Momentum operator $\hat{p}$ as a generator of space translation

$$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x} \rightarrow e^{i\hat{p}a/\hbar}$$

$$e^{i\hat{p}a/\hbar}\,\psi(x) = e^{a\frac{\partial}{\partial x}}\,\psi(x)$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!}\left(a\frac{d}{dx}\right)^n \psi(x)$$

$$= \psi(x) + a\frac{d\psi}{dx} + \frac{a^2}{2}\frac{d^2\psi}{dx^2} + \cdots$$

$$= \psi(x+a)$$

$\hat{T}_a = e^{i\hat{p}a/\hbar}$ generates space translation

$\hat{p} \rightarrow$ generator of space translation

$\hat{T}_a$ shifts the expectation value of position by 'a'.

[Recall $e^{iq\hat{x}/\hbar} \rightarrow$ shifts the expectation value of momentum by q]

Now consider a particle in a periodic potential

$$V(x+a) = V(x)$$

$$\hat{T}_a V(x) = V(x+a) = V(x)$$

$$[\hat{T}_a, V(\hat{x})]\,\varphi(x) = [\hat{T}_a V(\hat{x}) - V(\hat{x})\hat{T}_a]\,\varphi(x)$$

$$= V(\hat{x}+a)\,\varphi(x+a) - V(\hat{x})\,\varphi(x+a)$$

$$= V(\hat{x})\,\varphi(x+a) - V(\hat{x})\,\varphi(x+a)$$

$$= 0$$

$$\Rightarrow [\hat{T}_a, V(\hat{x})] = 0 \quad , \quad \text{Also } [\hat{T}_a, \hat{p}^2] = 0$$

$\Rightarrow [\hat{H}, \hat{T}_a] = [\frac{\hat{p}^2}{2m} + V(\hat{x}), \hat{T}_a] = 0$

$\hat{H}$, $\hat{T}_a$ have simultaneous eigenstates.

However $\hat{H}$ does not commute with $\hat{p}$!

$$\hat{p}\, V(x) = \frac{\hbar}{i}\frac{\partial}{\partial x} V(x) = \frac{\hbar}{i} V'(x)$$

$\hat{H}$, $\hat{p}$ do <u>not</u> have simultaneous eigenstates.

[$\hat{H}\,\phi_{E,q} = E\,\phi_{E,q}$

$\hat{T}_a\,\phi_{E,q} = e^{i\theta}\,\phi_{E,q}$

since $\hat{T}_a$ is unitary, its eigenvalues are pure phase.]

If $\psi(x)$ is a non-degenerate eigenstate of $\hat{H}$, then it is also an eigenstate of $\hat{T}_a$

$$\hat{T}_a \psi(x) = \psi(x+a) = e^{i\theta}\psi(x)$$

Since $V(x) = V(x+a) = V(x+2a) \ldots$

probability density should also be periodic

$$|\psi(x)|^2 = |\psi(x+a)|^2 = \ldots = |\psi(x+na)|^2$$

$$\hat{T}_n \psi_k(x) = \boxed{\psi_k(x+na) = e^{ikna}\psi(x)}$$

or simply $\psi(x+a) = e^{ika}\psi(x)$

Let us see how!

$$\psi(x+a) = e^{i\theta(a)}\psi(x)$$

$$\psi(x+2a) = e^{i\theta(a)}\psi(x+a) = e^{2i\theta(a)}\psi(x)$$

Again $\psi(x+2a) = e^{i\theta(2a)}\psi(x) \Rightarrow \theta(2a) = 2\theta(a)$

θ is linear in a $\Rightarrow \theta(a) = ka$

$$\boxed{\psi(x+a) = e^{ika}\,\psi(x)}$$ Bloch's theorem

Alternatively, $\boxed{\psi_k(x) = e^{ikx}\,u_k(x)}$, where $u_k(x)$ is periodic with the same periodicity of the lattice.

$$\boxed{u_k(x+a) = u_k(x)}$$

Verify: $\psi_k(x+a) = e^{ik(x+a)}\,u_k(x+a)$

$$= e^{ika}\,e^{ikx}\,u_k(x)$$

$$= e^{ika}\,\psi_k(x)$$

Bloch's theorem: For a particle moving in a potential with periodicity a i.e. $V(x+a) = V(x)$, the corresponding wave function is such that

$$\boxed{\begin{array}{l} \psi(x+a) = e^{ika}\,\psi(x) \\ \text{Alternatively,} \\ \psi_k(x) = e^{ikx}\,u_k(x), \text{ where} \\ u_k(x+a) = u_k(x) \end{array}}$$

$\psi_k(x) = e^{ikx}\,u_k(x)$ is NOT a momentum eigenstate

$$\hat{p}\,\psi_k(x) = \frac{\hbar}{i}\frac{\partial}{\partial x}\left[e^{ikx}\,u_k(x)\right] \neq \underbrace{c}_{\text{const.}}\,e^{ikx}\,u_k(x)$$

In the trivial case, $V(x) = V(x+a) \ldots = \text{const}$

$$\psi_k(x) = e^{ikx}, \quad u_k(x) = 1$$

$\downarrow$

momentum eigenstate $\Rightarrow$ free particle of momentum k.

Again, $\hat{T}_a \psi_k(x) = e^{i\alpha} \psi_k(x) = \psi_k(x+a)$

$$u_k(x) = e^{-ikx} \psi_k(x)$$

$$\Rightarrow \hat{T}_a u_k(x) = e^{-ik(x+a)} \psi_k(x+a)$$

$$= e^{-ik(x+a)} e^{i\alpha} \psi_k(x)$$

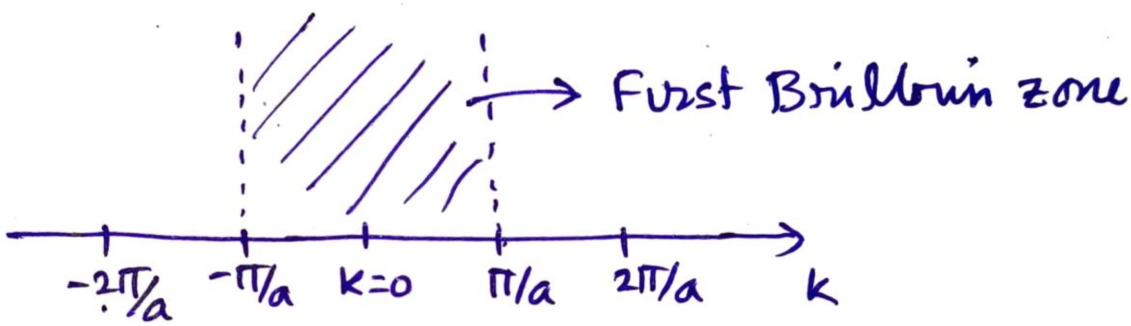
$$= e^{i(\alpha - ka)} e^{-ikx} \psi_k(x) = e^{i(\alpha - ka)} u_k(x)$$

$$\Rightarrow u_k(x+a) = e^{i(\alpha - ka)} u_k(x)$$

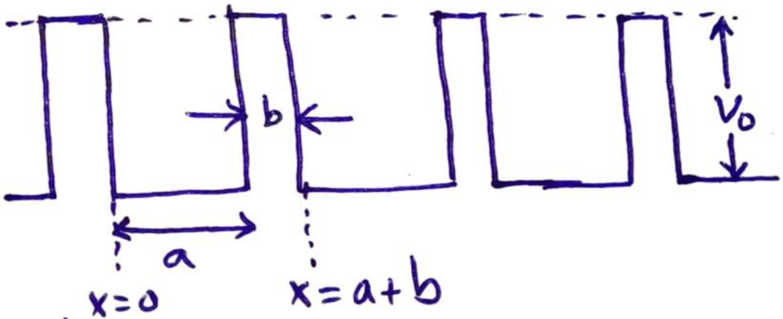
since $u_k(x+a) = u_k(x) \Rightarrow e^{i\alpha} = e^{ika}$

translate $k \to k + \frac{2\pi}{a} \Rightarrow e^{i\alpha}$ remains the same

convention : Restrict k to $-\frac{\pi}{a}$ to $+\frac{\pi}{a}$



Kronig-Penney model



Period of the potential $\rightarrow a+b$

Energy eigenvalue determined by boundary condition

$$\psi_k(a+b) = e^{ik(a+b)} \psi_k(0)$$

$\psi(0 \le x \le a)$: $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$, $V = 0$ for $0 \le x \le a$

$$\Rightarrow \boxed{\psi(x) = A e^{i\alpha x} + B e^{-i\alpha x}} \quad , \quad \alpha = \sqrt{\frac{2mE}{\hbar^2}}$$

$\psi(a<x<b)$: $\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(V_0 - E)\psi$

$$\Rightarrow \boxed{\psi(x) = C e^{\beta x} + D e^{-\beta x}} \quad , \quad \beta = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

B.C. : 1) ψ continuous at $x = a$

$$\Rightarrow A e^{i\alpha a} + B e^{-i\alpha a} = C e^{\beta a} + D e^{-\beta a}$$

2) $\frac{d\psi}{dx}$ continuous at $x = a$

$$\Rightarrow i\alpha e^{i\alpha a} A - i\alpha e^{-i\alpha a} B = \beta e^{\beta a} C - \beta e^{-\beta a} D$$

3) Using Bloch's theorem

$$\psi(a+b) = e^{ik(a+b)}\psi(0) = e^{ik(a+b)}(A+B)$$

$$\Rightarrow C e^{\beta(a+b)} + D e^{-\beta(a+b)} = e^{ik(a+b)}(A+B)$$

4) $\frac{d\psi}{dx}$ is continuous at $x = a+b$

$$\left.\frac{d\psi}{dx}\right|_{x=a+b} = e^{ik(a+b)} \left.\frac{d\psi}{dx}\right|_{x=0}$$

$$\Rightarrow \beta e^{\beta(a+b)} C - \beta e^{-\beta(a+b)} D = e^{ik(a+b)}\, i\alpha (A - B)$$

Solve for A, B, C, D $\Rightarrow$

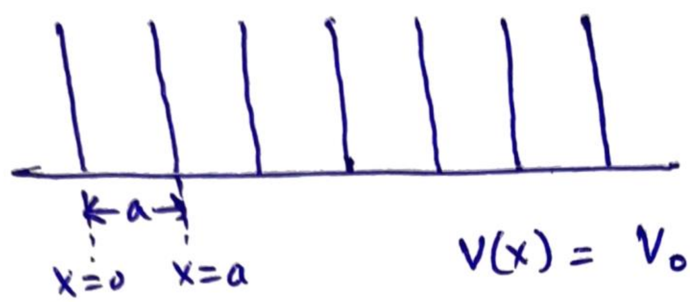
$$\begin{vmatrix} e^{i\alpha a} & e^{-i\alpha a} & -e^{\beta a} & -e^{-\beta a} \\ i\alpha e^{i\alpha a} & -i\alpha e^{-i\alpha a} & -\beta e^{\beta a} & \beta e^{-\beta a} \\ e^{ik(a+b)} & e^{ik(a+b)} & -e^{+\beta(a+b)} & -e^{-\beta(a+b)} \\ i\alpha e^{ik(a+b)} & -i\alpha e^{ik(a+b)} & -\beta e^{\beta(a+b)}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

The eqn will be satisfied for certain values of E for a given k

$f(\alpha, \beta, k) = 0 \Rightarrow$ plot E vs k in the 1st BZ.

dependent on E

We can simplify the model further. Take the limit where the barrier becomes higher and higher, while also squeezing the barrier width smaller and smaller $\rightarrow$ delta potential barrier



$$V(x) = V_0 \sum_n \delta(x - na)$$

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2} = 0 \qquad \text{for } 0 < x < a$$

$$\Rightarrow \psi(x) = A e^{i\beta x} + B e^{-i\beta x} \quad , \; 0 < x < a$$

$$\left.\begin{aligned} \psi(x=0) &= A + B \\ \left.\frac{d\psi}{dx}\right|_{x=0} &= i\beta(A - B) \end{aligned}\right\} \beta = \sqrt{\frac{2mE}{\hbar^2}}$$

Bloch's theorem $\rightarrow$ $\boxed{\psi(x = a+) = e^{ika}\psi(0) = e^{ika}(A+B)}$ -- ①

$$V = V_0 \delta(x - a)$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0 \delta(x-a)\psi = E\psi$$

Take $\lim_{\epsilon \to 0}$ $\int_{a-\epsilon}^{a+\epsilon} \ldots dx$ on both sides of the eqn

$$-\frac{\hbar^2}{2m}\left[\left.\frac{d\psi}{dx}\right|_{x=a+} - \left.\frac{d\psi}{dx}\right|_{x=a-}\right] + V_0\psi(a) = \int_{a-\epsilon}^{a+\epsilon} E\psi \, dx \rightarrow 0 \text{ as } \epsilon \to 0$$

$$\Rightarrow \boxed{\left.\frac{d\psi}{dx}\right|_{x=a+} - \left.\frac{d\psi}{dx}\right|_{x=a-} = \frac{2mV_0}{\hbar^2}\psi(a)} \quad \text{-- ②}$$

① $\Rightarrow$ $\psi(x=a+) = A e^{i\beta a} + B e^{-i\beta a} = e^{ika}(A+B)$

② $\Rightarrow$ $\underbrace{i\beta(A-B)}_{\left.\frac{d\psi}{dx}\right|_{x=0}} e^{ika} - i\beta(A e^{i\beta a} - B e^{-i\beta a}) = \frac{2mV_0}{\hbar^2} e^{ika}\psi(0)$

$$\Rightarrow \left(e^{ika} - e^{i\beta a}\right) A + \left(e^{ika} - e^{-i\beta a}\right) B = 0$$

and, $$\left(i\beta e^{ika} - i\beta e^{i\beta a} - \frac{2mV_0}{\hbar^2} e^{ika}\right) A + \left(-i\beta e^{ika} + i\beta e^{-i\beta a} - \frac{2mV_0}{\hbar^2} e^{ika}\right) B = 0$$

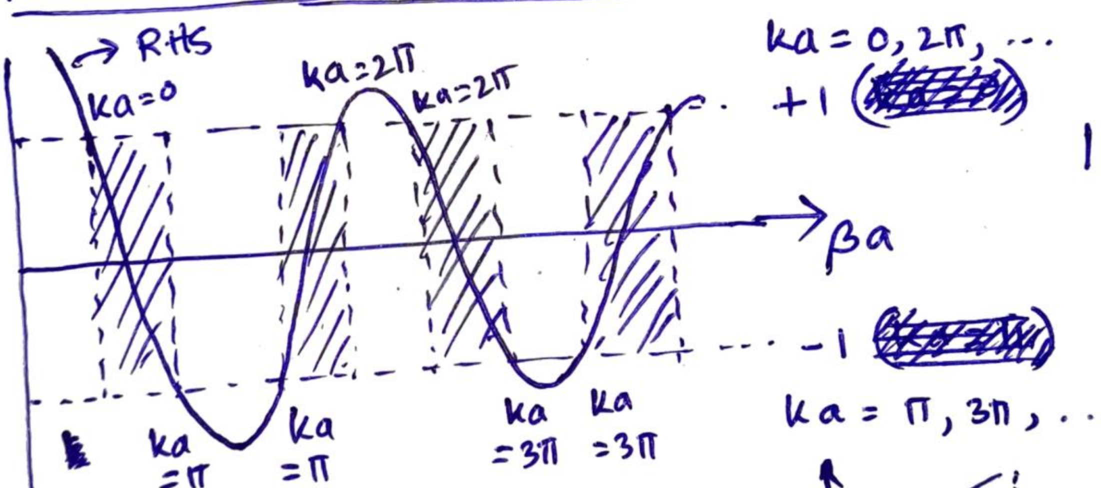
$\Rightarrow$ solve for A, B $\Rightarrow$

$$\left(e^{ika} - e^{i\beta a}\right)\left(-i\beta e^{ika} + i\beta e^{-i\beta a} - \frac{2mV_0}{\hbar^2} e^{ika}\right) - \left(i\beta e^{ika} - i\beta e^{i\beta a} - \frac{2mV_0}{\hbar^2} e^{ika}\right)\left(e^{ika} - e^{-i\beta a}\right) = 0$$

$$\Rightarrow \beta e^{2ika} + \beta - \beta e^{-i\beta a} e^{ika} - \beta e^{i\beta a} e^{ika} = \frac{2mV_0}{\hbar^2} e^{ika} \sin\beta a$$

$$\Rightarrow \beta e^{ika} + \beta e^{-ika} - \beta\left(e^{i\beta a} + e^{-i\beta a}\right) = \frac{2mV_0}{\hbar^2} \sin\beta a$$

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



$|\cos ka| \le 1$