

Wavefunction and Transmission Coefficient

Transmission coefficient:

$$T = \frac{J_{\text{trans}}}{J_{\text{inc}}} = \frac{V_R |\psi_N|^2}{V_L |1|^2} \leftarrow |e^{ikx}|^2 \quad \text{except } V \neq \frac{\hbar k}{m} \quad \text{in finite differences!}$$

$$J = \frac{\hbar}{m} \text{Im} \left\{ \psi^* \frac{d\psi}{dx} \right\} = \frac{\hbar}{2mi} \left\{ \psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right\} = \frac{\hbar}{2mi} \left(\psi_i^* \frac{\psi_{i+1} - \psi_i}{\Delta x} - \psi_i \frac{\psi_{i+1}^* - \psi_i^*}{\Delta x} \right)$$

If $\psi = e^{ikx}$,

$$J = \frac{\hbar}{2mi\Delta x} \left(e^{-ikx_i} (e^{ik(x_i+\Delta x)} - e^{ikx_i}) - e^{ikx_i} (e^{-ik(x+\Delta x)} - e^{-ikx_i}) \right)$$

$$= \frac{\hbar}{2mi\Delta x} (e^{ik\Delta x} - 1 - (e^{-ik\Delta x} - 1)) = \frac{\hbar}{m\Delta x} \left(\frac{e^{ik\Delta x} - e^{-ik\Delta x}}{2i} \right) = \frac{\hbar}{m\Delta x} \sin k\Delta x$$

$$\sim \frac{\hbar k}{m} \quad \text{for } \Delta x \rightarrow 0$$

Dispersion relation

In continuous spatial dimension, $E = \frac{\hbar^2 k^2}{2m}$ so $\omega(k) = \frac{\hbar k^2}{2m}$

In finite differences, we can use $v = \frac{d\omega}{dk}$:

$$\omega(k) = \int v dk = \int \frac{\hbar}{m\Delta x} \sin k\Delta x dk = -\frac{\hbar}{m\Delta x^2} \cos k\Delta x + \text{const.} \rightarrow \frac{\hbar}{m\Delta x^2} (1 - \cos k\Delta x)$$

$$\cos k\Delta x \sim 1 - \frac{(k\Delta x)^2}{2} \quad \text{so} \quad \omega(k) \sim \frac{\hbar}{m\Delta x^2} \left(1 - \left(1 - \frac{(k\Delta x)^2}{2} \right) \right) = \frac{\hbar k^2}{2m} \quad \checkmark$$

Recipe

1. Choose E

2. construct $\left[E \hat{I} - (\hat{H} + \hat{\Sigma}_L + \hat{\Sigma}_R) \right]$ and \vec{Q}

using $k_{R/L} = \sqrt{\frac{2m(E - V_{L/R})}{\hbar^2}}$

3. Calculate $\vec{\Psi} = \left[E \hat{I} - (\hat{H} + \hat{\Sigma}_L + \hat{\Sigma}_R) \right]^{-1} \vec{Q}$

4. Calculate $T(E) = \frac{V_R}{V_L} |\Psi_L|^2$ using $V_{R/L} = \frac{\hbar^2}{m \Delta x} \sin k_{R/L} \Delta x$

5. Go to #1 and repeat w/ different E

6. Plot $T(E)$ vs. E .

Comparison between methods

