Electronic Properties of the Material: Computational Approach
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Module No # 07
Lecture No # 32
Concept of Effective Mass

Hello, friends in this lecture, I already discussed the concept of hole in a periodic potential electron. Sometimes we have in a way as if it has a positive charge, which is termed as a whole. In this lecture, I am going to introduce another important concept; concept of effective mass.

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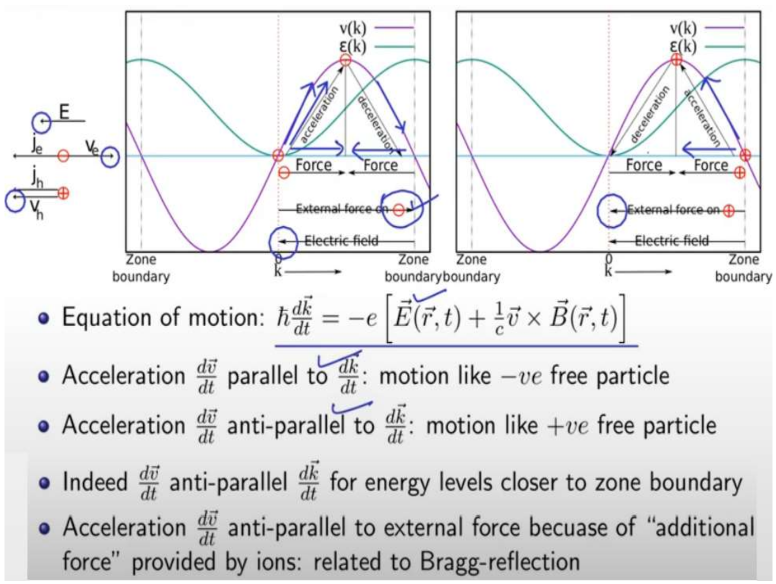

Let me start with a brief summary of electrons and holes say the electric field is in this direction. Since electrons are negatively charged, electrons will move in a direction opposite to the direction of the electric field. On the other hand since holes are positively charged, holes will move in a direction parallel to the electric field, however direction of current remains the same.

The motion of an electron is determined by the semi-classical equation of motion. Let us consider only electric field. Since the external electric field is in the negative direction, k is going to increase in the positive direction with time. There are 2 possible scenarios first one is velocity increasing as k increases. In this case, acceleration d v d t is parallel to d k d t. This is exactly what you would expect for a negatively charged free particle to accelerate in the direction of an external force.

This is the direction of external force on a negatively charged particle, which is same as the direction of acceleration in this region. A second possible scenario is velocity decreasing with increasing k. In this case, the electron decelerates in other words, acceleration is anti-parallel to d k d t. This is a rather strained situation where acceleration is the opposite of the external force. This is the direction of external force on a negatively charged particle and the direction of acceleration is the opposite of the external force in this region.

Let us try to understand the case of acceleration anti-parallel to d k d t. Instead of a negatively charged particle, if we consider a positively charged particle, this is what we would expect the particle to accelerate in the direction of the external electric field. As shown in this figure this is the direction of external force on a positively charged particle, and in this region acceleration is parallel to the direction of external force for a positively charged particle.

Thus, in this region, which is closer to the zone Center, we can describe the motion in the electric field as the motion of a negatively charged particle or electron. And in this region, which is closer to the zone boundary; we can describe the motion in the electric field as the motion of a positively charged particle or hole. However, keep in mind that positively charged holes are fictitious particles. We have introduced the idea for our convenience.

In reality, the acceleration of electrons is anti-parallel to the external force because the lattice provides some additional force which is associated with back reflection. Note that in this region, because the net force on electron is parallel to the external force due to the electric field and the electron accelerates in this region. However, in this region the net force on the electron is parallel to the external force due to the electric field and the result it decelerates.

However, instead of considering the motion of a negatively charged particle, if we consider the motion of a positively charged particle in an electric field. Then in this region the net force on whole is parallel to the external force. Thus instead of deceleration of electrons, we can equivalently represent this as acceleration of positively charged holes whether we prefer electron description or a whole description depends on our convenience.

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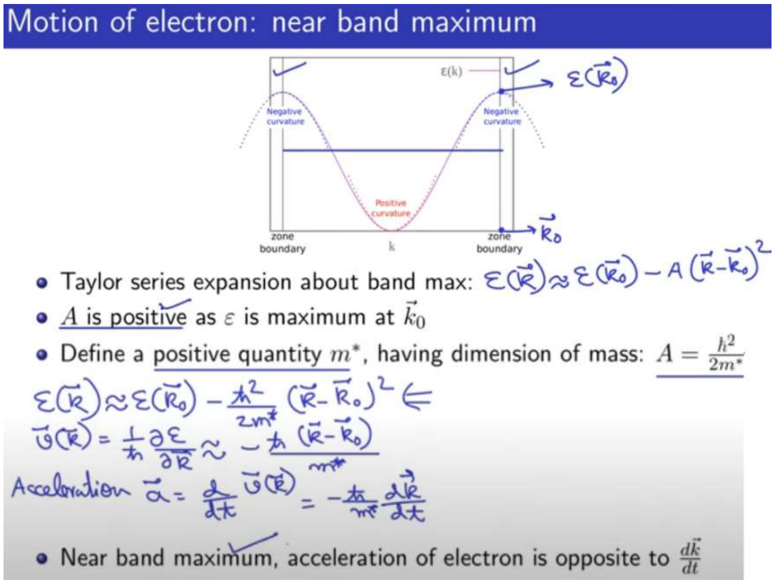

Let us discuss the motion of electrons near the band's maximum unoccupied levels, which lie near the top of the band. We do not know what the exact form of E k or energy dispersion. All we know is that E k is maximum at some point k naught, so this is the point k naught, and energy is maximum at this point. Now, we expand E k about the maximum point using Taylor series expansion.

So, this is energy as a function of K, which is approximately = E k naught. This is the energy maximum, and as we go away from this k naught, we just assume that the energy is decreasing quadratically. The linear term vanishes as we are expanding about the maximum point, and the first derivative of e k has to be equal to 0. Moreover since E k is maximum at naught, a; has to be positive. We define a positive quantity m star having a dimension of mass and we write a = h cross square divided by 2 m star.

Thus, we can rewrite this equation as E k is approximately equal to E k naught -h cross Square by 2m star k-k0 whole Square.

$$\varepsilon(\vec{k}) \approx \varepsilon(\overrightarrow{k_0}) - \frac{\hbar}{2m^*}\left(\vec{k} - \overrightarrow{k_0}\right)^2$$

Now we calculate the first derivative of e with respect to k to get the velocity v of k =1 by the h cross first derivative of energy with respect to k and from this equation we have -h cross square k-k naught divided by m star.

$$\text{Acceleration } \vec{a} = \frac{d\vec{k}}{dt} = -\frac{\hbar}{m^*}\frac{d\vec{k}}{dt}$$

And we can write acceleration a = d, d t of which is equal to -h bar divided by m star K naught is a constant, so we just have B k d t. Thus, near the band, maximum acceleration is opposite to B k d t.

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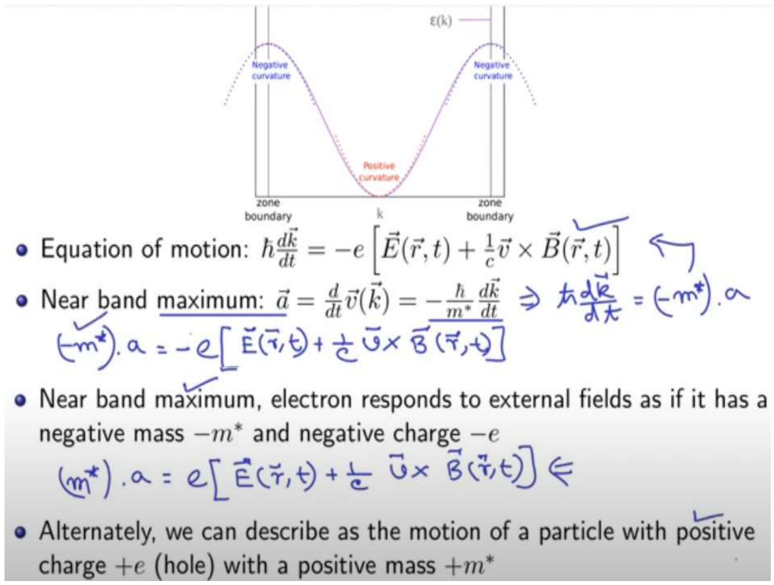

This is the semi-classical equation of motion. We have found that near band maximum the acceleration can be written as this and we can rewrite this as h cross d k d t = m star times a. Now we put it in this equation and we get - m star times a is equal to the force, thus near band maximum electrons response to external fields as if it has a negative mass of -m star and a negative charge of -e.

Now we can cancel the negative sign from both sides of the equation and write this as m star times a, = E times electric field + 1 by c v cross B. This equation is an alternate way of describing the previous equation. However, we are describing the motion of a particle with positive charge or whole with a positive mass m star.

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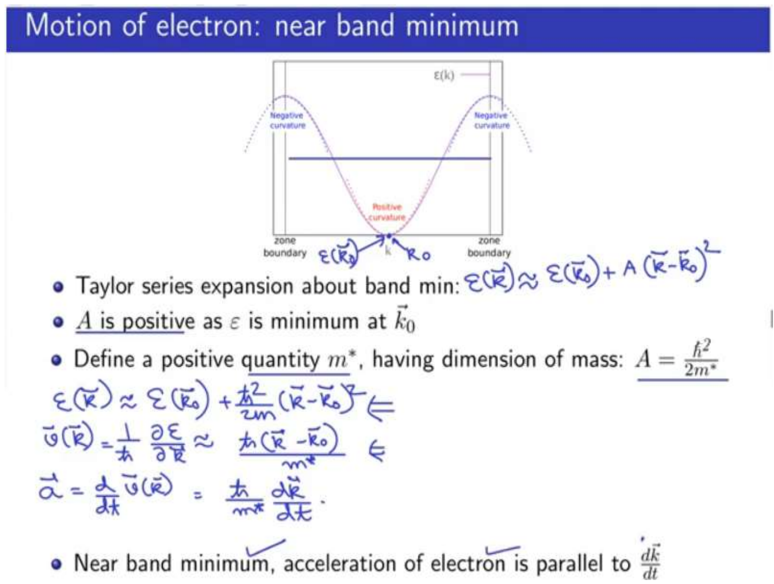

Now let us discuss the motion of electrons near band minimum. Thus previously, what we did was relevant for unoccupied levels, but now what we are going to do is relevant for occupied levels. We do not know what is the exact form of E k is. All we know is that E k is minimum at some point k naught, so this is the point k nught and E k naught is minimum at this point as we did before. We expand E of k about the minimum point k naught using Taylor series expansion,

So we write E k as E k naught, so this is the minimum energy and as we go away from the point k naught, energy increases quadratically. The linear term vanishes as we are expanding about a minimum point and the first derivative has to vanish moreover since E of k is minimum at k naught, a, has to be positive. Now we define a positive quantity m Star, which has a dimension of mass and right a = h cross Square divided by 2 times by replacing this in this equation,

We get E of k is E of k naught + h + square by 12 k-k naught whole Square. Now we calculate first derivative of e with respect to k to get the velocity. Velocity d of k is 1 by h Bar times the first derivative of E with respect to k, which is approximately = h cross k - k naught divided by m star. Now we derive the acceleration, which is equal to d, d t of v, by using this equation. We can write it as h bar by m star d k d t, thus near the band minimum acceleration of electron is parallel to d k d t.

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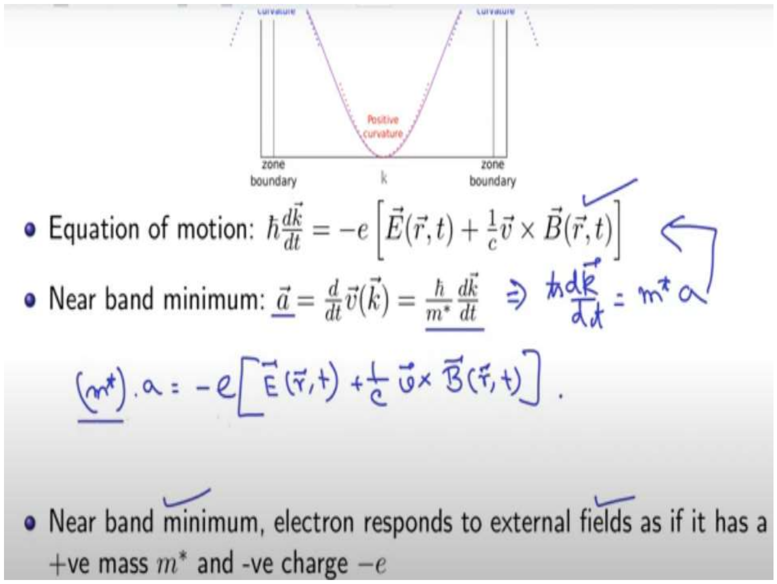

This is the semi-classical equation of motion. We have found that near band minimum acceleration can be written as h bar divided by m star times d k d t and we just rewrite this as h bar d k d t = m star times a. Replacing this in equation of motion we get m star times a = -e times the electric field +1 by c B cross your magnetic field. So near the band minimum electron responds to external field as if it has a positive mass m star and a negative charge – e.

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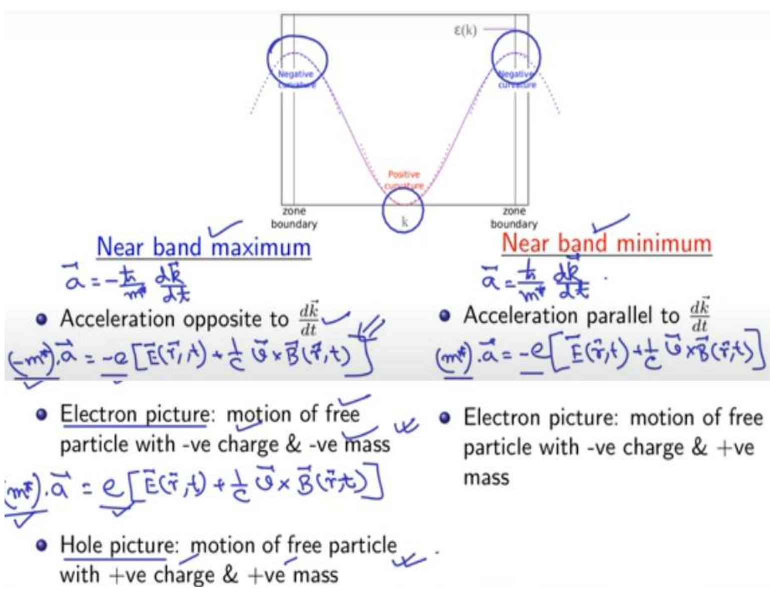

Let me quickly summaries' what I have done so far. In the case of free electrons, if we apply some external field, the acceleration is parallel to d k d t. However, in the case of block electrons, this is not necessarily true. If we look at a region near the band minimum that is in this region then it is very similar to the free electron picture. The acceleration is parallel to d k d t and we can write a = h bar by m star d k d t.

In this case, the equation of motion is m star, which has a dimension of mass times acceleration, is equal to external force. This looks like the motion of a free particle with a negative charge and positive mass. Now if we focus on a region near the back maximum, that is in this region and in this region. In this case, the acceleration is opposite to d k d t that is, we can write acceleration is = -h bar divided by m star d k d t where m star is the dimension of mass.

In this case, the equation of motion looks like -m star times acceleration is equals to external force. This looks like the motion of a free particle with a negative charge as well as negative mass. Thus, near the band maximum motion of an electron, this looks like the motion of a free particle with negative charge and a negative mass. However, it is more intuitive to write it as the motion of a free particle with a positive charge and positive mass.

From this equation, we can just cancel the negative sign from both the sides and we can write it as mass times acceleration is equal to e electric field + 1 by c velocity across the magnetic field. This is the motion of a free particle with positive charge and positive mass. Note that in the electron picture, charge remains negative but mass becomes negative. However, in the whole picture, mass remains positive but charge becomes positive near the band maximum we get to use either the electron picture or the whole picture. However, it is more common to use the whole description near the band maximum.

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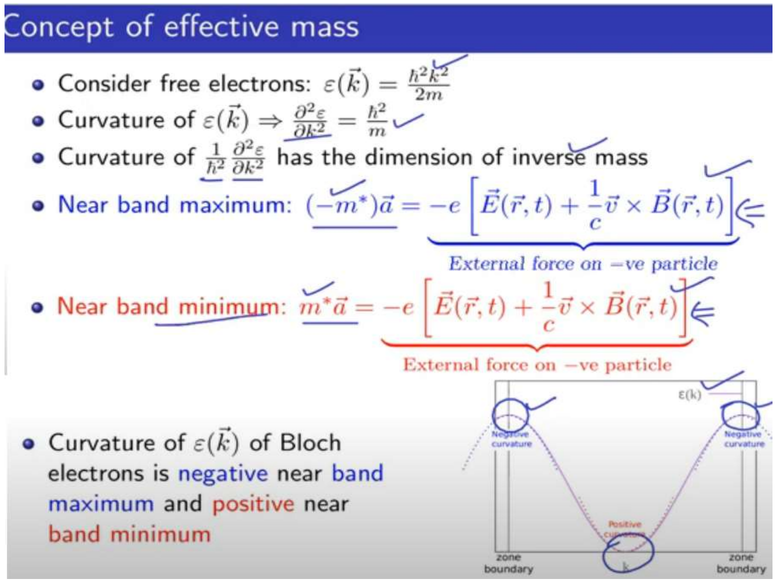

Now let me formally introduce the concept of effective mass. Let us start with the energy dispersion relation of free electrons E k = h cross square a square divided by 2 m. The curvature of E k curve for free electron is equal to h cross square divided by m. The curvature is given by the second derivative of the e k cruve with respect to k, thus 1 by h bar square times. The curvature has the dimension of inverse mass.

We have seen that near the band maximum, the equation of motion of an electron looks like this. The right-hand side is the low range force on a negatively charged particle the left hand side is - m star times acceleration, where m star is a positive number and it has a dimension of mass. Near band maximum it appears from the equation of motion that the mass of the electron is negative near the band minimum.

The equation of motion looks like this: the right hand side of the equation is the lower force on a negatively charged particle. On the left hand side, we have m star times acceleration, where m star is a positive number and it has a dimension of mass. In the case of band minimum m-star of electrons is positive. Now let us look at the E k curve of block electrons. The curvature is negative near the band maximum since the curvature of the E k curve is related to mass.

Negative curvature corresponds to negative effective mass in the case of states near the bank maximum. This agrees very well with the equation of motion near band maximum on the other hand, the curvature of the E k curve is positive near the band minimum, which corresponds to a positive effective mass. This also agrees very well with the equation of motion near the band minimum.

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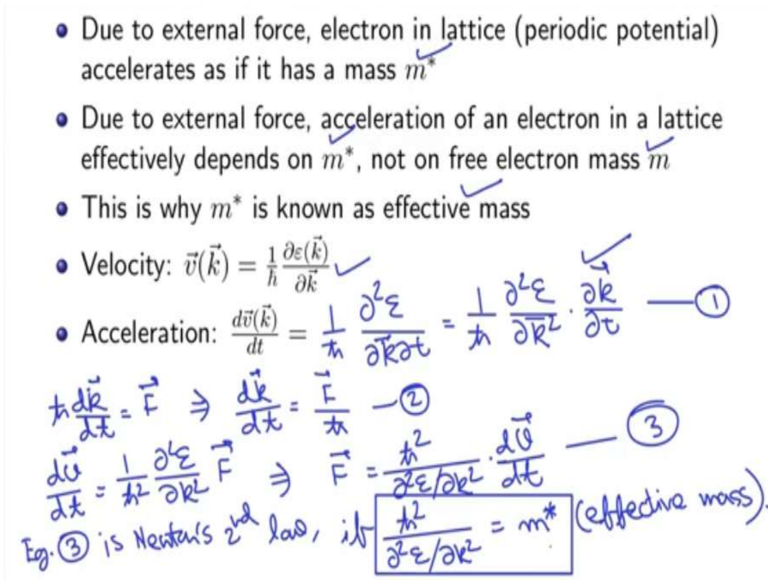

We have already seen the connection between curvature and the m-star of electrons m star has the dimension of mass, and we call it as effective mass. Let me explain why we call it an effective mass electron in a periodic potential accelerating relative to the lattice due to the external field as if the mass of the electron is m-star. Due to external force, the acceleration of an electron in a lattice effectively depends on m star and not on the free electron mass m which is a fundamental constant.

This is why m star is known as the effective mass velocity of an electron, which is the first derivative of energy with respect to gain. Now let us calculate acceleration, which is

$$\frac{d\vec{v}(\vec{k})}{dt} = \frac{1}{\hbar}\frac{\partial\varepsilon}{\partial\vec{k}\partial t} = \frac{1}{\hbar}\frac{\partial^2\varepsilon}{\partial\overrightarrow{k^2}}\frac{\partial\vec{k}}{\partial t} \qquad (1)$$

$$\hbar\frac{d\vec{k}}{dt} = \vec{F} \Rightarrow \frac{d\vec{k}}{dt} = \frac{\vec{F}}{\hbar} \qquad (2)$$

Now, replacing 2 in 1, we can write

$$\frac{d\vec{v}}{dt} = \frac{1}{\hbar^2}\frac{\partial^2\varepsilon}{\partial\overrightarrow{k^2}}\vec{F} \Rightarrow \vec{F} = \frac{\hbar^2}{\partial^2\varepsilon/\partial k^2}\frac{d\vec{v}}{dt} \qquad (3)$$

Note that equation 3 is Newton's second law if h + square divided by del to e del k square has a dimension of mass and this is what we call it as effective mass.

$$\vec{F} = \frac{\hbar^2}{\partial^2 \varepsilon / \partial k^2} = m^* (\text{effective mass})$$

So effective mass is related to the curvature of e k curve if the curvature is negative, as in the case of block electrons near the band maximum. The effective mass of an electron can either be negative in a periodic potential.

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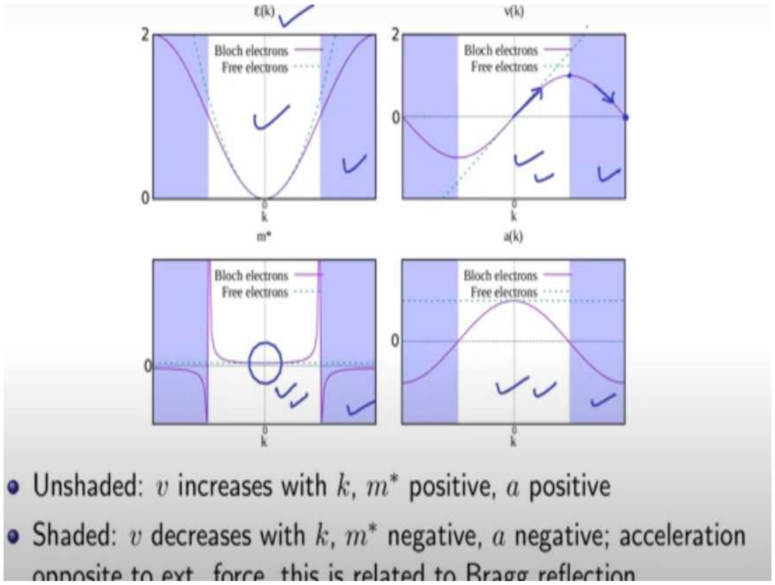

Using a simple E k diagram lets me summaries various concepts discussed so far. The solid line represents the E k curve for block electrons and the dashed line represents the E k curve for free electrons. The curves are drawn only in the possible doing zone. We can see that near the zone center, the E k curves of free and blocked electrons are identical, and the difference becomes prominent as we go away from the zone Center. The same is proof of the velocity. Velocity of block electrons is the same as free electron velocity near the zone Center.

Velocity increases with increasing k it reaches some maximum value and then it decreases and becomes 0 at the zone boundary. In the unshaded region of the first pillow in zone velocity increases with k m star is positive and equal to the free electron mass near the zone center and acceleration is positive. Thus in the unshaded region closer to the zone centered behavior of block electrons is somewhat similar to 3 electrons

On the other hand block electrons differ from free electrons significantly in the Shaded region velocity decreases with k m star is negative and acceleration is negative. That is acceleration is opposite to the external force which is related to the back reflection. In conclusion effect of periodic potential is manifested mainly near the zone boundary while free electron description remains valid near the zone Center.