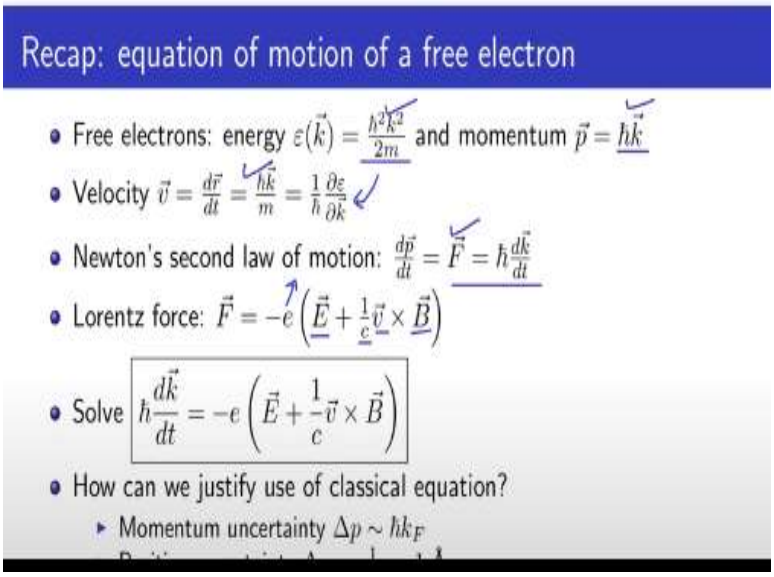
Electronic Properties of the Materials: Computational Approach
Prof. Somnath Bhowmick
Department of Materials Science and Engineering
Indian Institute of Technology, Kanpur

Module No # 06
Lecture No # 29
Semi classical Electron Dynamics: Part 1

Hello friends we already have salt allowed energy levels of electrons in a periodic potential these are known as block electrons. Now we would like to know how block electrons move when we apply an external electric or magnetic field. In this lecture i am going to introduce semi-classical model to solve the dynamics of block electrons in externally applied electric and magnetic field.

(Refer Slide Time: 00:45)

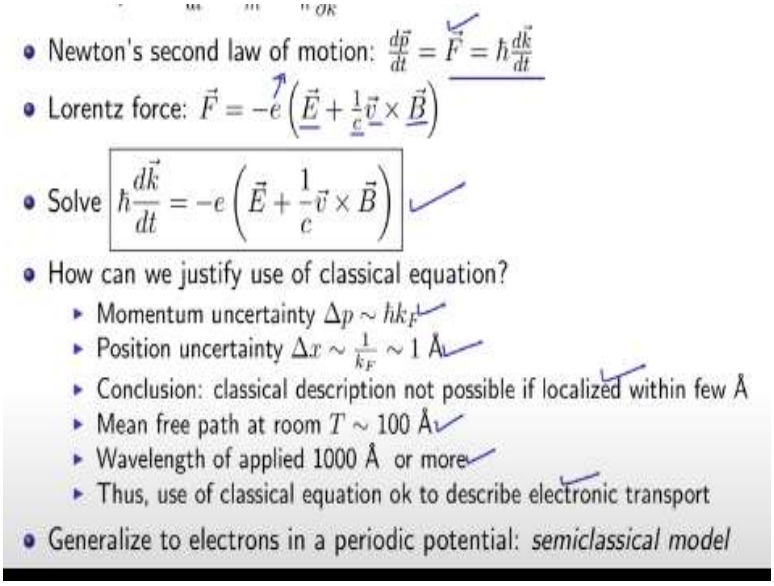


Before I start discussing about dynamics of block electrons let me briefly revisit what we did for 3 electrons. For free electrons energy Eigen value for a given wave vector k is h cross square k square divided by 2m and the momentum is h cross times k. Velocity of an electron is momentum divided by mass, that is h bar k divided by m using the energy dispersion relation we can further write the velocity as 1 by h bar del e del k.

Electrons collide with very heavy ionic cores and trajectory of an electron between collisions was calculated using Newton's second law of motion d p d t is equals to force. Now we replace p with h bar k and rewrite this equation as F = h bar times d k d t. For solar electron due to externally applied electric and magnetic field is given by the Lorentz force f = - e times E + 1 by c v cross B.

Where - e is the charge of an electron, E is the electric field, c is the speed of light, v is the velocity and b is the magnetic field. Thus we have to solve h bar d k d t = - e times E + 1 by c v cross B.

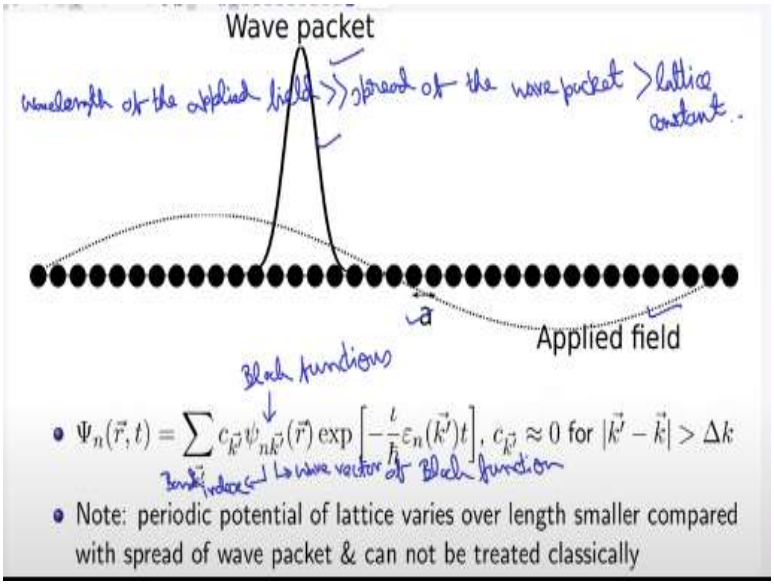
(Refer Slide Time: 02:49)



We justified the use of classical equation by using the following arguments. The momentum uncertainty of free electrons is of the order of h bar times k f; where k f is the farming wave factor. Corresponding position uncertainty is of the order of 1 angstrom thus according to Heisenberg uncertainty principle classical description is not possible if we are dealing with some length scale of the order of few Angstrom.

Now let us find out the length scales we are dealing with in electronic transport problem. Mean free path at root temperature is of the order of 100 Angstrom. Wavelength of externally applied field is of the order of 1000 angstrom or even more. Thus we are dealing with some length scale which is much larger than 1 angstrom as a result we are allowed to use classical equation to describe electronic transport. The classical approach used for free electrons has a simple generalization to electron in a periodic potential this is known as the semi-classical model.

(Refer Slide Time: 04:18)

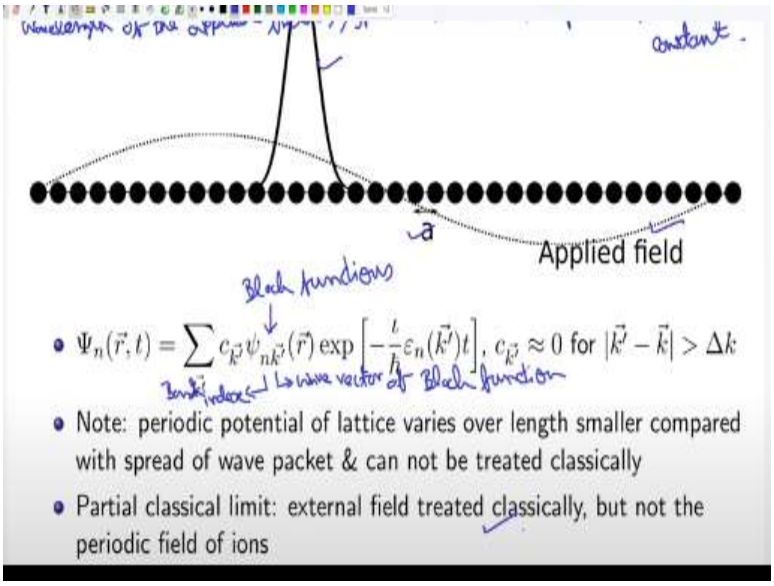


In this diagram I schematically show the situation described by the semi-classical model a, is the lattice constant the electron is described by a wave packet. We can construct such a wave packet by using several block functions of different k values for a given band of index f, so these are the block functions. K is the wave vector of function and n is the band index by controlling the spread of k values in the sum we can control the speed of the wave packet. The spread is typically few lattice parameters as shown in this diagram.

Semi-classical model describes a situation where the applied field varies slowly in space, compared to the periodic potential due to the underlying lattice. If, we associate some wavelength with the applied field then; wavelength of the applied field is much greater, than spread of the wave packet which is larger than the lattice constant. Note that period potential of lattice varies in a scale of the lattice parameter of a, which is much smaller than the state of the wave packet.

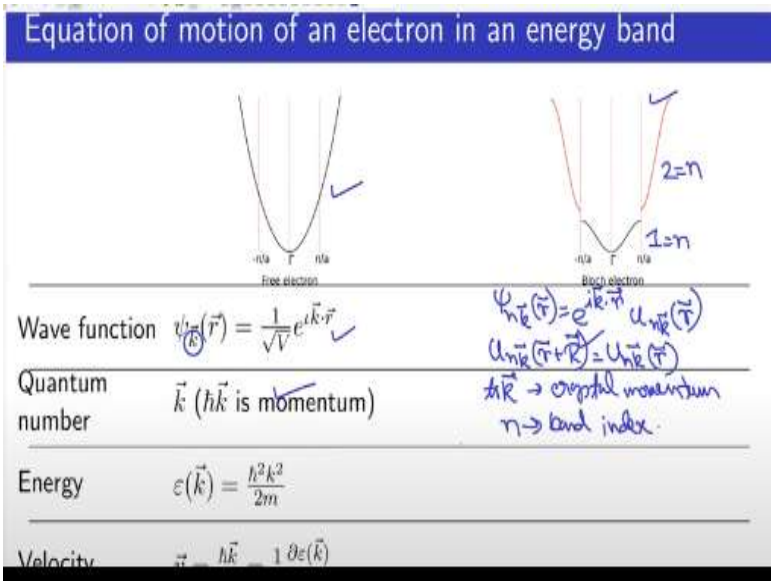
Thus the periodic potential cannot be treated classically, we indeed have solved time independent solving the equation in presence of periodic potential to get the energy of electrons in a periodic potential.

(Refer Slide Time: 07:04)



This is a partial classical limit because the external field is treated classically but not the periodic field of ions this is why we call it a semi-classical model.

(Refer Slide Time: 07:27)

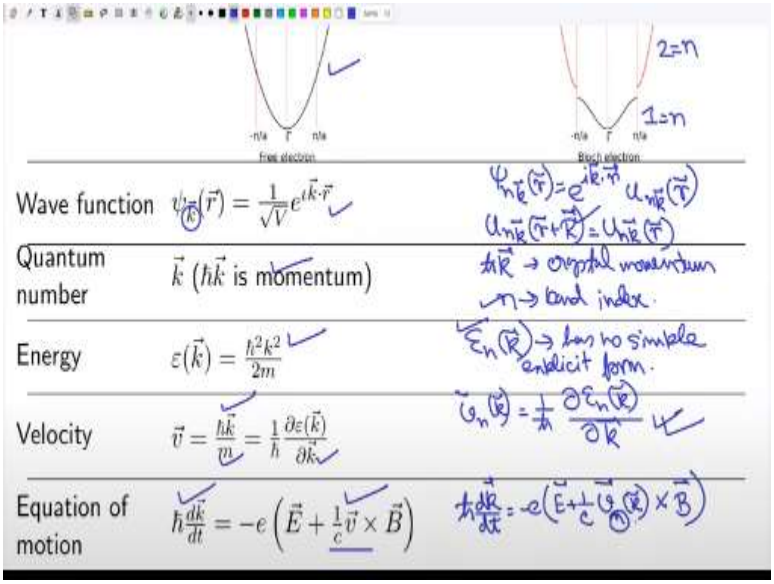


Let us derive the equation of motion of an electron in an energy band they look so similar to the free electron equations. That I am going to actually start with the free electron equations and show the minimal changes required to get the equation of motion of block electrons. This is the e versus k parabola for free electrons and this is the energy dispersion relation for block electrons plotted using extended zone scheme. I have shown just two bands in this figure band 1 and band 2.

Wave function of a free electron with wave vector k is given by psi k of r = 1 by square root of b times e power i k dot r. Wave function of a block electron is given by psi n k of r is equals to e power i k dot r this is same as the free electron part times some function u n a of r. The function u has no simple explicit form, the only general property it has is the periodicity of the direct lattice. That is u n k of r + R = u, where R is a lattice translation vector.

Note that in case of free electron wave function we have only one index k and h bar k is the momentum of 3 electrons. In case of block electrons we have 2 indices n and k, in this case h bar k is the crystal momentum, and n is the band index. N is equals to 1 for band 1, n is equals to 2 for band 2 excreta. In both the cases allowed values of k r obtained from periodic boundary condition, in case of block electrons m can be any positive integer.

(Refer Slide Time: 10:16)



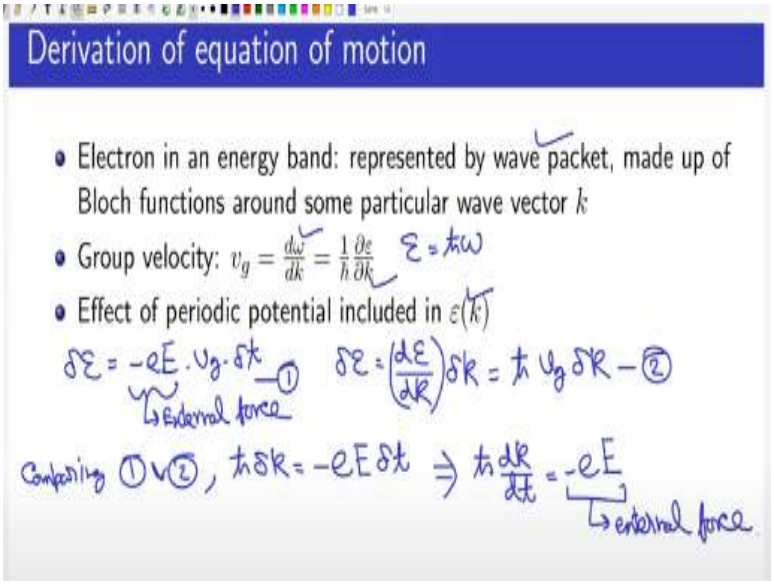
Energy of free electrons is a quadratic function of k, in case of block electrons for a given band index n e, n k is the energy but e n k has no simple explicit form. We have to solve time independent Schrodinger equation to get e n of k velocity of free electron is momenta divided by mass. In terms of energy dispersion relation it can be written as 1 by h bar del e del k. In case of block electrons energy depends on k as well as the band index can as shown here.

Thus velocity also depends on both wave vector k and band index n and can be written as v n k =1 by h del n l k del k. Comparing with the free electron equation we just have to add the band index in case of block electrons. Equation of motion for free electron can be obtained by equating rate

of change of momentum given by h bar times dk dt to the Lorentz force, this is directly from Newton's second law of motion.

In case of block electrons velocity v depends on band index and we rewrite the equation of motion as h bar times bk dt = - e e + 1 by c v n k cross b. Where; v n k is the velocity of block electron with wave vector k, and band index n given by this equation. Again comparing with the free electron equation of motion we just need to add the band index n to get the equation of motion for block electrons.

(Refer Slide Time: 13:24)



We got the equation of motion of electron in an energy band by doing minor changes to the free electron equation of motion. Let me show you a simple derivation of equation of motion for band electrons. This will also help us to understand the difference between free electrons and band electrons equation of motion which look so similar. Electron in an energy bank can be represented by a wave packet, made up of block functions around some particular wave vector k.

Let me show a simple 1d case by considering external electric field only extension to external magnetic field is straightforward. Group velocity of the wave packet is given by vg = d omega dk. And since e = h bar times omega we can write group velocity as 1 by h bar del v del k. Effect of periodic potential is included in energy dispersion relation e of k we can ignore band index for this particular derivation.

Say we apply some external electric field e work done by external electric field on the electron is given by

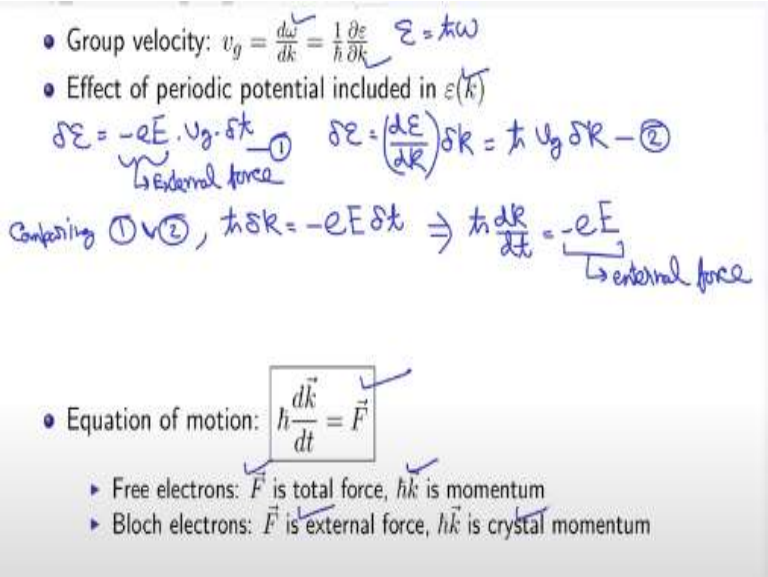
$\delta\varepsilon = -eEU_g\delta t$ (1)

Where small e is the charge of the electron E is the electric field vg is the group velocity and t is time note that $-eE$ is the external force. Now we can just write

$\delta\varepsilon = \frac{d\varepsilon}{dk}\delta k = \hbar v_g \delta k$ (2)

Now comparing 1 and 2 we get $\hbar\delta k = -eE\delta t$. And from this equation we can write $\hbar\frac{dk}{dt} = -eE$, note that this term is the external force.

(Refer Slide Time: 17:05)



Now I revert back to the 3d and write the equation of motion in this form, this equation has the same form for free electrons and electrons in an energy band. However there is a significant difference in case of free electrons f is the total force, and h bar k is the momentum. On the other hand in case of electrons in an energy band f is the external force and h bar k is the crystal momentum. Effect; of force on electrons due to the ions are included in the energy dispersion relation.

(Refer Slide Time: 17:51)

- Equation of motion:
  - $\frac{d\vec{r}}{dt} = \vec{v}_n(\vec{k}) = \frac{1}{\hbar}\frac{\partial \varepsilon_n(\vec{k})}{\partial \vec{k}}$
  - $\hbar\frac{d\vec{k}}{dt} = -e\left[\vec{E}(\vec{r},t) + \frac{1}{c}\vec{v}_n(\vec{k}) \times \vec{B}(\vec{r},t)\right]$
- Input: energy dispersion relation $\varepsilon_n(\vec{k})$, $\vec{E}(\vec{r},t)$ and $\vec{B}(\vec{r},t)$
  - $\vec{E}(\vec{r},t)$: externally applied electric field, field due to ions not included
  - Field due to ions incorporated in $\varepsilon_n(\vec{k})$, because periodic potential U is taken into account while solving for $\varepsilon_n(\vec{k})$
- An electron is described by a wave packet and it has (a) mean position $\vec{r}$, (b) mean wave vector $\vec{k}$ and (c) band index n
- Semi-classical model predicts how these three quantities change in the presence of external electric and magnetic field
  - Band index n: a constant of motion (ignore inter-band transition)
  - Time evolution of position and wave vector of an electron with a band index n given by two equations mentioned above

Now we know the equations of motion of the semi classical model. These equations look very similar to the free electron equations, only difference is we have to use actual energy dispersion for block electrons instead of free electron e k parabola. Let us focus on finer details of the semi-classical model. First let us understand what are the inputs to the model, we have to provide the energy dispersion relation e n k.

The model takes e n k as a given function and does not tell anything about how to compute them. The purpose of the model is to relate the band structure to the transport properties, using the semi-classical model one can get transport properties from a given band structure. One can also deduce features of the band structure from the observed transport properties using semi-classical model. Other than the energy dispersion semi-classical model requires two more inputs external electric field e, and external magnetic field b.

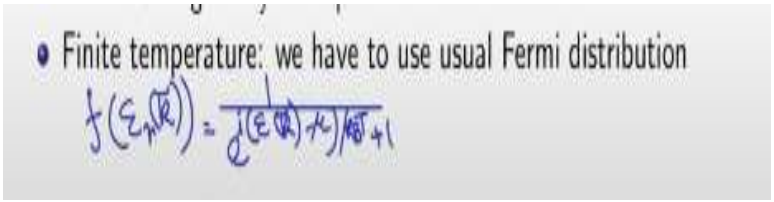
Note that there is some electric field because of the ions also however electric field due to the ions are not included in E. Fields due to the ions are already incorporated in energy dispersion e and k because we took into account the effect of periodic potential u y solving for n k. Thus all the effects of periodic potential is contained in the energy dispersion relation and semi-classical model has no other explicit information about the periodic potential of the ions.

An electron is described by a wave packet and it has a mean position r mean wave vector k and band index n. I call it mean position and mean wave vector because a wave packet has some spread

in real as well as wave vector space, as it has to satisfy Heisenberg uncertainty principle. Semi-classical model predicts how these three quantities are k and n change in the presence of external electric and magnetic field.

That index n is a constant of motion semi-classical model ignores possibility of any inter band transition. Time evolution of position and wave vector of an electron with a band index n is given by 2 equations mentioned here.

(Refer Slide Time: 21:05)

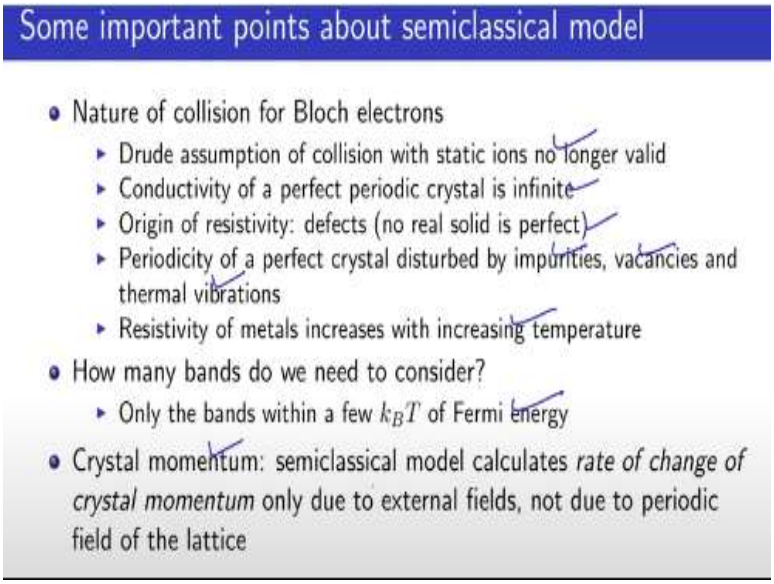


Effect of finite temperature can be incorporated by fermi distribution the same way we did for free electrons. Fermi distribution is given by

$$f\left(\varepsilon\left(\vec{k}\right)\right) = e^{1/(i(\varepsilon(\vec{k})-\mu)/k_B T+1)}$$

f e k = 1 divided by e power i e k – mu. Where mu is the chemical potential divided by k b t, kb is Boltzmann constant and t is temperature + 1, this is same as the case of a free electron. Now since these are block electrons we have to add the band index n.

(Refer Slide Time: 22:04)



Let us discuss about few more subtle points in semi-classical model, the first question that comes to our mind is what is the nature of collisions for block electrons. Assumed that electrons collide with heavy ionic cores, this is no longer valid for block electrons. Anyway it is difficult to justify electron iron collision based on the experimental fact that mean free path in metals is very large, much larger than inter atomic distance.

Block theory discards electron ion collision on theoretical ground as well, since block levels are stationary solution of Schrodinger equation in presence of periodic potential. If an electron in some block state has a non-zero velocity then that velocity will persist forever. Interactions of the electron with ions have already been taken care while solving the type independent Schrodinger equation; thus we cannot consider electronical collision anymore.

This leads to the conclusion that conductivity of a perfect crystal is infinite. Waves can propagate in a perfectly periodic lattice without attenuation, however if perfect periodicity is disrupted somehow then there is a problem. Electrical resistivity we observe in metals is because of defects, which disrupts the perfect periodicity. A defect can appear in the form of some impurity atom or in the form of some missing atom known as vacancies.

Even if we manage to eliminate effects completely by very careful processing technique still there will be thermal vibration induced distortions from the perfect periodicity. At finite temperature atoms by debt about their mean position in the lattice, this leads to disruption of perfect periodicity of the lattice, and this is why resistivity of metals increases with increasing temperature.

Next question is how many bands do, we need to consider in semi-classical model at p equal to 0 kelvin all the states above the fermi energy are vacant, even at finite temperature states with energy many cavity above the fermi energy remains unoccupied. Thus we need to consider only those bands having energies within a few k b t of fermi energy. Note that semi-classical model calculates rate of change of crystal momentum only due to external fields, not due to the periodic field of the lattice the effect of periodic field is embedded in energy dispersion regulation.