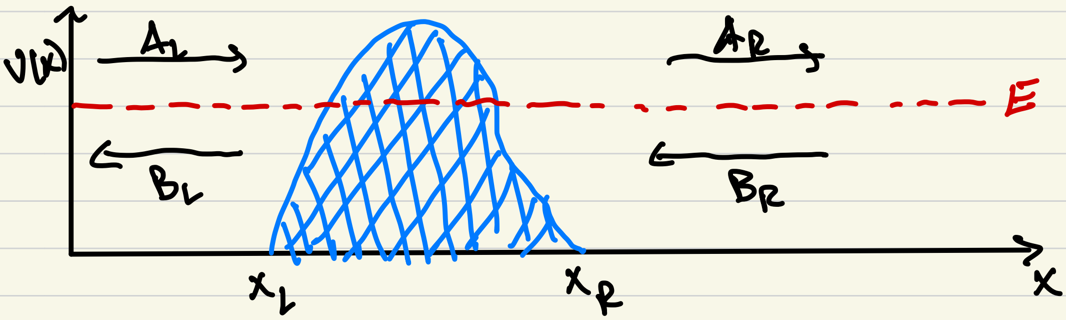
Alternative picture of 1D solid: Electrons tunneling through barriers

- Lets consider election impinging on some barrier:



- wave functions to left and right:

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

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

$q = \sqrt{\frac{2mE}{\hbar^2}}$ (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 $S(E)$:

outgoing

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

incoming

scattering

transfer

LHS

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

RHS

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

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

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

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

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

  * 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:

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

  * reflection coefficient:

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

  * transmission amplitude:

$$t = \frac{A_R}{A_L} = S_{11} + S_{12}\frac{B_L}{A_L} = S_{11} + S_{12}\left(-\frac{S_{21}}{S_{22}}\right) = \frac{1}{S_{22}}\left(S_{11}S_{22} - S_{12}S_{21}\right)$$

$$= \frac{1}{S_{22}} \det S = \boxed{\frac{1}{S_{22}}}$$

  * transmission coefficient:

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

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

$$= 1$$

  * So:

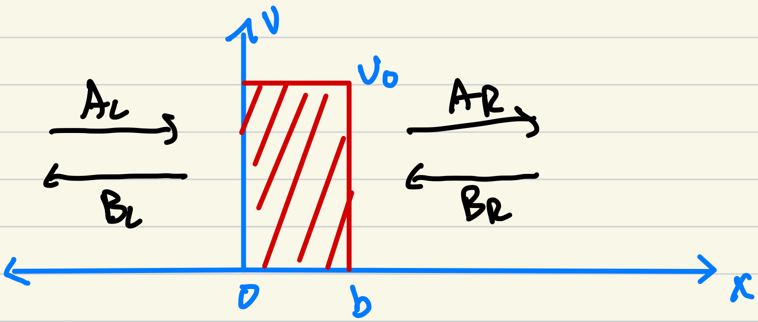
$$\boxed{S = \begin{pmatrix} 1/t^* & -r/t^* \\ -r/t & 1/t \end{pmatrix}}$$

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

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

– Returning to the square barrier:

$q = \sqrt{2mE/\hbar^2}$ $\beta = \sqrt{2m(E-V_0)/\hbar^2}$



$$\psi_L = A_L e^{iqx} + B_L e^{-iqx} \qquad x<0$$
$$\psi_I = A_I e^{\beta x} + B_I e^{-\beta x} \qquad 0<x<b$$
$$\psi_R = A_R e^{iqx} + B_R e^{-iqx} \qquad x>b$$

* Apply normal continuity conditions to get:

at $x=0$:
$$\begin{pmatrix} A_I \\ B_I \end{pmatrix} = \underbrace{\frac{1}{2\beta}\begin{pmatrix} iq+\beta & -iq+\beta \\ -iq+\beta & iq+\beta \end{pmatrix}}_{S'} \begin{pmatrix} A_L \\ B_L \end{pmatrix}$$

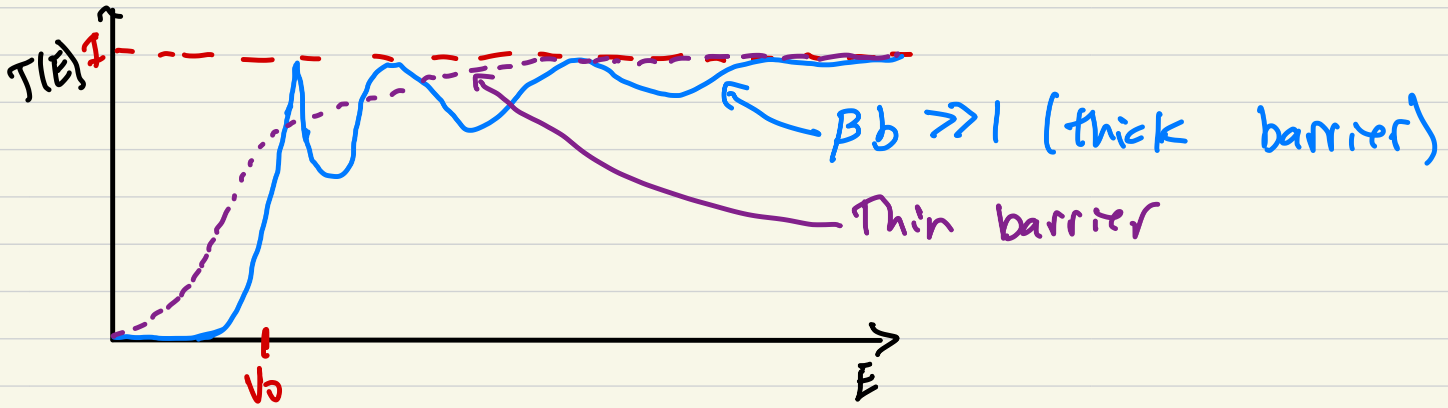
at $x=b$:
$$\begin{pmatrix} A_R \\ B_R \end{pmatrix} = \underbrace{\frac{1}{2iq}\begin{pmatrix} (iq+\beta)\, e^{(-iq+\beta)b} & (-iq-\beta)\, e^{(-iq-\beta)b} \\ (iq-\beta)\, e^{(iq+\beta)b} & (iq+\beta)\, e^{(iq-\beta)b} \end{pmatrix}}_{S''} \begin{pmatrix} A_I \\ B_I \end{pmatrix}$$

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

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

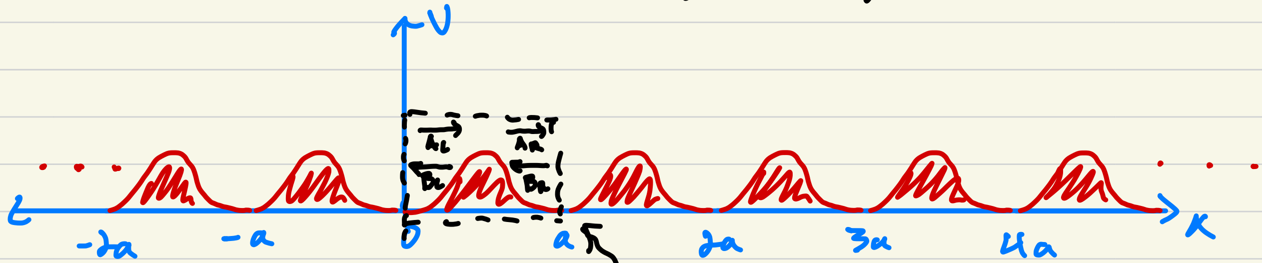
$$S_{12} = e^{-iqb}\,(-i)\,\frac{q^2+\beta^2}{2q\beta}\sinh(\beta b) = S_{21}^*$$

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



- Note: For $E > V_0$, $\sinh \to \sin$, $T=1$ 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:

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

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

- Boundary conditions required by Bloch's theorem:

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

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

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

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

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

$\Rightarrow$ 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

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

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