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Electron dynamics in an Electric field

When an ~~electron~~ electric field is applied to the solid, the electrons in the solid are accelerated. We can study their motions most easily in k-space. Suppose that an electric field $\mathcal{E}$ is applied to a given crystal. As a result, an electron in the crystal experiences a force $F = -e\mathcal{E}$ and hence a change in its energy. The rate of absorption of energy by the electron is

$$\frac{dE(k)}{dt} = -e\mathcal{E}\cdot v \qquad -(1)$$

where the term on the right is the expression for the power absorbed by a moving object. If we write

$$\frac{dE(k)}{dt} = \nabla_k E(k)\cdot\frac{dk}{dt} \qquad -(2)$$

We may write velocity of Bloch electron

$$v = \frac{1}{\hbar}\nabla_k E(k) \qquad -(3)$$

which states that the velocity of an e^- in state k is proportional to the gradient of the energy in k-space. Substituting (3) in (1) we get

$$\hbar\frac{dk}{dt} = -e\mathcal{E} = F \qquad -(4)$$

This shows that the rate of change of k is prop. to Electric force F.

This relation is known as the acceleration theorem.

In a Uniform electric field the semiclassical eq. of motion for k i.e.

$$\dot{r} = v_n(k) = \frac{1}{\hbar}\frac{\partial E_n(k)}{\partial k}$$

has the general solution

$$k(t) = k(0) - \frac{e\mathcal{E}t}{\hbar} \qquad -(5)$$

Thus in a time t every electron changes its ② wave vector by the same amount. This is consistent with our observation that applied fields can have no effect on a filled band in a semiclassical model.

Velocity of an electron at time t will be

$$v(k(t)) = v\left(k(0) - \frac{eEt}{\hbar}\right) \quad \text{— ⑥}$$

where $v(k)$ is periodic in the reciprocal lattice, the velocity is a bounded function of time. The k dependence of the velocity is plotted in one dim.

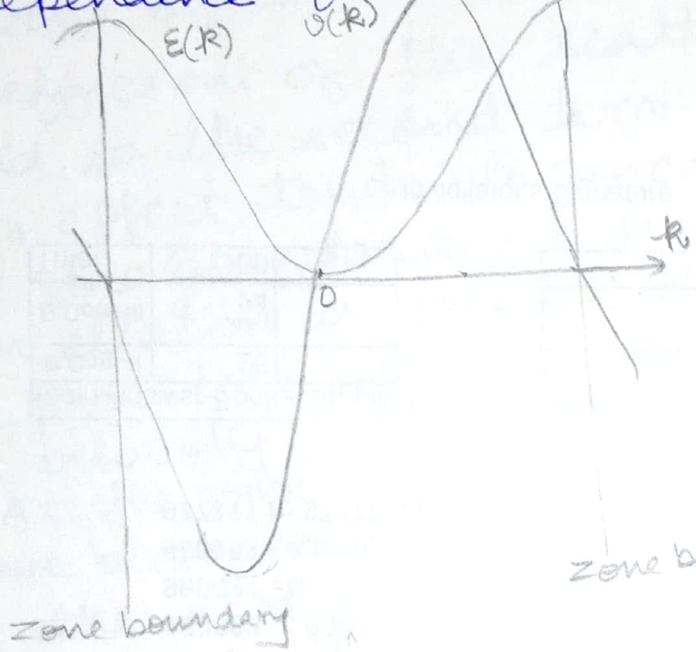

Fig. 1

Figure 1 shows a typical band structure in one dim. via eq. ⑤

we know that

$$v = \frac{1}{\hbar}\frac{\partial E}{\partial k} \quad \text{— ⑦}$$

i.e. velocity is prop. to the slope of the energy curve.

We see that as k varies from the origin to the edge of the zone, the velocity increases at first linearly, reaches a maximum, and then decreases to zero at the edge of the zone. The anomalous behaviour i.e. decrease in the velocity near the edge of the zone can have following explaination :-

Near the zone centre, the e^- may be represented by a single plane wave $\psi_k \sim e^{ikx}$ and hence $v = \frac{\hbar k}{m_0}$, explaining the linear region of fig. 1. However, as k increases, the scattering of the free wave by the lattice introduces a new left-traveling wave whose wave vector $k' = k - \frac{2\pi}{a}$ and which is to be superimposed on the original right traveling wave k.

Therefore, the electron is now represented by the $\psi_k \approx e^{ikx} + b e^{-i(2\pi/a - k)x}$ — (7)

b - coefficient found from perturbation theory -

The velocity of this wave is given by

$$v = \underbrace{\frac{\hbar k}{m_0}}_{\text{Contributions of right traveling wave}} - \underbrace{|b|^2 \frac{\hbar}{m_0}\left(\frac{2\pi}{a} - k\right)}_{\text{contribution of the left traveling wave}} \quad - (8)$$

At small k, the coefficient b is small and v is given by $\hbar k/m_0$. As k increases, however the coefficient of the scattered wave increases, and so the second term of (8) becomes appreciable. Its effect tends to cancel the first term. Near the zone boundaries, b is so large that resulting cancellation is greater than the increase in the first term, which leads to a net decrease in the velocity.

At the zone boundary itself $\left(k = \frac{\pi}{a}\right)$, the scattered wave becomes equal to the incident wave as a result of the strong Bragg reflection i.e. $b = 1$, which when substituted in (8) yields $v = 0$ in agreement with figure.