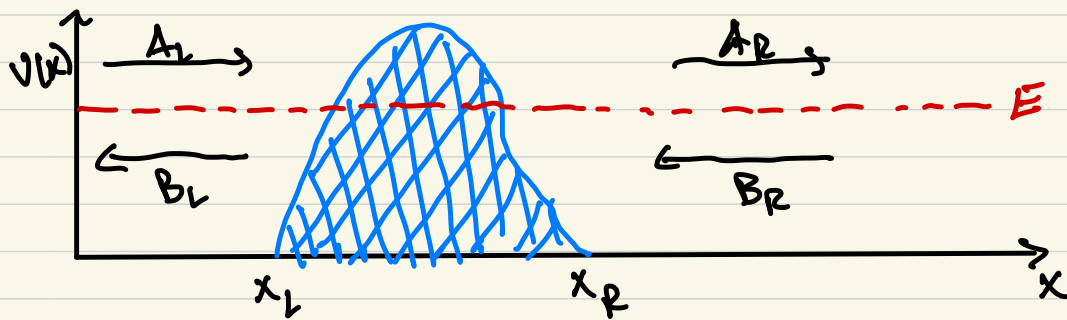


Alternative picture of 1D solid: Electrons tunneling through barriers

- Lets consider electron impinging on some barrier:



- Wave Functions to left and right:

$$\psi_L(x) = A_L e^{iqx} + B_L e^{-iqx} \quad x \leq x_L$$

$$\psi_R(x) = A_R e^{iqx} + B_R e^{-iqx} \quad x \geq x_R$$

$$q = \sqrt{\frac{2mE}{\hbar^2}} \quad (\text{free space outside of } x_L < x < x_R)$$

- We could proceed in the same way as the k.p. model: Write continuity conditions

* But we have not specified the form of $V(x)$

* Instead, just consider ψ outside of $x_L < x < x_R$

* Coefficients can be related by "Scattering" (or "transfer") matrix $S(E)$:

$$\begin{pmatrix} B_L \\ A_R \end{pmatrix} = \tilde{S}(E) \begin{pmatrix} A_L \\ B_R \end{pmatrix}$$

Labels: "outgoing" points to the left vector, "incoming" points to the right vector, "transfer" points to the matrix, "scattering" points to the matrix.

$$\begin{pmatrix} A_R \\ B_R \end{pmatrix} = S(E) \begin{pmatrix} A_L \\ B_L \end{pmatrix} = \begin{pmatrix} S_{11}(E) & S_{12}(E) \\ S_{21}(E) & S_{22}(E) \end{pmatrix} \begin{pmatrix} A_L \\ B_L \end{pmatrix}$$

Labels: "LHS" points to the left vector, "RHS" points to the right vector.

$$\Rightarrow A_R = S_{11} A_L + S_{12} B_L$$

$$B_R = S_{21} A_L + S_{22} B_L$$

- some general properties: (will work out for HW)

* complex conjugation provides solutions to S.E. w/ same E:

$$S_{11} = S_{22}^*, \quad S_{12} = S_{21}^*$$

* Can show that $\det S = 1 \Rightarrow S$ is unimodular

- consider wave impinging from left $\Rightarrow B_R = 0$

$$A_R = S_{11} A_L + S_{12} B_L$$

$$0 = S_{21} A_L + S_{22} B_L$$

* reflection amplitude: * reflection coefficient:

$$r = \frac{B_L}{A_L} = -\frac{S_{21}}{S_{22}}$$

$$R = r r^* = |r|^2 = \left| \frac{S_{21}}{S_{22}} \right|^2$$

* transmission amplitude:

$$\begin{aligned} t = \frac{A_R}{A_L} &= S_{11} + S_{12} \frac{B_L}{A_L} = S_{11} + S_{12} \left(-\frac{S_{21}}{S_{22}} \right) = \frac{1}{S_{22}} (S_{11} S_{22} - S_{12} S_{21}) \\ &= \frac{1}{S_{22}} \det S = \boxed{\frac{1}{S_{22}}} \end{aligned}$$

* transmission coefficient:

$$T = t t^* = \left| \frac{1}{S_{22}} \right|^2$$

$$\begin{aligned} * R + T &= \left| \frac{S_{21}}{S_{22}} \right|^2 + \left| \frac{1}{S_{22}} \right|^2 = \frac{1}{|S_{22}|^2} (|S_{21}|^2 + 1) = \frac{1}{|S_{22}|^2} (|S_{21}|^2 + |S_{22}|^2 - |S_{21}|^2) \\ &= 1 \end{aligned}$$

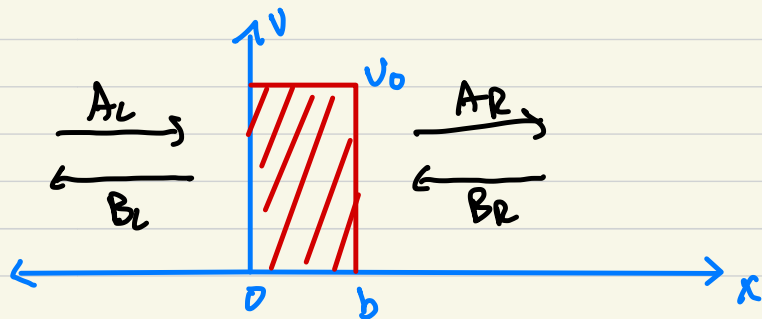
* So:

$$S = \begin{pmatrix} 1/t^* & -r/t^* \\ -r/t & 1/t \end{pmatrix}$$

- What if we shift $V(x) \rightarrow V(x-d)$? Extra phases e^{-iqd} :

$$S(d) = \begin{pmatrix} S_{11} & S_{12} e^{-2iqd} \\ S_{21} e^{2iqd} & S_{22} \end{pmatrix}$$

- Returning to the square barrier:



$$\psi_L = A_L e^{iqx} + B_L e^{-iqx} \quad x < 0$$

$$\psi_I = A_I e^{\beta x} + B_I e^{-\beta x} \quad 0 < x < b$$

$$\psi_R = A_R e^{iqx} + B_R e^{-iqx} \quad x > b$$

* Apply normal continuity conditions to get:

at $x=0$:

$$\begin{pmatrix} A_I \\ B_I \end{pmatrix} = \underbrace{\frac{1}{2\beta} \begin{pmatrix} iq + \beta & -iq + \beta \\ -iq + \beta & iq + \beta \end{pmatrix}}_{S'} \begin{pmatrix} A_L \\ B_L \end{pmatrix}$$

at $x=b$:

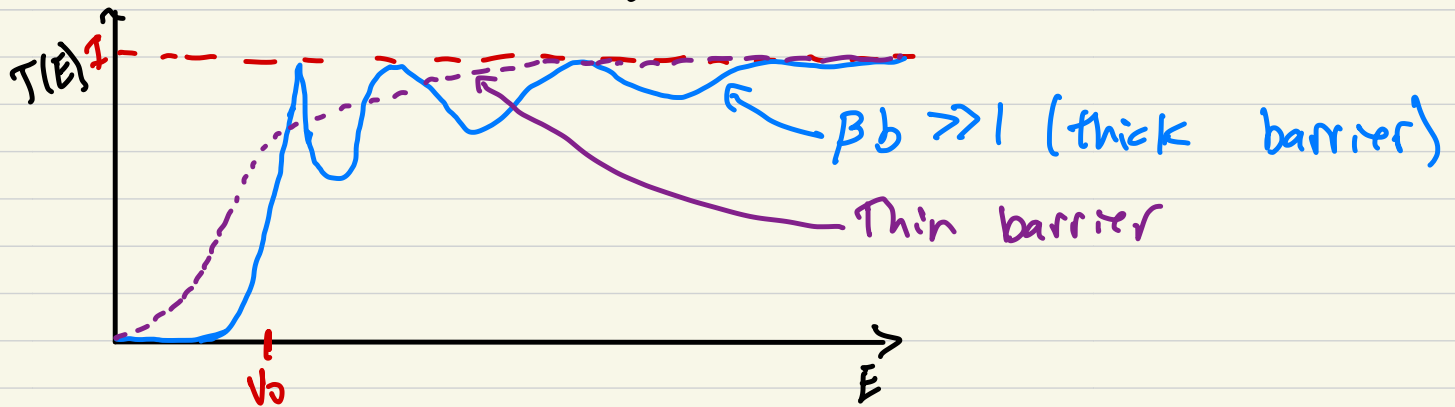
$$\begin{pmatrix} A_R \\ B_R \end{pmatrix} = \underbrace{\frac{1}{2iq} \begin{pmatrix} (iq + \beta) e^{(-iq + \beta)b} & (-iq - \beta) e^{(-iq - \beta)b} \\ (iq - \beta) e^{(iq + \beta)b} & (iq + \beta) e^{(iq - \beta)b} \end{pmatrix}}_{S''} \begin{pmatrix} A_I \\ B_I \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} A_R \\ B_R \end{pmatrix} = \underbrace{S'' \cdot S'}_S \begin{pmatrix} A_L \\ B_L \end{pmatrix}$$

$$\Rightarrow S_{11} = e^{-iqb} \left[\cosh(\beta b) + i \frac{q^2 - \beta^2}{2q\beta} \sinh(\beta b) \right] = S_{22}^*$$

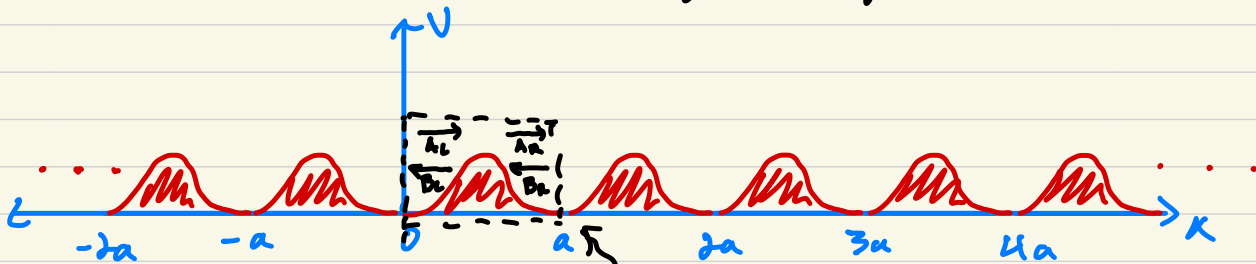
$$S_{12} = e^{-iqb} (-i) \frac{q^2 + \beta^2}{2q\beta} \sinh(\beta b) = S_{21}^*$$

$$* T = \frac{1}{|S_{11}|^2} = \left[1 + \frac{(1^2 + \beta^2)^2}{4 q^2 \beta^2} \sinh^2(\beta b) \right]^{-1}$$



• Note: For $E > V_0$, $\sinh \rightarrow \sin$, $T=1$ for $\beta b = \pi n$ ($n \in \mathbb{Z}$)

- Now consider tunneling through periodic potential:



* For one unit cell $0 \leq x \leq a$, using transfer matrix:

$$\psi_L(x) = A_L e^{iqx} + B_L e^{-iqx}$$

$$\psi_R(x) = (S_{11} A_L + S_{12} B_L) e^{iqx} + (S_{21} A_L + S_{22} B_L) e^{-iqx}$$

• Boundary conditions required by Bloch's theorem:

$$\psi_R(a) = e^{ika} \psi_L(0), \quad \left. \frac{d\psi_R}{dx} \right|_{x=a} = e^{ika} \left. \frac{d\psi_L}{dx} \right|_{x=0}$$

$$\Rightarrow \begin{pmatrix} S_{11} e^{ika} & S_{12} e^{ika} \\ S_{21} e^{-ika} & S_{22} e^{-ika} \end{pmatrix} \begin{pmatrix} A_L \\ B_L \end{pmatrix} = e^{ika} \begin{pmatrix} A_L \\ B_L \end{pmatrix}$$

- From prev page:

$$\overbrace{\begin{pmatrix} S_{11} e^{iqa} & S_{12} e^{iqa} \\ S_{21} e^{-iqa} & S_{22} e^{-iqa} \end{pmatrix}}^S \begin{pmatrix} A_L \\ B_L \end{pmatrix} = e^{ika} \begin{pmatrix} A_L \\ B_L \end{pmatrix}$$

$\Rightarrow e^{ika}$ is eigenvalue of S

\Rightarrow Since S is unimodular, e^{-ika} is other eigenvalue

\Rightarrow Trace of S is $e^{ika} + e^{-ika} = 2 \cos(ka)$

\Rightarrow Thus: $S_{11} e^{iqa} + S_{22} e^{-iqa} = 2 \cos(ka)$

- If we write: $S_{11} = \frac{1}{|t|} e^{i\phi}$, $\frac{1}{|t|} \cos(\phi + qa) = \cos(ka)$

\Rightarrow Allowed energies: $|\frac{1}{|t|} \cos(\phi + qa)| < 1$

\Rightarrow produces bands of allowed energies, w/ forbidden energy gaps

- Plug in S_{11} from square barrier case:

$$\left[\cosh(\beta b) + i \frac{q^2 - \beta^2}{2q\beta} \sinh(\beta b) \right] e^{iq(a-b)} + \text{c.c.} = 2 \cos(ka)$$

- Recall that $a - b = w$, where w was our square well width

$$\Rightarrow \cosh(\beta b) \cos(qw) - \frac{q^2 - \beta^2}{2q\beta} \sinh(\beta b) \sin(qw) = \cos ka$$

\Rightarrow Same compatibility condition for tunneling of Bloch-type wavefunctions as we saw before for K.P. model!!