Electrons in bands: Semiclassical Equations

Classical Mechanics (Hamiltonian ≡ Newtonian)

$$\dot{x} = \frac{\partial H(x,p)}{\partial p}$$

$$\Rightarrow \dot{x} = \frac{\partial}{\partial p}\left(\frac{p^2}{2m} + V(x)\right) = \frac{p}{m}$$

$$\dot{p} = -\frac{\partial H(x,p)}{\partial x}$$

$$\Rightarrow \dot{p} = -\frac{\partial}{\partial x}\left(\frac{p^2}{2m} + V(x)\right) = -V'(x) = F$$

Semiclassical Equations for *wavepackets* (electrons in bands)

$$\dot{x} = v = \frac{1}{\hbar}\frac{\partial E_k}{\partial k}$$

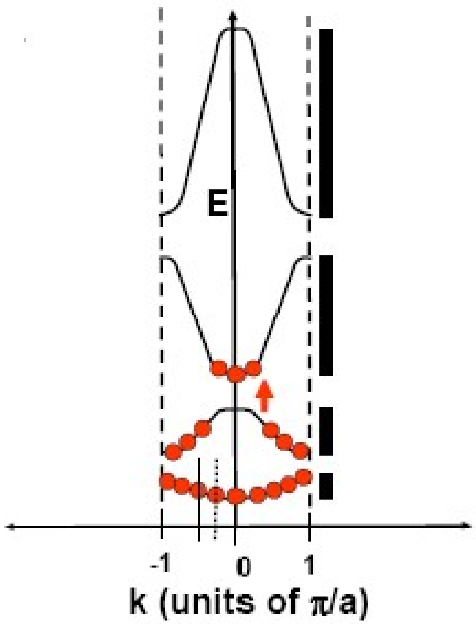
$$\Leftarrow v = \frac{\partial \omega_k}{\partial k}$$

External forces only $\hbar\dot{k} = F_{ext} = -e\mathcal{E}$

Internal forces (ionic potentials) included in E_k

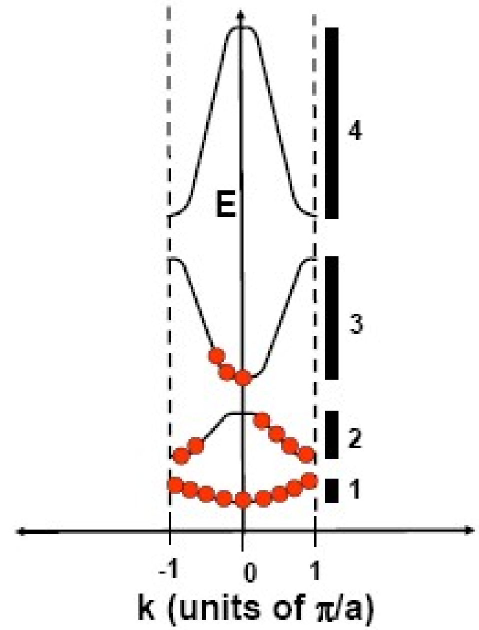
Wavepacket dynamics, no interband transitions
➔ small fields, slowly varying in space and time

Electrons in bands: effective mass



Electrons thermally excited from highest fully-occupied band (@ 0K) to lowest empty band (@ 0K)

Electrons motion under the influence of an external field given by semiclassical equations



$$v = \frac{d\omega}{dk} = \frac{1}{\hbar}\frac{dE}{dk}$$

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

$$F_{ext} = \frac{d\left(\hbar k\right)}{dt} = m^*\frac{dv}{dt}$$

Newton's Second

Effective mass

$$m^* = \left(\frac{1}{\hbar^2}\frac{d^2E}{dk^2}\right)^{-1}$$

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Artwork Sources:

1. en.wikipedia.org
2. iue.tuwien.ac.at
3. Souvik Mahapatra (IITB)