Network for Computational Nanotechnology (NCN)

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

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Scattering Matrix approach

Define our system: Double barrier

One matrix each for each interface: 4 S-matrices

Left Incident → Reflected → Right Incident → Transmitted

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.
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

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

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

- The solution in the well is:
  \[\psi_n(x) = A\sin\left(\frac{n\pi}{L_x} x\right), \quad n = 1, 2, 3, \ldots\]

- Plugging the normalized wave-functions back into the Schrödinger equation we find that energy levels are quantized.
  \[E_n = \frac{\hbar^2 \pi^2}{2mL_x^2} n^2\]
  \[n = 1, 2, 3, \ldots, \quad 0 < x < L_x\]
Double barrier & particle in a box

- 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.

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

\[ E_n = \frac{\hbar^2 \pi^2}{2 m L_{\text{well}}^2} n^2 \]

\[ n = 1, 2, 3, K \quad 0 < x < L_{\text{well}} \]
• 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