Solid State Electronics EC210
Arab Academy for Science and Technology
AAST – Cairo
Spring 2015

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

Lecture Notes Prepared by:
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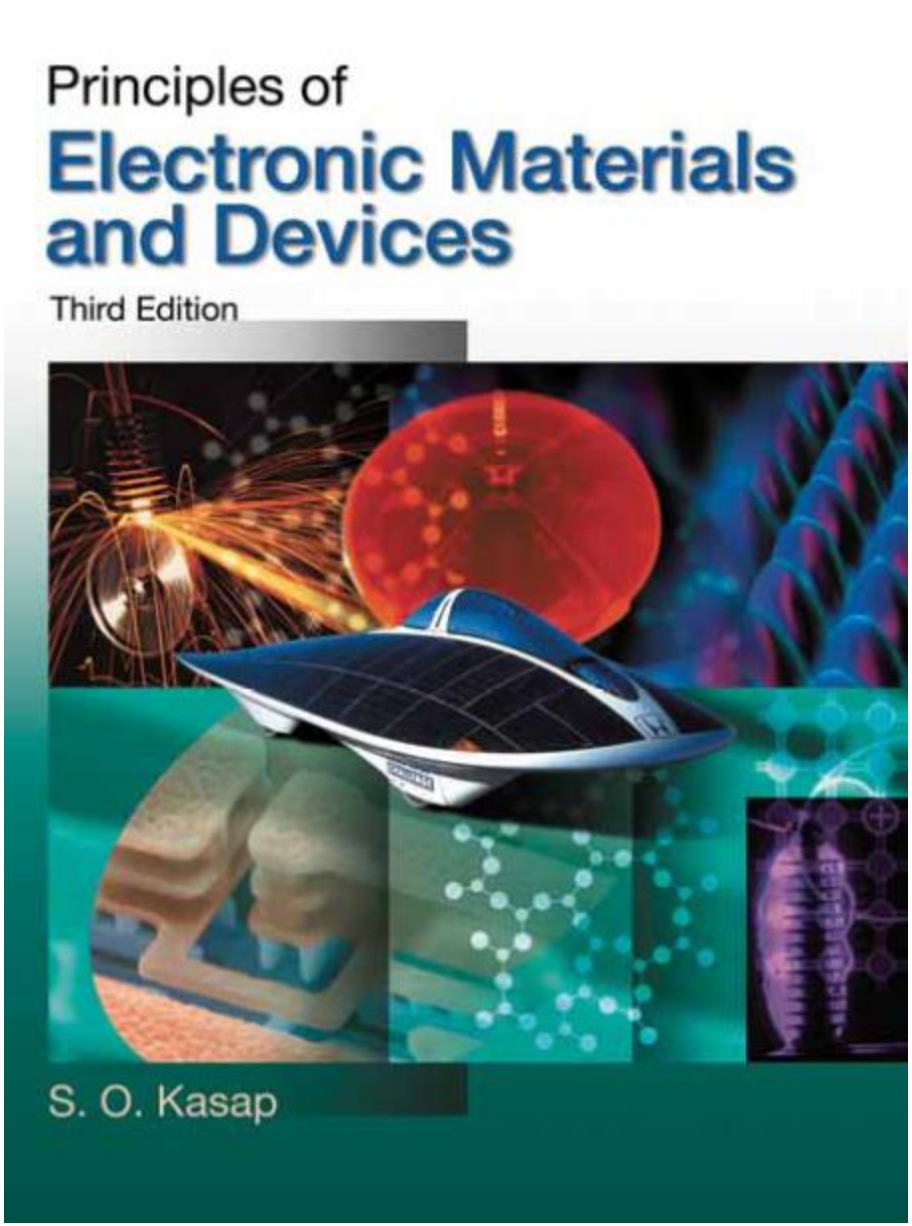

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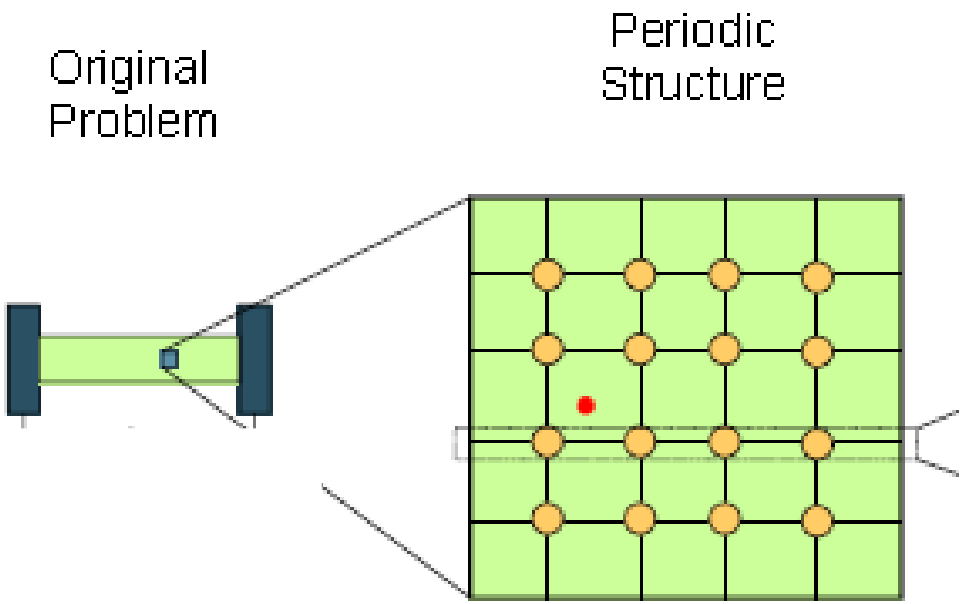
Pages

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

Particle in a Crystalline Solid (Periodic Potential)



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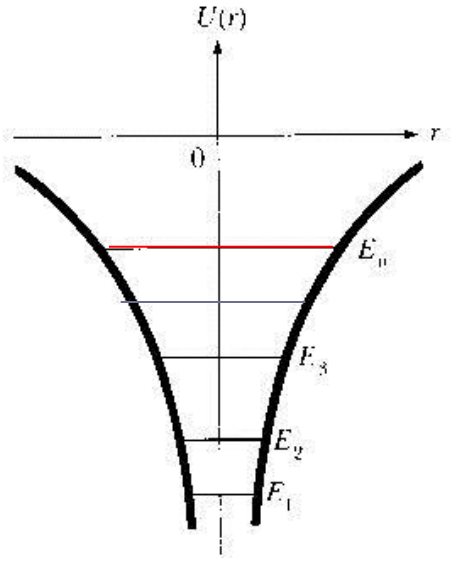
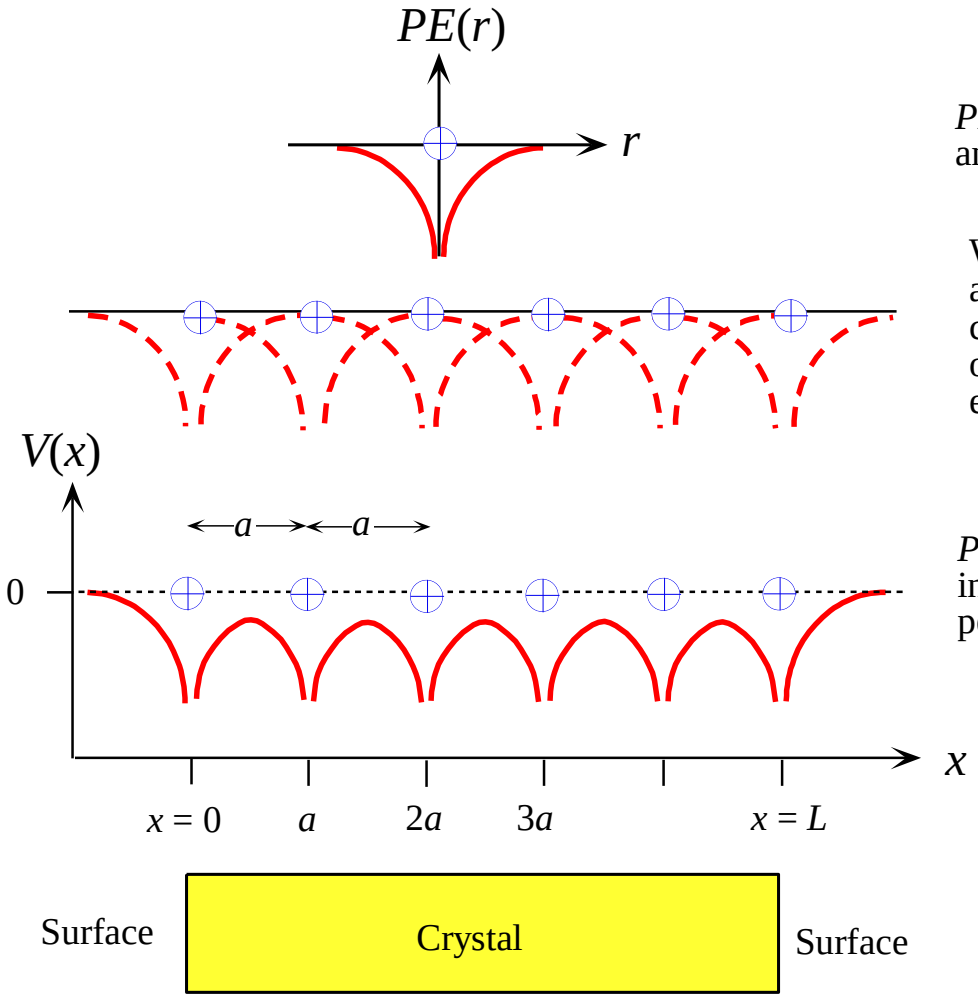
Remember for the Hydrogen atom



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



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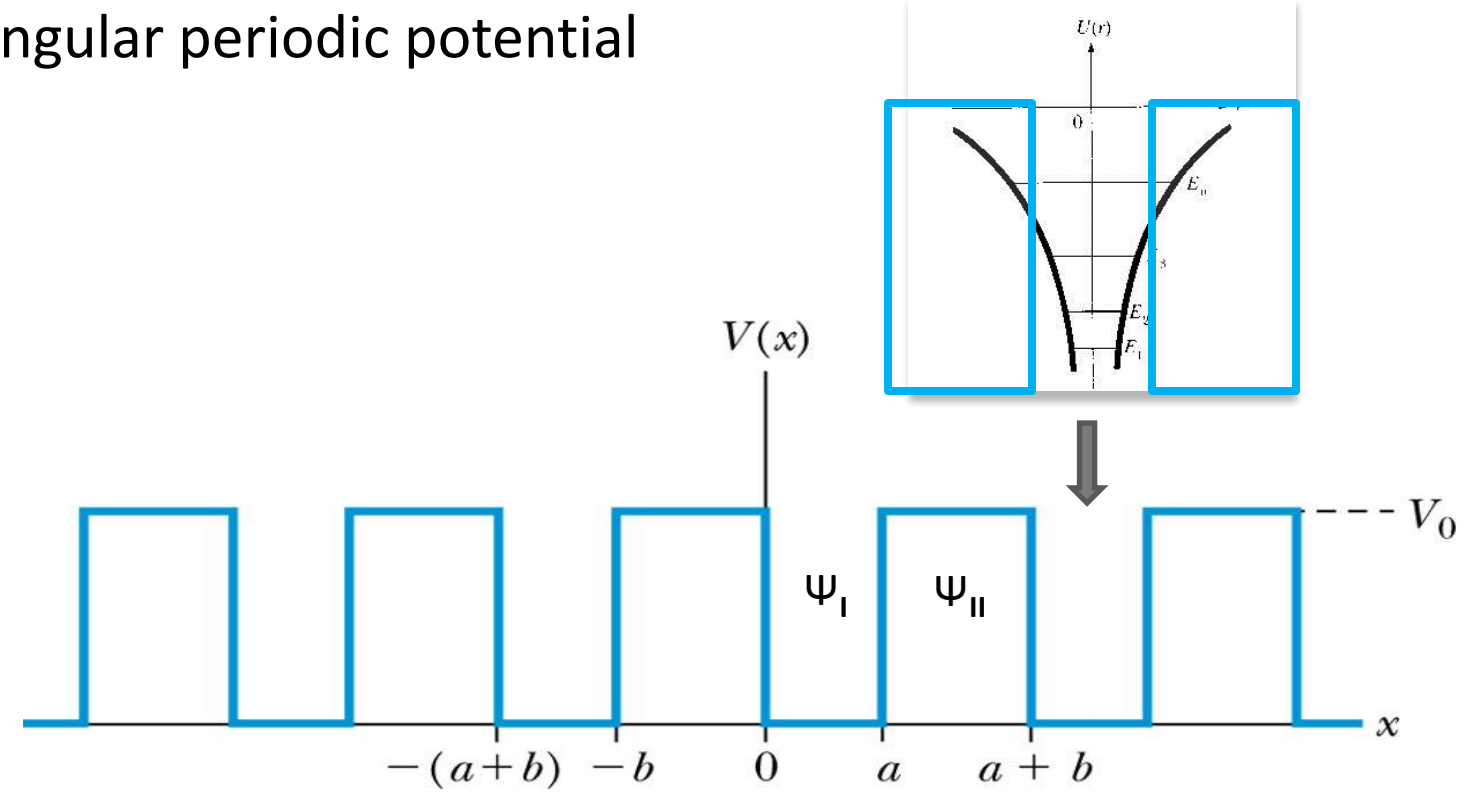
The electron *PE*, $V(x)$, inside the crsytal is periodic with the same periodicity as that of the crystal, *a*. Far away outside the crsytal, by choice, $V = 0$ (the electron is free and $PE = 0$).

Fig 5.48

Kronig-Penney Model

- Approximate crystal periodic Coulomb potential by rectangular periodic potential



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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 a unit cell base function $u(x)$:

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

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

- a can be replaced by na

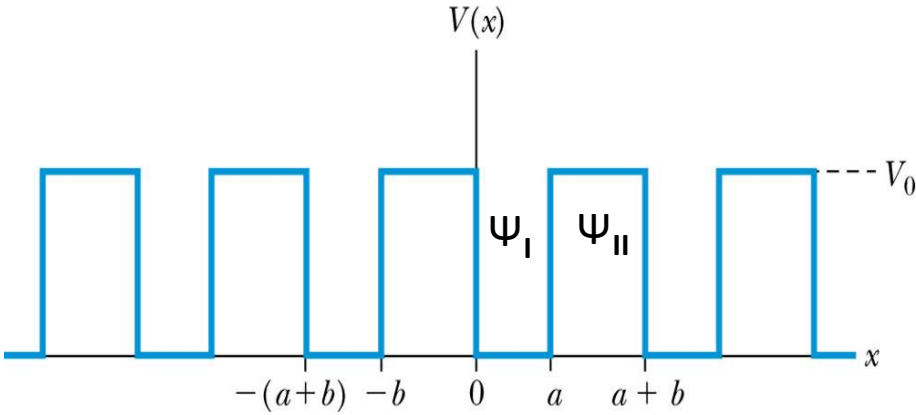
Wavefunction Periodic Boundary Conditions

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

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

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

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



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From Tunneling Lecture

Region I:

Free particle: $k^2 = \frac{2mE}{\hbar^2}$

$$\Psi_I(x) = Ae^{jkx} + Be^{-jkx}$$

Region II:

If $E < U_o$:

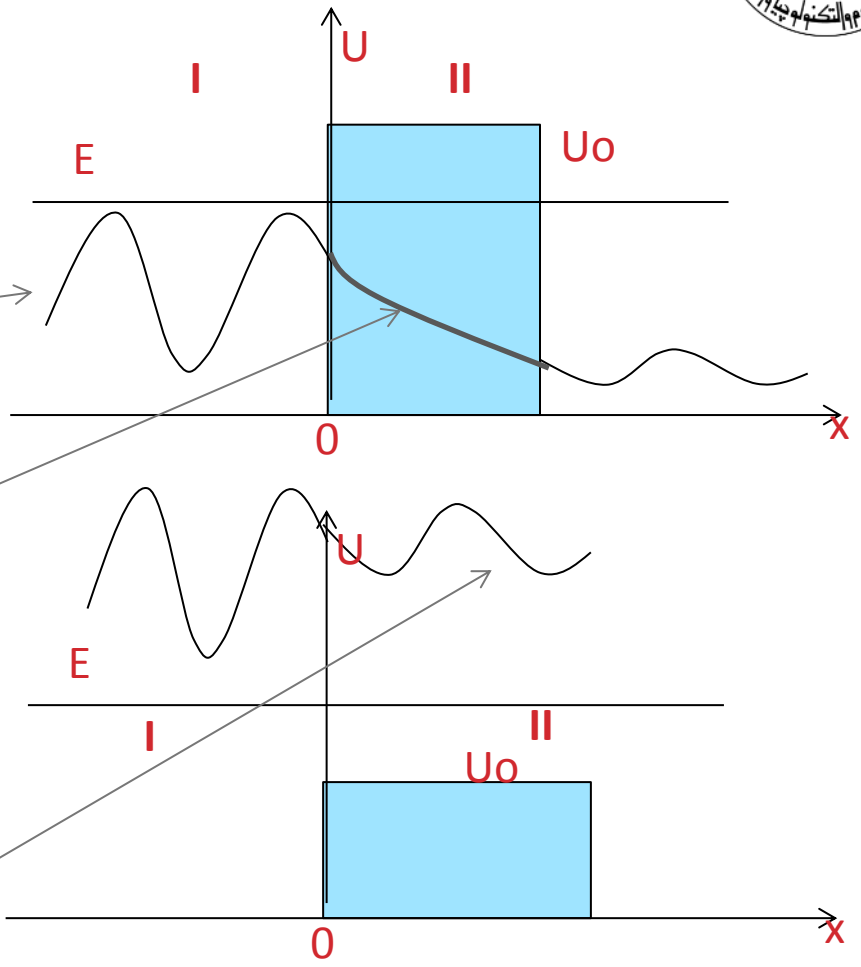
$$\alpha^2 = 2m(U_o - E)/\hbar^2$$

$$\Psi_{II}(x) = Ce^{\alpha x} + De^{-\alpha x}$$

If $E > U_o$:

$$k_{II}{}^2 = -\alpha^2 = 2m(E - U_o)/\hbar^2$$

$$\Psi_{II}(x) = Ce^{jk_{II}x} + De^{-jk_{II}x}$$



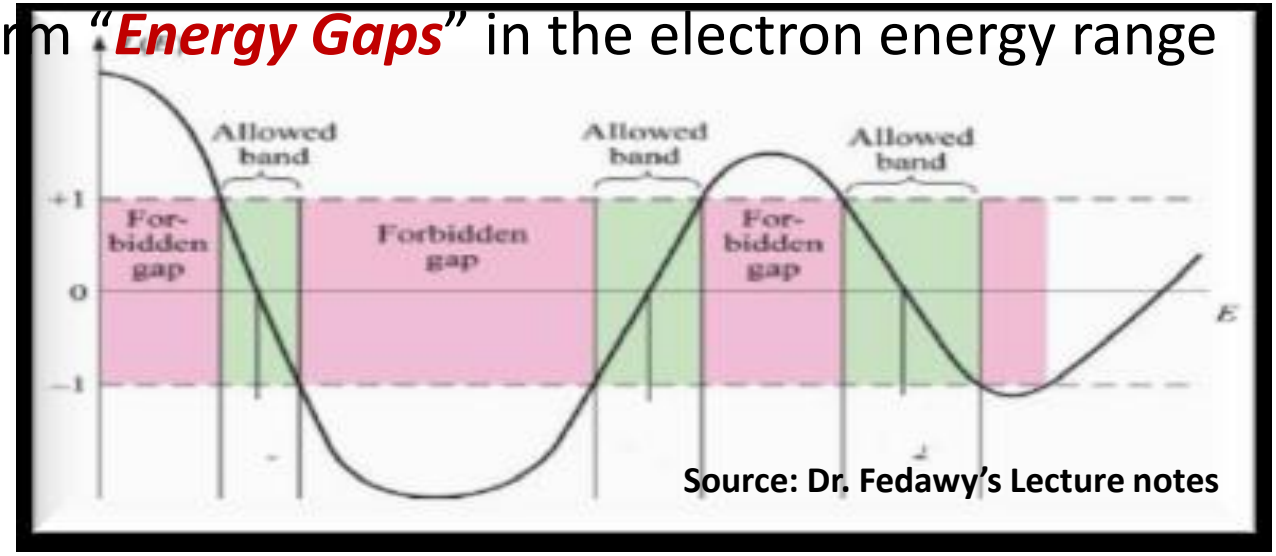
Kronig-Penney Solution: Allowed Energies

- The wavefunctions have solutions only in some allowed "continuous" ranges "or "***Bands***"of k:

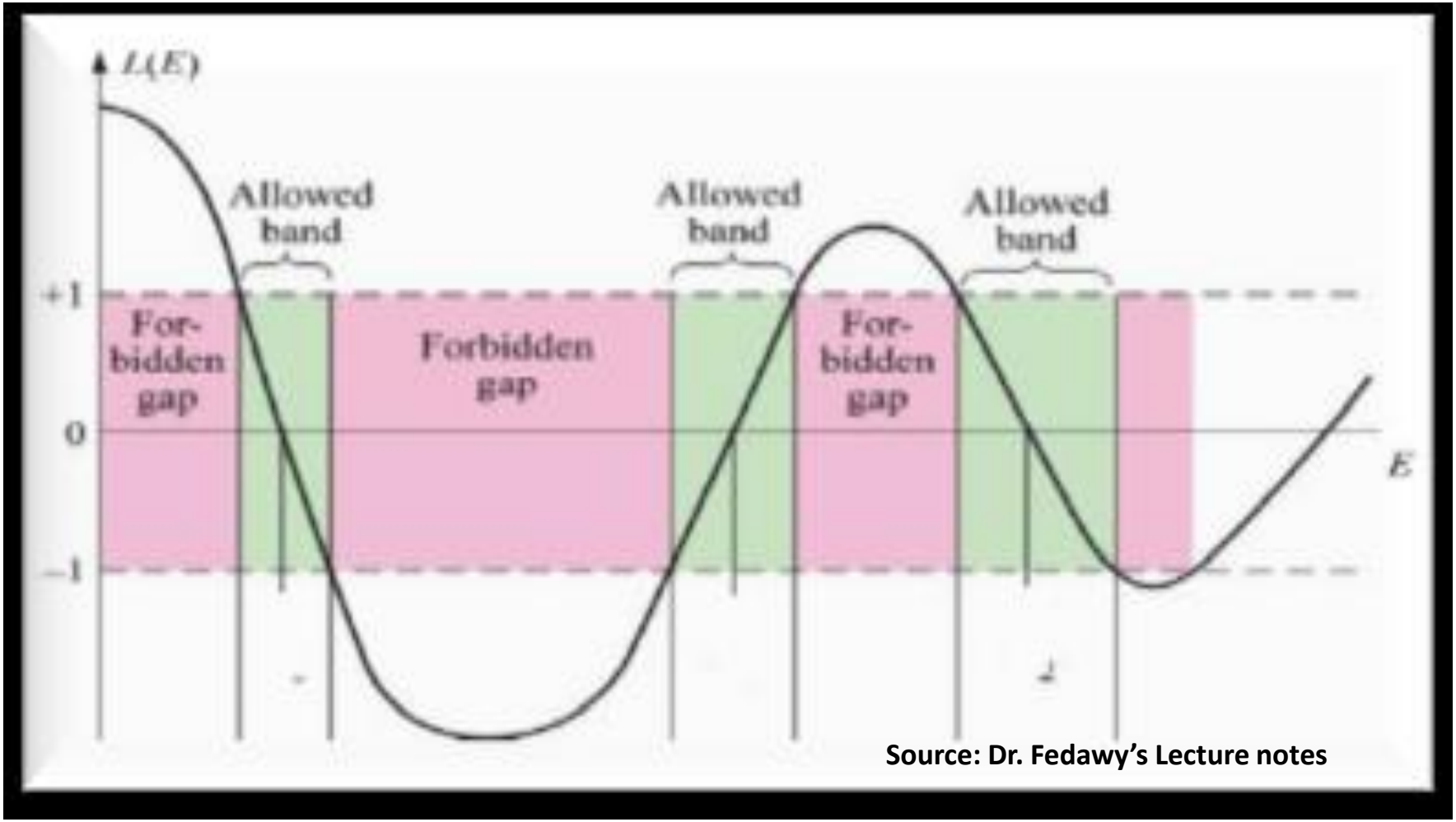
  → $\boldsymbol{E = \frac{k^2\hbar^2}{2m}}$ is **allowed**

- The solution is NOT allowed in other ranges of k:

  → Energies corresponding to these k are "Forbidden". i.e. form "***Energy Gaps***" in the electron energy range

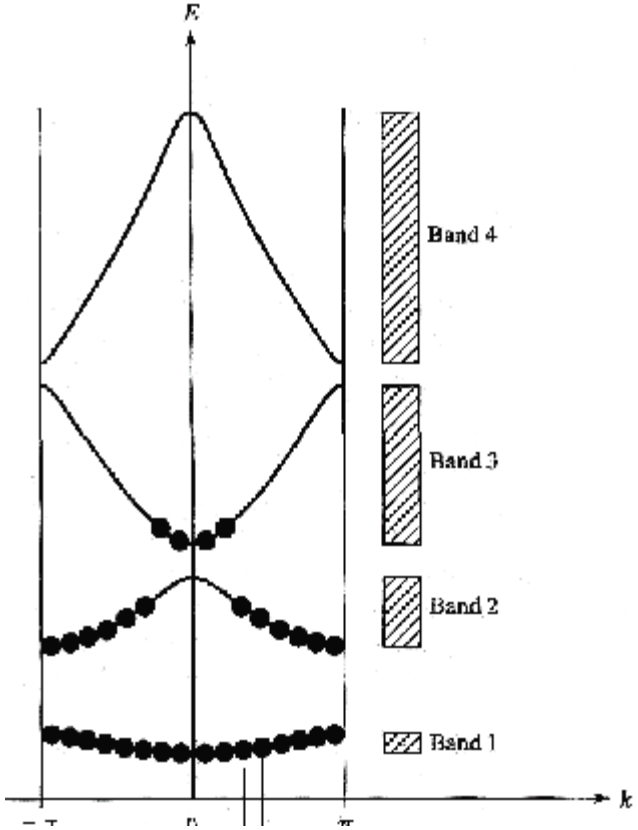


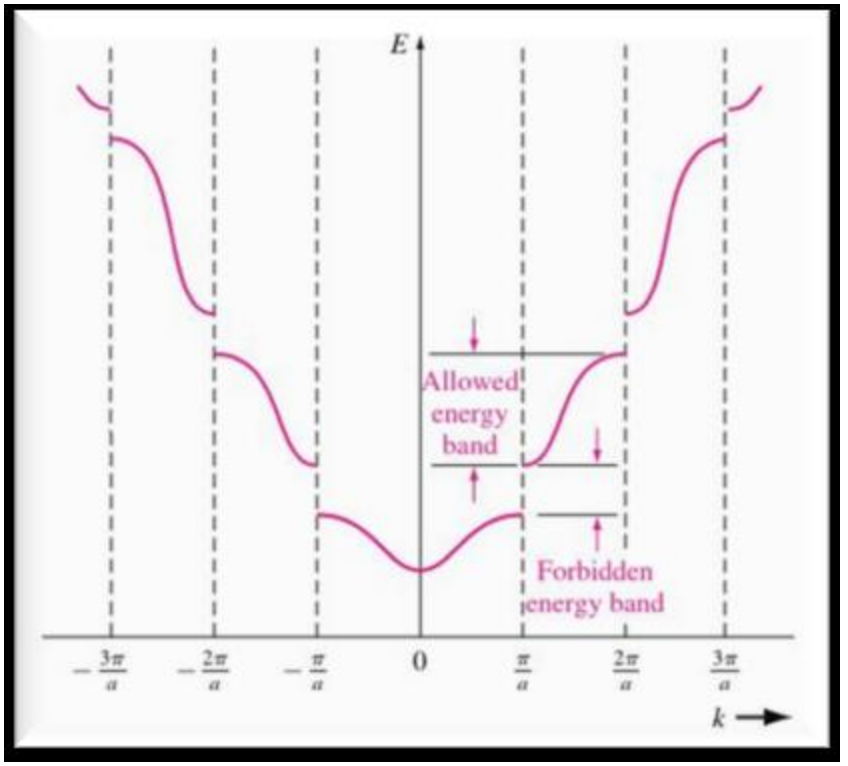
Kronig-Penney Solution: Allowed Energies



Source: Dr. Fedawy's Lecture notes

Kronig-Penney Model





Source: Dr. M. Fedawy's Lecture notes

Fig 4.52

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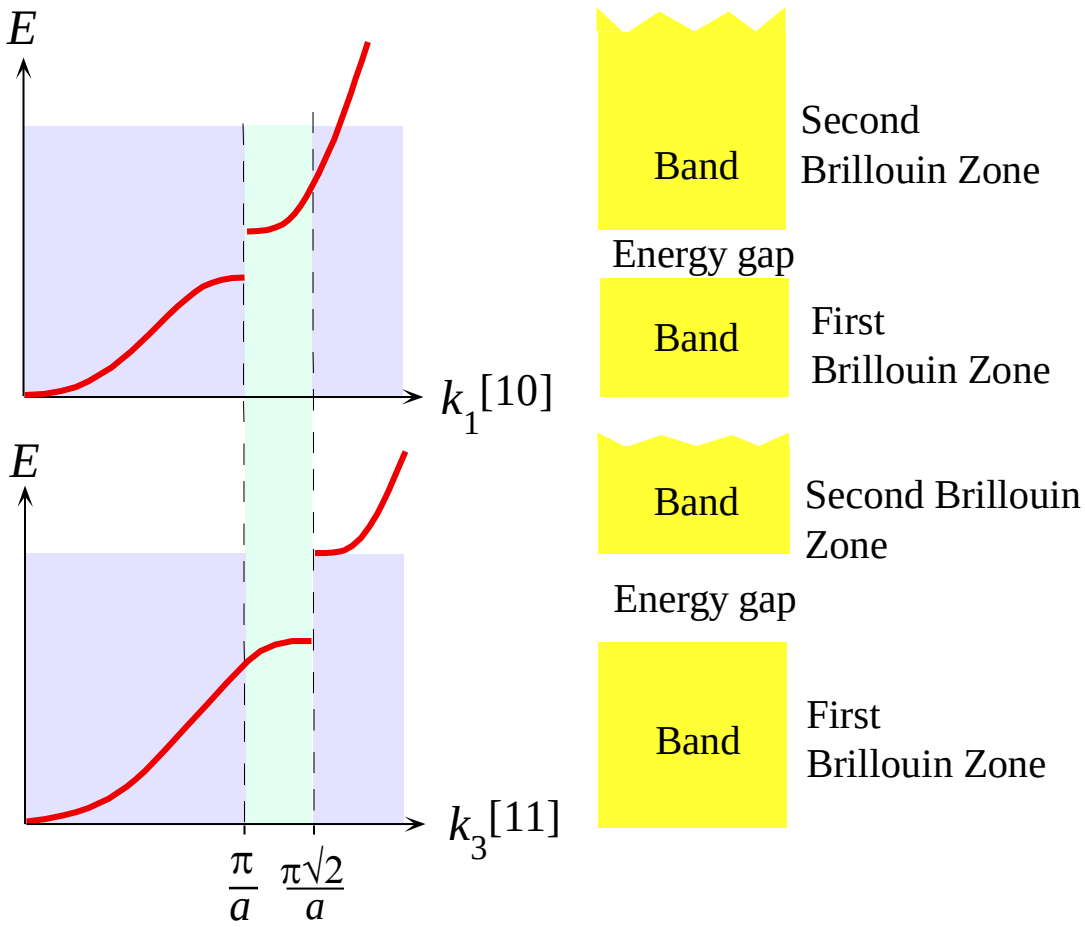

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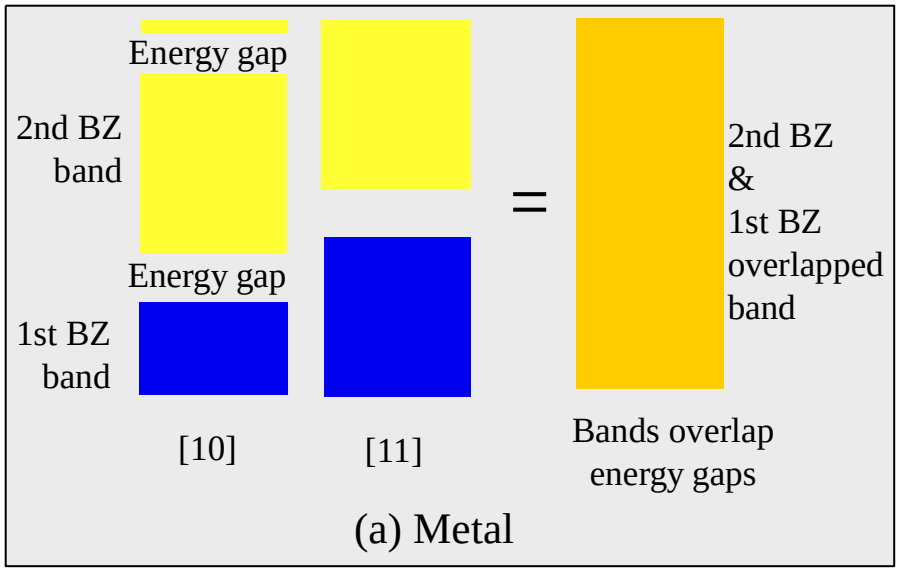
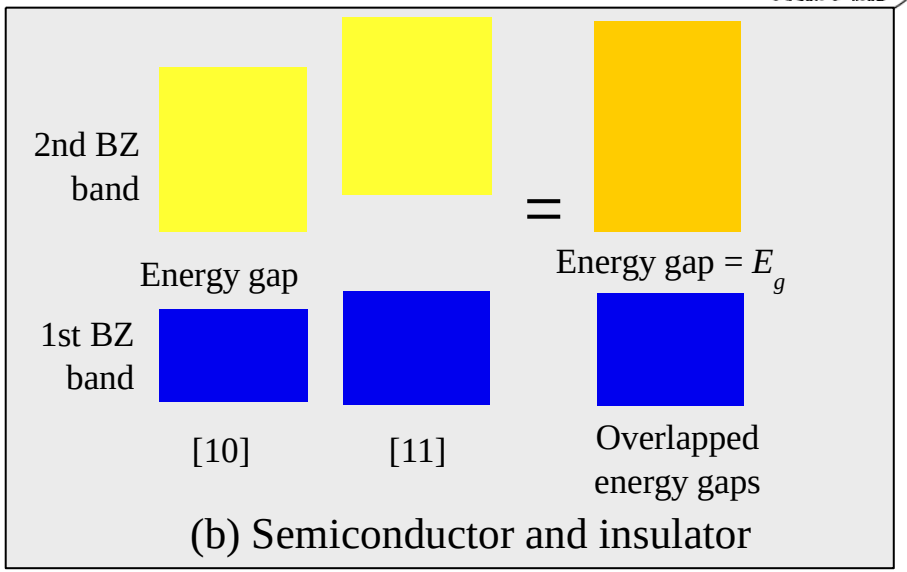
The *E-k* behavior for the electron along different directions in the two dimensional crystal. The energy gap along [10] is at π/a whereas it is at $\pi\sqrt{2}/a$ along [11].

Fig 4.54

Energy Gaps





(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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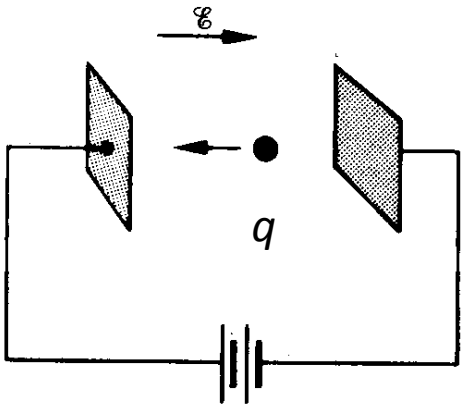
Fig 4.55

Effective Mass

In vacuum

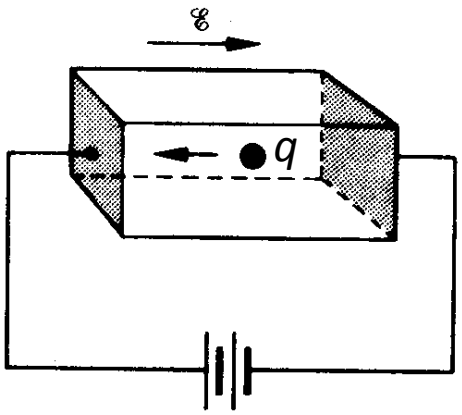


$F = q\,\varepsilon = m_o a$

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):

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

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

Acceleration:

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

Effective Mass:

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