Electronic Properties of the Materials: Computational Approach
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Module No # 06
Lecture No # 30
Semi classical Electron Dynamics: Part 2

Hello friends in this lecture we are going to continue our discussion on semi-classical electron dynamics. I already have introduced the main concepts and derived the equations of motion, in this lecture I am going to discuss about the limits of validity of semi-classical model.

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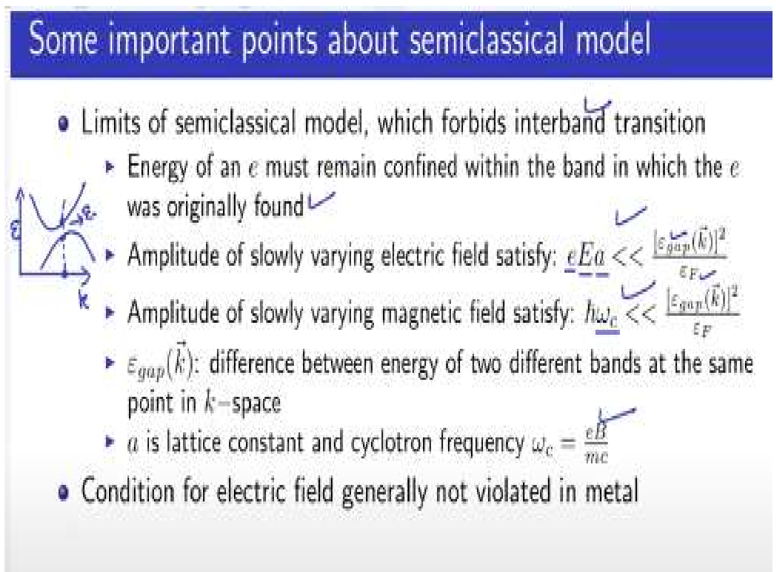

Let me describe the limits in which we can apply semi-classical model to describe dynamics of band electrons. In case of free electrons kinetic energy can increase continuously in uniform electric field. However keep in mind that semi-classical model for this inter band transition, thus energy of an electron must remain confined within the band in which the electron was originally found.

This can be ensured only if there is some gap between 2 bands at a given k value. For a particular value of k semi classical equations of motion for a band electron in the nth band remains valid provided the amplitude of the slowly varying electric field satisfies this condition and the amplitude of the slowly varying magnetic field satisfies this condition. Small e is the charge of electron, E is the amplitude of the electric field and small a is the lattice constant.

Omega c is the cyclotron frequency which is related to the external magnetic field strength d, e f is the fermi energy. Let me explain the term e gap; this is the difference between 2 adjacent bands at the same point in k space. For example let me draw 2 bands vertical axis is energy, and horizontal axis is wave vector, now the 2 bands are like this. Let us take a key point let us say here, energy gap between the 2 bands at this k point is equal to e gap.

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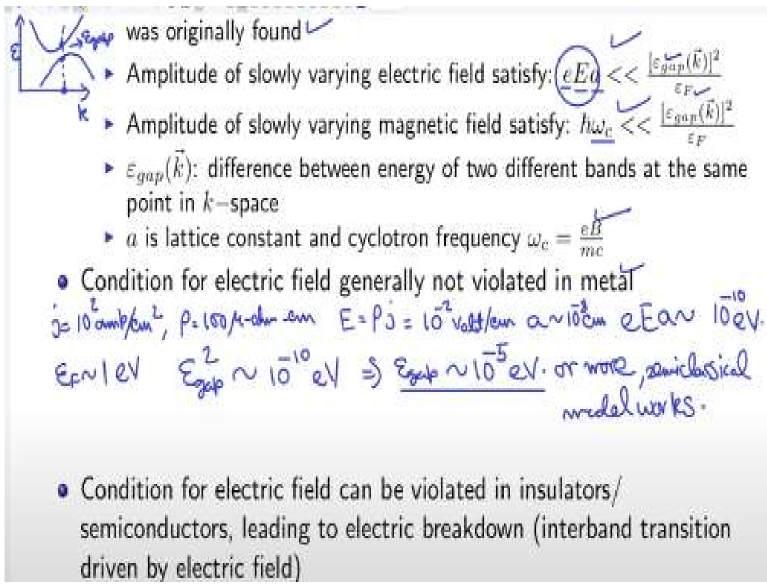

Let me prove that condition for electric field is not generally violated in a metal. Assumer current density j equal to 10 power 2 ampere per centimeter square and let us assume relatively large resistivity rho equal to 100 micro ohm centimeter. Thus the electric field strength e is equals to rho times j which is equal to 10 power - 2 volt but centimeter. Now a is of the order of 10 power - 8 centimeter in that case the quantity in the left hand side is equal to 10 power - 10 electron voltage.

Now fermi energy f is of the order of 1 electron volt then we can write e gap square is of the order of 10 power - 10 electron volt. Which implies that e gap is of the order of 10 power - 5 electron volt. Thus as long as e gap is 10 power - 5 electron volt or more it is safe to apply semi-classical model. Typical gap between 2 bands at a given k point in a metal is of the order of 10 power - 1 electron volt which is much larger than this limit, thus we can safely use semi-classical model for metals.

However in an insulator or semiconductor we can apply very large electric field, in that case condition for electric field is violated and we get external field induced internet transition this is known as electric breakdown.

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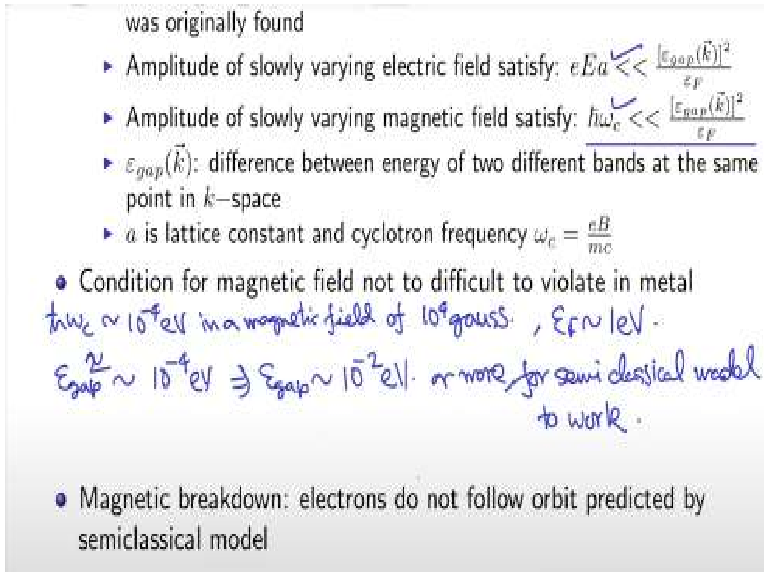

Now let me show that condition for magnetic field is not too difficult to be violated in a typical metal. Energy h cross omega c is cop the order of 10 power - 4 electron volt in r magnetic field of 10 power 4 gauss. Fermi energy is of the order of 1 electron volt thus from this equation we can write e gap square is of the order of 10 power - 4 electron volt which implies that e gap is of the order of 10 power - 2 electron volt.

Thus for semi-classical model to work gap between 2 bands at a given k point must be 10 power - 2 electron volt or more. Note that gap needed for electric field to satisfy this equation was only 10 power - 5 electron volt; thus in case of magnetic field gap needed between 2 bands for semi-classical model to remain valid is much higher.

A gap of less than 10 power - 2 electron volt between 2 bands at a k point in a metal is not very uncommon. If this condition fails then electron makes inter band transition and do not follow orbit predicted by semi-classical model this is known as magnetic breakdown.

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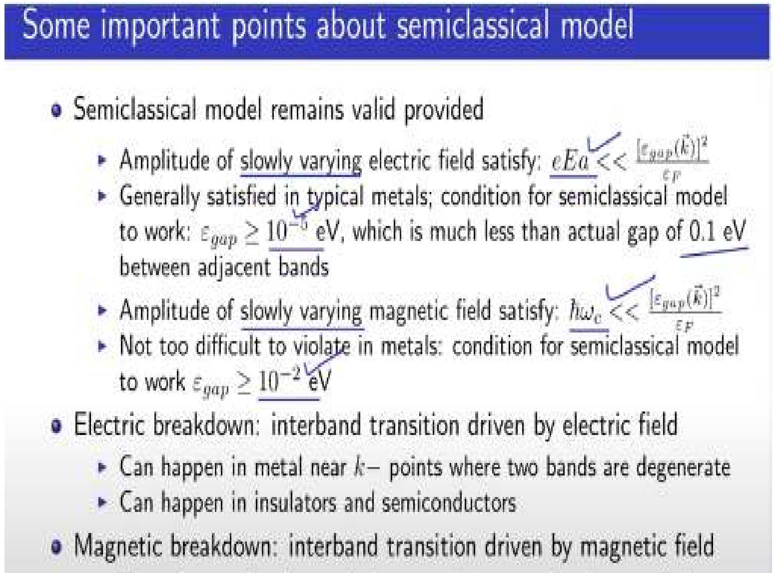

(refer time: 08:07) let me summarize the limits of validity of semi-classical model. Amplitude of the slowly varying electric field must satisfy this condition by slowly varying i mean that wavelength of the electric field is much higher than the spread of the wave packet which describes the electron. For a typical metal left hand side of the equation is 10 power - 10 electron volt and fermi energy is of the order of 1 electron volt.

Thus if the gap between successive bands at a given k point is more than 10 power - 5 electron volt we can apply semi classical model. Typically in a metal gap between 2 successive bands that are given k point is 0.1, electron volt. Thus we can safely apply semi-classical dynamics in case of a metal under some external electric field.

Amplitude of the slowly varying magnetic field must satisfy this condition again by slowly varying i mean the wavelength of the applied magnetic field is much larger than the spread of the wave packet that describes the electron. Each part omega c where omega c is the cyclotron frequency is of the order of 10 power - 4 electron volt in a field of 10 power 4 gauss and fermi energies of the order of 1 electron volt in a metal.

Thus gap between 2 adjacent bands has to be 10 power - 2 electron volt for semi classical model to be valid. Note that the gap needed for validity of the semi-classical model for magnetic field is much larger than that of electric field. Thus we have to be more careful about the validity of the semi-classical model where we are apply external magnetic field.

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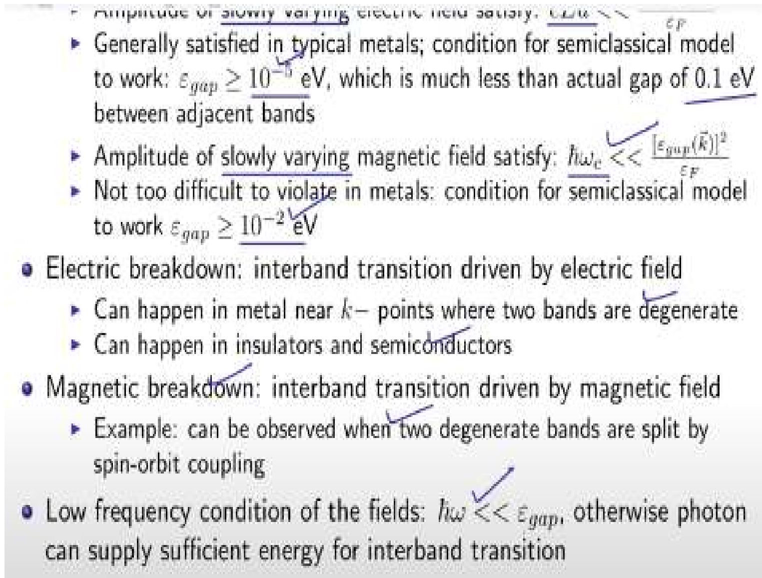

Electric breakdown is a phenomenon which leads to inter band transition driven by electric field. In case of electric breakdown we can no longer apply semi-classical dynamics. This can happen in metals near k points where 2 bands are degenerate, such that the gap between, 2 bands fall below 10 power - 5 electron volt. In case of insulators or semiconductors electric breakdown can happen if we apply very large electric field.

Magnetic breakdown is a phenomena which leads to intervene transition driven by external magnetic field. In case of magnetic breakdown semi-classical dynamics does not work and electrons do not follow orbit predicted by semi-classical dynamics. Magnetic breakdown is more often observed in metals than electric breakdown, because gap between adjacent energy bands should be more than 10 power - 2 electron volt to stop magnetic breakdown.

However gap between adjacent bands can fall below 10 power - 2 electron volt in case of 2 degenerate bands split by spin orbit coupling. In addition to the conditions on the amplitude of the applied electric and magnetic fields we also have to add a low frequency condition on the fields. Such that h bar omega is much less than e gap otherwise a single photon can supply sufficient energy to produce an inter band transition.

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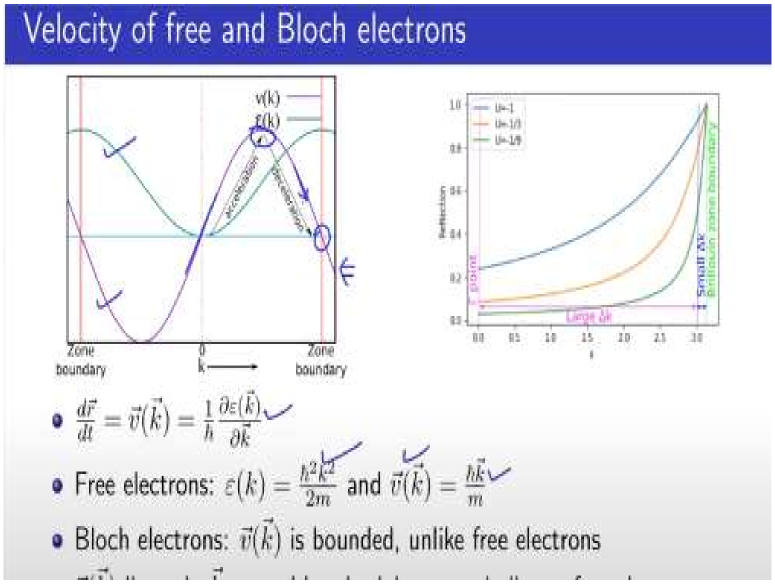

Let us compare the velocity of block and free electrons velocity is given by the first derivative of energy. In case of free electrons energy dispersion relation is h cross square, k square by 2m, and as a result velocity is h cross k divided by m. Thus in case of free electrons velocity increases linearly with k. Let us see what happens in case of block electrons, i am going to consider a simple 1d case which is sufficient to explain the most important concepts.

This is how the energy dispersion relation looks like in case of block electrons. First derivative of e k curve is the velocity of block electrons plotted as a function of k, in this figure. Note that unlike free electrons velocity of block electrons have some upper and lower bound. Interestingly near the band minimum velocity is linear in k which is similar to the free electrons.

For example in this region velocity of block electrons appears similar to velocity of free electrons and increases linearly with k. It attains a maximum value in this region and then it starts to decrease and drops to 0 at the zone boundary. This implies that between maximum of v and zone boundary velocity decreases with increasing k. This is exactly opposite to the case of free electrons where velocity always increases with increasing k.

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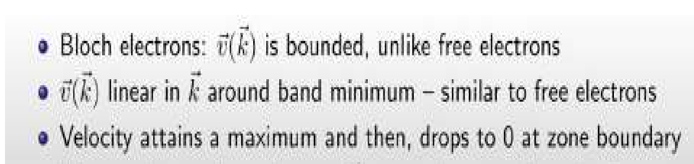

Why does that electron slow down near the zone boundary this is related to brag reflection as k approaches zone boundary the electron is increasingly likely to be drag reflected back in the opposite direction. This is the plot showing reflection increases in a periodic potential as k approaches the zone boundary. Note that how the model is taken into account additional forces other than the external field exerted by the periodic potential. Although it is not explicit in the semi-classical model but it is included in energy dispersion relation.

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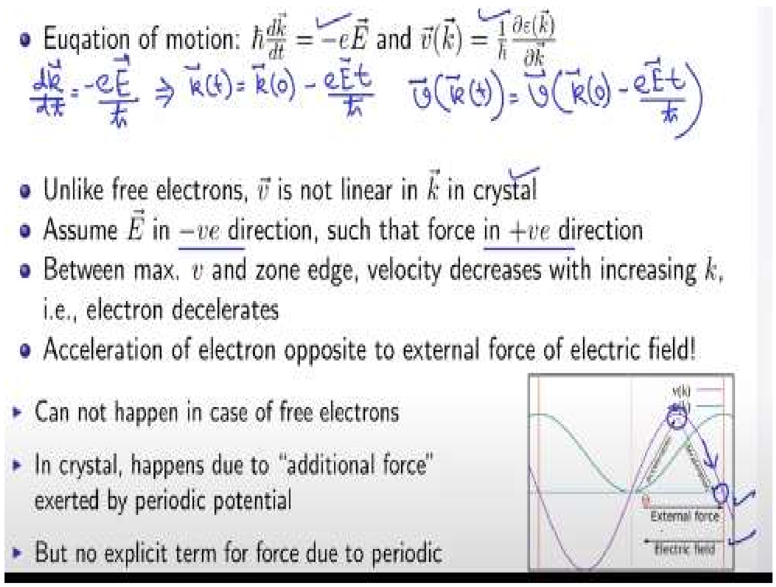

Let us now solve motion of a block electron in dc electric field using semi-classical equations of motion. We rewrite the first equation as d k, d t = to - e times e divided by h bar; where small e is the charge of electron and E is the electric field. And solving this equation we can write k of t = k at 0 - e E t by h by. Thus velocity at time p is given by v of k at time t = v of k at time 0 - e e t by h bar, unlike free electrons v is not linear in k in a free star.

Now let us assume that e is applied in the negative direction such that the force is in the positive direction as shown in this figure. Between maximum of v and the zone boundary velocity decreases with increasing k that is the electron decelerates in this region. This implies that acceleration of the electron is opposite to the external force of electric field.

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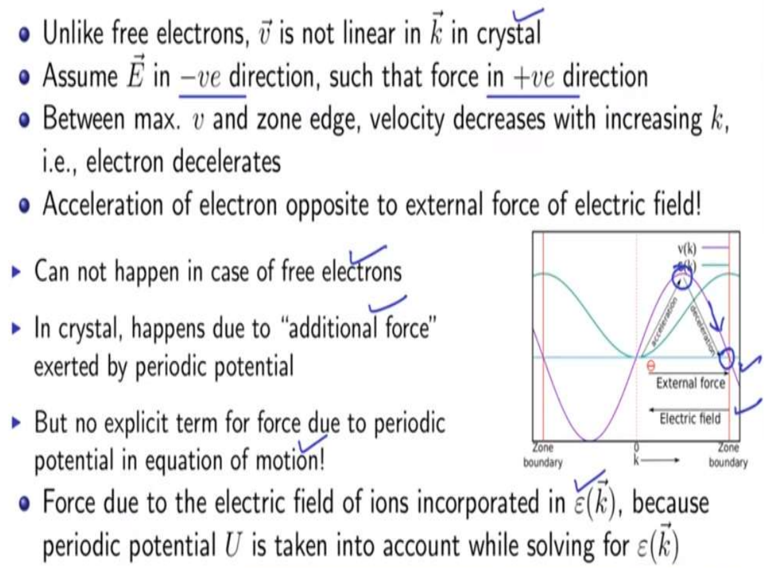

Such a thing cannot happen in case of free electrons, in crystal this happens due to additional force exerted by the periodic potential. But remember that there is no explicit term for force due to periodic potential in equation of motion. Force due to the electric field of ions is incorporated in the energy dispersion, because periodic potential u is already taken into account while solving the time independent Schrodinger equation to get the energies of block electrons.

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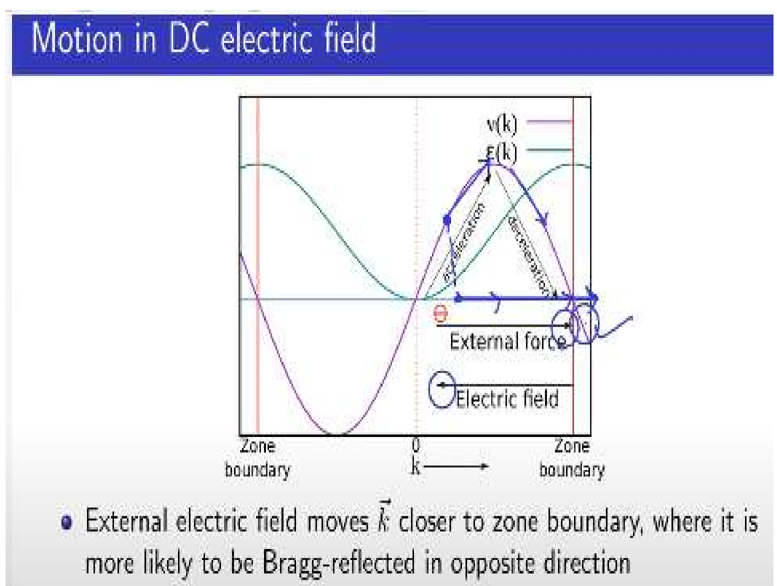

In principle we can find some extraordinary phenomena in case of electron in a periodic potential remember that we have applied a dc field in this direction, such that electrons experience a force in the opposite direction. Say the electron has an initial k somewhere here and the corresponding velocity is this because of the external field k starts to change in this direction. As a result velocity increases initially it reaches a maximum value and then it starts decreasing in this region.

Finally as the value of k reaches the zone boundary the velocity becomes 0, if k changes further then the velocity becomes negative in this region. This implies that the electron is moving in the opposite direction and as a result direction of current also reverses, however keep in mind that we have applied a dc field.

Thus if an electron can manage to travel a distance in k space which is more than the dimension of the zone boundary then we can actually get an alternating current in a dc field, this is known as block oscillation. Such an extraordinary phenomenon can never happen for free electrons.

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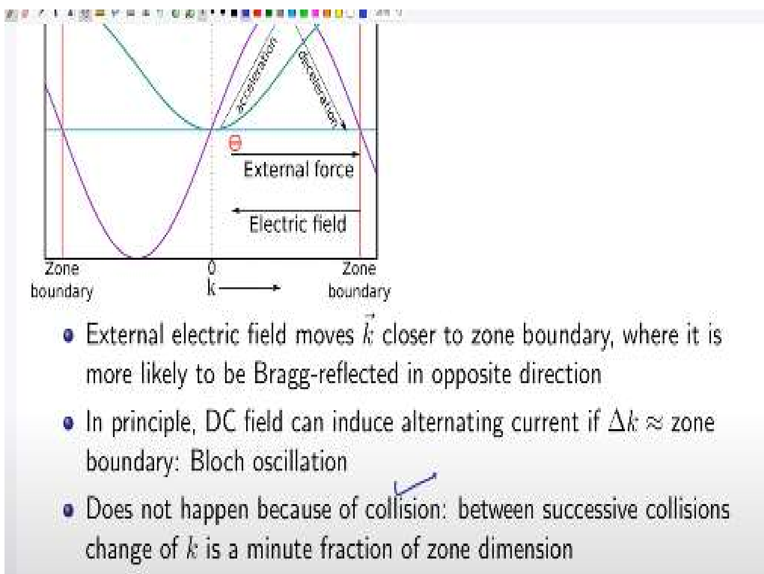

However; block oscillation is not observed experimentally because of collision or scattering. The change of wave vector between 2 collision is only a small fraction of the zone dimension the electron will be scattered much before the change of k due to the electric field becomes equivalent to the zone dimension. Remember that semi-classical model does not discard collision or scattering.

The only difference between Drude model and semi-classical electron dynamics model is the nature of pollution in Drude model electrons collide with heavy ions. In semi-classical model wave packets get scattered as there are defects in the crystal which destroys perfect periodicity of a lattice. Even if you manage to prepare a defect free crystal thermal vibrations of atoms about their mean position in a lattice can disrupt perfect periodicity leading to the scattering of electron wave packets.

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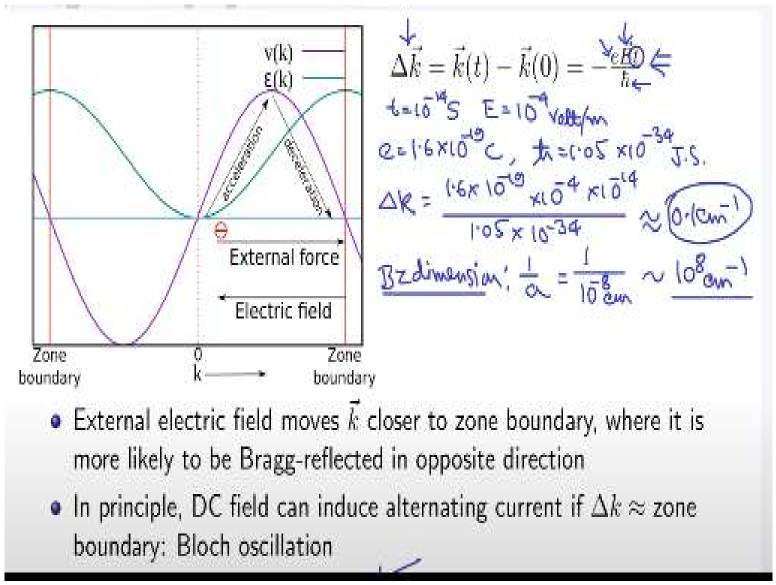

Let me prove that change of k between 2 collisions is very small compared to the zone dimension. In order to do this we have to estimate the change of k between 2 scattering events this is how k changes as we apply an external electric field. E is the charge of electron which is a fundamental constant and h bar is the reduced plan's constant. However, t it is known experimentally that time between 2; collision is of the order of 10 power - 14 second.

Let us assume the electric field strength to be 10 power - 4 volt per meter charge of electron is 1.6 into 10 power - 19 Coulomb reduced lungs constant is 1.05 into 10 power - 34 joule second. Putting all these values in this equation we get the magnitude of delta k which is equal to; and this turns out to be approximately equal to 0.1 centimeter inverse. Now Brillouin zone dimension is inverse of the lattice parameter and lattice parameter is of the order of 1 angstrom which is 10 power - 8 centimeter.

Thus Brillouin zone dimension is of the order of 10 power 8 centimeter inverse. Thus change of delta k is really small then compared to the zone dimension and we do not see block oscillations experimentally for this reason.