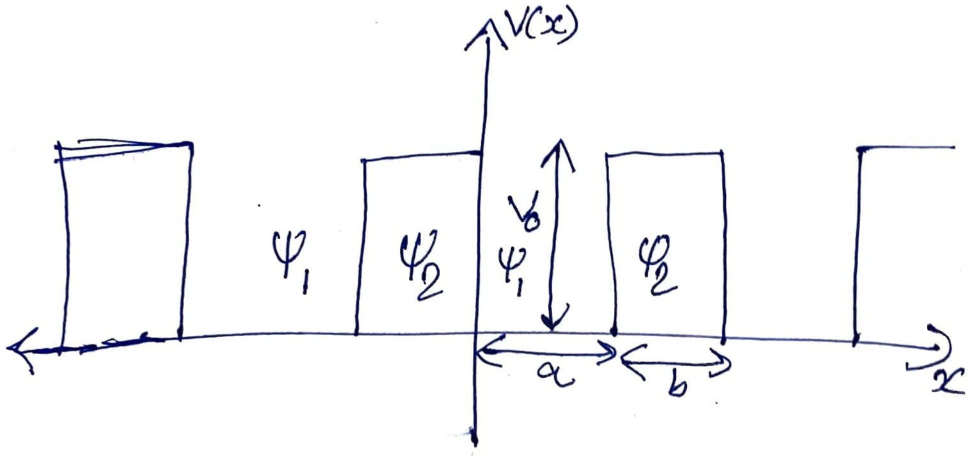
SARTHAK
Q3
7061086009

In Kronig-Penney model, we consider a single electron moving in a one-dimensional crystal with Potential energy being a periodic array of square wells.



TISE gives $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left[E - V(x)\right]\psi = 0$

For $0 < x < a \Rightarrow V(x) = 0$

$a < x < b \Rightarrow V(x) = V_0$

$\therefore$

$$\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} = -E\psi_1$$

&

$$\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} = V_0\psi_2 - E\psi_2$$

SARTHAK
Q3
7061086009

Now we exploit the Bloch theorem:

$$H = -\frac{\hbar^2 \nabla^2}{2m} + V(r)$$ where $V(r)$ is periodic

$$\Downarrow$$

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

$\therefore$ Putting $\psi_1(x) = u_1(x) e^{ikx}$

& $\psi_2(x) = u_2(x) e^{ikx}$

gives:

$$\frac{d^2(u_1(x))}{dx^2} + 2ik \frac{d(u_1(x))}{dx} + (\alpha^2 - k^2) u_1(x) = 0$$

for $0 < x < a$

&

$$\frac{d^2 u_2}{dx^2} + 2ik \frac{du_2}{dx} - (\beta^2 + k^2) u_2 = 0$$

for $a < x < b$
or
$-b < x < 0$

where $\alpha = \sqrt{\frac{2mE}{\hbar^2}}$ & $\beta = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$

SARTHAK
Q3
7061086009

Solving the two DEs gives:

$$u_1(x) = Ae^{i(\alpha-k)x} + Be^{-i(\alpha+k)x}$$

$$u_2(x) = Ce^{(\beta-ik)x} + De^{-(\beta+ik)x}$$

Now we apply the boundary conditions:

$$u_1(0) = u_2(0)$$

$$u_1(a) = u_2(-b)$$

$$\left(\frac{du_1}{dx}\right)_{x=0} = \left(\frac{du_2}{dx}\right)_{x=0}$$

& $$\left(\frac{du_1}{dx}\right)_{x=a} = \left(\frac{du_2}{dx}\right)_{x=-b}$$

Applying these conditions shall lead us to:

$$\boxed{\frac{\beta^2-\alpha^2}{2\alpha\beta}\sinh(\beta b)\sin(\alpha a) + \cosh(\beta b)\cos(\alpha a) = \cos k(a+b)}$$

SARTHAK
Q3
2061086009

We make a further simplification by assuming $b \to 0$ as $V_0 \to \infty$, i.e. potential barrier as a delta funcⁿ.

This gives

$$\frac{mV_0 b}{\hbar^2 \alpha} \sin \alpha a + \cos \alpha a = \cos ka$$

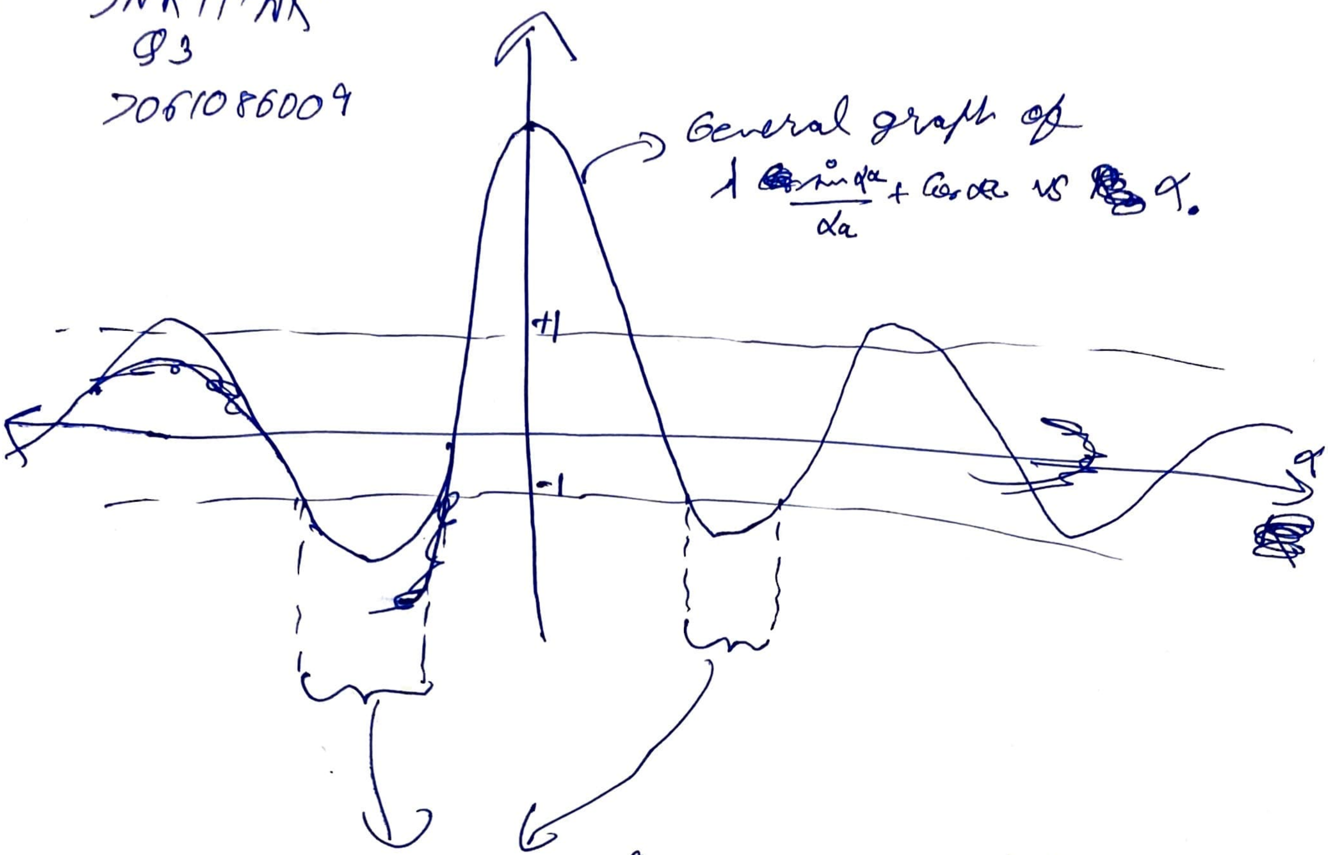
$$\Rightarrow \boxed{\frac{mV_0 ba}{\hbar^2} \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka}$$

Since $-1 \leq \cos ka \leq 1$, $\therefore$ only several energy bands are allowed (only those which make LHS lie b/w -1 & 1)

As α is directly related to energy since $\alpha = \sqrt{\frac{2mE}{\hbar^2}}$.

SARTHAK
Q3
7061086004

→ General graph of $\lambda \frac{\sin \alpha a}{\alpha a} + \cos \alpha a$ vs α.



These portions where $\lambda \frac{\sin \alpha a}{\alpha a} + \cos \alpha a$ become < -1 or > 1 are forbidden regions.

For very weak potentials:

$V_0 \to 0$

$\Rightarrow \cos \alpha a = \cos ka \Rightarrow \alpha = k \Rightarrow E = \frac{\hbar^2 \alpha^2}{2m}$

$\Downarrow$

free electron case. $E = \frac{\hbar^2 k^2}{2m}$

∴ As barrier strength decreases, allowed bands get wider.

For very large potentials :

$$V_0 \to \infty$$

$$\Downarrow$$

$$\frac{\sin a\alpha}{a\alpha} \to 0 \Rightarrow a\alpha = n\pi$$

$$\Rightarrow \alpha = \frac{n\pi}{a}$$

$$\Rightarrow E = \frac{\hbar^2\alpha^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$$

where $n = 0, 1, 2, 3, \ldots$

discrete possible energy levels (Not bands).

SARTHAK
03
7061086009