A Python-Based Simulation Framework for Visualizing Nanoscale Quantum Transport

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***Abstract*—This research paper aims to examine one-dimensional and two-dimensional Tight Binding Models, and the effects of disorder and magnetic field disruptions on these systems. We propose a software simulation to examine these effects and present a fully functional web application to allow for open inquiry. We intend for this paper to be a beginner's introduction into nanomaterials and quantum physics-related applications in quantum transport. We detail the related Hamiltonians and mathematical equations related to the Quantum Hall Effect and Anderson Localization with rigor.**

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

I. Introduction

Quantum transport in mesoscopic systems presents a fertile ground for both theoretical exploration and applied nanoengineering. Classical models of conduction fail at nanoscales, necessitating quantum mechanical treatments. This paper develops a tight-binding-based simulation tool and web interface for exploring the effects of disorder and magnetic fields on quantum transport in 1D and 2D lattices.

II. Methods

A. Theoretical Framework

The Hamiltonian is the operator that represents the total energy (kinetic + potential) of a quantum system. It allows us to solve the Schrödinger equation:

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

which governs the time evolution of the wavefunction $\Psi(t)$.

The tight-binding model (TBM) approximates electron behavior in solids by assuming electrons are localized on lattice sites and hop between neighboring sites. In 1D, the Hamiltonian is:

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

Here, ε_i is the on-site potential, $c_i^\dagger$ and c_i are fermionic creation and annihilation operators, and t_{ij} is the hopping amplitude.

These operators obey 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 $n_i = c_i^\dagger c_i$ measures the occupancy at site i. The hopping term allows electron motion across sites.

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:

$$H = \sum_{i,j} \varepsilon_{i,j} c_{i,j}^\dagger c_{i,j} - \sum_{\langle (i,j),(i',j')\rangle} t_{(i,j)(i',j')} c_{i,j}^\dagger c_{i',j'} + \text{h.c.} \tag{4}$$

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:

[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:

$$|\psi(x)| \sim e^{-x/\xi} \tag{5}$$

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:

$$t_{ij} \to t_{ij} e^{i\phi_{ij}}, \quad \phi_{ij} = \frac{2\pi}{\Phi_0} \int_i^j \vec{A} \cdot d\vec{l} \tag{6}$$

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

$$E_n = \hbar\omega_c(n + \frac{1}{2}), \quad \omega_c = \frac{eB}{m} \tag{7}$$

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

G. Quantum Transport Formalism

Transport is described by the Landauer formula:

$$G(E) = \frac{e^2}{h} T(E) \tag{8}$$

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

$$T(E) = \text{Tr}(S_{RL}^\dagger S_{RL}) \tag{9}$$

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.

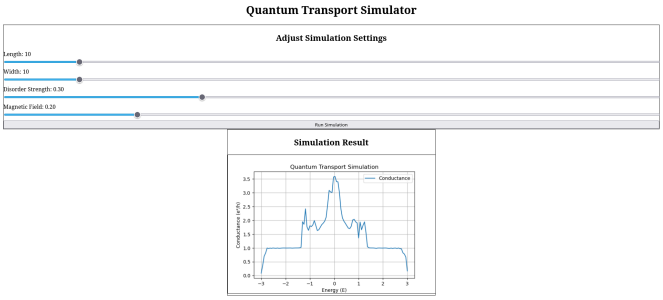

Fig. 1. User interface for adjusting lattice parameters and visualizing conductance.

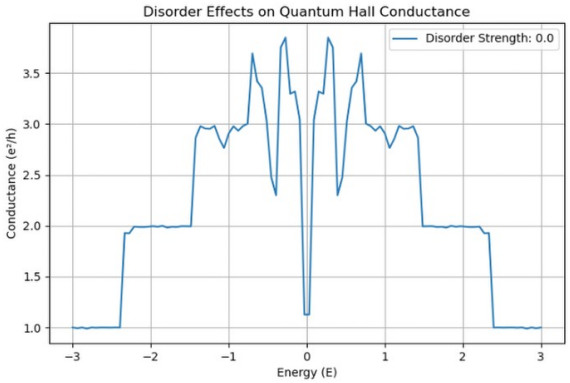

Fig. 2. Sample simulation output: conductance vs energy with disorder strength 0 in the QHE regime.

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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