Analytical and Numerical Solution of the Double Barrier Problem

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Exercise Background

Tunneling is fully quantum-mechanical effect that does not have classical analog. Tunneling has revolutionized surface science by its utilization in scanning tunneling microscopes. In some device applications tunneling is required for the operation of the device (Resonant tunneling diodes, EEPROMs – floating gate memories), but in some cases it leads to unwanted power dissipation, such as gate leakage in both MOS and Schottky transistors. Resonant tunneling diodes, due to the tunneling current at small biases exhibit negative differential resistance region and, thus, are suitable for oscillators. Because of this, it is very important to understand tunneling in double-barrier structure.

Exercise Objectives

You will understand the following after completing this assignment:

1. Analytical and numerical analysis of double barrier structure using the Piece-Wise Constant Potential Barrier tool (PCPBT).

2. Analyze multiple-barrier structures, the interactions between the wells and the formation of bands.

Relevant Literature

The following references may be useful for further study:

1. D. K. Ferry, *Quantum Mechanics: An Introduction for Device Physicists and Electrical Engineers* (Institute of Physics Publishing, London, 2001).

2. H. Mizuta, T.Tanoue, *The Physics and Applications of Resonant Tunneling Diodes* Cambridge University Press (1995)

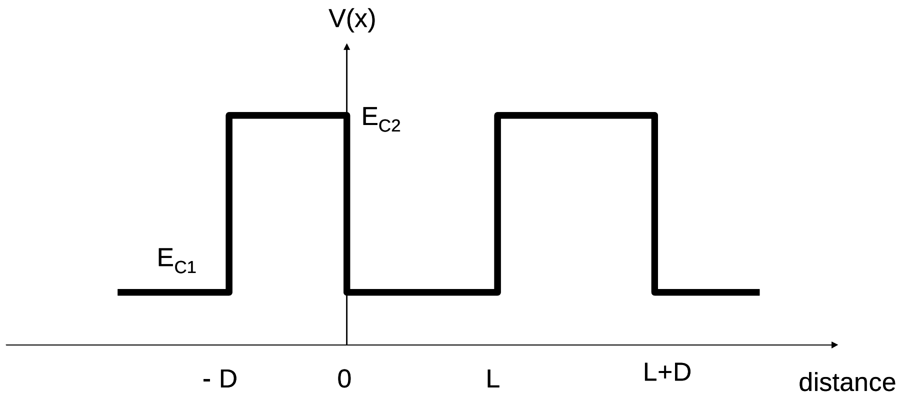
3. R. Tsu, *Superlattice to Nanoelectronics*, Elsevier Science; (2005)

4. A. Shik, *Quantum Wells: Physics & Electronics of Two dimensional Systems*, World Scientific Publishing Company; (1997)

5. B. Nag, *Physics of Quantum Well Devices*, Springer; (2001)

Exercise: <u>Analytical solution to the double barrier problem</u>:

1) Consider a double barrier structure where $E_{c1} - E_{c2} = -0.3eV$:



Show by simple wave function matching at every interface or by the transfer matrix method that the overall transmission coefficient can be written as:

$$T_{2B} = |t_{2B}|^2 \quad \text{where,} \quad t_{2B} = \frac{t_B{}^2 e^{ik_1 L}}{1 - r^2{}_B e^{i2k_1 L}}$$

t_{2B} is the overall transmission coefficient. Hence prove that $T_{2B} = \left[1 + \frac{4R_B}{T_B}\sin^2(k_1 L - \theta)\right]^{-1}$

where

$$r_B{}^2 = R_B e^{-i2\theta},$$
$$t_B{}^2 = T_B$$

2) Numerical solutions to multi-barrier transmission – use the PCPBT tool on nanoHUB.org to solve these problems: http://nanohub.org/tools/pcpbt. You can also access the same tool inside abacus http://nanohub.org/tools/abacus .

2a) Double Barrier:
- A) Plot the transmission and reflection coefficients for:
  V=1eV, Well width = 10nm, barriers thickness = 8nm.
- B) Comment on the spacing of the transmission peaks.
- C) Comment on the peak widths.
  Look for the difference of the transmission coefficients.
- D) Comment on the position of the transmission peaks.
- E) Comment on the reflection coefficient.
- F) Plot the composite "Potential Profile, Transmission data and Band structure" (the first available output) - comment on the energy positions of the resonances – compare to a particle in a box problem – how big is the equivalent box and what is the effective mass in the box?
- G) Compare your answer in F to the plot entitled "Band structure".

2b) Double Barrier:
Plot the transmission and reflection coefficients for two different structures:
- i) V=0.4eV, Well width = 6nm, barrier thickness = 2nm.

ii) V=0.2eV, Well width = 6nm, barrier thickness = 2nm, set the maximum energy range above the barriers from 0.1eV to 0.3eV

A) Plot the first tool output “Potential Profile, Transmission and Band structure”, click the “All” button on the bottom left.

B) Comment on the qualitative difference in the transmission coefficients

C) There is an “above the barrier” modulation for the case ii) – comment on the implications of that for electrons moving above the barriers.

2c) Multiple barriers – restart the PCPBT to get the default values back
As geometry chose “n potential barriers with same length”
Run for the following case:

i) 10 barriers, 1eV barrier, 2nm barrier width, well potential 0eV, well width 6nm, barrier effective mass 0.067, well effective mass 0.067, the energy extension above the barrier to 2.0eV

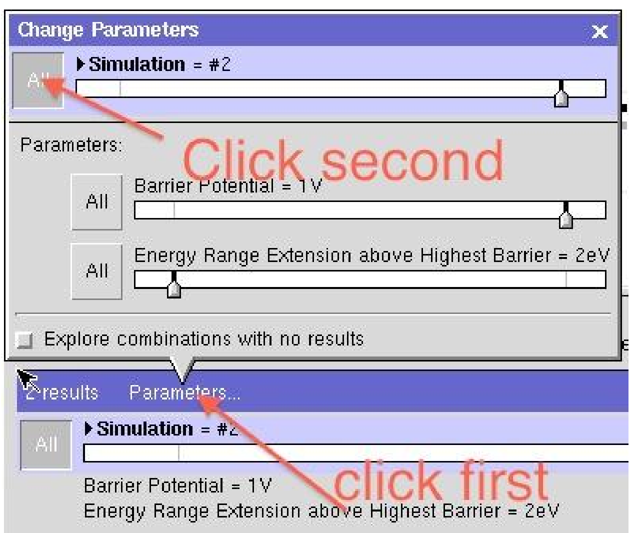
A) for case i) comment on the discreteness / selectiveness of the lower energy bands and the “shape” of the resonance positions as they occur.

B) same as A) but for the resonances above the barriers.

C) for case i) comment on the separation of the bands in terms of energy.

D) Run another case:

ii) same as i) but set the barrier height to 0.4V and the energy extension above the barrier to 2.6 eV. Since you changed 2 parameters a comparison is a bit more complicated. Click on “Parameters” and the “All” as indicated on the figure below:



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Now compare the output “Resonance Peaks vs. Occurrence”.
Comment on the “dispersion of states” you see in the two cases.