Quantum Tunneling

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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.

Exercise Objectives

The objective of this exercise is to:

1. Calculate analytically the tunneling coefficient for a single barrier.

2. Verify the analytical results obtained by simulating a potential barrier using the Piece-Wise-Constant Potential Barrier Tool (PCPBT).

Relevant Literature

You can look-up the following text to help unravel some of the mysteries behind tunneling.

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

2. M. Razavy, *Quantum Theory of Tunneling*, World Scientific Publishing Company (2003)

Exercise: <u>Quantum Tunneling</u>

1) This question deals with quantum tunneling. We want to solve the Schrödinger equation with the following potential barrier

$$V(x) = \begin{cases} E_{c1} = 0 & x < 0 \\ U = E_{c2} & 0 < x < D \\ E_{c1} = 0 & x > D \end{cases} \qquad E > E_{c2} = U$$

Consider a wave packet incident from the left, for which we have the following possible general solution:

$$\Psi(x) = \begin{cases} \exp(ikx) + \mathrm{Re}\,xp(-ikx) & x < 0 \\ A\exp(iqx) + B\exp(-iqx) & 0 < x < D \\ T\exp(ikx) & x > D \end{cases}$$

1a) By matching the wave function and the derivative of the wave functions at x=0 and x=L, show that:

$$\frac{A+B}{A-B} = \frac{\exp(-iqD) + \exp(iqD) + \frac{k}{q}\left(\exp(-iqD) - \exp(iqD)\right)}{\exp(-iqD) - \exp(iqD) + \frac{k}{q}\left(\exp(-iqD) + \exp(iqD)\right)} \equiv C$$

$$\mathrm{R} = \frac{\mathrm{Ck - q}}{\mathrm{Ck + q}}$$

1b) The transmission probability is given by $T = 1 - |R|^2$. Assuming U=0.2eV, L=10nm, plot T as a function of energy from 0eV to 0.5eV.

Plot T assuming L=1nm now. Comment which case resembles the classical case. You can verify your results with the PCPBT tool on the nanoHUB (http://nanohub.org/tools/pcpbt).
You can also access the same tool inside ABACUS http://nanohub.org/tools/abacus.

1c) Show that the single barrier transmission coefficient can be expressed as:

$$T_B = |t_B|^2 = \frac{T^2}{1 + R^2 - 2R\cos 2k_2 D}$$

corresponding to a reflection coefficient R;

$$R_B = |r_B|^2 = \frac{2R(1 - \cos 2k_2 D)}{1 + R^2 - 2R\cos 2k_2 D}$$

where T and R are, respectively, the transmission and reflection coefficients for a single potential step. The subscript "B" is used to denote scattering parameters of the barrier as a whole.