Solid State Electronics EC210
Arab Academy for Science and Technology
AAST – Cairo
Fall 2014

Lecture 8
Band Theory: Kronig-Penny Model and Effective Mass

Lecture Notes Prepared by:
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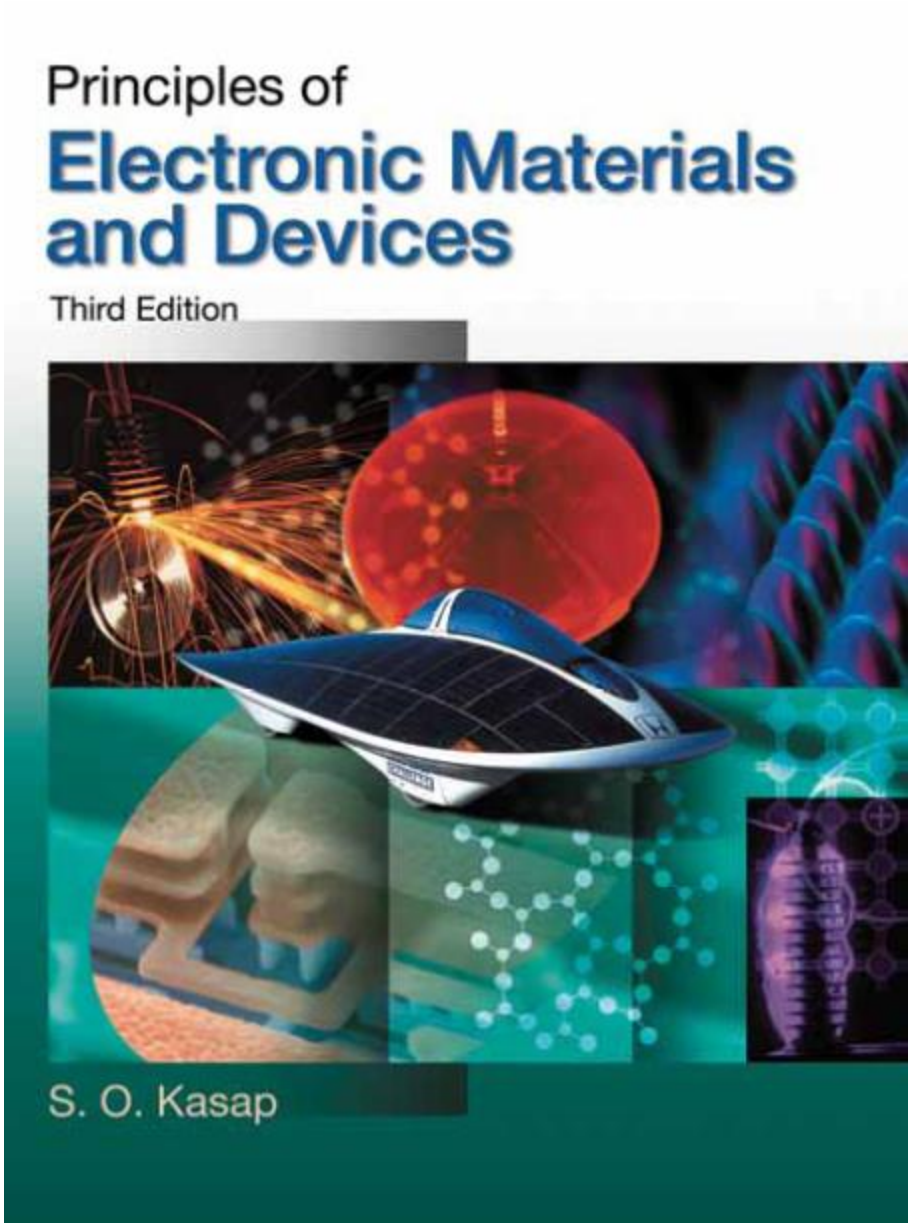

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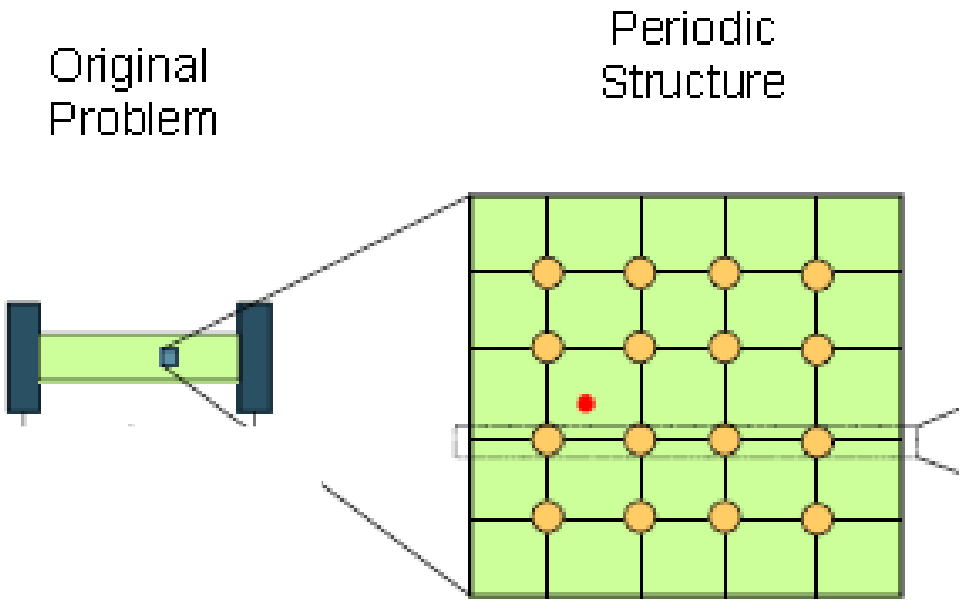
Pages

- Kasap:
  - P.355 (Kronig Penny)
  - P.303-304, p. 454-455 (Effective Mass)

Particle in a Crystalline Solid (Periodic Potential)



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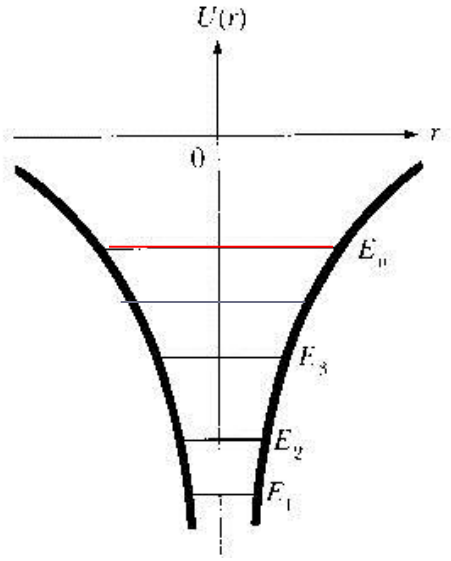
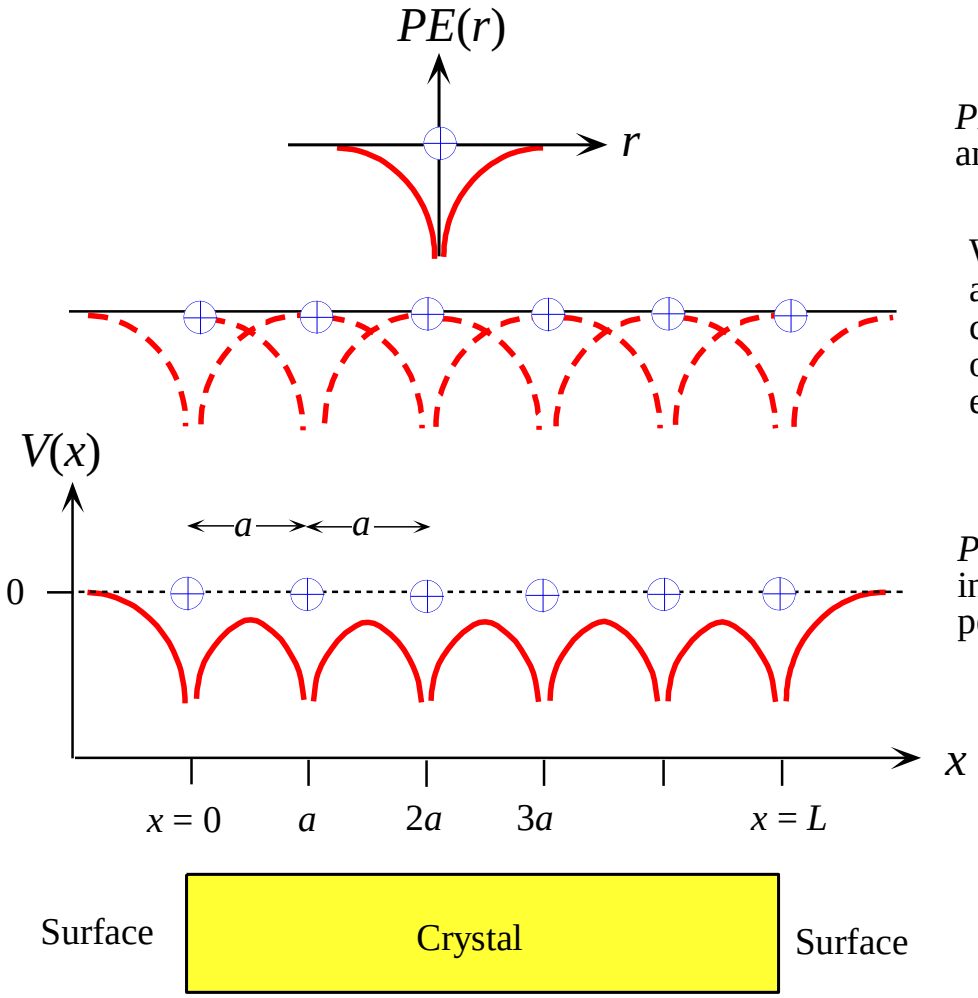
Remember for the Hydrogen atom



$$U(r) = -\frac{1}{4\pi\varepsilon_0}\frac{e^2}{r}$$



PE of the electron around an isolated atom

When *N* atoms are arranged to form the crystal then there is an overlap of individual electron *PE* functions.

PE of the electron, $V(x)$, inside the crystal is periodic with a period *a*.

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The electron *PE*, $V(x)$, inside the crsytal is periodic with the same periodicity as that of the crystal, *a*. Far away outside the crsytal, by choice, $V = 0$ (the electron is free and $PE = 0$).

Bloch's Waves

If a periodic potential with period "a" can be defined as:

$$U(x+a) = U(x)$$

Then the wavefunction is periodic, and can be defined in terms of base function:

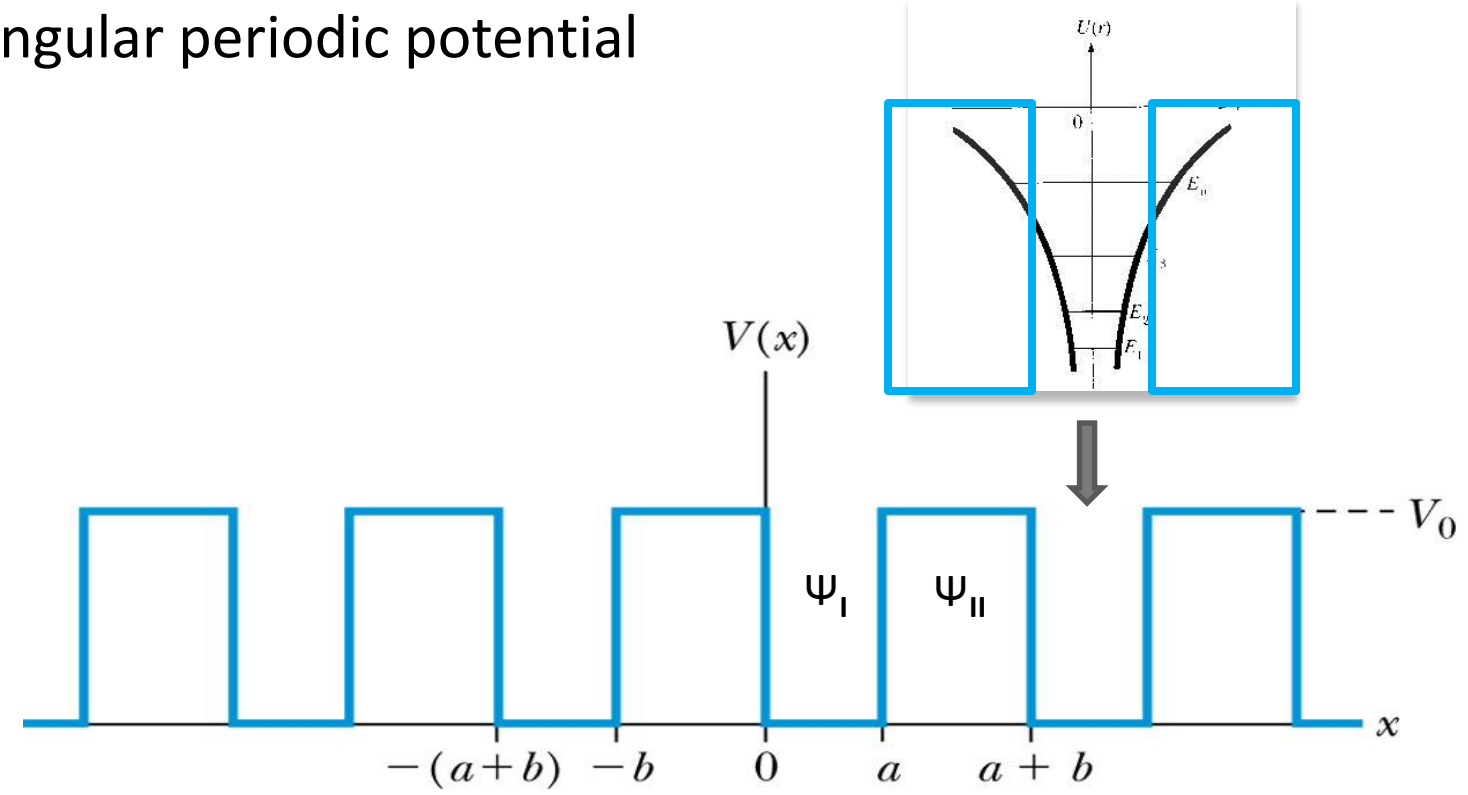
$$\Psi(x+a) = e^{ika}\,\Psi(x)$$

$$\Psi(x) = e^{ikx}u(x)$$

- a can be replace by na

Kronig-Penney Model

- Approximate crystal periodic Coulomb potential by rectangular periodic potential



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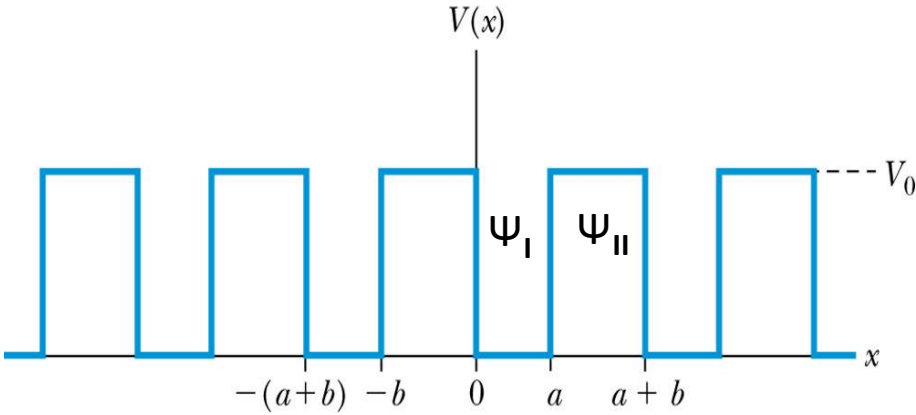
Wavefunction Periodic Boundary Conditions

$$\Psi_I(0) = \Psi_{II}(0)$$

$$\frac{d\Psi_I(0)}{dx} = \frac{d\Psi_{II}(0)}{dx}$$

$$\Psi_I(a) = e^{ik(a+b)}\Psi_{II}(-b)$$

$$\frac{d\Psi_I(a)}{dx} = e^{ik(a+b)}\,\frac{d\Psi_{II}(-b)}{dx}$$



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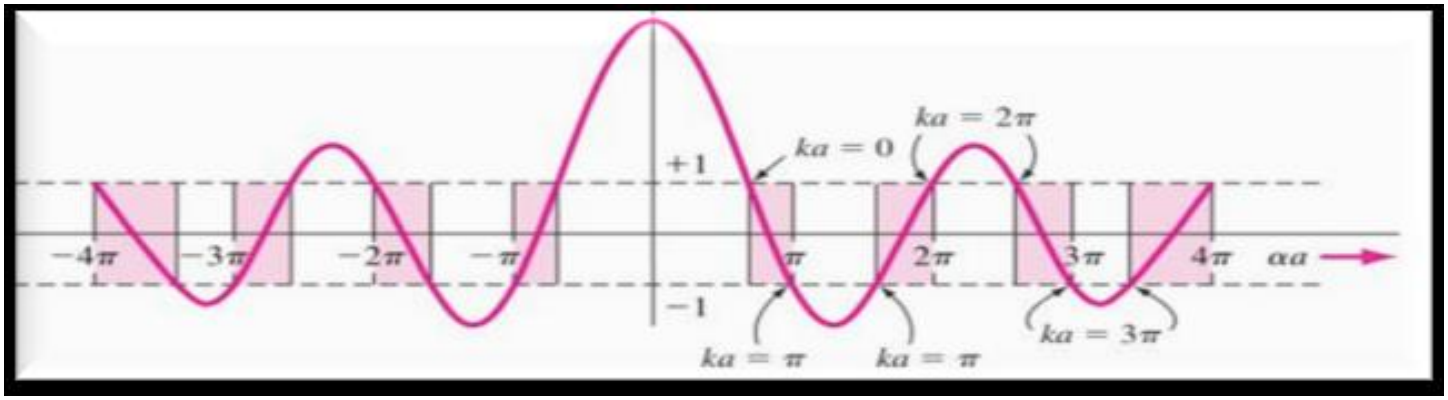
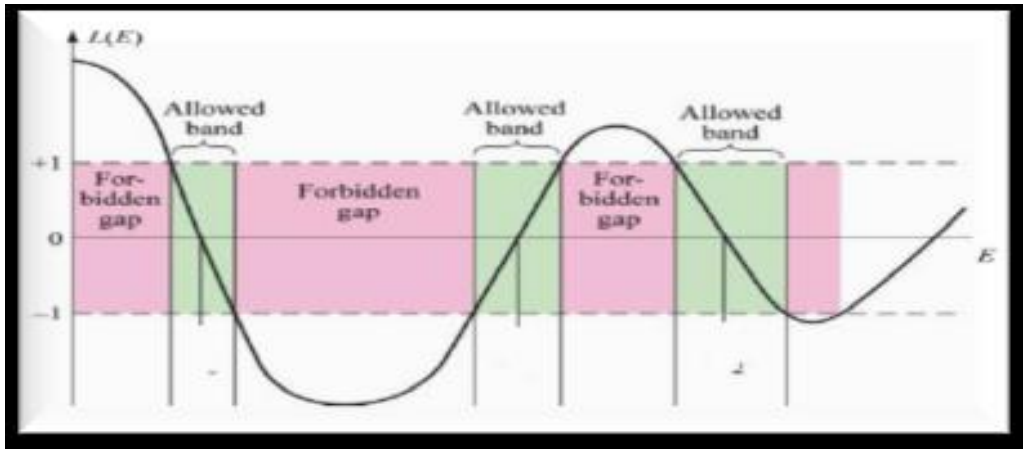
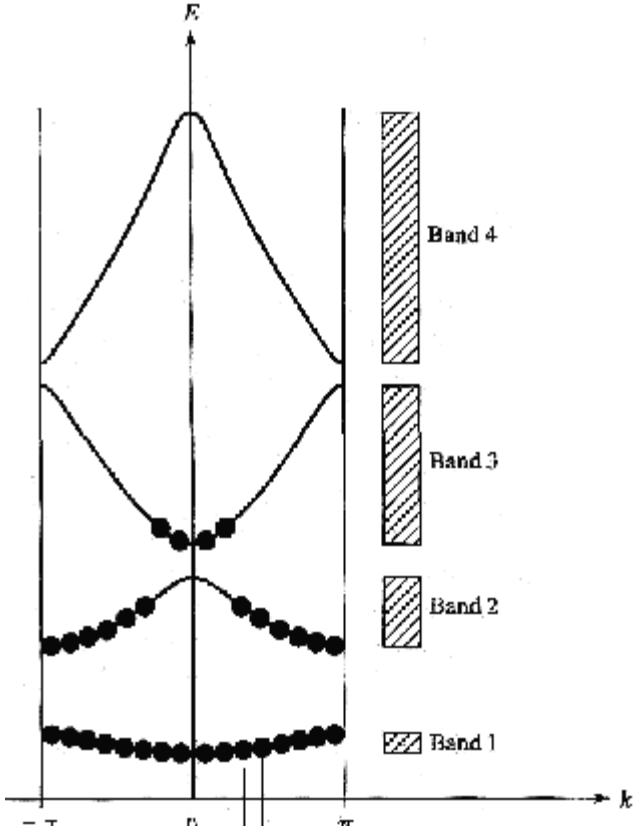
K-P Solution: Allowed Energies

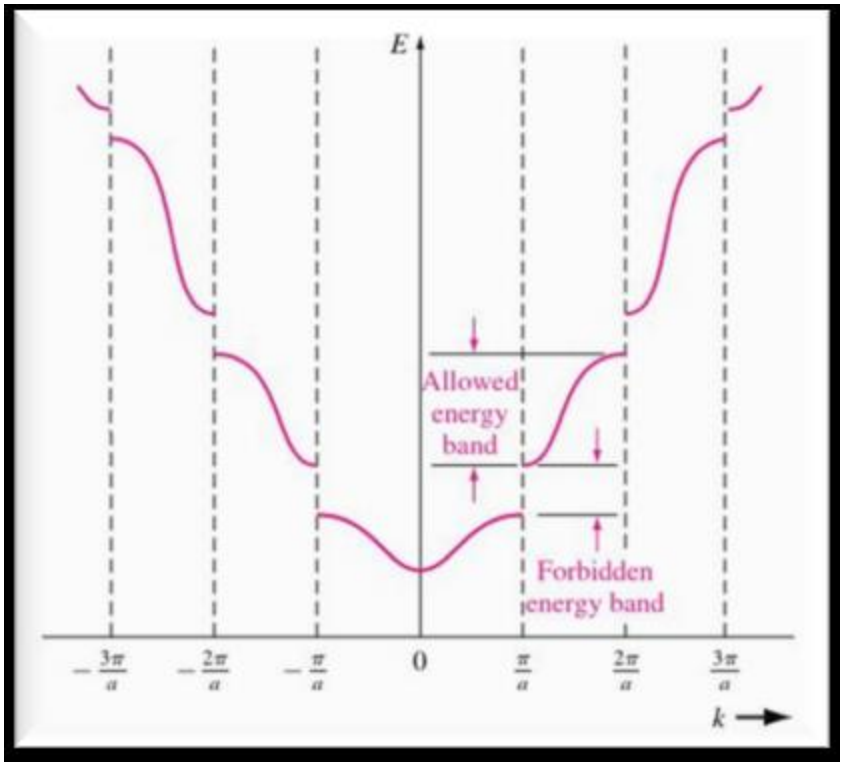




Source: Dr. Fedawy's Lecture notes

Kronig-Penney Model





Source: Dr. M. Fedawy's Lecture notes

Fig 4.52

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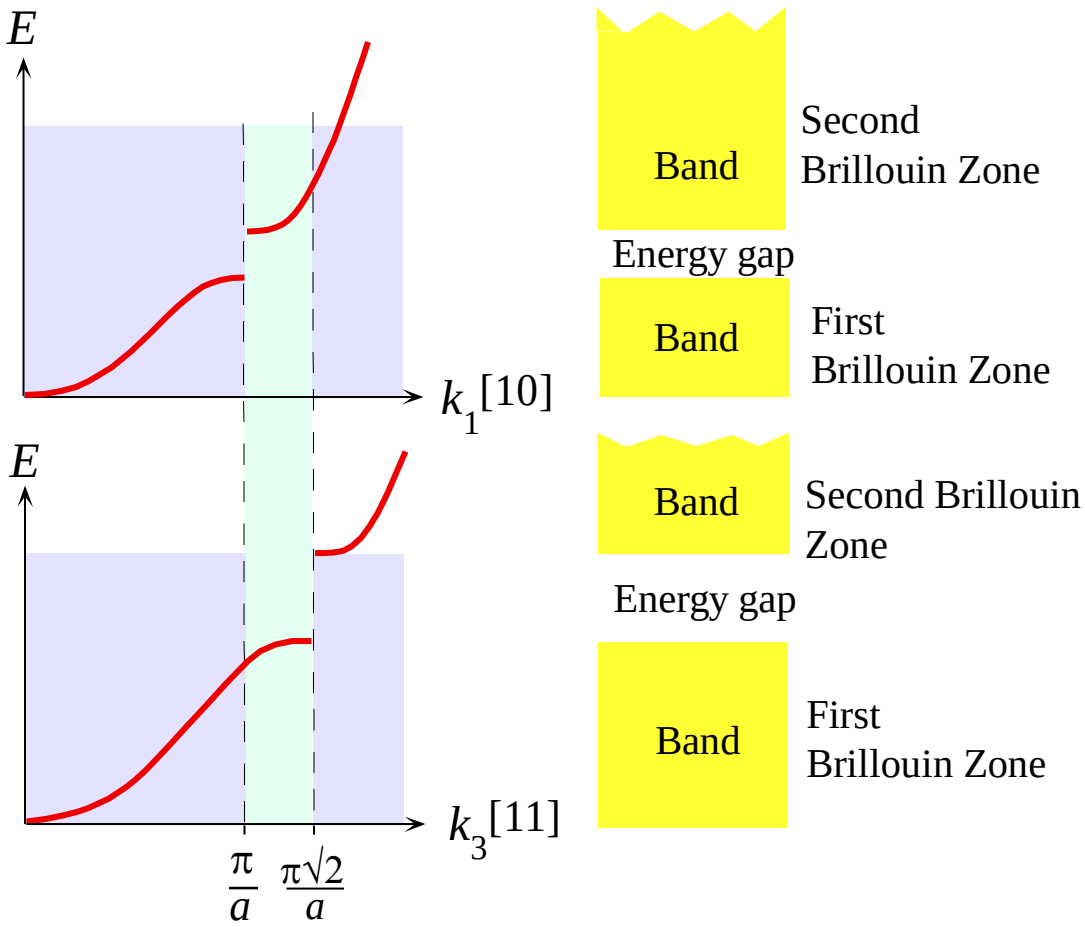

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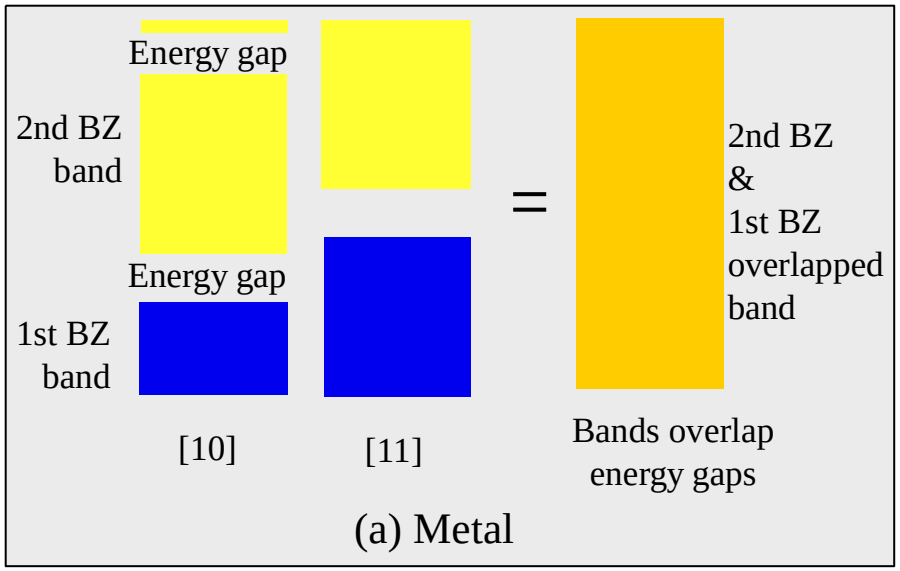
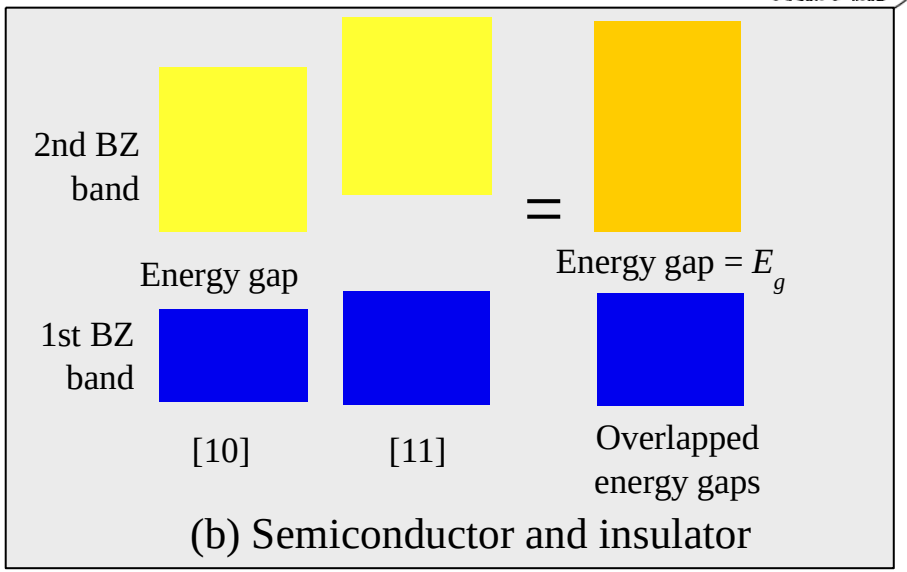
The *E-k* behavior for the electron along different directions in the two dimensional crystal. The energy gap along [10] is at π/a whereas it is at $\pi\sqrt{2}/a$ along [11].

Fig 4.54





(a) Metal: For the electron in a metal there is no apparent energy gap because the 2nd BZ (Brillouin Zone) along [10] overlaps the 1st BZ along [11]. Bands overlap the energy gaps. Thus the electron can always find any energy by changing its direction.
(b) Semiconductor or insulator: For the electron in a semiconductor there is an energy gap arising from the overlap of the energy gaps along [10] and [11] directions. The electron can never have an energy within this energy gap, E_g.

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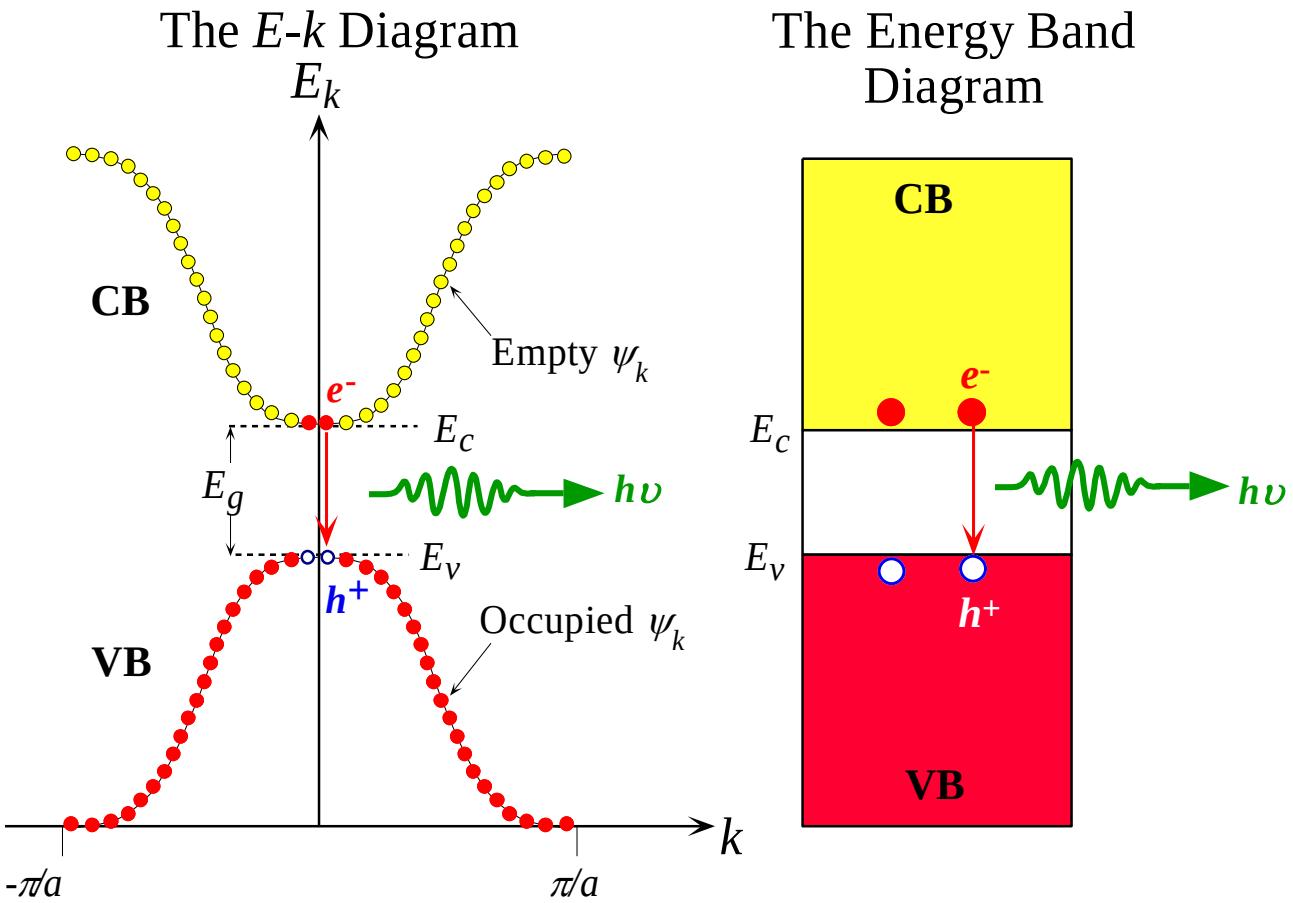
Fig 4.55



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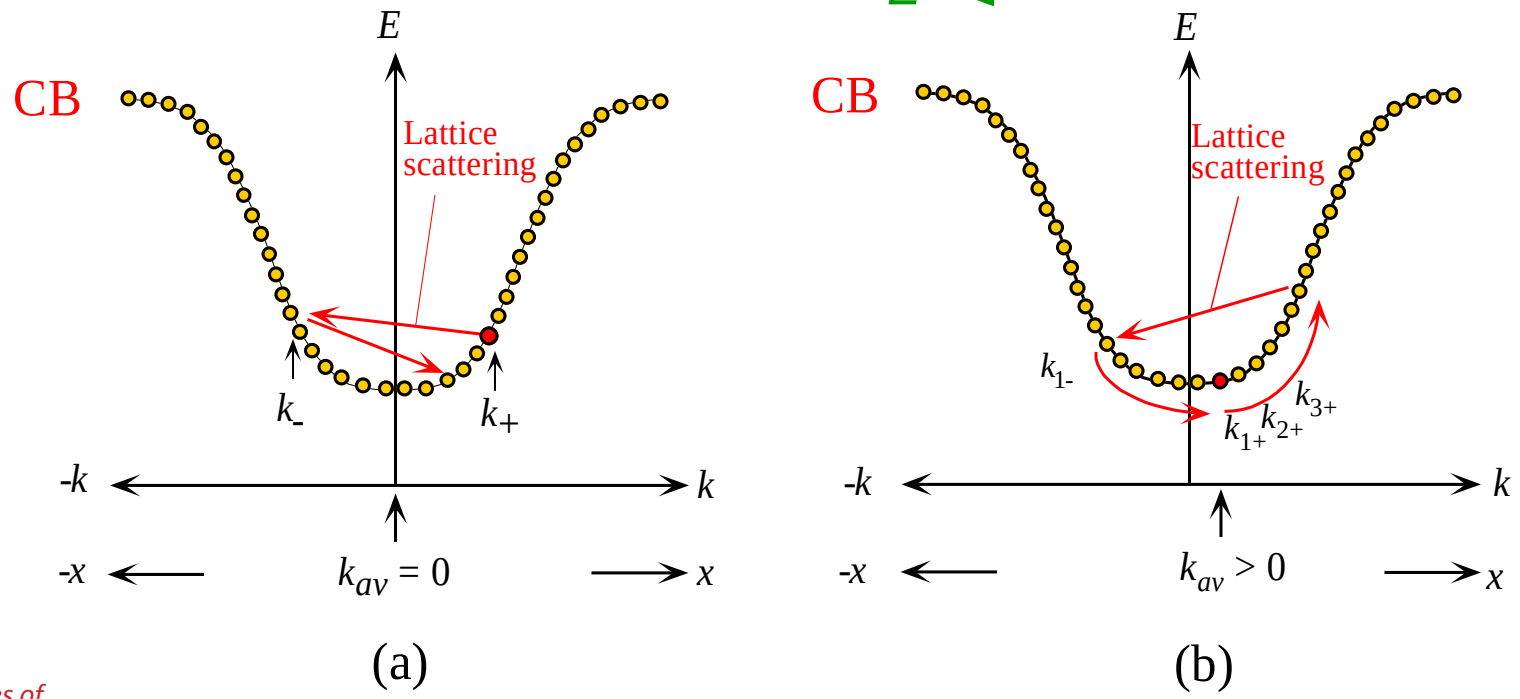
The E-k diagram of a direct bandgap semiconductor such as GaAs. The E-k curve consists of many discrete points each point corresponding to a possible state, wavefunction y k(x), that is allowed to exist in the crystal. The points are so close that we normally draw the E-k relationship as a continuous curve. In the energy range Ev to Ec there are no points (yk(x) solutions).



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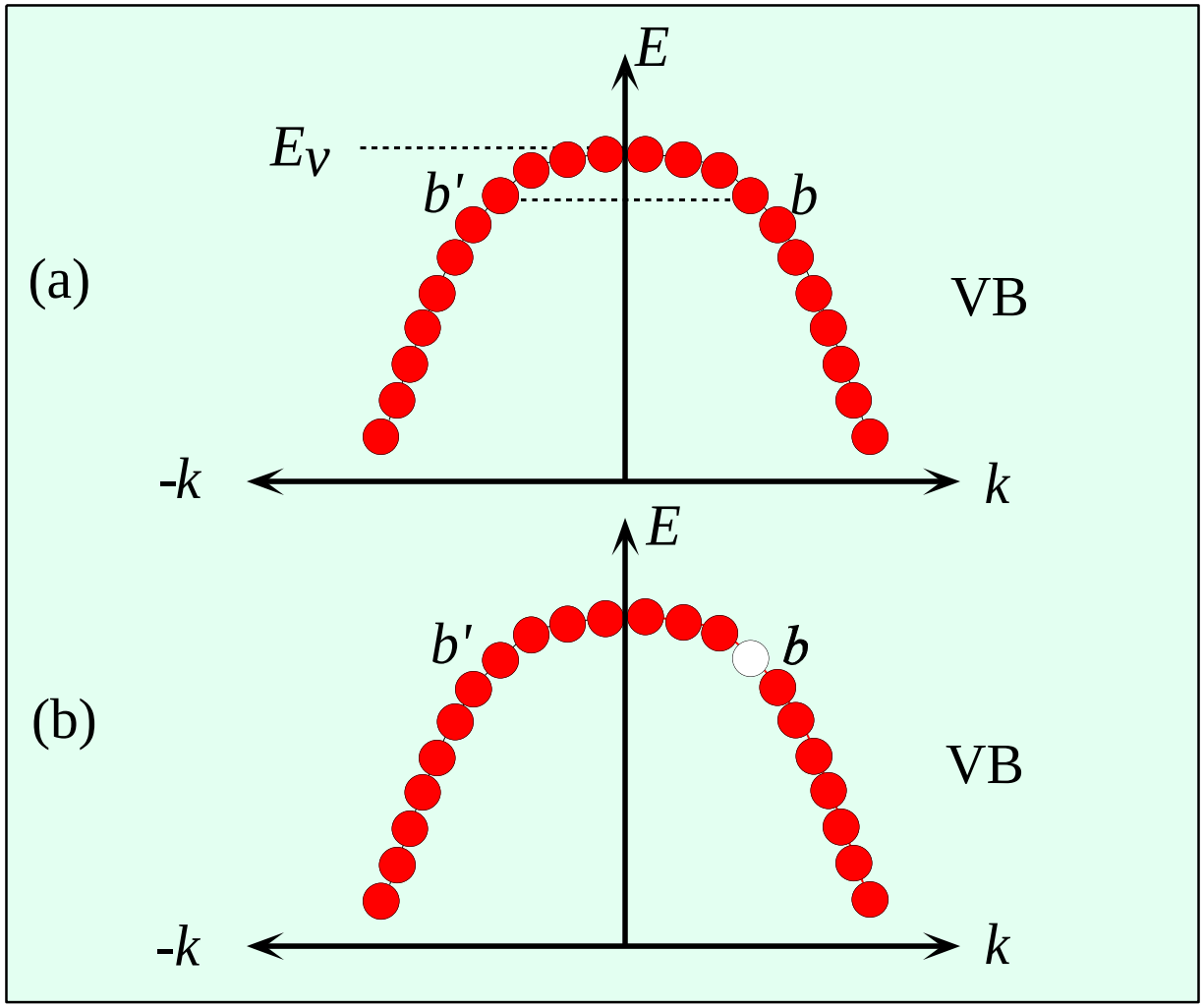
(a) In the absence of a field, over a long time, average of all k values is zero, there is no net momentum in any one particular direction. (b) In the presence of a field E in the $-x$ direction, the electron accelerates in the $+x$ direction increasing its k value along x until it is scattered to a random k value. Over a long time, average of all k values is along the $+x$ direction. Thus the electron drifts along $+x$.



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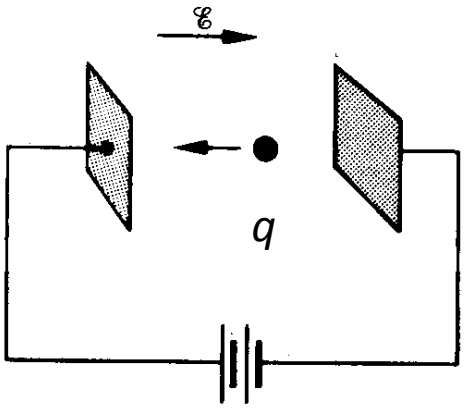
(a) In a full valence band there is no net contribution to the current. There are equal numbers of electrons (e.g. at *b* and *b'*) with opposite momenta. (b) If there is an empty state (*hole*) at *b* at the top of the band then the electron at *b'* contributes to the current.

Fig 5.52

Effective Mass

In vacuum

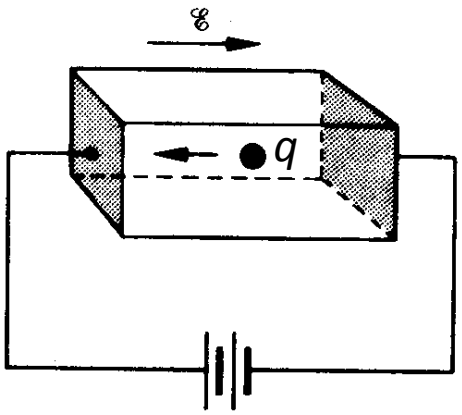


$F = q\,\varepsilon = m_o a$

where

m_o is the electron mass

In semiconductor



$F_{ext} = (-q)\mathbf{E}$

$F_{ext} + F_{int} = m_o a$

$F_{ext} = m_n^* a$

where

m_n^* is the electron effective mass

Effective Mass

Group Velocity defined as the velocity of the wavefunction of the electrons (analogous to speed of sinusoidal wave):

$$v_g = \frac{dx}{dt} = \frac{d\omega}{dk}$$

$$\omega = E/\hbar \rightarrow vg = \frac{1}{\hbar}\frac{dE}{dk}$$

$$\rightarrow dE = vg\,\hbar\,dk, \qquad dx = v_g\,dt$$

$$dE = F_{ext}\,dx = F_{ext}\,vg\,dt$$

$$F_{ext} = \frac{1}{v_g}\frac{dE}{dt} \rightarrow F_{ext} = \hbar\frac{dk}{dt}$$

Effective Mass (2)

Acceleration:

$$a = \frac{dv_g}{dt} = \frac{d}{dt}\left[\frac{1}{\hbar}\frac{dE}{dk}\right] = \frac{1}{\hbar}\frac{d}{dk}\left[\frac{dE}{dt}\right] = \frac{1}{\hbar}\frac{d}{dk}\left[\frac{dE}{dk}\frac{dk}{dt}\right]$$

$$a = \frac{1}{\hbar}\frac{d^2E}{dk^2}\frac{dk}{dt} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}\hbar\frac{dk}{dt} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}F_{ext}$$

Using $F_{ext} = m^* a$

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