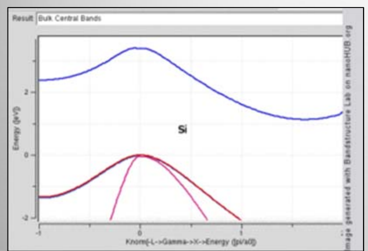
Dr. Gregory W. Clark
Manchester University

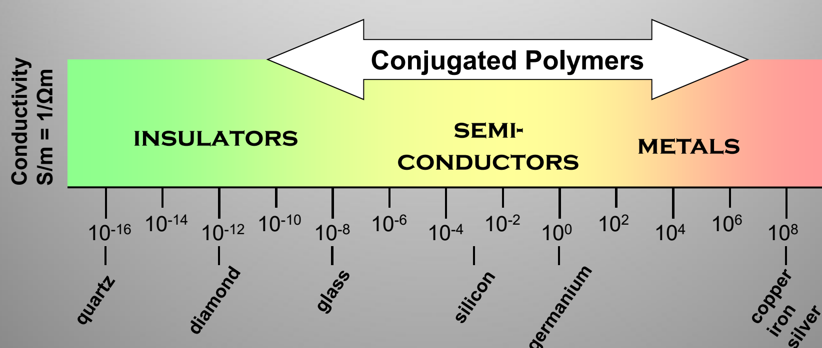


PHYS432

Materials Physics

Electrical conductivity

- Wide range of values!
- Early attempts to model:
  - Drude: free electron gas
  - Sommerfeld: quantum free electron gas



Group Velocity

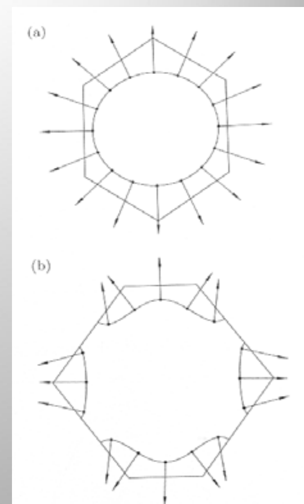
In 1-D: $$v = \frac{d\omega}{dk} = \frac{1}{\hbar}\frac{dE}{dk}$$

$$E = \hbar\omega$$

In 3-D: $$\vec{v} = \frac{1}{\hbar}\vec{\nabla}_k E$$

where

$$\vec{\nabla}_k \equiv \sum_i \hat{e}_i \frac{\partial}{\partial k_i}$$



velocity is perpendicular to Fermi surface

Equation of Motion

$$\vec{F}_{ext} = \frac{d\vec{p}}{dt}$$

- Can relate external forces to wavevector via: $$\vec{F}_{ext} = \hbar\frac{d\vec{k}}{dt}$$
- Can relate acceleration to: $$\vec{a} = \left[\frac{1}{\hbar^2}\frac{d^2E}{dk^2}\right]\vec{F}_{ext}$$
- So that we can define the ***effective mass***: $$m^* = \left[\frac{1}{\hbar^2}\frac{d^2E}{dk^2}\right]^{-1}$$

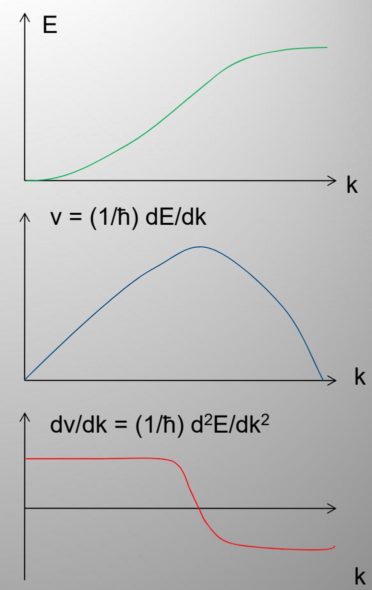
Particle behaves as if has mass m^* in external force

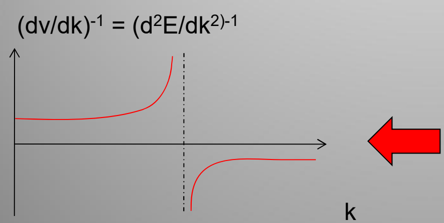
Can discern form experiments involving cyclotron resonance

Effective Mass

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

- Can be + (E vs. k concave up), - (E vs. k concave down) or infinite (inflection points).





Effective Mass

- Frequently negative near FBZ boundary
- An e^- with $m^* < 0$ can be thought of as a hole with $m_p^* > 0$

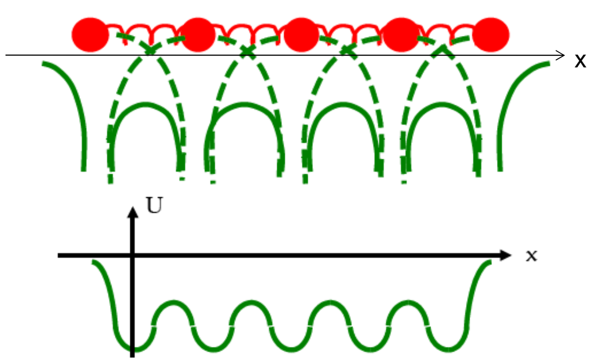
In 3-D: Effective Mass Tensor

$$\vec{F}_{ext} = \vec{\vec{m}}^* \, \vec{a} \quad \text{where} \quad \left(\frac{1}{m^*}\right)_{ij} = \left[\frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_i \partial k_j}\right]$$

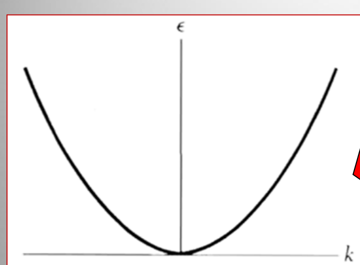
- Acceleration, in general, not parallel to external force

	m_e^*/m_e	m_h^*/m_e
InSb	0.014	0.4
InAs	0.022	0.4
Ge	0.60	0.28
Si	0.43	0.54
GaAs	0.065	0.5
Na	1.2	
Cu	0.99	
Zn	0.85	

Electrons in solid

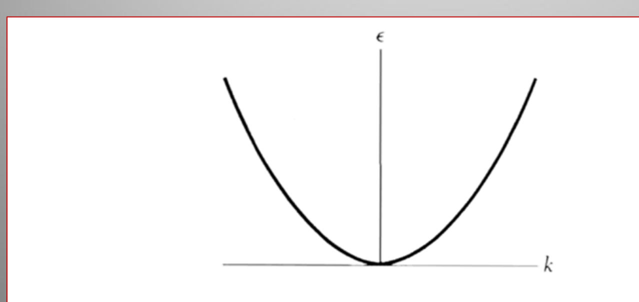


Band Structure



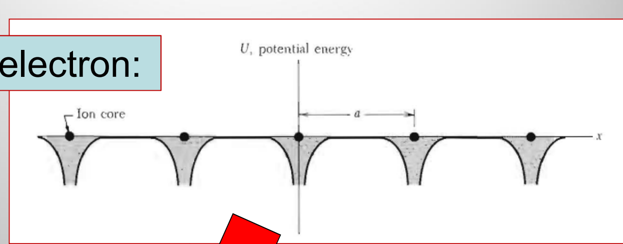
Free electron:

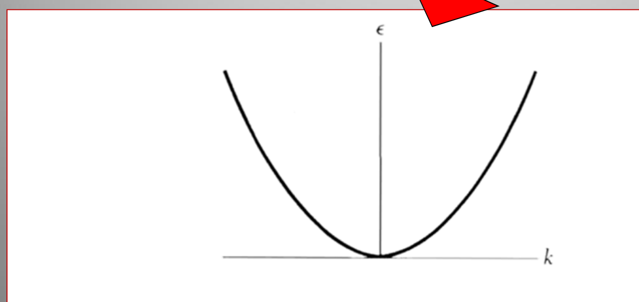
$$E = \frac{\hbar^2 k^2}{2m}$$



Band Structure

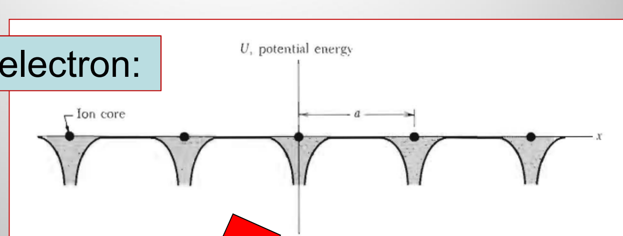
Nearly free electron:

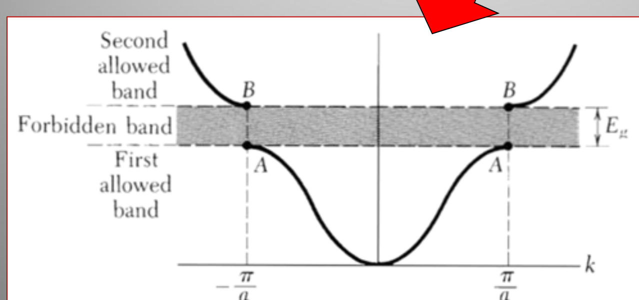




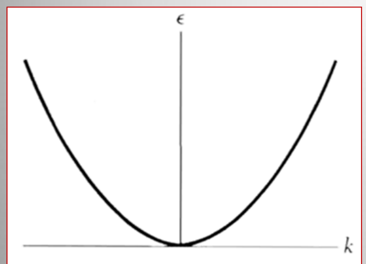
Band Structure

Nearly free electron:



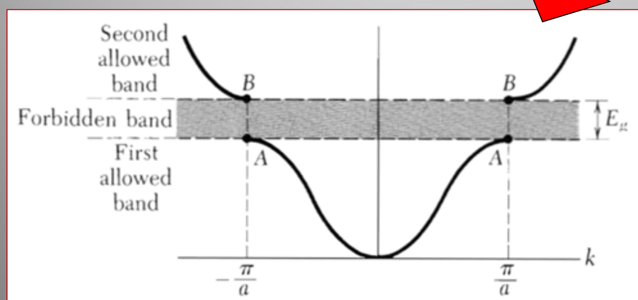


Band Structure

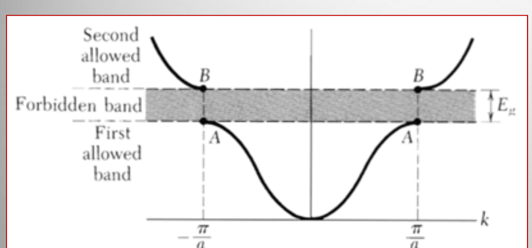


Nearly free electron:

$$E_g = \int dx\, U(x)\, [|\psi_+(x)|^2 - |\psi_-(x)|^2]$$



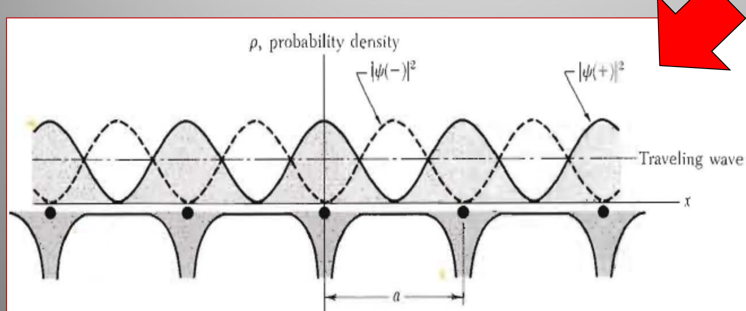
Band Structure



Nearly free electron:

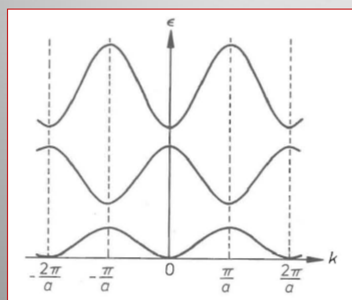
$$|\psi_+(x)|^2 = 2A^2 \cos^2(\pi\, x / a)$$

$$|\psi_-(x)|^2 = 2A^2 \sin^2(\pi\, x / a)$$

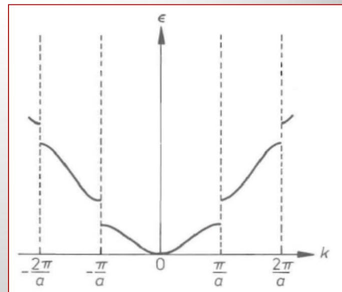


Band Structure

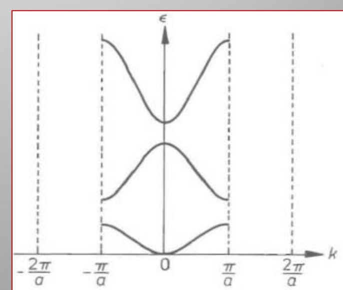
- Visualizing the gaps



Repeated zone scheme



Extended zone scheme

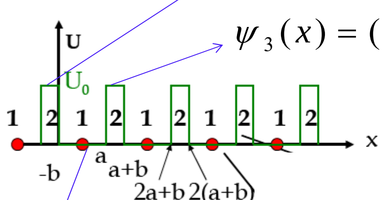


Reduced zone scheme

Kronig-Penning Model

$$\psi_2(x) = Ce^{Qx} + De^{-Qx}$$

$$\psi_3(x) = (Ce^{Qx} + De^{-Qx})e^{ik(a+b)}$$



$$\psi_1(x) = Ae^{iKx} + Be^{-iKx}$$

Boundary Conditions:

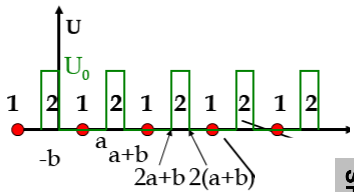
$$\psi_1(0) = \psi_2(0)$$

$$\frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx}$$

$$\psi_1(a) = \psi_3(a) = \psi_2(-b)e^{ik(a+b)}$$

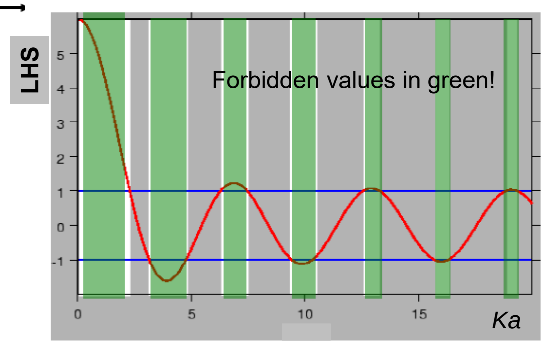
$$\frac{d\psi_1(a)}{dx} = \frac{d\psi_3(a)}{dx} = \frac{d\psi_2(-b)}{dx}e^{ik(a+b)}$$

Kronig-Penning Model

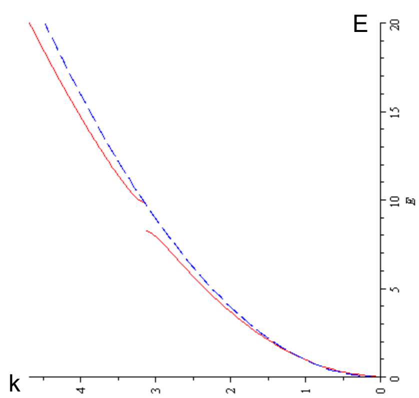


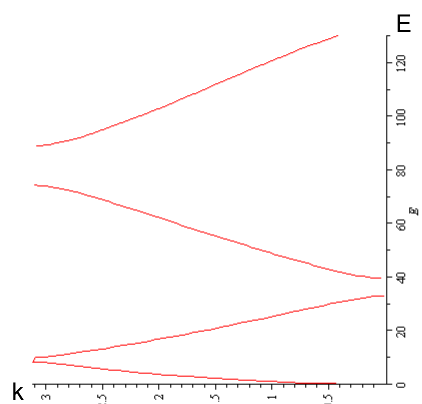
Delta function limit:

$$(Q^2 b / 2K) \sin Ka + \cos Ka = \cos ka$$



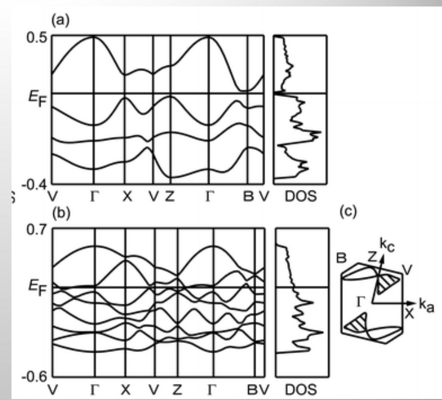
Kronig-Penning Model

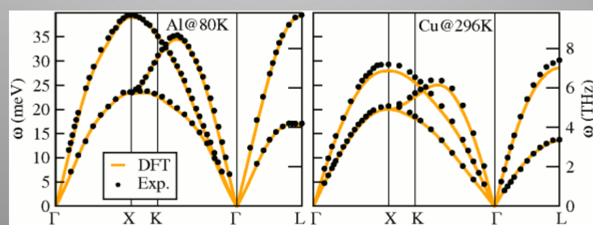




Band Structure

- See text!
- P. 88





Fermi Surface

- Copper