Dynamics of Electrons in a Crystal Lattice

- we defined a particle as a wave packet
- the uncertainty relation for k and x: $\Delta k \cdot \Delta x \sim 1$
- an electron is localized within the region $\Delta x \sim 1/\Delta k$
- The ψ - function of the electron can be represented in the form of the sum of plane waves of the kind $e^{i\mathbf{kr}}$, which values of wave numbers are within the limits of Δk

•Δk is not great, and the superposition of the plane waves forms a wave packet

$$v_{gr} = \frac{d\omega}{dk}$$

the velocity of an electron in a crystal

- v_{gr} is the velocity of the electron in a crystal. Taking into consideration the equation for energy $E = \hbar\omega$, we find this velocity

$$v_{gr} = \frac{1}{\hbar}\frac{dE}{dk}$$

work

- an electric field is imposed on a crystal, apart from the forces of crystalline lattice *F crystal*, the electron experiences the electric force $F = eE$. During the time dt this force does the work $dA = Fv_{gr}\, dt$ on the electron

$$dA = \frac{F}{\hbar}\frac{dE}{dk}dt$$

energy

- This work provides an increment of the energy of the electron in the crystal; *dA* = *dE*. Taking into account *dE* = (*dE*/*dk*) *dk*, we get

$$\frac{dE}{dk}dk = \frac{F}{\hbar}\frac{dE}{dk}dt$$

whence it follows that

$$\frac{dk}{dt} = \frac{F}{\hbar}$$

acceleration of the electron

$$\frac{dv_{gr}}{dt}\ \frac{1}{\hbar}\frac{d}{dt}\left(\frac{dE}{dk}\right)=\frac{1}{\hbar}\frac{d^2E}{dk^2}\frac{dk}{dt}$$

$$\frac{dv_{gr}}{dt}=\frac{1}{\hbar}\frac{d^2E}{dk^2}\frac{F}{\hbar}$$

$$\left(\frac{\hbar^2}{d^2E/dk^2}\right)\frac{dv_{gr}}{dt}=F$$

effective mass

$$m\frac{dv}{dt} = F$$

we arrive at the conclusion that the expression

$$m^* = \frac{\hbar^2}{d^2E/dk^2}$$

plays the part of the mass with respect to the external force. In this connection, the quantity given by (*4.45) is called the effective mass* of an electron in a crystal.

Behavior of the effective mass

- Near the bottom of the band (see the points *A* and *A'* $m^* \approx m$
- At the point of inflection (point *B) the second derivative of E* is zero. Consequently, *m** becomes infinite.
- Near the ceiling of the allowed band (point *C*), the derivative is *d*2*E/dk*2 < 0