# Solid State Simulation Techniques.
## Resonant Tunnel Diodes (RTD) Simulation.

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## 1 Introduction

The aim of this homework is to perform a numerical simulation of a Resonant Tunneling Diode (RTD) based on a combination of different layers of GaAs and AlGaAs. The RTD is a nano-electronic device whose operation relies fundamentally on the wave nature of electrons and the quantum tunneling effect.

To model this system, we assume ballistic transport, ignoring interactions with phonons or photons. Additionally, we treat the lateral dimensions of the device as infinite, allowing us to reduce the problem to 1D transport perpendicular to the layers. Under these approximations, the electron behavior is governed by the time-independent envelope Schrödinger [1, 2]:

$$\left[-\frac{\hbar^2}{2m^*}\frac{d^2}{dx^2} + E_c(x)\right]\psi(x) = E\psi(x), \tag{1}$$

where $m^*$ is the effective mass of the electron (assumed constant $0.063m_0$ for both , with $m_0$ being the free electron mass), $E_c(x)$ is the conduction band potential profile, and $E$ is the electron energy.

Using the Numerov method to solve this equation numerically, we aim to:

1. Compute the transmission coefficient $T(E)$ for a double-barrier potential.
2. Calculate the macroscopic Current-Voltage (I-V) characteristic using the Landauer-Büttiker formalism.
3. Simulate a multi-barrier structure to demonstrate the formation of energy bands, analogous to the Kronig-Penney model.

## 2 Theory Questions

**Question 1.** *The state that describes the electron within the three-dimensional crystal is of the form:*

$$\Psi_E(x, y, z) = \Psi_{E_x}(x) \cdot \frac{1}{\sqrt{2}} e^{ik_y y} \cdot \frac{1}{\sqrt{2}} e^{ik_z z}. \tag{2}$$

*What are the advantages and limitations of the previous wave functions to describe an electron in a semiconductor crystal? Do they have temporary dependency?*

The primary advantage of this wave function form is the simplification of the problem by means of separation of variables. By assuming the lateral dimensions of the device ($y$ and $z$) are very large compared to the electron's wavelength, we can treat the electron's motion in these directions as free, allowing us to decouple the complex longitudinal transport from the lateral motion. The problem then reduces from a difficult three-dimensional equation to a manageable one-dimensional Schrödinger equation along the $x$-axis (the direction where transport occurs). The lateral parts become simple

plane waves ($\frac{1}{\sqrt{2\pi}}e^{ik_y y}$ and $\frac{1}{\sqrt{2\pi}}e^{ik_z z}$), representing free motion that does not affect the tunneling probabilities determined by $\Psi_{E_x}(x)$.

On the other hand, the limitations arise from the idealizations required to make this model solvable:

- We use the ballistic transport approximation in our model to ignore inelastic scattering: we assume the electron does not interact with phonons, photons, or other electrons, but in reality, these interactions can cause energy loss and decoherence.
- The electron is treated as a single coherent particle: we assume that its coherence time is much larger than the transit time across the device. If the device were too long, phase-breaking events would occur, which randomize the wavefunction phase and destroy the interference effects that cause resonant tunneling.
- The model assumes the conduction band is isotropic and parabolic, and uses a single effective mass ($m^* = 0.063m_0$) for the entire device, ignoring non-parabolic behaviour or effective mass mismatches at interfaces.

Finally, regarding whether this state have time dependency or not, we can say that mathematically yes, it has, but for physical observables, it does not. The wave function $\Psi_E(\vec{r})$ presented is the solution to the Time-Independent Schrödinger Equation (TISE):

$$\hat{H}\Psi_E = E\Psi_E \qquad \Rightarrow \qquad \Psi(\vec{r},t) = \Psi_E(\vec{r}) \cdot e^{-iEt/\hbar}.$$

However, because we are dealing with a stationary state, any physical observable, such as the probability density $|\Psi|^2$ or the current density $J$, is independent of time (the time phase factors cancel out upon taking the modulus squared). Therefore, this model describes a steady-state system where the DC current is constant.

**Question 2.** *Demonstrate that the total current of the state is*

$$J(E) = \frac{q\hbar}{m}\frac{|t(k_+)|^2}{8\pi^2}k_+.$$

*Why is the current independent of position?*

We start with the standard quantum mechanical definition of the probability current $\vec{J}$:

$$\vec{J} = \frac{q\hbar}{2mi}\left(\Psi^*\vec{\nabla}\Psi - \Psi\vec{\nabla}\Psi^*\right).$$

Since we are analyzing transport through the device, we focus on the current flowing in the $x$-direction (perpendicular to the layers). Assuming unit incidence, the solution to the envelope equation in this direction takes the following form:

$$\Psi_{E_x}(x) = \frac{1}{\sqrt{2\pi}}\begin{cases} e^{ik_- x} + r(k_-)e^{-ik_- x} & \text{(Source)} \\ t(k_+)e^{ik_+ x} & \text{(Drain)} \end{cases}$$

We consider the wavefunction in the right reservoir (Drain), where the electron has been transmitted, and substitute it into the definition of the current density:

$$\begin{aligned} J_x &= \frac{q\hbar}{2mi}\left(\Psi^*\partial_x\Psi - \Psi\partial_x\Psi^*\right) = \frac{q\hbar}{2mi}\left(\Psi^*\Psi(ik_+) - \Psi\Psi^*(-ik_+)\right) \\ &= \frac{q\hbar k_+}{m}|\Psi(\vec{r})|^2. \end{aligned}$$

The probability density $|\Psi|^2$ is simply given by

$$|\Psi|^2 = \left|\frac{t(k_+)}{(2\pi)^{3/2}}\right|^2 \underbrace{|e^{i(\vec{k}\cdot\vec{r})}|^2}_{1} = \frac{|t(k_+)|^2}{(2\pi)^3} = \frac{|t(k_+)|^2}{8\pi^3}.$$

Finally, substituting this back into the expression for $J_x$, we arrive at the desired result:

$$J(E) = \frac{q\hbar k_+}{m} \frac{|t(k_+)|^2}{8\pi^3}. \tag{3}$$

Why is the current independent of the position? It is a direct consequence of charge conservation in a steady-state system. Since the wavefunction $\Psi_E$ is an energy eigenstate of the TISE, the probability density $\rho = |\Psi|^2$ is constant in time ($\frac{\partial \rho}{\partial t} = 0$). Applying the continuity equation:

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{J} = 0 \quad \Rightarrow \quad \vec{\nabla} \cdot \vec{J} = 0.$$

This implies that $J_x$ must be constant throughout the device.

# 3 Numerical Simulation

## 3.1 Part 1: Transmission Coefficient $T(E)$

### 3.1.1 Strategy

To simulate the quantum transport, we discretize the spatial domain with a step size $\Delta x = 1$ Å. The Schrödinger equation (1) is rearranged into a form suitable for numerical integration:

$$\frac{d^2\psi}{dx^2} = \frac{2m^*}{\hbar^2}[V(x) - E]\psi(x) = f(x)\psi(x). \tag{4}$$

To solve this second-order differential equation, we employ the Numerov method, given that there is not first-order [3].
The physical problem involves an electron incident from the left (Source) that may be reflected or transmitted to the right (Drain). The scattering states take then the general form:

$$\psi(x) = \begin{cases} Ae^{ik_L x} + Be^{-ik_L x} & x < 0 \quad \text{(Source)} \\ Ce^{ik_R x} & x > L \quad \text{(Drain)} \end{cases} \tag{5}$$

We are looking to find the transmission coefficient $T \propto |C/A|^2$, but we do not know the reflection coefficient $B$ a priori, making forward integration difficult.
Instead, we use a *backward integration* strategy:

1. We invert the problem: we assume a normalized transmitted wave at the drain boundary: $\psi_{right} = 1 \cdot e^{ik_R x}$.

2. We initialize the last two points of the grid, $\psi(N)$ and $\psi(N-1)$, using this plane wave assumption.

3. We use the Numerov relation which allows us to find $\psi_{n-1}$ given $\psi_n$ and $\psi_{n+1}$:

$$\psi_{n-1} = \frac{\left(2 + \frac{10\Delta x^2}{12} f_n\right)\psi_n - \left(1 - \frac{\Delta x^2}{12} f_{n+1}\right)\psi_{n+1}}{1 - \frac{\Delta x^2}{12} f_{n-1}}. \tag{6}$$

   Using it, we integrate backwards from the Drain to the Source.

4. Once we reach the Source ($x < 0$), the calculated numerical function $\psi_{num}$ represents the specific superposition of incident and reflected waves required to produce exactly one unit of transmitted amplitude.

At the left boundary (Source), the numerical wavefunction $\psi_{num}$ and its numerical derivative $\psi'_{num}$ must match the analytical scattering form:

$$\psi_{num}(x) = Ae^{ik_L x} + Be^{-ik_L x} \tag{7}$$

$$\psi'_{num}(x) = ik_L Ae^{ik_L x} - ik_L Be^{-ik_L x} \tag{8}$$

To extract the incident amplitude $A$, we eliminate the reflection term $B$. We multiply Eq. (7) by $ik_L$ and add it to Eq. (8):

$$\begin{aligned} ik_L\psi_{num} + \psi'_{num} &= (ik_L A e^{ik_L x} + ik_L B e^{-ik_L x}) + (ik_L A e^{ik_L x} - ik_L B e^{-ik_L x}) \\ &= 2ik_L A e^{ik_L x}. \end{aligned}$$

Solving for $A$:

$$A = \frac{1}{2} e^{-ik_L x} \left( \psi_{num}(x) + \frac{\psi'_{num}(x)}{ik_L} \right). \tag{9}$$

This derivation allows us to compute exactly how much incident wave amplitude was required to produce our assumed output (a unit transmitted amplitude).

Finally, the transmission coefficient is defined as the ratio of the transmitted to the incident probability fluxes. Taking into account that we might have different group velocities in the source and drain (if potential bias $V \neq 0$), we obtain:

$$T(E) = \frac{v_R}{v_L} \frac{|\psi_{trans}|^2}{|\psi_{inc}|^2} = \frac{k_R}{k_L} \frac{|1|^2}{|A|^2}. \tag{10}$$

This calculation is repeated for every energy step in the simulation loop.

### 3.1.2 Results

Using the methodology described above, we computed the transmission spectrum for the symmetric double-barrier structure at equilibrium ($V = 0$). The results, shown in Figure 1, display a sharp resonant peak where $T(E) \to 1$, despite the electron energy being significantly lower than the barrier height ($E < V_0$).

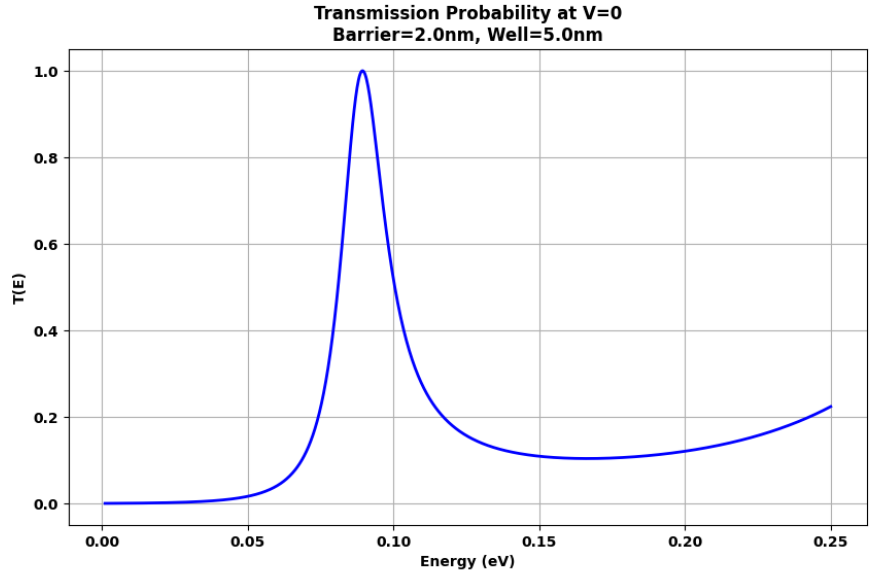



Figure 1: Computed Transmission Coefficient $T(E)$ for the Double Barrier Structure at zero bias ($V = 0$). Simulation parameters: Barrier width $W_{barrier} = 2$ nm, Well width $W_{well} = 5$ nm, Barrier height $V_0 = 0.3$ eV, Effective mass $m^* = 0.063m_0$, and Temperature $T = 298$ K.

This phenomenon arises because the central quantum well have discrete quasi-bound energy levels. When the energy of an incident electron matches one of these specific eigenenergies, the portion of the wave that tunnels into the well undergoes multiple internal reflections between the two barriers. At resonance, these reflections interfere constructively, causing the wavefunction amplitude to build up significantly inside the well.

Simultaneously, the waves leaking back towards the source interfere destructively with the direct reflection of the incident wave. This effectively cancels out the total reflection coefficient ($R \to 0$). In this way, despite the barriers being classically "opaque", the electron builds up a high probability density inside the well and tunnels through to the drain with near 100% probability.

## 3.2 Part 2: I-V Characteristic

### 3.2.1 Strategy

Once we have determined the transmission coefficient $T(E, V)$ for a specific potential profile, we can now calculate the macroscopic current flowing through the device using the Landauer-Büttiker formalism [1].

To obtain the Current-Voltage (I-V) characteristic, we compute the current density $J(V)$ by integrating the transmission coefficient over the full range of incident energies, weighted by a logarithmic function. Its mathematical expression is given by:

$$J(V) = \frac{qmk_BT}{2\pi^2\hbar^3} \int_0^\infty T(E,V) \ln \left\{ \frac{1 + \exp\left(\frac{E_{fe}(V) - E}{k_BT}\right)}{1 + \exp\left(\frac{E_{fc}(V) - E}{k_BT}\right)} \right\} dE. \tag{11}$$

Physically, the logarithmic term serves as "the energy window available for transport". It represents the difference in carrier populations between the source ($E_{fe}$) and drain ($E_{fc}$) Fermi levels. When these levels are misaligned by an applied voltage, this window opens, allowing current to flow proportional to $T(E, V)$.

Finally, the total current $I(V)$ is obtained by multiplying the calculated density by the cross-sectional area of the device:

$$I(V) = J(V) \times \text{Area}. \tag{12}$$

To simulate the I-V characteristic numerically, we perform a sweep over the applied voltage $V$ from 0 to a final value $V_{final}$. For each voltage step, the simulation proceeds as follows:

1. First, we modify the potential profile $V(x)$ to account for the applied bias. The model assumes that the leads (emitter and collector) are highly conductive regions where the potential remains flat. Therefore, the entire voltage drop $V$ is assumed to occur linearly across the resistive active region (the barriers and the well), effectively "tilting" the band diagram.

2. Simultaneously, the bias voltage creates an imbalance between the reservoirs. We model this by fixing the source Fermi level ($E_{fe}$) and lowering the drain Fermi level ($E_{fc}$) by an amount equal to the applied voltage ($E_{fe} - E_{fc} = V$). This difference opens the energy window within which current can flow.

3. Because the potential profile changes with the voltage, the transmission coefficient $T(E, V)$ is voltage-dependent. We must recalculate it for the new tilted potential over the entire energy range. Finally, we integrate the product of this new transmission spectrum and the logarithmic term in Eq. 11 to obtain the total macroscopic current for that specific voltage point.

By repeating this process for increasing values of $V$, we construct the full I-V characteristic of the diode.

### 3.2.2 Results

The simulation yields the I-V curve displayed below. The most interesting feature is the appearance of a region of Negative Differential Resistance (NDR), where the current decreases despite an increase in voltage.

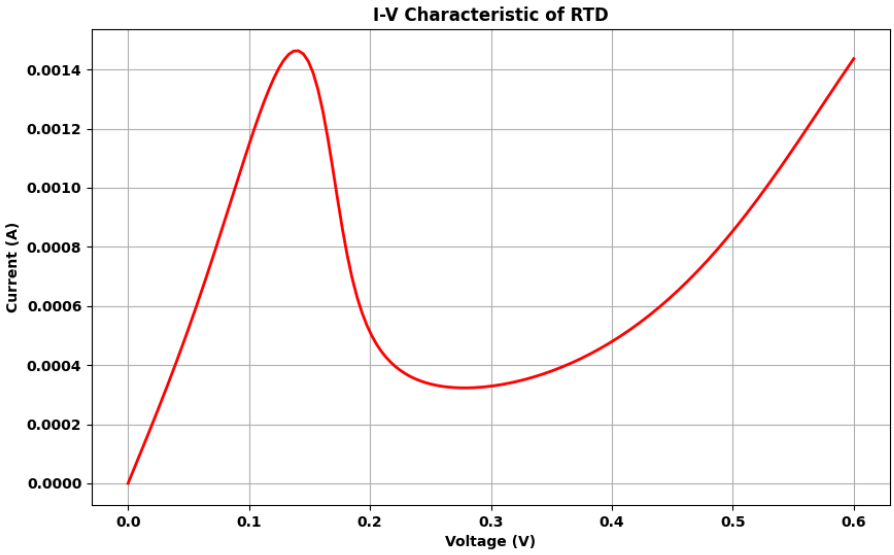



Figure 2: I-V Characteristic of the RTD calculated using the Landauer-Büttiker formalism. Simulation parameters: Barrier width $W_{barrier} = 2$ nm, Well width $W_{well} = 5$ nm, Barrier height $V_0 = 0.3$ eV, Effective mass $m^* = 0.063m_0$, Temperature $T = 298$ K, Fermi energy $E_F = 0.005$ eV, and Device Area $A = 10^{-12}$ m$^2$.

This phenomenon has a clear physical origin: at equilibrium, the Fermi levels of the source and drain are aligned, and no net current flows though the device. But when we apply a bias voltage, we drive the system out of equilibrium, shifting the energy levels of the quantum well relative to the emitter. The current reaches a maximum value when the resonant energy level inside the well aligns perfectly with the energy of the incident electrons in the emitter (maximum transmission).

However, as the voltage increases further (and the potential energy of the well continues to drop), the resonant energy is eventually pulled below the conduction band edge of the emitter. Although it might seem intuitive that the higher-energy incident electrons could simply drop into these lower energy states, such a transition is forbidden in our model. Relaxing into a lower energy level would require dissipating excess energy (e.g., through collisions), which explicitly contradicts our assumption of ballistic transport where total energy is strictly conserved. Consequently, the resonant tunneling path is effectively blocked, causing the current to drop sharply to a minimum and creating the negative slope observed in the I-V curve.

Finally, we discuss how useful these Negative Differential Resistors can be in practice. In a standard resistor, current rises with voltage, always dissipating power; but in the NDR region, the opposite happens: increasing voltage reduces current. This behavior thus creates "negative differential electrical power" ($\Delta V \cdot \Delta I < 0$) in which, instead of consuming signal energy like a normal resistor, the RTD effectively generates it. We can use this to cancel out the natural energy losses (positive resistance) of other circuit components, allowing the device to drive continuous, self-sustained oscillations without external [2].

## 3.3 Part 3: Band Structure from transmission coefficient

### 3.3.1 Strategy

We now explore the transition from the discrete quantum states of a single well (analogous to an isolated atom) to the continuous energy bands of a solid crystal. To do this, we simulate a multi-barrier structure, which acts as a finite approximation of the Kronig-Penney model. This model provides the theoretical basis for understanding how a periodic arrangement of atoms naturally creates "allowed"

and "forbidden" energy ranges.

In order to do this, we adapted our existing simulation code to handle an arbitrary number of barriers $N$, and computed the transmission coefficient spectrum for increasing values of $N$.

### 3.3.2 Results

The resulting transmission spectra in Fig. 3 reveal a clear trend. For the simplest case of $N = 2$ (a single quantum well), we observe a sharp, discrete resonant peak (where $T \to 1$) corresponding to an isolated energy level, analogous to the discrete orbitals of a single atom.

As we increase the count to $N = 5$, we see that the main peak start splitting into a cluster of separate sub-peaks. This happens because the wavefunctions in adjacent wells begin to interact and couple with each other, a phenomenon resembling the hybridization of molecular orbitals. For $N = 10$ and $N = 20$, the cluster densify and merge almost completely, becoming a broad, continuous region. This transition beautifully demonstrates the origin of the solid-state band structure:

- The allowed (conduction) bands are regions where transmission is near unity ($T \approx 1$), corresponding to energy ranges where electrons propagate freely through the lattice (Bloch states).
- The forbidden (band) gaps are regions where transmission drops to zero, corresponding to energy ranges where the wave interferes destructively and decays rapidly, allowing no electronic state propagation.

This numerical experiment thus shows how macroscopic electronic properties emerge directly from the quantum mechanical coupling of microscopic potential wells.

## 4 Conclusions

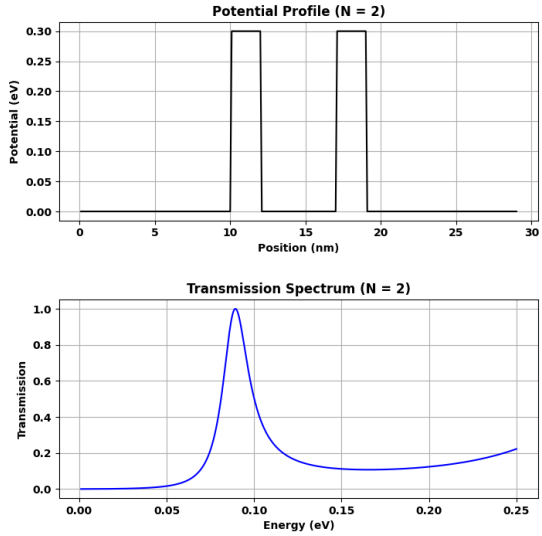
This simulation successfully modeled the quantum transport of an RTD using the Numerov method and the Landauer-Büttiker formalism. We reproduced the characteristic Negative Differential Resistance (NDR) region essential for device applications and demonstrated the emergence of continuous energy bands from discrete states in multi-barrier systems. These results confirm the effectiveness of the ballistic transport model for describing semiconductor heterostructures.

## References

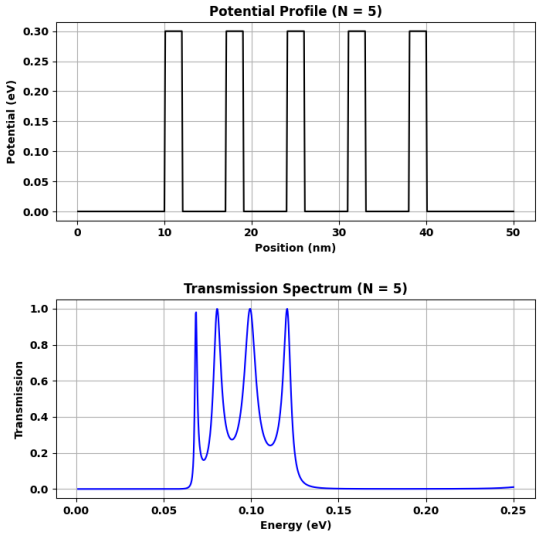
[1] Supriyo Datta. *Quantum Transport: Atom to Transistor*. Cambridge University Press, New York, 2005.

[2] D. K. Ferry, X. Oriols, and J. Weinbub. *Quantum Transport in Semiconductor Devices: Simulation Using Particles*. IOP Ebooks. IOP Publishing, 2023.

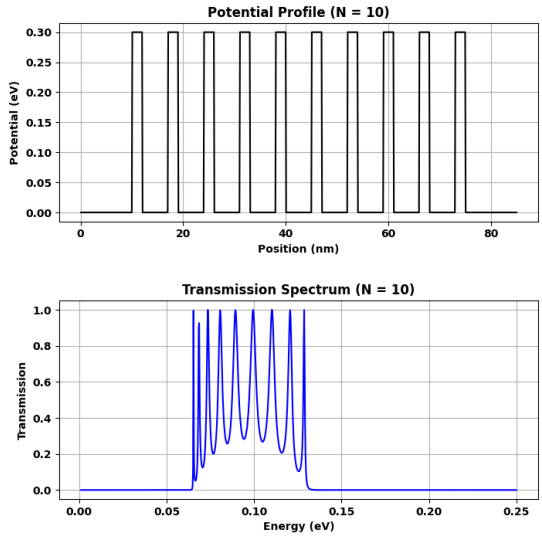
[3] Jos Thijssen. *Computational Physics*. Cambridge University Press, New York, 2nd edition, 2012.



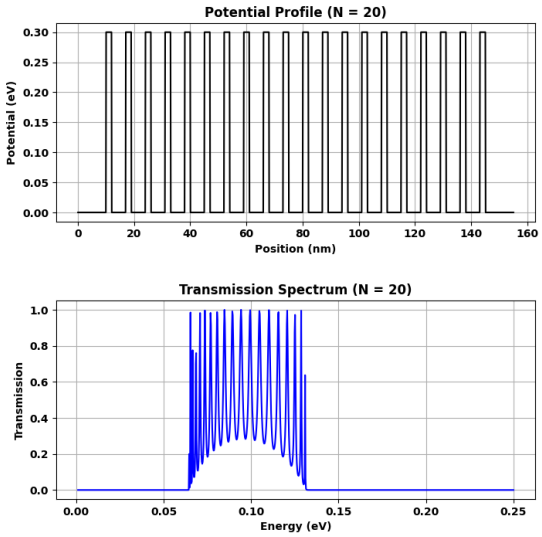

(a) $N = 2$ Barriers




(b) $N = 5$ Barriers




(c) $N = 10$ Barriers




(d) $N = 20$ Barriers

Figure 3: Evolution of the transmission spectrum for a multi-barrier structure with $N = 2$, $N = 5$, $N = 10$, and $N = 20$ barriers.

# A Python Simulation Code

Below is the complete Python code used to generate the transmission spectra, I-V characteristics, and multi-barrier band structure simulations presented in this report.

```
import numpy as np
import matplotlib.pyplot as plt

#
    ================================================================================

# HOMEWORK 3: RESONANT TUNNELING DIODE (RTD) SIMULATION
#
```

```
    ================================================================================


#
    --------------------------------------------------------------------------------
# PHYSICAL CONSTANTS & PARAMETERS
#
    --------------------------------------------------------------------------------
Dx = 1e-10              # Spatial step (1 Angstrom)
L_device = 2e-8         # Simulation Box length (large enough to include the
    Reservoirs/Leads)
                        # ensuring electrons behave as free waves before and
                            after hitting the barriers.
m = 0.063 * 9.109e-31   # Effective electron mass (kg)
h_bar = 1.054e-34       # Reduced Planck constant (J s)
qe = 1.6e-19            # Electron charge (C)
Kb = 1.38e-23           # Boltzmann constant (J/K)
T = 298                 # Temperature (K)
Area = 1e-12            # Cross-sectional area (m^2)

# Geometry parameters
W_barrier = 4e-9        # 4 nm
W_well = 10e-9          # 10 nm
V0 = 0.3                # Barrier height/Potential offset (eV)
Ef = 0.005              # Fermi energy (eV)

#
    --------------------------------------------------------------------------------
# SPATIAL GRID SETUP (FOR PARTS 1 & 2)
#
    --------------------------------------------------------------------------------
xpoints = int(np.floor(L_device / Dx))
# x = np.arange(1, xpoints + 1) * Dx

# Define indices for the Double Barrier Structure V(x)
# Center the device in the simulation box
center_idx = xpoints // 2
half_well_pts = int((W_well / 2) / Dx)
barrier_pts = int(W_barrier / Dx)

# Define (Symmetric) Barrier Regions
# Left Barrier: [start_B1, end_B1]
end_B1 = center_idx - half_well_pts
start_B1 = end_B1 - barrier_pts

# Right Barrier: [start_B2, end_B2]
start_B2 = center_idx + half_well_pts
end_B2 = start_B2 + barrier_pts

# Initial Potential (V=0)
U0 = np.zeros(xpoints)
U0[start_B1:end_B1] = V0 * qe  # Left Barrier
U0[start_B2:end_B2] = V0 * qe  # Right Barrier

#
    --------------------------------------------------------------------------------
```

```
# HELPER FUNCTIONS
#
    ------------------------------------------------------------------------


def get_transmission(Energy, Potential):
    """
    Calculates Transmission T(E) using the Numerov Method for a given
       Potential profile.

    Inputs:
    :Energy: Energy values (in eV)
    :Potential: Potential Energy V(x) (in Joules)
    """
    N_points = len(Potential)
    x = np.arange(1, N_points + 1) * Dx

    T_prob = np.zeros(len(Energy))

    # Numerov Constants (for Equation 1)
    A = (10 * Dx**2) / 12
    AA = Dx**2 / 12
    const_factor = (2 * m) / h_bar**2

    for i, E in enumerate(Energy):
        E_joule = E * qe

        # We ensure E > U at boundaries (leads) to avoid k being imaginary
        if E_joule <= Potential[0] or E_joule <= Potential[-1]:
            T_prob[i] = 0.0
            continue

        # Wavevectors in extremes (scattering states): k = sqrt(2m(E-V)) /
           h_bar
        k_left = np.sqrt(const_factor * (E_joule - Potential[0]))
        k_right = np.sqrt(const_factor * (E_joule - Potential[-1]))

        # Numerov Function: f(x) = 2m/h^2 * (V(x) - E)
        # Equation to be solved: psi'' = f(x)psi.
        func_numerov = const_factor * (Potential - E_joule)

        # Initialize Wavefunction (first two points at right boundary)
        # We assume outgoing plane waves on the right are prop. to exp(i *
           k_right * x) (scattering state)
        # This is the same as assuming a wave has successfully transmited to
            the right side
        psi = np.zeros(N_points, dtype=complex)
        psi[-1] = np.exp(1j * k_right * x[-1])
        psi[-2] = np.exp(1j * k_right * x[-2])

        # Backward Integration from Right to Left (Equation 1)
        for j in range(N_points - 3, -1, -1):
            term1 = (2 + A * func_numerov[j+1]) * psi[j+1]
            term2 = (1 - AA * func_numerov[j+2]) * psi[j+2]
            denom = (1 - AA * func_numerov[j])
            psi[j] = (term1 - term2) / denom

        # Now let's match boundary conditions at the left side:
        # Psi_left = A * exp(ikx) + B * exp(-ikx)
        # We want T = (k_right / k_left) * |Amplitude_Transmitted|^2 / |
           Amplitude_Incident|^2
```

```
        #           = (k_right / k_left) * (1 / |A|^2)
        # We need to isolate A. We do it using Psi_left and Psi'_Left = ik * A * exp(ikx) -ik * B * exp(-ikx)
        # Knowing Psi and Psi', we have two unkowns A and B --> A = ... = (1/2) exp(-ikx) (Psi(x) + Psi'(x) / (ik))

        # First, we get numerical values for psi and psi' in a safe point (not at the edges)
        idx_match = 5
        psi_val = psi[idx_match]
        # Finite difference derivative: dpsi/dx
        d_psi = (psi[idx_match+1] - psi[idx_match]) / Dx

        # Second, we get the incident amplitude with the derived formula above:
        A_inc = 0.5 * np.exp(-1j * k_left * x[idx_match]) * (psi_val + d_psi / (1j * k_left))

        if np.abs(A_inc) == 0:
            T_prob[i] = 0
        else:
            T_prob[i] = (k_right / k_left) / (np.abs(A_inc)**2)

    return T_prob

def simulate_multibarrier(num_barriers, W_b=4e-9, W_w=10e-9, V_height=0.3):
    """
    Constructs a potential with 'num_barriers' and computes its transmission coeff.

    Returns:
        :x_new: set of new points for the simulation
        :U_multi: Potential Multi-barrier profile
        :T_multi: Transmission coeffs
    """
    # Define region for computation
    # Device length = (N * Barrier) + (N-1 * Well)
    device_active_len = (num_barriers * W_b) + ((num_barriers - 1) * W_w)

    # Add leads on both sides (10 nm each)
    L_leads = 10e-9
    L_total = device_active_len + 2 * L_leads

    xpoints_new = int(np.floor(L_total / Dx))
    x_new = np.arange(1, xpoints_new + 1) * Dx

    # Potential
    U_multi = np.zeros(xpoints_new)

    current_pos_idx = int(L_leads / Dx)     # start painting the potential at the end of the left lead
    barrier_width = int(W_b / Dx)
    well_width = int(W_w / Dx)

    for k in range(num_barriers):
        start = current_pos_idx
        end = start + barrier_width
        U_multi[start:end] = V_height * qe

        # move current position to the next barrier position start
        current_pos_idx = end + well_width
```

```
162
163     # Compute Transmission coeff
164     T_multi = get_transmission(Energies, U_multi)
165
166     return x_new, U_multi, T_multi
167
168
169 #
    ------------------------------------------------------------------------
170 # PART 1: TRANSMISSION COEFFICIENT (V=0)
171 #
    ------------------------------------------------------------------------
172
173 # Energy Grid
174 E_max = 0.5 # eV (Up to barrier height + bit more)
175 E_steps = 5000
176 Energies = np.linspace(0.001, E_max, E_steps)
177
178 # Plotting T(E) for V=0 first (no bias)
179 T_zero_bias = get_transmission(Energies, U0)
180
181 plt.figure(figsize=(10, 6))
182 plt.plot(Energies, T_zero_bias, 'b-', linewidth=2)
183 plt.title(f'Transmission Probability at V=0\nBarrier={W_barrier*1e9}nm, Well
    ={W_well*1e9}nm')
184 plt.xlabel('Energy (eV)')
185 plt.ylabel('T(E)')
186 plt.grid(True)
187 plt.show()
188
189 #
    ------------------------------------------------------------------------
190 # PART 2: I-V CHARACTERISTIC
191 #
    ------------------------------------------------------------------------
192
193 # Voltage Grid
194 V_max = 0.6 # max value enough to see the negative slope region, in Volts
195 V_steps = 150
196 Voltages = np.linspace(0, V_max, V_steps)
197 Currents = np.zeros(V_steps)
198
199 # Active region (where voltage drops) defined by:
200 start_active = start_B1
201 end_active = end_B2
202 points_active = end_active - start_active       # number of points in the
    active region
203
204 for i, Vb in enumerate(Voltages):
205     # 1. Tilt Potential in the active region
206     # Left reservoir has V = 0, while right one has V = - Vb = constant
207     U_bias = U0.copy()
208     U_bias[end_active:] = U_bias[end_active:] - (Vb * qe)
209
210     # Create (linear) voltage drop in active region as Vb * fraction
211     # fraction = 0 at the start, and = 1 at the end
212     points_slope = np.arange(points_active)
```

```
    fraction = (points_slope / points_active)
    voltage_drop = (Vb * qe) * fraction
    U_bias[start_active:end_active] -= voltage_drop

    # 2. Calculate T(E, V) for this specific (tilted) potential profile
    Trans_V = get_transmission(Energies, U_bias)

    # 3. Define chemical potentials (energy window)
    mu_L = Ef           # Source fixed
    mu_R = Ef - Vb      # Drain drops by Vb

    # 4. Equation 3 (to compute J(V))
    # Note Energies are in eV, so we multiply by qe -> Joules
    arg_L = (mu_L - Energies) * qe / (Kb * T)
    arg_R = (mu_R - Energies) * qe / (Kb * T)

    integrand = Trans_V * np.log( (1 + np.exp(arg_L)) / (1 + np.exp(arg_R)))
    integral = np.trapezoid(integrand, Energies) * qe   # Numerical
       integration (in Joules)

    J_V = (qe * m * Kb * T) / (2 * np.pi**2 * h_bar**3) * integral

    Currents[i] = J_V * Area


plt.figure(figsize=(10, 6))
plt.plot(Voltages, Currents, 'r-', linewidth=2)
plt.title('I-V Characteristic of RTD')
plt.xlabel('Voltage (V)')
plt.ylabel('Current (A)')
plt.grid(True)
plt.show()

#
   ------------------------------------------------------------------------

# PART 3: BAND STRUCTURE (MULTI-BARRIER)
#
   ------------------------------------------------------------------------


# Plotting Band Structure Development
N_values = [2, 5, 10, 20]

for i, N in enumerate(N_values):
    x_mb, U_mb, T_mb = simulate_multibarrier(N, W_barrier, W_well, V0)

    plt.figure(figsize=(8, 8))

    # Potential Plots
    plt.subplot(2, 1, 1)
    plt.plot(x_mb * 1e9, U_mb / qe, 'k-')
    plt.title('Potential Profile (N = ' + str(N) + ')')
    plt.ylabel('Potential (eV)')
    plt.xlabel('Position (nm)')
    plt.grid(True)

    # Transmission Plots
    plt.subplot(2, 1, 2)
    plt.plot(Energies, T_mb, 'b-')
    plt.title('Transmission Spectrum (N = ' + str(N) + ')')
```

```
    plt.ylabel('Transmission')
    plt.xlabel('Energy (eV)')
    plt.grid(True)

    plt.subplots_adjust(hspace=0.4)
    plt.show()
```

Listing 1: Python script for RTD and Band Structure Simulation