Hofstadter Butterflies and Anderson Localization in 2D Lattices

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Motivation & Goals

- Study 2D materials and common Euclidean lattice structures
- Simulate magnetic field effects
- **Motivation**: Existing tools, i.e. HofstadterTools, are limited and difficult to interpret

Goal: Create generalizable code for physically realizable 2D lattice simulations

Introduction: Theory

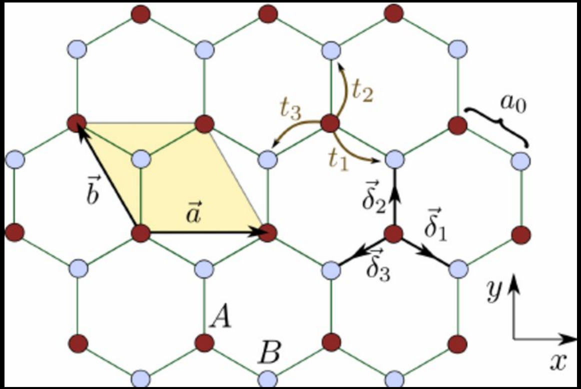
Suppose we take an atom

→ orbitals are eigenfunctions of corresponding Hamiltonian

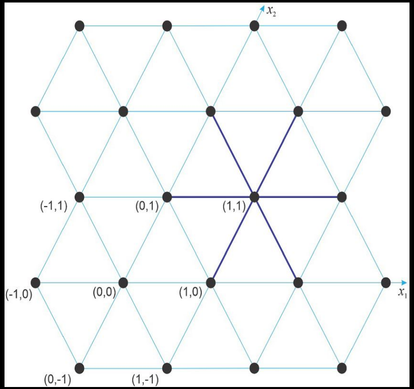
But what if we configure our atom with other atoms in a crystalline structure?

→ *How do we describe the energy of this system?*

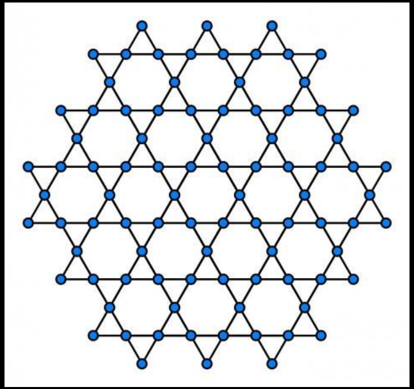
Introduction: 2D Lattices



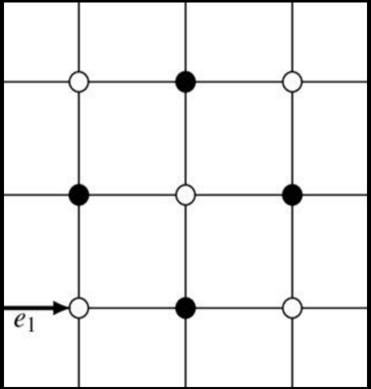
Honeycomb



Triangular



Kagome



Square

Tight-Binding Model

- **Tight-Binding Hamiltonian:** Describes lattices in absence of external interactions while accounting for hopping

$$H = \underbrace{\omega_0 \sum_i a_i^\dagger a_i}_{\text{all latice sites}} - \underbrace{t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i)}_{\text{hopping between nearest neighbors}}$$

Anderson Localization: Theory

What happens if our lattices become disordered?

- If system passes a disorder threshold,
  - certain materials may undergo a phase transition from conductor to insulator
  - electronic wavefunctions become localized and exponentially decay — they're essentially trapped because of constructive interference

$$\psi(x)\ e^{-x\,/\,\eta}$$

- Anderson Hamiltonian: Describe electron localization

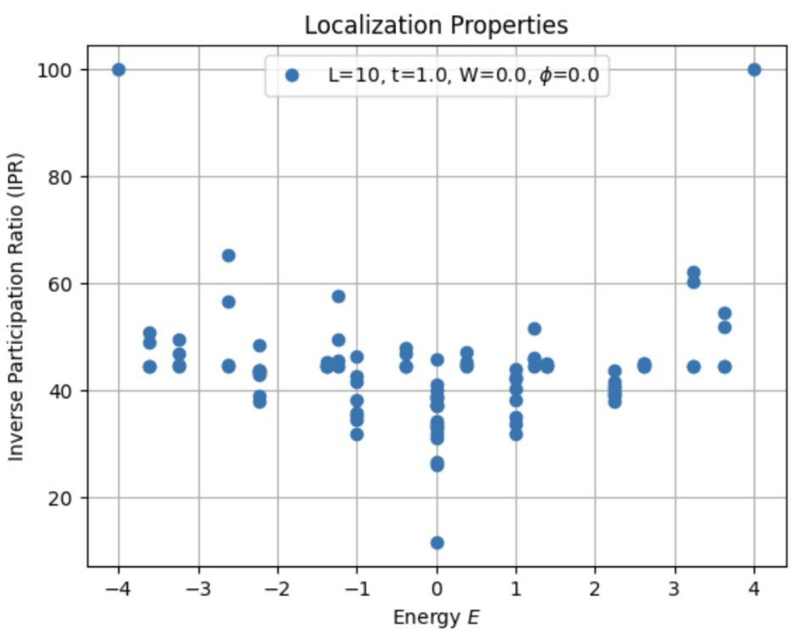
$$H = W\sum_{n}(\epsilon_n c_n^{\dagger} c_n) + t\sum(c_n^{\dagger} c_m + h\,.\,c)$$

Inverse Participation Ratio (IPR)

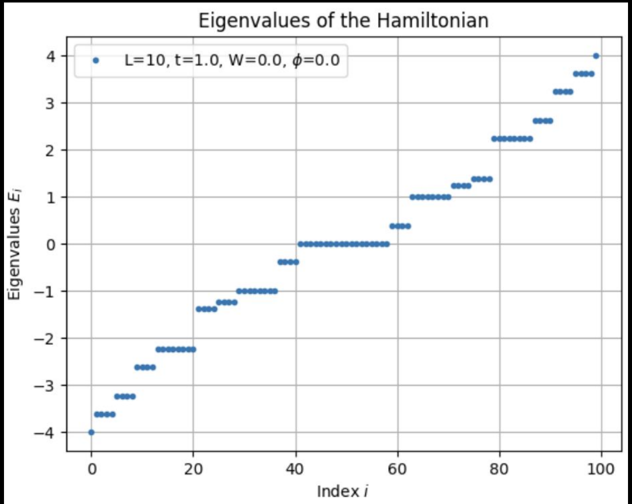
- **IPR**: Estimate of localization length

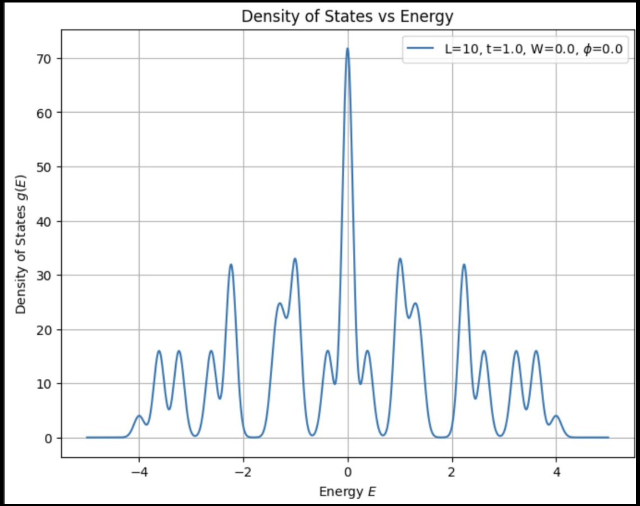
Recall: $\psi(x)\ e^{-x\,/\,\eta}$

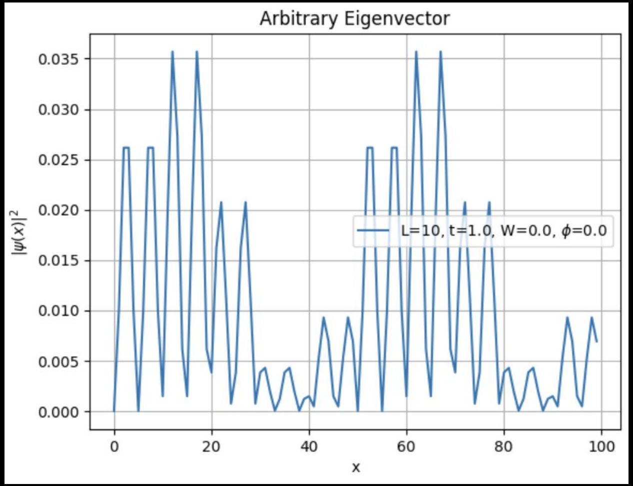
$$IPR = \frac{(\sum_x |\psi(x)|^2)^2}{\sum_x |\psi(x)|^4}$$



For square lattice


Eigenvalues of the Hamiltonian
L=10, t=1.0, W=0.0, ϕ=0.0
Eigenvalues E_i
Index i


Density of States vs Energy
L=10, t=1.0, W=0.0, ϕ=0.0
Density of States $g(E)$
Energy E


Arbitrary Eigenvector
L=10, t=1.0, W=0.0, ϕ=0.0
$|\psi(x)|^2$
x

Hofstadter Butterflies: Theory

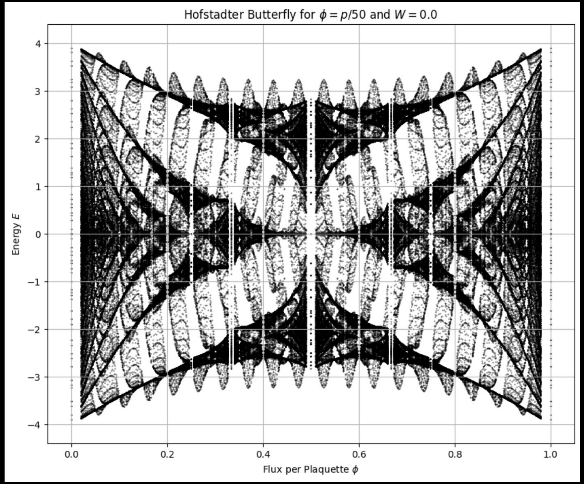
What happens when we apply a perpendicular, uniform magnetic field onto a lattice?

- Peierls phase
  - Accounts for: Magnetic flux through each plaquette; relevant changes in boundary conditions

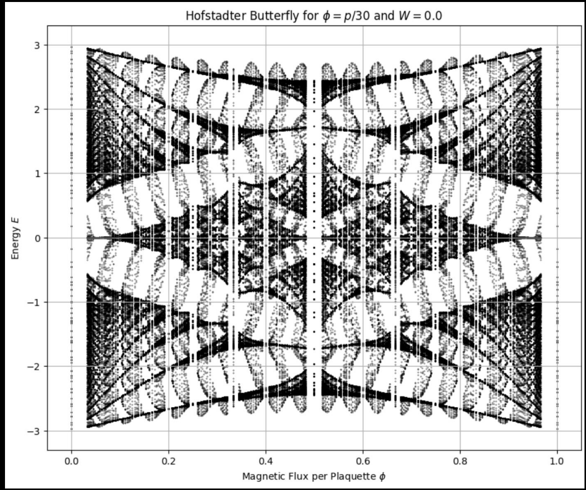
- Magnetic flux ratio: $\Phi = p / q$
  - p and q are coprime integers
  - Plot of energies as function of Φ leads to fractal pattern!

Hofstadter Butterflies: Results

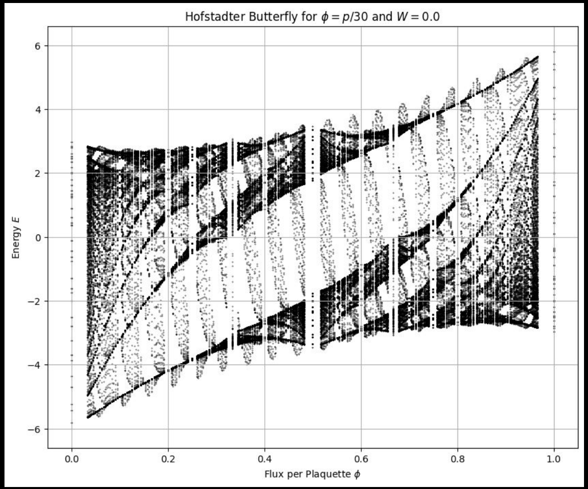
- Method:
  - Choose max value for q
  - Iterate through all coprime p, q pairs up to q_{max}
  - Reconstruct hamiltonian for each consequent Φ



Square lattice



Honeycomb lattice



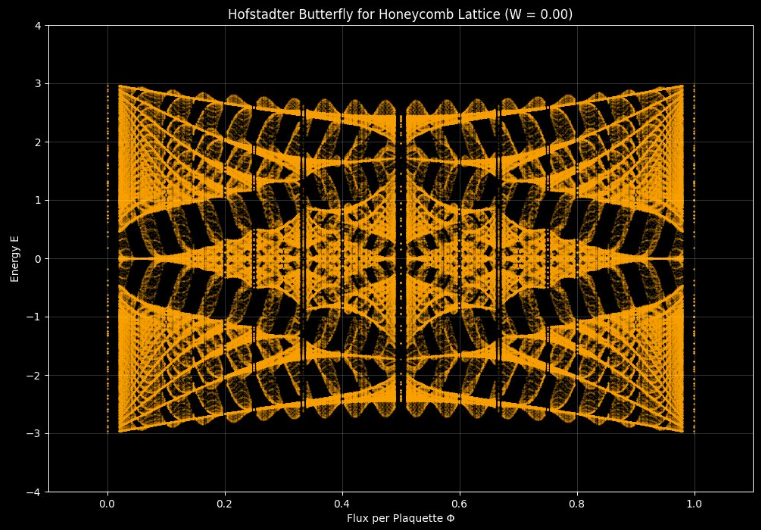
Triangular lattice

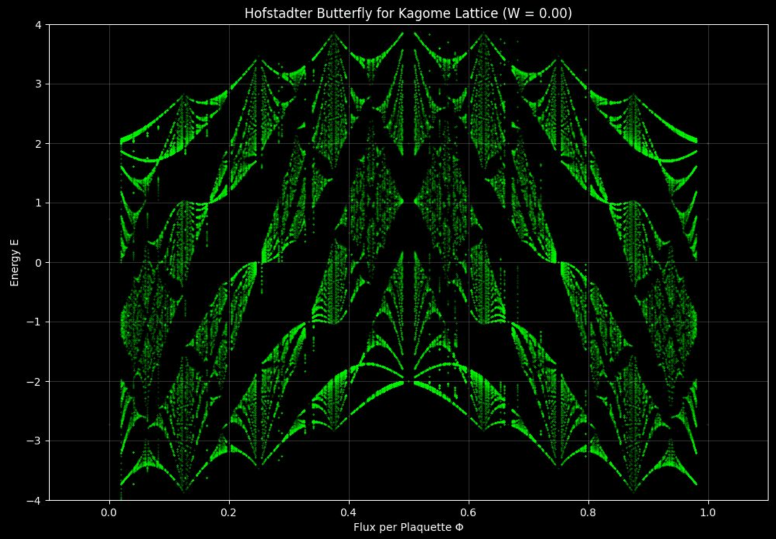
Plots were verified with the literature

Hofstadter Butterflies: Disorder

- **Interesting Result:** Presence of disorder kills the butterfly structure which has been observed in the literature

In the high-disorder limit, some butterfly-like pattern may persist





Summary

- <u>Achievements</u>: simulate basic tight-binding hamiltonians specific to the most common, physically realizable 2D lattice types found in materials
  - **No reliance on crystal momentum** → extend code to cases where Bloch's theorem no longer holds
  - Support for **magnetic field** → may investigate quantum hall effect
  - Visualize effect of **disorder** on butterfly structure

- <u>Potential applications:</u>
  - Simulating graphene (twisted-bilayer graphene)
  - Hyperbolic Circuit QED
  - Realizing the quantum hall effect in moiré materials

Future Directions

- Support for hyperbolic cases
- Open boundary conditions
- Extensions for quantum hall effect
- Additional parameters for specific materials

Questions?

Thank you Dr. William Gilpin and course staff for support throughout the semester!