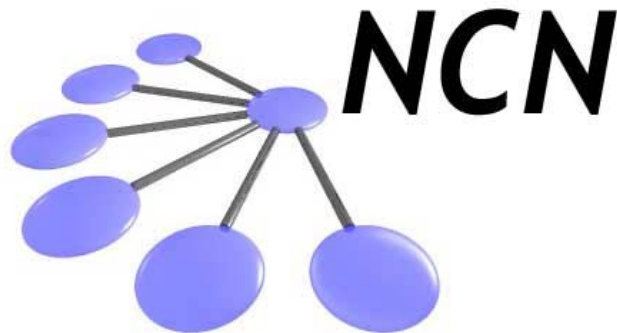


# *Network for Computational Nanotechnology (NCN)*

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

## **Open 1D Systems: Transmission through Double Barrier Structures - Resonant Tunneling**

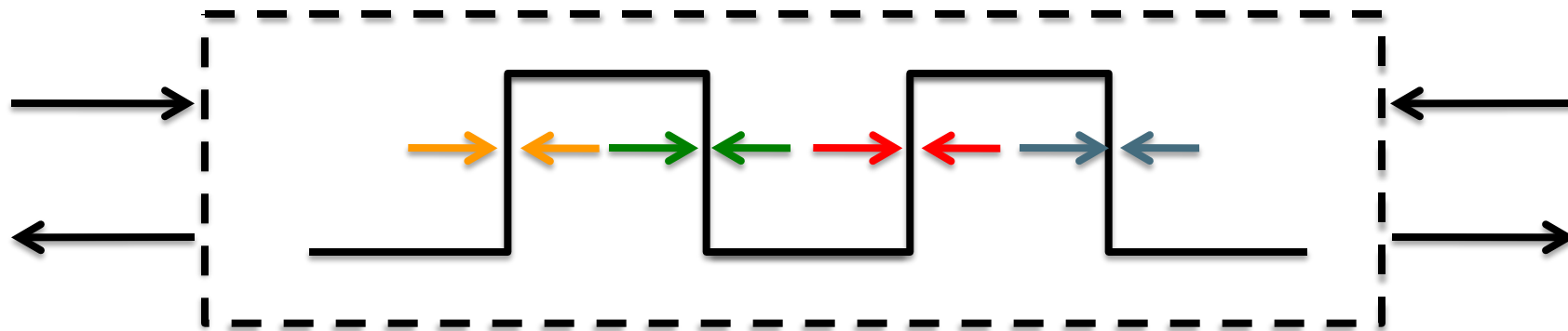


Gerhard Klimeck,  
Dragica Vasileska,  
Samarth Agarwal

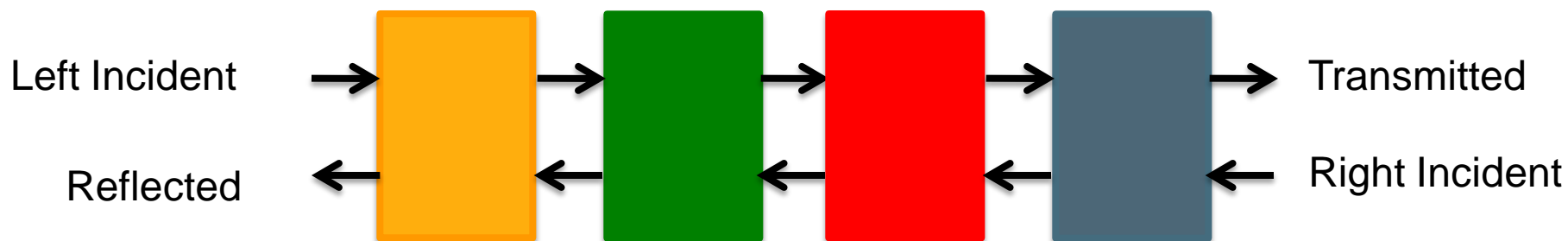
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# Scattering Matrix approach

Define our system : Double barrier



One matrix each for each interface: 4 S-matrices

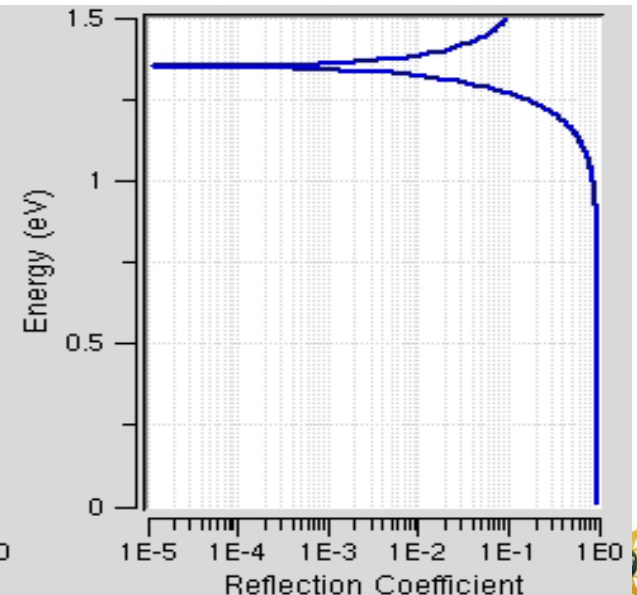
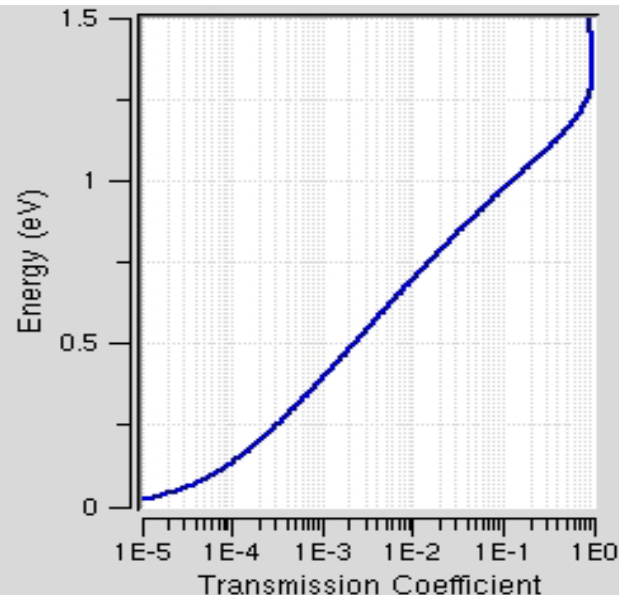
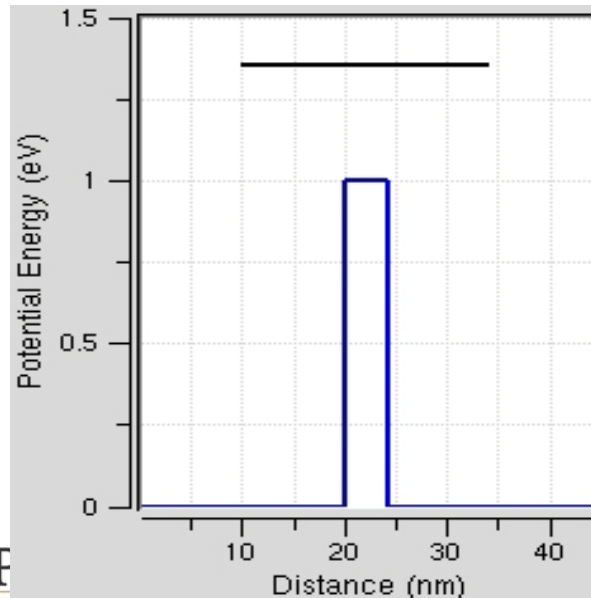


No particles lost!

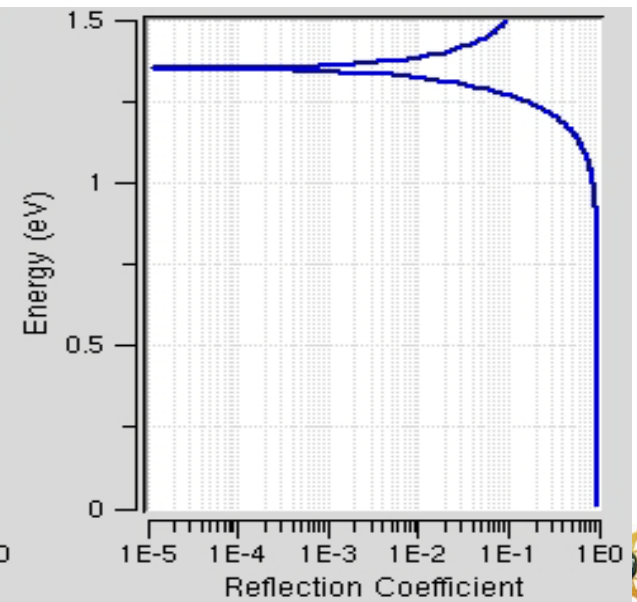
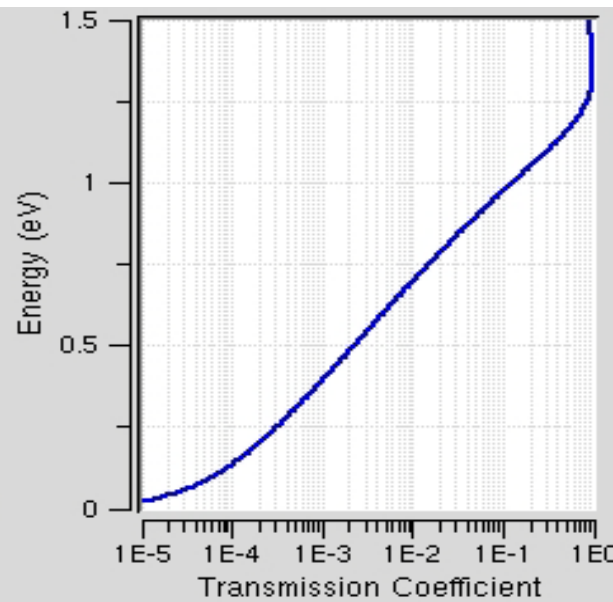
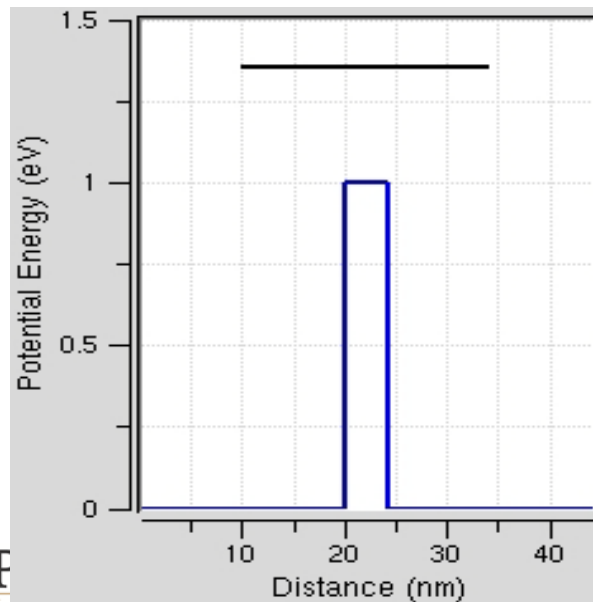
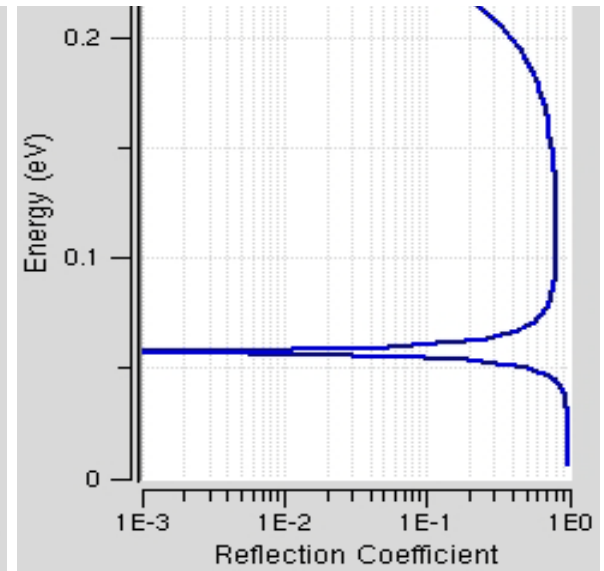
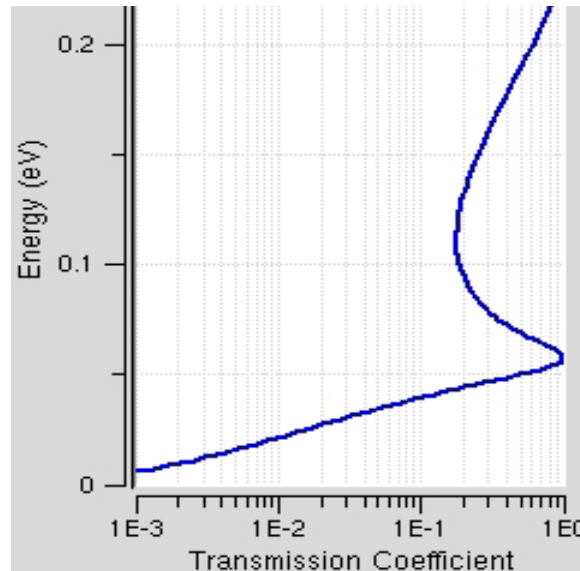
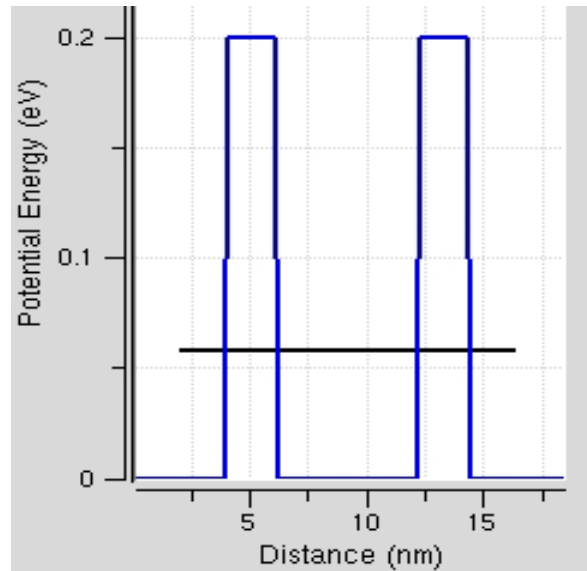
Typically Left Incident wave is normalized to one.

Right incident is assumed to be zero.

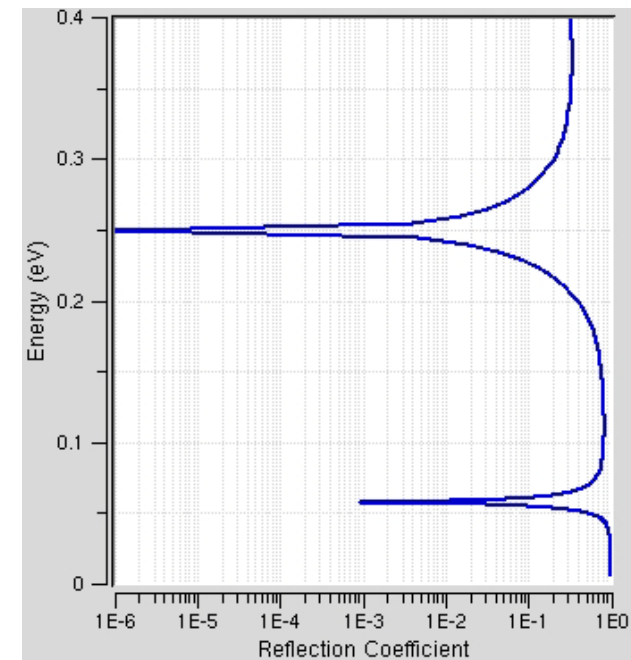
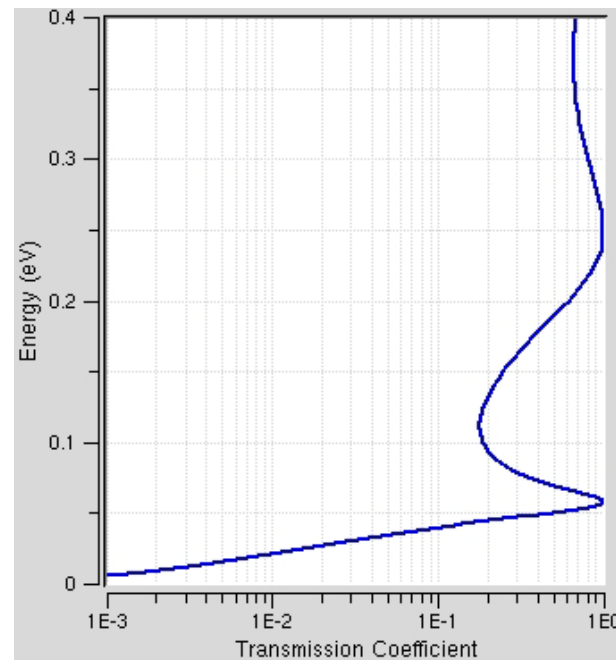
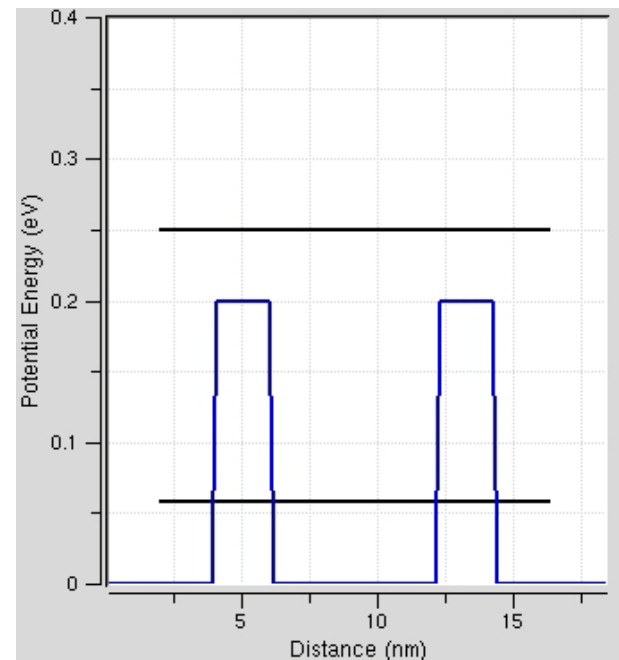
- Transmission is finite under the barrier – tunneling!
- Transmission above the barrier is not perfect unity!
- Quasi-bound state above the barrier.  
Transmission goes to one.



- Double barriers allow a transmission probability of one / unity for discrete energies
- (reflection probability of zero) for some energies below the barrier height.
- This is in sharp contrast to the single barrier case
- Cannot be predicted by classical physics.

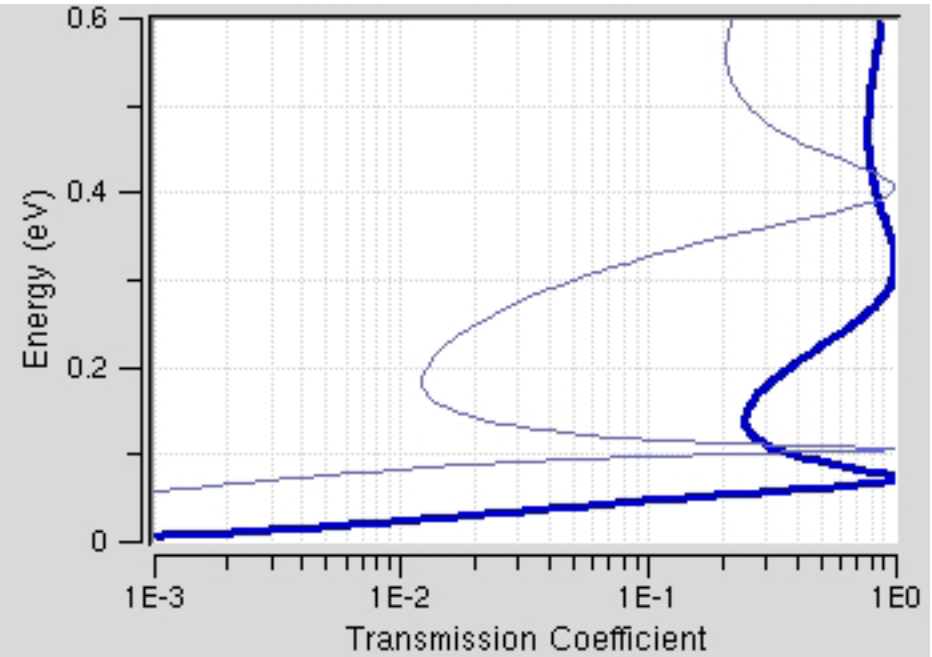
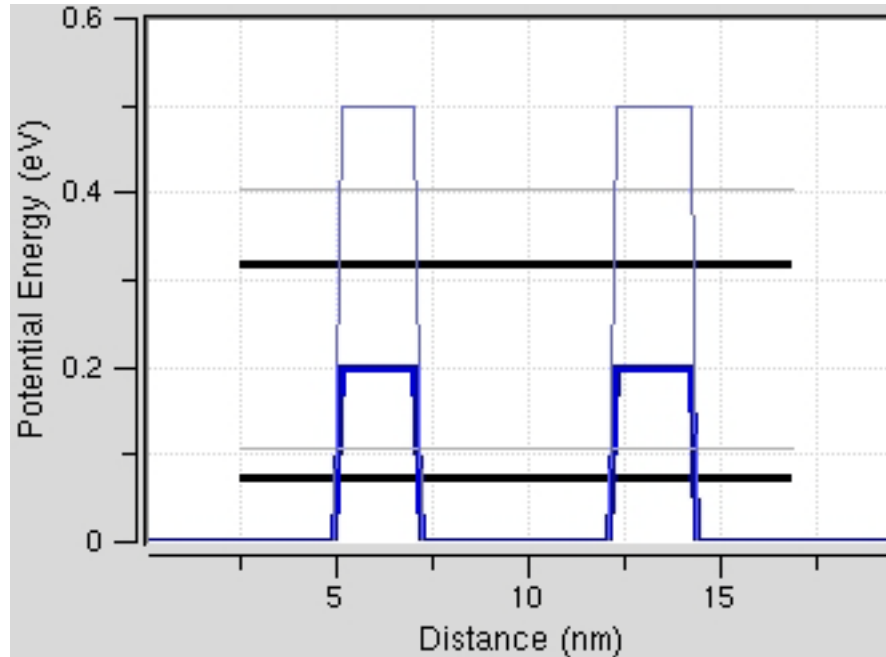


# Double barrier: Quasi-bound states



- In addition to states inside the well, there could be states above the barrier height.
- States above the barrier height are quasi-bound or weakly bound.
- How strongly bound a state is can be seen by the width of the transmission peak.
- The transmission peak of the quasi-bound state is much broader than the peak for the state inside the well.

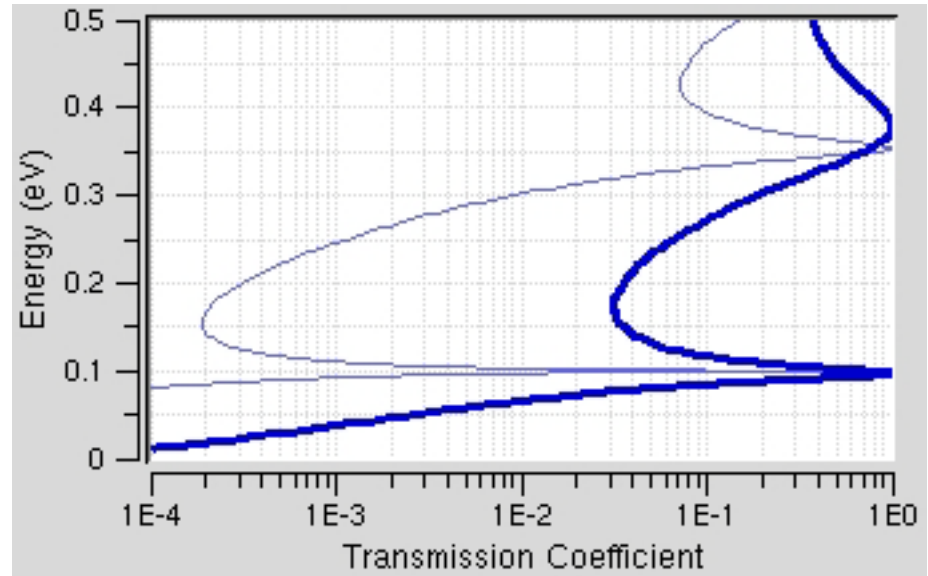
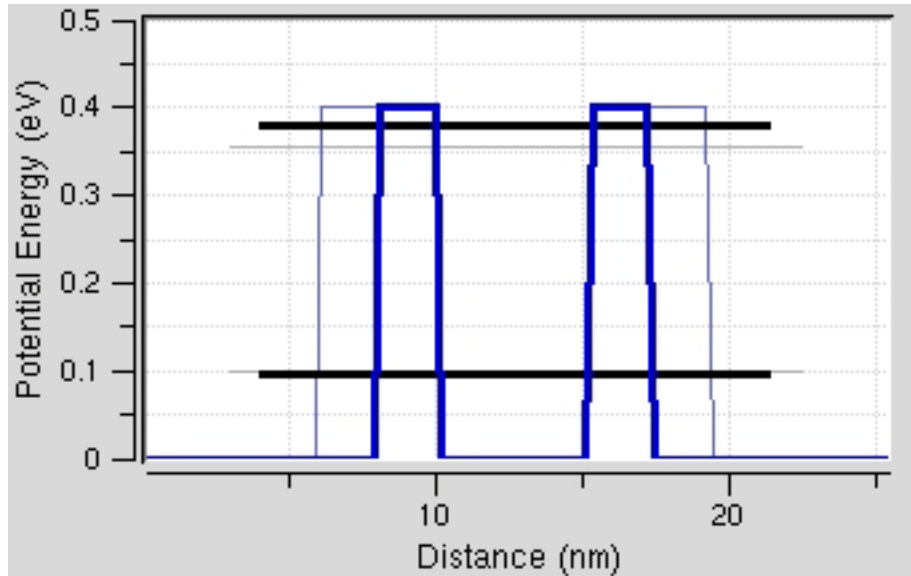
## Effect of barrier height



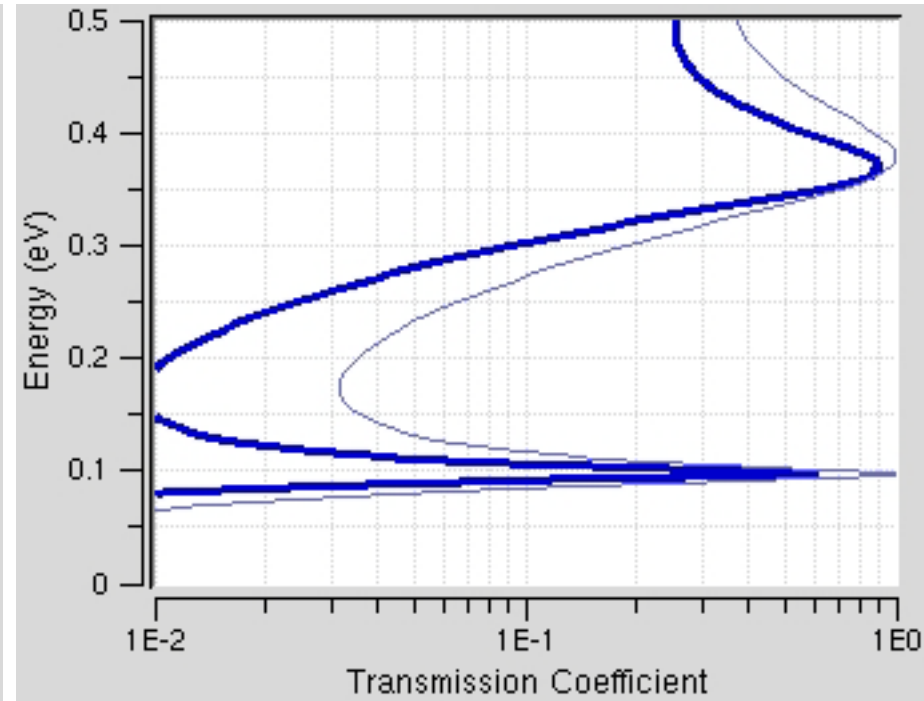
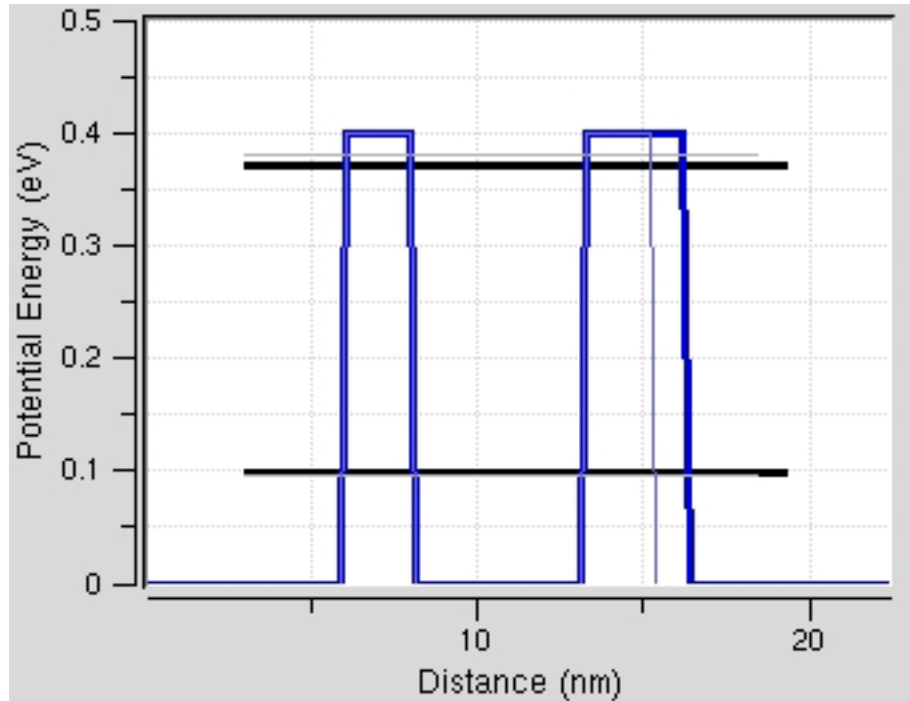
- Increasing the barrier height makes the resonance sharper.
- By increasing the barrier height, the confinement in the well is made stronger, increasing the lifetime of the resonance.
- A longer lifetime corresponds to a sharper resonance.



## Effect of barrier thickness

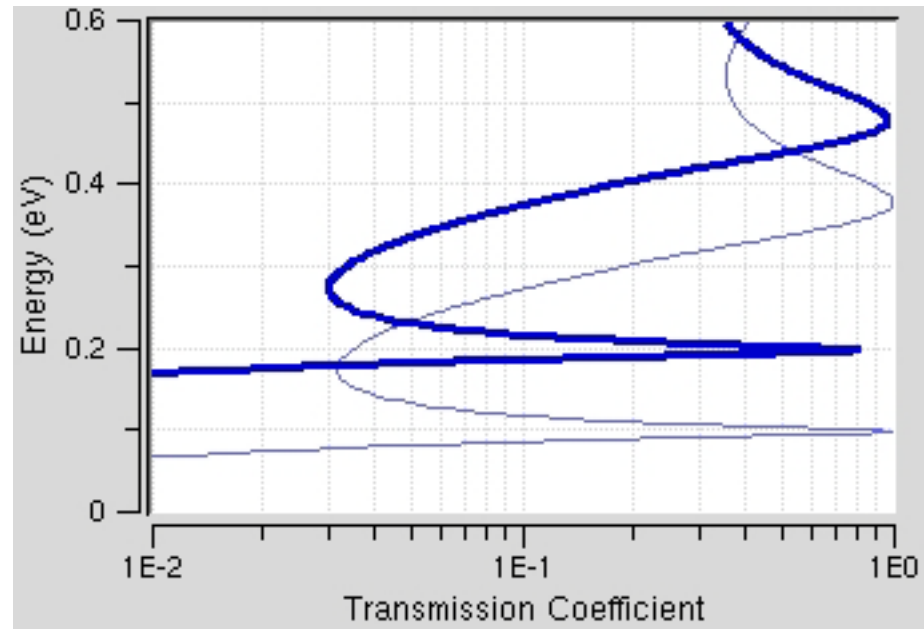
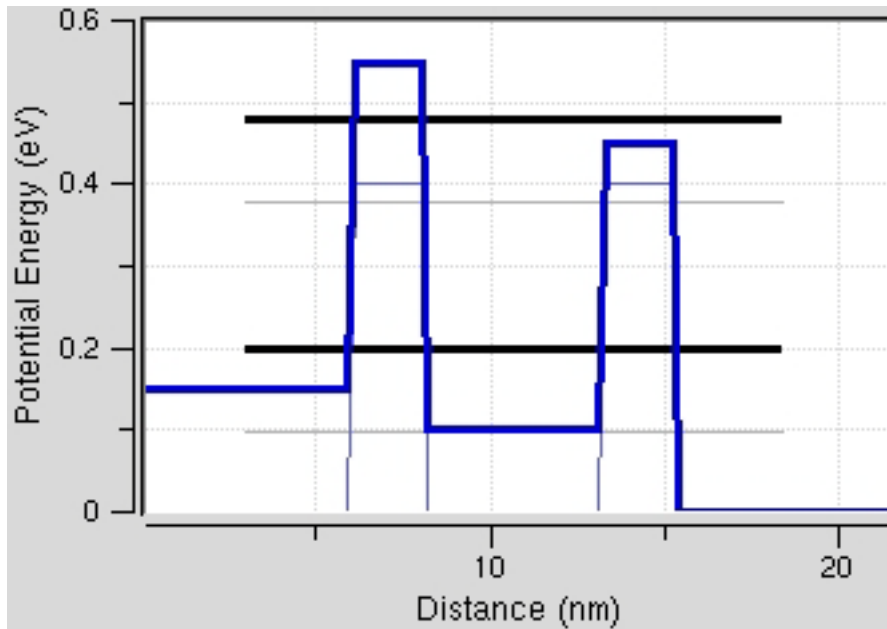


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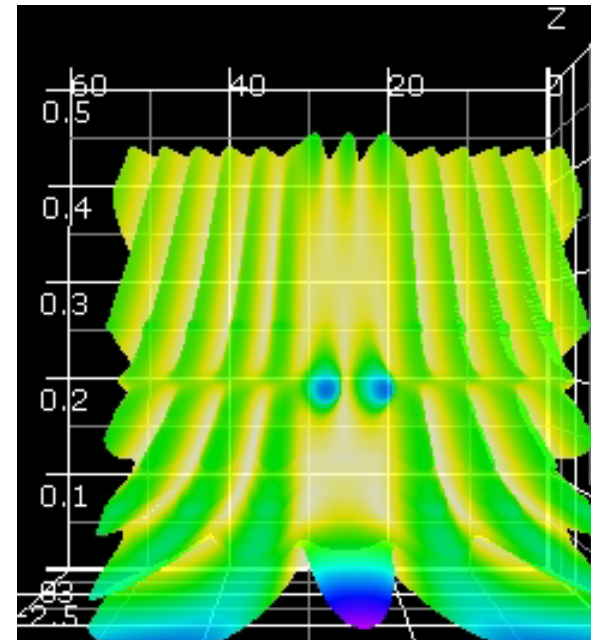
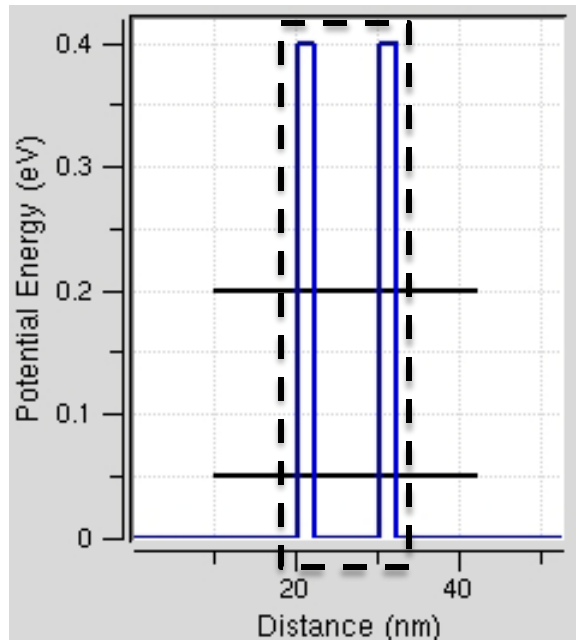
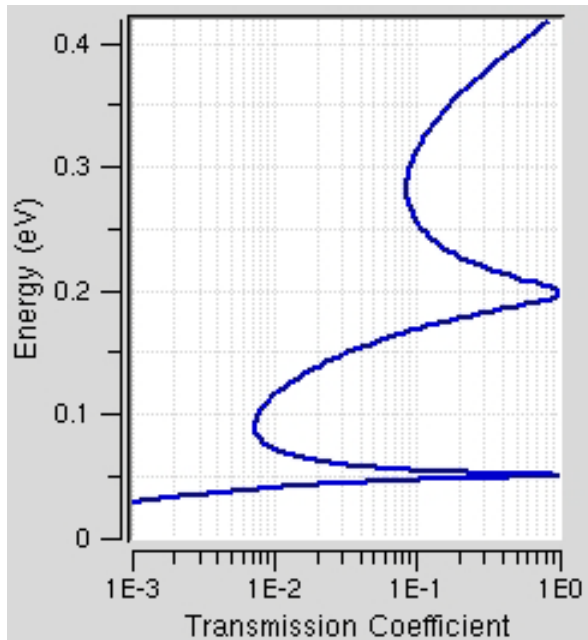
- Transmission in the symmetric case goes to one for resonance energies.
- Transmission in the non-symmetric case (second barrier is thicker) does not go to one for resonance energies.
- Current in the non-symmetric case will always be less than the symmetric case.





- Symmetric structure (no bias) exhibit unity transmission on resonance.
- Potential drop introduces asymmetry  
=> transmission never reaches unity anymore
- Increased asymmetry reduces resonance transmission / current.

# Double barrier energy levels Vs Closed system



The well region in the double barrier case can be thought of as a particle in a box.

# Particle in a box

- The time independent Schrödinger equation is

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x)\psi(x) = E\psi(x) \quad \text{where, } V(x) = \begin{cases} 0 & 0 < x < L_x \\ \infty & \text{elsewhere} \end{cases}$$

- The solution in the well is:

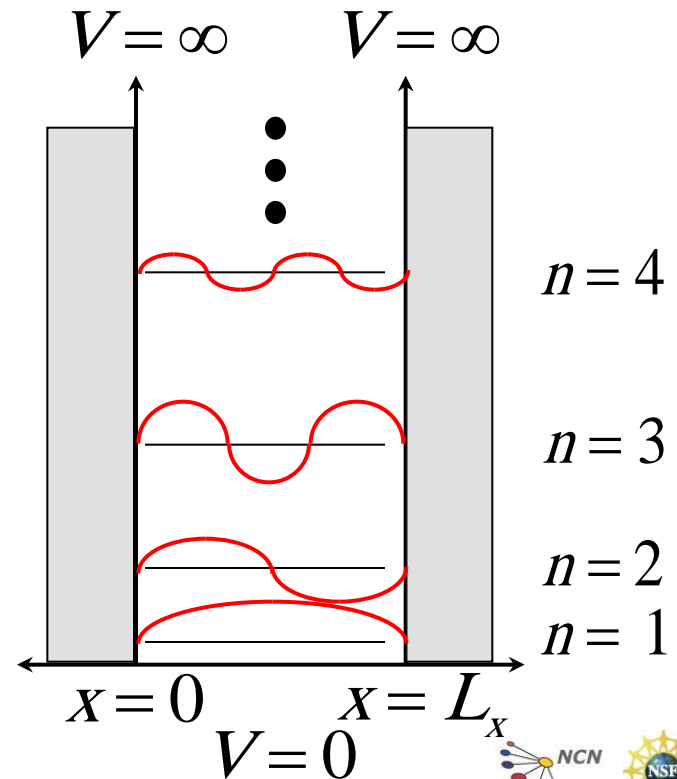
$$\psi_n(x) = A \sin\left(\frac{n\pi}{L_x} x\right), \quad n = 1, 2, 3, \dots$$

- Plugging the normalized wave-functions back into the Schrödinger equation we find that energy levels are quantized.

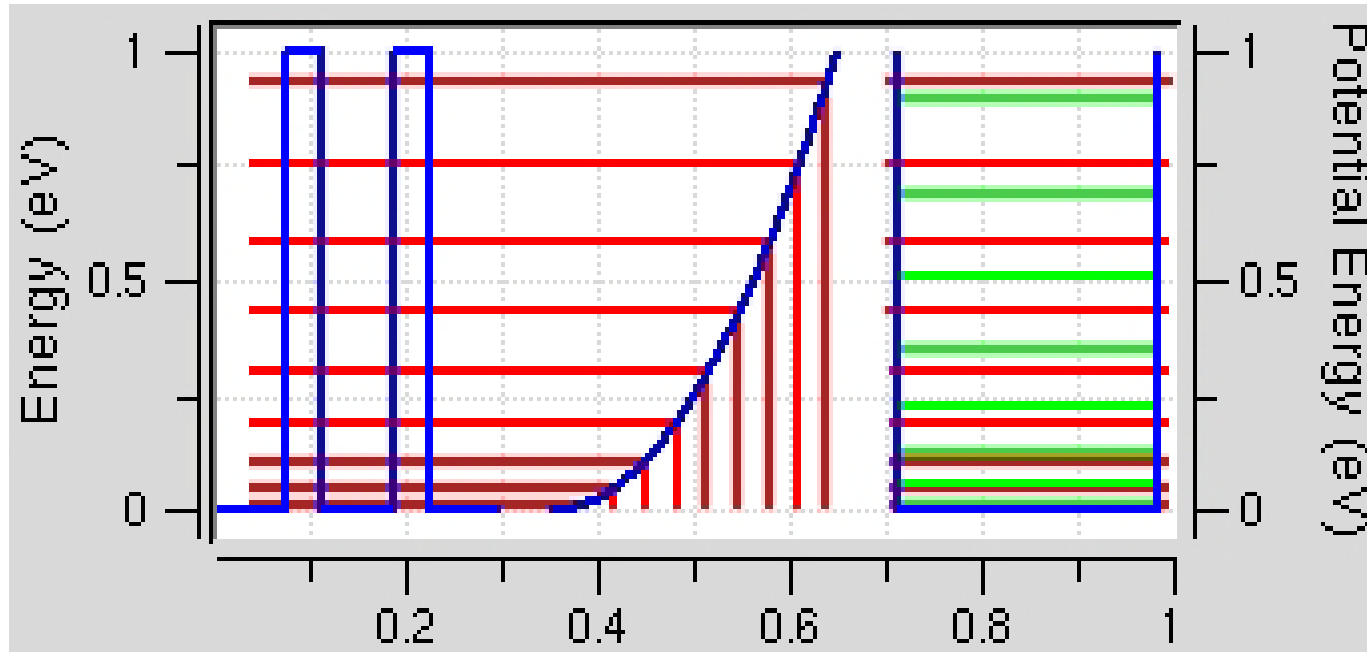
$$\psi_n(x) = \sqrt{\frac{2}{L_x}} \sin\left(\frac{n\pi}{L_x} x\right)$$

$$E_n = \frac{\hbar^2 \pi^2}{2mL_x^2} n^2$$

$$n = 1, 2, 3, \dots, \quad 0 < x < L_x$$



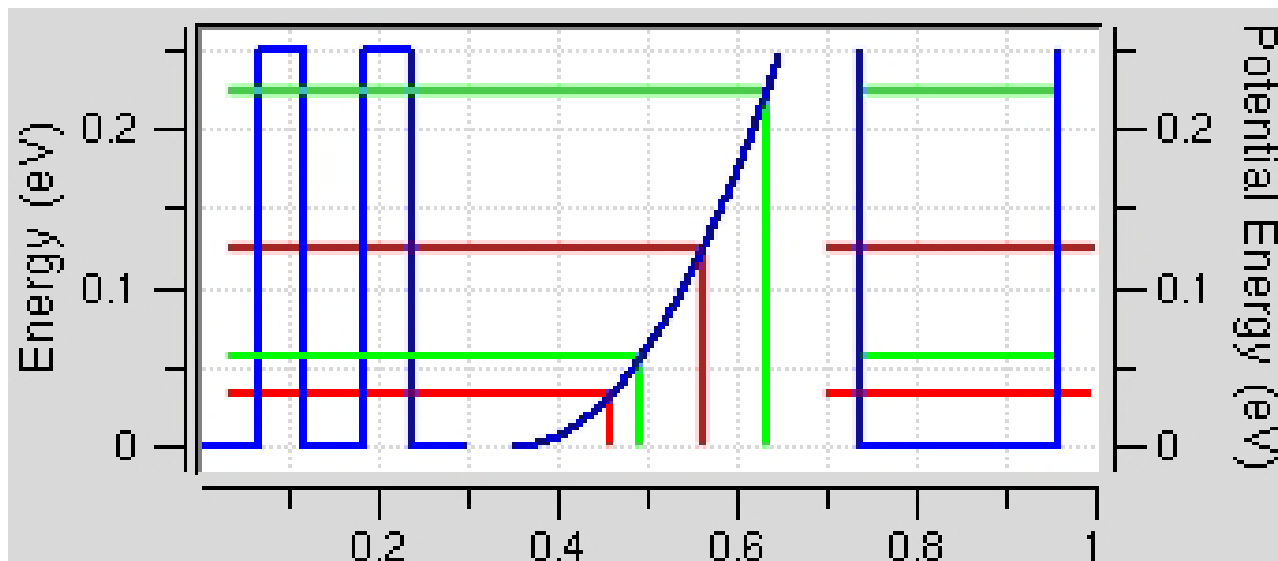
# Double barrier & particle in a box



- Green: Particle in a box energies.
- Red: Double barrier energies

- Double barrier: Thick Barriers(10nm), Tall Barriers(1eV), Well(20nm).
- First few resonance energies match well with the particle in a box energies.
- The well region resembles the particle in a box setup.

# Open systems Vs closed systems



- Green: Particle in a box energies.
- Red: Double barrier energies

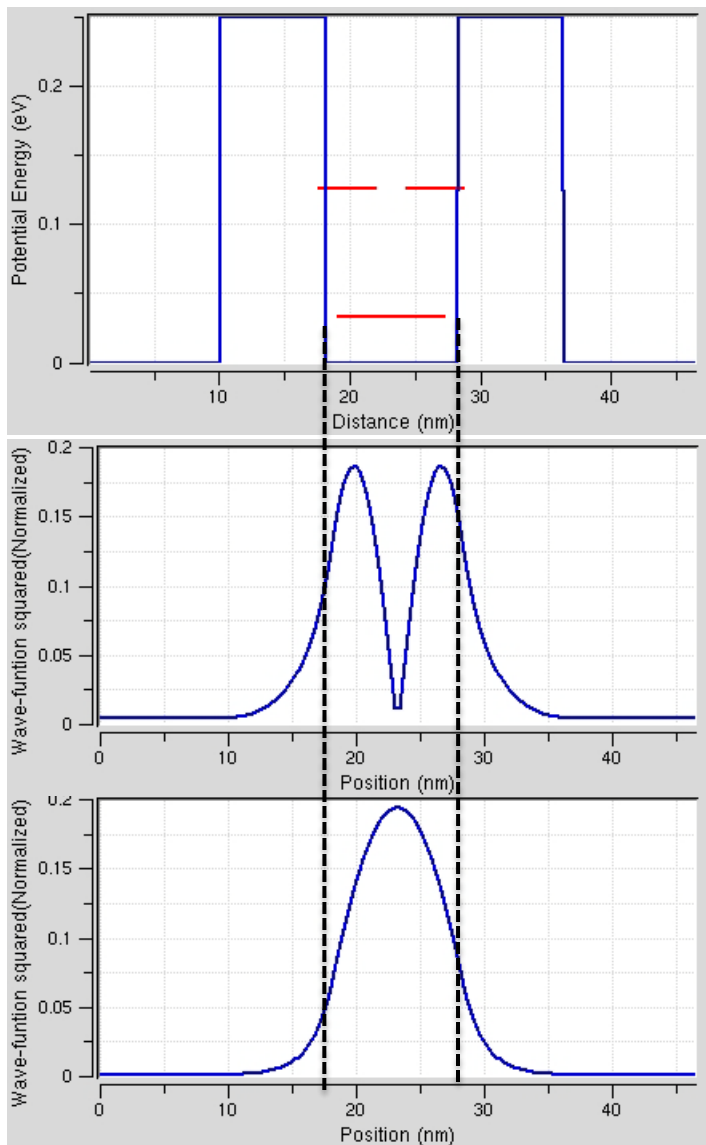
- Double barrier: Thinner Barriers(8nm), Shorter Barriers(0.25eV), Well(10nm).
- Even the first resonance energy does not match with the particle in a box energy.
- The well region does not resemble a particle in a box.
- A double barrier structure is an OPEN system, particle in a box is a CLOSED system.

## Reason for deviation?

Potential profile and resonance energies using tight-binding.

First excited state wave-function amplitude using tight binding.

Ground state wave-function amplitude using tight binding.



- Wave-function penetrates into the barrier region.
- The effective length of the well region is modified.
- The effective length of the well is crucial in determining the energy levels in the closed system.

$$E_n = \frac{h^2 \pi^2}{2mL_{well}^2} n^2$$

$$n = 1, 2, 3, \dots, \quad 0 < x < L_{well}$$



- Double barrier structures can show unity transmission for energies **BELOW** the barrier height

» Resonant Tunneling

- Resonance can be associated with a quasi bound state

» Can relate the bound state to a particle in a box  
 » State has a finite lifetime / resonance width  
 » Open and closed systems differ significantly for realistic barrier heights/widths

- Increasing barrier heights and widths:

» Increases resonance lifetime / electron residence time  
 » Sharpens the resonance width

- Asymmetric barriers

» Reduce the unity transmission

