

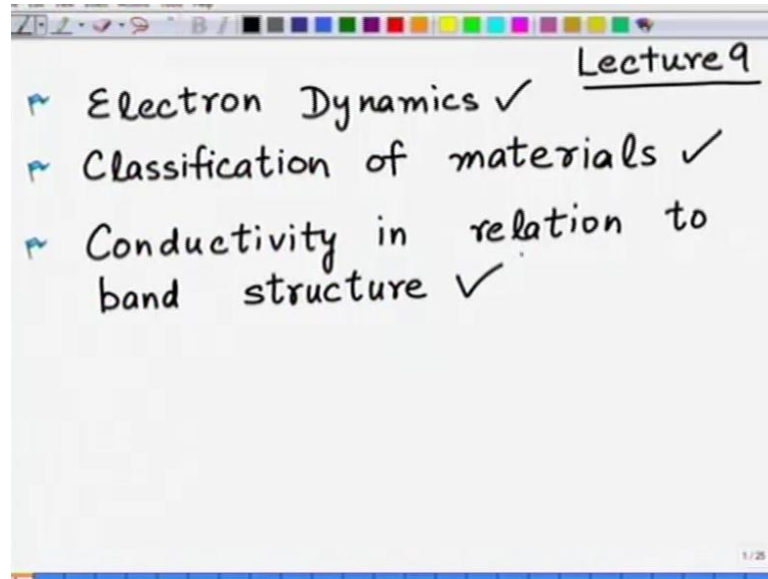
Optoelectronic Materials and Devices
Prof. Dr. Deepak Gupta
Department of Materials Science and Engineering
Indian Institute of Technology, Kanpur

Module - 1
Electronic Structure of Materials
Lecture - 9
Electron dynamics

Welcome to lecture number 9. So, let us see what we going to do today. Let us see from the context of what we finished. Yesterday, we plotted E versus k diagram. We go to the point where we could... Last lecture, we were able to reduce E k diagram into first bullion zone. Also, I gave you idea of what periodic potential would do by looking at one dimensional Kronig Penney model. That one dimensional model told us that if we apply a potential, which is neither too small in comparison to the electron energy nor it is too high that means tending to infinity.

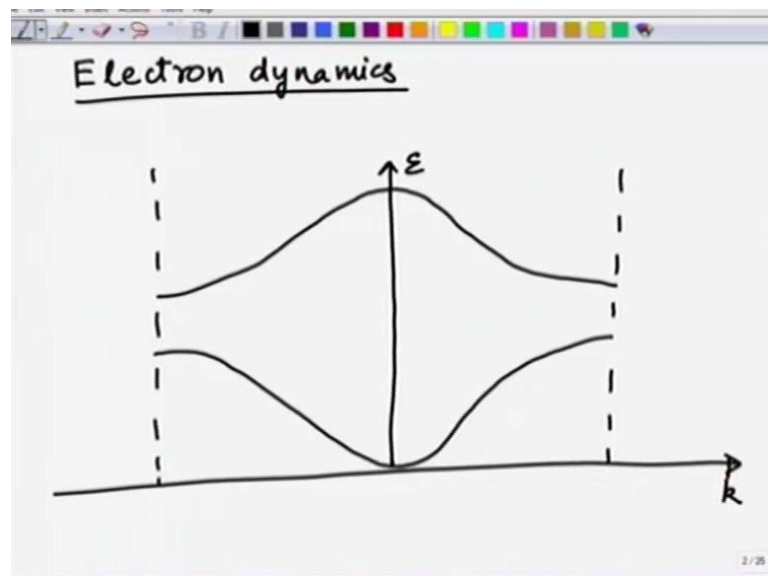
Then, in that case, we have a possibility of either having a metal where there is a no band gap or it is also possible. Well, if it is some reasonable potential, periodic potential, in that case, we could have a band gap opening up. There is a band gap meaning this allowed energy is for electrons. That means the n states case states, case states, where electron, which electron cannot have. So, those are that leads to, sorry, I rephrase my words actually not disallowed case states rather the disallowed energies case states are possible. But, there are certain, this energy ranges, which electron cannot have. So, that is what we called as band gap. We saw periodic potential leading to band gap.

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So, now knowing that origin of band gap and those we can E k diagrams. So, in order to do so using E k diagram, first thing I will do today is electron dynamics. Then, we will again start looking at the classification of materials, and following that, we will start looking at conductivity of materials in relation to the band structure. Let us see how far we go with respect to this particular topic. Then, we will continue if we do not finish, we will continue in the next lecture also.

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So, let us start with electron dynamics. What do we mean by that? What we saw was that if I plot again energy versus k; if I again plot energy versus k, this is energy and this is within this possible n zone. Now, I will always plot only everything in possible n zone and where it is symmetric, I did not need to plot both halves, I could have plotted only one half, but anyways for sake of completeness, let us do that.

What do we see? We see that we had two types of energy curves; one which was like this, after this nearly the free electron theory, where we found that band gap opens up, we found or bless droid the way it was, we found that the curves were of these two forms. The shape of the curves was something like this. There were two types of curves. We had either concave downwards or concave upwards or you can talk in terms of convexity, but anyways either way these are the two types of curves for E versus k we saw.

Now, given these curves, this type of curves, what is the kind of information which we can get on motion of electrons from these curves? Can we derive anything from it? That is what we want to see. That is what is called as electron dynamics. In order to do that, let us look at it, this following form.

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The image shows a whiteboard with handwritten mathematical equations. At the top, the wave function is given as $\Psi(\vec{r}, t) = \psi(\vec{r}) e^{j\omega t}$. An arrow points from the ω term to the text "average (group) velocity of the wave packets". Below this, the velocity vector \vec{v} is defined as $\vec{v} = \frac{\partial \omega}{\partial \vec{k}} = \vec{\nabla}_{\vec{k}} \omega$. This is then expanded into its components: $= \frac{\partial \omega}{\partial k_1} \hat{x}_1 + \frac{\partial \omega}{\partial k_2} \hat{x}_2 + \frac{\partial \omega}{\partial k_3} \hat{x}_3$. A bracket is drawn under the three terms. At the bottom, the unit vectors are defined: $(\hat{x}_1 \equiv \hat{x}, \hat{x}_2 \equiv \hat{y}, \hat{x}_3 \equiv \hat{z})$ and $1 \equiv x, 2 \equiv y, 3 \equiv z$.

If I look at the total wave function, which is this total wave function, it is function of position and time. I have already said. In front of that, I am solving for the special part time dependence is already assumed. We had said that this wave function would look

like something like this. This is the quantity we have been along solving. We had assumed the time dependence to be of the form $e^{j\omega t}$. That is what we had assumed. That is why, I have, did separated the time dependent part of the Schrodinger equation from the special part of the Schrodinger equation.

I been solving only this, only the special part because the time dependence form was already known each part $e^{j\omega t}$. Anyways, I construct the whole wave function. The reason is that what we are going to see is there what first thing we want is if we think of electron as a wave, the energy is transmitted through the group velocity. That means the in velocity of the wave packet.

If I look at the wave, if I look at the group velocity average, which is group velocity of the wave packets, but that quantity is simply v is this. It is the velocity by which the energy is transmitted transferred is travelling. So, if that velocity is simply given by the dispersion relationship that is $\frac{d\omega}{dk}$ vector, which in another form can be written as gradient with respect to k of ω . So, you take gradient that means this. If you want to expand it out further, then you can write it as $\frac{d\omega}{dk_1} \hat{x}_1$ or $\frac{d\omega}{dk_2} \hat{x}_2$ plus $\frac{d\omega}{dk_3} \hat{x}_3$.

What is the $\hat{x}_1, \hat{x}_2, \hat{x}_3$? I hope you know understand \hat{x}_1 . For example, in Cartesian co-ordinate system, where \hat{x}_1 would be equivalent to \hat{x} and \hat{x}_2 would be equal to \hat{y} and \hat{x}_3 would be equal to \hat{z} meaning, thereby let us 1, 2, 3 or 1 implies x and 2 implies y and 3 implies z meaning, thereby that the 3 notations I am using 1, 2, 3 is really or the symbol from the orthogonal co-ordinates. If it is Cartesian, then it is x, y, z . In the way, I have written, expanded of course, it is implies this Cartesian co-ordinate system here.

So, therefore, it is x, y, z . That is how I have written the group velocity. So, that is the velocity by which; average velocity with which this electron transferring energy. So, that is dispersion relationship which is given here. Now, why did I do this? What I really want to do is this is what I want to determine this is what I want to determine? Now, let us look at this.

I want to do it in terms of energy and k . However, I want because I want to relate it to this diagram. Here, this diagram is given here. I want to relate the velocity of electron

through this diagram. So, in order to do so, let us see what is an energy operator? We are going to next page. Let us forget the energy operator.

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Energy operator $\equiv -\frac{\hbar}{j} \frac{\partial}{\partial t}$

$-\frac{\hbar}{j} \frac{\partial}{\partial t} \Psi(\vec{r}, t) = \epsilon \Psi(\vec{r}, t)$
 $\Psi(\vec{r}) e^{j\omega t}$

$\boxed{\epsilon = \hbar \omega}$

$\omega = \frac{1}{\hbar} \epsilon$

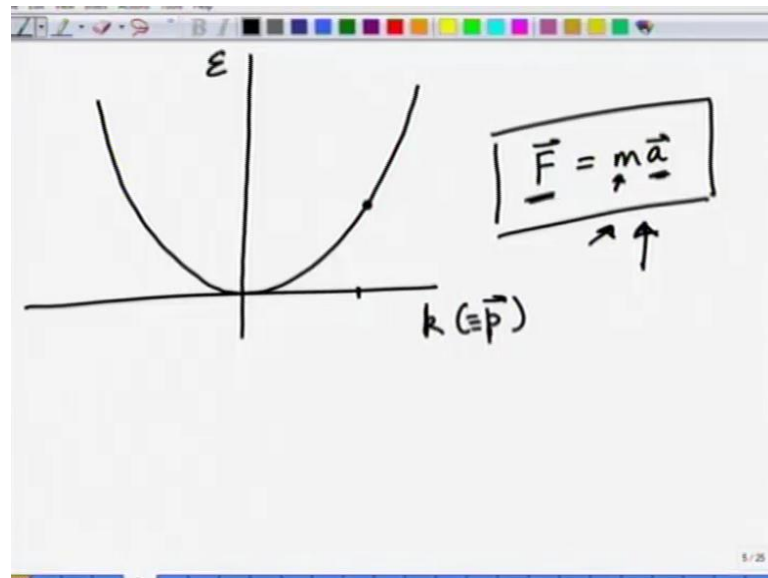
$\vec{v} = \frac{1}{\hbar} \vec{\nabla}_k \epsilon = \frac{1}{\hbar} \frac{\partial \epsilon}{\partial \vec{k}}$ $\left[v_i = \frac{1}{\hbar} \frac{\partial \epsilon}{\partial k_i} \right]$
 $i = 1, 2 \text{ or } 3$

What is the energy operator? Energy operator, we call was this operator was simply minus h bar by j del by del t. So, if I operate this, apply this operator minus h bar j to my del del t to psi of r comma t. Then, I will get my, I will get my energy times this wave function. In what, I will get? What is the energy? It means go ahead, substitute in this wave function. Remember, this dependence is e to power time; dependence is e to power j omega t.

So, this is equal to psi r j omega t. Go ahead, substitute in there. What would you find? You will find that energy would simply be equal to h bar omega. Simply, this is the co relationship from this, which will come out that. Energy is equal to h bar omega. What is that mean? That means omega is 1 over h bar of energy. Therefore, this quantity, the velocity, average velocity, the group velocity would be equal to 1 by h bar of gradient of energy or 1 over h bar, whichever way you like to write of energy.

In fact, I could write in indicial notation because I am going to use this very soon. So, I can write the component, the ith component, i being equal to 1, 2 or 3. I could write this as h del energy by del k i. I could simply write it like this, where i is equal to 1, 2 or 3. So, that is the component, velocity components written out in indicial notations.

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So, that is the relationship that is very important. So, what is that tell you. That tells you that if I, if I have a E versus k curve, if I have a E versus k curve, then if this is the curve E versus k, let us say is E versus k curve, then in that case, if an electron occupies the particular k site, if an electron occupies the particular k site, its velocity can be determined through this slope of E versus k curve.

E versus slope of E versus k curve tells us the velocity. Notice what are we trying to do? At the end of the day, we have energy versus k relationship. Remember, what is k? I have already said that relates to momentum k relates to, is related to momentum though i will prove this more clearly today so in principle we can do the entire dynamic symptoms of energy and momentum space.

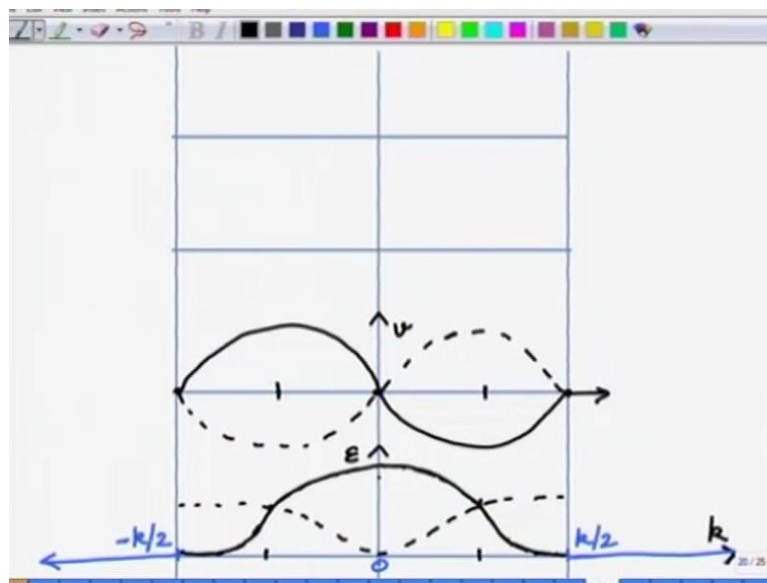
Now, since what we are trying to do is that since, we are quite comfortable with Newton's law, which is force equal to mass times acceleration, this force being the external force which we applied. Again, that I want to know what is the acceleration produced if I knew mass. Now, this is the relationship that I want to do, which is classical particle would follow.

Since, I am quite comfortable doing this kind of dynamics F equal to $m a$, what we have achieved as E versus k curve from quantum mechanical quantum mechanical calculations? What we attempting now to do is fit this quantum mechanical calculations into this form into this form. Once we do so, then for future we do not need to start

calculating based on E versus k, but a lot of electro dynamics in that case can be done based on Newtonian type of mechanics.

That is the interest and that is why we are trying to define certain parameters here. So, in that context, you can see that I can define a quantity called velocity, which simply is the slope of E versus k diagram. Of course, 1 by \hbar factor is also there. So, we can take the slope of E versus k diagram and define the, define the velocity. So, let us do that. Let us plot this diagram out first.

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As we go along, let us keep plotting it. What I am going to is that I will take and draw a big line right in the center. I will draw a big line like this. Then, let us so, plot this. So, I am, what I am going to do is I am going within the first bullion zone. One of this is k axis. So, this is my k axis. This is k equal to 0. This is let us say, some direction k by 2 and minus k by 2 meaning, thereby that I have drawn everything in the, I am going to draw everything in first bullion zone. Only remember, I already have, let me first plot the energy curves.

So, energy curves are two kinds. I have already thought about this. So, let us say the energy curves are something like this. So, energy curves go have a form, which is something like this. This one shape and other shape, I am not looking at the scale. I am just showing you the scale, the shape of these curves. So, I am going to on top of this

draw the other form of it also which was something like this. That meant it is inverted shape. So, that was like this slightly of what has shape like this 2 shapes of energy.

So, I am plotting right here. I am plotting the energy. So, now, based on this, I can now start plotting velocity curves. So, if I plot the velocity curve, let me plot it like this. Let me draw another line like this. So, let it drawn in the line here, which is this line. Another axis same k axis we are drawing and on this now, suppose that I want to draw velocity. So, velocity is derivative of E versus k curve. So, we can clearly start seeing the velocity.

What happens is if I look at the dash time, so dash time of curve, and then that case we start with somewhere here and somewhere here and up to here, up to this point. We have a maximum or first as the slope is negative, so velocity is negative. So, it goes something like this goes through a maximum here and then goes through, goes through a behavior like this and around here y corresponding to this point corresponding to this point.

This point is corresponding to this point is where we have go through a maximum. So, this is a nature of velocity corresponding to the dash curve where it is 0. Here it is 0, here it is 0. Similarly, I can draw it for the solid one, solid lines also. If I draw for the solid line again, the slope is 0 here. Slope is 0 here, slope is 0 here for dash line as should I pointed here, here and here.

So, now, for solid line, if I plot it, then it will be the same way for the solid line. It will look like something like this. This is how it will look like solid line. This I have just plotted velocity. Remember, velocity is if of electron if a site is occupied, if it is not occupied obviously, there is no question of velocity. Then, though there is a relationship something called E versus slope of E versus k curve though, there is slope of E versus k , but electron must be on that site. To considerate velocity, let us talk about its velocity. So, that is the velocity. Let us proceed further little bit. So, this is what where we were we are just shows you the plot of this E versus k curve, which is the velocity. Now, I am going to start looking at something slightly more.

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What is the relation between external force & $\hbar \vec{k}$

if \vec{F} is the external force

$$\vec{v} \cdot \vec{F} = \frac{dE}{dt} \quad E(\vec{k}) \equiv E(k_1, k_2, k_3)$$
$$dE = \frac{\partial E}{\partial k_1} dk_1 + \frac{\partial E}{\partial k_2} dk_2 + \frac{\partial E}{\partial k_3} dk_3$$
$$\frac{dE}{dt} = \frac{\partial E}{\partial k_1} \frac{dk_1}{dt} + \frac{\partial E}{\partial k_2} \frac{dk_2}{dt} + \frac{\partial E}{\partial k_3} \frac{dk_3}{dt}$$

Let us look at what is the, what is the relation between external force. Keyword is external here external force and quantity called $\hbar k$. I have already given you the answer that this quantity $\hbar k$ represents crystal momentum. I use the word crystal momentum earlier to suggest that it behaves as a momentum to an external force. This, I just had stated much earlier in free electron case. I said that $\hbar k$ is exactly the momentum of the electron. In passing, I said in general it is called crystal momentum because in other cases also, where $\hbar k$ not necessarily is the momentum, yet it behaves like a momentum to external force. What does that mean?

What I am going to show to you if F is the, if F is the external force, this is external force. In that case, external force that is applied in that case, what is this quantity called $v \cdot F$? Clearly, that is rate of change of energy that you know very well. Rate of change of energy is dE/dt , not $\text{del } E \text{ del } t$, but dE/dt is what this quantity is. Remember, what E is? E is a function of k or in expanded form, you will write E as a function of k_1, k_2 and k_3 , 1, 2, 3 representing x, y, z . For example, it is in Cartesian co-ordinate system.

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The image shows a whiteboard with the following handwritten equations and text:

$$\vec{v} \cdot \vec{F} = \frac{dE}{dt} = \frac{\partial E}{\partial \vec{k}} \cdot \frac{d\vec{k}}{dt}$$

$$= \underbrace{\frac{1}{\hbar} \frac{\partial E}{\partial \vec{k}}}_{\vec{v}} \cdot \underbrace{\hbar \frac{d\vec{k}}{dt}}_{\vec{F}}$$

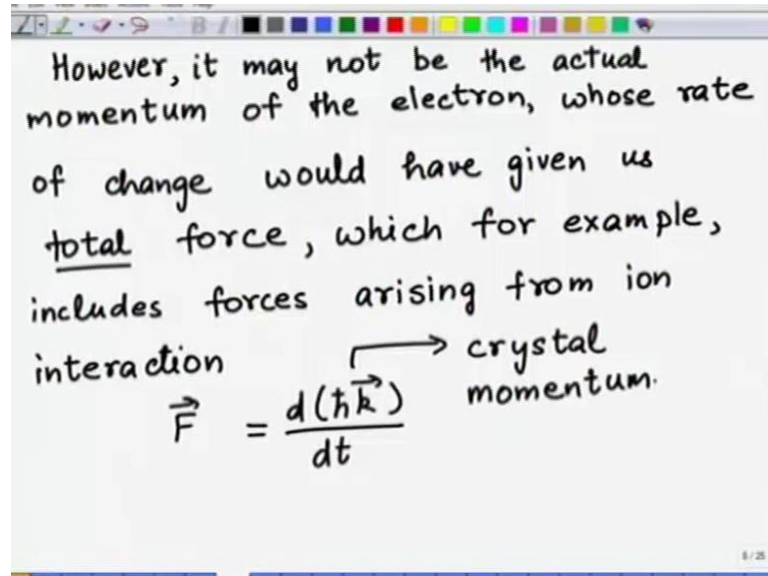
$$\vec{F} = \hbar \frac{d\vec{k}}{dt} = \frac{d(\hbar \vec{k})}{dt} \quad \text{like}$$

hence $\hbar \vec{k}$ must be the momentum whose rate of change is external force on a electron

So, this is E or k 1, k 2, k 3 are in direction. So, x, y and z, so there is a E versus k. So, if I want to calculate this, let us do that. So, let us let us write it down explicitly this time. So, d E quantity clearly is equal to del E by del k 1 d k 1 plus del E by del k 2 d k 2 plus del E by del k 3 d k 3. Therefore, d E d E d t is del E by del k 1 d k 1 d t plus del E by del k 2 d k 2 d t plus del E del k 3 d k 3 by d t, which I could write as del del E by del k vector dot d k d d k d t.

So, I can write this quantity as follows. Now, if I further introduce this 1 over h del E del k and dot product with h bar d k d d t remember, this quantity is equal to d E d t which is v dot F. What do you recognize? This quantity as we have just shown that this quantity is nothing but v. so, what is this quantity? So, what is this quantity? Clearly therefore, this quantity must be F. This quantity must be F. Therefore, in other words, F is equal to h bar d k d t total derivative equal to h bar k d d t. So, hence h k must be the momentum whose rate of change is external force. I should say momentum like whose rate of change is external force on an electron. So, it should behave like a momentum of the electron.

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However, it may not be the actual momentum of the electron, whose rate of change would have given us total force, which for example, includes forces arising from ion interaction. So, they are internal forces for example, arising from ion interaction. So, that is what electron experiences. So, and F is the external force that is applied. These are total forces, some of these 2 forces. Rate of change of momentum, actual momentum is then equal to total force, but this quantity $\hbar k$ behaves like a momentum for external force. So, its rate of change is simply equal to F , which is external force \times which is just the external force. Hence, we call this quantity as crystal momentum.

Now, I hope it becomes really clear that in case of free electron theory since there were no interactions, there were no ion interactions, and therefore, the force experienced by electron was only the external force. Hence, $\hbar k$ was also the actual momentum of the electron. But, in general $\hbar k$ quantity will not be the actual momentum, but it just behaves like momentum to external force. That said, let us move further and start looking at the acceleration.

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What is the relation between external force & $\hbar \vec{k}$

if \vec{F} is the external force

$$\vec{v} \cdot \vec{F} = \frac{dE}{dt} \quad E(\vec{k}) \equiv E(k_1, k_2, k_3)$$
$$\frac{dE}{dt} = \frac{\partial E}{\partial k_1} \frac{dk_1}{dt} + \frac{\partial E}{\partial k_2} \frac{dk_2}{dt} + \frac{\partial E}{\partial k_3} \frac{dk_3}{dt}$$
$$\rightarrow \frac{dE}{dt} = \frac{\partial E}{\partial k_1} \frac{dk_1}{dt} + \frac{\partial E}{\partial k_2} \frac{dk_2}{dt} + \frac{\partial E}{\partial k_3} \frac{dk_3}{dt}$$

So, I want to look at the acceleration of electron when external force F is applied. So, let us start looking at that acceleration of an electron when external force is applied. Now, you see where we heading towards. We are trying to find a relationship between F of time. F is equal to $m a$, for an electron in terms of $E k$ diagram because we have $E k$ diagram.

Given $E k$ diagram, I want to do the dynamics. $E k$ diagram gives me all the information through the quantum mechanics, which is what I want to do. Then, I will not reduce it back to a classical like particle called F equal to $m a$, which behaves, which follows m equal to $m a$. Hence, at the again my calculations would become easy as I am trying to fit that $E k$ data into F equal to $m a$ type expression.

So, let us do that. So, acceleration as before we will define as quantity called $d v d t$. We already know what v is. So, let us do that. Let us start doing this part. Now, what I am going to do is I am going to start using indicial notation. So, let us start from here. What I will write is v of i , i being 1 2 or 3 is $\frac{1}{\hbar} \frac{\partial E}{\partial k_i}$. For those of you again, I keep writing here. We are more comfortable with vector notation where that is quantity is simply $\nabla_{\vec{k}} E$.

If you prefer this way, then we can write it as follows anyways or if you wish which is equivalent say v is equal to $\frac{1}{\hbar}$ gradients with respect to k of energy. If that is the case, let us find what is what this quantity is $d v d t$ total derivative i . We want to find

out. Remember, we will do the same exercise that we did for energy in this page. On this page, we did this exercise. We wrote dE . Then, we calculated total derivative through this expression, in this expression.

Now, instead of total derivative of energy, we are going to take total derivative of, total derivative of ∇ , this whole quantity here, this ∇E by ∇k_i . We will take a total derivative of this with respect to time. We will therefore, replace energy by this whole quantity in there. So, in there, in that case, I will write dv_i/dt as equal to $1/\hbar$ d/dt of ∇E by ∇k_i . Therefore, we are going to take the total derivative of it. So, what do we do?

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$$\frac{dv_i}{dt} = \frac{1}{\hbar} \sum_j \frac{\partial}{\partial k_j} \left(\frac{\partial E}{\partial k_i} \right) \frac{dk_j}{dt} \quad j=1,2,3$$

changing the order of differentiation

$$\begin{aligned} \frac{dv_i}{dt} &= \frac{1}{\hbar} \sum_j \frac{\partial^2 E}{\partial k_i \partial k_j} \frac{dk_j}{dt} \\ &= \frac{1}{\hbar^2} \frac{\partial}{\partial k_i} \sum_j \frac{\partial E}{\partial k_j} \frac{\hbar dk_j}{dt} \\ &= \frac{1}{\hbar^2} \frac{\partial}{\partial k_i} \sum_j \frac{\partial E}{\partial k_j} F_j \end{aligned}$$

So, same way we will write this as $1/\hbar$. Since, we want to take total derivative, so we will write this as summation over j which is going there. ∇ by ∇k_i of this quantity ∇E by ∇k_j is what we will do here. So, if you want, I can write this as vector here, $d\nabla/dt$. Therefore, we write it as $1/\hbar$ d/dt of ∇E by ∇k and d/dt of this, d/dt of this quantity ∇ . I can write this as equal to, equal to $1/\hbar$ d/dt of this quantity. I should write also simultaneously with this a dk_j/dt . Notice, I have done basically same thing. I have taken, essentially expand it out. I have written dE in this. I have replaced E by ∇E by ∇k_i .

Then, of course, you can see. This is, then ∇ by ∇k_1 ∇ by ∇k_2 ∇ by ∇k_3 and dk_3/dt , which is what exactly I have done here that the summation is over j . That

means j takes a value of 1, 2, 3. So, you can sum this over j equal to 1, 2, 3. So, j is equal to 1, 2 and 3. So, this is this quantity which is changing this order of differentiation, it is changing the order of differentiation. I can write this quantity as $\frac{d v_i}{d t}$ as equal to $\frac{1}{\hbar^2}$ summation $\nabla_{k_i}^2 E$ by ∇_{k_j} j being conducted first and $d t$ if I write it like this. Then, I can further write it like this as $\frac{1}{\hbar^2}$ I made it square.

Now, and this summation is over j and what I am going to do is I am going to take this ∇_{k_i} out ∇_{k_i} out. I am going to write this as summation over j of what quantities $\nabla_{k_j} E$ and $\frac{d k_j}{d t}$. So, this is the quantity. Remember, \hbar should also be put in there. So, I should put \hbar in there as this quantity. Now, clearly what do you associate this with this quantity is simply the j -th component of the force j component of force. So, force is 1, 2, 3.

Remember here $\frac{d k_j}{d t}$ is the force. So, this is the j -th component of the force. So, I can write this as. Remember, this has been possible because this force does not depend on k_i . So, it is derivative with respect to k_i is 0. This force is external force. So, I write this as $\frac{1}{\hbar^2}$ ∇_{k_i} . I am going to write this quantity. Therefore, as summation over j of what $\nabla_{k_j} E$ F_j .

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$$\frac{d v_i}{d t} = \frac{1}{\hbar^2} \frac{\partial}{\partial k_i} [(\nabla_{\mathbf{k}} E) \cdot \vec{F}]$$

$$\Rightarrow \frac{d \vec{v}}{d t} = \frac{1}{\hbar^2} \left\{ \nabla_{\mathbf{k}} [(\nabla_{\mathbf{k}} E) \cdot \vec{F}] \right\}$$

$$a_i = \frac{1}{\hbar^2} \frac{\partial}{\partial k_i} \sum_j \frac{\partial E}{\partial k_j} F_j$$

Now, I am going to write it. Alternatively, I will write this as $\frac{1}{\hbar^2}$ ∇_{k_i} of I am going to write this as now dot F I am going to write this as dot F , which is

this. This is a gradient taken with respect to k . Here is a gradient taken with respect to k and dot F will give me this summation, this summation quantity right here. These are the 3 components I am going to get. So, if I get this, I can have of course, write as also this. I can write in a different form.

In vector form, I can write it this as 1 over \hbar square gradient with respect to k of that is what little algebra was. But, what do you see? What you see is that something interesting that you can begin to see from right here either right here or right here. You have these 2 points. You can write here or right here. Just focus your attention here. What does that mean? Notice that I can write therefore, a i component of acceleration is equal to 1 over \hbar square ∇ by ∇ k_i times summation over j of ∇E by ∇k_j F_j . I am basically reproducing this equation here j . I am basically reproducing this equation right here.

What does that mean? That means that acceleration in direction i , i being 1, 2, 3, so x , y , z if you wish, you reduce by forces, which are not necessarily in direction i . So, that means since j can take the values of 1, this j can take a value of 1, 2 or 3. Therefore, a force in direction 2 or direction 3 will also produce an acceleration, which is in direction i . So, that is a , that is the difference and that is what we need to keep track of. So, if you keep track of this, the way we will do it is there as follows. Therefore, I am going to define this quantity a_i .

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$$a_i = \frac{1}{\hbar^2} \sum_j \frac{\partial^2 E}{\partial k_i \partial k_j} \hbar \frac{dk_j}{dt}$$

$$= \sum_j \left[\frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j} \right] F_j$$

$$\frac{1}{m_{ij}} = \left[\frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j} \right]$$

$$a_i = \sum_j \frac{1}{m_{ij}} F_j$$

$$a_i = \frac{F_i}{m}$$

Classical particle

We use this equation right here. We will use this equation right from here itself. Let us pick it off from here. Let us take it off from here $\frac{1}{h} \frac{d^2 v}{dt^2}$. Acceleration this a_i quantity as being equal to $\frac{1}{h} \frac{d^2 E}{dk_i}$ second derivative $\frac{d^2 E}{dk_i dk_j}$ plus pick this equation from here. So, acceleration is equal to $\frac{1}{h}$. In fact, I will make it $\frac{1}{h^2} \frac{d^2 E}{dk_i dk_j}$. I will write \bar{h} . Of course, $\frac{d^2 E}{dk_i dk_j}$ by $\frac{d^2 E}{dt^2}$, which is what it was $\frac{d^2 v}{dt^2}$. In this, I have inserted, made this square. I have made this h^2 . I have inserted h right here. Introduce a h here. So, that is fine. That is the only thing that I have made difference I have made.

Therefore, I am going to write this as this. Of course, there is a summation and of course, there is a summation over j like you see here, this summation right here, this summation over j . so, I can write this as quantity, which is equal to summation $\frac{1}{h^2} \frac{d^2 E}{dk_i dk_j}$, this whole thing times F_j . This summation is over j . So, I am, let me define a quantity call m_{ij} . What it means? Forget about it for a minute that quantity. Let us define as $\frac{1}{m_{ij}}$ or $\frac{1}{m_{ij}}$ inverse of this quantity. Let us define inverse of this quantity m_{ij} as equal to $\frac{1}{h^2} \frac{d^2 E}{dk_i dk_j}$.

So, if that is the case, I can write a_i . I substitute a_i as summation over j . Then, I can write this quantity as $\frac{1}{m_{ij}} F_j$. So, what do you see? So, what we see is remember Newton's law or classical particle follows a_i equal to F_i by mass, a mass that is what a classical particle follow. Essentially therefore, I have just defined a quantity called effective mass. So, if I have E versus k curve, if I have a E versus k curve, then its second derivative once with respect to k_i or there is respect to k_j , then gives me a component. Now, it is a 9 components thing. So, this is a tensor. So, this is rank 2 tensor m_{ij} .

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$$\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{m_{11}} & \frac{1}{m_{12}} & \frac{1}{m_{13}} \\ \frac{1}{m_{21}} & \frac{1}{m_{22}} & \frac{1}{m_{23}} \\ \frac{1}{m_{31}} & \frac{1}{m_{32}} & \frac{1}{m_{33}} \end{pmatrix} \begin{pmatrix} F_1 \\ F_2 \\ F_3 \end{pmatrix}$$

if we use principle axes, in that case m_{ij} ($i \neq j$) vanish and only m_{ii} survives

$$m_{ii}^* = \left[\frac{1}{\hbar^2} \frac{\partial^2 \epsilon}{\partial k_i^2} \right]^{-1}$$

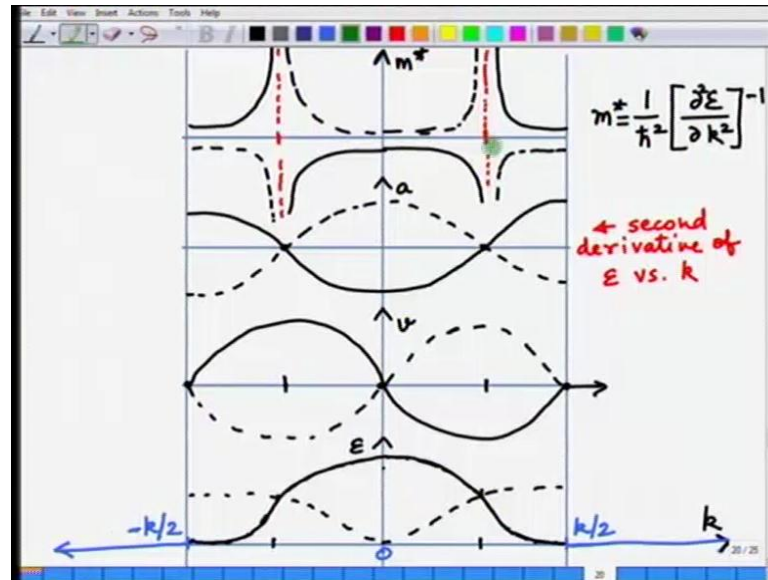
So, this is effective essentially. Therefore, I have something called this a_1, a_2, a_3 . The 3 components are equal to $1/m_{11}, 1/m_{12}, 1/m_{13}, 1/m_{21}, 1/m_{22}, 1/m_{23}, 1/m_{31}, 1/m_{32}, 1/m_{33}, F_1, F_2, F_3$. Now, I have got a behavior like a classical particle except that I have to introduce an effective mass tensor. This m_{ij} of course, is a quantity given by this. So, if I find essentially from E versus k diagram, I can find effective mass. Once I know the effective mass, then I can also draw essentially.

In that case, I can, I will also draw; extract what the effective mass is. Once I have active mass, then I can apply that to force equal to mass time acceleration kind of behavior and then use it further except in the last. Let us make a small simplification. If we use principle axis in that case $m_{ij}, i \neq j$ vanish and only m_{ii} survives. That means only the diagonal component survives if I choose the principle axis. So, if I chose, in fact, that is the definition of principle axis. So, if I chose the axis such that all the all, only the diagonal elements survive.

In that case, I can write, I can, let me put a star n here to denote that this is not electrons mass necessarily, but it represents a , this represents essentially an effective mass. So, in that case, I can define an effective mass m_i . Now, since we have only diagonal components, in that case, I can define this quantity as $1/\hbar^2 \partial^2 E / \partial k_i^2$ inverse. Of course, of this inverse of this k_i square second derivative that means

say inverse of second derivative of E versus k curve gives E the effective mass of the electron. Effective mass of the electron meaning that mass, which can be put in to force is equal to mass times acceleration, this kind of equation. So, what is that?

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So, now, let us go back and start plotting all these quantities in the graph. If this is the velocity, then I can plot acceleration. So, let us plot acceleration as derivative of velocity. So, let us do this part first. So, just draw this line right here. This is a line for drawing my acceleration. Then, clearly in this case, the solid line will be here. I have derivative derivative goes to 0. Derivative of velocity goes to 0 here and derivative of velocity goes to here. So, it is going to go to 0 here. It is going to go to 0 here.

So, I am going to draw this like this. The solid line goes, therefore something like this. The acceleration, therefore behaves something like this and for the dotted lines, for a shape of energy curve like this. Then, this here somewhat like this where the maximum minimum and zeroes are. This is my acceleration, is what I plotted as acceleration. Now, of course, you know that already said that if you take a second derivative $\hbar^2 \frac{\partial^2 E}{\partial k^2}$ and take inverse of it and inverse of that, then that gives me effective mass. That gives me effective mass of the electron. Also, let us plot effective mass of the electron. Let us do that right here. So, how does that behave? Just put it right here. How does that behave?

So, as I see and in this case also, right here are my 2 points here. What happens? Where does slope, where the slope goes to 0? This slope is a slope second derivative of E. Remember, this represents acceleration. So, this acceleration is a quantity, which is equal to essentially second derivative. Acceleration is the second derivative of velocity or second derivative of energy. So, this is the second derivative. I have plotted second derivative of energy versus k curve.

Remember, that is what energy versus acceleration. If I take inverse of that, then if I take inverse of that, then that gives me effective mass. So, wherever it goes to 0, wherever this second derivative goes to 0, that is where I am going to effective mass going to plus infinity or minus infinity. So, that means where where? 0 is here. 0 is here. Something will happen. I need to take the inverse. I need to calculate the inverse of this curve.

What I am basically trying to plot? So, let us do that for solid line. So, there now, as we go along, this second derivative is decreasing. So, inverse of this is along this solid line from here to here. This this quantity is second derivative. It is decreasing that means inverse of it would be increasing. Here, it will be going towards infinity. So, if I draw it like this right here the dotted lines here, the dotted lines here, some dotted lines here, then what I should see is a behavior. Somewhere this should go and go towards should towards infinity. Similarly, what should happen if I look at it? Similarly, what should happen of this side also that it is decreasing decreasing, decreasing along this side.

It is decreasing. Therefore, inverse of it must be increasing. What about here? On this side, I should have as I am going this way from here either oppose here to here on solid line. This second derivative is increasing. The second derivative is increasing. Then, the second derivative is increasing. Then, inverse of it should be decreasing. So, that means that my behavior here should be something like this. Similarly, on this side, it is going towards minus infinity. So, the mass, the second derivative of this effective mass I am plotting here, effective mass that I am trying to plot here m^* is what I am trying to plot and hence, this behavior.

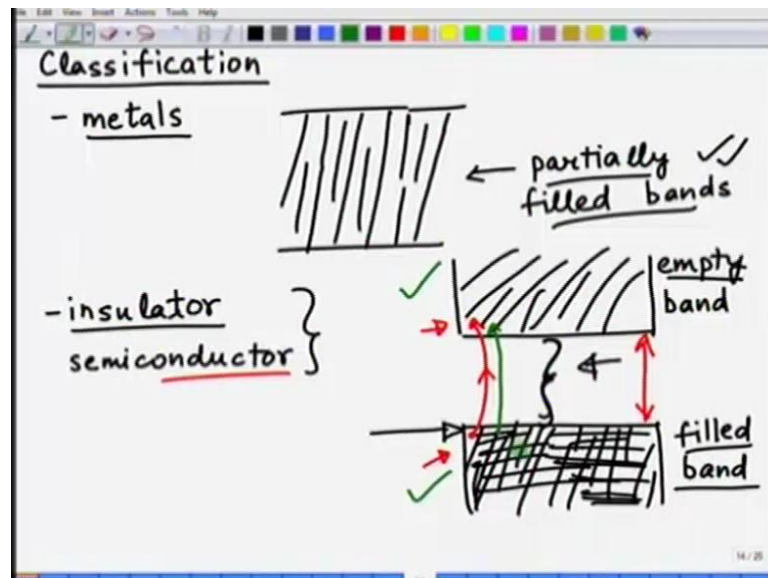
Similarly, you can see for the dotted lines. I can draw it for the dotted lines. It will be here like this exactly opposite of this. This is how it will be and shooting towards infinity here. So, this is strange. Add these inflection points. Add these inflection points of energy versus k curves. As the energy versus k curve adds the inflection points, we find

that effective mass shoots up towards either process infinity or minus infinity. That is strange. So, remember that this is effective mass. This is not real mass of the electron. So, this a fitted mass so that we can use f equal to m a type of equation.

In this context, you see effective mass behaving in a strange manner. This has a consequence. I will shortly in the next lecture, I will begin to explain what is this consequence of this particular effective, this kind of behavior effective mass. It has a consequence. We will see that. We will introduce a term called a hole, a hole also in order to explain some of these phenomena. Therefore, why I do this? Now, you can see that I having E k curve, E k diagram, I wanted to tell you what the utility is...

That is that there is lot more utility in optical sides also which we have to do, but on the dynamic side, you can say from you can see from E verses k curve, you can extract all the dynamical parameters, whatever is required for dynamics F equal to m a time of m a type of dynamics. You can extract all that information from E k diagram. That is the power of E k diagrams. Hence, we had been doing all along, for so along this E k diagram. So, having done this part now, what I am going to do is start with showing it E k diagram or E k diagram, also the direct parameter.

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Let us start again with classification of materials, which we have already done. But, we repeat and we introduce the idea of conductivity again in context of what you have done of E k diagram, what you have done from dynamics and the behavior, the velocity, the

acceleration etcetera in context of band diagram after looking for classification of materials. Then, we start looking at the conductivity relation to diagram. You will see that we will use all these ideas together.

So, let us start looking at classification of materials first. We are going to define as metals. Of course, it is clear and I am just repeating myself, which we did in yesterday's in previous lecture. What we have in metals? We found that metal; we found that we had continuous energy levels of the label. We had continuous energy levels label. Second thing is that we had for example, if we have a alkali metal which has 1 electron per atom, then that I will go through the details of it in the next lecture again.

Then, it will fill the band partially. It is a continuous band. Then, it is filling up completely. If I have a continuous band, then I have a very wide band available that means allowed energies are there. When I start putting electrons on them, I put electrons up to certain level. After that, I run out of all the electrons. All the other energy states are empty. The point is that is a partially filled band. That is not completely full. That has a consequence metal. I am saying is a large conductivity because of that reason.

Therefore, as I start looking at what is in insulator, you already know insulator is a material which has very, very low conductivity. It cannot conduct. So, what is what is that mean? That means that insulators and I should see it would context of semiconductor itself, a conductor itself. These, both of these necessarily have a band gap that means this is allowed energies. This is, these are the allowed energies right here and these are allowed energies these are allowed energies and these are allowed energies.

In both these systems, we find that electrons fill up to this level. That means that one of the bands is completely full, completely filled band at 0 k, at least at 0 k, at 0 k completely filled, band. Here, a band gap is not allowed energies and an empty band. Such a material is always insulator. Such a material is always insulator. Remember. Unlike partially filled band, I have a completely filled band.

Though there is an empty band, but there is a separation between them. So, a band gap is right here, which we did not have in case of metals. But, here we do. We have a gap in there. This band is completely full up to this point. It is empty here. The consequence of that is that this material cannot conduct. It is a insulator and that I need to explain to you in terms of when I explain conductivity in terms of, but I am just classifying the

materials. I am telling you the features of it. You will see because of these features, such materials will be insulators.

Such materials will be semi semiconductors. Such materials will be metals. If somehow at some high temperature, it is some electron is able to jump, make a jump from here to here, and then what do we do here? Then, we have this band also becoming slightly partially empty if you wish because some electrons are left. This is some. Therefore, it is completely filled band. Similarly, this is not since some electrons jump from here on to this particular band.

Therefore, this particular band is not completely empty, but it has some electrons in there. In such a case, we start getting some conductivity. Those are the materials, which we call as semiconductors. If however this gap, which is here is very, very large, if this gap is very, very large, for example, in diamond. It is 5.3 electron volts. In that case, even room temperature or some high temperature is not sufficient enough to cause these electrons to jump here over to this empty band. As a consequence, this material remains continuous to remain insulator.

So, semiconductor or insulator is a relative term at 0 k. All of these will be insulators. You go to higher little higher temperature say room temperature, then in that case, in case of semiconductors, since this gap is small, some electrons can jump up jump over both these bands. Therefore, become partially filled this one top and one bottom become partially filled. Some electrons are left.

Hence, they began to conduct. Hence, we call it semiconductor, whereas is in case of insulators since the jump is not be possible even at room temperature. Hence, it will not be able to conduct. Now, what I need to do is, in next lecture, establish for you that how, so why it is that only partially filled bands conduct? So, that is what we will start in the next lecture.

Thank you.