Nalanda Open University

M.SC Part-1

Course : Physics

Paper : 7

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Topic- Condensed Matter (Kronig-Penny Model)

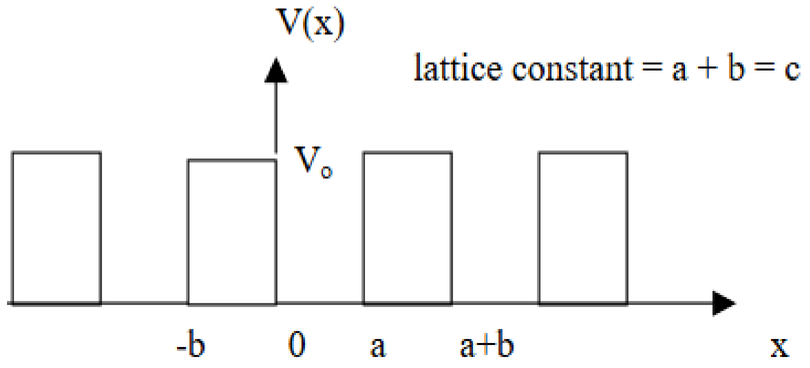
Kronig - Penny Model

The Kronig -Penney model is a solvable problem in quantum mechanics that can either be viewed as an approximation of an electron in a 1D crystal potential or a generalization of a potential-barrier problem to a 1D chain of potential barriers. The problem consists of a particle inside an array of equally spaced potential wells or potential barriers, all which have the same width and depth/height.

This can be viewed as a simple model for a 1D monoatomic crystal, which is characterized by electrons existing around positively charged nuclei, each equally spaced from its neighbor.

Most significantly, solutions to the Kronig-Penney model manifest ‘band gaps’ (a band of energies that electrons cannot assume) , which are physically seen in real materials, most notably in semiconductors.

Consider the following idealized crystal potential:



We assume $E < V_o$

for $0 \le x \le a$:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$$

and

$$\psi = A\sin\alpha x + B\cos\alpha x \qquad \frac{d\psi}{dx} = A\alpha\cos\alpha x - B\alpha\sin\alpha x \qquad \alpha = \frac{\sqrt{2mE}}{\hbar}$$

and for $-b \le x \le 0$:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_o)\psi = 0$$

Solution is periodic, barrier of limited thickness - solution does not continue decaying to zero. There is tunneling between wells.

$$\psi = C\sinh(\gamma x) + D\cosh(\gamma x) \qquad \frac{d\psi}{dx} = C\gamma\cosh(\gamma x) + D\gamma\sinh(\gamma x)$$

$$\gamma = \frac{\sqrt{2m(V_o - E)}}{\hbar}$$

ψ must be continuous at $x = 0$, so $B = D$.

Also, $\frac{d\psi}{dx}$ must be continuous at $x = 0$, so $A\alpha = C\gamma$ or $C = (\alpha/\gamma)A$

From Bloch's theorem (Periodic potential)

$$\psi(x) = U(x)e^{jkx}$$

and

$$\psi(a) = e^{jk(a+b)}\psi(-b)$$

$$\frac{d\psi}{dx}\Big|_a = e^{jk(a+b)}\frac{d\psi}{dx}\Big|_{-b}$$

Therefore

$$A\sin\alpha a + B\cos\alpha a = e^{jk(a+b)}(A\sinh(-\gamma b) + B\sinh(-\gamma b))$$

$$A\left[\sin(\alpha c) + \frac{\alpha}{\gamma}e^{jk(a+b)}\sinh(\gamma b)\right] + B\left[\cos(\alpha c) - e^{jk(a+b)}\cosh(\gamma b)\right] = 0 \qquad (1)$$

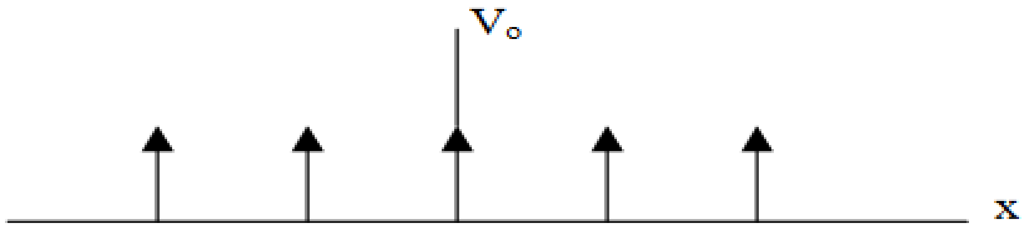
and

$$A\alpha\left[\cos(\alpha c) - e^{jk(a+b)}\cosh(\gamma b)\right] + B\left[-\alpha\sin(\alpha c) + \gamma e^{jk(a+b)}\sinh(\gamma b)\right] = 0 \qquad (2)$$

Equations (1) and (2) have a non-trivial solution (i.e. a solution other than A=B=0 only if

$$\frac{\gamma^2 - \alpha^2}{2\alpha\gamma}\sin(\alpha c)\sinh(\gamma b) + \cos(\alpha c)\cosh(\gamma b) = \cos(k(b + c)) \qquad (3)$$

At this point it is convenient to consider the special case in which b->0 and V_o-> infinity (makes things a little simpler – no problem for E>V_o transition) while the product $V_o b$ remains constant.

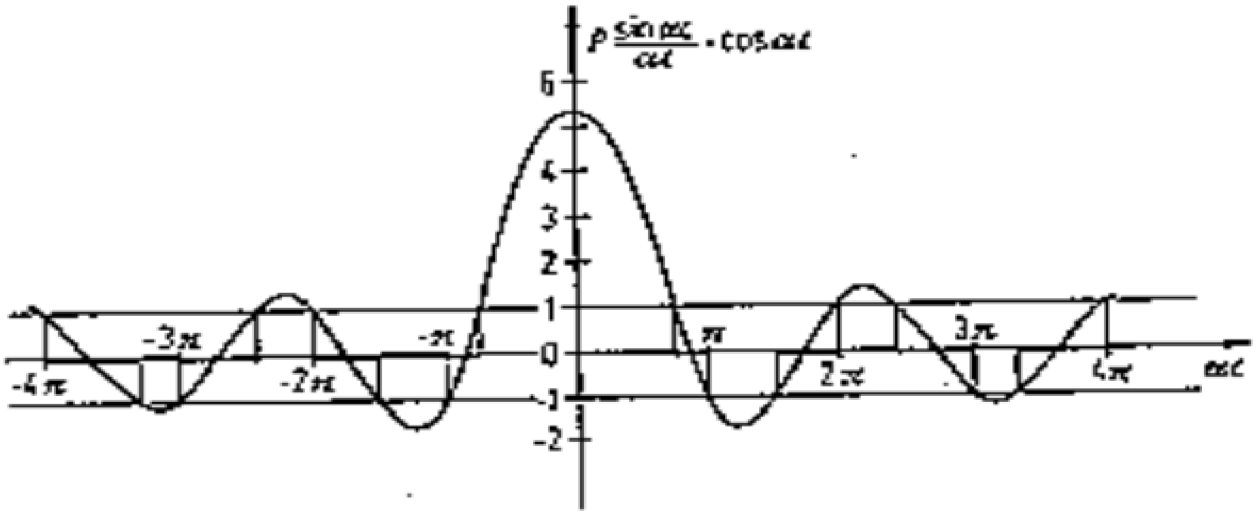


Delta Function Potential

Letting $P = (mV_o bc)/H^2$, (3) becomes

$$\frac{\frac{P}{\alpha c}\sin(\alpha c) + \cos(\alpha c)}{\text{(term i)}} = \frac{\cos(kc)}{\text{(term ii)}}$$

This can be solved graphically. Solutions for P = 3π/2 (corresponding to a high barrier) are shown below. We plot (i) and (ii) as function of αc.

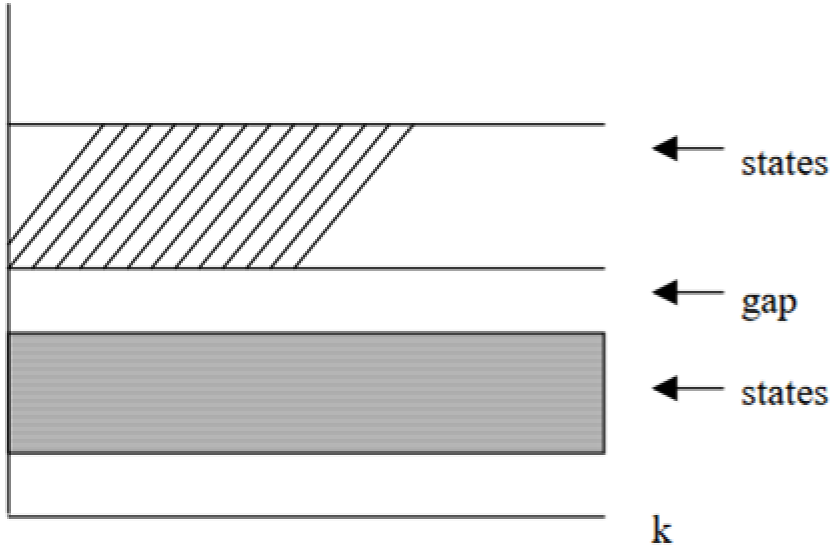


We can only have a Solution for this when

$$\frac{P}{\alpha c}\sin(\alpha c) + \cos(\alpha c) \leq 1$$

and as cos(kc) ≤ 1 always we have a valid solution for ranges of αc which implies a valid solution for particular energy regions.

E

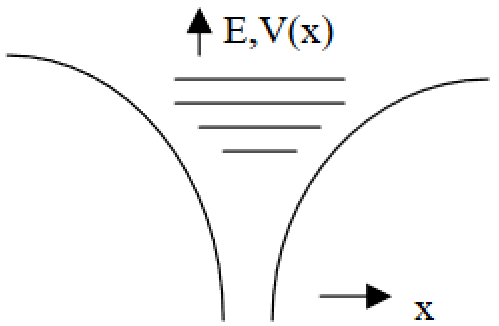


We therefore find there are α's for which there is no valid K. As $E = \frac{\hbar^2}{2m}\alpha^2$

This means there are disallowed regions of energy, i.e., energy gaps.

Energies and wave functions for electrons in crystal (periodic potential V(x))

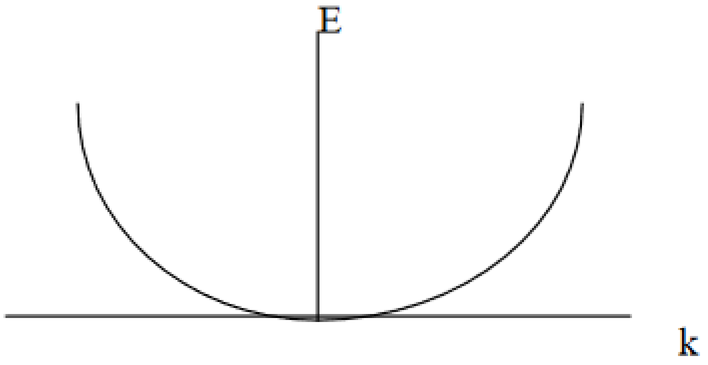
a) Isolated Potential well



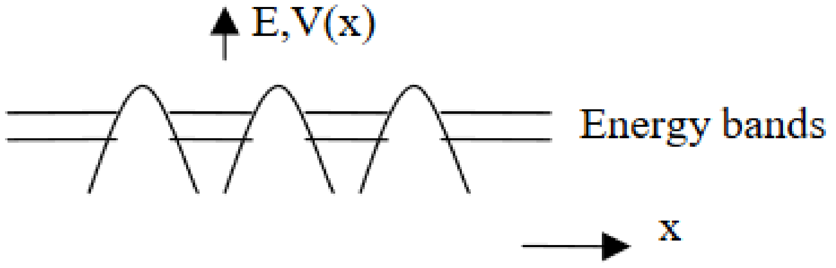
- only discrete energies E allowed
- wave functions are standing waves

b) Free Electrons $\psi(x) = Ce^{jkx}$ $\Psi(x,t) = Ce^{j(kx-\omega t)}$

- plane wave solutions
- any energy allowed: $E = \frac{\hbar^2 k^2}{2m}$
- Parabolic E versus k



c) Periodic Potential



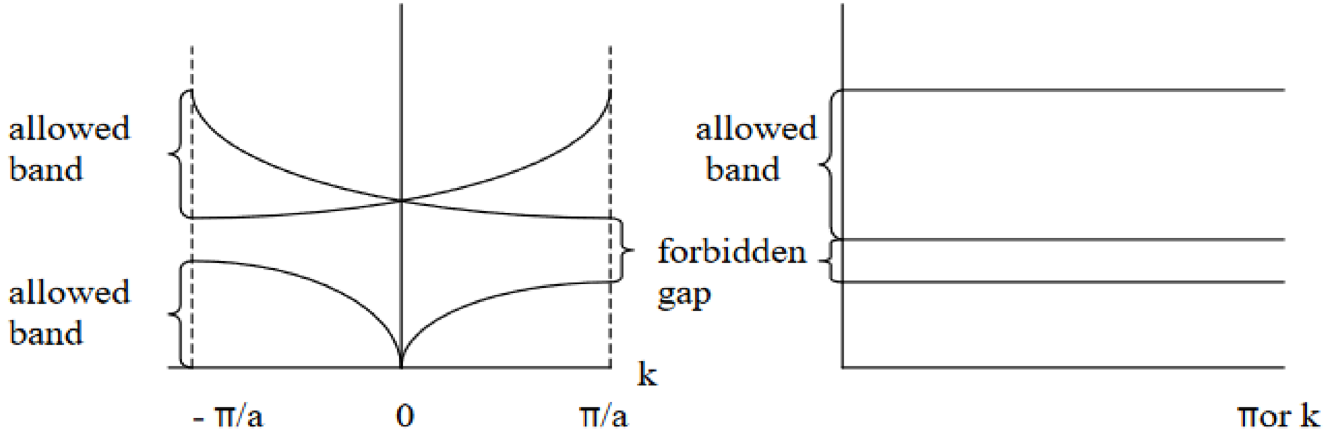
- ability of electrons to tunnel between barrier walls spreads out the discrete energy levels seen for isolated wells into bands

- We fine a number of bands of energies are allowed.
- We have restricted K values: $(-\pi / a \leq k \leq \pi / a)$
- The wave functions are Block waves: $\psi_k(x) = U_k(x)Ce^{jkx}$

$\psi_k(x,t) = U_k(x)e^{j(kx-\omega t)}$ - which is modulated travelling wave

- Waves functions act like free electrons (almost)

Simplified energy diagram:



General results from Kronig-Penney model:

- if potential barrier between wells is strong, energy bands are narrowed and spaced far apart

(Corresponds to crystals in which electrons are tightly bond to ion cores, and wavefunctions do not overlap much with adjacent cores. Also true for lowest energy bands)

- if potential barrier between wells is weak, energy bands are wide and spaced close together (this is typically situation for metals with weakly bond electrons – e.g. alkali metals. Here the “nearly free” electron model works well.)