

Exploring Competing Quantum Effects in Disordered 2D Systems: A Simulation Framework

Senuri Rupasinghe

February 15, 2025

Abstract

This report presents the development and analysis of a quantum transport simulation tool aimed at visualizing conductance in disordered 2D lattice systems under the influence of magnetic fields. By implementing the tight-binding model with Kwant, incorporating Anderson disorder and Peierls phase, and visualizing conductance via the Landauer formula, this project enables interactive exploration of localization and quantized conductance phenomena.

1 Introduction

Quantum transport in mesoscopic systems presents a fertile ground for both theoretical exploration and applied nanoengineering. As devices shrink to nanometer scales, classical approximations of electron behavior break down, and quantum coherence, interference, and tunneling dominate transport behavior.

This project aims to create an intuitive, web-based visualization tool to simulate and observe how disorder (Anderson localization) and magnetic fields (Quantum Hall regime) affect electron transport. We implement a tight-binding Hamiltonian model on a 2D lattice using Kwant, simulate conductance through the Landauer-Büttiker formalism, and enable parameter control via a React.js frontend.

2 Methods

2.1 Theoretical Foundation

Tight-Binding Hamiltonian in 2D

We model a square lattice using a nearest-neighbor tight-binding model:

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

Where:

- ε_i is the on-site energy, randomized to simulate disorder.
- c_i^\dagger, c_i are the fermionic creation and annihilation operators, obeying the Pauli exclusion principle.
- t_{ij} is the hopping amplitude, typically set to 1 (or $e^{i\phi}$ under a magnetic field).

The Pauli exclusion principle is naturally embedded via the anticommutation relations:

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

The number operator $n_i = c_i^\dagger c_i$ gives the occupation at site i , and the kinetic energy arises from hopping terms. The **h.c.** ensures Hermiticity by adding the conjugate term $t_{ji}^* c_j^\dagger c_i$.

Quantum Transport Formalism

The Landauer-Büttiker formalism relates conductance to transmission:

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

Where:

- $T(E)$ is the transmission probability.
- $\frac{e^2}{h}$ is the conductance quantum.

In finite temperature scenarios:

$$G = \frac{e^2}{h} \int T(E) \left(-\frac{\partial f(E)}{\partial E} \right) dE$$

Where $f(E)$ is the Fermi-Dirac distribution. Kwant computes $T(E)$ via the scattering matrix S :

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

Disorder: Anderson Localization

We model disorder with a uniformly distributed random on-site energy:

$$\varepsilon_i \in [-W, W]$$

Disorder causes exponential localization of wavefunctions, hindering transport:

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

Where ξ is the localization length.

Magnetic Field: Quantum Hall Effect

We incorporate magnetic field via the Peierls substitution:

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

For a constant perpendicular field in the Landau gauge $\vec{A} = (0, Bx, 0)$, the phase becomes:

$$\phi_{ij} = 2\pi Bx$$

This results in quantized Landau levels:

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

which manifest as conductance plateaus in transport.

Information on Transport Regions

- **Left Lead:** Source of coherent electrons.
- **Scattering Region:** Central region with disorder/magnetic effects.
- **Right Lead:** Acts as electron drain.

Note on 1D vs 2D

In 1D, any nonzero disorder causes Anderson localization. In 2D, the situation is richer: a magnetic field introduces topological effects like Landau levels and edge states, yielding quantized transport behavior.

2.2 Software Implementation

Backend: Built with FastAPI. Kwant simulates the quantum system and computes the conductance over a range of energies. Plots are returned as base64-encoded PNGs.

Frontend: Built with Vite + React.js + TailwindCSS. Users can adjust simulation parameters (lattice size, disorder, magnetic field) via sliders and observe updated plots.

Tech Stack:

- Python, Kwant, NumPy, Matplotlib
- FastAPI (Backend API)
- React.js, TailwindCSS (Frontend UI)

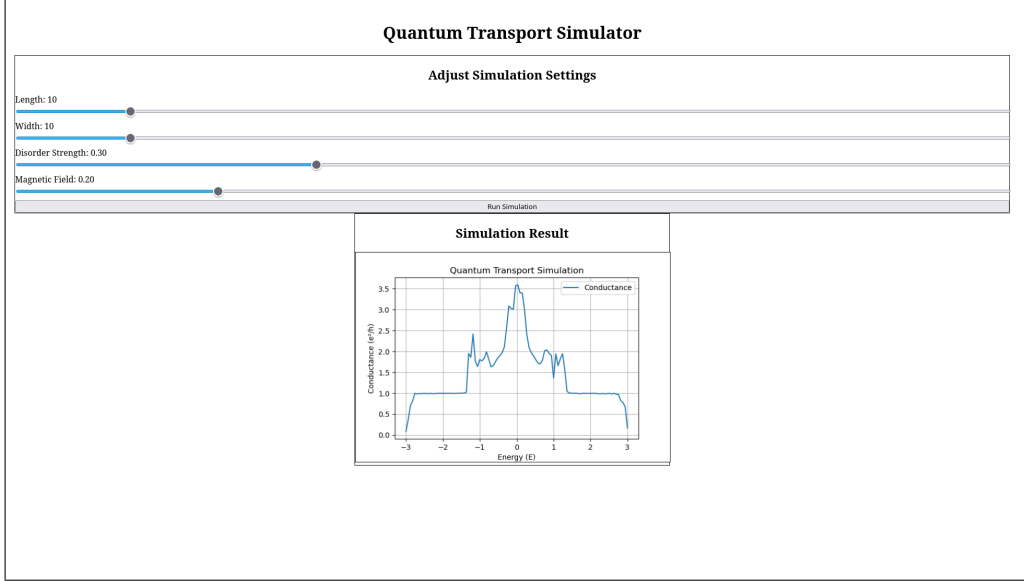


Figure 1: Frontend interface for interactively configuring simulation parameters and viewing conductance plots.

3 Results

Example plots from the simulation show:

- **Clean system:** Smooth conductance profile with peaks near the band edges.
- **Disordered system:** Fluctuations and suppression of conductance due to localization.
- **Magnetic field:** Formation of quantized plateaus and conductance spikes (Quantum Hall effect).
- **Combined effects:** Interplay between disorder and field strength modulates transport properties.

4 Discussion

The combination of theoretical modeling and interactive visualization helps demystify concepts like:

- Role of phase coherence in quantum transport.
- Why disorder localizes wavefunctions (exponential decay).
- How magnetic field introduces chirality and topological effects.

The simulation reproduces known physical behaviors such as Anderson localization and the emergence of Landau levels, making it useful for educational and research purposes.

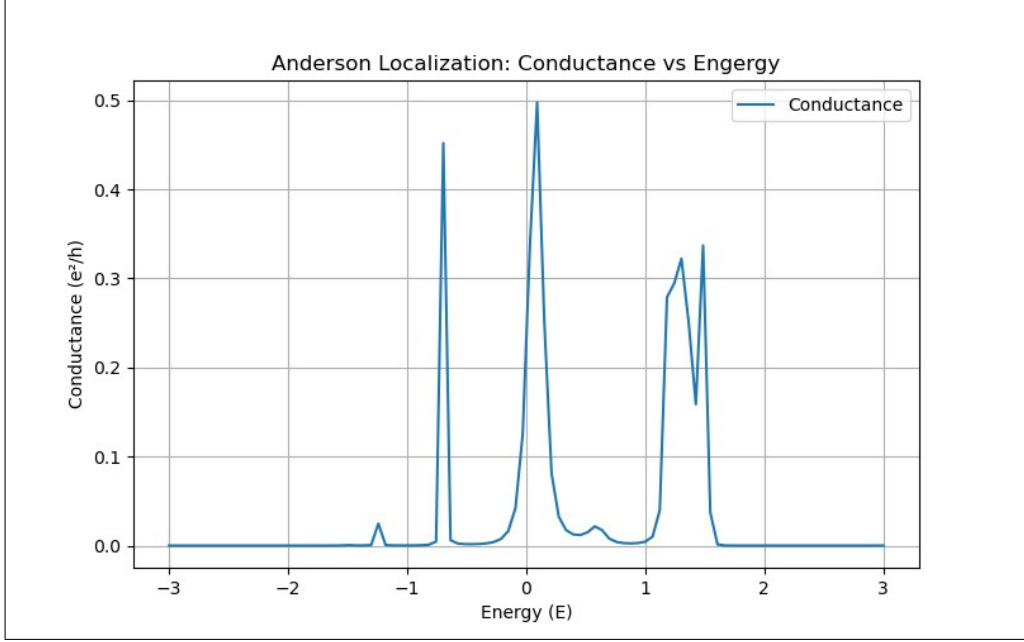


Figure 2: Anderson Localization in 1D.

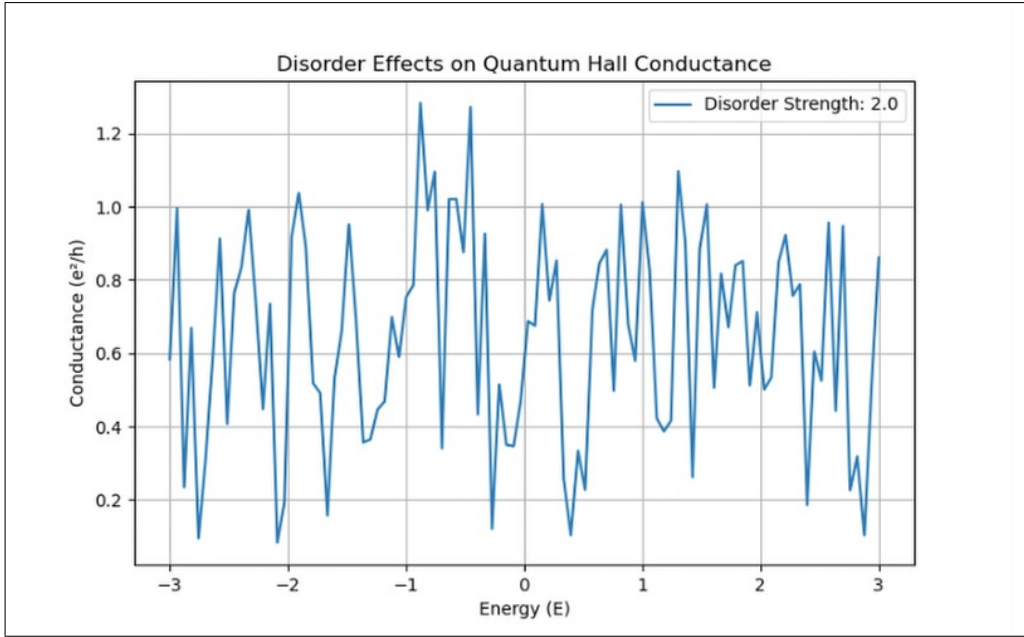


Figure 3: Competing Effects: Disorder in Quantum Hall Effect

5 Conclusion

We presented a quantum transport simulation platform enabling exploration of tight-binding systems under the effects of disorder and magnetic fields. Through visualization and tunable parameters, users can gain intuitive understanding of key quantum phenomena. This tool lays a foundation for extensions to more exotic lattice geometries (e.g., graphene), interac-

tions, or time-dependent dynamics.

References

1. S. Datta, *Electronic Transport in Mesoscopic Systems*, Cambridge University Press.
2. M. Z. Hasan and C. L. Kane, “Colloquium: Topological insulators,” *Rev. Mod. Phys.* 82, 3045 (2010).
3. Kwant Documentation: <https://kwant-project.org/doc/1.4/tutorial>
4. D. J. Thouless et al., “Quantized Hall Conductance in a Two-Dimensional Periodic Potential,” *Phys. Rev. Lett.* 49, 405 (1982).