Effective Mass

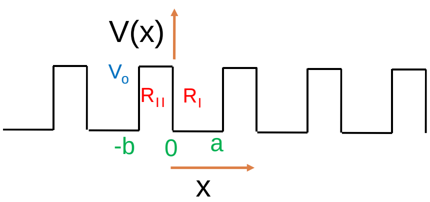
$$a = \frac{dv}{dt} = \frac{1}{\hbar}\frac{d}{dt}\left(\frac{dE}{dk}\right)$$

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

$$m^* \equiv \frac{\hbar^2}{\dfrac{d^2E}{dk^2}}$$

In all the above relations E vs. k relationship is critical as this determines the dynamical behavior of electron in the solid. This relationship is called Band-Structure of the Solid.

Kronig- Penny Model



$V = 0$ for $0 \le x < a$ $\quad R_I$

$V = V_o$ for $-b \le x < 0;\ V_o > 0$ $\quad R_{II}$

The potential structure is repeated infinitely. Clearly

$$V\left[x + n\left(a + b\right)\right] = V\left(x\right)$$

Consider an electron with $E < V_o$.

Solutions

$$\phi_I = Ae^{ik_1x} + Be^{-ik_1x}; \ \hbar k_1 \equiv \sqrt{2mE}$$
$$\phi_{II} = Ce^{\alpha x} + De^{-\alpha x}; \ \ \hbar\alpha \equiv \sqrt{2m(V_o - E)}$$

Boundary Conditions at x=0

$$A + B - C - D = 0$$
$$ik_1A - ik_1B - \alpha C + \alpha D = 0$$

How many more regions should we create and how many boundary conditions should we match?

Bloch's law applied

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

Note: k is different from k_1. In Bloch theorem, it is k, which is called wave vector not k_1. The term k_1 represents only energy. Wave vector k is same irrespective of the region.

$$Ae^{ik_1a} + Be^{-ik_1a}$$
$$-\left(Ce^{-\alpha b} + De^{\alpha b}\right)e^{ik(a+b)} = 0$$
$$Aik_1e^{ik_1a} - ik_1Be^{-ik_1a}$$
$$-\alpha\left(Ce^{-\alpha b} - De^{\alpha b}\right)e^{ik(a+b)} = 0$$

$$A + B - C - D = 0$$
$$ik_1 A - ik_1 B - \alpha C + \alpha D = 0$$
$$Ae^{ik_1 a} + Be^{-ik_1 a}$$
$$-\left(Ce^{-\alpha b} + De^{\alpha b}\right) e^{ik(a+b)} = 0$$
$$Aik_1 e^{ik_1 a} - ik_1 Be^{-ik_1 a}$$
$$-\alpha\left(Ce^{-\alpha b} - De^{\alpha b}\right) e^{ik(a+b)} = 0$$

$$\begin{vmatrix} 1 & 1 & -1 & -1 \\ ik_1 & -ik_1 & -\alpha & \alpha \\ e^{ik_1 a} & e^{-ik_1 a} & -e^{-ab}e^{ik(a+b)} & -e^{ab}e^{ik(a+b)} \\ ik_1 e^{ik_1 a} & -ik_1 e^{-ik_1 a} & -\alpha e^{-ab}e^{ik(a+b)} & \alpha e^{-ab}e^{ik(a+b)} \end{vmatrix} = 0$$

$$\left[\frac{\alpha^2 - k_1^{\,2}}{2\alpha k_1}\right] \sinh \alpha b \sin k_1 a$$
$$+ \cosh \alpha b \cos k_1 a = \cos k(a+b)$$

In the limit

$V_o \to \infty \;\&\; b \to 0$

Such that

$V_0 b = \text{constant}$

This equation can be simplified.

$$P\frac{\sin k_1 a}{k_1 a} + \cos k_1 a = \cos ka$$
$$\hbar k_1 = \sqrt{2mE}$$
$$P = \frac{m\left(V_o b\right)a}{\hbar^2}$$

Note: We use a single block wave vector for all the regions unlike step potentials that we had dealt earlier.

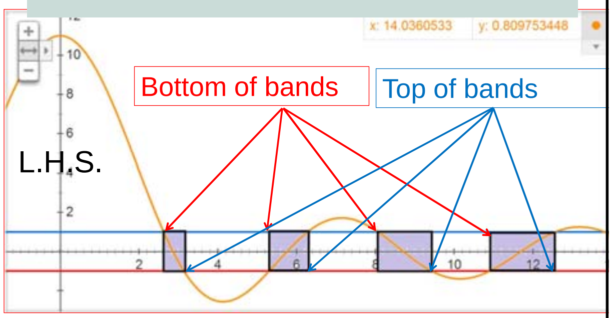
For $k_1 a \to 0$ L.H.S.= $1 + P$

For $k_1 a = \pi$ L.H.S.= -1

For $k_1 a = 2\pi$ L.H.S.= $+1$

Note: Energy depends on k_1.

Allowed Bands



$k_1 a$

Important Features

- The solution gives allowed band of energies separated by not-allowed gaps.
- Width of the band increases as energy increases.

Top of the bands

The top of the energy band corresponds to

$$k_1 = \frac{n\pi}{a}$$

$$\varepsilon_{n,t} = \frac{n^2\hbar^2\pi^2}{2ma^2}$$

Other Features

- The energy of the bottom of the band would depend on *P*.
- For $P \to \infty$, the bands would reduce to a single level.

E-k Relationship

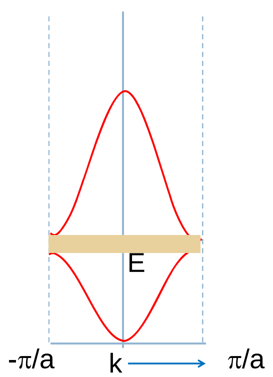
- Assign a value of *k* within each band.
- There are multiple ways the *k* can be assigned.

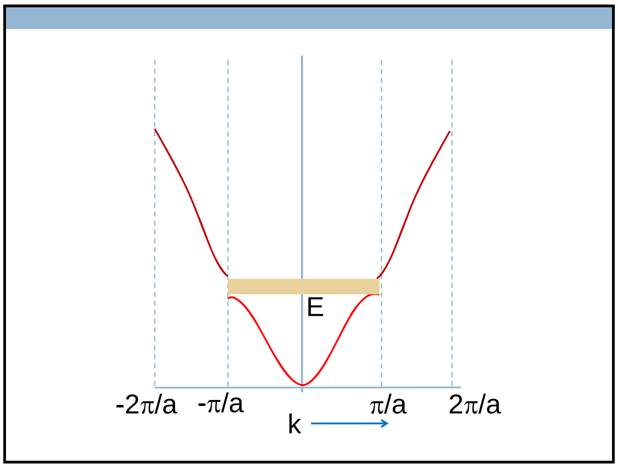
Two Conventions

- Start from zero value of *k* and let it increase continually, as we go from one band to another.(Extended Zone Scheme).
- Restrict the k values to

$$-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$$

(Reduced Zone Scheme)




E
-2π/a
-π/a
π/a
2π/a
k