QE4. Quantum Solid-state Physics

Semiconducting devices:

- Kronig – Penney Model
- Effective mass

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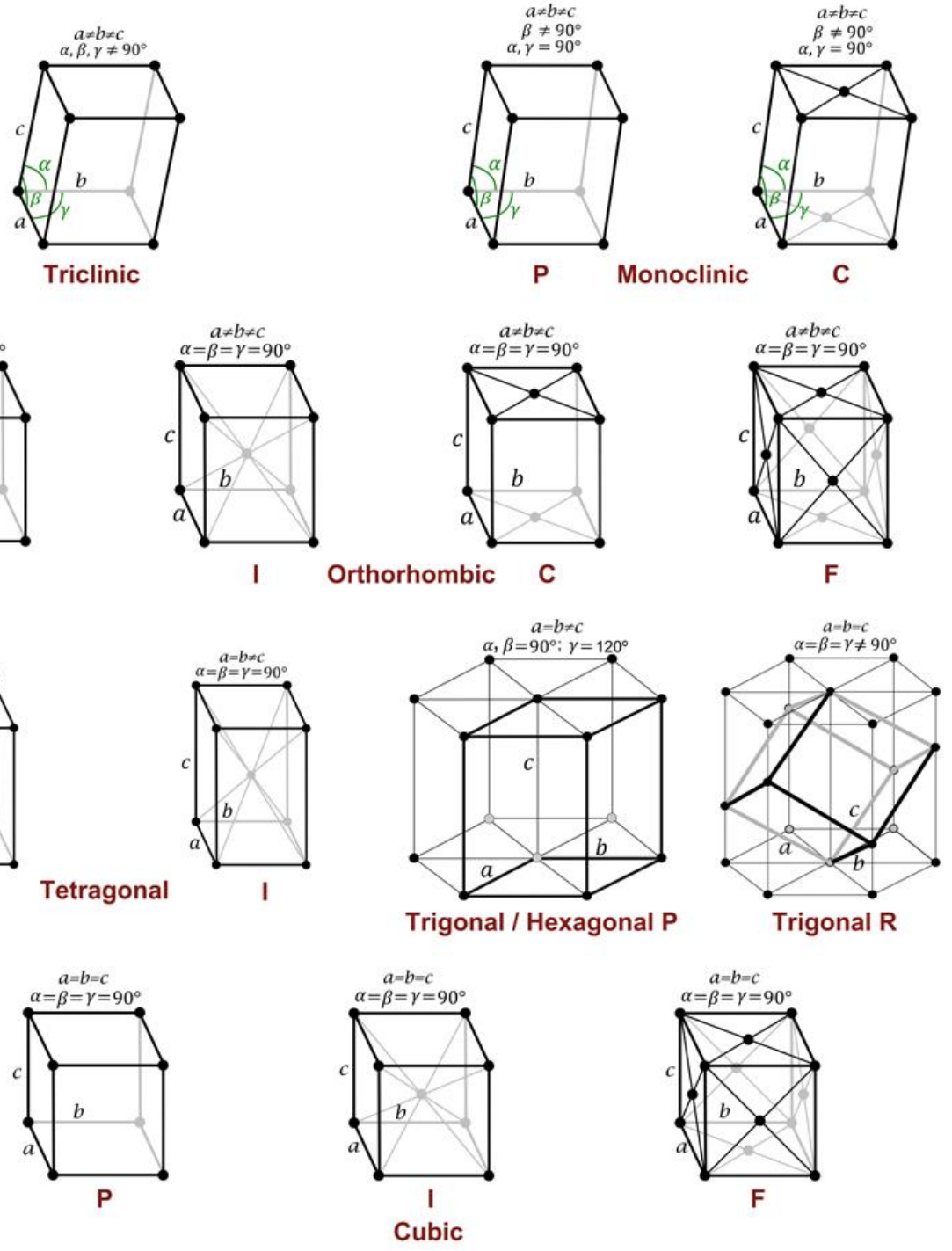
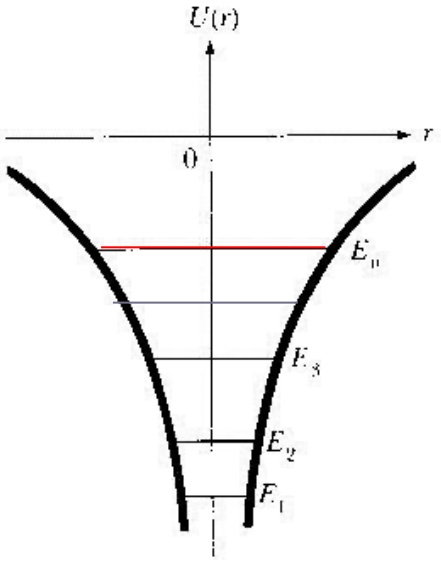
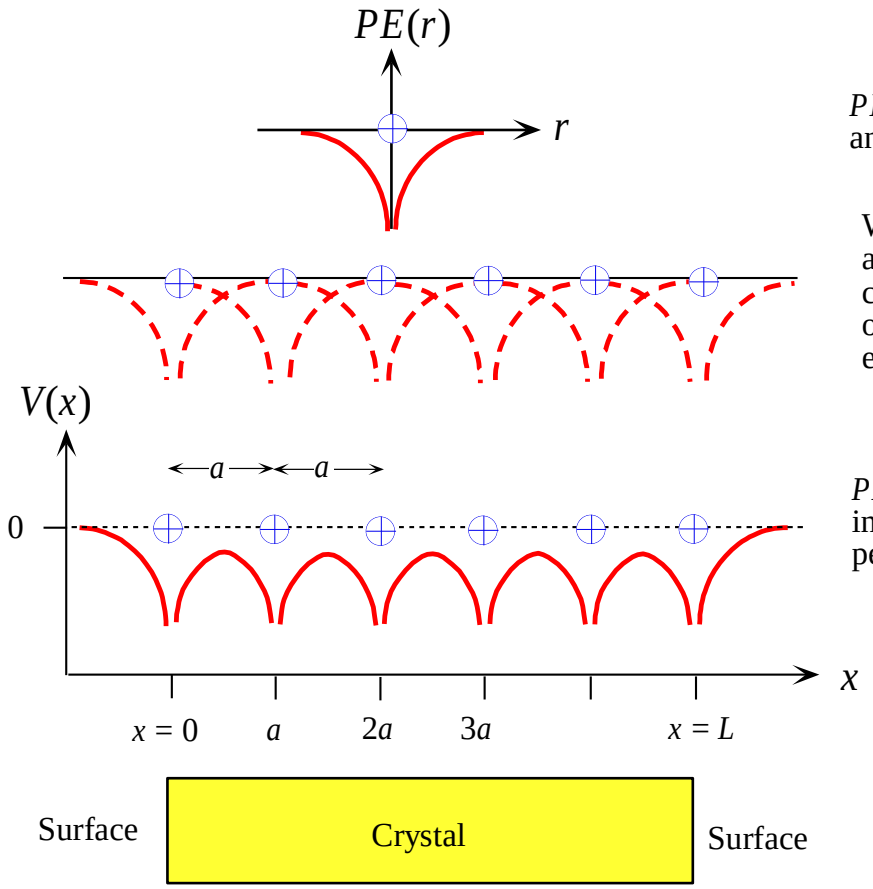
The 14 basic Bravais Lattices



Atomic Potential – Linear Array of Atoms



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



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*.

$$V(r) = \sum_n \frac{-qe^2}{4\pi\varepsilon_0 |r - na|}$$

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

Bloch Theory - Bloch's Waves (1D)

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

$$U(x+a) = U(x) = U(x+\mathrm{n}a)$$

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

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

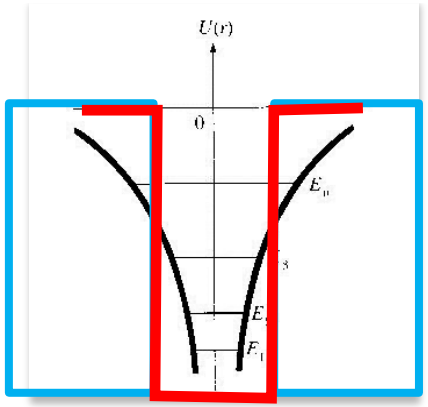
Where $$\Psi(x) = e^{ikx}u(x)$$

Kronig-Penney Model

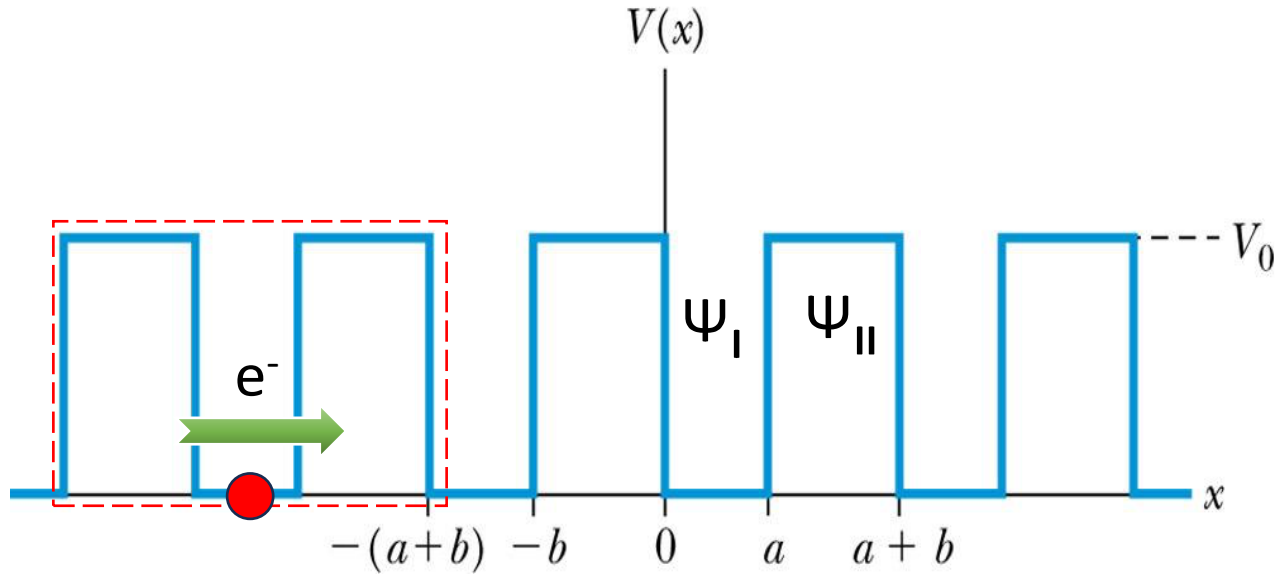
Approximate crystal periodic Coulomb potential by rectangular periodic potential

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x)$$

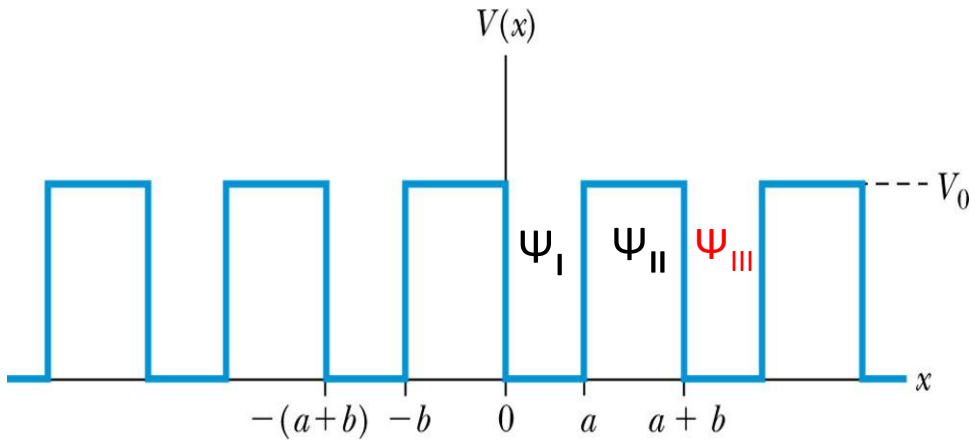
Single Atom



Linear Array of Atoms



Wavefunction Periodic Boundary Conditions



Region I: $\Psi_{\mathrm{I}} = Ae^{iKx} + Be^{-iKx}$

Region II: $\Psi_{\mathrm{II}} = Ce^{iQx} + De^{-iQx}$

Region III: Connected to Ψ_{II} via Bloch's Theorem

$$\Psi_{\mathrm{III}} = e^{ik(a+b)}\Psi_{\mathrm{II}}$$

$$K = \sqrt{\frac{2m}{\hbar^2}(E - V)} = \sqrt{\frac{2m}{\hbar^2}E} \qquad Q = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

Periodic Conditions

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

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

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

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

Solve the systems of 4 linear equations

Boundary between II and I, at $x = 0$

1) $\psi_{II}(x = 0) = \psi_{I}(x = 0)$

$$Ce^{0} + De^{0} = Ae^{0} + Be^{0} \rightarrow \underline{A + B = C + D}$$

2) $\psi'_{II}(x = 0) = \psi'_{I}(x = 0)$

$$QC - QD = iKA - iKB \rightarrow \underline{iK(A - B) = Q(C - D)}$$

Boundary between I and III, at $x = a$

3) $\psi_{I}(x = a) = \psi_{III}(x = a) = e^{ik(a+b)}\psi_{II}(x = -b)$

$$\underline{Ae^{iKa} + Be^{-iKa} = e^{ik(a+b)}[Ce^{-Qb} + De^{Qb}]}$$

$$0 = \begin{pmatrix} & M & \end{pmatrix}\begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix}$$

4) $\psi'_{I}(x = a) = \psi'_{III}(x = a) = e^{ik(a+b)}\psi_{II}{}'(x = -b)$

$$\underline{AiKe^{iKa} - BiKe^{-iKa} = e^{ik(a+b)}[CQe^{-Qb} - DQe^{Qb}]}$$

K-P Solution – Allowed energies and gaps

$$\boxed{\frac{Q^2 - K^2}{2QK}\sinh(Qb)\sin(Ka) + \cosh(Qb)\cos(Ka) = \cos[k(a+b)]}$$

Q and K have E in them, so in principle, given a k we can solve for E to get *E(k)*.
In practice must be done numerically.

$$K^2(a+b)^2 = \frac{2mE(a+b)^2}{\hbar^2} = 0.262468\ E_0(a_0+b_0)^2 = \varepsilon$$

$$Q^2(a+b)^2 = \frac{2m(U-E)(a+b)^2}{\hbar^2} = 0.262468\ (U_0 - E_0)(a_0+b_0)^2 = u - \varepsilon$$

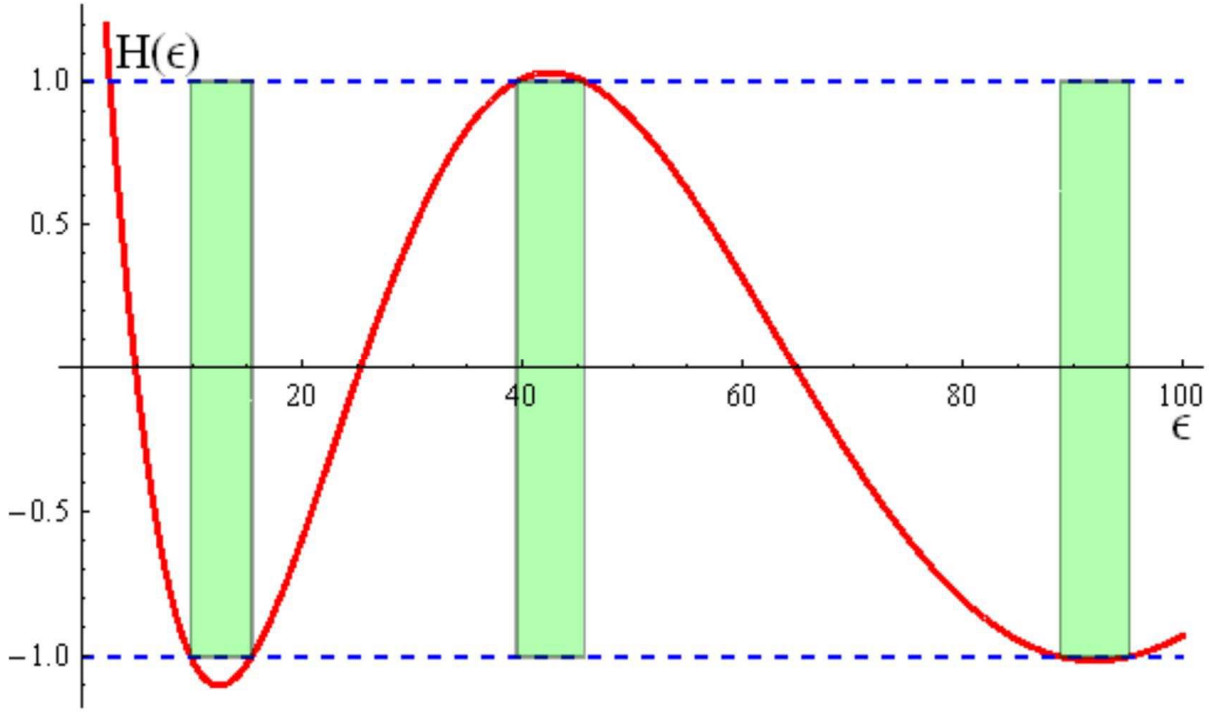
$$k(a+b) = \kappa$$

K-P Solution – Allowed energies and gaps

$$\frac{Q^2 - K^2}{2QK}\sinh(Qb)\sin(Ka) + \cosh(Qb)\cos(Ka) = \cos[k(a+b)]$$

$$H(\varepsilon) = \cos[\frac{\sqrt{\varepsilon}}{1+\alpha}]\cosh(\frac{\alpha\sqrt{u-\varepsilon}}{1+\alpha}] + \frac{(u-2\varepsilon)}{2\sqrt{u-\varepsilon}\sqrt{\varepsilon}}\sin(\frac{\sqrt{\varepsilon}}{1+\alpha})\sinh[\frac{\alpha\sqrt{u-\varepsilon}}{1+\alpha}] = \cos(\kappa)$$

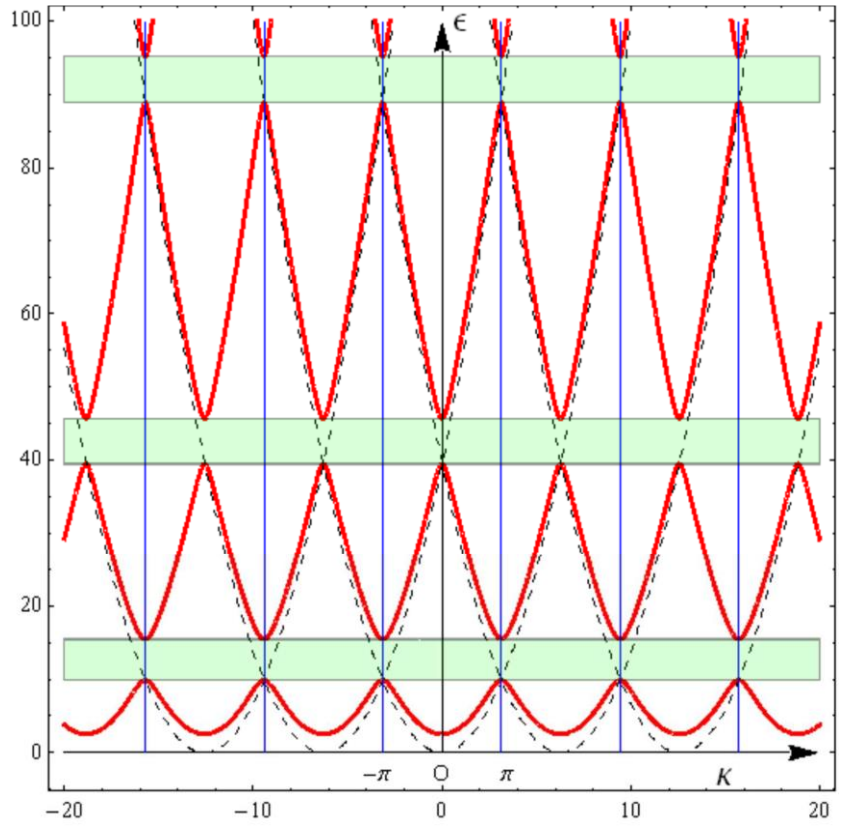
K-P Solution – Allowed energies and gaps

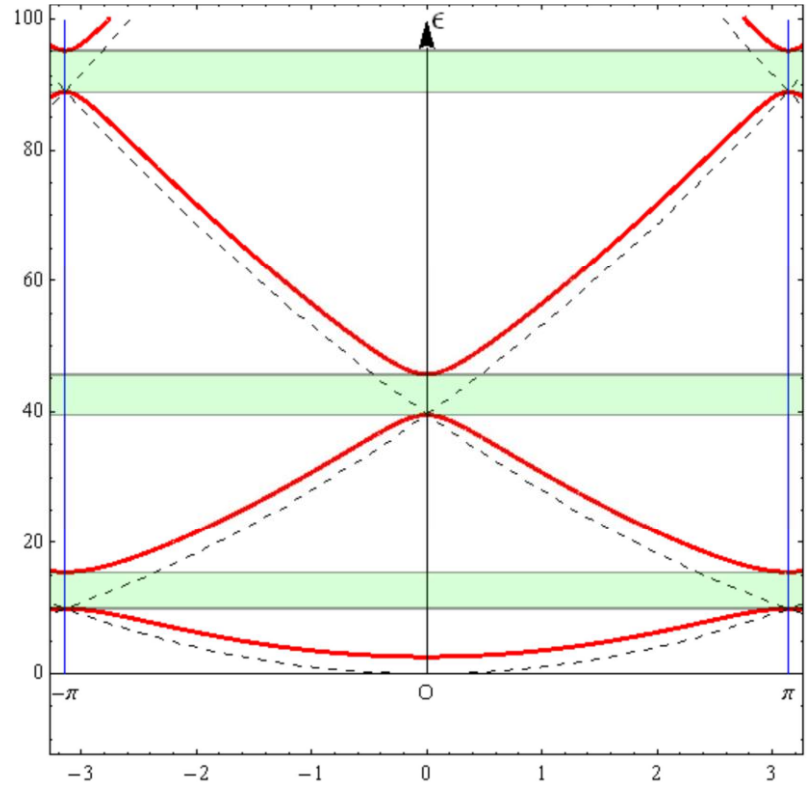


The right hand side of the Kronig-Penney expression, H(ε) as a function of ε, where u = 100. α = b/a = 0.1/3. The energy gap exists in the green zone where |H(ε)|>1. ε = (9.87507 - 15.4575). ε= (39.5002 - 45.6691), ε = (88.8754 - 95.1686), and ε = (158.0 - 164.288).

The energy gap width (Δε) is the same

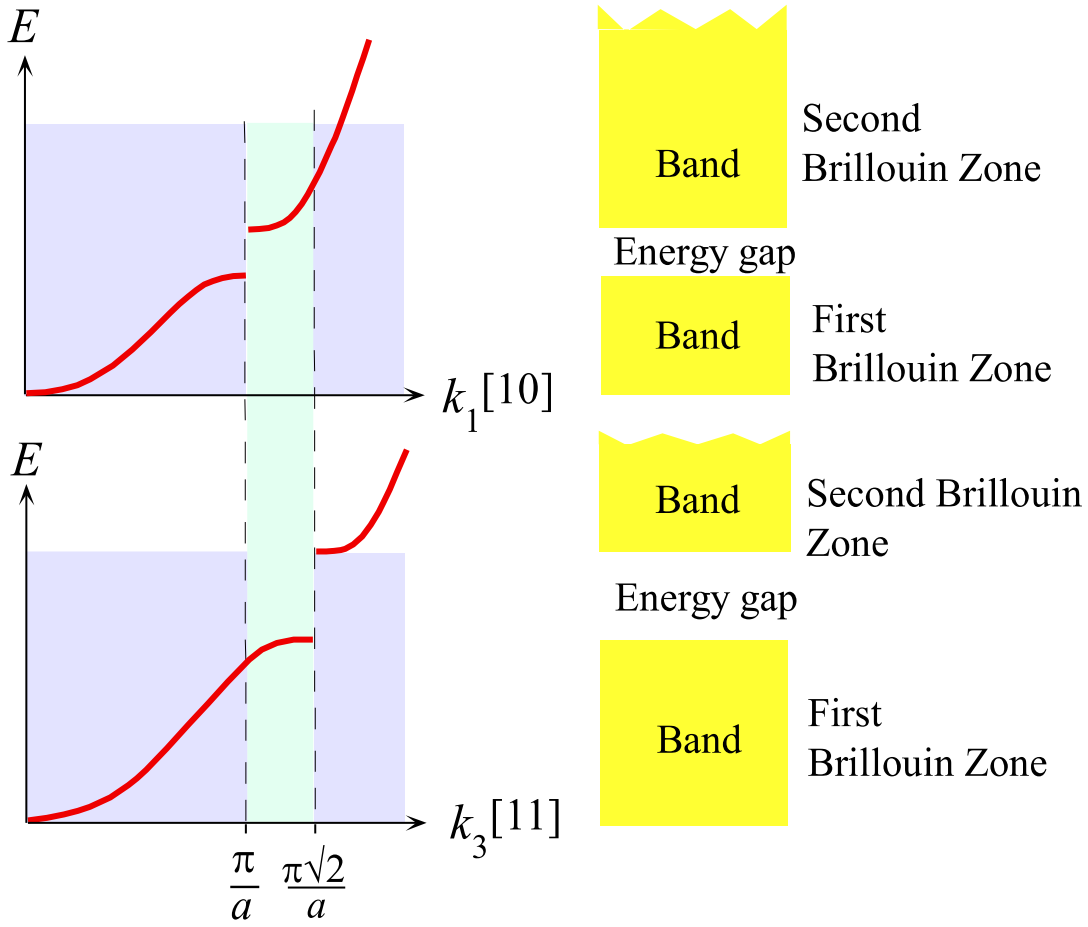
$E - k$ Diagrams (energy dispersion diagrams)





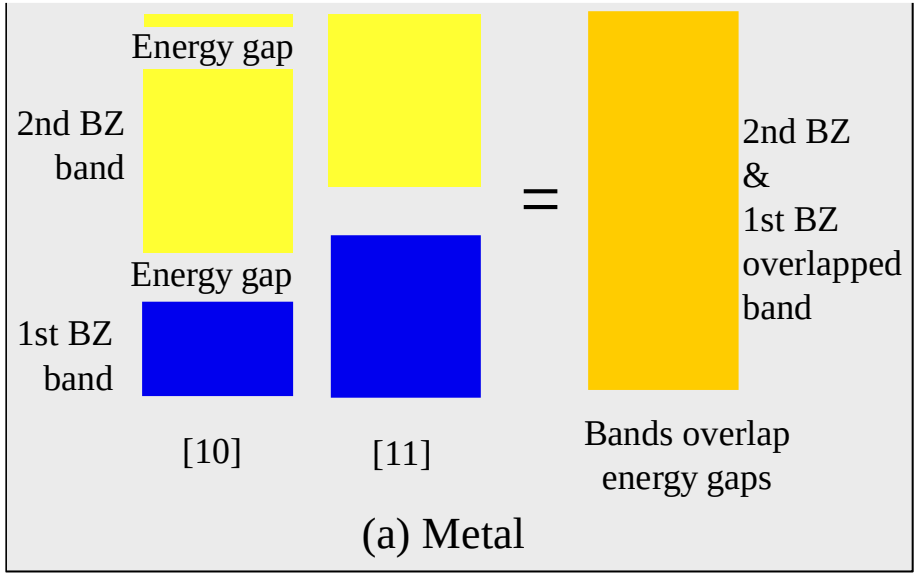
Kronig-Penney energy band in the reduced zone scheme. b/a = 0.1/3. u = 100.

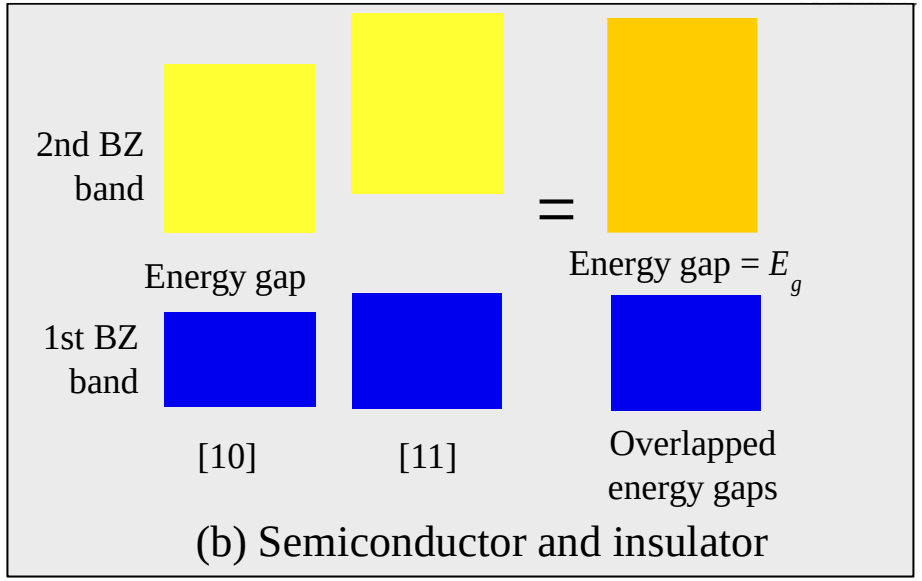
$E - k$ Diagrams (energy dispersion diagrams)



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 π √2/a along [11].

$E - k$ Diagrams (energy dispersion diagrams)

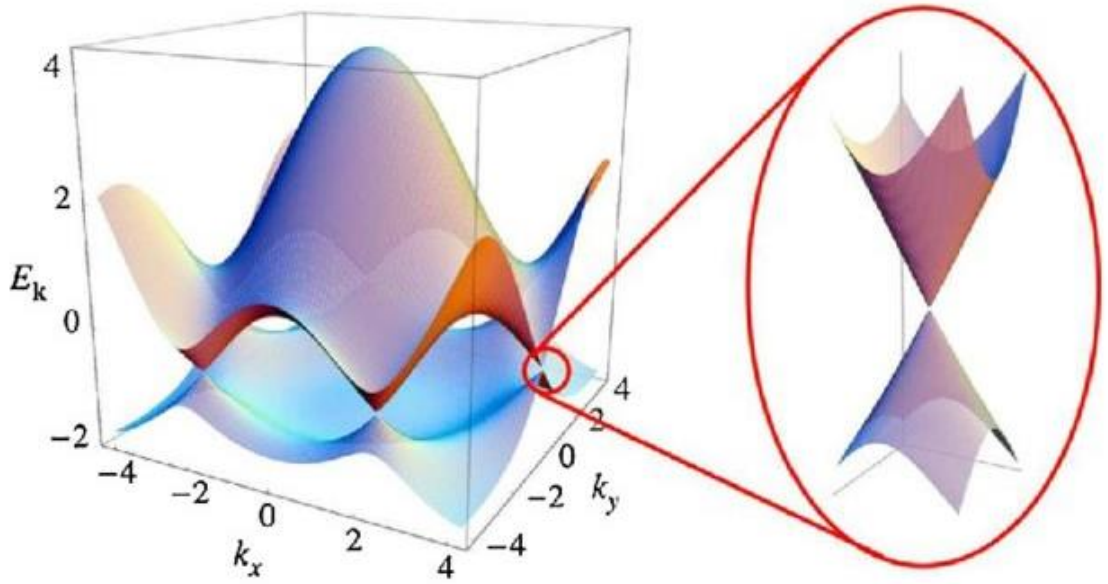




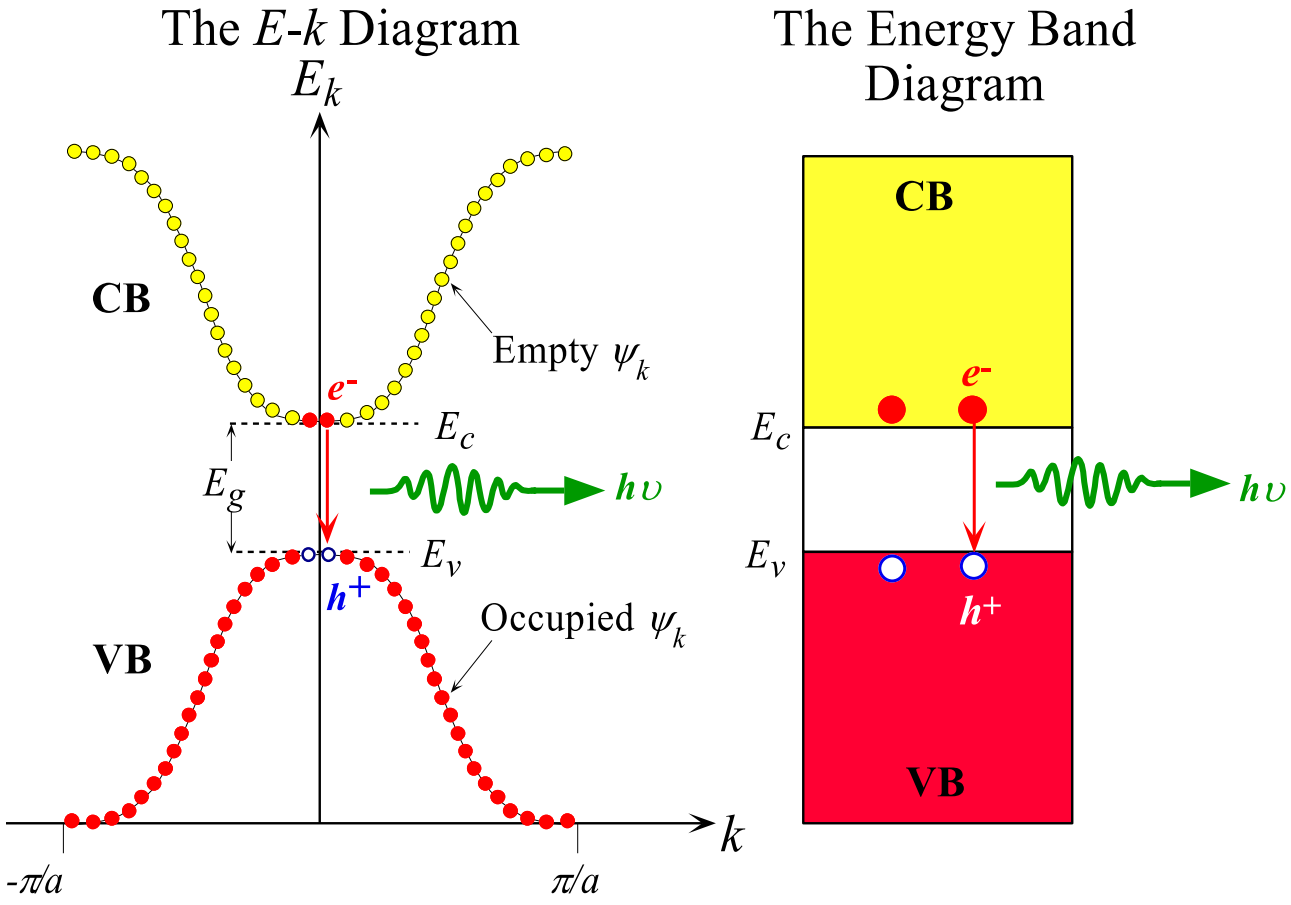
(a) Metal: For the electron in a metal there is no apparent energy gap because the 2nd BZ (Brillouin Zone) along [10] overlaps the 1st BZ along [11]. Bands overlap the energy gaps. Thus the electron can always find any energy by changing its direction.

(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, Eg.

Zero bandgap - Graphene

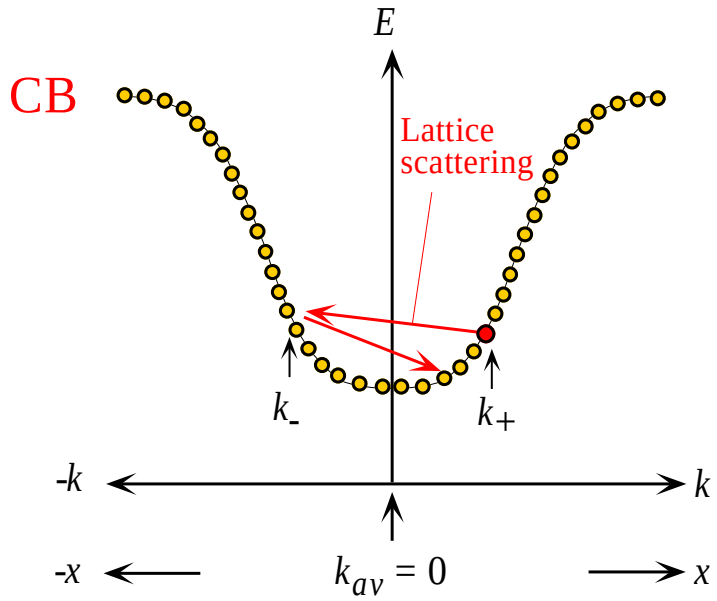


E – *k* Diagrams (energy dispersion diagrams)

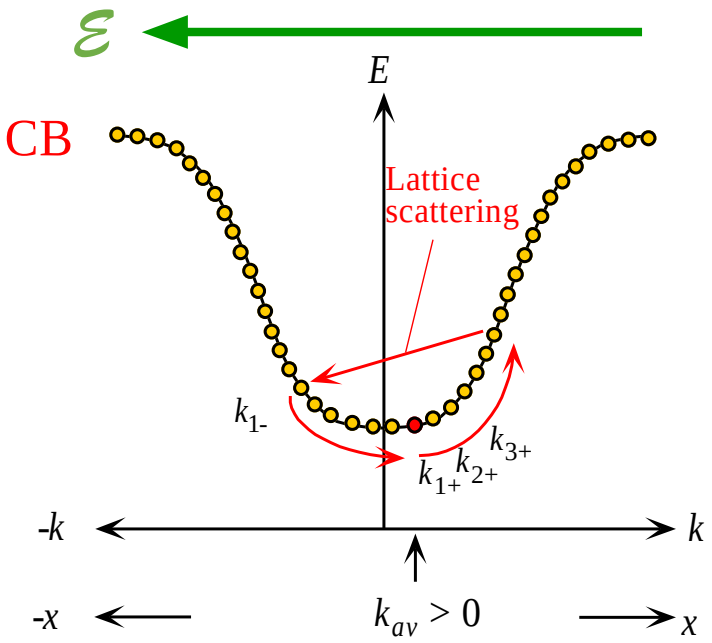


The E-k diagram of a direct bandgap semiconductor such as GaAs. The E-k curve consists of many discrete points each point corresponding to a possible state, wavefunction $\psi_k(x)$, that is allowed to exist in the crystal. The points are so close that we normally draw the E-k relationship as a continuous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

$E - k$ Diagrams – Electric field

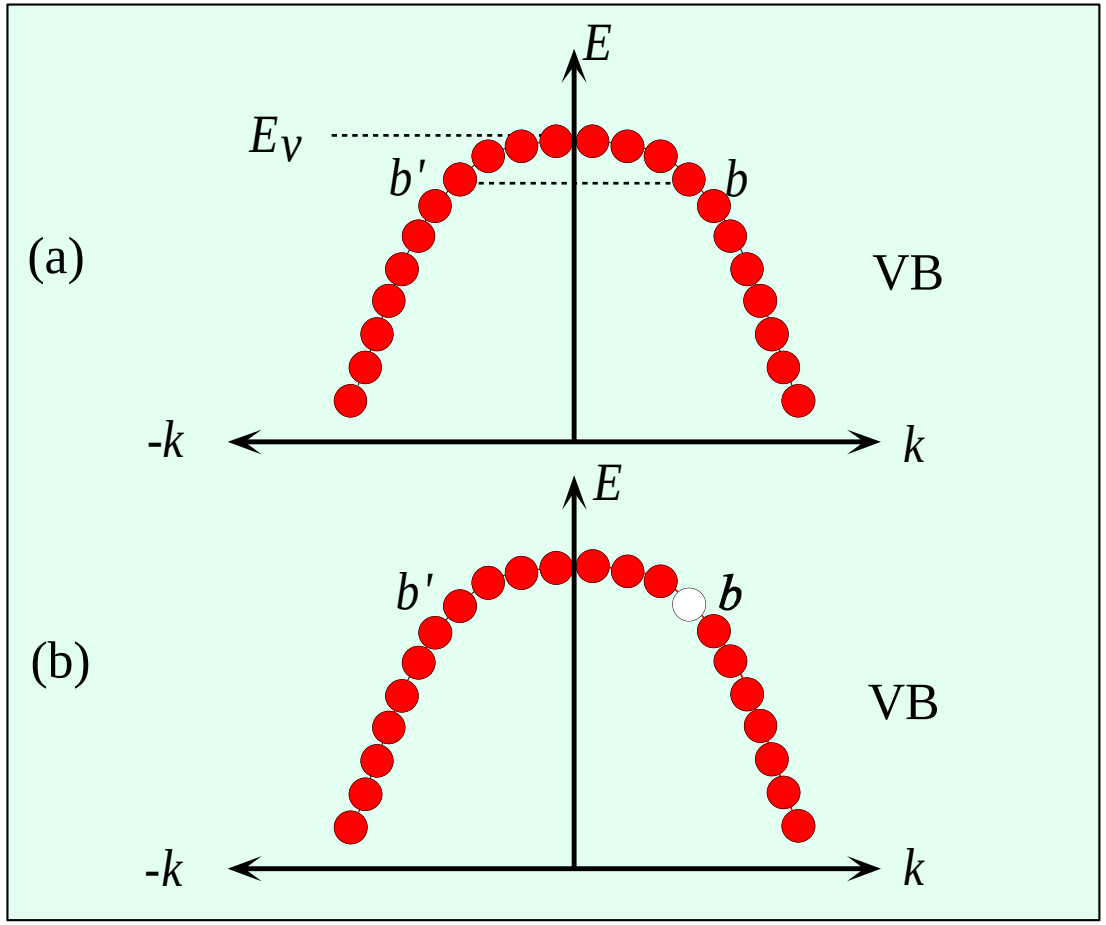


(a) In the absence of a field, over a long time, average of all k values is zero, there is no net momentum in any one particular direction.



(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.

$E - k$ Diagrams – Hole movement

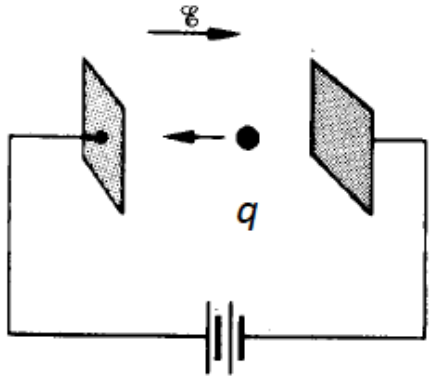


(a) In a full valence band there is no net contribution to the current. There are equal numbers of electrons (e.g. at b and b') with opposite momenta.

(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.

Effective mass

In vacuum

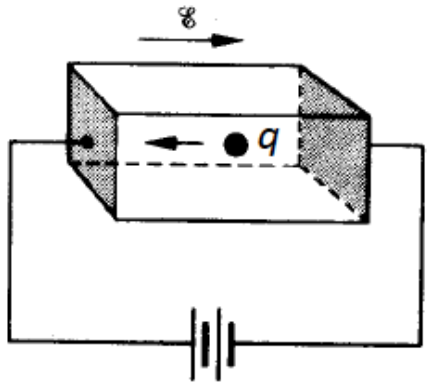


$F = q\,\varepsilon = m_o a$

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

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

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

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

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

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

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

Effective Mass

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

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

But $F_{ext} = m^* \alpha$, thus :

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

The End

THANK YOU

E-class Support

Lesson	Kassap	Hanson
1		Chap.5
2		
3		