RESONANT TUNNELING DIODE SIMULATOR USING NON-EQUILIBRIUM GREEN'S FUNCTION FORMALISM

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Abstract. Observing the numerical solutions of the Time-Dependent Schrödinger equation using different methods of computation gave one image on how to model particles. This article investigates how quantum effects can be captured and implemented within different systems, to see how quantum mechanics can be used to create components. In particular, I look into the numerical simulation of resonant tunneling diodes (RTDs) using the Non-Equilibrium Green's Function (NEGF) formalism and explaining how quantum tunneling can be leveraged to create diodes. RTDs are quantum devices exhibiting negative differential resistance (NDR) due to coherent tunneling through double-barrier heterostructures. Starting from the time-independent Schrödinger equation, we derive the discretized Hamiltonian using finite differences, introduce the concept of Green's functions for open quantum systems, and establish the self-energy formalism to model semi-infinite leads. The Landauer-Büttiker formula is employed to compute the current-voltage characteristics. Our implementation demonstrates the characteristic N-shaped I-V curve with peak-to-valley ratios consistent with experimental observations in GaAs/AlGaAs heterostructures.

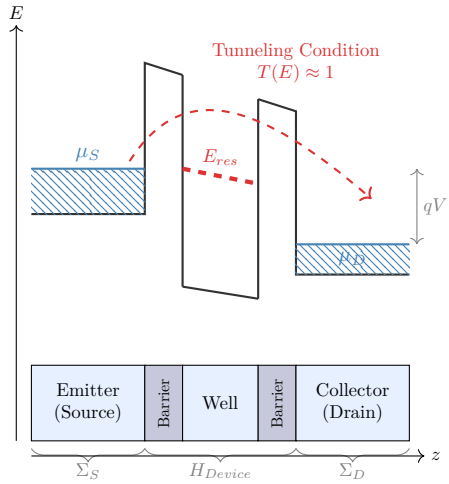
Introduction. Resonant tunneling diodes (RTDs) are quantum devices that exploiting the nature of electrons to achieve a resonance in current - voltage (Tsu and Esaki 1973; Chang, Esaki, and Tsu 1974). This phenomenon arises from quantum-mechanical tunneling through a double-barrier structure, where electrons can only traverse the device efficiently when their energy aligns with states in the quantum well.

The simulation of such nanoscale devices requires a quantum transport framework that accounts for the open nature of the system—electrons can enter and leave through contacts. The Non-Equilibrium Green's Function (NEGF) formalism provides exactly this capability, offering a rigorous contact coupling, and non-equilibrium carrier distributions (Datta 1995, 2005; Braggio, Carrega, and Ferraro 2023).

In this work, we develop a complete NEGF-based simulator for RTDs in Julia, following the theoretical framework established by Datta and others (Datta 2005; Lake et al. 1997; Camsari, Chowdhury, and Datta 2020). We begin with the mathematical foundations of Green's functions, proceed through the discretization of the Schrödinger equation, and culminate in the computation of current-voltage characteristics using the Landauer-Büttiker formula (Landauer 1957; Büttiker 1986).

Foundations.

The Resonant Tunneling Diode Structure. A typical RTD consists of a quantum well sandwiched between two potential barriers, often realized using semiconductor materials like GaAs/AlGaAs. The device is connected to a source and a drain, and depending on the bias voltage, electrons can tunnel through the barriers when their energy matches the resonant levels in the well.



Simulation Map:
Σ_S: Source Self-Energy (Inflow)
Σ_D: Drain Self-Energy (Outflow)
H_D: Hamiltonian (Barriers + Well)

Mathematic base - Green's Functions for Differential Equations.

Definition 0.1 (Green's Function). *Let L be a linear differential operator acting on differentiable functions in some domain $\Omega \subset \mathbb{R}^n$. The Green's function $(x, s) \to G(x; s)$ associated with L is the solution to*

$$LG(x; s) = \delta(x - s) \tag{0.1}$$

where $x \to \delta(x - s)$ is the Dirac delta distribution centered at s and $x \in \Omega$.

In other words, the Green's function represents the response of the system described by L to a point source located at s.

Green's functions, given the inhomogeneous equation

$$L\Psi(x) = f(x), \tag{0.2}$$

offer solutions that can be expressed as a convolution,

$$\Psi = x \to \int_\Omega G(x; s) f(s)\, ds. \tag{0.3}$$

Remark 0.2. The Green's function depends on the operator L and the boundary conditions, but not on the forcing term f. This separation makes Green's functions particularly useful for quantum transport, where we don't always know where the excitation can come from [@economo2006].

The Time-Independent Schrödinger Equation. For a particle of mass m in a potential V, the time-independent Schrödinger equation (TISE) in 1-D reads

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\Psi(x) = E\Psi(x), \tag{0.4}$$

which we rewrite as

$$(E - H_0)\Psi(x) = 0, \tag{0.5}$$

where $H_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$ is the Hamiltonian operator.

The Green's function for the free-particle Hamiltonian satisfies

$$(E - H_0)G(x, x') = \delta(x - x'). \tag{0.6}$$

Rearranging with $H_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$ and defining $k = \sqrt{2mE}/\hbar$, we obtain

$$\left(\frac{d^2}{dx^2} + k^2\right)G(x, x') = \frac{2m}{\hbar^2}\delta(x - x'). \tag{0.7}$$

For $v = \hbar k/m$.

This gives the **Retarded Green's Function**:

$$G^R(x, x') \approx \frac{-i}{\hbar v}e^{ik|x-x'|}$$

The Problem of Non-Invertibility. A fundamental issue arises: the operator $(E - H_0)$ is not invertible for real energies $E > 0$. For a linear operator A to be invertible, it must be a bijection, as a result, because the homogeneous equation $(E - H_0)\Psi = 0$ admits plane-wave solutions $\Psi(x) \sim e^{\pm ikx}$, and E lies in the continuous spectrum of H_0. The operator is not invertible.

THEOREM 0.3 (Limiting Absorption Principle). *To obtain a unique, physically meaningful Green's function, we introduce an infinitesimal imaginary part to the energy,*

$$E \to E + i\eta, \quad \eta \to 0^+. \tag{0.8}$$

This regularization selects the outgoing-wave (retarded) solution and ensures the operator is invertible.

The retarded Green's function is thus defined as

$$G^R = \lim_{\eta \to 0^+}(E + i\eta - H)^{-1}. \tag{0.9}$$

Sommerfeld Radiation Condition. The Sommerfeld radiation condition requires that waves propagate outward from sources (not inward from infinity), and is expressed as:

$$\lim_{|x|\to\infty} |x|^{\frac{n-1}{2}}\left(\frac{\partial\Psi}{\partial|x|} - ik\Psi\right) = 0. \tag{0.10}$$

For outgoing waves $\Psi(x) \sim e^{ikx}$ as $x \to +\infty$:

$$\frac{\partial}{\partial x}e^{ikx} - ik \cdot e^{ikx} = ike^{ikx} - ike^{ikx} = 0 \quad \text{Condition is verified.} \tag{0.11}$$

On the other hand, incoming waves e^{-ikx} violate this condition. The limiting absorption principle (0.8) automatically enforces Sommerfeld's condition.

Solving (0.7) via Fourier transform and contour integration yields the retarded Green's function in one dimension:

$$G^R(x,x') = -\frac{im}{\hbar^2 k} e^{ik|x-x'|} = -\frac{i}{\hbar v} e^{ik|x-x'|}, \tag{0.12}$$

Discretization of the Hamiltonian.

Finite Difference Approximation. Instead of working with the continuous spatial domain, we discretize space onto a uniform grid with spacing a. Let $x_i = i \cdot a$ where $i \in [1, N]$ for some $N \in \mathbb{N}$ and denote $\Psi_i = \Psi(x_i)$.

Using Taylor expansion:

$$\Psi(x+a) \approx \Psi(x) + a\Psi'(x) + \frac{a^2}{2}\Psi''(x) + O(a^3), \tag{0.13}$$

$$\Psi(x-a) \approx \Psi(x) - a\Psi'(x) + \frac{a^2}{2}\Psi''(x) + O(a^3). \tag{0.14}$$

Adding these expressions and solving for the second derivative:

$$\left.\frac{d^2\Psi}{dx^2}\right|_{x_i} \approx \frac{\Psi_{i+1} - 2\Psi_i + \Psi_{i-1}}{a^2}. \tag{0.15}$$

The Discrete Schrödinger Equation. Substituting (0.15) into the TISE (0.4):

$$-\frac{\hbar^2}{2m}\left[\frac{\Psi_{i+1} - 2\Psi_i + \Psi_{i-1}}{a^2}\right] + V_i\Psi_i = E\Psi_i. \tag{0.16}$$

Definition 0.4 (Hopping Parameter). *We define the hopping parameter*

$$t = \frac{\hbar^2}{2m^* a^2}, \tag{0.17}$$

where $m^* = m_{eff} \cdot m_0$ is the effective electron mass in the semiconductor.

Rearranging:

$$E\Psi_i = (2t + V_i)\Psi_i - t\Psi_{i+1} - t\Psi_{i-1}, \tag{0.18}$$

or equivalently:

$$(E - 2t - V_i)\Psi_i + t\Psi_{i+1} + t\Psi_{i-1} = 0. \tag{0.19}$$

The Device Hamiltonian Matrix. Equation (0.18) can be written in matrix form $(E\mathbf{I} - \mathbf{H}_D)\mathbf{\Psi} = 0$, where the device Hamiltonian $\mathbf{H}_D$ is the tridiagonal matrix:

$$\mathbf{H}_D = \begin{pmatrix} 2t+V_1 & -t & 0 & \cdots & 0 \\ -t & 2t+V_2 & -t & \cdots & 0 \\ 0 & -t & 2t+V_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & -t \\ 0 & 0 & 0 & -t & 2t+V_N \end{pmatrix}. \tag{0.20}$$

This tight-binding representation captures the kinetic energy (off-diagonal terms $-t$) and potential energy (diagonal terms V_i) of electrons on the discrete lattice.

Open Quantum Systems and Self-Energy.

Device-Lead Partitioning. An RTD is an open system: electrons are injected from a source contact and collected at a drain contact. To model this, we partition the full Hamiltonian into three regions (Datta 2005; Braggio, Carrega, and Ferraro 2023):

$$\mathbf{H} = \begin{pmatrix} \mathbf{H}_S & \boldsymbol{\tau}_S^\dagger & \mathbf{0} \\ \boldsymbol{\tau}_S & \mathbf{H}_D & \boldsymbol{\tau}_D \\ \mathbf{0} & \boldsymbol{\tau}_D^\dagger & \mathbf{H}_{Dr} \end{pmatrix}, \tag{0.21}$$

where:

- $\mathbf{H}_S$: Hamiltonian of the semi-infinite source lead
- $\mathbf{H}_D$: Hamiltonian of the device region (our region of interest)
- $\mathbf{H}_{Dr}$: Hamiltonian of the semi-infinite drain lead
- $\boldsymbol{\tau}_{S,D}$: Coupling matrices between device and leads

Considering that

$$\mathcal{H} = \mathcal{H}_S \oplus \mathcal{H}_D \oplus \mathcal{H}_d$$

We can define a base of the Hilbert, decomposed as,

$$\mathcal{B} = \underbrace{\{|s_i\rangle\}_{i=1}^{N_S}}_{\text{Basis of } \mathcal{H}_S} \cup \underbrace{\{|d_j\rangle\}_{j=1}^{N_D}}_{\text{Basis of } \mathcal{H}_D} \cup \underbrace{\{|k_l\rangle\}_{l=1}^{N_d}}_{\text{Basis of } \mathcal{H}_d}$$

Given the spatial ordering of our basis, the subspaces $\mathcal{H}_S$ and $\mathcal{H}_d$ are "separated" by $\mathcal{H}_D$.

This implies that there is no direct coupling between source and drain, mathematically expressed as,

$$H_{Sd} = P_S \hat{H} P_d = \mathbf{0}$$

Because,

$$\forall |u\rangle \in \mathcal{H}_S, \forall |v\rangle \in \mathcal{H}_d \implies \langle u|\hat{H}|v\rangle = 0$$

Hence, the Hamiltonian matrix in the basis $\mathcal{B}$ takes the block form, where τ_{SD} maps $\mathcal{H}_S \to \mathcal{H}_D$

$$[H]_{\mathcal{B}} = \begin{pmatrix} H_S & \tau_{SD}^\dagger & \mathbf{0} \\ \tau_{SD} & H_D & \tau_{Dd} \\ \mathbf{0} & \tau_{Dd}^\dagger & H_d \end{pmatrix}$$

The explicit form of the Green's function matrix, $\mathbf{G}(E) = [E\mathbf{I} - \mathbf{H}]^{-1}$, is obtained by direct inversion of the discretized Hamiltonian. By performing a blockwise Gaussian elimination, we can demonstrate that the Green's function acquires a dense block structure. Consequently, we admit the following form for $\mathbf{G}$, where the non-zero off-diagonal blocks $\mathbf{G}_{Sd}$ and $\mathbf{G}_{dS}$ rigorously capture the quantum mechanical tunneling probability between the theoretically disconnected leads

$$G = \begin{bmatrix} G_S & G_{SD} & G_{Sd} \\ G_{DS} & G_D & G_{Dd} \\ G_{dS} & G_{dD} & G_d \end{bmatrix} \begin{matrix} \leftarrow \text{End in Source} \\ \leftarrow \text{End in Device} \\ \leftarrow \text{End in Drain} \end{matrix}$$

Derivation of the Self-Energy. The Green's function equation $(E\mathbf{I} - \mathbf{H})\mathbf{G} = \mathbf{I}$ becomes a coupled system. Focusing on the device region, we seek $\mathbf{G}_D$ by eliminating the lead degrees of freedom.

From the source hamitonian 1^{st} row-block and 2^{nd} column-block:

$$(E\mathbf{I} - \mathbf{H}_S)\mathbf{G}_{SD} - \boldsymbol{\tau}_S^\dagger \mathbf{G}_D = \mathbf{0} \tag{0.22}$$

$$\Rightarrow \mathbf{G}_{SD} = (E\mathbf{I} - \mathbf{H}_S)^{-1}\boldsymbol{\tau}_S^\dagger \mathbf{G}_D = \mathbf{g}_S^R \boldsymbol{\tau}_S^\dagger \mathbf{G}_D, \tag{0.23}$$

where $\mathbf{g}_S^R = (E\mathbf{I} - \mathbf{H}_S)^{-1}$ is the surface Green's function of the source material.

Substituting into the device equation and performing similar algebra for the drain, we arrive at the effective device Green's function,

$$\mathbf{G}_D^R = \left[E\mathbf{I} - \mathbf{H}_D - \boldsymbol{\Sigma}_S - \boldsymbol{\Sigma}_D\right]^{-1}, \tag{0.24}$$

where the **self-energies** are defined as:

$$\boldsymbol{\Sigma}_S = \boldsymbol{\tau}_S^\dagger \mathbf{g}_S^R \boldsymbol{\tau}_S, \quad \boldsymbol{\Sigma}_D = \boldsymbol{\tau}_D \mathbf{g}_D^R \boldsymbol{\tau}_D^\dagger. \tag{0.25}$$

Remark 0.5. The self-energy $\Sigma = \Delta - i\Gamma/2$ help describe the open boundary conditions. With the real component, Δ, shifting the resonant levels, while the imaginary component, Γ, represents the electron escape rate into the leads, resulting in level broadening.

Self-Energy for 1D Semi-Infinite Leads. A semi-infinite lead $\mathcal{L}$ is defined as a quantum mechanical system modeled on the Hilbert space $\mathcal{H}_L$, spanned by an orthonormal basis of spatially ordered states $\{|n\rangle\}_{n=0}^{-\infty}$

We now derive the computational expression of the self-energy Σ by considering the boundary conditions at the interface.

Consider the interface between the device (site 1) and the semi-infinite source lead. The discrete Schrödinger equation for the first site of the device is,

$$(E - \epsilon_1)\psi_1 + t\psi_2 + t\psi_0 = 0. \tag{0.26}$$

We must express ψ_0 solely in terms of ψ_1.

In the semi-infinite lead (with uniform potential $V = 0$ and on-site energy $\epsilon_0 = 2t$), the wavefunction must satisfy the retarded boundary condition, meaning it propagates away from the device. We assume a plane-wave solution;

$$\psi_n \propto e^{ikna} \implies \psi_0 = \psi_1 e^{ika} \tag{0.27}$$

where a is the lattice constant and k is the longitudinal wavevector.

Substituting this boundary condition back into Eq. (0.26):

$$(E - \epsilon_1)\psi_1 + t\psi_2 + t(\psi_1 e^{ika}) = 0 \tag{0.28}$$

Rearranging to group the terms acting on ψ_1:

$$(E - \epsilon_1 - \Sigma_S)\psi_1 + t\psi_2 = 0 \tag{0.29}$$

Here, the coupling to the semi-infinite lead gives the self-energy,

$$\Sigma_S(E) = -te^{ika} \tag{0.30}$$

Expressing k in terms of energy via the dispersion relation $E = 2t(1 - \cos(ka)) \approx \hbar^2 k^2 / 2m^*$ (parabolic band approximation):

$$\Sigma_S(E) = -t \exp(ik_S a), \quad k_S = \frac{\sqrt{2m^* E}}{\hbar}. \tag{0.31}$$

Similarly, for the drain contact under bias V, the band bottom is shifted by $-qV$, yielding:

$$\Sigma_D(E) = -t \exp(ik_D a), \quad k_D = \frac{\sqrt{2m^*(E + qV)}}{\hbar}. \tag{0.32}$$

Broadening Matrices. The coupling strength between device and leads is characterized by the broadening matrices

They give the resonant states within the device and the injection/extraction rates of charge carriers at the boundaries

$$\mathbf{\Gamma}_S = i(\mathbf{\Sigma}_S - \mathbf{\Sigma}_S^\dagger) = -2\,\mathrm{Im}(\mathbf{\Sigma}_S), \tag{0.33}$$

and similarly for $\mathbf{\Gamma}_D$. For propagating modes ($E > 0$), the broadening is:

$$\Gamma_{S,D} = 2t \sin(k_{S,D} a). \tag{0.34}$$

Spectral Representation and Physical Interpretation.

Spectral Theorem. For a Hermitian Hamiltonian $\mathbf{H}$ with eigenstates $|\psi_n\rangle$ and eigenvalues ϵ_n, the spectral theorem gives:

$$\mathbf{H} = \sum_n \epsilon_n |\psi_n\rangle\langle\psi_n|, \quad \mathbf{I} = \sum_n |\psi_n\rangle\langle\psi_n|. \tag{0.35}$$

The retarded Green's function admits the spectral representation:

$$\mathbf{G}^R(E) = \sum_n \frac{|\psi_n\rangle\langle\psi_n|}{E - \epsilon_n + i\eta}. \tag{0.36}$$

This reveals that $\mathbf{G}^R$ has poles at the eigenenergies ϵ_n, and the residues are the projection operators onto the corresponding eigenstates.

Local Density of States. For the sake of computation, we will use a formula giving the local density of states from the Green's function.

The imaginary part of the diagonal Green's function elements gives the local density of states,

$$A(x_i, E) = -\frac{1}{\pi} \mathrm{Im}\left[G_{ii}^R(E)\right] = \sum_n |\psi_n(x_i)|^2 \delta(E - \epsilon_n). \tag{0.37}$$

Indicating where electrons can exist in the device at a given energy.

Quantum Transport and Current.

Heisenberg Equation of Motion. To derive the current, we use the Heisenberg picture where operators evolve in time, for some operator $\hat{A}$,

$$\frac{d\hat{A}_H(t)}{dt} = \frac{i}{\hbar}[\mathbf{H}, \hat{A}_H(t)] + \left(\frac{\partial \hat{A}_S}{\partial t}\right)_H . \tag{0.38}$$

Where $[\cdot, \cdot]$ is the commutator and the subscript H denotes Heisenberg representation and S the Schrödinger representation.

The current from the source is related to the rate of change of the number operator $\hat{N}_S$ in the source,

$$I_S = -e\frac{d\langle \hat{N}_S \rangle}{dt}. \tag{0.39}$$

Since $[\hat{N}_S, \mathbf{H}_S] = 0$ (particle number is conserved), only the coupling terms $\boldsymbol{\tau}$ contribute. Detailed derivation (Meir and Wingreen 1992; Haug and Jauho 2008) yields,

Schrödinger equation for Source state,

$$i\hbar\frac{d}{dt}|\Phi_S\rangle = H_S|\Phi_S\rangle + \tau_S^\dagger|\Psi\rangle \tag{0.40}$$

Which can be rearranged to,

the conjugate expression,

$$\frac{d}{dt}\langle\Phi_S| = -\frac{1}{i\hbar}\langle\Phi_S|H_S - \frac{1}{i\hbar}\langle\Psi|\tau_S \tag{0.41}$$

Hence,

$$\frac{d}{dt}\langle\Phi_S|\Phi_S\rangle = \left(\frac{d}{dt}\langle\Phi_S|\right)|\Phi_S\rangle + \langle\Phi_S|\left(\frac{d}{dt}|\Phi_S\rangle\right) \tag{0.42}$$

Substituting the previous expressions, we get,

$$\frac{1}{i\hbar}\left(\langle\Phi_S|\tau_S^\dagger|\Psi\rangle - \langle\Psi|\tau_S|\Phi_S\rangle\right) \tag{0.43}$$

Definition 0.6 (Expectation value in Statistical Physics). *In a quantum state $|\Psi\rangle$, the expected value an observable A is $\langle\Psi|\hat{A}|\Psi\rangle$. For a mixed state described by a density matrix ρ,*

$$\langle\hat{A}\rangle = Tr(\rho\hat{A}) \tag{0.44}$$

Hence, the current from the source lead can be expressed as,

$$I_S = -\frac{e}{\hbar}\mathrm{Tr}\left(\langle\Psi|\tau_S|\Phi_S\rangle - \langle\Phi_S|\tau_S^\dagger|\Psi\rangle\right) \tag{0.45}$$

I_S gives the current flowing into and out from the source. A similar expression holds for the drain current I_D.

Let us determine the transmission function $T(E)$, which quantifies the probability of electrons transmitting from source to drain at energy E.

$$1 = T(E) + R(E) \quad \Rightarrow \quad R(E) = 1 - T(E)$$

Hence, the reflection function $R(E)$ gives the probability of electrons being reflected back into the source.

$$R(E) \cdot f_S = (1 - T) f_S$$

Meanwhile, the electrons transmitted to the drain are given by,

$$T(E) \cdot f_D$$

The electrons coming from the source and drain leads are described by the Fermi-Dirac distributions $f_S(E)$ and $f_D(E)$, respectively.

$$\text{Flow in} \propto 1 \cdot f_S$$

Hence in summary we recover an expression resembling the Landauer-Büttiker Formula of the net flow of electrons from source to drain,

$$I_{net} \propto T(E)[f_S(E) - f_D(E)]$$

Transmission Function. For coherent transport (no inelastic scattering), the current can be expressed in terms of the transmission function (Datta 2005):

$$T(E) = \mathrm{Tr}\left[\mathbf{\Gamma}_S \mathbf{G}^R \mathbf{\Gamma}_D \mathbf{G}^A\right], \tag{0.46}$$

where $\mathbf{G}^A = (\mathbf{G}^R)^\dagger$ is the advanced Green's function.

For our 1D system with single-channel leads, this simplifies to:

$$T(E) = \Gamma_S \Gamma_D |G^R_{1,N}|^2, \tag{0.47}$$

where $G^R_{1,N}$ is the corner element of the Green's function connecting the first site (source) to the last site (drain).

Landauer-Büttiker Formula. The total current is obtained by integrating the transmission over energy, weighted by the difference in Fermi-Dirac distributions (Landauer 1957; Büttiker 1986):

$$I(V) = \frac{2e}{h} \int_{-\infty}^{+\infty} T(E, V) \left[f_S(E) - f_D(E)\right] dE, \tag{0.48}$$

Where the factor of 2 accounts for spin degeneracy. f_S and f_D are the Fermi-Dirac distributions with chemical potentials $\mu_S = E_F$ and $\mu_D = E_F - eV$.

$$f_{S,D}(E) = \frac{1}{1 + \exp\left(\frac{E - \mu_{S,D}}{k_B T}\right)} \tag{0.49}$$

The Landauer formula has a beautiful physical interpretation: current is proportional to the number of conducting channels (T) times the difference in occupation ($f_S - f_D$).

Numerical Implementation in Julia.

Device Parameters. For a GaAs/AlGaAs RTD, we use the following parameters:

Parameter	Symbol	Value	Units
Grid points	N	200	-
Device length	L	50	nm
Effective mass	m^*/m_0	0.067	-
Barrier height	U_b	0.3	eV
Barrier width	w_b	3	nm
Well width	w_w	5	nm
Temperature	T	300	K
Fermi energy	E_F	0.1	eV

The hopping parameter evaluates to $t = \hbar^2/(2m^*a^2) \approx 0.9$ eV for grid spacing $a \approx 0.25$ nm.

Algorithm Overview. The algorithm consists of nested loops over applied bias voltages and energy values to compute the I-V characteristic. Starting by defining the device Hamiltonian within a grid and the potential profile then followed by a calculation for each energy the correspondant Green's function and transmision, before accumulating the current via the Landauer formula.

The Recursive Green's Function algorithm (Sancho, Sancho, and Rubio 1985) can compute $G^R_{1,N}$ in $O(N)$ time instead of $O(N^3)$ for full inversion. However, for simplicity, we use direct inversion here.

Results and Discussion.

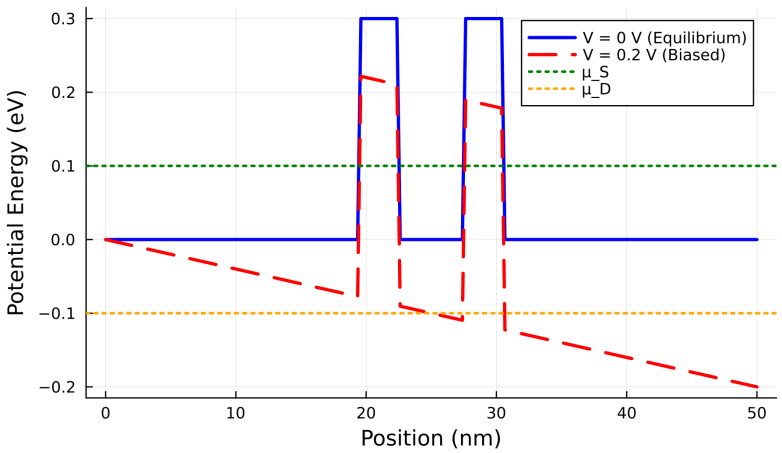


Figure 0.1: Double-barrier potential profile at equilibrium (solid) and under bias (dashed).

Double-Barrier Potential Profile. Figure 0.1 shows the RTD potential: two 3 nm barriers of height 0.3 eV enclosing a 5 nm GaAs quantum well.

Physics of Resonant Tunneling. Resonant tunneling arises from constructive quantum interference.

When an electron wave encounters the double-barrier structure, it partially gets transmitted through the barrier and partially reflected back. The part of the wave transmitted will bounce between the barriers and eventually tunnel out once they interfere constructively at certain energies.

At resonance, the coherent sum yields $T \approx 1$.

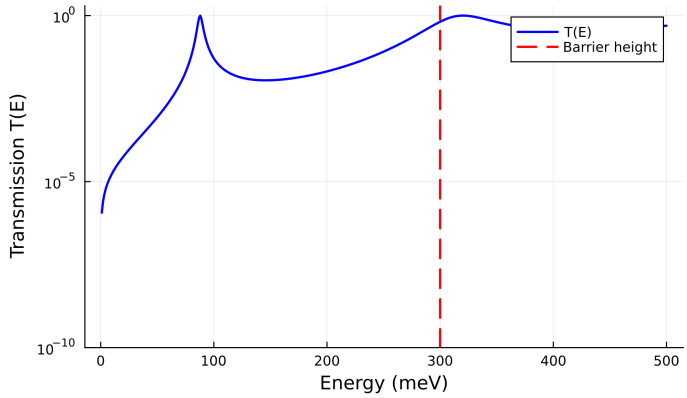


Figure 0.2: Transmission coefficient $T(E)$ showing sharp resonant peaks at quasi-bound state energies below the barrier height.

Transmission Spectrum. Figure 0.2 displays $T(E)$ at equilibrium, $E \approx 50$–100 meV correspond to quasi-bound states in the well.

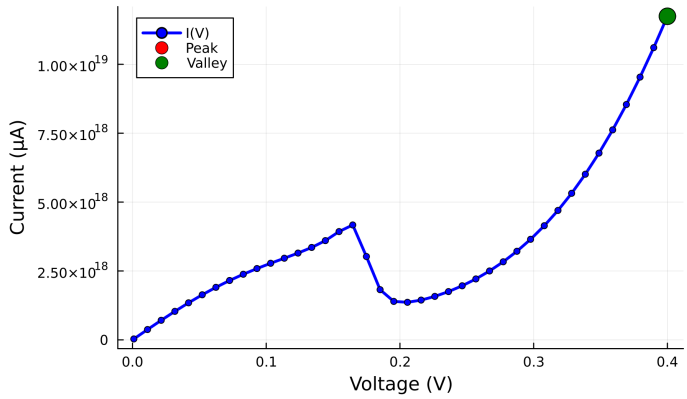


Figure 0.3: Current-voltage characteristic exhibiting negative differential resistance (NDR) between peak and valley.

I-V Characteristics. Figure 0.3 shows the I-V curve:

The Maximum current occurs when the resonant state aligns optimally with incoming electrons from the emitter.

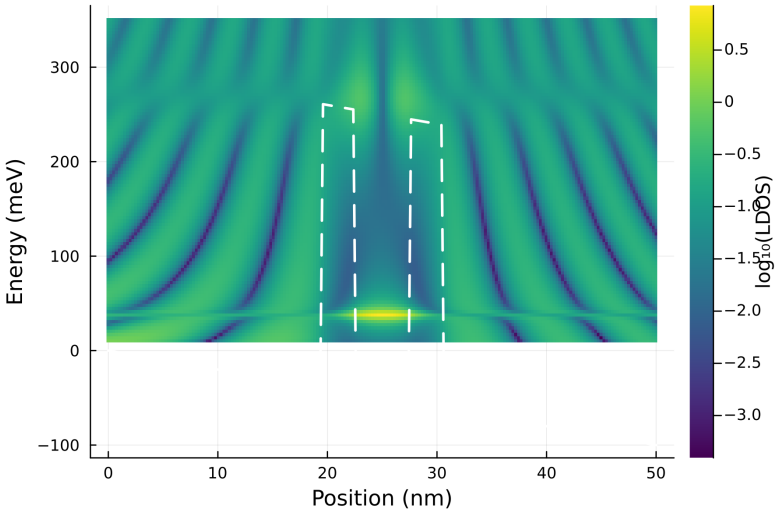


Figure 0.4: Local density of states $A(x, E)$ showing enhanced probability density in the quantum well at resonant energies.

Local Density of States. Figure 0.4 reveals the spatial structure of quasi-bound states: electron density is localized within the well at resonant energies.

Conclusion. We have presented an implementation of NEGF-based quantum transport simulation for resonant tunneling diodes, and tried deriving most of the equations and make sense from basic quantum mechanics, material physics and statistical physics. Starting from the Schrödinger equation, Green's function formalism, and the Landauer-Büttiker approach we developed a working simulator in Julia that reproduces the essential physics of RTDs.

The NEGF formalism provides a powerful and extensible framework for quantum device simulation. Future extensions could include, modelling coupling that comes from electrostatics. and possibly an extension to 2D/3D geometries for more realistic structure. Or perhaps looking into ways to get a transient response.

The complete Julia implementation is available as an interactive Jupyter notebook, enabling exploration of parameter space and visualization of the underlying quantum physics.

Acknowledgments. The foundational texts where those of Datta (Datta 1995, 2005) and the tutorial by Braggio et al. (Braggio, Carrega, and Ferraro 2023) which greatly informed this work, and gave not only the idea but also the rigor needed to implement this simulator.

References.

Braggio, A., M. Carrega, and D. Ferraro. 2023. "A Tutorial on the NEGF Method for Electron Transport in Devices and Defective Materials." *The European Physical Journal B* 96: 147. https://doi.org/10.1140/epjb/s10051-023-00580-5.

Büttiker, M. 1986. "Four-Terminal Phase-Coherent Conductance." *Physical Review Letters* 57 (14): 1761–64. https://doi.org/10.1103/PhysRevLett.57.1761.

Camsari, Kerem Y., Shuvro Chowdhury, and Supriyo Datta. 2020. "The Non-Equilibrium Green Function (NEGF) Method." *arXiv Preprint*.

Chang, L. L., L. Esaki, and R. Tsu. 1974. "Resonant Tunneling in Semiconductor Double Barriers." *Applied Physics Letters* 24 (12): 593–95. https://doi.org/10.1063/1.1655067.

Datta, Supriyo. 1995. "Electronic Transport in Mesoscopic Systems." https://doi.org/10.1017/CBO9780511805776.

———. 2005. "Quantum Transport: Atom to Transistor." https://doi.org/10.1017/CBO9781139164313.

Haug, Hartmut, and Antti-Pekka Jauho. 2008. "Quantum Kinetics in Transport and Optics of Semiconductors," Springer series in solid-state sciences,. https://doi.org/10.1007/978-3-540-73564-9.

Lake, Roger, Gerhard Klimeck, R. Chris Bowen, and Dejan Jovanovic. 1997. "Single and Multiband Modeling of Quantum Electron Transport Through Layered Semiconductor Devices." *Journal of Applied Physics* 81: 7845–69. https://doi.org/10.1063/1.365394.

Landauer, Rolf. 1957. "Spatial Variation of Currents and Fields Due to Localized Scatterers in Metallic Conduction." *IBM Journal of Research and Development* 1 (3): 223–31. https://doi.org/10.1147/rd.13.0223.

Meir, Yigal, and Ned S. Wingreen. 1992. "Landauer Formula for the Current Through an Interacting Electron Region." *Physical Review Letters* 68 (16): 2512–15. https://doi.org/10.1103/PhysRevLett.68.2512.

Sancho, M. P. López, J. M. López Sancho, and J. Rubio. 1985. "Highly Convergent Schemes for the Calculation of Bulk and Surface Green Functions." *Journal of Physics F: Metal Physics* 15 (4): 851–58. https://doi.org/10.1088/0305-4608/15/4/009.

Tsu, R., and L. Esaki. 1973. "Tunneling in a Finite Superlattice." *Applied Physics Letters* 22 (11): 562–64. https://doi.org/10.1063/1.1654509.