Calculation of current-voltage characteristic of a resonant-tunneling diode (RTD) and using the adiabatic approximation for simulation of conductance quantization in quantum point contact (QPC)

Simulations of quantum transport in nanoscopic systems
Nanomaterials Engineering

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Contents

Aim

The aim of the exercise was to simulate quantum transport phenomena in two types of nanodevices — a resonant-tunneling diode (RTD) and a quantum point contact (QPC). The main goals were to calculate the current-voltage characteristic of a resonant-tunneling diode and simulate conductance quantization in a quantum point contact using the adiabatic approximation.

1 Methods

Calculations were carried out in *Python* using the *NumPy* and *Matplotlib* libraries, along with *linalg* functions from *SciPy*. The complete code is available in the GitHub repository.

2 Results

The exercise is divided into three main tasks: 1) calculating transmission and reflection coefficients through a single potential barrier using the transfer matrix method, assuming constant and spatially varying effective mass; 2) simulating the current-voltage characteristic of a resonant-tunneling diode based on transmission data; 3) calculating quantized conductance of a quantum point contact within the adiabatic approximation using the Landauer formula.

2.1 Transmission through a Single Potential Barrier

Figure 1 shows the transmission and reflection coefficients for a single potential barrier assuming constant effective mass $m_{eff} = 0.27$ eV. In comparison, Figure 2 presents the transmission and reflection coefficients for the same barrier, but now accounting for spatially varying effective mass. Compared to the constant mass case, the results exhibit noticeable differences, highlighting the influence of material composition on quantum transport.

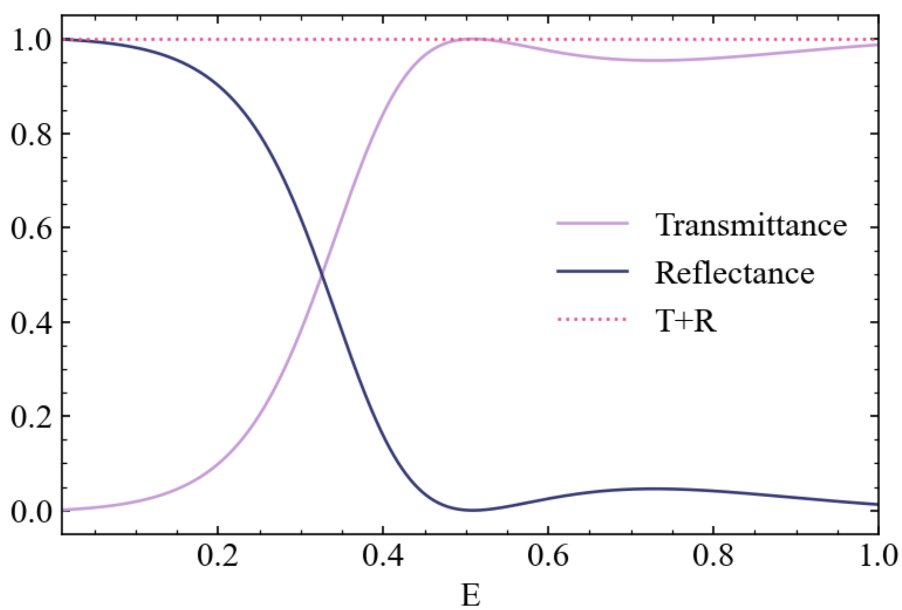

Figure 1: Transmission and reflection coefficient through potential barrier with constant effective mass as a function of energy. The dashed orange line shows the analytical solution.

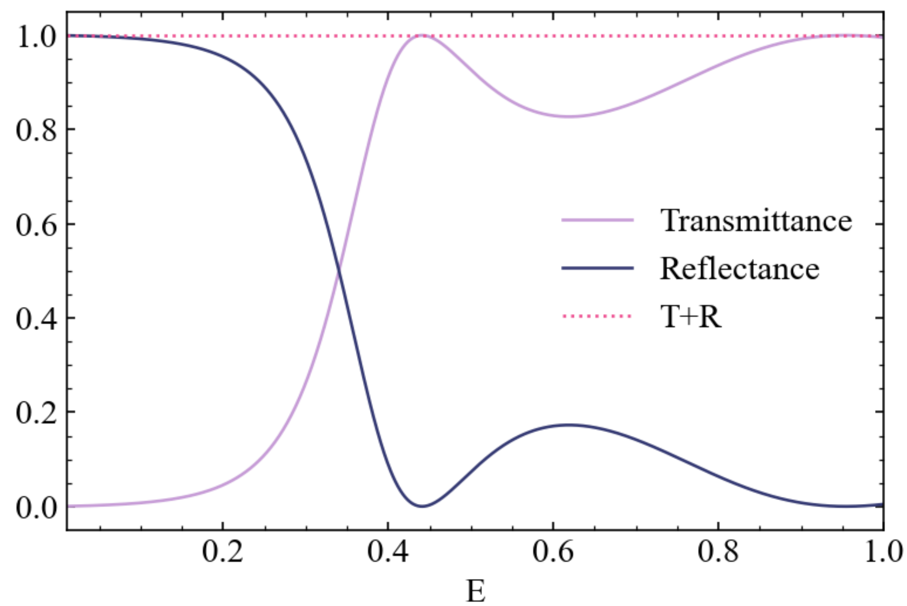

Figure 2: Transmission and reflection coefficient through potential barrier with spatially varying effective mass as a function of energy.

2.2 Resonant-Tunneling Diode Current-Voltage Characteristics

Figure 3 illustrates the transmission and reflection coefficients for a double-barrier potential, modeling a resonant-tunneling diode. Sharp peaks in the transmission spectrum indicate the presence of resonant energy states, where the probability of tunneling is significantly enhanced.

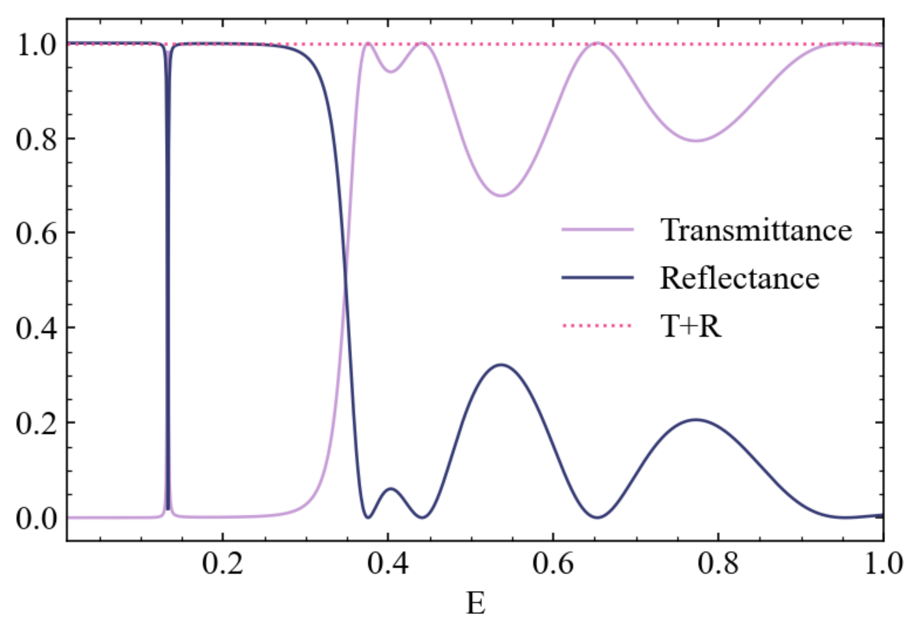

Figure 3: Transmission and reflection coefficient through a double potential barrier with spatially varying effective mass as a function of energy.

Figure 4 displays a potential profile under a bias voltage equal to 0.05 eV.

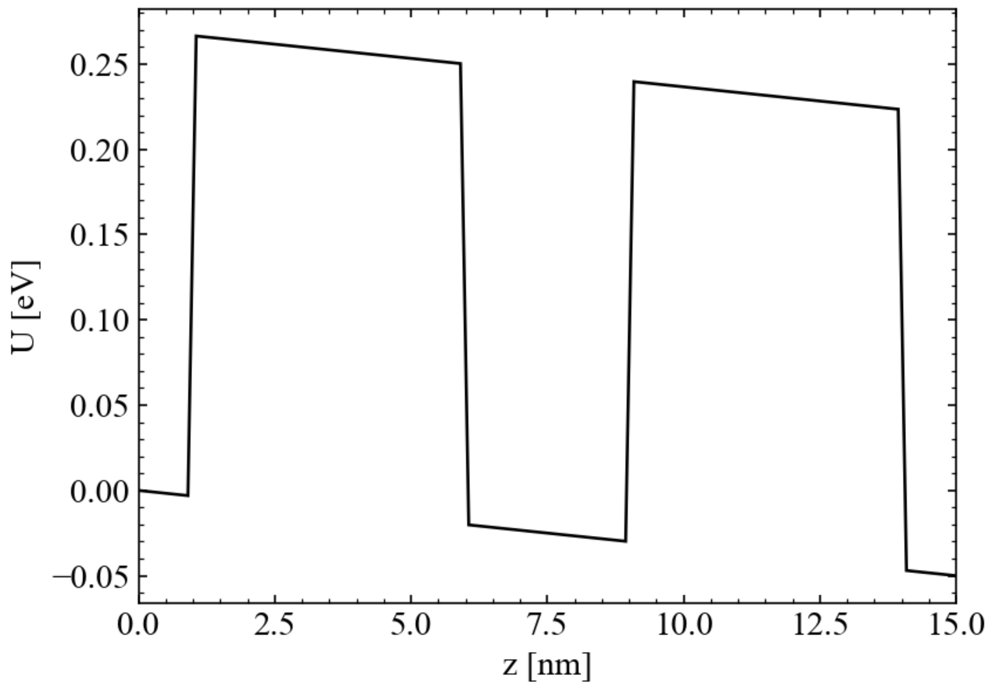

Figure 4: Profile of potential under bias conditions.

The calculated curve of current-voltage characteristic (Fig. 5) is very similar to curve presented in scientific papers.

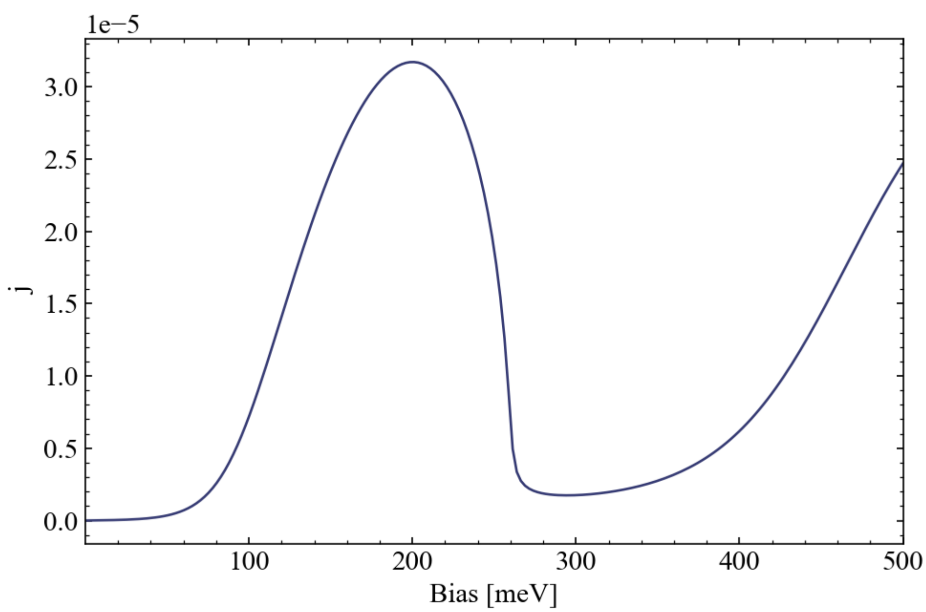

Figure 5: Current-voltage characteristic of a resonant-tunneling diode, assuming temperature 77 K.

2.3 Conductance Quantization in Quantum Point Contact

Figure 6 presents the two-dimensional potential profile of the quantum point contact (QPC), shaped by gate voltages. The geometry of potential effectively narrows the conduction channel, allowing only certain transverse modes to contribute to transport.

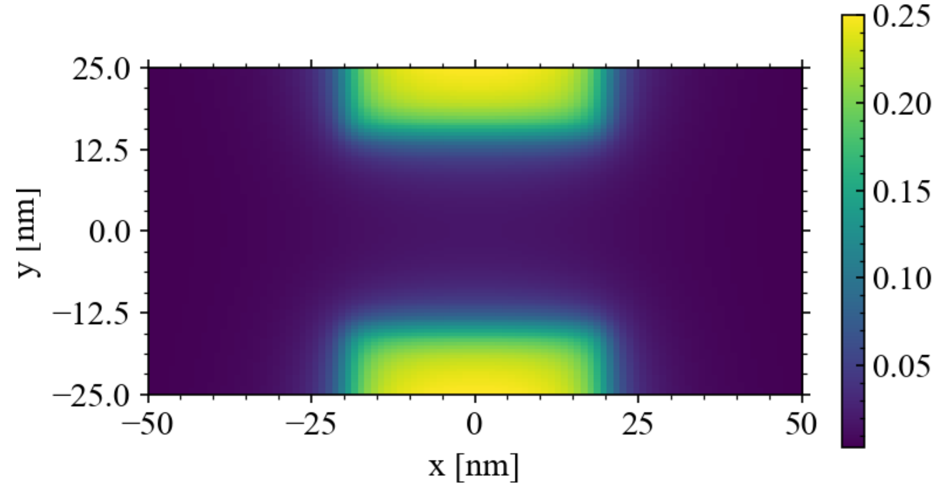

Figure 6: Potential profile of the QPC.

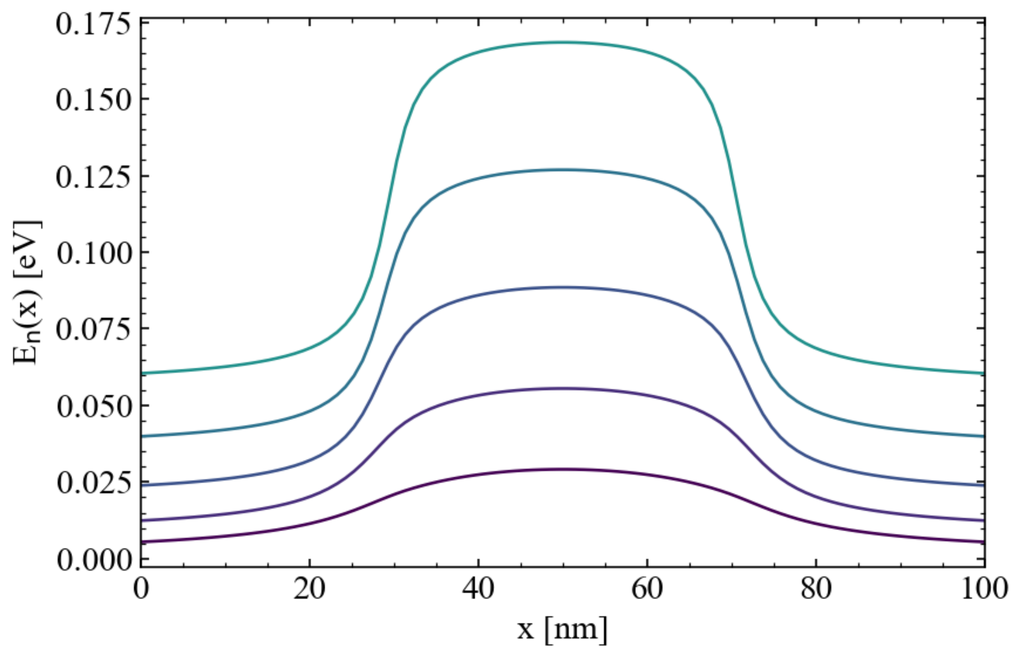

Figure 7: The effective potential $E_n(x)$ for n = 1, 2, 3, 4, 5.

The step-like behavior of QPC conductance (Fig. 8 and 9) is a clear signature of it quantization, arising from the discrete number of propagating modes available at each energy level.

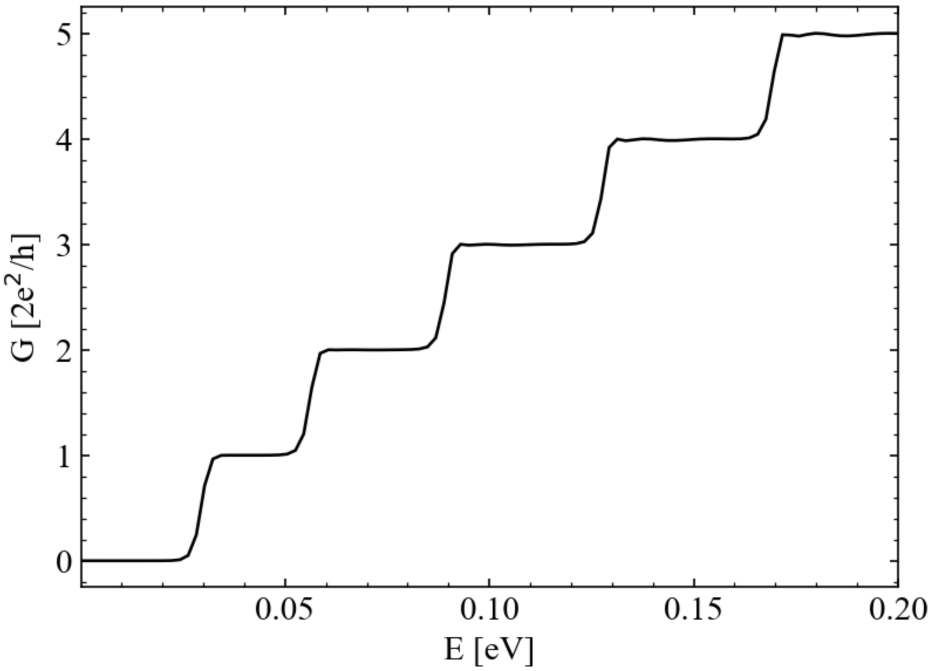

Figure 8: The QPC conductance as a function of incident electron energy.

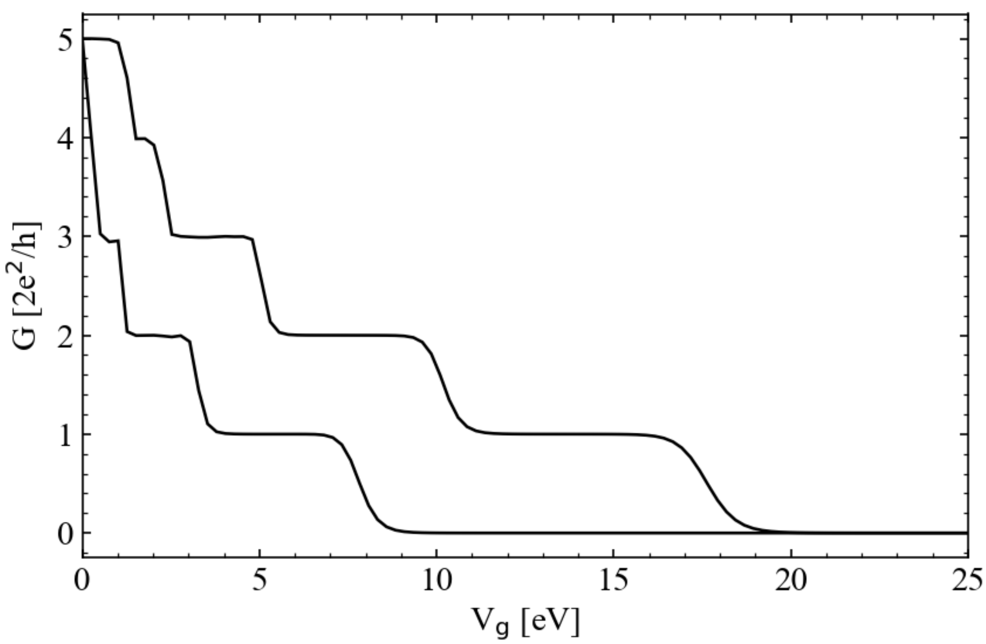

Figure 9: The QPC conductance as a function of the gate voltage Vg at incident electron energy E = 50 meV and 100 meV.