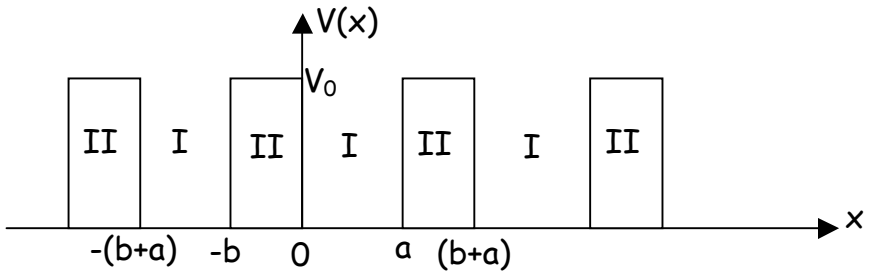
The Kronig-Penney one-dimensional model

Purpose: to demonstrate that in solids, where many atoms stay closely, the interference between atoms will create allowed and forbidden bands of energy for electrons.

To simplify the analysis, we only consider a one-dimensional system where atoms are aligned and equally spaced. This constructs a one-dimensional potential function:



Where V_0 is the value of potential barrier; *a* and *b* are lattice constant, represent distance between atoms.

For an electron traveling in the x-direction in free-space, the general solution of the wave equation is,

$$\psi(x) = \exp(jkx)$$

Now, within this periodic potential structure, the solution should be modified,

$$\psi(x) = u(x)\exp(jkx)$$

Bring this assumed solution back to the Schrodinger equation,

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

In region I, where V(x) = 0, we have,

$$\frac{d^2u_1(x)}{dx^2} + 2jk\frac{du_1(x)}{dx} - (k^2 - \alpha^2)u_1(x) = 0 \qquad (1)$$

where $\alpha^2 = 2mE/\hbar^2$

In region II, where V(x) = V_0, we have,

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

where $\beta^2 = \frac{2m}{\hbar^2}(E - V_0) = \alpha^2 - \frac{2mV_0}{\hbar^2}$

Equations (1) and (2) are two new equations for envelop $u_1(x)$ and $u_2(x)$ in regions I and II, respectively.

The general solutions for (1) and (2) is,

$u_1(x) = Ae^{j(\alpha-k)x} + Be^{-j(\alpha+k)x}$ For region I (0 < x < a)

$u_2(x) = Ce^{j(\beta-k)x} + De^{-j(\beta+k)x}$ For region II (-b < x < 0)

Boundary conditions:

Field continuity $u_1(0) = u_2(0)$

$$\left.\frac{du_1}{dx}\right|_{x=0} = \left.\frac{du2}{dx}\right|_{x=0}$$

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

$$\left.\frac{du_1}{dx}\right|_{x=a} = \left.\frac{du2}{dx}\right|_{x=-b}$$

This results in 4 equations for coefficients A, B, C, and D,

$$A + B - C - D = 0$$

$$(\alpha - k)A - (\alpha + k)B - (\beta - k)C + (\beta - k)D = 0$$

$$Ae^{j(\alpha-k)a} + Be^{-j(\alpha+k)a} - Ce^{-j(\beta-k)b} - De^{j(\beta+k)b} = 0$$

$$(\alpha-k)Ae^{j(\alpha-k)a}-(\alpha+k)Be^{-j(\alpha+k)a}-(\beta-k)Ce^{-j(\beta-k)b}+(\beta+k)De^{j(\beta+k)b}=0$$

In order to have nontrivial solutions for A, B, C, and D, the determinant must be zero. That is

$$\begin{vmatrix} 1 & 1 & -1 & -1 \\ (\alpha-k) & -(\alpha+k) & -(\beta-k) & (\beta+k) \\ e^{j(\alpha-k)a} & e^{-j(\alpha+k)a} & e^{-j(\beta-k)b} & e^{j(\beta+k)b} \\ (\alpha-k)e^{j(\alpha-k)a} & -(\alpha+k)e^{-j(\alpha+k)a} & -(\beta-k)e^{-j(\beta-k)b} & (\beta+k)e^{j(\beta+k)b} \end{vmatrix}=0$$

This is equivalent to,

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

We are mostly interested in the case of $V_0 > E$ (electrons are bounded inside the crystal structure). In this case,

$$\beta^2=\frac{2m}{\hbar^2}(E-V_0)<0 \text{ and } \beta=j\sqrt{\frac{2m}{\hbar^2}(V_0-E)}=j\gamma$$

where γ is real and,

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

To further simplify the analysis, we assume δ-type potential barriers with $V_0=\infty$, $b=0$ and $V_0 b = u$, which is a constant,

Then,
$$\gamma b=b\sqrt{\frac{2m}{\hbar^2}V_0}=b\sqrt{\frac{2m}{\hbar^2}}\frac{u}{\sqrt{V_0}}\to 0$$

$$\cosh(\gamma b)\to 1 \text{ and } \sinh(\gamma b)\to \gamma b$$

$$\frac{\gamma^2-\alpha^2}{2\alpha\gamma}\sinh(\gamma b)\to\frac{\gamma}{2\alpha}\gamma b=\frac{1}{2\alpha}\frac{2m}{\hbar^2}V_0 b=\frac{mu}{\alpha\hbar^2}$$

Therefore, we have,

$$\frac{mV_0ba}{\hbar^2}\frac{\sin(\alpha a)}{\alpha a}+\cos(\alpha a)=\cos(ka)$$

or, $$M\frac{\sin(\alpha a)}{\alpha a}+\cos(\alpha a)=\cos(ka) \qquad (3)$$

where $M \equiv \frac{mV_0ba}{\hbar^2}$

On the right-hand-side of equation (3),

$$-1<\cos(ka)<1$$

While on the left-hand-side of equation (3), the value of $M\frac{\sin(\alpha a)}{\alpha a}+\cos(\alpha a)$ is not bounded within ±1.

Therefore, in order to have non-trivial solution of equation (3), the parameter $\alpha=\sqrt{2mE}/\hbar^2$ or ultimately the electron energy **E** only has certain allowed values, while other values are forbidden.

This gives an explanation of allowed and forbidden energy bands:

Allowed energy band: $$\left|M\frac{\sin(\alpha a)}{\alpha a}+\cos(\alpha a)\right|\le 1$$

Forbidden energy band: $$\left|M\frac{\sin(\alpha a)}{\alpha a}+\cos(\alpha a)\right|>1$$

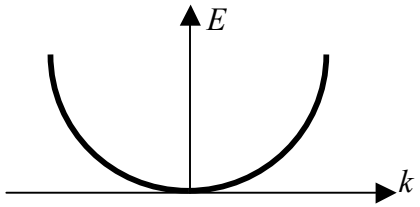
Although $M\frac{\sin(\alpha a)}{\alpha a}+\cos(\alpha a)=\cos(ka)$ can be solved numerically, we only look at two extreme cases:

(1) No periodic potential barrier $V_0 = 0$ or $V_0b = 0$ and M=0,

Equation (3) becomes, $\cos(\alpha a)=\cos(ka)$

Therefore $\alpha = k$

that is, $\frac{\sqrt{2mE}}{\hbar} = k$ or, $E = \frac{k^2\hbar^2}{2m}$



Obviously any E-value is allowed, no restriction.

(2) Very high periodic potential barrier $V_0 b \gg 1$ and therefore, $M \gg 1$.

Equation (3) becomes, $M\frac{\sin(\alpha a)}{\alpha a} = \cos(ka)$

Since $M \gg 1$, the solutions can only be found around $\sin(\alpha a) = 0$, or,

$$\alpha \equiv \frac{\sqrt{2mE}}{\hbar} = \pm\frac{n\pi}{a} \quad \text{with n = 1, 2, 3....}$$

That is,

$$E = \left(\frac{n\pi}{a}\right)^2 \frac{\hbar^2}{2m} \quad \text{with n = 1, 2, 3....}$$

Obviously, E has only discrete values.