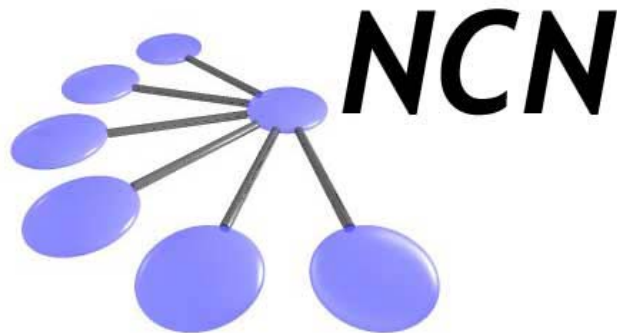


Network for Computational Nanotechnology (NCN)

UC Berkeley, Univ. of Illinois, Norfolk State, Northwestern, Purdue, UTEP

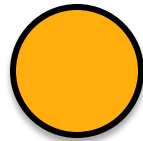
Open 1D Systems: Reflection at and Transmission over 1 Step



Gerhard Klimeck,
Dragica Vasileska,
Samarth Agarwal

PURDUE
UNIVERSITY

Stationary states for a free particle



$$V(x) = 0$$

TISE for a free particle.

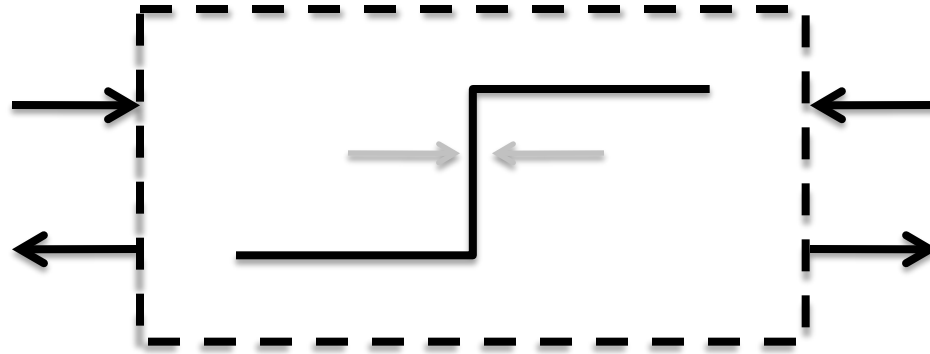
$$\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + E\psi(x) = 0$$

Solution: $\psi(x) = Ae^{ikx} + Be^{-ikx}, \quad k = \sqrt{\frac{2mE}{\hbar^2}}$

All positive energies are allowed and are doubly degenerate.

Scattering Matrix approach

Define our system : Step potential



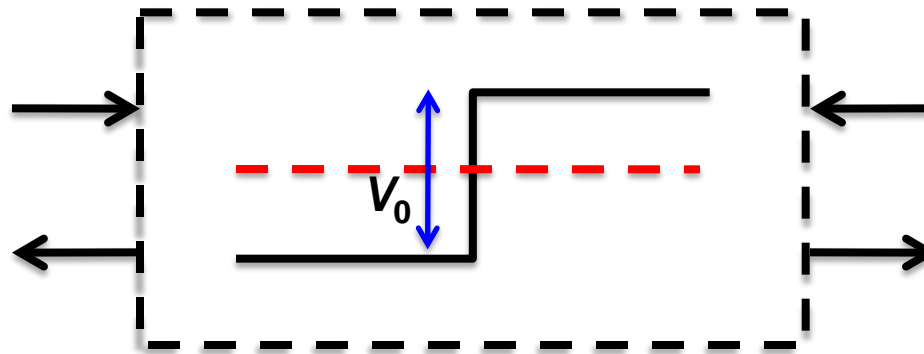
One matrix represents our system: S-matrix



No particles lost! Typically $A_1=1$ and $A_2=0$.

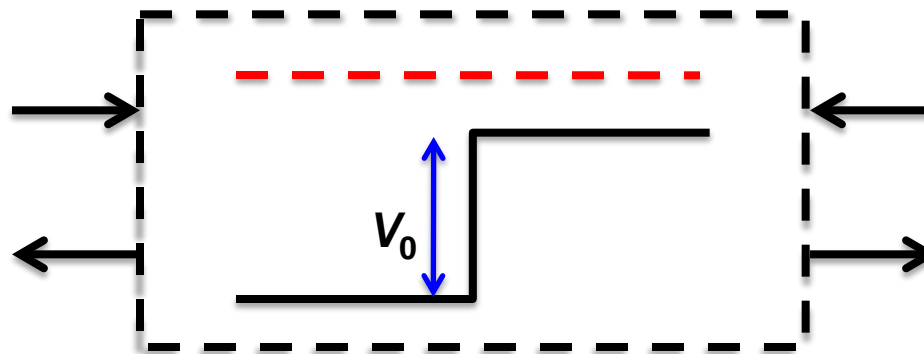
S-matrix: Cases

Case 1: $E < V_0$



Waves reflected

Case 2: $E > V_0$

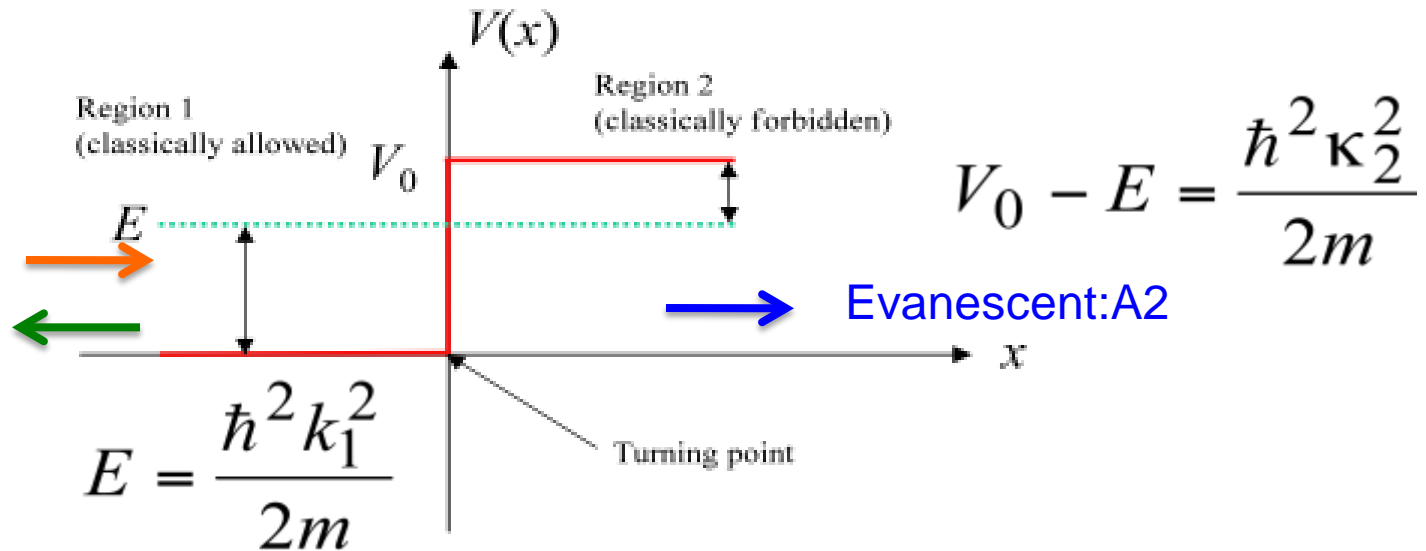


Waves transmitted
and reflected

Potential Step: $E < V_0$

$$E < V_0$$

Incident: A1
Reflected: B1



Wave-function in each region.

$$\psi(x) = \begin{cases} \underline{A}^{(1)} e^{ik_1 x} + \underline{B}^{(1)} e^{-ik_1 x} = \psi_1(x), & k_1 = \sqrt{\frac{2mE}{\hbar^2}} \\ \underline{A}^{(2)} e^{-\kappa_2 x} = \psi_2(x), & \kappa_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \end{cases}$$

Potential Step: Boundary Conditions

Match wave-functions and the derivatives at each turning point.

$$\begin{cases} \psi_1(0) = \psi_2(0) \\ \left. \frac{d\psi_1(x)}{dx} \right|_{x=0} = \left. \frac{d\psi_2(x)}{dx} \right|_{x=0} \end{cases}$$

We obtain:

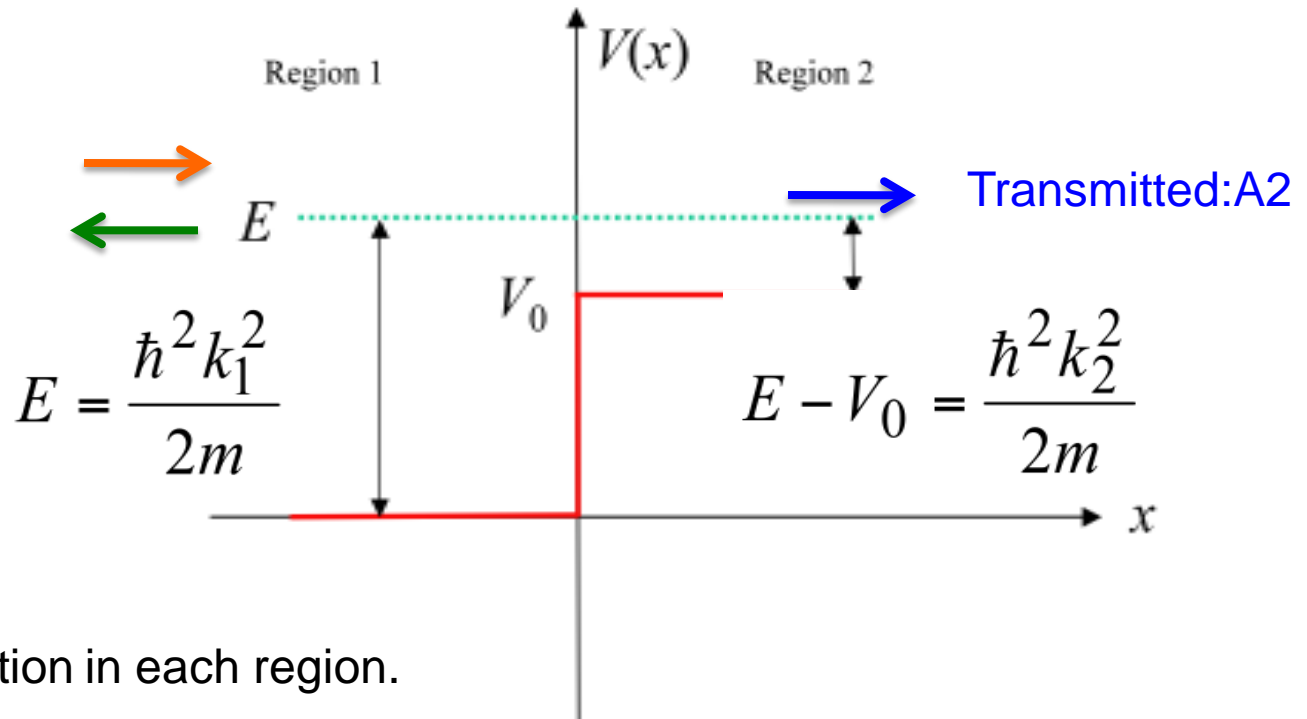
- Region 1: Standing Waves
- Region 2: Evanescent Waves
- Classical Physics will also give this result
- No probability associated with evanescent waves.

$$\begin{cases} B^{(1)} = \frac{k_1 - i\kappa_2}{k_1 + i\kappa_2} A^{(1)} \\ A^{(2)} = \frac{2k_1}{k_1 + i\kappa_2} A^{(1)} \end{cases}$$

Potential Step: $E > V_0$

Incident: A1
Reflected: B1

$$E > V_0$$



Wave-function in each region.

$$\psi(x) = \begin{cases} \underline{A}^{(1)} e^{ik_1 x} + \underline{B}^{(1)} e^{-ik_1 x} = \psi_1(x), & k_1 = \sqrt{\frac{2mE}{\hbar^2}} \\ \underline{A}^{(2)} e^{ik_2 x} = \psi_2(x), & k_2 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}} \end{cases}$$

Potential Step: Boundary Conditions

Match wave-functions and the derivatives at each turning point.

$$\left\{ \begin{array}{l} \psi_1(0) = \psi_2(0) \\ \left. \frac{d\psi_1(x)}{dx} \right|_{x=0} = \left. \frac{d\psi_2(x)}{dx} \right|_{x=0} \end{array} \right. \quad \left\{ \begin{array}{l} B^{(1)} = \frac{k_1 - k_2}{k_1 + k_2} A^{(1)} \\ A^{(2)} = \frac{2k_1}{k_1 + k_2} A^{(1)} \end{array} \right.$$

We can conclude: $\psi(x) = \begin{cases} \text{incident wave + reflected wave} & \rightarrow \text{source} \\ \text{transmitted wave} & \rightarrow \text{detector} \end{cases}$

We get,

$$\psi(x) = \begin{cases} A^{(1)} e^{ik_1 x} + \rho(E) A^{(1)} e^{-ik_1 x} = \psi_1(x), & x < 0 \\ \tau(E) A^{(1)} e^{ik_2 x} = \psi_2(x), & x \geq 0 \end{cases}$$

$$\rho(E) = B^{(1)} / A^{(1)} \quad \tau(E) = A^{(2)} / A^{(1)}$$

Probability Current given by,

$$J(x) = -\frac{ie\hbar}{2m} \left(\frac{\partial \psi^*}{\partial x} \psi - \psi^* \frac{\partial \psi}{\partial x} \right)$$

We get,

$$J_1 = -\frac{e\hbar k_1}{2m} \left[1 - |\rho(E)|^2 \right] |A^{(1)}|^2 = J_{inc} + J_{ref}, \quad x < 0$$

$$J_2 = -\frac{e\hbar k_2}{2m} |\tau(E)|^2 |A^{(1)}|^2 = J_{trans}, \quad x \geq 0$$

Reflection probability: (Reflected)/(Incident)

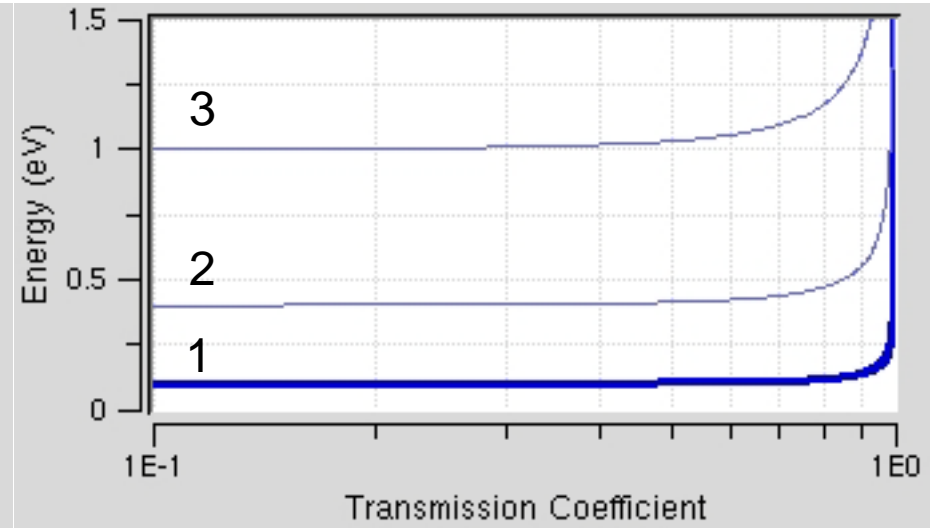
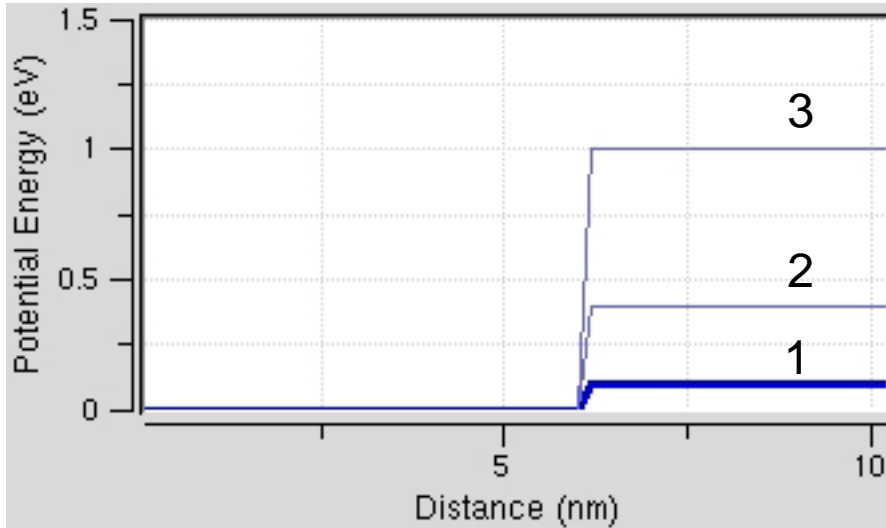
$$R(E) = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2$$

Transmission probability: (Transmission)/(Incident)

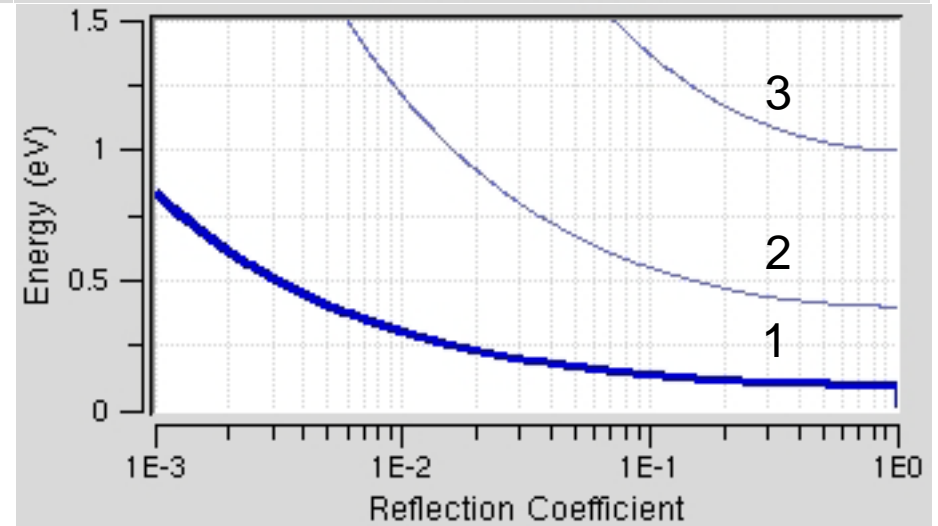
$$T(E) = \frac{4k_1 k_2}{(k_1 + k_2)^2}$$

Results do not agree with classical physics.

Transmission and Reflection



- Transmission not unity immediately above step.
- As the height of the step is increased the transmission takes longer to go from zero to one.
- The gradual change of transmission from zero to one is not comprehended by classical physics.
- This gradual change can be understood in terms of the nature of the propagation constant in the two regions.



Key Messages

- Electron wave can penetrate into a barrier
- Electron wave is not completely transmitted above a barrier
- There is a finite reflection above the barrier

