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The University of Texas at Austin

HOW TO TRAIN YOUR ELECTRON

Anderson localization on the lattice & random graphs

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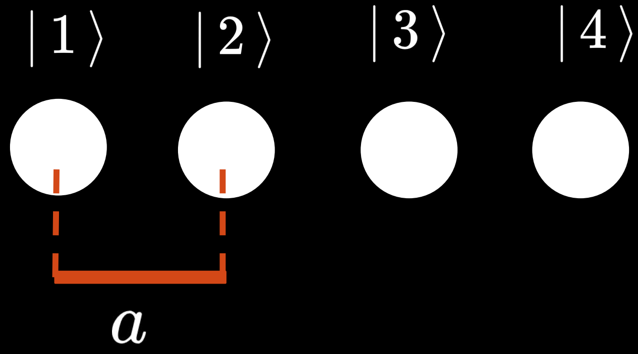
The Tight Binding Model

- **Goal:** understand how an electron behaves in a material
- For simplicity, think of an electron on an atomic ring:
  - The n$^{\text{th}}$ atom has a single orbital, labelled $|n\rangle$
  - We represent the wavefunction in the site basis
  - The electron can hop between nearby sites



Simon, Steven. “Solid State Basics,” *Oxford University Press*, 2013.

The Tight Binding Hamiltonian

- The tight binding hamiltonian:

$$\langle n|H|m\rangle = H_{n,m} = \underbrace{\epsilon_0 \delta_{n,m}}_{\text{binding}} \underbrace{- t(\delta_{n+1,m} + \delta_{n-1,m})}_{\text{hopping}}$$

- where ϵ_0 refers to the energy at a site and *t* is the hopping parameter
- Hamiltonian ~ Time Evolution
- This is typically diffusive!!

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Numerical Approach

- Given a hamiltonian, we can time evolve the wave function:

$$|\psi(t)\rangle \;=\; \exp\left(-iHt/\hbar\right)|\psi(0)\rangle$$

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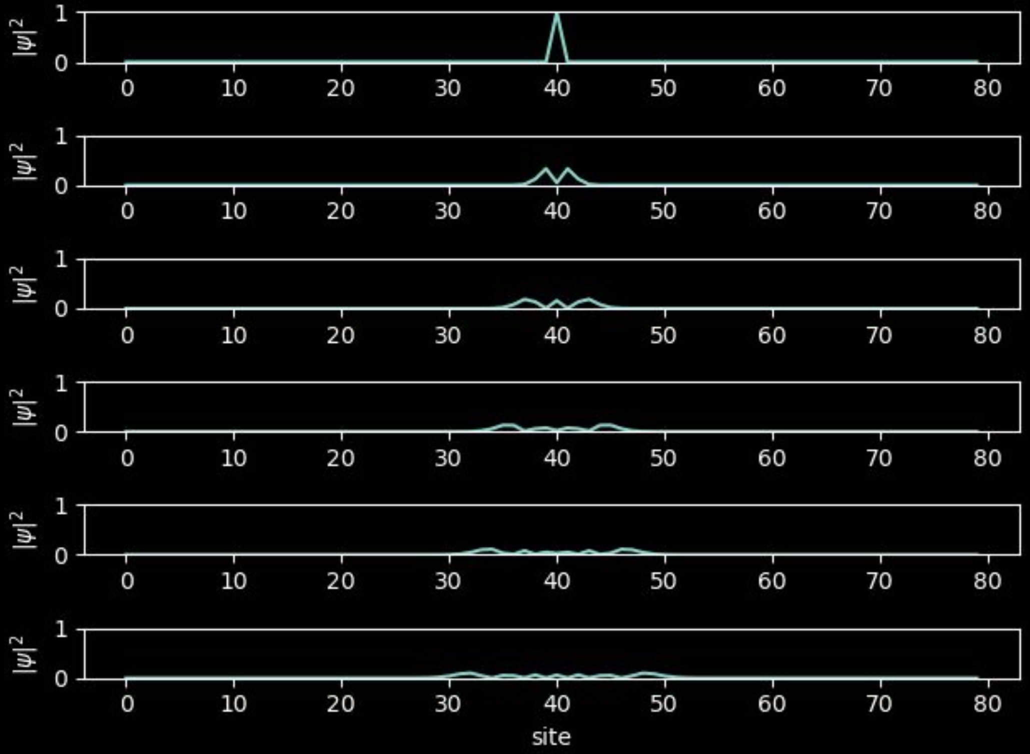

Anderson Localization

- **Counterintuitively, we can get localization by modifying tight binding.**

$$\langle n|H|m\rangle = H_{n,m} = \underbrace{\epsilon_0 \delta_{n,m}}_{\text{binding}} \underbrace{- t(\delta_{n+1,m} + \delta_{n-1,m})}_{\text{hopping}}$$

- Key idea: randomly sample values of ϵ from a uniform distribution from [-*W*, *W*]
  - Randomizing the diagonal of *H*
  - Represents a disordered material
  - Larger *W* = more localized

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Anderson Localization on the Ring

$W = 0$ $W = 10$

Anderson Localization on a Graph

- We can identify the hopping term with the adjacency matrix of a graph

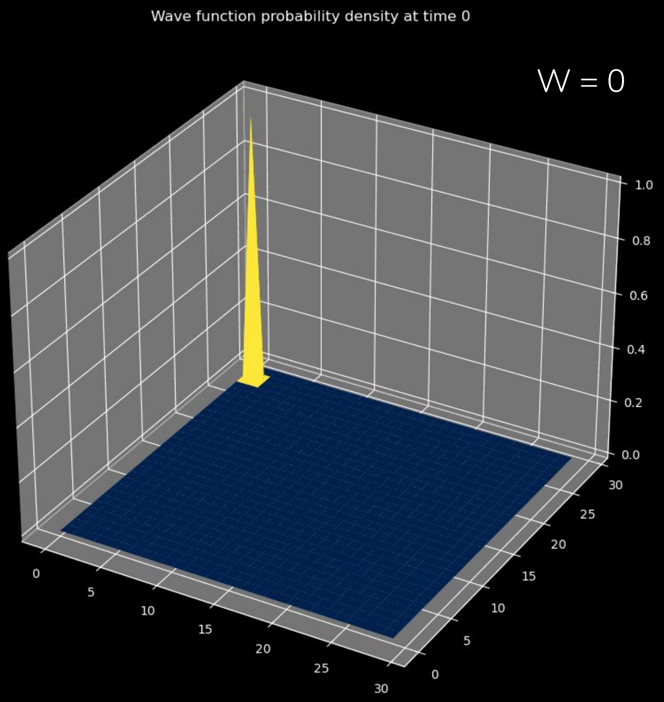
$$\langle n|H|m\rangle = H_{n,m} = \underbrace{\epsilon_0\delta_{n,m}}_{\text{binding}} \underbrace{- t(\delta_{n+1,m} + \delta_{n-1,m})}_{\text{hopping}}$$

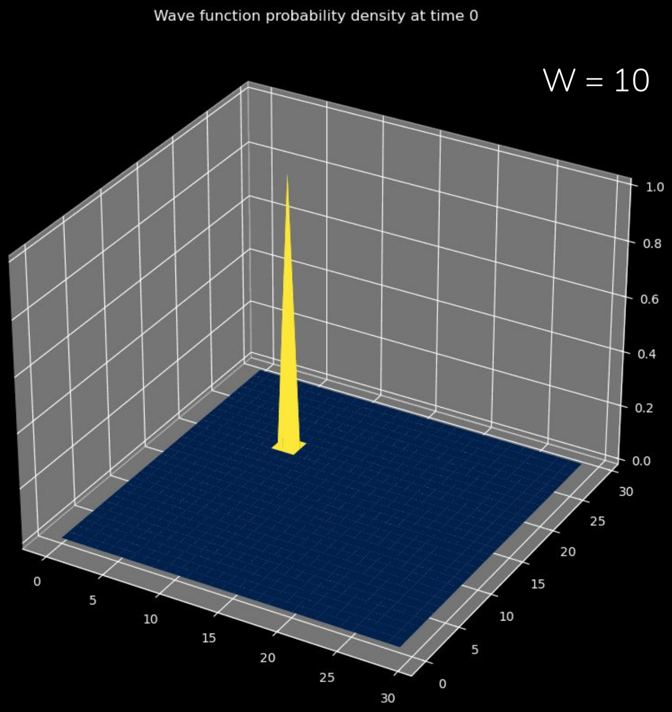
- This allows us to extend to more interesting configurations*

*we assume periodic boundary conditions

Anderson Localization on a Periodic Lattice

- Consider a 2D lattice with periodic boundary conditions.
- For low W, the wave function diffuses. For high W, we see localization



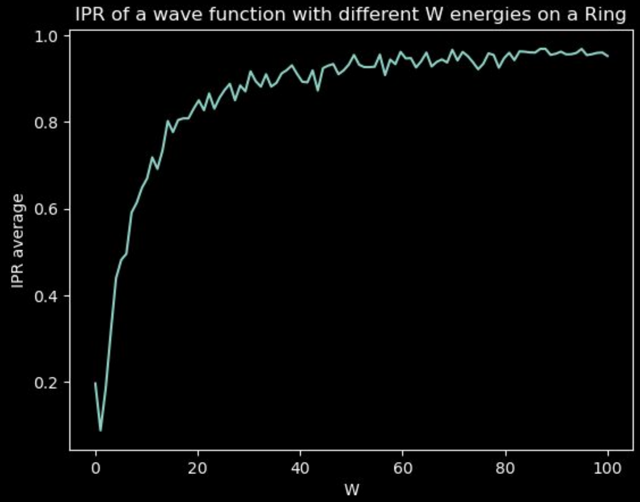


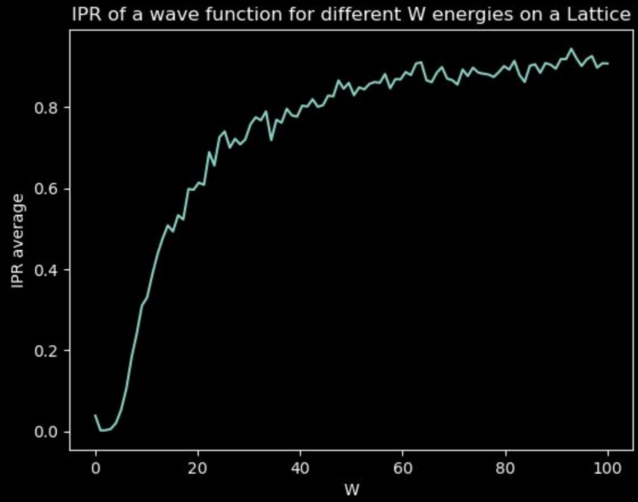
Inverse Participation Ratio (IPR)

- IPR is a rough measure of localization. IPR of 1 means fully localized.

$$IPR = \sum_n |\psi(n)|^4$$

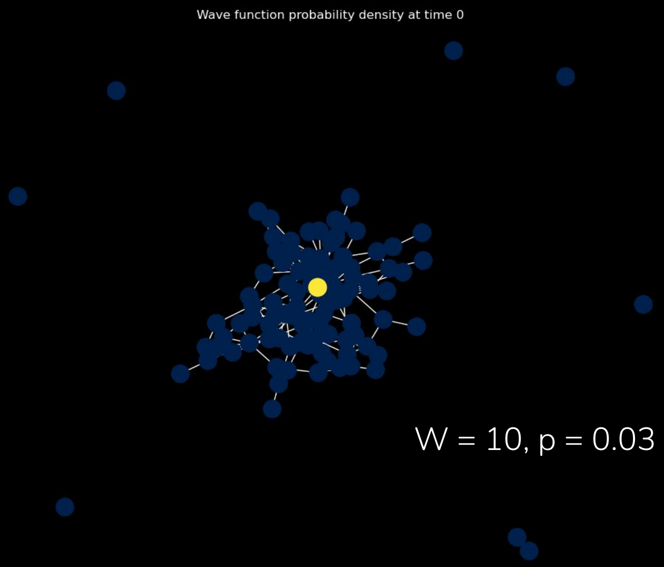
- As W increases, the localization also tends to increase.



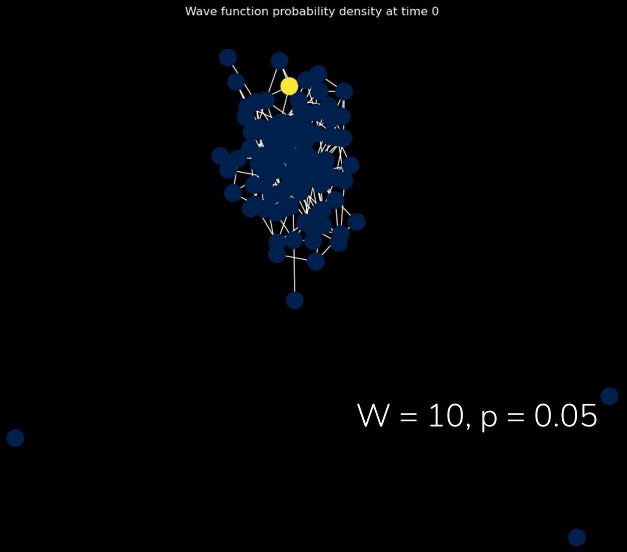


Random Graphs

- We generalize even more by simulating the behavior of a wave function on Erdős–Rényi graphs (where you're given a node set and each possible edge is generated with probability p)



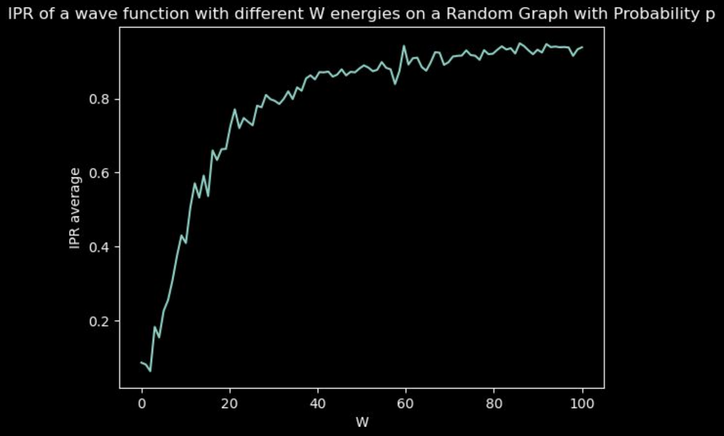
W = 10, p = 0.03

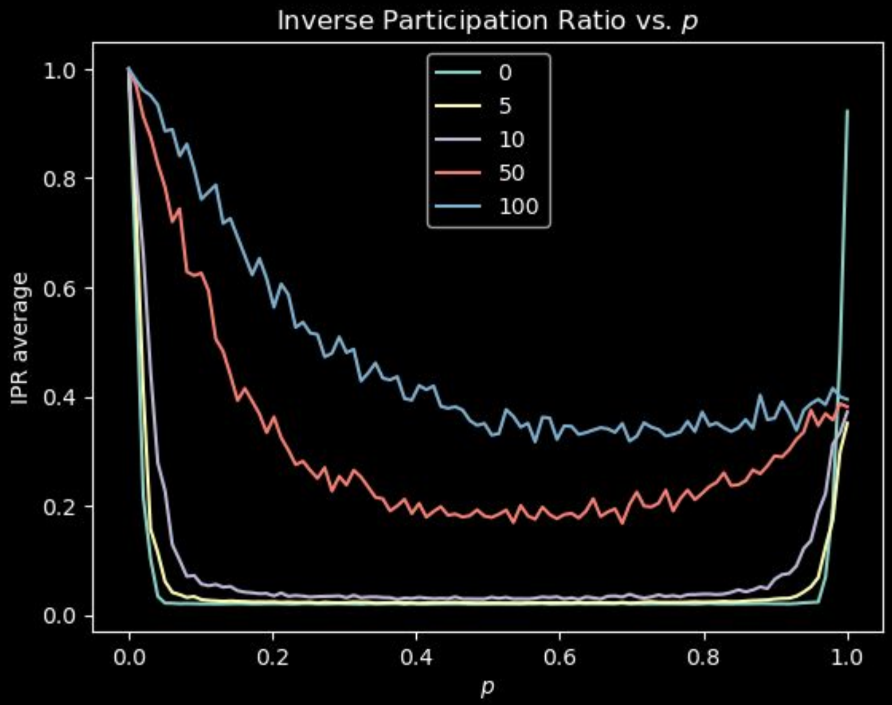


W = 10, p = 0.05

IPR vs. p for different W values

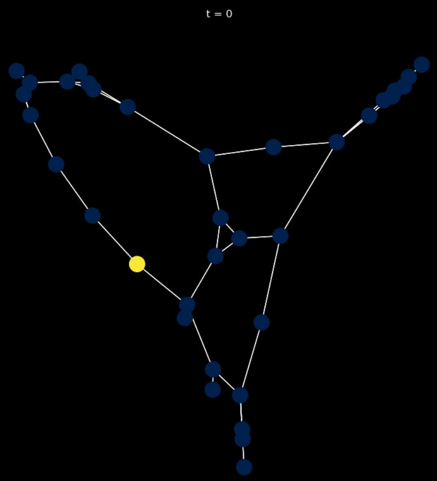
- It's harder to see localization for random graphs, so we lean on IPR more heavily.
- We're interested in how localization changes as the graph becomes more connected (i.e. p increases).



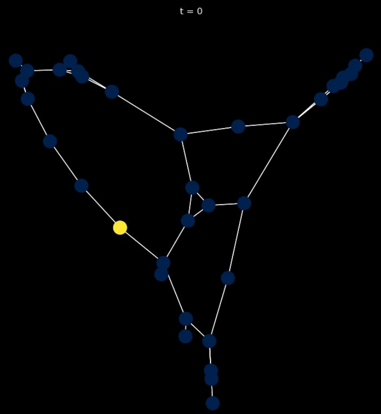


Sparse Graphs

- In a restricted domain, do structural (e.g., symmetry) properties of the graph influence localization parameters?



W = 0



W = 18.7

Future Directions

- Correlating & extending analytical predictions made for regular random graphs to specific properties of adjacency matrices.
- Why does the IPR vs. W graph dip in the beginning instead of just increasing?
- Why does the IPR vs. p graph increase at the end?
- Investigate time-dependence of IPR, e.g. test whether noise in IPR vs. W graph disappears over IPR averaged over multiple time points
- Investigate different boundary conditions and connections between nodes

Questions?

- Thank you Dr. Gilpin, Anthony, and Edoardo for the fun semester!