Introduction to Solid State Physics
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Lecture - 66
Semiclassical dynamics of a particle in a band and Bloch oscillations

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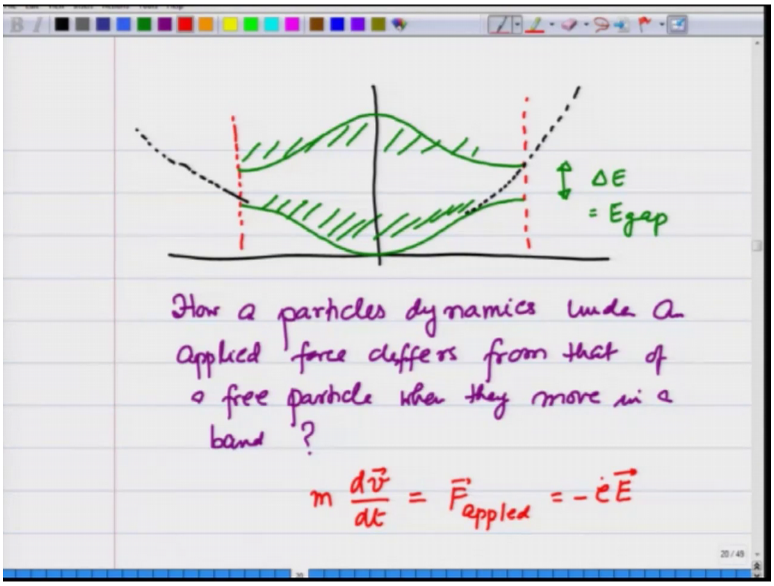

So, far we obtained bands in different manners and what you have understood that when a particle moves in a periodic potential it takes energies continuously in a band and then there is some energy gap and another band and so this we have gotten through two or three different pictures. This is quite different from the case of free electrons where the energy is continuous as shown here by this black dashed curve.

So, what we have is these bands of energies with energy gap delta E E gap in between like the energy levels in an atom have some difference between them. Now the question is that how a particles dynamics under an applied force differs from that of a free particle when they move in a band. This is the question I am going to raise and this question is important because earlier when professor Satyajit Banerjee taught you conductivity and things like those, under free electron approximation the equation of motion that was used was that dv dt that is a velocity of an electron changed according to Newton's laws.

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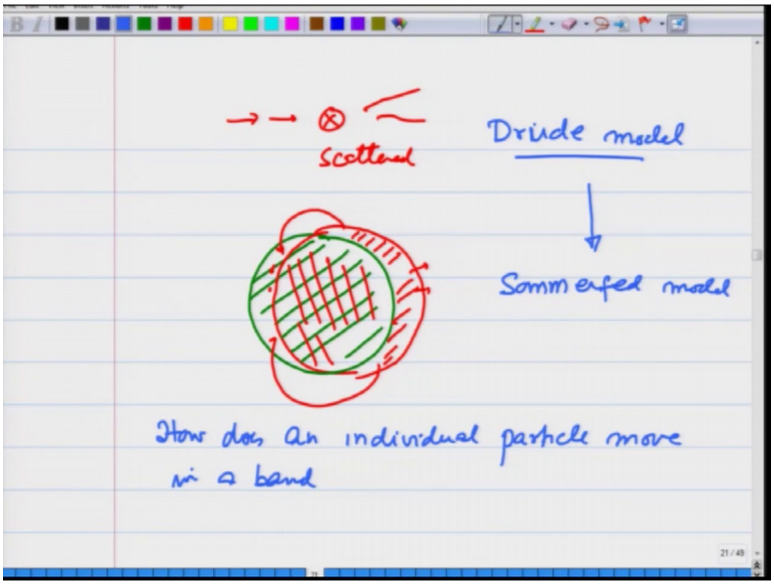

So, I am going to multiply this by m this was equal to F applied, which in the case of an electric field became minus e the electric field applied E and then particle could move under this force accelerating until it was scattered and then something happened. So, this was a picture that you started with right in the beginning of the course in Drude model and then this was generalized to Sommerfed model, where instead of these each particle moving with same velocity and each particle being scattered we had a Fermi sphere which was filled. And when a field was applied this Fermi sphere shifted because of the applied field and because of then scattering.

Now, these electrons out here that gain velocity when they got scattered they could not go anywhere else, but only to those states which were empty. So, either they will go out, then they will gain energy or they get scattered and they could not come to this region which is overlapping in this region they could not come. The only region they could come to was here. They are gave larger scattering lengths. So, this is the picture that we drew.

In this lecture I am not concerned with this collective conductivity instead what I am asking is how does an individual particle move in a band and this will give some new concepts once I understand how an individual particle moves then I can obviously generalize to a collection of particles and calculate the current and all that, but initially I have no scattering nothing just a particle in a band and I am applying an external force and I want to understand how it moves. Is it any different from free particle? So, before I do that let me just review what we did in free particle.

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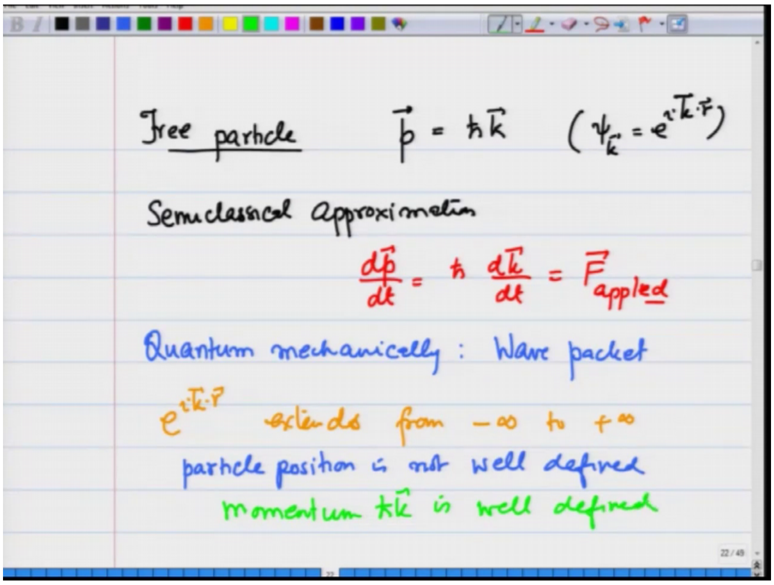

In a free particle the momentum of the particle p was given as h cross k where k is arises from this wave function e raised to i k dot r and in semi classical approximation and I will explain in a minute why I am calling semi classical approximation. I had dp dt is equal to h cross d k dt equals F applied. I am calling it semi classical approximation because when I look at these particles quantum mechanically then to locate a particle I actually have to make a wave packet.

Why? Because the plane wave e raised to i k dot r is extending from minus infinity to plus infinity and therefore, the part of the position is not well defined. So, for the plane wave the particle position is not well defined and what is well defined is the momentum h cross k is indeed well defined.

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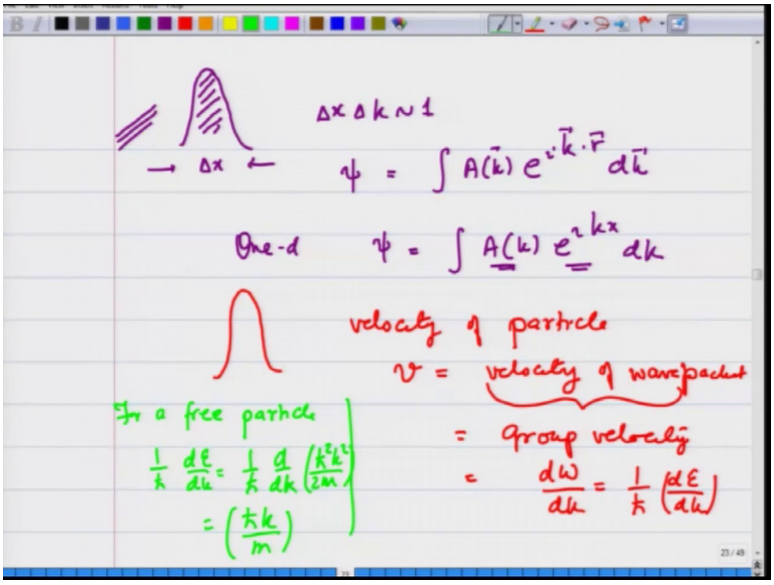

So, what we do is we make a wave packet. We make a wave packet within which we say that the particle can be localized within this sum delta x and delta x, delta k is of the order of 1 by uncertainty principle. So, its momentum is also spread in some small interval so that delta k delta x is equal to 1 and the wave packet psi is given as an integral A k e raised to i k dot r d k and let me specialize to one d so that things are easy, it is A k e raised to i k x d k that means, what I am doing physically is I am taking many many plane waves with different case and with different amplitudes and mixing them up so that all of them add up at one place and cancel at other places and that gives rise to a wave packet.

For the wave packet the velocity of particle v is related to the velocity of wave packet. They are in fact equal and velocity of wave packet is known as the group velocity which is given as d omega d k or 1 over h cross d energy d k. This is a review of quantum mechanics on the side I am going to show you that for a free particle 1 over h cross d e d k will be equal to 1 over h cross d by d k of h cross square k square over 2 m which comes out to be h cross k over m which is the velocity of the particle and this is same as the group velocity. And then when we apply the force and in one d I will remove the vector sign force is nothing, but h cross d k d t.

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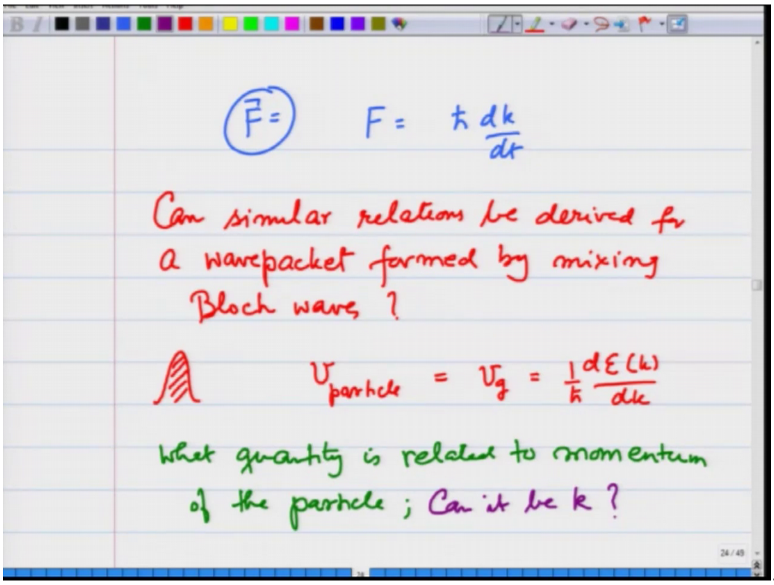

The question we now ask is can similar relations be derived for a wave packet formed by mixing Bloch waves? Why Bloch waves because now stationary state for a particle is given by a Bloch wave and if I combine these Bloch waves I may be able to localize a particle in a wave packet. So, first thing is if I want to see a particle moving, I need to localize it in a wave packet and then see what relations are. The question is can v particle then be related to v group that is d E k d k 1 over h cross for a band and then what quantity is related to momentum of the particle can it be k.

So, the answer to both these questions is in the affirmative and this is indeed. So, and this is what we are going to do in this lecture.

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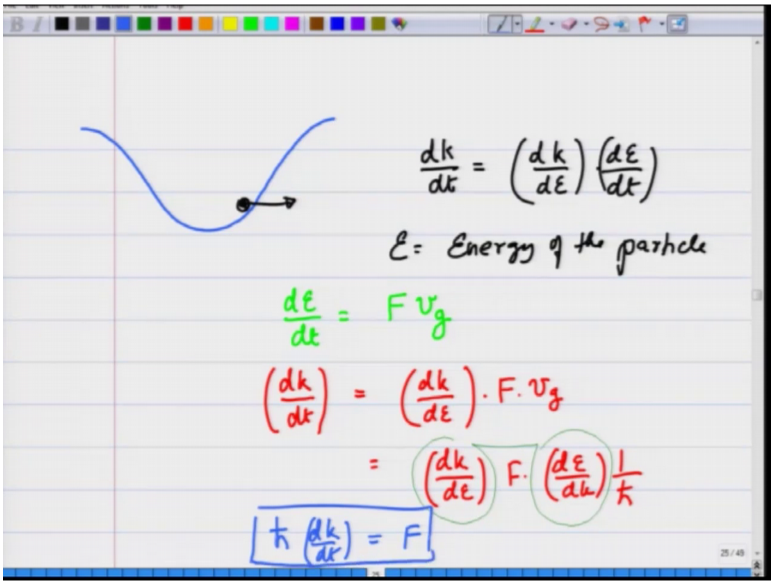

So, first let us see if I apply a force on a particle moving in a band and. So, the particle was somewhere here and I apply a force in the right direction. As I apply the force is going to change energy. Let us calculate how is k is going to change; d k d t, I can write as d k d E and d E dt where E is the energy of the particle. How does the energy of a particle change? The energy of the particle d E dt is going to change by the force applied times a velocity the particle which we said is v group.

So, this is going to change as F times v group therefore, d k d t, I am again writing everything in one d which can be easily generalized to three d, but one d is easy to visualize is d k d E times the force applied times v group and v group is F times d E d k 1 over h cross. Now you see these two quantities here, d k d E with d E d k gives me 1 and therefore, I end up getting the result that h cross d k dt is equal to F.

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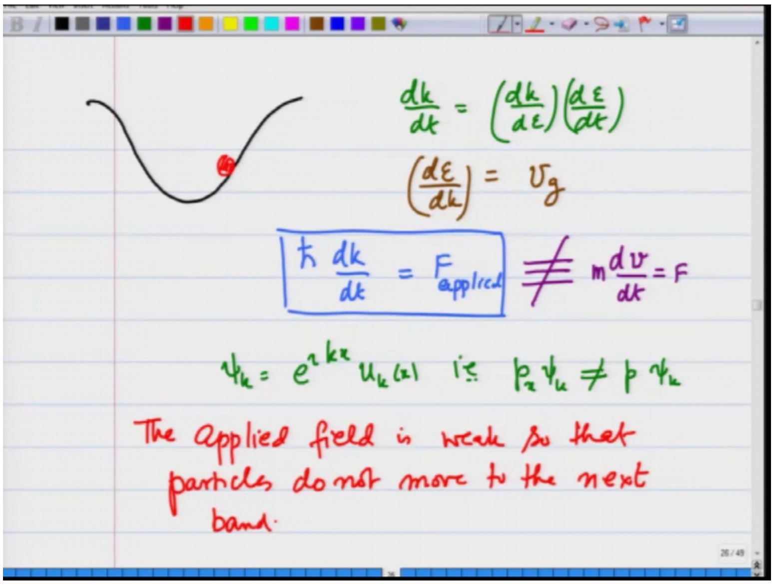

Again making this picture band and a particle moving in this through d k dt equals d k d E d e dt and realizing that d E d k is v group. We found relationship that h cross d k dt is equal to force applied.

Let me also be explicit, let me write this applied. Notice that the relationship is in terms of h cross and k, not the velocity. So, this is not equivalent to dv dt times m equals F. This is not equivalent to that because now things are moving in a band so because v as m v is not h cross k. Why is m v not h cross k? Because psi k which is e raised to i k x u k x is not a momentum of eigenstate. That is p x psi k is not equal to some p momentum time psi k. It is not and therefore, the two relationships are not equal what is happening when you apply a force the k a wave vector of the particle changes and when the wave vector changes, it moves in the band. Now, what we are going to assume is that the applied field is weak so that particles do not move to the next band.

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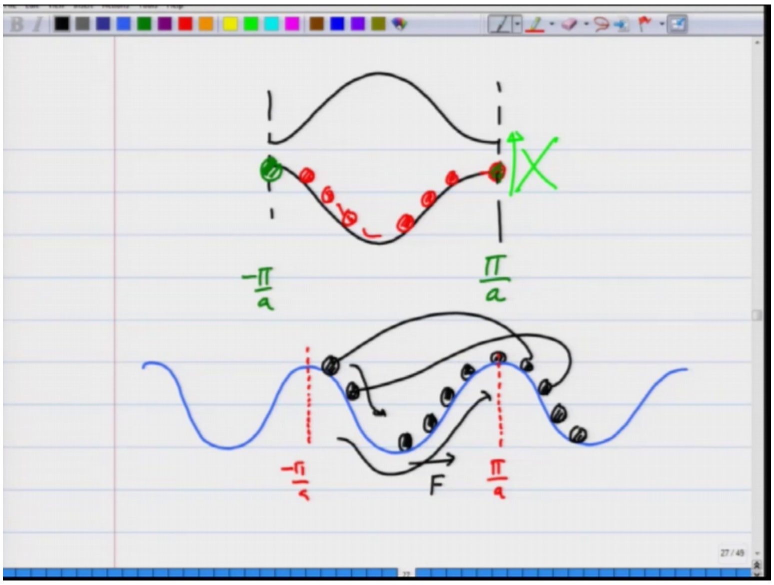

And what that means, is let me explain the next slide if I have a band like this and a higher band like this, a particle can move from here to here as you apply the field, but this is not allowed field is quite weak. So, as k increases, energy increases. Now what happens when the particle reaches of end of the brillouin zone which we show by pi by a. What we have learnt is that as it reaches here this point is equivalent to the point on the left minus pi by a.

So, I can think of this particle reaching here is same as particle reaching as minus pi by a and then it starts all over again coming this way, k increases and then it goes there and comes back. You can also see this in extended zone scheme. If I look at this band, it is like this and the band extends from minus pi by a to pi by a and as a particle moves up the band by increasing k. If I apply a force to the right, it reaches the top and then it starts coming down, k is increasing, but that is same, this point is equivalent to the point out here. This point is equivalent to point out here that is the same as if the motion is taking place like this.

So, what is this particle doing? It is going like this, coming back again, coming back again, it is performing a periodic motion. This is quite different from what happens to a free particle.

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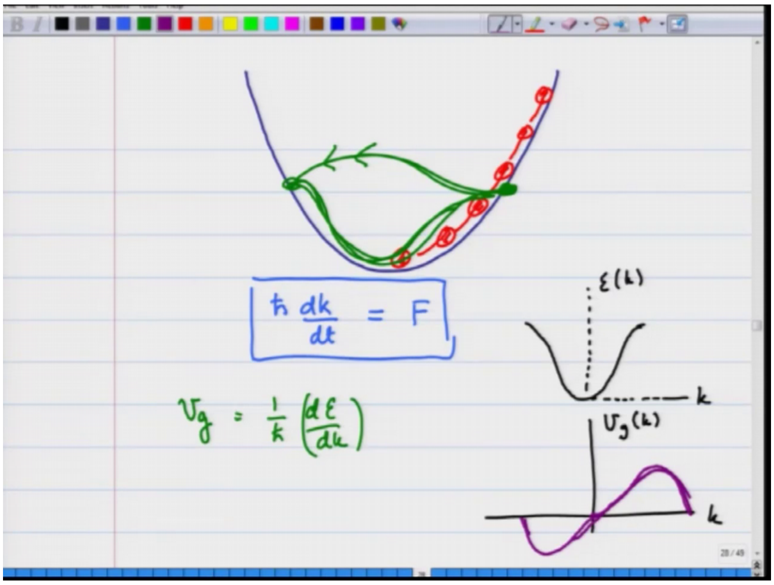

In a free particle where the energy spectrum is continuous a particle moving would keep increasing is k and increasing this energy not anymore in this band it comes here and goes back here and it starts all over again, comes back here starts all over again. It is performing a periodic motion let us now do this mathematically.

So, what we have found is that h cross d k dt is force F. What about the velocity of the particle? Velocity we said is v group which is 1 over h cross dE dk. So, how would it look? Let us see it on the side I am going to make here on the right side of the screen a band. So, let me make that band like this. This is E k versus k. And if I look at the slope of this band, it will give me v group velocity or velocity of this particle and that will be 0 at this point at k equals 0 then it increases and then again becomes 0 and this point is equivalent to the point at minus pi by a and here the velocity starts from 0 goes negative and then comes back here.

So, as you see this particle it will be performing this motion, as velocity increases goes to 0 then it becomes negative. So, it will be going back and then again its velocity will become zero and it will be coming forward.

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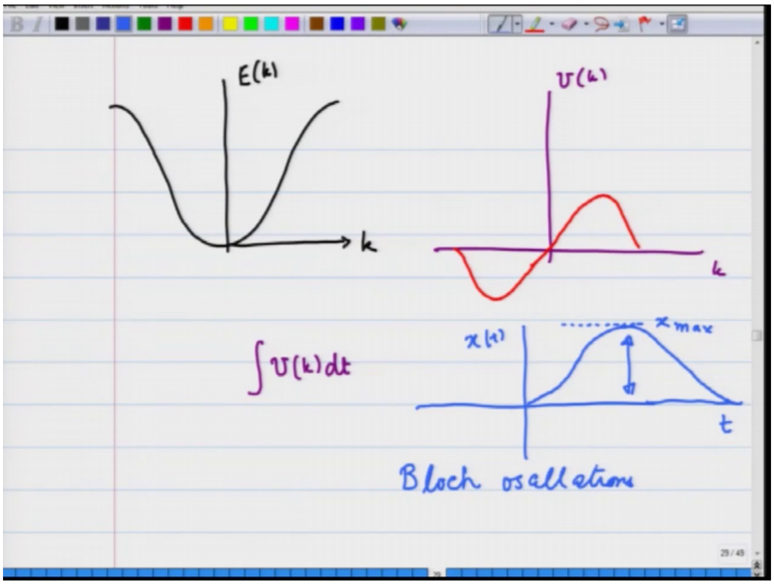

So, let us make these pictures again here is the band E k versus k. The corresponding velocity, if I plot v k versus k it is, like this and then if I were to plot integral v k dt that is a displacement of the particle. Let us do that. How would it look? It would look initially we will increase, become large and then it will slow down go to a maximum and then the velocity is negative then it comes back.

So, this is versus t. This is x t and then it starts all over again. So, it will be oscillating back and forth going to a x max and then returns, comes back to where it started from and then starts all over again. So, it will be performing an oscillatory motion and these are known as Bloch oscillations.

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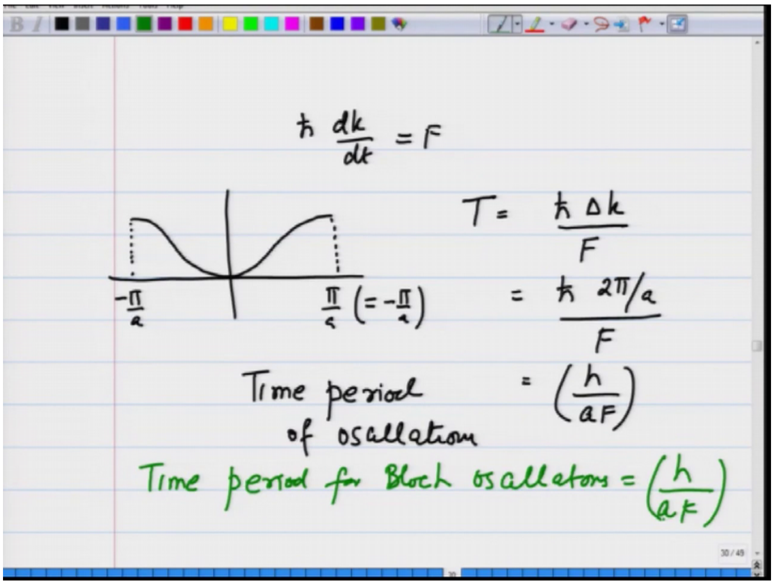

So, if I were to look at again h cross d k over dt equals F, then in this band how much time would the particle take from going from minus pi by a to pi by a and pi by a is again equivalent to minus pi by a and that will be the time of oscillations of these particles.

So, the time T would be equal to h cross delta k over F which will be h cross delta k has become 2 pi by a over F and this will be h over a F. This is the time period of oscillations. It is in this time that will complete an oscillation. It will go to some x maximum, come back to its original position and this is the time period we have calculated. So, time period for is h the Planck's constant divided by the lattice spacing a F.

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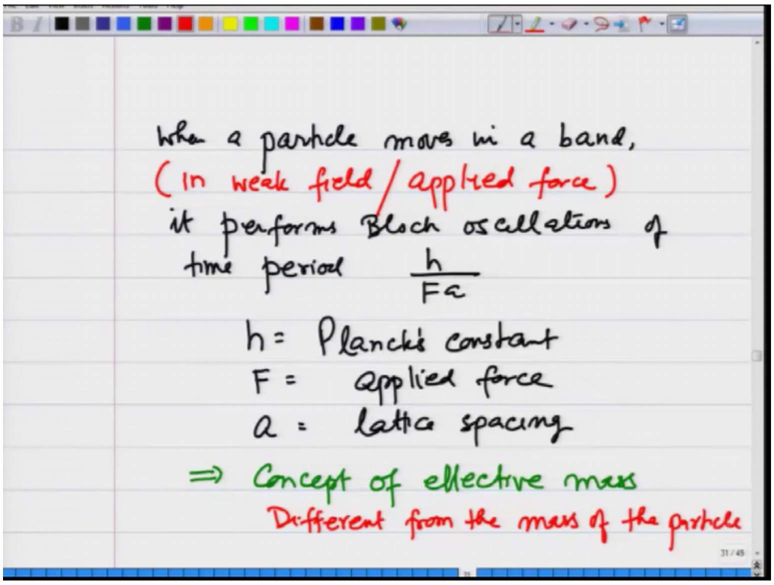

So, what we have learnt that when a particle moves in a band and let me qualify in weak field or applied force performs Bloch oscillations of time period h over F a where h is Planck's constant, F is applied force and a is the lattice spacing.

So, this is very different from the free electrons where they keep moving in one direction. Now this also leads to the concept of effective mass in a band which is different from the mass of the particle and let me show you how.

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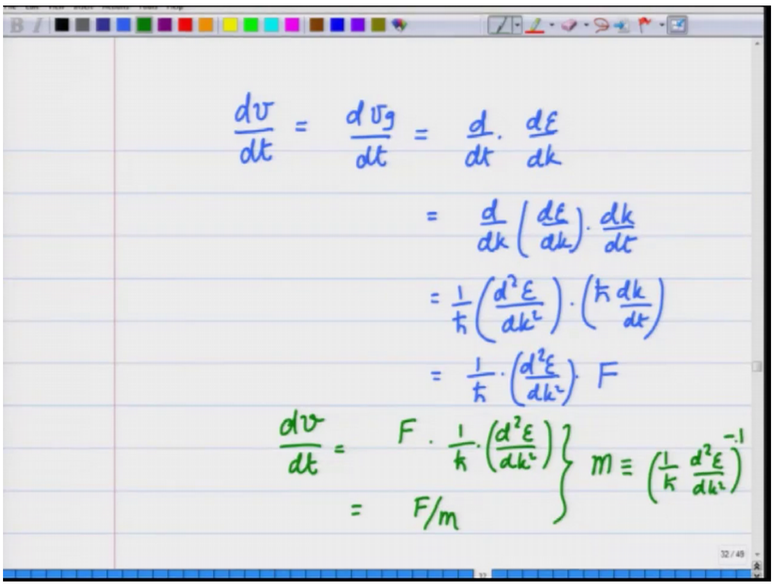

So, if I were to calculate the rate of change of velocity of a particle, it will be same as dv g dt where v g is the group velocity and this will be d by dt of d E by dk which I can change to d by dk of dE by dk dk dt. This is d 2 E by d k square times d k dt which I can write h cross d k dt and 1 over h cross outside.

This is 1 over h cross d 2 E by d k square times F. So, I see that dv dt of the particle is F times 1 over h cross d 2 E by d k square. Compare this with F over m, then you see that m is equivalent to 1 over h cross d 2 E by d k square inverse.

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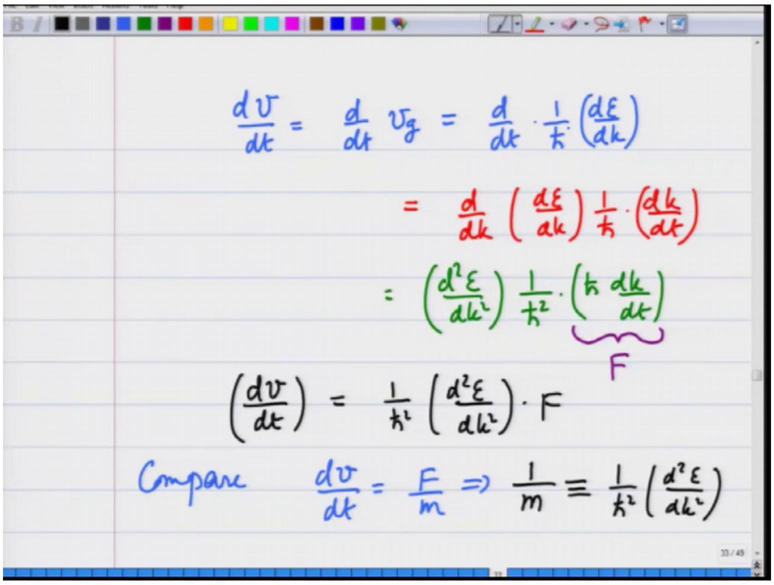

So, to understand the concept of effective mass let us calculate dv dt for the particle which will be the same as d by dt of its group velocity which I can write as d by dt of 1 over h cross d E d k. This can be written as d by d k of d E d k 1 over h cross d k d t. I can further write this as d 2 E by d k square 1 over h cross square h cross d k by dt and the last thing we have already derived this is nothing, but the applied force.

So, I can write finally, that dv dt of the particle is 1 over h cross square d 2 E by d k square times F and if I compare with dv dt equals F over m this implies that the mass of the particle 1 over m is equivalent to 1 over h cross square d 2 E by d k square it depends on the second derivative of the energy with respect to k.

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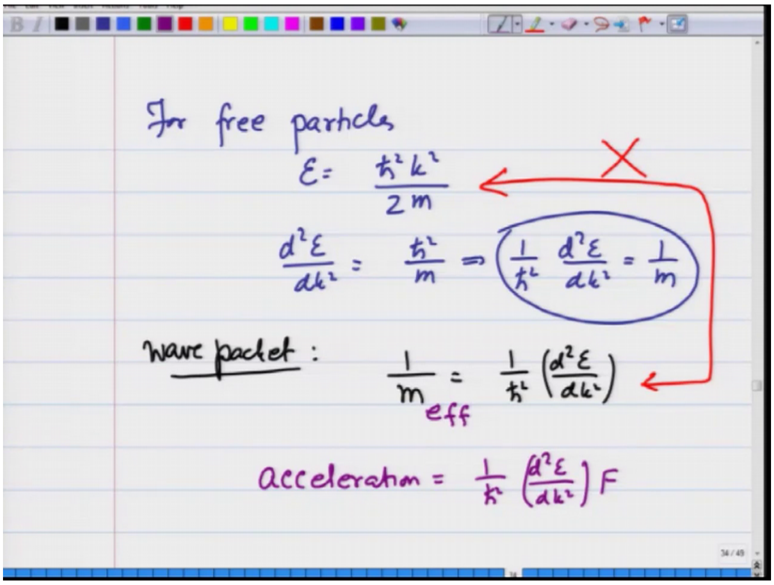

Let us see if this is true for free particles E is h cross square k square over 2 m. So, d 2 E by d k square comes out to be h cross square over m and this implies 1 over h cross square d 2 E by d k square is 1 over m. And what we are finding is, even when we make a wave packet by mixing these Bloch waves even then the mass effectively can be seen as 1 over h cross square d 2 E by d k square, but E versus k relationship is not like this. It is not like this and therefore, this mass is necessarily different from the free electron mass and therefore, we call it effective mass of the particle. This is how massive the particle appears to be when you apply a force.

So that is acceleration, is equal to 1 over h cross square d 2 E by d k square F and this effective mass is the quantity that will appear when we consider transport of electricity or current in a solid system where the current is carried by electrons they will respond as if the mass is this effective mass and not the free mass. We will discuss it more when we come to discuss semiconductors. So, in the next lecture what I am going to show you some experiments where these Bloch oscillations have been demonstrated and that will give you a feel for what the motion in a band is like.

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Equality of the expectation value of the velocity of an electron in a Bloch state and the group velocity

The group velocity v_g of a wavepacket is given as

$$v_g = \frac{d\omega}{dk}$$

where $\omega = E/\hbar$, and E is the energy of the particle associated with the wavepacket. This means

$$v_g = \frac{1}{\hbar}\frac{dE}{dk}$$

Let us now calculate the derivative of the energy with respect to k and show that the resulting expression is indeed the expectation value of the velocity operator.

The energy $E(k)$ is the expectation value

$$E(k) = \frac{1}{N}\int_0^L e^{-ikx}u_k^*(x)H\, e^{ikx}u_k(x)\, dx$$

where the Hamiltonian H is

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

The action of operator $-\frac{\partial^2}{\partial x^2}$ on $e^{ikx}u_k(x)$ gives

$$e^{ikx}\left(k + \frac{1}{i}\frac{\partial}{\partial x}\right)^2 u_k(x)$$

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Therefore $u_k(x)$ satisfies the Schrodinger equation

$$\left[\frac{\hbar^2}{2m}\left(k + \frac{1}{i}\frac{\partial}{\partial x}\right)^2 + V(x)\right]u_k(x) = E(k)u_k(x)$$

Thus the energy can be written as

$$E(k) = \int_{UnitCell} u_k^*(x)\left[\frac{\hbar^2}{2m}\left(k + \frac{1}{i}\frac{\partial}{\partial x}\right)^2 + V(x)\right]u_k(x)dx$$

Now taking the derivative of $E(k)$ with respect to k we get

$$\frac{\partial E(k)}{\partial k} = \int_{UnitCell}\frac{\partial u_k^*(x)}{\partial k}\left[\frac{\hbar^2}{2m}\left(k + \frac{1}{i}\frac{\partial}{\partial x}\right)^2 + V(x)\right]u_k(x)dx$$

$$+\int_{UnitCell} u_k^*(x)\left[\frac{\hbar^2}{2m}\left(k + \frac{1}{i}\frac{\partial}{\partial x}\right)^2 + V(x)\right]\frac{\partial u_k(x)}{\partial k}dx$$

$$+\int_{Unit\ Cell} u_k^*(x)\frac{\hbar^2}{m}\left(k + \frac{1}{i}\frac{\partial}{\partial x}\right)u_k(x)dx$$

Using the Hermitian nature of the Hamiltonian, the first two terms can be combined to get

$$\int_{UnitCell}\frac{\partial u_k^*(x)}{\partial k}\left[\frac{\hbar^2}{2m}\left(k + \frac{1}{i}\frac{\partial}{\partial x}\right)^2 + V(x)\right]u_k(x)dx$$

$$+\int_{UnitCell} u_k^*(x)\left[\frac{\hbar^2}{2m}\left(k + \frac{1}{i}\frac{\partial}{\partial x}\right)^2 + V(x)\right]\frac{\partial u_k(x)}{\partial k}dx$$

$$= E(k)\frac{\partial}{\partial k}\int_{UnitCell}|u_k(x)|^2\, dx$$

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Since $\int_{UnitCell}|u_k(x)|^2\,dx = 1$, the right hand side of the equation above vanishes. Thus we get

$$\frac{\partial E(k)}{\partial k} = \int_{Unit\ Cell} u_k^*(x)\frac{\hbar^2}{m}\left(k+\frac{1}{i}\frac{\partial}{\partial x}\right)u_k(x)dx$$

This can be rewritten as

$$\frac{1}{\hbar}\frac{\partial E(k)}{\partial k} = \int_{Unit\ Cell} e^{-ikx}u_k^*(x)\frac{\hbar}{m}\frac{1}{i}\frac{\partial}{\partial x}e^{ikx}u_k(x)dx$$

Now using the normalized wavefunction (normalized over N cells)

$$\psi_k(x) = \frac{1}{\sqrt{N}}e^{ikx}u_k(x)$$

The expression above is

$$\frac{1}{\hbar}\frac{\partial E(k)}{\partial k} = \int_0^L \psi_k^*(x)\frac{\hbar}{m}\frac{1}{i}\frac{\partial}{\partial x}\psi_k(x)dx$$

which is the expectation value of the velocity operator. This shows that the expectation value of the velocity operator is indeed the group velocity v_g.

Right now I stop here and I will come back with the experiment results in the next lecture that will complete the material covered in this week.

Thank you.