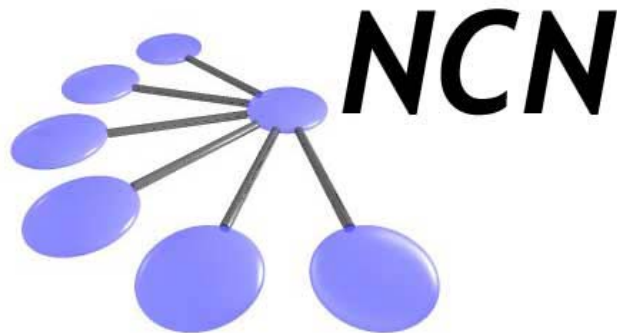


Network for Computational Nanotechnology (NCN)

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

Open 1D Systems: Transmission through & over 1 Barrier

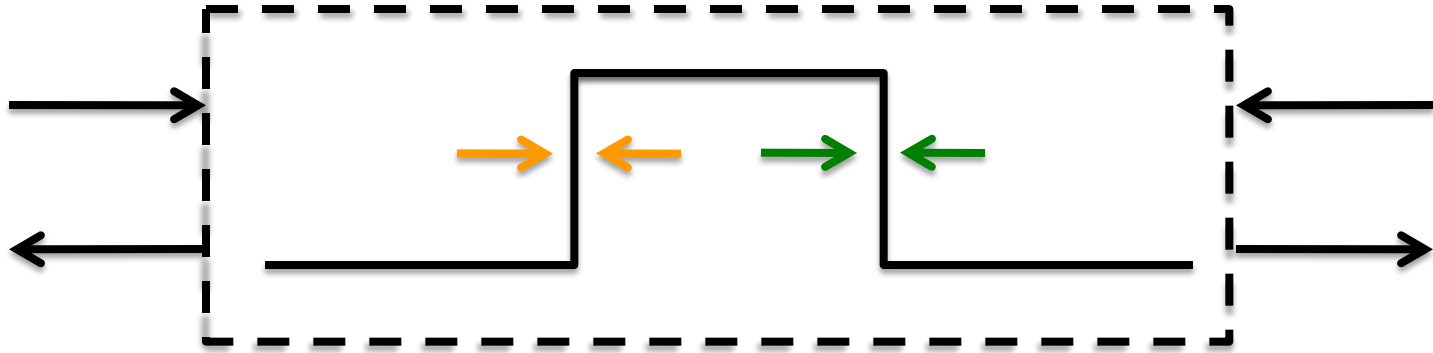


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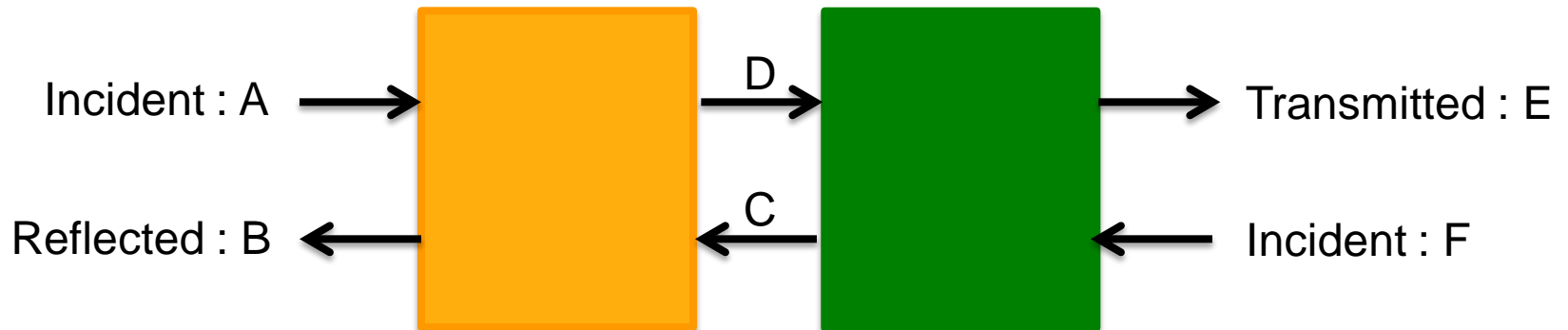
PURDUE
UNIVERSITY

Scattering Matrix approach

Define our system : Single barrier

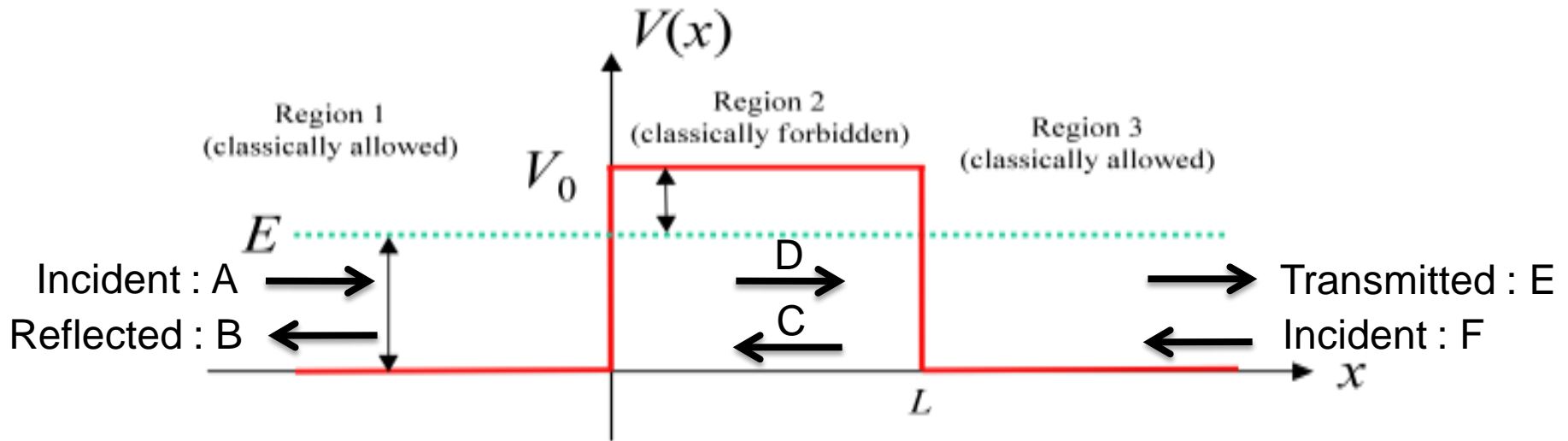


One matrix each for each interface: 2 S-matrices



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

Tunneling through a single barrier



Wave-function each region,

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx}$$

$$\psi_2(x) = Ce^{-\gamma x} + De^{\gamma x}$$

$$\psi_3(x) = Ee^{ikx} + Fe^{-ikx}$$

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

Single barrier case

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

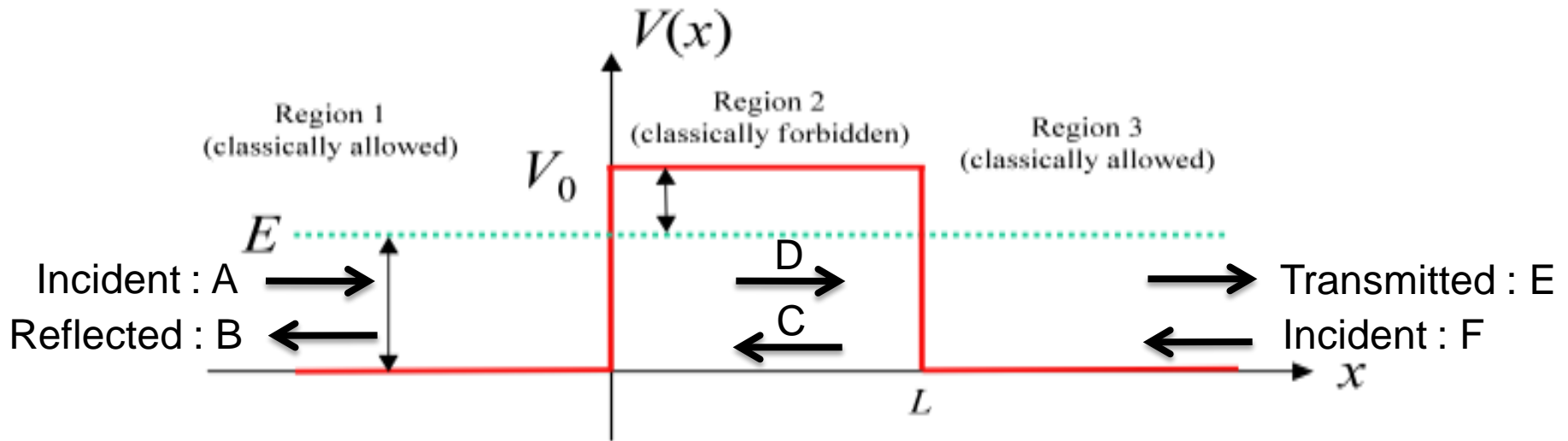
$$\psi_1(0) = \psi_2(0) \quad \rightarrow \quad A + B = C + D$$

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

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

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

Tunneling through a single barrier



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

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,

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

Case: $E < V_0$

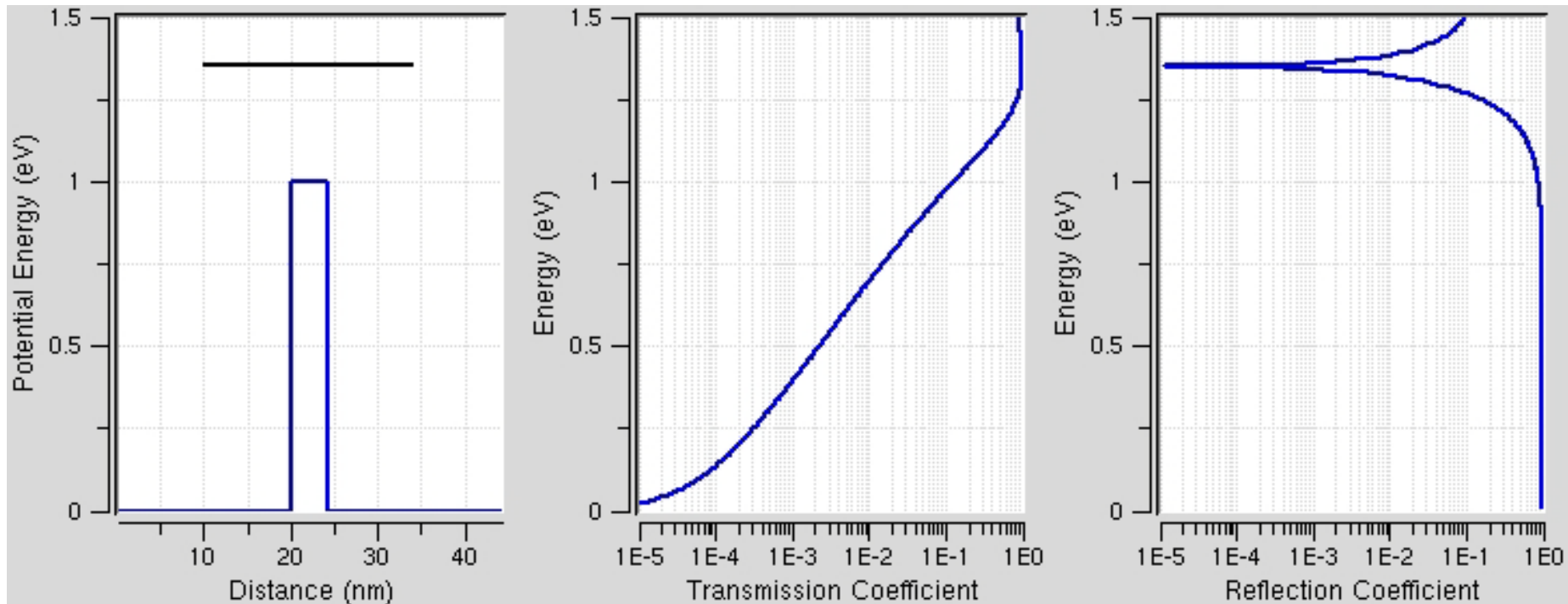
Case (γL large): Strong barrier

$$T(E) = \left[1 + \left(\frac{\gamma^2 + k^2}{2k\gamma} \right)^2 \text{sh}^2(\gamma L) \right]^{-1} \quad T(E) \approx \left(\frac{4k\gamma}{k^2 + \gamma^2} \right)^2 \exp(-2\gamma L)$$

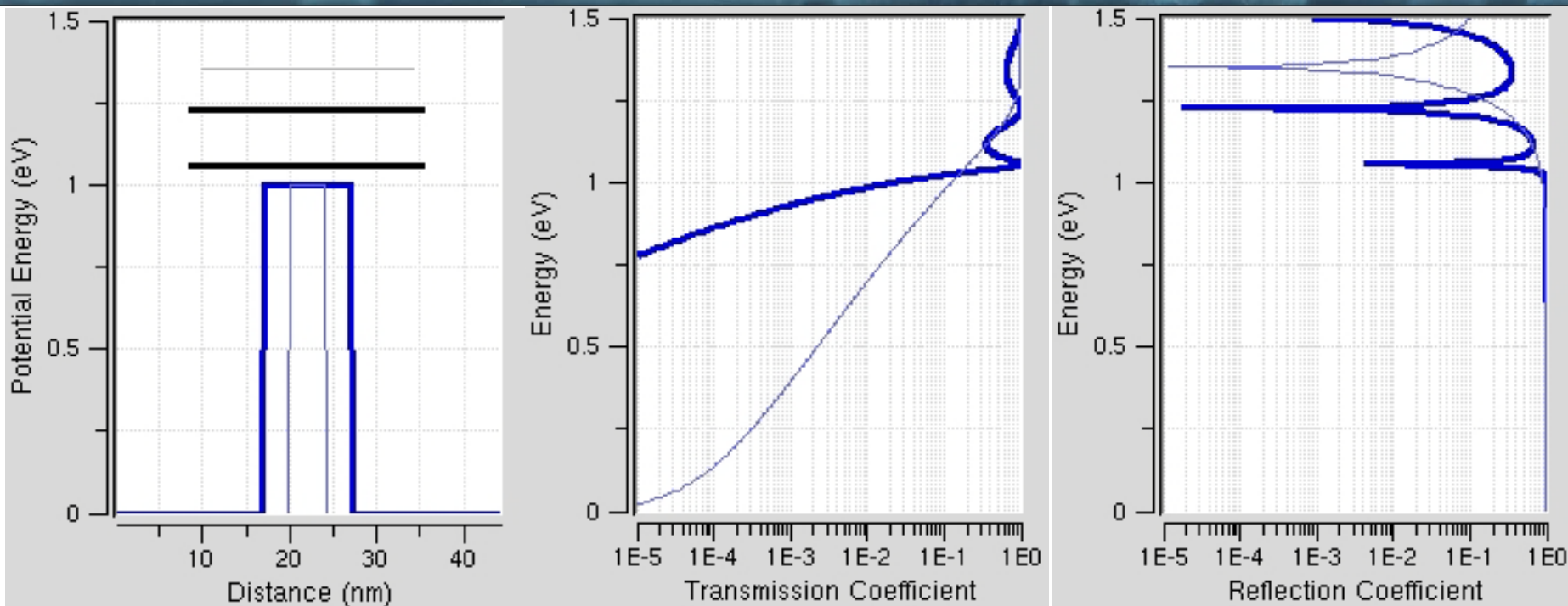
Case ($\gamma L \ll 1$): Weak barrier

Case: $E > V_0$

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

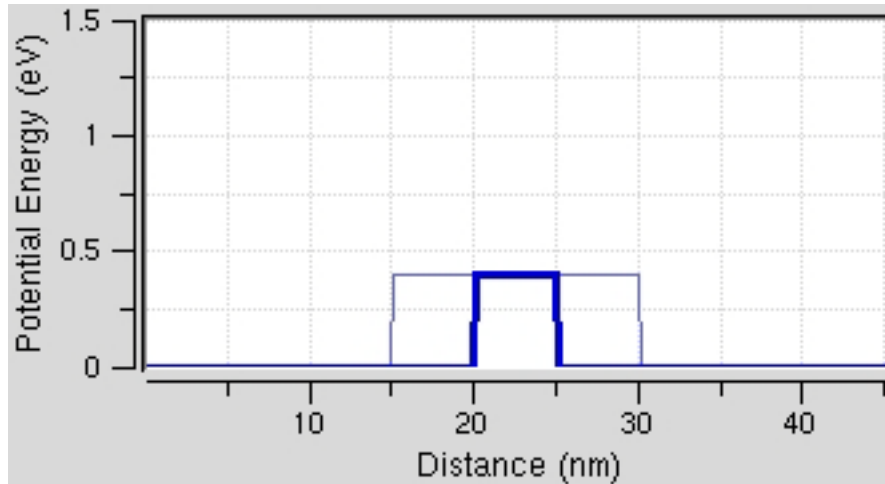


- Transmission is finite under the barrier – tunneling!
- Transmission above the barrier is not perfect unity!
- Quasi-bound state above the barrier.
Transmission goes to one.

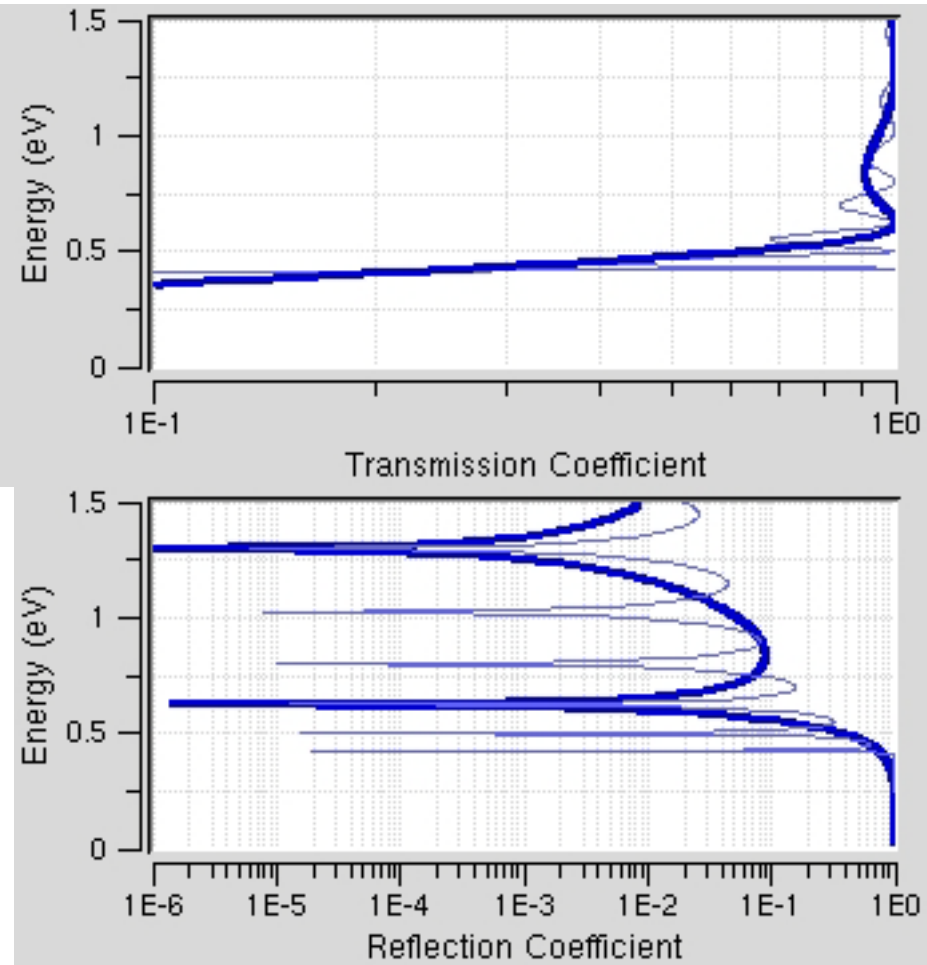


- Increased barrier width reduces tunneling probability
- Thicker barrier increase the reflection probability below the barrier height.
- Quasi-bound states occur for the thicker barrier too.

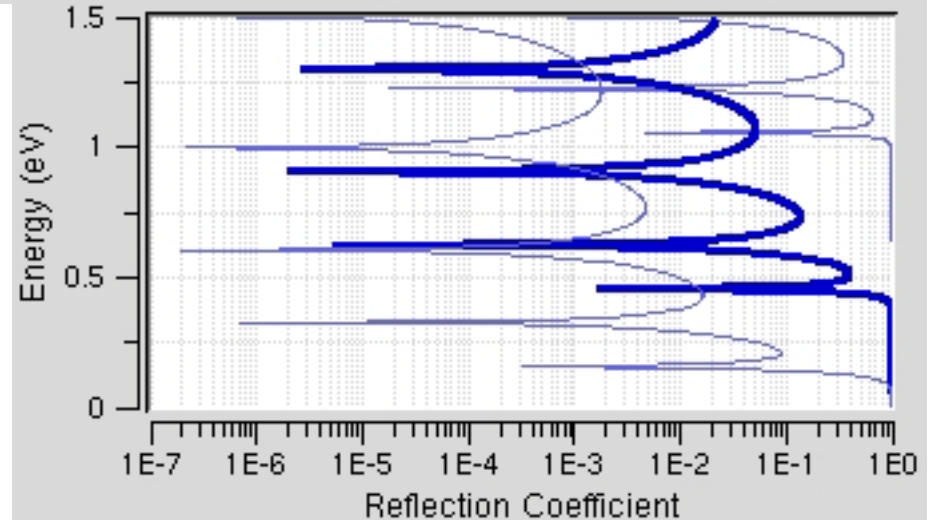
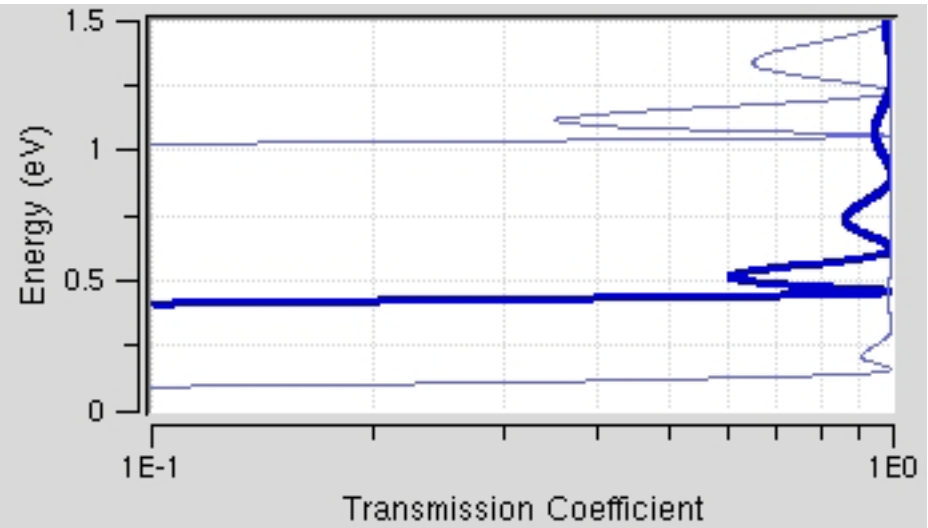
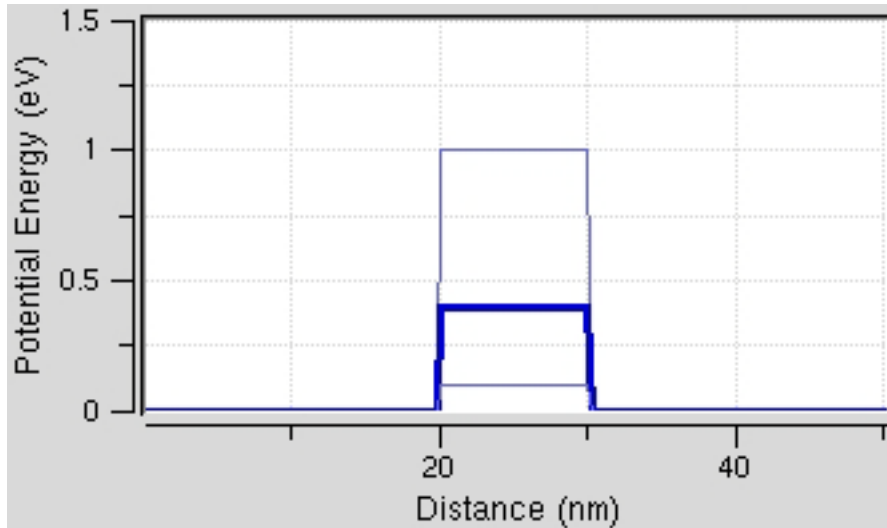
Effect of barrier thickness above the barrier



- Increased barrier width increases oscillation frequency in transmission and reflection.
- Quasi-bound states above the barrier due to 2 reflections.

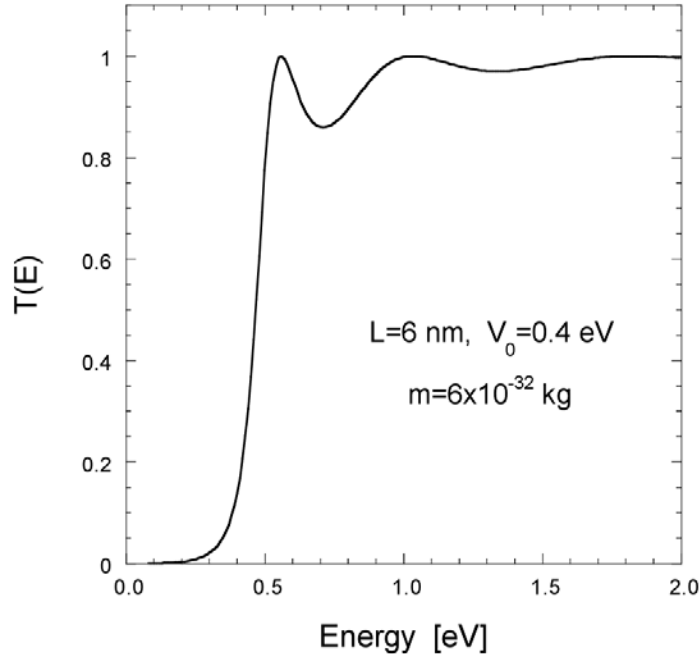


Effect of barrier height

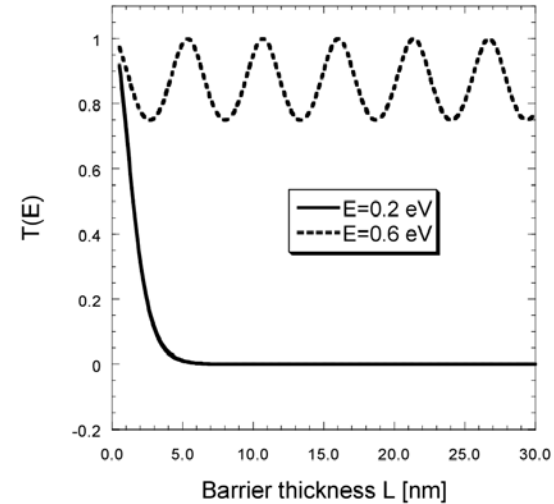


- Increasing the barrier height does not have a significant effect on the modulation frequency above the barrier height.
- Oscillations are strongly related to barrier width but not height!

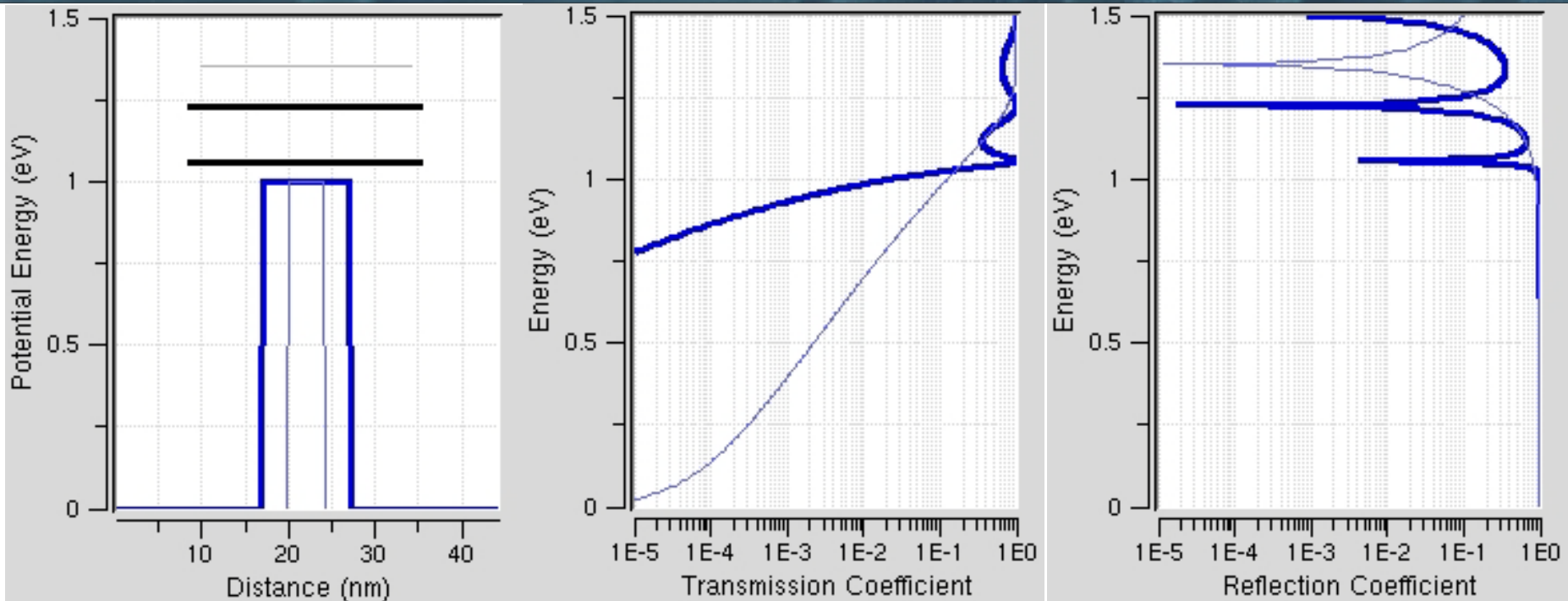
T(E) for a given geometry



T(E) for different lengths



- $E < V_0$: Classical Physics: $T(E)=0$,
Quantum Physics: a hyperbolic increase.
- $E > V_0$: 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.



- 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