

# Computational Non-Equilibrium Green's Function Formalism

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## 1 Self-Consistent Field (SCF)

### 1.1 Introduction

The self-consistent field (SCF) method is a fundamental technique in quantum mechanics for solving problems involving multi-electron systems. It works by repeatedly calculating the electron density and electrostatic potential of the system, using a combination of quantum transport equations and electrostatic constraints. This method is especially valuable in the field of nanoelectronics, where quantum effects play a major role.

### 1.2 SCF Procedure

The SCF procedure involves two key components:

- **Electrostatic Potential:** Solved using the Poisson equation, which describes the relationship between charge density and potential.
- **Quantum Transport:** Solved using the Non-Equilibrium Green's Function (NEGF) formalism to determine the electronic properties.

The electrostatic potential  $U$  is given by:

$$U = U_{\text{Laplace}} + q^2 \frac{\Delta N}{C_E}, \quad (1)$$

where:

- $U_{\text{Laplace}}$ : Potential due to external contacts and gates (calculated using Laplace's equation).
- $\Delta N = N - N_0$ : Change in electron density.
- $C_E$ : Electrostatic capacitance of the system.

### 1.3 Iterative Procedure for SCF

To solve for  $U$  and  $N$  self-consistently, an iterative process is used:

1. Initialize  $U$ : Start with an initial guess for  $U$ .
2. Solve for  $N$ : Use the quantum transport equation to compute the electron density:

$$N = \int_{-\infty}^{\infty} dE D_{\epsilon}(E - U) \frac{\gamma_1 f_1(E) + \gamma_2 f_2(E)}{\gamma_1 + \gamma_2},$$

where  $D_{\epsilon}(E)$  is the density of states (DOS) and  $\gamma_{1,2}$  are broadening terms from contacts.

3. Update  $U$ : Update the potential using:

$$U = U_{\text{Laplace}} + q^2 \frac{(N - N_0)}{C_E}.$$

4. Repeat: Iterate until  $U$  converges within a specified tolerance (e.g.,  $|U_{\text{new}} - U_{\text{old}}| < \epsilon$ ).

### 1.4 Example: Quantum Dot

For a quantum dot with a single energy level at  $\epsilon$ , the current is computed using:

$$I = q \int_{-\infty}^{\infty} T(E) [f_1(E) - f_2(E)] dE,$$

where  $T(E)$  is the transmission function:

$$T(E) = \frac{\gamma_1 \gamma_2}{(E - \epsilon - U)^2 + (\gamma_1 + \gamma_2)^2}.$$

The iterative SCF method ensures  $U$  is consistent with the charge distribution.

## 2 Basis Functions

### 2.1 Introduction

Basis functions are essential in quantum mechanics and computational modeling, as they break down complex wavefunctions into simpler, well-defined components. Here I explored the concepts and practical uses of basis functions, highlighting their importance in building Hamiltonians and solving eigenvalue problems in quantum transport.

### 2.2 Wavefunction Representation

The wavefunction  $\psi(\mathbf{r})$  of a quantum system is expressed as a linear combination of basis functions  $u_m(\mathbf{r})$ :

$$\psi(\mathbf{r}) = \sum_m \phi_m u_m(\mathbf{r}), \quad (2)$$

where:

- $u_m(\mathbf{r})$ : Basis functions, chosen based on the system's properties (e.g., plane waves, atomic orbitals).
- $\phi_m$ : Expansion coefficients to be determined.

This representation reduces complex quantum problems to manageable matrix equations.

## 2.3 Matrix Formulation

Substituting the basis expansion into the Schrödinger equation:

$$H\psi = E\psi,$$

leads to a generalized eigenvalue problem:

$$H\Phi = E S \Phi, \quad (3)$$

where:

- $H_{mn} = \int u_m^* H u_n d\mathbf{r}$ : Matrix elements of the Hamiltonian.
- $S_{mn} = \int u_m^* u_n d\mathbf{r}$ : Overlap matrix, accounting for non-orthogonality of the basis functions.
- $E$ : Eigenvalue matrix representing energy levels.
- $\Phi$ : Column vector of coefficients  $\phi_m$ .

## 2.4 Computational Aspects

**Choice of Basis Functions:** The accuracy and efficiency of calculations depend on the choice of our basis functions like:

- Plane Waves: Ideal for periodic systems.
- Atomic Orbitals: Suitable for localized systems, such as molecules.
- Gaussian Functions: Commonly used in quantum chemistry for molecular systems.

**Orthogonalization:** Non-orthogonal basis functions require the overlap matrix  $S$  for proper normalization. If  $S$  is ill-conditioned, numerical issues may arise, requiring orthogonalization techniques:

$$\tilde{u}_m = \sum_n (S^{-1/2})_{mn} u_n.$$

## 2.5 Equilibrium Density Matrix

The equilibrium density matrix can be expressed in terms of the basis functions:

$$\rho = \sum_{m,n} \rho_{mn} u_m^*(\mathbf{r}) u_n(\mathbf{r}), \quad (4)$$

where  $\rho_{mn}$  are the matrix elements of the density matrix:

$$\rho_{mn} = \int_{-\infty}^{\infty} \frac{dE}{2\pi} G^<(E)_{mn}.$$

## 2.6 Applications to Quantum Transport

The construction of the Hamiltonian and overlap matrices using basis functions forms the foundation of the Non-Equilibrium Green's Function (NEGF) formalism:

- Hamiltonian: Encodes the system's energy levels and coupling.
- Density of States: Calculated using the Green's functions derived from the Hamiltonian and basis functions.
- Transmission Function: Dependent on the coupling matrices, constructed using the chosen basis.

## 3 Bandstructure

### 3.1 Introduction

Bandstructure is a fundamental concept in quantum mechanics and solid-state physics, describing the relationship between the energy of electrons and their wavevector  $k$  in periodic solids. This chapter focuses on the theoretical foundation of bandstructure and its computational applications, particularly its role in quantum transport.

### 3.2 Bloch's Theorem

In a periodic potential, the electron wavefunction can be expressed using Bloch's theorem:

$$\psi_k(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_k(\mathbf{r}), \quad (5)$$

where:

- $\psi_k(\mathbf{r})$ : Electron wavefunction.
- $e^{i\mathbf{k}\cdot\mathbf{r}}$ : Plane wave factor.
- $u_k(\mathbf{r})$ : Periodic function with the periodicity of the lattice.

This theorem reduces the problem to solving the Schrödinger equation within a single unit cell of the crystal lattice.

### 3.3 Hamiltonian Matrix Construction

The Hamiltonian for a periodic solid is constructed using basis functions and accounts for interactions within and between unit cells. For a given wavevector  $\mathbf{k}$ , the Hamiltonian matrix  $H(\mathbf{k})$  is given by:

$$H_{mn}(\mathbf{k}) = \int u_m^*(\mathbf{r})H u_n(\mathbf{r})e^{i\mathbf{k}\cdot(\mathbf{r}_m-\mathbf{r}_n)}d\mathbf{r}, \quad (6)$$

where  $\mathbf{r}_m$  and  $\mathbf{r}_n$  are the positions of the basis functions.

### 3.4 Energy Dispersion Relation

The eigenvalues of the Hamiltonian matrix provide the energy dispersion relation  $E(\mathbf{k})$ :

$$H(\mathbf{k})\Phi = E(\mathbf{k})S\Phi, \quad (7)$$

where:

- $H(\mathbf{k})$ : Hamiltonian matrix for wavevector  $\mathbf{k}$ .
- $S$ : Overlap matrix (if the basis functions are non-orthogonal).
- $E(\mathbf{k})$ : Eigenvalue matrix representing energy levels.
- $\Phi$ : Eigenvector matrix.

### 3.5 Applications to Quantum Transport

The bandstructure provides critical information for quantum transport calculations, including:

- Density of States (DOS): The DOS is derived from the bandstructure and determines the availability of electronic states at a given energy.
- Effective Mass: The curvature of  $E(\mathbf{k})$  determines the effective mass of carriers, influencing their mobility and conductivity.
- Transmission Function: The bandstructure helps identify transmission modes for electrons traveling through a material.

### 3.6 Effect of Spin-Orbit Coupling

Spin-orbit coupling introduces additional terms in the Hamiltonian, splitting degenerate states. For example, in materials like GaAs, this effect is critical for understanding spin transport and spintronic devices.

### 3.7 Computational Aspects

**Numerical Diagonalization:** For a given  $\mathbf{k}$ , the Hamiltonian matrix is numerically diagonalized to obtain eigenvalues and eigenvectors. The procedure is repeated across the Brillouin zone to construct the full bandstructure.

**Visualization:** Bandstructure is typically visualized as  $E$  vs.  $\mathbf{k}$ , highlighting features like band gaps and dispersion relations.

## 4 Subbands

### 4.1 Introduction

Subbands arise in low-dimensional systems where quantum confinement restricts the motion of electrons in one or more spatial directions. Here I will focus on the theoretical understanding of subbands and their role in determining the electronic and transport properties of quantum wells, wires, and dots.

## 4.2 Quantum Confinement

When electrons are confined in a specific direction, their motion becomes quantized. For example, in a quantum well with confinement along the  $z$ -direction, the allowed wavevectors  $k_z$  are discrete:

$$k_z = \frac{n\pi}{L_z}, \quad n = 1, 2, 3, \dots, \quad (8)$$

where  $L_z$  is the width of the quantum well.

This quantization leads to the formation of subbands, where each subband corresponds to a discrete energy level in the confined direction.

## 4.3 Density of States (DOS)

The density of states (DOS) is significantly modified in low-dimensional systems:

- 3D Systems: DOS increases with the square root of energy:  $D(E) \propto \sqrt{E}$ .
- 2D Systems: DOS is constant for each subband:  $D(E) \propto \text{constant}$ .
- 1D Systems: DOS diverges at the subband edges:  $D(E) \propto \frac{1}{\sqrt{E-E_c}}$ , where  $E_c$  is the subband edge.
- 0D Systems: DOS consists of delta functions, representing discrete energy levels.

## 4.4 Subband Energy Levels

For a particle in a box of width  $L$ , the energy levels are given by:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2m^* L^2}, \quad n = 1, 2, 3, \dots, \quad (9)$$

where  $m^*$  is the effective mass of the electron.

In quantum wires or dots, confinement in additional directions leads to further quantization, resulting in fewer available states and enhanced quantum effects.

## 4.5 Transport Properties

The number of subbands that contribute to transport determines the conductance of a system. For a quantum wire, the conductance is quantized as:

$$G = M(E)G_0, \quad (10)$$

where:

- $M(E)$ : Number of subbands (or modes) at energy  $E$ .
- $G_0 = \frac{2q^2}{h}$ : Quantum of conductance.

## 4.6 Velocity of Subband Electrons

The group velocity of electrons in a subband is given by:

$$v_g = \frac{1}{\hbar} \frac{\partial E}{\partial k}. \quad (11)$$

This velocity plays a critical role in determining the transport properties, as it affects the current flow in the system.

## 4.7 Applications to Quantum Transport

Subbands influence the following aspects of quantum transport:

- **Conductance Quantization:** The stepwise increase in conductance as more subbands contribute to transport.
- **Thermoelectric Effects:** Subband structure impacts the Seebeck coefficient and thermoelectric efficiency.
- **Optical Properties:** Subbands dictate the absorption and emission spectra in quantum wells and dots.

## 4.8 Computational Aspects

**Numerical Calculation of Subband Structure:** The subband energies and wavefunctions are computed by solving the Schrödinger equation numerically, often using methods like finite differences or finite elements.

**Visualization of DOS:** The DOS for subbands is plotted as a function of energy, showing features like peaks in 1D systems and constant values in 2D systems.

# 5 Coherent Transport Using NEGF

## 5.1 Introduction

In this chapter, we explore the Non-Equilibrium Green's Function (NEGF) formalism to model coherent electron transport in nanoscale systems. By leveraging insights from earlier chapters, including the concepts of self-consistent field (Chapter 3), basis functions (Chapter 4), bandstructure (Chapter 5), and subbands (Chapter 6), we develop a comprehensive framework for analyzing quantum transport.

## 5.2 Theoretical Framework

**Hamiltonian Construction** The system's Hamiltonian  $H$  is constructed using basis functions to represent the quantum device. For periodic systems, the Hamiltonian depends on the wavevector  $\mathbf{k}$ :

$$H_{mn}(\mathbf{k}) = \int u_m^*(\mathbf{r}) H u_n(\mathbf{r}) e^{i\mathbf{k} \cdot (\mathbf{r}_m - \mathbf{r}_n)} d\mathbf{r}, \quad (12)$$

where  $u_m(\mathbf{r})$  are the basis functions, and the integral is taken over the spatial domain.

The overlap matrix  $S$ , as discussed in basis function, accounts for non-orthogonality and ensures proper normalization:

$$S_{mn} = \int u_m^*(\mathbf{r}) u_n(\mathbf{r}) d\mathbf{r}. \quad (13)$$

**Subbands and Mode Contributions** As learned in bandstructures, the electronic structure of low-dimensional systems results in discrete subbands. The number of subbands  $M(E)$  contributing to transport determines the conductance of the device. Each subband corresponds to a mode, and their energies  $E_n$  are determined by:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2m^* L^2}, \quad n = 1, 2, 3, \dots, \quad (14)$$

where  $m^*$  is the effective mass of the electron and  $L$  is the confinement width.

**Self-Consistency** As discussed in Chapter 3, the potential  $U$  within the device must be determined self-consistently. The iterative self-consistent field (SCF) approach updates  $U$  using the electron density  $N$ :

$$U = U_{\text{Laplace}} + q^2 \frac{N - N_0}{C_E}, \quad (15)$$

where:

- $U_{\text{Laplace}}$ : Potential due to external contacts and gates.
- $N$ : Electron density.
- $C_E$ : Electrostatic capacitance of the system.

The density  $N$  is computed from the Green's functions, as explained below.

### 5.3 NEGF Formalism

The NEGF formalism provides a powerful framework for computing electron transport properties, including the Green's functions  $G$ , transmission  $T(E)$ , and current  $I$ .

**Green's Functions** The retarded Green's function  $G^r$  is computed as:

$$G^r(E) = [EI - H - \Sigma_1^r - \Sigma_2^r]^{-1}, \quad (16)$$

where:

- $H$ : Device Hamiltonian.
- $\Sigma_1^r, \Sigma_2^r$ : Retarded self-energies due to coupling with the source and drain leads.
- $E$ : Energy.

The lesser Green's function  $G^<$  is computed as:

$$G^<(E) = G^r [\Gamma_1 f_1(E) + \Gamma_2 f_2(E)] G^{r\dagger}, \quad (17)$$

where  $\Gamma_{1,2} = i(\Sigma_{1,2}^r - \Sigma_{1,2}^{r\dagger})$  are the broadening matrices and  $f_{1,2}(E)$  are the Fermi functions of the source and drain, respectively.



**Transmission Function** The transmission coefficient  $T(E)$  is computed using:

$$T(E) = \text{Tr} [\Gamma_1 G^r \Gamma_2 G^{r\dagger}] . \quad (18)$$

This function quantifies the probability of electron transport through the device at a given energy  $E$ .

**Current Calculation** The current  $I$  is computed using the Landauer formula:

$$I = \frac{2q}{h} \int_{-\infty}^{\infty} T(E) [f_1(E) - f_2(E)] dE, \quad (19)$$

where:

- $q$ : Electron charge.
- $h$ : Planck's constant.
- $f_1(E), f_2(E)$ : Fermi-Dirac distributions of the source and drain leads.

## 5.4 Computational Implementation

**Hamiltonian and Overlap Matrices:** Using basis functions from Chapter 4, construct  $H$  and  $S$  matrices. For periodic systems, incorporate  $\mathbf{k}$ -dependent terms as discussed in Chapter 5.

**Self-Energy Matrices:** Calculate  $\Sigma_1^r$  and  $\Sigma_2^r$  for the source and drain leads, typically using semi-infinite lead models.

**Green's Function Solver:** Solve for  $G^r$  and  $G^<$  using numerical matrix inversion and multiplications.

**Transmission and Current:** Integrate  $T(E)$  over the energy range using numerical techniques (e.g., trapezoidal or Gaussian quadrature) to compute  $I$ .

## 5.5 Conclusion

This chapter integrates the theoretical foundations from earlier chapters to model coherent transport in quantum devices. By combining the NEGF formalism with concepts like self-consistency, basis functions, bandstructure, and subbands, I develop a powerful framework for understanding and predicting nanoscale transport phenomena.

# 6 Numerical Analysis and Visualization

To deepen our understanding of the quantum transport phenomena described in the NEGF formalism, several numerical simulations were conducted. These simulations illustrate key concepts such as the density of states (DOS), transmission function, local density of states (LDOS), subband contributions, potential profile updates, bandstructure, and conductance quantization. The theoretical background and corresponding plots are detailed below. For codes click [here](#).

## 6.1 Density of States (DOS)

The density of states quantifies the number of available electronic states at a given energy. Using the retarded Green's function  $G^r(E)$ , the DOS is calculated as:

$$D(E) = -\frac{1}{\pi} \text{Im} (\text{Tr} [G^r(E)]) . \quad (20)$$

The plot in Figure 1 demonstrates the DOS for a tight-binding Hamiltonian system. Peaks in the DOS correspond to energy levels where states are highly available.

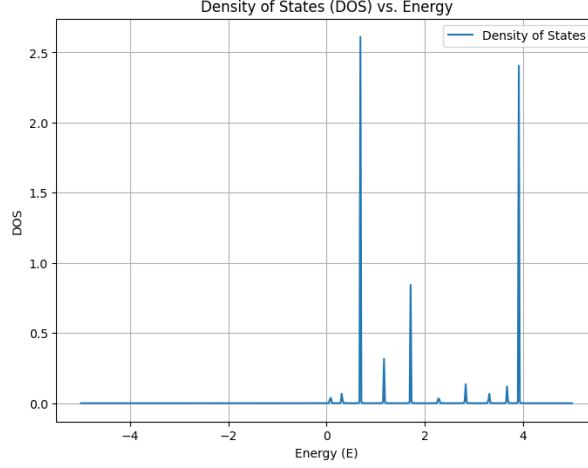


Figure 1: Density of States (DOS) vs. Energy for a tight-binding Hamiltonian.

## 6.2 Local Density of States (LDOS)

The local density of states (LDOS) describes the spatial distribution of available states at specific energies. It is computed as:

$$\text{LDOS}_i(E) = -\frac{1}{\pi} \text{Im} [G_{ii}^r(E)] . \quad (21)$$

Figure 2 shows the LDOS for selected sites in the system, highlighting spatial variations in electronic states.

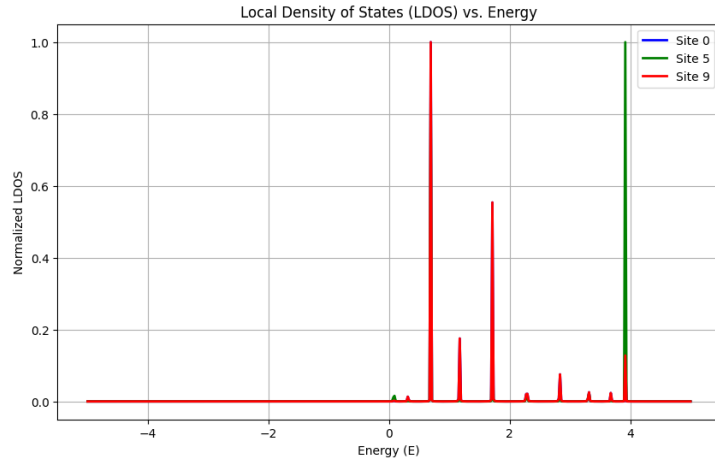


Figure 2: Local Density of States (LDOS) vs. Energy for selected sites in the device.

### 6.3 Transmission Function

The transmission function  $T(E)$  quantifies the probability of electrons traversing the device. It is computed as:

$$T(E) = \text{Tr} [\Gamma_1 G^r \Gamma_2 G^{r\dagger}] , \quad (22)$$

where  $\Gamma_{1,2}$  are the broadening matrices for the source and drain leads. The plot in Figure 3 shows how transmission varies with energy.

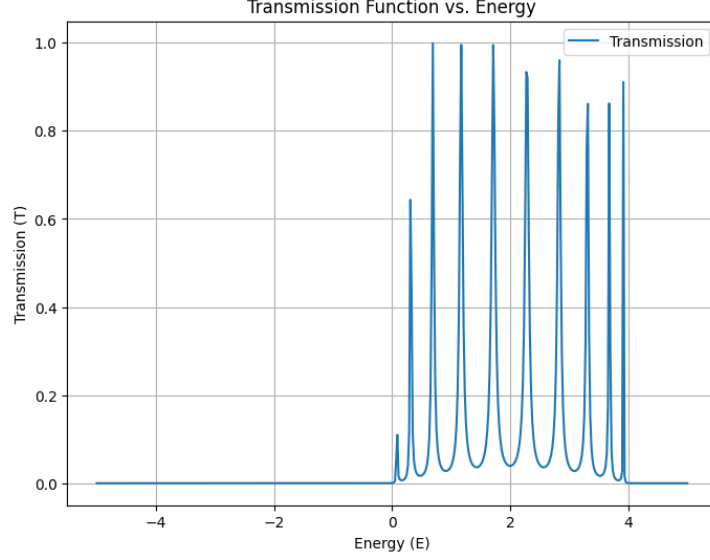


Figure 3: Transmission Function vs. Energy for a device coupled to source and drain leads.

### 6.4 Subband Contributions to Transmission

For systems with discrete subbands (Chapter 6), each subband contributes to the total transmission. Subband contributions are modeled as Lorentzian peaks centered around subband energies. The transmission function for a multi-subband system is shown in Figure 4.

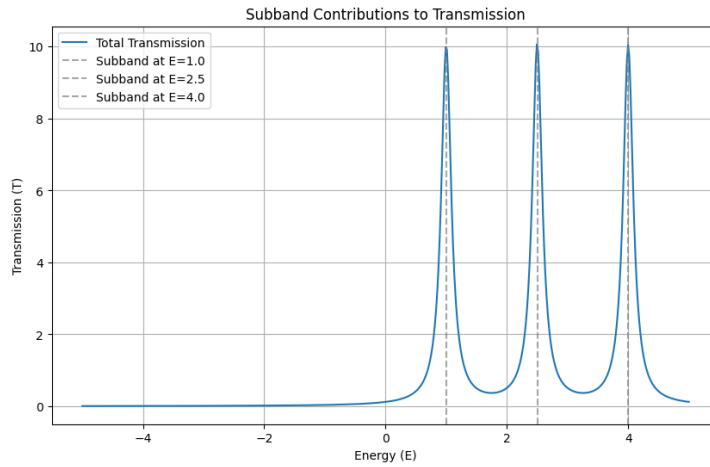


Figure 4: Subband Contributions to Transmission. Vertical lines indicate subband energies.

## 6.5 Potential Profile Update (SCF)

The potential profile in a quantum device is updated self-consistently using the SCF method described in Chapter 3. The updated potential  $U(x)$  is given by:

$$U(x) = U_{\text{external}} + \frac{q^2}{C_E} [N(x) - N_0(x)]. \quad (23)$$

Figure 5 illustrates the converged potential profile after iterative updates.

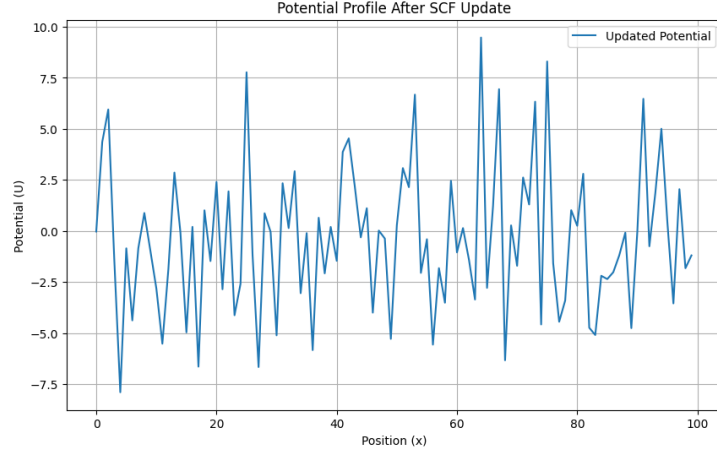


Figure 5: Converged Potential Profile in the quantum device after SCF updates.

## 6.6 Bandstructure Visualization

The bandstructure of a periodic system provides insights into energy dispersion relationships. For a 1D tight-binding chain, the bandstructure is given by:

$$E(k) = 2t \cos(k), \quad (24)$$

where  $t$  is the hopping parameter and  $k$  is the wavevector. Figure 6 shows the energy dispersion relation for such a system.

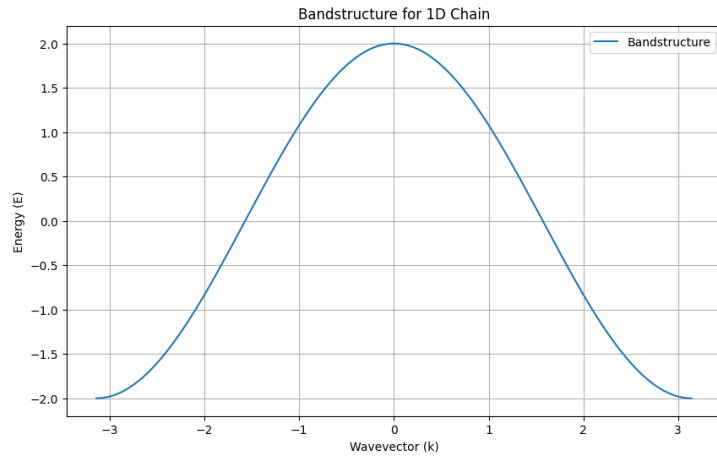


Figure 6: Bandstructure for a 1D periodic tight-binding chain.

## 6.7 Conductance Quantization

The conductance  $G$  is quantized in systems with discrete subbands (Chapter 6):

$$G = M(E)G_0, \quad G_0 = \frac{2q^2}{h}, \quad (25)$$

where  $M(E)$  is the number of modes at energy  $E$ . Figure 7 demonstrates the stepwise increase in conductance as subbands are populated.

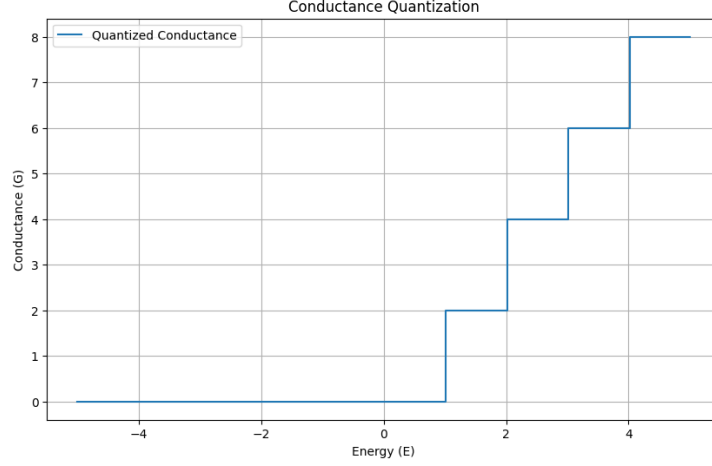


Figure 7: Conductance Quantization showing stepwise increases with energy.

## 6.8 Current-Voltage Characteristics (I-V)

Using the Landauer formula, the current  $I$  is computed as:

$$I = \frac{2q}{h} \int_{-\infty}^{\infty} T(E) [f_1(E) - f_2(E)] dE, \quad (26)$$

where  $f_1(E)$  and  $f_2(E)$  are the Fermi-Dirac distributions of the source and drain, respectively. Figure 8 illustrates the I-V characteristics for varying source-drain biases.

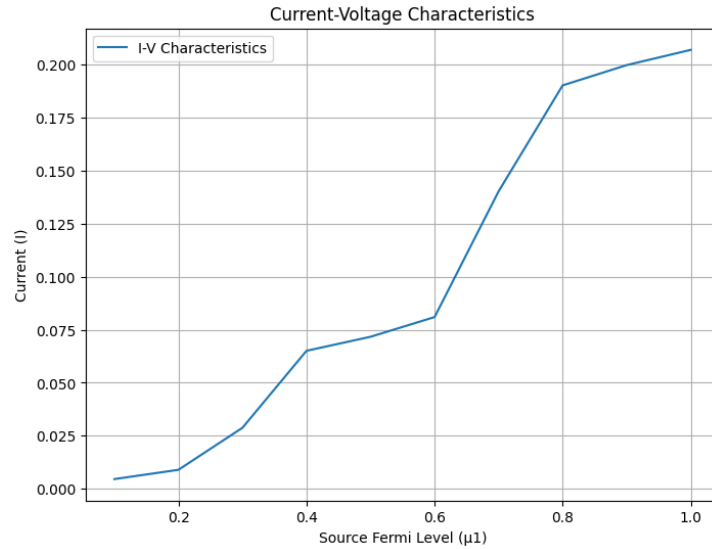


Figure 8: Current-Voltage (I-V) Characteristics showing the non-linear behavior at larger biases.