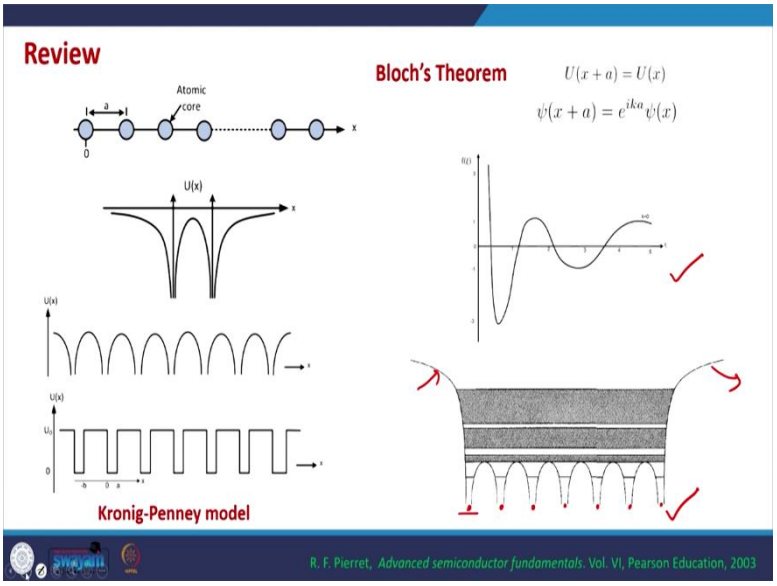
Physics of Nanoscale Devices
Prof. Vishvendra Singh Poonia
Department of Electronics and Communication Engineering
Indian Institute of Technology, Roorkee

Lecture - 08
Bands, Effective Mass, DOS

Hello, everyone. Hope all of you are doing well, in today's class we will conclude our discussion on energy bands and we will try to understand the notion of effective mass. And, before going into that discussion let me quickly summarize what we discussed in the last class.

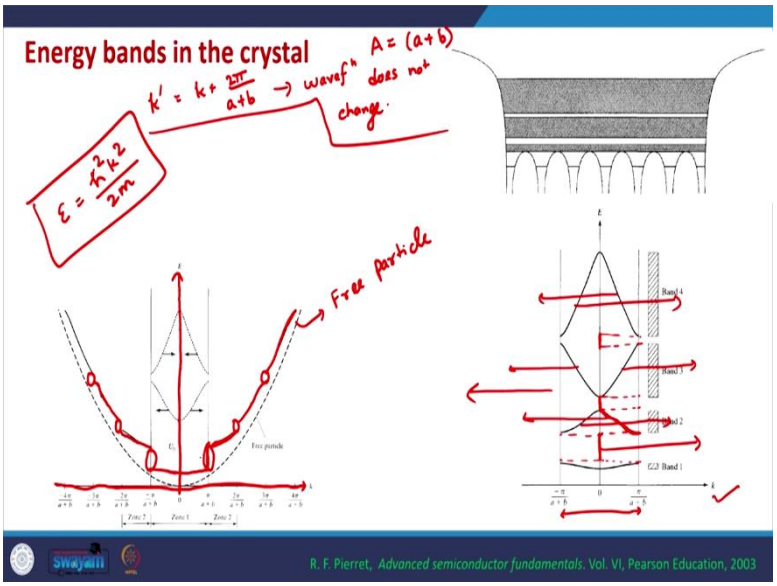
(Refer Slide Time: 00:48)



In the last discussion, we saw that the K- P model solution gives a constraint which naturally tells us that there are certain energy values in a solid which are disallowed for the electron to take. And, there is a certain energy range which the electron can take in a solid ok, and this is the graphical representation of the constraint the function that is there in the solution of the K-P model.

And, this is the intuitive picture of allowed and disallowed energy values of electrons in a solid. This is the crystal momentum, these are the edges of the crystal, these are atomic cores here. So, that is why the potential energy of the electron is going to negative infinity at these points and these shaded regions these are the allowed energy values that the electron can take in the solid ok.

(Refer Slide Time: 01:54)



So, now, extending this discussion if we plot the e values the electronic energy values and the k values, this is what we get basically. This is the plot that we obtain. And as we discussed in the last class there are certain conditions that naturally come from the solution of the that naturally come from the Bloch's theorem which we can see from its derivation.

But, which we can also see from the statement of the Bloch's theorem and one of those conditions says that all k values can be all sort of all k values lie in a range of 0 - 2π by period of the potential profile or from $-\frac{\pi}{A}\ to\ \frac{\pi}{A}$, where capital A is the period of the potential profile. In our solution the period of the potential profile is capital A is (a+b).

So, all possible k values will be between $-\frac{\pi}{a+b}\ to\ \frac{\pi}{a+b}$ and corresponding to these k values we will have many energy values basically. The solution of the Schrodinger equation and Bloch's theorem statement of the Bloch's theorem also sort of conveyed that tthere will be an energy range for which no k value will exist and, this we can see from here.

So, these energy ranges this y-axis is the energy axis, x-axis is the k-axis these highlighted portions on the energy axis, these are the energy range these are the energy values which do not have valid wave function of electrons which means the electrons cannot take these energy values in the solids or there is no k-value corresponding to these e values and these are also known as the band gaps. Because this is a gap in the energy axis, this is the gap where no electron can exist on the energy axis, ok.

Also, one of the conditions that we also studied that if we shift the k value by 2π/period of the potential profile, the wave function remains the same basically the wave function does not change. It corresponds to essentially the same wave function, ok. So, this will sort of tell us by making use of this condition we will see that there is an alternative way of representing or alternative way of visualizing the E-k relationship for a 1D solid and which is essentially can be given by this.

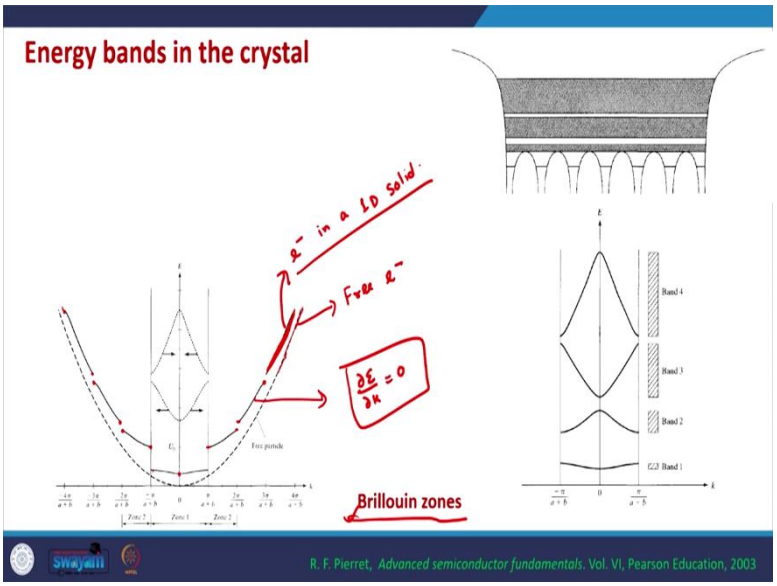
So, what we can do is we can now shift this plot by $2\pi/(a+b)$ in either direction left or right. So, that is what we do and if we shift this to the left by $\frac{2\pi}{A}$ and this to the right by $\frac{2\pi}{A}$ this to the right this to the left by $\frac{2\pi}{A}$ and this to the left, this to the right by $\frac{4\pi}{A}$ here it is $\frac{4\pi}{a+b}$ this is what we obtain.

Here y-axis is the energy axis and x-axis is the k-axis and on this E-k axis system, this is the allowed values of energies as a function of k. And, as is also clear from this plot, certain energy values for example, this range of energy values these are the disallowed energy values or the band gaps of the solid, ok.

So, this is so to say this is the first band, this is the second band, this is the first band gap the band gap between band number 1 and band number 2, this is third band, this is fourth band which we can easily visualize here ok. Along with this there is a plot of E-k relationship for a free particle as well.

If you recall from one of our previous discussions for a free particle E is related to k as $\frac{\hbar^2 k^2}{2m}$. So, it is a parabolic relationship which we can also see here ok.

(Refer Slide Time: 07:44)



So, we have the E-k relationship for a free particle free electron. So, to say electron which is free from all the interactions and we have E-k relationship for an electron in a 1D solid. As you can see for higher energy values for when the energies are quite high the E-k relationship for the electron in the solid and the E-k relationship for the free electron they approach to each other, basically they converge.

So, what it means is, that if an electron has extremely high energy then it is quite like a free particle free electron ok, but the E-k relationship for electrons in solid in a 1D solid and a free electron is quite different for low energy values for the low energy electrons when the electronic energy is not so high.

What it means is low energy electron means that the electron is confined in the solid. Electron is tightly confined or not I would not say tightly because that word has been used in a different context. Electron does not have too much of energy to sort of move away from atomic course, but it is still moving in the solid. It is not like a free electron, but it is moving inside the solid.

And, for low energy values, the E-k relationship between E-k relationship for a 1D solid and for free electrons are very different as we can see here. So, this is one observation and with this we also comes the notion of the Brillouin zone. So, Brillouin is not the precise pronunciation of this word. This is a French name, but still for the sake of better sort of understanding I will use the Brillouin pronunciation.

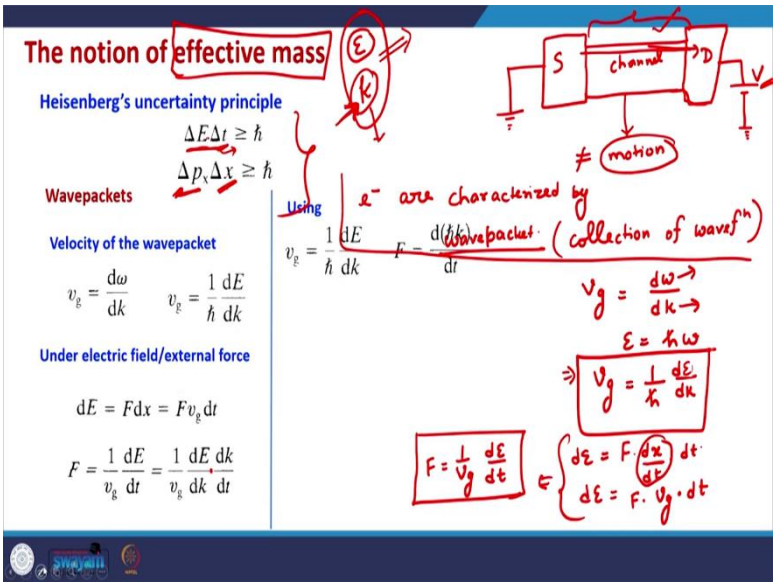
Brillouin zone is a set of k values corresponding to an energy band. So, the set of k values which correspond to first energy band they are known as Brillouin zone 1, similarly corresponding to energy band 2 they are Brillouin zone 2, similarly corresponding to third band they are Brillouin zone 3. This is how this is defined.

And, this is very important concept in solid state physics and generally whenever we analyze a new material whose property we do not know beforehand, we first try to find out the relationship between E and k for that material. So, that tells us a lot about how electrons will behave in that new material. So, this notion of E-k relationship notion of Brillouin zone it is quite important for understanding the nature of electrons in solids.

There is a one more point here for an electron in a solid although we did not do it mathematically a precise analytical solution we did not do here most of after a stage we are using a graphical solution for the sake of better understanding, but at the boundaries of Brillouin zones $\frac{\partial E}{\partial k}$ is 0. What it means is that at these points, these boundary points the gradient of E-k plot is 0 ok, also at this point.

So, this notion, this idea will be useful for us in the next discussion which is the discussion on effectiveness. So, this is essentially the broad idea of energy bands in a solid how the energy bands arise in a solid and that is a consequence of periodic potential in solids and using K-P model we can see that we can visualize that mathematically as well as graphically ok.

(Refer Slide Time: 12:56)



So, but we at the outset, in the beginning our aim was to understand how the electrons will behave and what I mean by behave is how the electrons will be transported in a device or the transport behavior of electrons in a device.

And, we started with a simple two terminal device like this where we have two contacts source and drain contacts in between we have a channel region. And, we saw that the channel region is becoming smaller and smaller in modern devices. Generally, we apply a positive voltage on the drain terminal which makes electrons flow from source to drain or a current from drain to source.

So,in this we need to know how electrons are travelling, we need to know about the motion of the electrons. So far, our discussion has been primarily focused on what is the allowed energy value that the electron can take in a solid or in a particular environment and what are the k values that electrons can take in a solid or in a particle in a box situation or as a free particle.

So, our discussion so far has been focused on the allowed energy values or the k values. So, in that sense we have solved the Schrodinger equation, where the energy and momentum are precisely defined. So, energy of the electron is precisely defined and the momentum of the electron is also precisely defined, but that is not sufficient for understanding the motion of electrons in actual solid.

So, we cannot understand the motion of electrons in solid using this and the reason for that is that quantum mechanics has another principle which is a consequence of the measurement of quantum mechanics that this principle is known as Heisenberg's uncertainty principle.

And what it says is that there is a set of complementary variables there are many complementary variables in quantum mechanics which cannot be measured simultaneously and these variables are known as complementary variables or conjugate variables.

So, energy and time is one such pair if we know about the energy of an electron precisely we cannot say about it is sort of motion about it is dynamics. If we know the position or if we know the momentum of the electron precisely we cannot tell about the position exact

location of the electron and this is known as the Heisenberg's uncertainty principle and this is the mathematical inequality that captures the Heisenberg's uncertainty principle.

What it says is that the uncertainty in energy and uncertainty in time to which we can precisely measure an electron is always greater than equal to h bar and similarly, the product of uncertainty of momentum and product momentum and position is greater than equal to h bar.

So, what it means is that if we precisely try to measure the momentum, the uncertainty in position will be high and similarly, if we try to precisely find out at a certain time where the electron is, how it is behaving, what is its wave function, its energy will not be well defined.

But, in our discussion up to this point, we have sort of precisely defined the energy and precisely defined the momentum of the electron which is momentum of the electron is related to the this k parameter, the wave number parameter basically. So, based on the discussion that we have done so far, we cannot sort of visualize we cannot understand the motion of electrons in actual solids.

Although, building on this, this is the building block, this the discussions that we have done so far is the building block of our understanding of electrons and in this context this notion of effective mass basically arises. So, we will see that what it is for a single wave function as we have seen the energy and momentum is precisely defined.

But, if we have an electron for example, if we in this device an electron is starting from the source going through channel up to drain, we have an idea or we have basically determined the path of the electron we have electron which is confined in certain dimension of the space which is confined between source and drain. So, if the electron is in channel, it is confined in a certain length.

So, what it means is that now there is some clarity about the position of the electron. So, in that sense the momentum of the electron cannot be precisely defined. There will be uncertainty in the momentum, uncertainty in the k values as well. Similarly, if we want to understand what is the position of electron at a certain time at a precisely at a certain instant its energy cannot be precisely defined.

So, that is why, generally in all practical devices in all sort of for all practical purposes where the electron is we know that electron exist in this regime of space in this for example, in channel in this region of space in that case a single wave function cannot describe the electron because a single wave function has precisely defined energy and k values. And, now the energy in k values energy in momentum values are not precisely defined because some clarity is there about the position and the time, ok.

So, that is why in all practical devices, in most of the practical devices the electrons are characterized by a bunch of wave functions. Electrons will have wave functions corresponding to different energy values so that the energy uncertainty will be there and this bunch of wave functions is known as the wave packet. This term appears in classical wave mechanics as well.

So, in practical devices when we have some clarity about the position of the electron, generally the electron will be characterized by electrons will be defined by a collection of wave functions or by a wave packet. So, a wave packet is essentially collection of wave functions corresponding to different energy or k values.

So, I hope this point is clear that in an actual device where we have clarity about the position and timing of the electron that at this time the electron is moving from this to that. Although, we might not know where that is precisely located the electron is precisely located, but in that case energy and momentum will not be precisely defined. So, we cannot define electron by a single wave function and that is why the electron will be defined by a collection of wave function or wave packets.

Now, we have wave packets of different energies, different momentums and that will make sort of a bunch of waves and that bunch of waves or wave packet will move with certain velocity that is known as the velocity of the wave packet. And, from the classical mechanics dispersion relationship, the velocity of the wave packet is given by the dispersion relation v_g, the group velocity of the wave packet is given by $\frac{d\omega}{dk}$ where ω is the frequency central frequency and k is the central wave number of the wave packet.

So, the wave packet will consist of waves which will have frequencies centered around ω for our case energy equals $\hbar\omega$ which means v_g is $\frac{1dE}{\hbar dk}$. So, please keep in mind here we are trying to understand the motion of electron, how the electron actually moves in a solid or

in a device when they are confined or when they are in a actual device like they are moving in a channel. And, in that case we borrow some ideas from classical wave mechanics like the idea of a wave packet and its group velocity the notion of the group velocity.

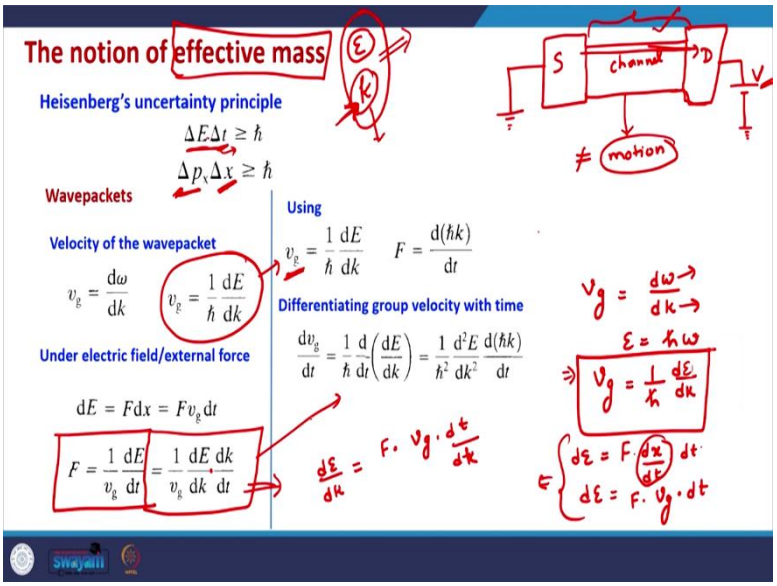
And, now, we will try to see if we apply a voltage on the device or electric field on the device which will exert a force on the electron electric force in the electron how this wave packet will move. So, that is what we will try to see here. And, so, if we apply a force F by virtue of a applied voltage using a battery the amount of work done by this force will be F times dx where dx is the distance or the displacement of the electron.

So, this will also be the change in energy, amount of work done will be equal to the change in energy of the electron. So, the change in energy of electron will be dE equals Fdx and dx can be written as $v_g$dt. So, dx by dt will be the velocity which is the velocity of electron wave packet in the group velocity times dt. So, this dx by dt will be v_g. And, in this case this expression will be dE equals F times v_g times dt. So, this implies that F will be equal to $\frac{1}{V_g}\frac{dE}{dt}$, ok.

So, this is the relationship that we obtained and this can further be expanded as dE by dt can be written as dE by dk times dk by dt by multiplying and dividing by dk, ok. So, now, we use this relationship between the group velocity, velocity of the wave packet and the energy as we derived earlier.

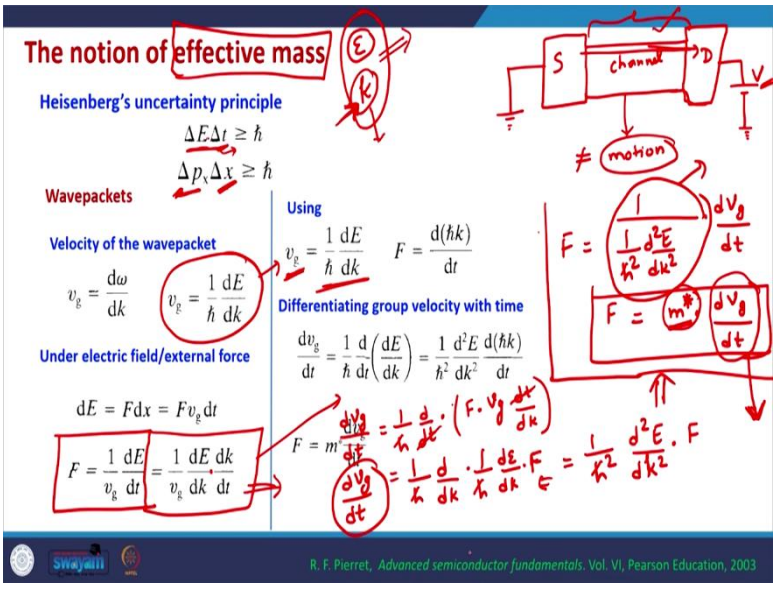
So, we have this relationship between the applied force and the v_g or it can also be written as $\frac{1}{V_g}\frac{dE}{dk}\frac{dk}{dt}$.

(Refer Slide Time: 25:51)



So, by using this expression $\frac{1dE}{\hbar dk}$ and writing $\frac{dE}{dk}$ from this expression from. So, from this expression $\frac{dE}{dk}$ will be $Fv_g\frac{dk}{dt}$ ok. So, this is the expression for the relationship betweenv_g and $\frac{dE}{dk}$ and so if we differentiate this expression with respect to t, then we obtain $\frac{dv_g}{dt} = \frac{1}{\hbar}\frac{d}{dt}(\frac{dE}{dk})$.

(Refer Slide Time: 27:05)



And, now, this $\frac{dE}{dk}$ can be written from this equation ,from using this equation we can write $\frac{dE}{dk}$. And, that will give us basically $\frac{dv_g}{dt} = \frac{1}{\hbar}\frac{d}{dt}(\frac{dE}{dk})$ can be written as $Fv_g\frac{dt}{dk}$ and $\frac{d}{dt}$ goes away. $\frac{1}{\hbar}\frac{d}{dk}(Fv_g)$ by writing v_g as $\frac{1}{\hbar}\frac{dE}{dk}F$.

So, by using this expression we can deduce the relationship between the this $\frac{dv_g}{dt}$ is like acceleration in classical mechanics, the relationship between the force and the acceleration. So, this ultimately turns out to be $\frac{1}{\hbar^2}(\frac{d^2E}{dk^2})F$ ok.

So, if we equate this with so, in this case from here we can write force is equal to $\frac{1}{\frac{1}{\hbar^2}(\frac{d^2E}{dk^2})}\frac{dv_g}{dt}$.

And, this first term can now be written as like a modified mass because if we write, it like a modified mass it will be like our classical motion equation classical equation of motion, Newtonian equation classical mechanics equation of motion.

So, in this case F, the applied force, is basically the acceleration of the electronic wave packet times a parameter which we write as m^* we do not call it the mass of the electron. It is not the mass of the electron, it is a modified mass and this is known as the effective mass of the electron and it is defined as the $\frac{1}{\frac{1}{\hbar^2}(\frac{d^2E}{dk^2})}$ by this parameter basically.

And, this is an important result because now, in a way the quantum mechanical treatment of the electron in solid has been encapsulated in the idea of the effective mass here. And, by encapsulating the quantum mechanics in the notion of effective mass we can now use the classical equation of motion to find out the effect of an applied voltage or applied force on the electron, ok.

So, that way it is quite an elegant concept because it simplifies the understanding and the calculations. So, we just need to sort of instead of using the mass of electron we need to use effective mass of electrons and at many places we can still use our classical concepts, if we properly define the group velocity or the electronic wave packet, ok.

So, I will recommend you to read more about the notion of effective mass from especially from the text by Robert Pierret, titled as Advanced Semiconductor Fundamentals. This book discusses the K-P model, the E-k relationship for solids and this idea of effective

mass in a very concise and very simple way, easy to understand way. And, please go through this and I will see you in the next class.

Thank you for your attention.