

A Python-Based Simulation Framework for Visualizing Nanoscale Quantum Transport

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Abstract—This work presents a Python-based simulation framework and web application for visualizing quantum transport phenomena in nanoscale systems, focusing on one- and two-dimensional tight-binding models. We explore how disorder and external magnetic fields affect electron transport using the Landauer-Büttiker formalism, with calculations performed via the Kwant software package. The platform allows real-time parameter tuning and conductance visualization, enabling users to study Anderson localization in 1D chains and quantized conductance plateaus in 2D systems under magnetic fields. Our results demonstrate the suppression of transport due to disorder and the emergence of Landau level-induced quantization, providing a pedagogical and exploratory tool for students and researchers interested in quantum materials and mesoscopic physics.

Index Terms—quantum transport, tight-binding model, Anderson localization, quantum Hall effect, simulation, Kwant

I. INTRODUCTION

Quantum transport in mesoscopic systems is a central topic in condensed matter physics, particularly as devices shrink to nanoscale dimensions where classical descriptions of conduction break down. In this regime, quantum coherence, wave interference, and discrete energy levels dominate electron behavior, requiring the use of quantum mechanical models such as the tight-binding approximation and scattering theory.

Accurate modeling of these systems is crucial not only for fundamental research, but also for designing novel materials and quantum devices. However, many computational tools for quantum transport—while powerful—are often inaccessible to newcomers due to steep learning curves or lack of interactive visualization.

This paper introduces a simulation framework and accompanying web application aimed at making quantum transport phenomena more accessible to learners and researchers. Built using Python and Kwant, and delivered through a FastAPI backend with a React frontend, the tool allows users to visualize how disorder and magnetic fields affect conductance in one- and two-dimensional tight-binding models. By simulating conductance in real time using the Landauer-Büttiker formalism and presenting the results through an interactive interface, our framework serves both as a research tool and a pedagogical aid. We focus particularly on phenomena such as Anderson localization and the integer quantum Hall effect,

both of which offer rich insights into the interplay between symmetry, topology, and disorder.

The modular design of our platform enables future extensions to more complex systems, including multi-terminal geometries, spinful tight-binding models, and topological phases beyond the quantum Hall regime. In particular, it can be adapted to simulate superconducting systems by incorporating particle-hole symmetry through the Bogoliubov-de Gennes formalism, paving the way for studies of Majorana modes and proximity-induced superconductivity.

II. METHODS

A. Theoretical Framework

At the core of our model is the *tight-binding approximation*, a widely used method for describing quantum particles (typically electrons) in a lattice. In this framework, electrons are assumed to be strongly localized around atomic sites, and their dynamics arise from quantum tunneling (hopping) between neighboring sites. The tight-binding Hamiltonian captures both the on-site potential energy and inter-site hopping terms.

The dynamics of the quantum system are governed by the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} \Psi(t) = H \Psi(t), \quad (1)$$

where $\Psi(t)$ is the time-dependent quantum state and H is the Hamiltonian operator encoding the system's total energy. In tight-binding systems, $\Psi(t)$ is typically expanded in a discrete basis of localized orbitals associated with each lattice site.

Assuming a system of *non-interacting spinless fermions*, the Hamiltonian can also be expressed in *second quantization*, where the basic objects are not wavefunctions (as in first quantization), but operators that create and annihilate particles at given lattice sites. In one dimension, the tight-binding Hamiltonian takes the form:

$$H = \sum_i \varepsilon_i c_i^\dagger c_i - \sum_{\langle i,j \rangle} t_{ij} c_i^\dagger c_j + \text{h.c.} \quad (2)$$

where:

- ε_i is the on-site energy at site i ,
- c_i^\dagger and c_i are the fermionic creation and annihilation operators at site i ,

- t_{ij} is the hopping amplitude between neighboring sites i and j ,
- “h.c.” denotes the Hermitian conjugate to ensure a Hermitian Hamiltonian.

These operators obey the canonical fermionic anticommutation relations:

$$\{c_i, c_j^\dagger\} = \delta_{ij}, \quad \{c_i, c_j\} = 0 = \{c_i^\dagger, c_j^\dagger\}. \quad (3)$$

The number operator $\hat{n}_i = c_i^\dagger c_i$ measures the occupancy at site i . The hopping term $c_i^\dagger c_j$ describes an electron moving from site j to site i , while the on-site term reflects local potential energy.

The tight-binding model is particularly powerful for exploring phenomena such as Anderson localization and quantum interference. In such systems, spatial variation of ε_i introduces disorder, while magnetic fields can be included via complex Peierls phases on the hopping terms (discussed in Section II-F).

Throughout this work, we compute transport properties using the *scattering matrix formalism*, where energy-resolved transmission coefficients are obtained from the system’s S -matrix and inserted into the Landauer formula to calculate conductance. These calculations are implemented using the Kwant software package.

In numerical simulations, the abstract operator Hamiltonian is represented as a finite matrix acting on a discrete Hilbert space. For a tight-binding chain with N sites, this leads to a sparse matrix whose structure encodes the system’s connectivity and boundary conditions. Below is the Hamiltonian matrix for a simple case with three sites and uniform parameters:

$$H = \begin{bmatrix} \varepsilon & -t & 0 \\ -t & \varepsilon & -t \\ 0 & -t & \varepsilon \end{bmatrix} \quad (4)$$

This tridiagonal structure is characteristic of 1D chains with nearest-neighbor hopping.

B. Comparison: 1D vs 2D Hamiltonians

In the 1D tight-binding model, electrons are confined to hopping along a linear chain. The hopping terms only connect each site to its nearest neighbor on the left and right. The Hamiltonian contains on-site energy terms and hopping terms between adjacent sites. The 1D system is especially sensitive to disorder: any non-zero disorder strength leads to Anderson localization.

In contrast, the 2D tight-binding model expands this concept to a square lattice. Each site is now connected to its neighbors in both the x and y directions. The Hamiltonian becomes:

$$H = \sum_{i,j} \varepsilon_{i,j} c_{i,j}^\dagger c_{i,j} - \sum_{\langle(i,j),(i',j')\rangle} t_{(i,j)(i',j')} c_{i,j}^\dagger c_{i',j'} + \text{h.c.} \quad (5)$$

This richer connectivity allows for the manifestation of new phenomena, such as cyclotron orbits and Landau level quantization in the presence of a magnetic field. It also means that disorder has a more complex impact, as localization can occur differently along the two axes. Additionally, the 2D model

allows for breaking time-reversal symmetry via magnetic flux, enabling quantum Hall physics.

C. Physical Apparatus Simulated

We model a quantum transport setup composed of three regions: the left lead (electron source), the central scattering region, and the right lead (electron drain). Electrons are injected from the left lead, propagate through the central disordered or magnetically perturbed region, and exit through the right lead. The full structure behaves as:

$$[\text{Left Lead}] - [\text{Scattering Region}] - [\text{Right Lead}]$$

The left and right leads act as ideal electron reservoirs that maintain a constant chemical potential and inject electrons into the system. The scattering region is finite in size and hosts the disorder and magnetic field perturbations we wish to study. Conductance is calculated by tracking how much of an incoming wave from the left lead is transmitted to the right lead.

D. Lead and Boundary Handling in Kwant

Kwant handles leads by requiring them to be translationally invariant and infinite in extent. The user defines a unit cell and symmetry direction, and Kwant replicates the unit cell to model an ideal semi-infinite lead. These leads are connected to a finite central region (the scattering region), forming a complete system. Internally, Kwant uses recursive Green’s function or wavefunction matching techniques to solve for the system’s scattering matrix. Boundary conditions are carefully enforced at lead-scatter junctions to ensure continuity and current conservation.

E. Anderson Localization

In disordered systems, random on-site potentials cause destructive interference of wavefunctions, leading to localization:

$$|\psi(x)| \sim e^{-x/\xi} \quad (6)$$

where ξ is the localization length. Even weak disorder in 1D systems causes exponential localization, leading to suppressed conductance.

F. Magnetic Field and Quantum Hall Effect

To model a perpendicular magnetic field in a 2D TBM, we apply the Peierls substitution:

$$t_{ij} \rightarrow t_{ij} e^{i\phi_{ij}}, \quad \phi_{ij} = \frac{2\pi}{\Phi_0} \int_i^j \vec{A} \cdot d\vec{l} \quad (7)$$

In Landau gauge $\vec{A} = (0, Bx, 0)$, the phase becomes $\phi = 2\pi Bx$. The result is quantized Landau levels:

$$E_n = \hbar\omega_c(n + \frac{1}{2}), \quad \omega_c = \frac{eB}{m} \quad (8)$$

These give rise to conductance plateaus observed in the quantum Hall effect.

G. Quantum Transport Formalism

Transport is described by the Landauer formula:

$$G(E) = \frac{e^2}{h} T(E) \quad (9)$$

where $T(E)$ is the energy-dependent transmission. Kwant computes $T(E)$ from the scattering matrix S :

$$T(E) = \text{Tr}(S_{RL}^\dagger S_{RL}) \quad (10)$$

H. Software Design

The core of our application is implemented in Python and powered by Kwant. A FastAPI backend defines the API interface, where clients can submit parameters (system length, width, disorder strength, magnetic field). The backend uses these inputs to construct a Kwant system, attach leads, and finalize the lattice. It then sweeps through energy values, calculating transmission probabilities using Kwant's scattering matrix tools. The resulting conductance vs energy data is plotted using Matplotlib and returned to the frontend as a base64-encoded image. A React.js frontend, styled with Tailwind CSS, receives this image and renders it alongside interactive sliders for user input. Each time the user updates a parameter and submits a new simulation, the frontend sends a POST request to the backend and updates the plot accordingly. This architecture enables fast feedback and exploration of transport phenomena.

III. RESULTS

Our first simulations focus on 1D chains with increasing disorder. We observe rapid decay of conductance as disorder increases. In 2D systems with a magnetic field, we observe the emergence of plateaus in conductance due to Landau levels. When disorder is added to this system, conductance degrades, and the quantum Hall effect is eventually suppressed.

IV. DISCUSSION

These results validate theoretical expectations: disorder induces localization while magnetic fields create quantized energy levels. Competing effects can be visualized, such as localization competing against topologically protected transport.

V. CONCLUSION

We developed a Python-based quantum transport simulation tool with a frontend for interactive exploration. It demonstrates localization, quantum Hall effects, and their interplay in disordered lattices. The tool can be extended for use in research and teaching.

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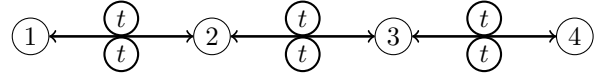


Fig. 1. 1D tight-binding chain with nearest-neighbor hopping amplitude t between lattice sites.

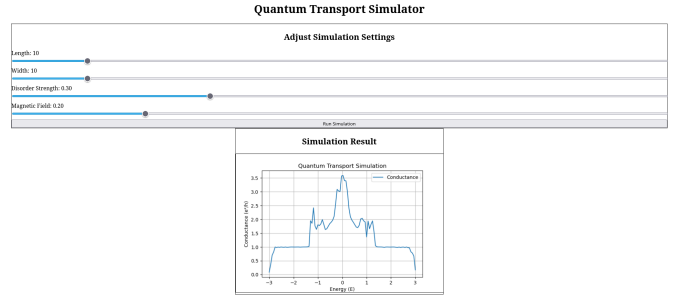


Fig. 2. User interface for adjusting lattice parameters and visualizing conductance.

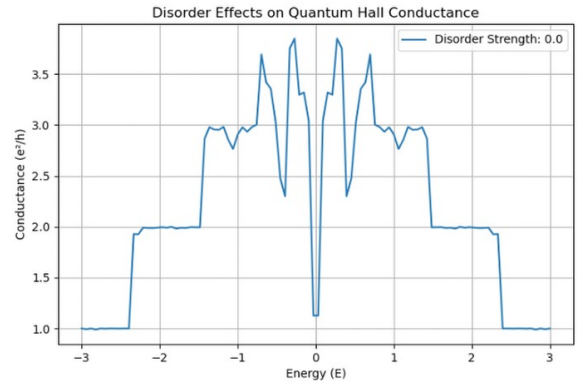


Fig. 3. Sample simulation output: conductance vs energy with disorder strength 0 in the QHE regime.