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: Transmission through & over 1 Barrier

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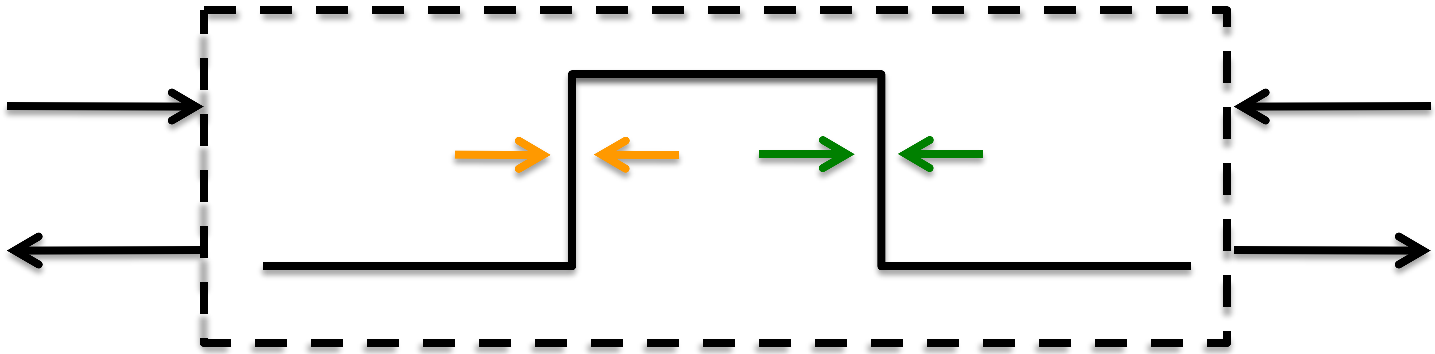
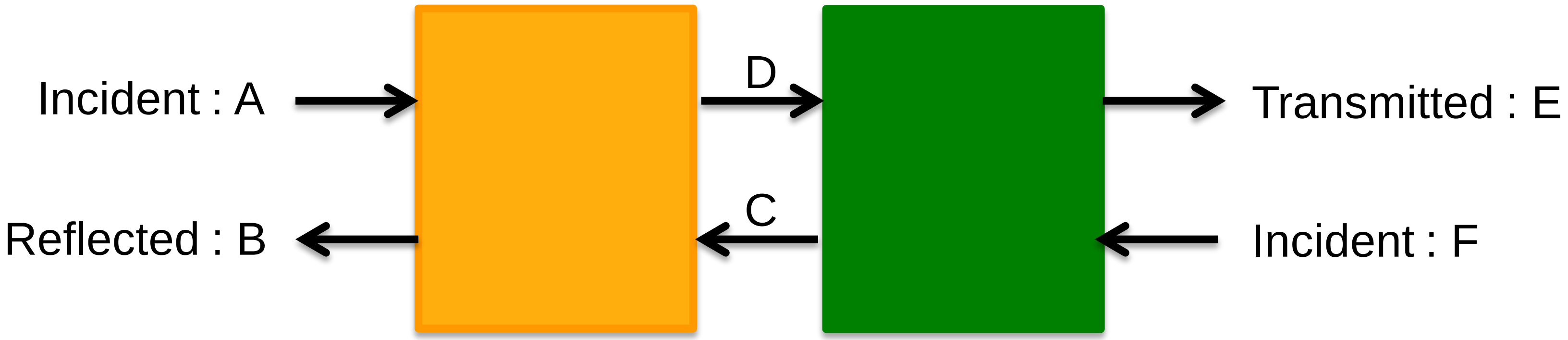
Scattering Matrix approach

Define our system : Single barrier

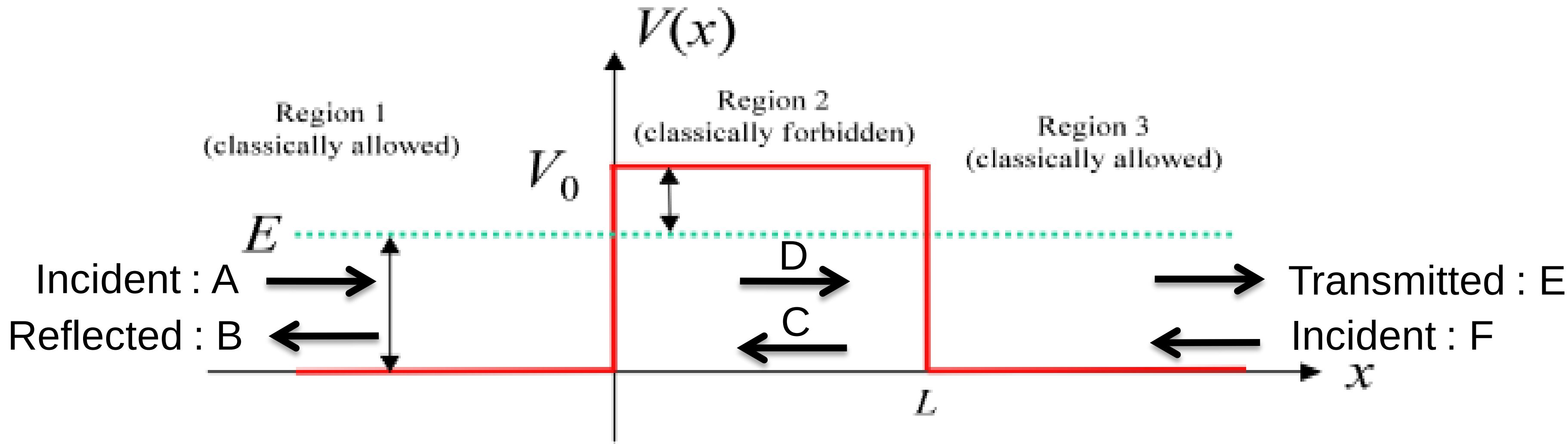


One matrix each for each interface: 2 S-matrices



No particles lost! Typically A=1 and F=0.

Tunneling through a single barrier



Wave-function each region,

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx}$$
$$\psi_2(x) = Ce^{-\gamma x} + De^{\gamma x}$$
$$\psi_3(x) = Ee^{ikx} + Fe^{-ikx}$$

$$k = \sqrt{\frac{2mE}{\hbar^2}} \qquad \gamma = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

Single barrier case

Applying boundary conditions at each interface (x=0 and x=L) gives,

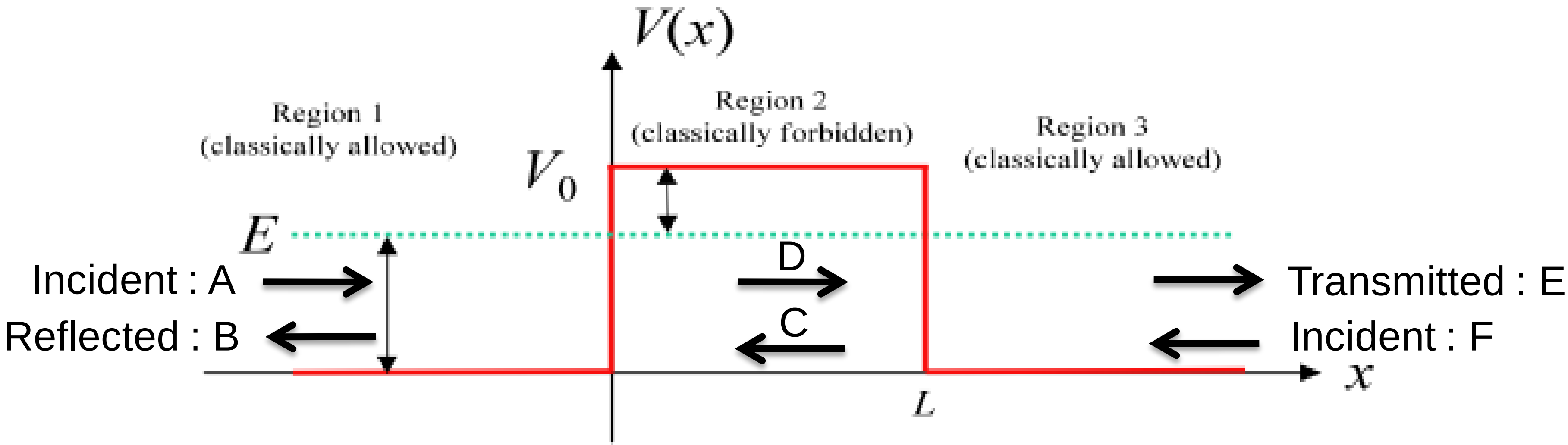
$$\psi_1(0) = \psi_2(0) \quad \rightarrow \quad A + B = C + D$$

$$\psi_1'(0) = \psi_2'(0) \quad \rightarrow ik(A - B) = -\gamma(C - D)$$

$$\psi_2(L) = \psi_3(L) \quad \rightarrow \quad Ce^{-\gamma L} + De^{\gamma L} = Ee^{ikL} + Fe^{-ikL}$$

$$\psi_2'(L) = \psi_3'(L) \quad \rightarrow \quad -\gamma\left(Ce^{-\gamma L} - De^{\gamma L}\right) = ik\left(Ee^{ikL} - Fe^{-ikL}\right)$$

Tunneling through a single barrier



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Which in matrix can be written as,

$$\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} \frac{1}{2}\left(1 + i\frac{\gamma}{k}\right) & \frac{1}{2}\left(1 - i\frac{\gamma}{k}\right) \\ \frac{1}{2}\left(1 - i\frac{\gamma}{k}\right) & \frac{1}{2}\left(1 + i\frac{\gamma}{k}\right) \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = M_1 \begin{bmatrix} C \\ D \end{bmatrix}$$

$$\begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} \frac{1}{2}\left(1 - i\frac{k}{\gamma}\right)e^{(ik+\gamma)L} & \frac{1}{2}\left(1 + i\frac{k}{\gamma}\right)e^{-(ik-\gamma)L} \\ \frac{1}{2}\left(1 + i\frac{k}{\gamma}\right)e^{(ik-\gamma)L} & \frac{1}{2}\left(1 - i\frac{k}{\gamma}\right)e^{-(ik+\gamma)L} \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix} = M_2 \begin{bmatrix} E \\ F \end{bmatrix}$$

Single barrier case

Transmission can be found using the relations between unknown constants,

$$T(E) = \left|\frac{E}{A}\right|^2 = \frac{1}{|m_{11}|^2} \qquad \begin{bmatrix} A \\ B \end{bmatrix} = M_1 \begin{bmatrix} C \\ D \end{bmatrix} = M_1 M_2 \begin{bmatrix} E \\ F \end{bmatrix} = M \begin{bmatrix} E \\ F \end{bmatrix}$$

Case: $E<V_o$

$$T(E) = \left[1 + \left(\frac{\gamma^2 + k^2}{2k\gamma}\right)^2 sh^2(\gamma L)\right]^{-1}$$

Case(γL large): Strong barrier

$$T(E) \approx \left(\frac{4k\gamma}{k^2 + \gamma^2}\right)^2 \exp(-2\gamma L)$$

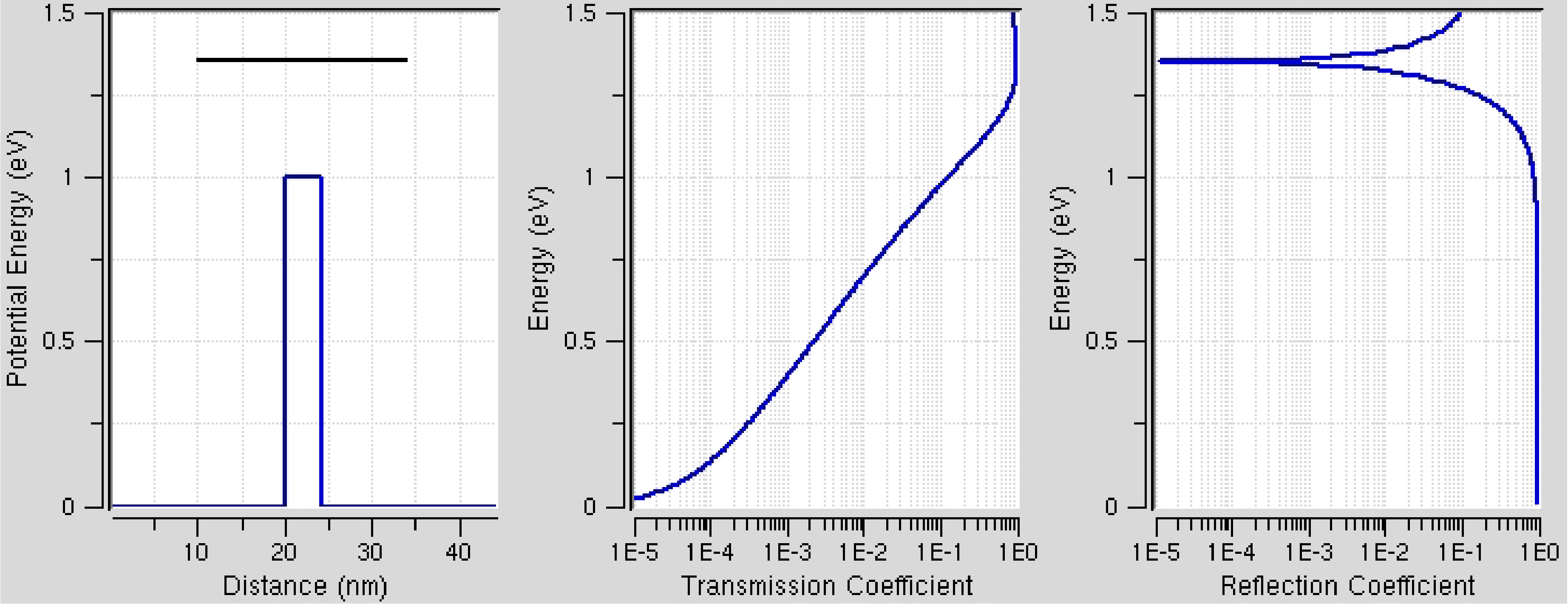
Case(γL<<1): Weak barrier

$$T(E) \approx \frac{1}{1 + (kL/2)^2}$$

Case: $E>V_o$

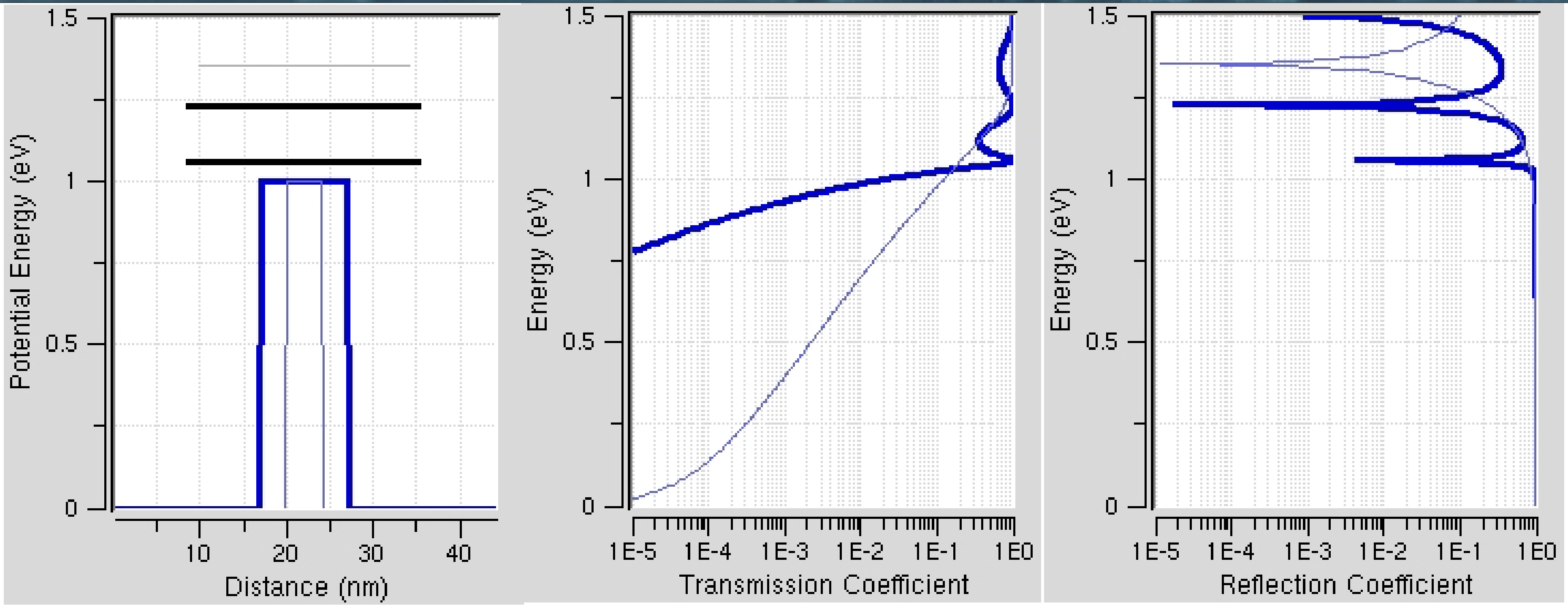
$$T(E) = \left[1 + \left(\frac{k^2 - k_2^2}{2kk_2}\right)^2 \sin^2(k_2 L)\right]^{-1}$$

Single barrier : Concepts



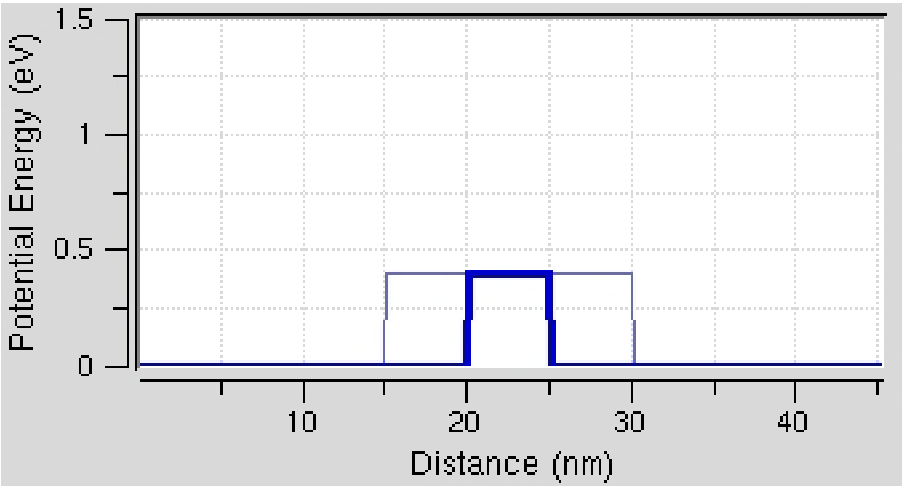
- Transmission is finite under the barrier – tunneling!
- Transmission above the barrier is not perfect unity!
- Quasi-bound state above the barrier.
  Transmission goes to one.

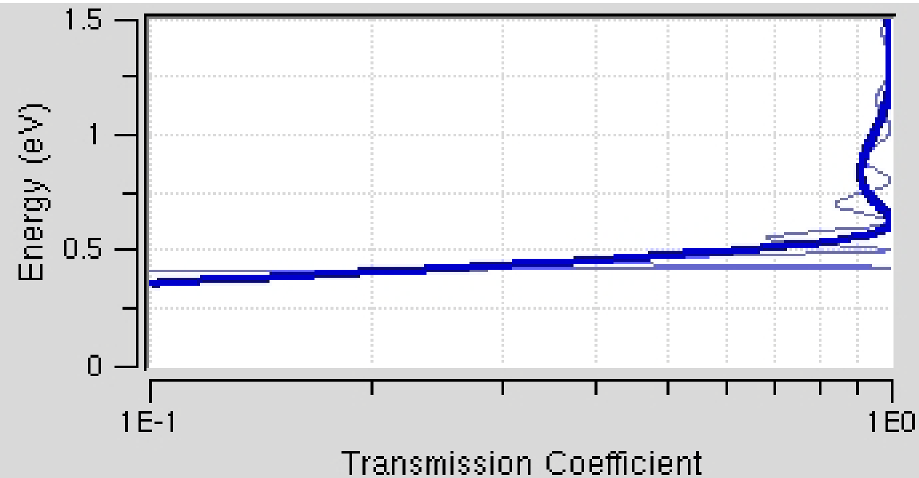
Effect of barrier thickness below the barrier

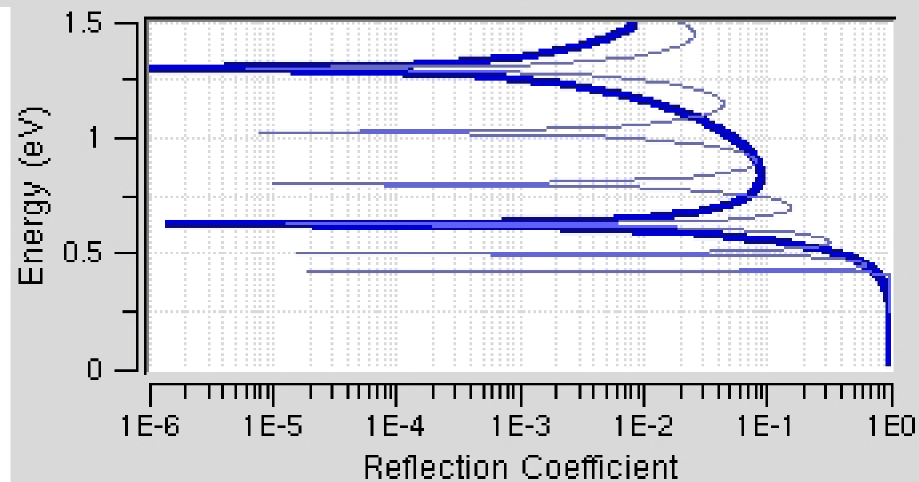


- Increased barrier width reduces tunneling probability
- Thicker barrier increase the reflection probability below the barrier height.
- Quasi-bound states occur for the thicker barrier too.

Effect of barrier thickness above the barrier



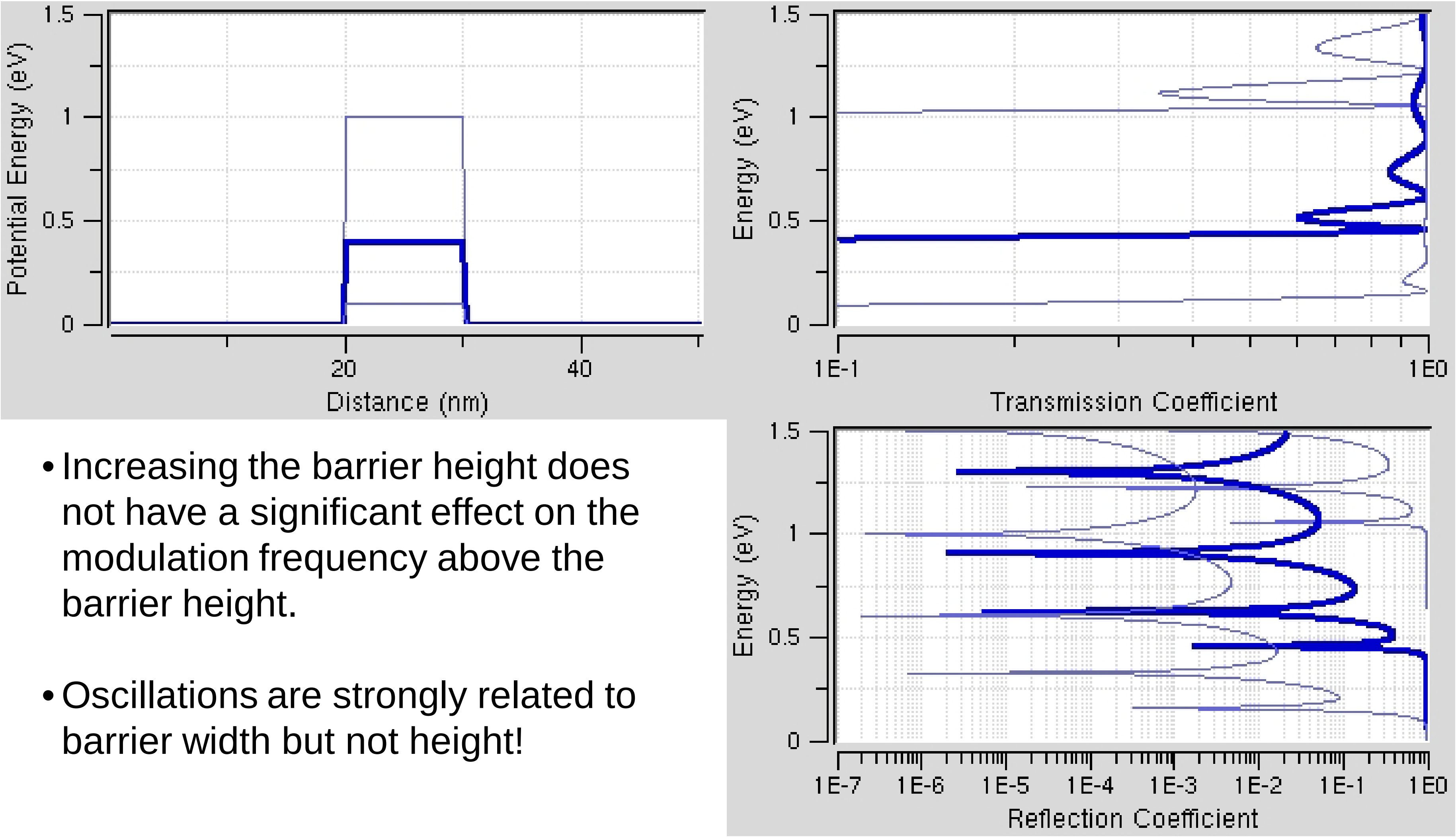




- Increased barrier width increases oscillation frequency in transmission and reflection.

- Quasi-bound states above the barrier due to 2 reflections.

Effect of barrier height

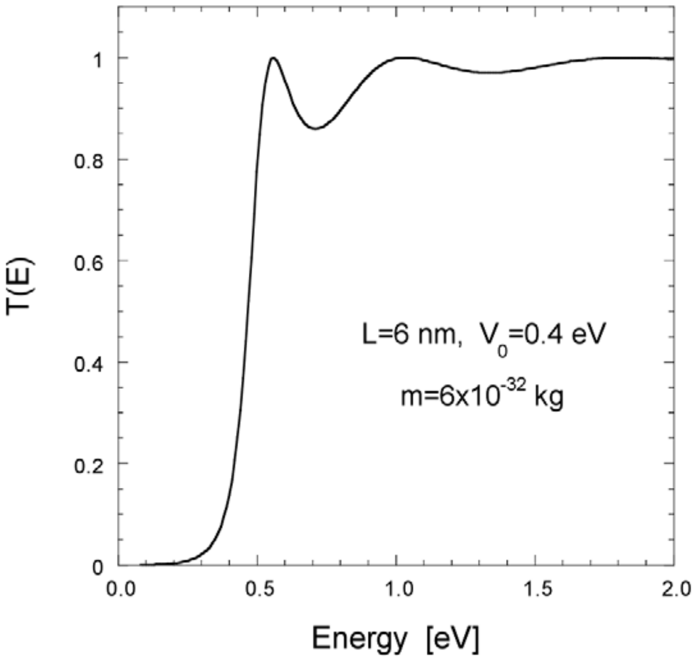


- Increasing the barrier height does not have a significant effect on the modulation frequency above the barrier height.

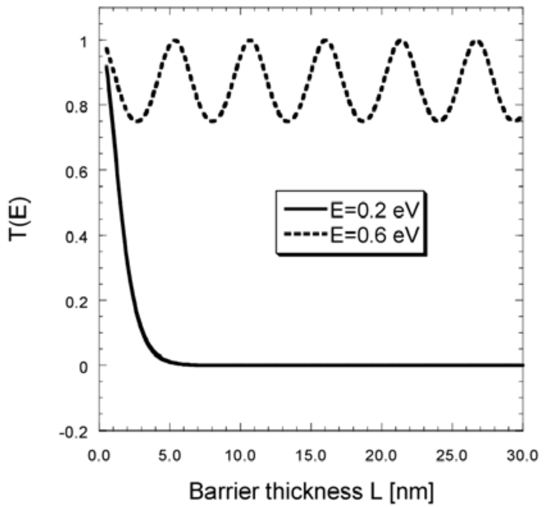
- Oscillations are strongly related to barrier width but not height!

Single barrier case: Discussion

T(E) for a given geometry

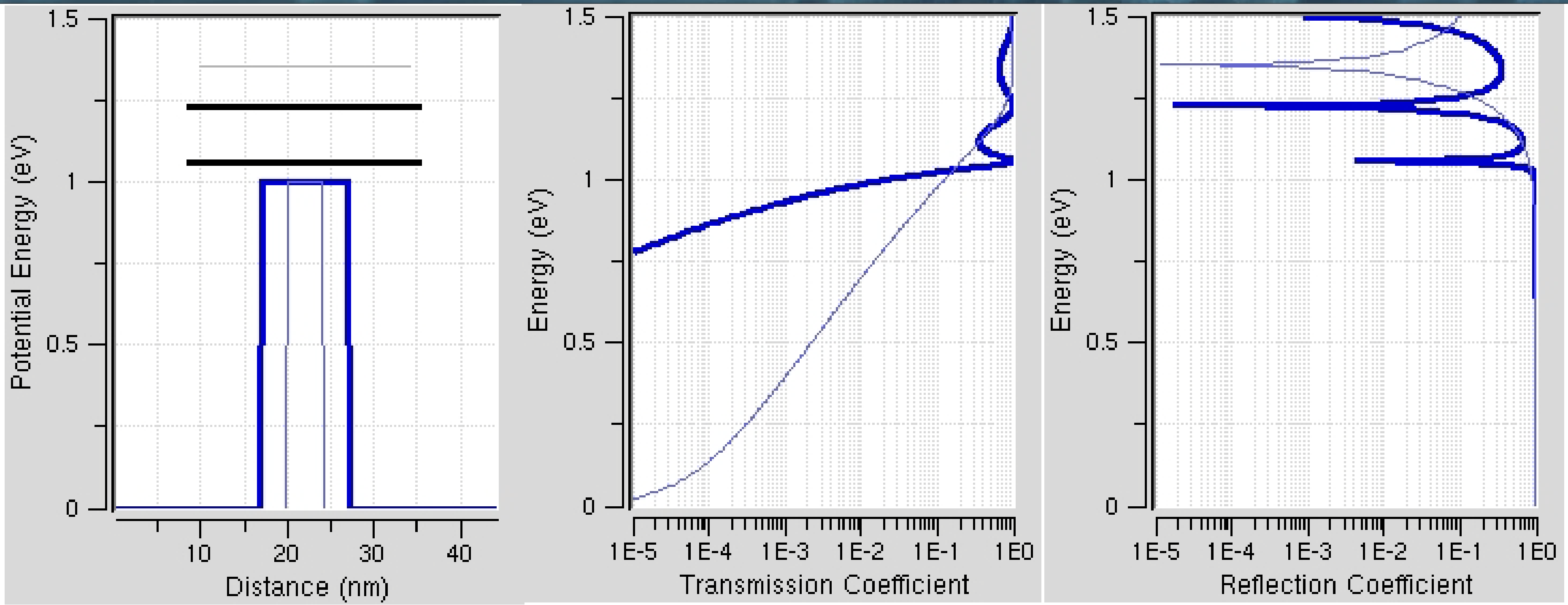


T(E) for different lengths



- $E<V_o$: Classical Physics: T(E)=0,
  Quantum Physics: a hyperbolic increase.
- $E>V_o$: Classical Physics: T(E)=1,
  Quantum Physics: total transmission at discrete energies only.
  Only barriers of certain width will transmit all particles at a given energies.

Single Barrier - Key Summary



- Quantum wavefunctions can tunnel through barriers
- Tunneling is reduced with increasing barrier height and width
- Transmission above the barrier is not unity
  - » 2 interfaces cause constructive and destructive interference
  - » Quasi bound states are formed that result in unity transmission