Kronig Penney Model

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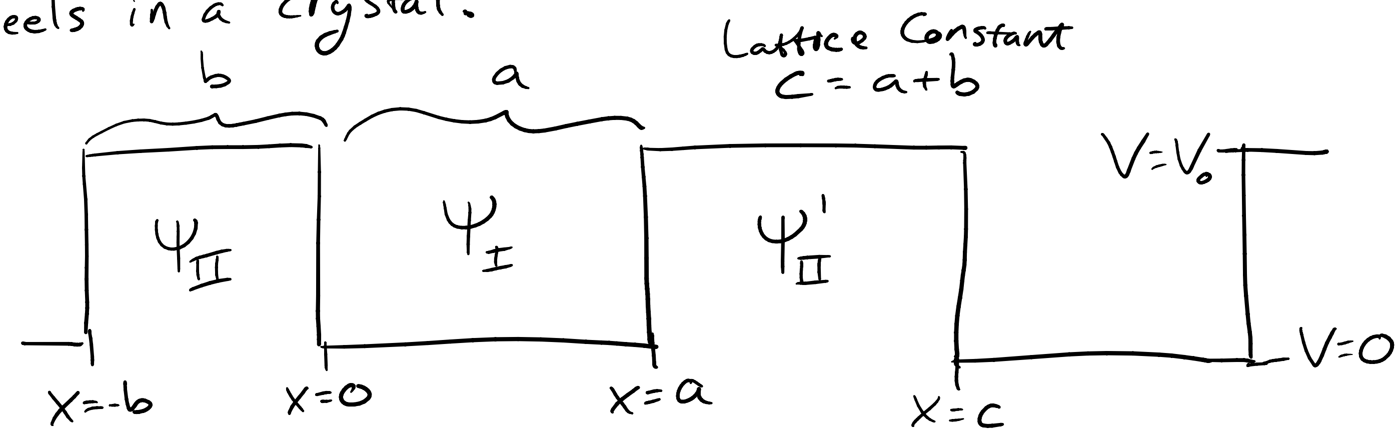
The Kronig-Penney model consists of a periodic lattice of finite square wells. It serves as a very simple model for the potential an electron feels in a crystal.



According to Schrödinger's equation, the eigenstates obey:

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

In our case $V(x)$ is piecewise constant:

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

If we want to find solutions with energy, E, where

$$0 \leq E \leq V_0$$

Then the solutions in each region are:

$$\psi_I = Ae^{i\alpha x} + Be^{-i\alpha x} \qquad \psi_{II} = Ce^{\beta x} + De^{-\beta x}$$

$$\alpha = \sqrt{\frac{E2m}{\hbar^2}} \qquad \beta = \sqrt{\frac{(V_0 - E)2m}{\hbar^2}}$$

In order to make more progress, we need to apply the appropriate boundary conditions.

There are two boundaries, at $x=0$ + $x=a$.

1) $\psi_I(x=0) = \psi_{II}(x=0)$ 3) $\psi_I(x=a) = \psi'_{II}(x=a)$

2) $\left.\frac{d\psi_I}{dx}\right|_{x=0} = \left.\frac{d\psi_{II}}{dx}\right|_{x=0}$ 4) $\left.\frac{d\psi_I}{dx}\right|_{x=a} = \left.\frac{d\psi'_{II}}{dx}\right|_{x=a}$

So we need $\psi'_{II}(x)$, which we can get from Bloch's Theorem, which says that for a potential that obeys $V(x+c) = V(x)$, the wave function obeys

$$\psi(x+c) = e^{ikc}\psi(x)$$

This implies that the wavefunction can be written as:

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

where $u(x+c) = u(x)$ (Periodic)

$$u_I = Ae^{i(\alpha-k)x} + Be^{-i(\alpha+k)x}, \quad u_{II} = Ce^{(\beta-ik)x} + De^{-(\beta+ik)x}$$

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So boundary conditions 3) and 4) become

3) $u_I(x=a) = u_{II}'(x=a) = u_{II}(x=-b)$

4) $\left.\dfrac{du_I}{dx}\right|_{x=a} = \left.\dfrac{du_{II}}{dx}\right|_{x=-b}$

These boundary conditions yield

1) $A + B = C + D$

2) $i\alpha A - i\alpha B = \beta C - \beta D$

3) $Ae^{i(\alpha-k)a} + Be^{-i(\alpha+k)a} = Ce^{(ik-\beta)b} + De^{(ik+\beta)b}$

4) $Ai(\alpha-k)e^{i(\alpha-k)a} - Bi(\alpha+k)e^{-i(\alpha+k)a}$
$= C(\beta-ik)e^{-(\beta-ik)b} - D(\beta+ik)e^{(\beta+ik)b}$

Writing this as a matrix equation yields:

$$\begin{bmatrix} 1 & 1 & -1 & -1 \\ i\alpha & -i\alpha & -\beta & +\beta \\ e^{i(\alpha-k)a} & e^{-i(\alpha+k)a} & -e^{(ik-\beta)b} & -e^{(ik+\beta)b} \\ i(\alpha-k)e^{i(\alpha-k)a} & -i(\alpha+k)e^{-i(\alpha+k)a} & -(\beta-ik)e^{(ik-\beta)b} & (\beta+ik)e^{(ik+\beta)b} \end{bmatrix} \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix}$$

$$i(\alpha-k)e^{i(\alpha-k)a} \quad -i(\alpha+k)e^{-i(\alpha+k)a} \quad -(\beta-ik)e^{(ik-\beta)b} \quad (\beta+ik)e^{(ik+\beta)b}$$

$$= 0$$

<u>Note</u> Enforcing Bloch's Theorem, equations 3) + 4), automatically means that the wavefunctions obey the appropriate continuity and smoothness conditions at every other well. So by solving these equations, we find the wavefunction at every point in the lattice.