nanoHUB online simulation and more

an NCN project

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

NCN

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Stationary states for a free particle

TISE for a free particle.

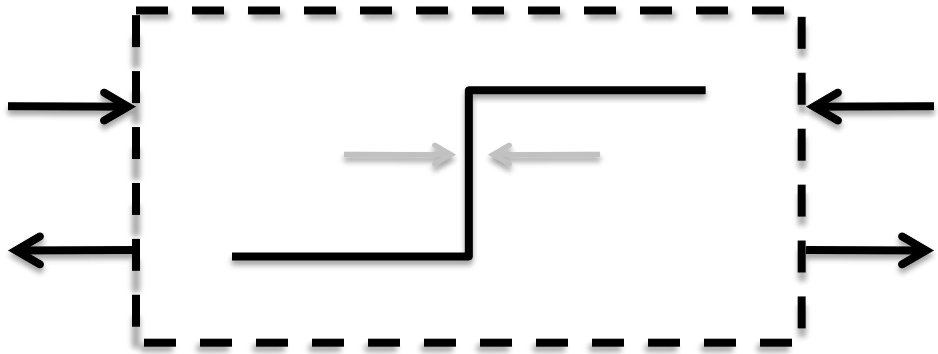
$$\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + E\psi(x) = 0$$

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

Incident:A1

Reflected:B1

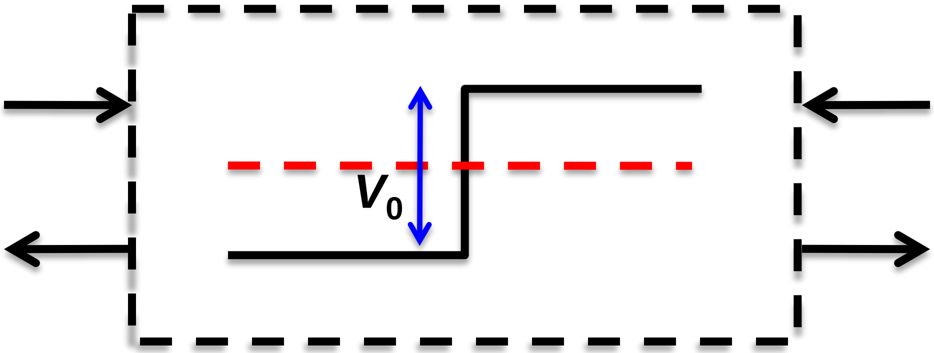
Incident:A2

Transmitted:B2

No particles lost! Typically A1=1 and A2=0.

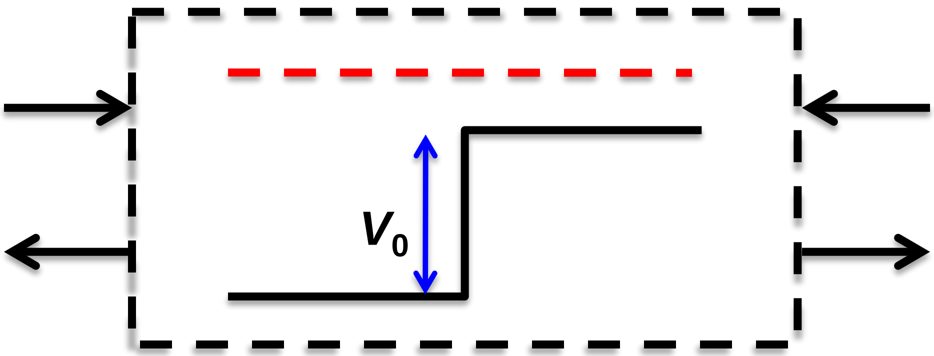
S-matrix: Cases

Case 1: $E<V_0$



Waves reflected

Case 2: $E>V_0$



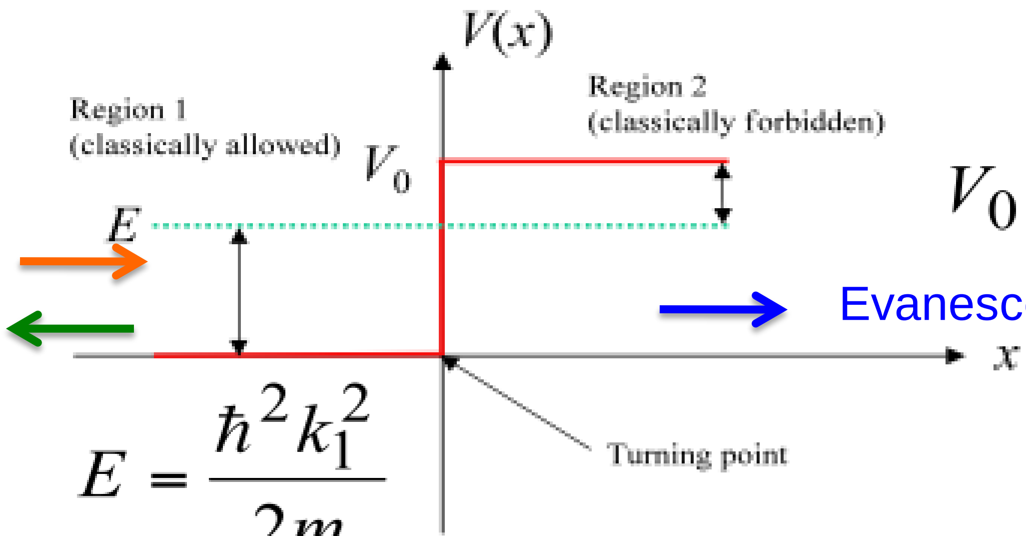
Waves transmitted and reflected

Potential Step:E<Vo

***E*$<V_0$**

Incident:A1

Reflected:B1



Evanescent:A2

$$V_0 - E = \frac{\hbar^2 \kappa_2^2}{2m}$$

$$E = \frac{\hbar^2 k_1^2}{2m}$$

Wave-function in each region.

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

Potential Step: Boundary Conditions

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

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

We obtain:

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

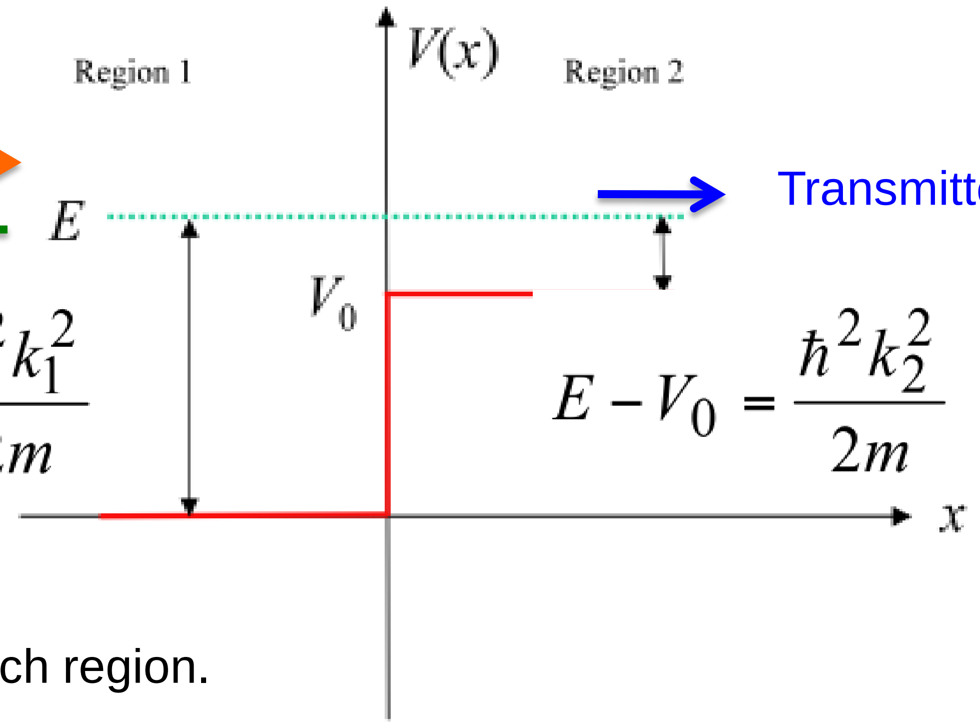
$$\begin{cases} B^{(1)} = \dfrac{k_1 - i\kappa_2}{k_1 + i\kappa_2} A^{(1)} \\ A^{(2)} = \dfrac{2k_1}{k_1 + i\kappa_2} A^{(1)} \end{cases}$$

Potential Step: E>Vo

Incident:A1

Reflected:B1

Transmitted:A2



E>V $_0$

$$E = \frac{\hbar^2 k_1^2}{2m}$$

$$E - V_0 = \frac{\hbar^2 k_2^2}{2m}$$

Wave-function in each region.

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

Potential Step: Boundary Conditions

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

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

We can conclude:

$$\psi(x) = \begin{cases} \textbf{incident wave + reflected wave} & \rightarrow \textbf{source} \\ \textbf{transmitted wave} & \rightarrow \textbf{detector} \end{cases}$$

We get,

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

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

Analysis

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,

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

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

Reflection probability: (Reflected)/(Incident)

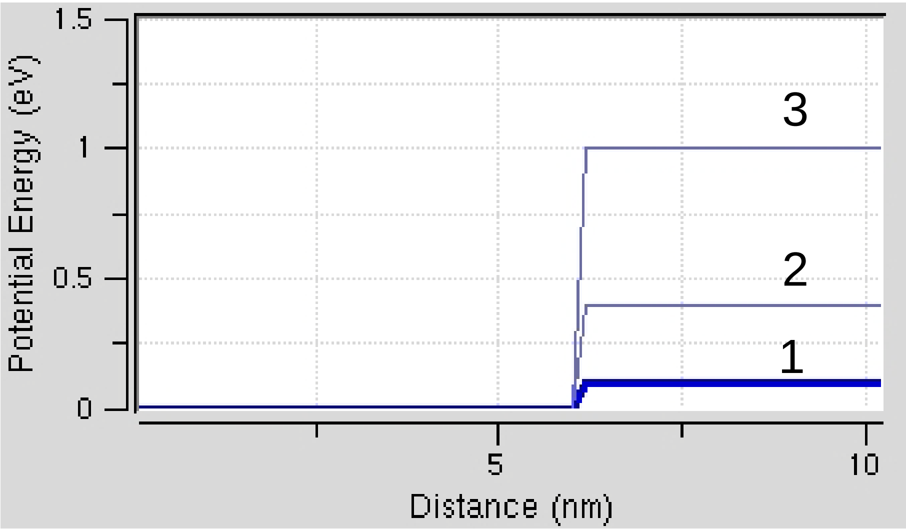
$$R(E) = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$$

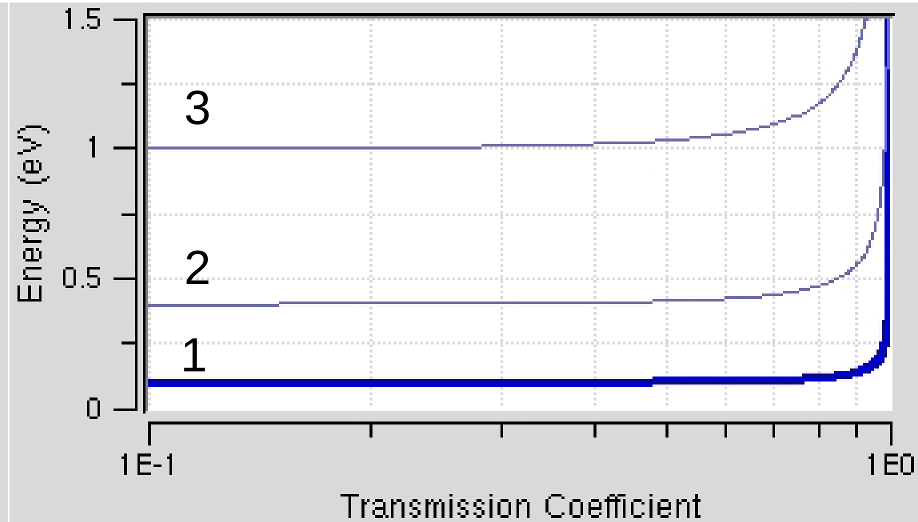
Transmission probability: (Transmission)/(Incident)

$$T(E) = \frac{4k_1k_2}{(k_1 + k_2)^2}$$

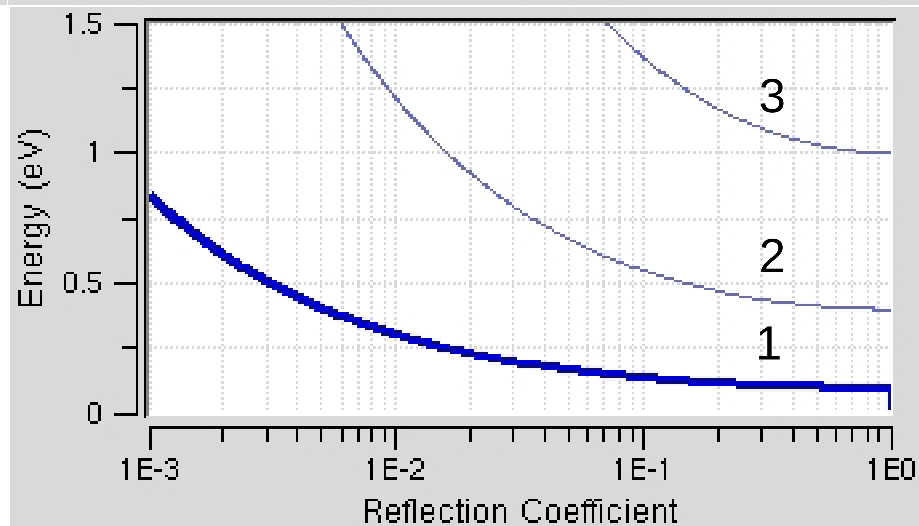
Results do not agree with classical physics.

Transmission and Reflection



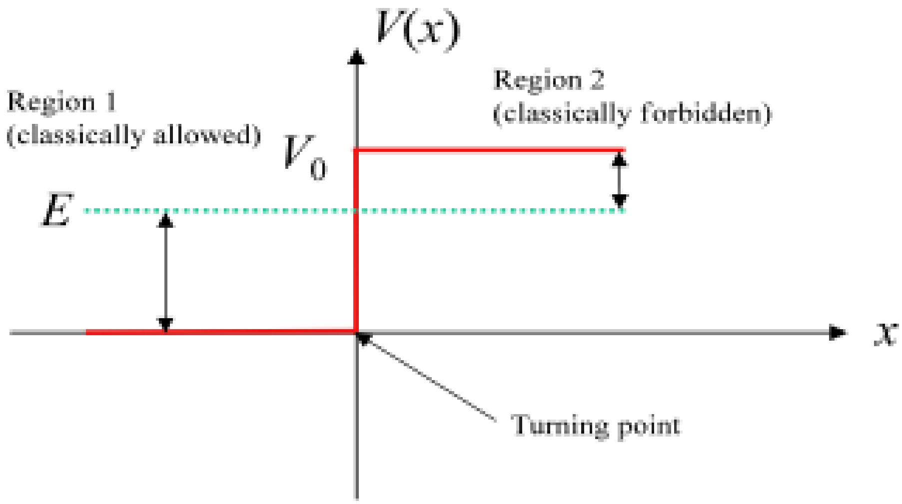


- Transmission not unity immediately above step.
- As the height of the step is increased the transmission takes longer to go from zero to one.
- The gradual change of transmission from zero to one is not comprehended by classical physics.
- This gradual change can be understood in terms of the nature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