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. In addition to transport spectra, the framework includes a wavefunction inspection feature that visualizes the spatial probability density $|\psi(x, y)|^2$ of eigenstates near a user-selected energy, offering insight into localization behavior and the spatial structure of transmitting states. Our results demonstrate the suppression of transport due to disorder, the emergence of Landau level–induced quantization, and the correspondence between spatially extended eigenstates and high-conductance regimes, 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:

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

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:

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

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:

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

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.

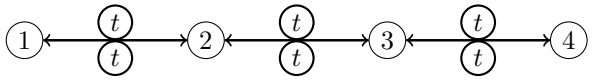

Fig. 1. 1D tight-binding chain with nearest-neighbor hopping amplitude t between lattice sites.

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:

$$H = \begin{bmatrix} \varepsilon & -t & 0 \\ -t & \varepsilon & -t \\ 0 & -t & \varepsilon \end{bmatrix} \tag{4}$$

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

B. Comparison: 1D vs 2D Hamiltonians

Building on the general Hamiltonian structure introduced in the previous section, we now compare how dimensionality—specifically 1D versus 2D lattice geometry—affects the physical behavior of quantum systems.

The tight-binding model naturally generalizes from one-dimensional (1D) chains to two-dimensional (2D) lattices, allowing for the exploration of richer physical phenomena.

In the 1D case, electrons can only hop to adjacent sites along a linear chain. The tight-binding Hamiltonian contains on-site potential terms and hopping terms between nearest neighbors to the left and right. As described earlier, this yields a tridiagonal matrix structure. The limited connectivity in 1D makes these systems especially sensitive to disorder: even infinitesimally weak disorder leads to Anderson localization, where wavefunctions become exponentially localized and conductance decays rapidly with system size.

In contrast, the 2D tight-binding model extends this concept to a square lattice, where each site can connect to neighbors in both the x and y directions. The Hamiltonian becomes:

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

Here, (i, j) indexes the lattice sites in two dimensions. The increased connectivity allows for more complex dynamics, including interference patterns, closed-loop trajectories, and orbital motion.

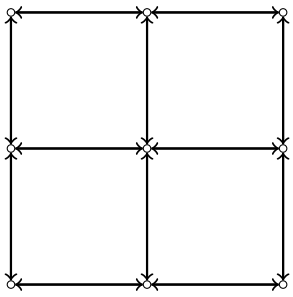

Fig. 2. 2D tight-binding lattice with nearest-neighbor hopping in both x and y directions.

To model the effect of a magnetic field $\vec{B}$ in a lattice system, we apply the Peierls substitution to the hopping terms. Each hopping amplitude acquires a complex phase determined by the magnetic vector potential $\vec{A}$:

$$t_{ij} \to t_{ij} \exp\left(\frac{2\pi i}{\Phi_0} \int_{\vec{r}_i}^{\vec{r}_j} \vec{A} \cdot d\vec{l} \right), \tag{6}$$

where $\Phi_0 = h/e$ is the magnetic flux quantum, and the line integral is taken along the path from site i to site j. This phase ensures gauge-invariant coupling of electrons to the external magnetic field in the lattice model.

After applying the Peierls substitution, the tight-binding Hamiltonian in 2D becomes:

$$H = \sum_{i,j} \varepsilon_{i,j}\, c_{i,j}^\dagger c_{i,j} - \sum_{\langle (i,j),(i',j') \rangle} t\, e^{i\phi_{(i,j)(i',j')}}\, c_{i,j}^\dagger c_{i',j'} + \text{h.c.} \tag{7}$$

Here, $\phi_{(i,j)(i',j')}$ is the Peierls phase associated with hopping from site (i, j) to (i', j'), and encodes the influence of the magnetic field through the vector potential. This phase modifies the interference properties of electron wavefunctions across the lattice, leading to new quantum phenomena such as Landau level quantization and edge state formation.

This phase accumulation depends on the vector potential and causes the system to lose time-reversal symmetry—that is,

the system no longer behaves identically when the direction of time is reversed. As a result, electrons experience a Lorentz-like force that bends their trajectories into circular orbits, analogous to classical cyclotron motion.

When the system is large enough, this circular motion becomes quantized, leading to discrete energy levels known as *Landau levels*. These are a direct quantum manifestation of cyclotron orbits and represent the allowed energies of an electron in a magnetic field.

In a finite 2D lattice with open boundaries, these Landau levels are not the whole story. At the edges of the system, special conducting states—called *chiral edge states*—appear. These edge states propagate in a single direction (i.e., they are chiral), and are spatially localized near the system's boundary. Unlike bulk states, they do not reflect or scatter backward, even in the presence of weak disorder or impurities.

This remarkable robustness arises from the system's underlying topological structure. Specifically, the bulk energy bands acquire a nontrivial topology, which is mathematically characterized by an integer known as the *Chern number*. As long as the energy lies within a bulk gap (between Landau levels), the number of conducting edge modes equals the Chern number. These edge states are said to be *topologically protected*, meaning they cannot be removed or localized without a fundamental change in the system's global band structure—such as closing the energy gap.

To illustrate the matrix structure in 2D, consider a 2×2 lattice with open boundary conditions and uniform parameters. The Hamiltonian matrix is:

$$H = \begin{bmatrix} \varepsilon & -t & -t & 0 \\ -t & \varepsilon & 0 & -t \\ -t & 0 & \varepsilon & -t \\ 0 & -t & -t & \varepsilon \end{bmatrix} \tag{8}$$

This form reflects the increased connectivity: each site may be coupled to up to four neighbors (left, right, up, down), leading to a sparsely filled but more complex matrix structure.

To explore these phenomena numerically, we construct finite tight-binding lattices with leads, simulating electron injection and transmission using the formalism described above. This setup is detailed in the following section.

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:

[Left Lead] – [Scattering Region] – [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:

$$|\psi(x)| \sim e^{-x/\xi} \tag{9}$$

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:

$$t_{ij} \to t_{ij} e^{i\phi_{ij}}, \quad \phi_{ij} = \frac{2\pi}{\Phi_0} \int_i^j \vec{A} \cdot d\vec{l} \tag{10}$$

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

$$E_n = \hbar\omega_c(n + \frac{1}{2}), \quad \omega_c = \frac{eB}{m} \tag{11}$$

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

G. Quantum Transport Formalism

Transport is described by the Landauer formula:

$$G(E) = \frac{e^2}{h} T(E) \tag{12}$$

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

$$T(E) = \text{Tr}(S_{RL}^\dagger S_{RL}) \tag{13}$$

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.

In addition to conductance visualization, the framework now includes a wavefunction inspection feature. For a user-specified target energy, the backend identifies the eigenstate whose eigenvalue is closest to that energy and computes the corresponding probability density $|\psi(x, y)|$. This density is plotted as a 2D heatmap over the lattice, allowing users to inspect the spatial structure of quantum states — including whether they are extended across the device (indicative of high transmission) or localized due to disorder. This feature provides complementary insight to the conductance plot, enabling direct correlation between energy-resolved transport properties and spatial wavefunction behavior.

III. Results

Our first simulations focus on 1D chains with increasing disorder. We observe rapid decay of conductance as disorder increases, consistent with Anderson localization. In 2D systems with a magnetic field, we observe the emergence of conductance plateaus due to Landau level quantization. As disorder is introduced, conductance degrades and eventually suppresses the quantum Hall effect. Using the wavefunction viewer, we confirm that high-transmission energies correspond to eigenstates that are spatially extended across the device, while low-transmission energies are associated with strongly localized states, validating the physical origin of transport suppression.

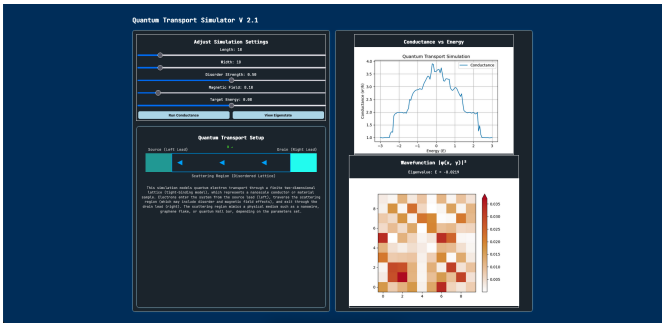

Fig. 3. User interface for adjusting lattice parameters and visualizing conductance and wavefunction plot.

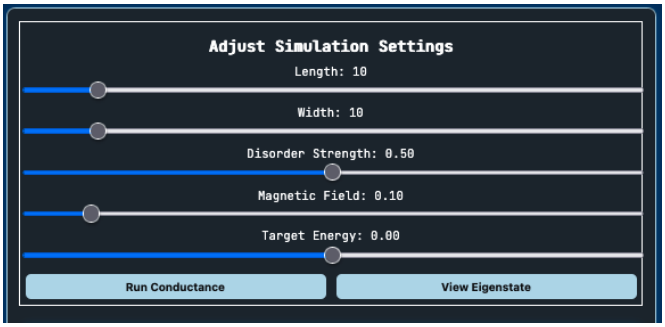

Fig. 4. Interactive simulation panel in the web application frontend. Users specify lattice dimensions, disorder strength, magnetic field, and a target energy to compute both conductance spectra and wavefunction profiles.

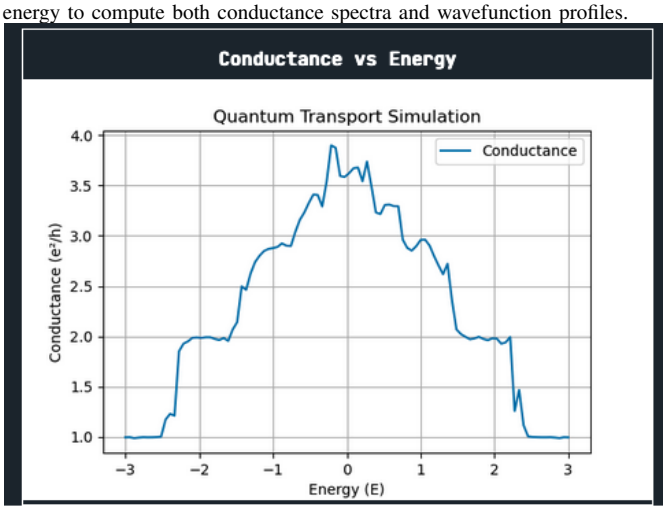

Fig. 5. Simulated conductance vs energy for a 10×10 lattice with disorder strength 0.5 and magnetic field 0.1. The conductance exhibits energy-dependent fluctuations due to quantum interference and partial localization, with multiple transmission channels contributing near the center of the band.

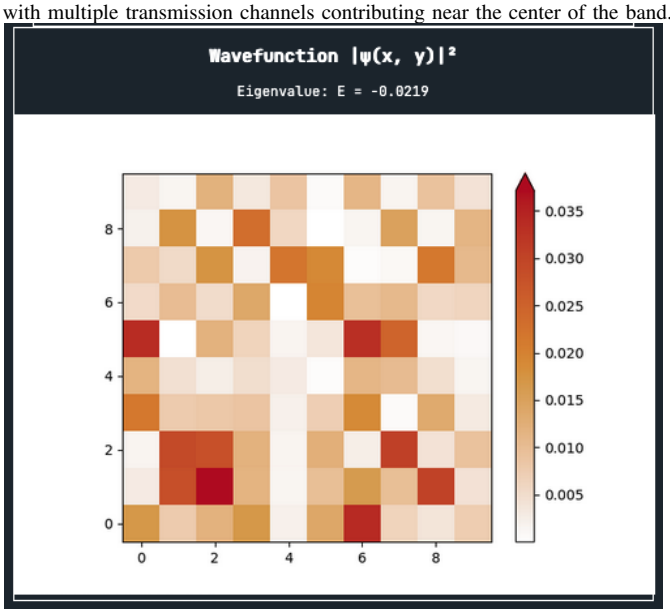

Fig. 6. Spatial probability density $|\psi(x, y)|^2$ of the eigenstate closest to energy $E = 0$, under the same simulation conditions as the conductance plot. The wavefunction is partially delocalized, suggesting moderate transmission at this energy despite the presence of disorder.

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. The wavefunction viewer reinforces these findings by directly visualizing how extended and localized quantum states emerge under different disorder and magnetic field conditions.

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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