Physics of Nanoscale Devices
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Lecture - 09
Effective Mass, DOS

Hello everyone. Today, we will conclude our discussion of Effective Mass and if time permits, we will start the discussion of Density of states in Solids particularly in electronic devices.

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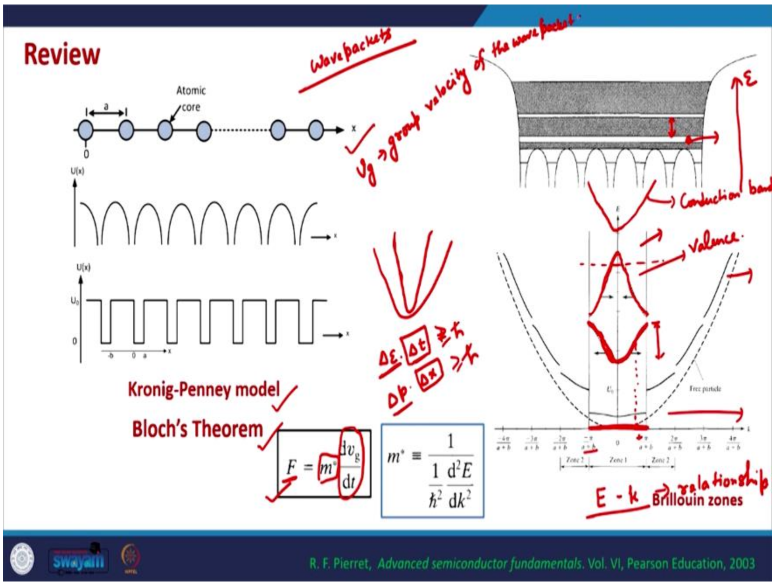

So, let me quickly review what we have been discussing so far. We are trying to understand how electrons behave in nanoscale devices how electrons behave when they are confined in extremely small regions of spaces, which is the case in our devices; in our modern devices where the channel length is of few nanometer length. And in order to understand that we started the discussion on electrons in a 1D solid.

And in order to understand the behavior of electrons in a 1D solid we need to solve the Schrodinger equation in a 1D solid and that is done by using the so, called Kronig-Penney model this is also known as KP model. Using KP model and by invoking Bloch's theorem we deduce that in solids electrons can occupy certain ranges of energies. So, this is the energy axis and electrons can occupy certain energy ranges and there are certain ranges, which the electrons cannot occupy.

So, the allowed electronics energy states are known as the energy bands and the disallowed energy range is known as the band gap. And this is what we deduced from our mathematical and graphical analysis of the solution of KP model basically. In this figure we analyze the relationship between energy and crystal momentum k the so called E k relationship for solids, E k relationship for solids.

What we see here is that there are two ways of representing E k relationship one is the so, called reduced zone representation and in which we can we plot E values corresponding to the k values in the range of$-\frac{\pi}{a+b}$ to $\frac{\pi}{a+b}$. So, as we saw during our discussion of Bloch's theorem we concluded that all possible or the complete set of k values lie in the range of 2π by period of the potential profile.

And here the period of the potential profile was a plus b so, the complete set of distinct k values lie in the range from $-\frac{\pi}{a+b}$ to $\frac{\pi}{a+b}$. And when we plot E k relationship in this range $\frac{2\pi}{a+b}$range this representation is known as the reduced zone representation of the solids. But we also saw that if we add $\frac{2\pi}{a+b}$ to any k value that will give the same wave function. So, we can equivalently have an extended zone representation in which k values are continuously increasing and we are seeing energy as a function of k when k values are continuously increasing.

So, these two are equivalent way of representing the E k relationship and various in this case these allowed values of energies. So, for example, this is the E k plot this is a part of E k plot. So, what it signifies is that this range of energies electrons can take and the corresponding k values will be these. So, corresponding to this point we will have the k value to be this ok. So, this is known as 1 electron band and corresponding to a band the set of k values is known as Brillouin zones.

So,by this also we can also find out Brillouin zones from the E k relationship. This can be easily visualized in case of 1D particles in case of 1D solids it can be easily graphically analyzed, but in case of 2D and 3D solids the visualization becomes difficult because the plot E k plot becomes 3D and 4D actually.

So, for 2D solids E k plot is 3D and for 3D solids it is 4D. So, this visualization becomes difficult so, that is why we are trying to understand these concepts in 1D case so, that the understanding or the visualization is simpler and we can grasp as many concepts as possible. So, this is about the bands and Brillouin zones one more thing here that we need to notice is that between two bands so, this is one band and this is another band. Similarly, we will have another band possibly like this another band will be like this ok.

So, the band which is the highest occupied band or the band up to which electrons exist in a solid is generally known as the valence band. So, in this case if electrons are taking energy for example, up to this value which means that at t equal to 0 kelvin all the electronic states up to this energy value are filled. So, this band will be known as the valence band and the band just above this band will be known as the conduction band. This is generally how we define valence band and conduction bands.

The bands can be even more complicated, sometimes there might be overlapping bands we can have E k relationship in which two bands might be like this, which means that the E k relationship the E and k values which satisfy the Kronig Penney constraint or which give a valid Schrodinger equation solution they can give rise to E k values which can have a plot like this ok.

So, there are multiple possibilities in which electrons can occupy energies corresponding to k values in solids, ok. After this idea we discussed the idea of effective mass and the notion of effective mass comes from the fact that the solution of Schrodinger equation is done for a given value of E and we have a certain value of k for which we analyze the wave functions for which we obtain the wave functions.

So, in a way in Schrodinger equation solutions we get fixed k values and fixed E values and because of the Heisenberg's uncertainty principle when the energy is fixed the time evolution will be uncertain which means the time uncertainty in the particle would be there. And similarly, if k value is fixed the position uncertainty will be there in the particle.

But in actual devices where we know that electron will be travelling through the device at a given time. So, we broadly know that electron will have a certain position at a certain time in that case we cannot have a definite value of E defined for the electron, which means for most practical purposes we cannot have a single wave function of electron in the devices.

So, in devices we will have many electronic wave a bunch of wave functions describing the electron and these bunch of wave these various wave functions in that bunch of wave functions will have different energies. So, that is known as the wave packet. So, if one wave packet will have many waves corresponding to a given energy and given k value ok. So, that is why we actually need to deal with wave packets in our devices.

And as soon as we deal with the notion of wave packets this is the equation that we obtain. We obtain a relationship between an applied force and a parameter m star and v g where v g is the group velocity of the wave packet. And this is a very important idea actually this relationship is extremely important because if you recall this relationship looks exactly like the Newton's second law of motion.

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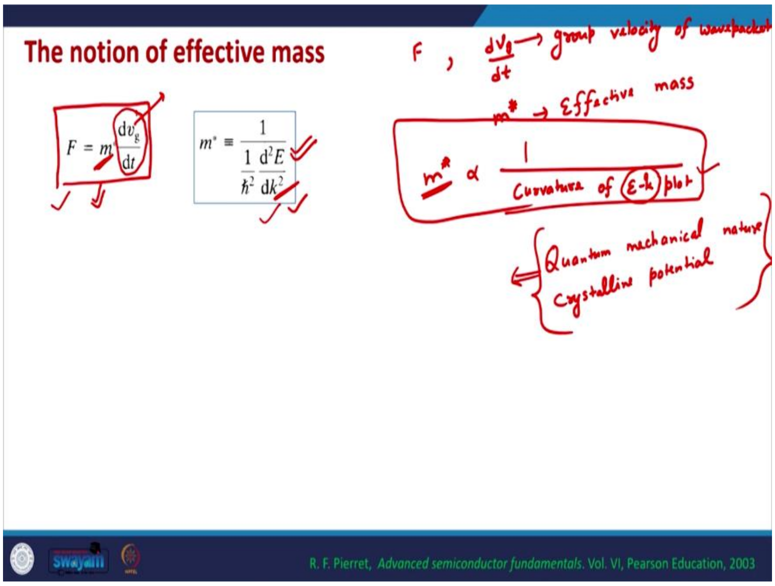

So, this is the relationship between the applied force and the $\frac{dv_g}{dt}$. So, in case of classical particle v_g is the velocity of the particle in case of electron wave packet v_g is the group velocity of the wave packet. And m^* is defined in this way m^* is by drawing parallels between this equation and Newton's second law of motion m^* is known as the effective mass of electron or we can also say this is the effective mass of the electron wave packet.

So, now we can use an equation which is exactly like Newton's second law of motion, but instead of using mass we need to use effective mass m^*, which is given by this relationship and instead of using the particle velocity v we need to use v_g which is the group velocity of electron wave packet ok. But this is an important result because as you can see the mass or the so called effective mass here it depends on the E k relationship. It is in fact; m^* is inversely proportional to the curvature of the E k plot.

So, $\frac{d^2E}{dk^2}$ is the curvature of E k plot. So, the effective mass of electronic wave packet is inversely proportional to the curvature of the E k diagram for an electron in solids. The advantage of having this kind of equation is that. Now, we can treat electron almost like a classical particle, but the mass will be taken as the effective mass which we need to draw from E k plot and the E k plot comes from the quantum mechanical solution. And the velocity we need to take as the group velocity of wave packet instead of the velocity of a particle ok.

So, in a way the quantum mechanics which is encapsulated in the E k plots is captured by the effective mass of the electron ok. So, this equation $\mathrm{F} = m^* \frac{dv_g}{dt}$ is very useful because now the quantum mechanical nature of electron the quantum mechanical nature and crystalline potential. This periodic potential due to crystal due to the solid this can be captured in the idea of the effective mass and the group velocity of electron, ok.

So, as you might have already seen that in many you might have already come across some books on this idea already where they do not deal with quantum mechanics directly instead they define effective mass and the group velocity. And they start the analysis of electronic devices from this point by considering the electron as a classical particle.

But by instead of using electronic mass they use effective mass and that is a valid actually that is a fairly good treatment of electrons. So, this is an extremely useful equation in electronic analysis because we cannot always solve Schrodinger equation for electrons in solids that is extremely difficult job. So, that is why having this idea of effective mass this sort of helps us analyze electronic behavior and devices to a great extent.

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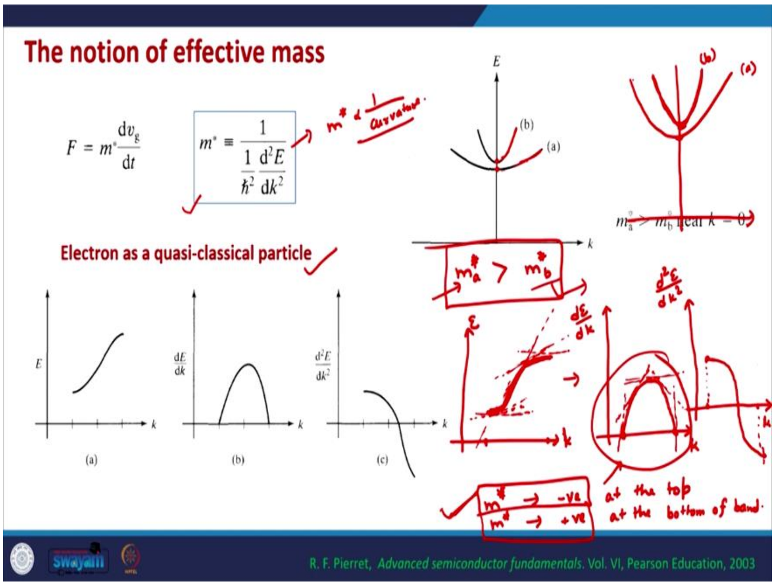

So, now we will see, what are the implications of this equation? The first implication is that now the electron can be considered as a quasi-classical particle and there is an interesting scenario which can arise which actually arises in many solids. So, for example, if a solid has E k relationship in which the E k plots are like this.

So, we have the E k relationship in which there are two curves very close to each other, but these curves have different curvature so, to say. So, let us say this is curve a this is curve b and if we just focus on the bottom of this band, these are two bands essentially. So, if you focus on the bottom of these bands and if we try to calculate the effective mass of electrons at the bottom of these bands we will see we see from this equation that m star is inversely proportional to the curvature.

And as you might have already guessed the curvature of this plot a is less as compared to the curvature of plot b. Plot b is having more curvature and that can be mathematically deduced as well if we have the exact expression for exact relationship between E and k for these two bands. The curvature or $\frac{d^2E}{dk^2}$ for b would be more as compared to curvature of plot a.

Which means the effective mass of electrons at the bottom of band a will be more than effective mass of electrons at the bottom of band b because the curvature of a is less effective mass would be more, curvature of b is more effective mass would be less as compared to a. So, electrons behave differently in these two different bands although their energies are quite similar.

So, the energy of electron at the bottom of band a and the energy of electron at the bottom of band b is almost the same it is very close they are very close to each other, but they behave differently when a force is applied on the system. Electron a behaves as a heavy particle and electron b behave as a or electrons in b behave as light particles, ok.

So, this is one interesting observation that we can deduce from the notion of effective mass and E k plots. Second thing is as you have seen in for example, in the E k relationship for solids you have seen that generally the bands take this kind of shape. So, the bands in a 1D solid they take this kind of a shape.

Similarly, this shape would be there the exactly similar shape would be there in 2D and 3D solids. So, the bands have this kind of shape. So, on the E k plot if we draw the E k plot the bands will be having this kind of shape. So, this is the E k relationship this is the bottom of the band this is the top of the band ok.

So, at the bottom of the band and at the top of the band the curvature might be the same actually. So, we will see that if we differentiate E with respect to k and plot it as a function of k so, if we plot from this plot if we plot $\frac{dE}{dk}$ as a function of k the curvature at this point the curvature is basically the tangent at the bottom of the band it is the curvature is 0. As we start moving away from the bottom of the band it starts increasing the curvature takes maximum value at this point where it is a positive value.

Then again, the curvature or the tangent starts taking less the value of the tangent starts reducing and finally, at the top of the band we again have $\frac{dE}{dk}$ to be 0. So , for example, if this is the bottom of the band and this is the top of the band the curvature at this point bottom of the band is 0 it gradually increases to a maximum value and again it decreases to 0 at the top of the band. So, the curvature at bottom is 0 top is 0 and in between it gradually increases to a maximum value and again goes to 0 as we approach the top of the band.

So, for this E k relationship this is the relationship between $\frac{dE}{dk}$ and using the same logic if we plot $\frac{d^2E}{dk^2}$ which means the relationship between the curvature of this plot as a function of k. So, $\frac{d^2E}{dk^2}$ is the curvature of this plot. So, if this is the bottom of the band this is the top of the band the curvature here as you can see curvature is tangent it is positive, the curvature the value of the curve or the value of the gradient of this plot starts reducing.

At this point the value of the gradient tends to 0 after this point the gradient starts becoming negative and at this point it takes even more negative value. So, the gradient of this plot which will be the curvature of E k plot is first positive then it decreases goes to 0 and then it becomes negative and then goes to a more negative value. So, this $\frac{d^2E}{dk^2}$ plot will be first it is positive in the middle it goes to 0 and then it becomes a negative value something like this and as you have already guessed effective mass is inversely proportional to the curvature.

So, at the bottom of the band curvature is positive at the top of the band the curvature is negative. This negative curvature implies that the effective mass will be negative at the top and positive curvature at the bottom of the band implies that effective mass will be positive at the bottom of the band. So, this notion of negative mass is entirely new for us actually in classical mechanics we cannot have negative mass for a particle.

But in actual solids at the top of the band when we apply a force electrons behave as if they are having a negative mass and what does that mean? Electrons accelerate in opposite direction to a classical particle electrons will accelerate in electron will move in a direction opposite to the direction of a classical particle. Had the classical particle been in the same situation now the electron moves in opposite direction to that.

So, this is an entirely quantum mechanical idea this comes from the E k plot which basically comes from the solution of the Schrodinger equation that electrons behave as if they are having a negative effective mass. And that is a very important result and the notion of holes in solids, in semiconductors that essentially comes from this analysis ok.

So, that is why this idea of effective mass is extremely useful because by defining effective mass we can do away with our quantum mechanical analysis we can avoid doing quantum mechanics for the device at least for the transport. And, but at the same time this idea results in such kind of implications where the electrons effective mass can be negative and it can behave a particle.

It can behave like a particle which is opposite to a classical particle which moves opposite to a classical particle in same situation and that is why and that is where this idea of holes come from in solid state devices. So, this is broadly what the idea of effective mass is.

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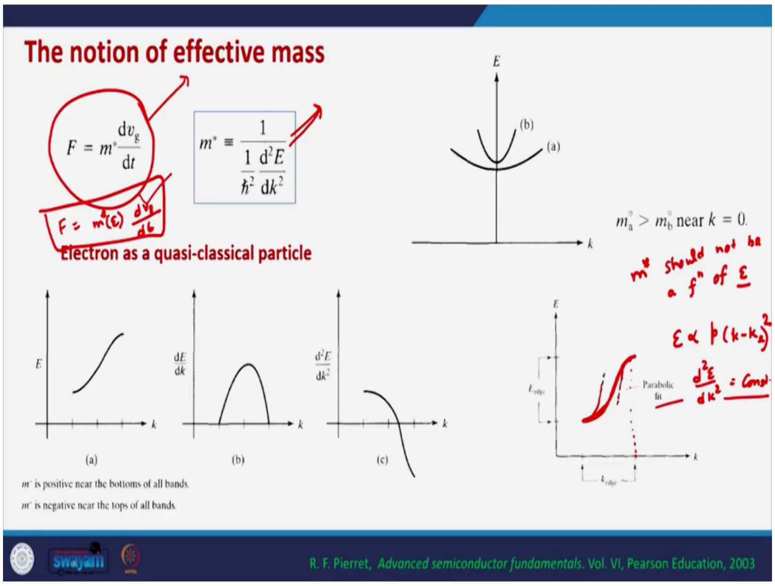

A last point in this notion is that we cannot always use the idea of effective mass or we cannot always use this equation for our analysis. There are certain constraints or certain conditions in which this equation or the idea of effective mass can be used to analyze electrons behavior in solids and one of these things is that effective mass should not be a function of E.

So, for example, in a certain E k regime if effective mass is a function of E in that case this idea cannot be used properly because then it will give rise to many complications in calculation. So, if effective mass changes with E then this equation will not be very useful because it again we will need to go back to the E k plots and ultimately we will we would need to do the quantum mechanical calculations for the device.

So, that is why if we observe a typical band like this at the bottom of the band and at the top of the band this band is quite like a parabolic band. So, this is as you might have already observed also in the E k plot for 1D solid this is the typical band structure that we see and just at the bottom of the band and just at the top of the band this band structure can be approximated by a parabola. So, at the bottom of the band and at the top of the band it can be approximated by a parabola.

And what is the advantage of parabolic approximation so, if the bands can be approximated by a parabola in a certain regime. So, for example, at this k value if we can assume that or if we can approximate the bands to be parabola which means the relationship between E and k is square relationship and there would be a constant let us say p here in that case $\frac{d^2E}{dk^2}$ would be constant.

So, in those regimes of E k plot where the plot can be approximated by a parabola there the effective mass is independent of energy the effective mass is constant. And in those regimes if electrons are having those energies and k values E and k values. In that case this equation can be directly used and the idea of effective mass is highly applicable and highly useful and simple as well.

So, these are few things that we need to keep in mind these two things differential masses of electrons and even the negative mass of electron this comes from the idea of effective mass. And here we talked about the applicability of the idea of effective mass and this equation of motion when a force is applied to a system. So, this basically concludes our discussion on the effective mass and electronics equation of motion in actual solids which we started with our discussion of quantum mechanics.

So, we have discussed basic postulates of quantum mechanics ,we have discussed how electrons behave when electrons are confined in a certain regime of space. We then discussed how electrons behave in 1D solids and in that discussion the idea of bands and band gaps that naturally comes up. We also analyzed blocks theorem which is an extremely important theorem in solid state physics.

Then we saw how we can sort of deduce the idea of effective mass from that analysis, which is a very simple concept, but which also encapsulates the quantum mechanical nature and the crystalline potential of the solids. So, we do not need to worry about the periodic potential of crystals and quantum mechanical nature of electrons if the effective mass of the electrons is properly defined in a device ok. So, all this discussion was done in order to understand the transport of electrons in devices and in order to understand the idea of density of states in the devices.

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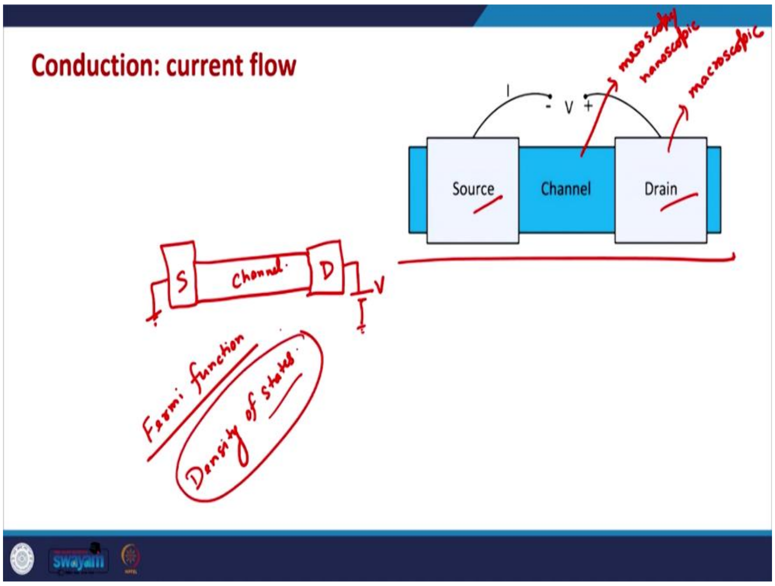

So, you might recall from one of our earlier classes if this is a two-terminal device in a two terminal device where we have a source a drain and a channel region. And generally, the source is grounded we apply a positive voltage on the drain and a flow of electrons start in the device, the electrons start moving from source to drain basically.

So, in these kind of devices , this is the outline of the device modern devices in this device in these devices the source and the drain regions are they are still bulk material like the material that used to be have in other words that have macroscopic dimensions. And the channel is now mesoscopic or nanoscopic channel is now nanoscale.

So, the electronic concentration in source and drain this can be easily defined by defining the Fermi function by the Fermi function in source and drains, but the electronic distribution in channel can be understood from the idea of density of states. Because in a small region electrons cannot occupy a continuous energy electrons cannot take continuous energy values, electrons will have discrete energy values and moreover in solids we have seen that there may be bands and band gaps in the solids.

So, we need to see how many electrons can exist in the channel and how they are distributed in the channel and that is defined by the idea of density of states. So, this idea of density of states which basically captures the allowed electronic states in the channel and how many sort of how many states are there, what are bands and band gaps in the channel this is basically captured by the density of states and this is what we will discuss in our next class. So, see you in the next class.

Thank you.