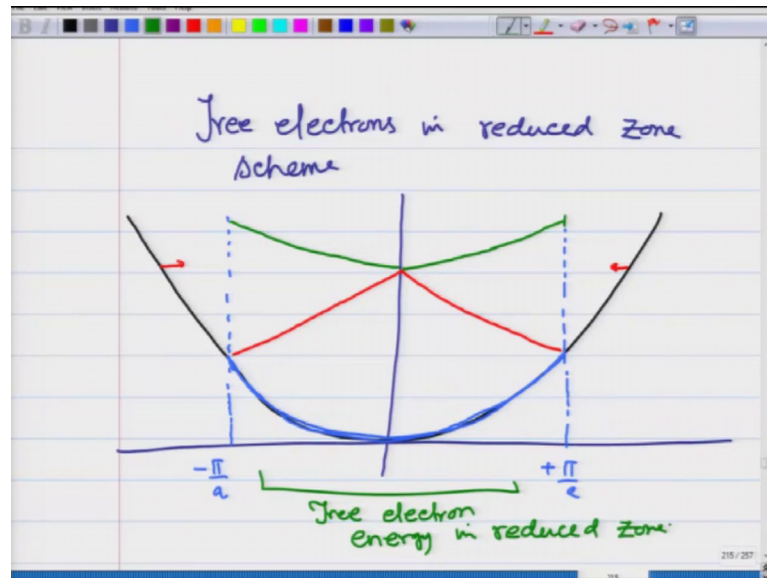
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I will just make the bands now within the first Brillouin zone. Since the band repeats itself is either a minimum or a maximum at the zone boundary and therefore, $E(k)$ versus k has slope equal to 0 at zone boundaries very important point.

Now, I said this in the context of 1d the same thing happens in 2d or 3d also except that this is slightly more subtle because you have to now think of the band structure in 3 dimensions, I will comment on that a little later.

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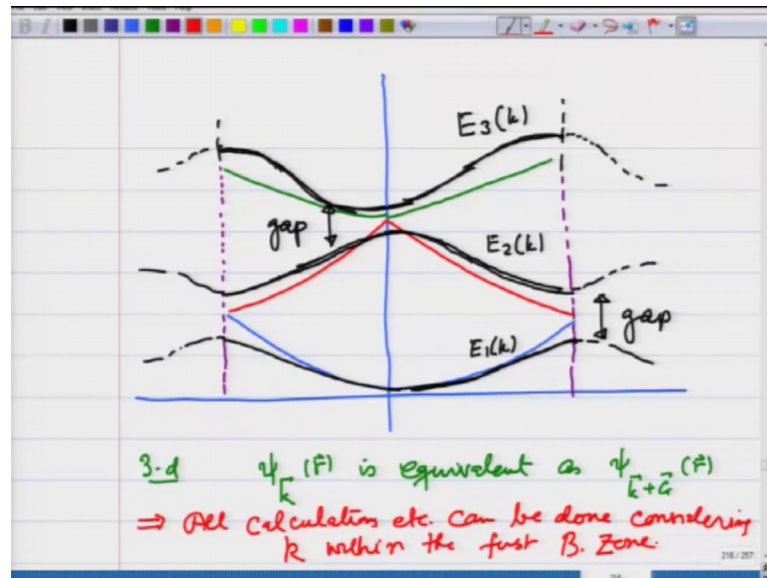


It will be interesting to see what happens if I look at the free electrons in reduced zone scheme. So, let us do that I have this curve of free electrons in the reduced zone scheme and the extended zone scheme and suppose now I say I want to bring it to the reduced zone scheme. I may want to do that before I even apply the Bloch's theorem or the perturbation theory or nearly free electron model if I do that.

So, in the first zone the zone is shown here with blue lines. So, this is extending from minus pi by a to plus pi by a, in the first zone which I have been making with blue the energy diagram looks like I have shown with blue out here.

For the second zone I will bring this fellow back by $2\pi/a$ and fellow from the left hand side to right moving it by $2\pi/a$ and the curve would look like this. In the third zone again I will do the same thing and as I will leave for you to see the curve would look like this. So, this is what I made within this is free electron energy in reduced zone, let me repeat it in the next slide.

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So, what I have done is I have taken these free electron energies and plotted them in the first zone by translating all the energy curves. So, they look like this the third zone look like this and so on. Now let us see what happens, when I turn on the perturbation or turn on that weak potential this curve starts developing a gap I am showing it by black now a gap near the zone boundary the upper one will go up and it becomes smooth near the zone boundary.

The next one again will become smooth near the zone boundary and become perpendicular to the zone boundary its slope near the zone boundary. So, this is E_3 k E_2 k E_1 k and here are the gaps here is the gap. So, you see very clearly if I put all this nearly free electron model free electron energy in the first zone, and then I apply the perturbation or the periodic potential how the bands evolve within the first Brillouin zone itself. And then of course, if you want to make it in the extended zone scheme you can always extend it.

So, I have given you a picture of how we can think of all the wave functions in a periodic structure being equivalent if they are wave vectors \mathbf{k} differ by a reciprocal space vector I have shown it in 1d and 3d also the same thing happens. So, in 3d $\psi_{\mathbf{k}}$ vector \mathbf{r} is equivalent. In fact, the same right as $\psi_{\mathbf{k}+\mathbf{G}}$ \mathbf{r} and therefore, I can make all the pictures energies and everything within the first Brillouin zone.

So, let us write that also and this implies all calculations etcetera can be done considering k within the first Brillouin zone two for 3d also having discussed this.

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Significance of wavevector \vec{k} , k

Question: In free electrons $\hbar\vec{k}$ gives the momentum of the electron

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

$$\vec{p} \psi_{\vec{k}}(\vec{r}) = \frac{\hbar}{i} \vec{\nabla} C_N e^{i\vec{k}\cdot\vec{r}}$$

$$= (\hbar\vec{k}) \psi_{\vec{k}}(\vec{r})$$

$$\vec{p} \psi_{\vec{k}}(\vec{r}) = \frac{\hbar}{i} \vec{\nabla} (e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r}))$$

$$\neq \vec{p}_0 \psi_{\vec{k}}(\vec{r})$$

Now, let us understand the significance of wave vector k in 3d and k in 1d. Question in free electrons k or \hbar cross k to be precise gives the momentum of the electron under consideration. Because here when I have $\psi_{\vec{k}}(\vec{r})$ which is some normalization constant C_N raised to $i\vec{k}\cdot\vec{r}$ if I apply the momentum operator to $\psi_{\vec{k}}(\vec{r})$ this is \hbar cross over i gradient of $C_N e^{i\vec{k}\cdot\vec{r}}$ it gives me \hbar cross k times the wave function $\psi_{\vec{k}}(\vec{r})$. So, this is a momentum eigen function and therefore, it gives the momentum of the electron. On the other hand if I look at momentum operating on $\psi_{\vec{k}}(\vec{r})$ of the Bloch form, it is \hbar cross over i del operating on $e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r})$ and this is not equal to some vector \vec{p}_0 let us say times $\psi_{\vec{k}}(\vec{r})$.

Therefore it's not a momentum eigen function. So, question is in the free electron this gives \hbar cross k gives the momentum of the electron what happens in a Bloch electron case. So, let me complete this question.

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Question: What does \vec{k} specify in case of an electron in a periodic potential

In case of free electron $\hbar\vec{k}$ is the momentum of an electron

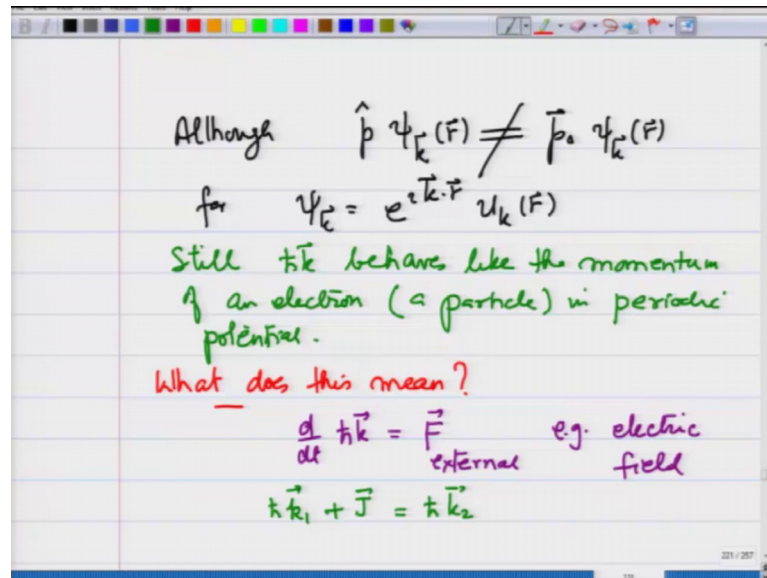
$$\psi_{\vec{k}} = e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r}) \text{ in 3d}$$
$$= e^{ikx} u_{\vec{k}}(x) \text{ in 1d}$$

Answer: $\hbar\vec{k}$ behaves exactly like the momentum of an electron

So, what does k specify in case of an electron in a periodic potential I am continuing this question from last slide. So, I will just previous slide, so, I will just say this is question continue. So, we just saw that in case of free electrons \hbar cross k is the momentum of an electron and the question we are raising it what about when the wave function is $\psi_{\vec{k}}$ of the form $e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r})$ or in 1d it is of the form $e^{ikx} u_{\vec{k}}(x)$ in 1d.

I am right now not proving anything, but the answer to this is \hbar cross k behaves exactly like the momentum of an electron or the particle in a periodic lattice; so, that is the answer.

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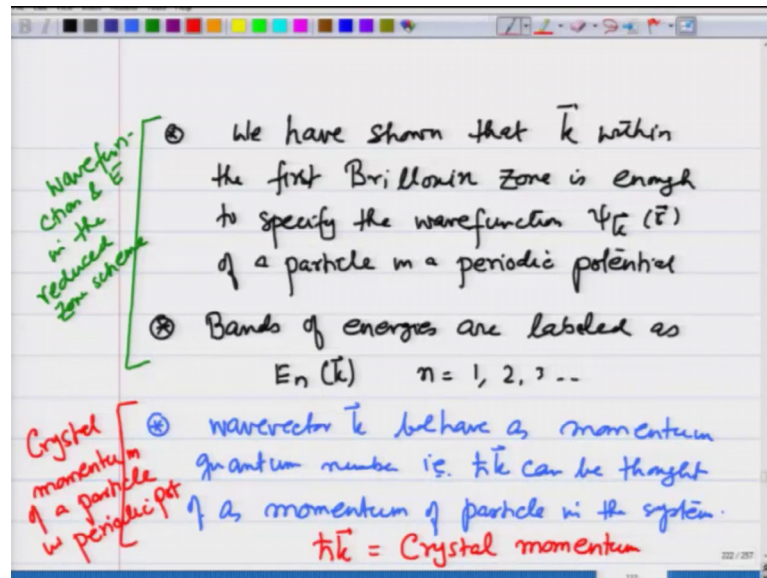


So, although \hat{p} operator $\psi_{\vec{k}}(\vec{r})$ is not equal to some p_0 which is the eigenvalue for the momentum $\psi_{\vec{k}}(\vec{r})$ for $\psi_{\vec{k}} = e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r})$. So, its not a momentum eigenstate still $\hbar\vec{k}$ behaves like a momentum of an electron whose wave function we are writing or a particle in periodic potential. what does this mean? So, question is although I am saying that it is behaving like the momentum what does this mean?

This means that if I take $\frac{d}{dt}$ of $\hbar\vec{k}$ for an electron or particle moving in a periodic system, this will be equal to the external force. And let me tell you why I am calling this external force this is external to the system; that means, its not including that periodic potential, but the force that I am applying from outside, it could be the electric field for example, an electric field.

So, that is one way that you know think of this as a momentum. The other thing is that, it is conserved if I have some impulse imparted to this electron through phonons through whatever right this will give you $\hbar\vec{k}_2$. So, it is in these two ways that it behaves like momentum and we will see examples of this later when we do little bit of transport.

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So, to conclude this lecture, we have shown that k within the first Brillouin zone is enough to specify the wave function $\psi_{\vec{k}}(\vec{r})$ or $\psi_{\vec{k} + \vec{g}}$ it does not matter the wave function of a particle in a periodic potential. Number 2 what we have shown is therefore, bands of energies are labeled as $E_n(\vec{k})$; \vec{k} is in the first Brillouin zone each band now is given this index n ; n equals 1 2 3 and so on.

And we showed through the example of the free electron and nearly free electron energy curves how everything gets reduced in the first Brillouin zone and the wave vector k behaves as momentum quantum number that is $\hbar k$ can be thought of as momentum of particle in the system.

And therefore, $\hbar k$ now let me give you the name also is given the name $\hbar k$ is given the name of crystal momentum. So, we have introduced the idea of crystal momentum also. So, let me on the side show this, this part is the wave function and energy in the reduced zone scheme and the second part is the introduction of crystal momentum of a particle in periodic potential.

So, these are the new things that we have introduced, in the next lecture, we will see how we count the number of states in a band and how the gaps lead to the behavior of metals insulators and semiconductors.

Thank you.