Effects of Weak Disorder on Electron Diffusion in 2D Lattices

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Background

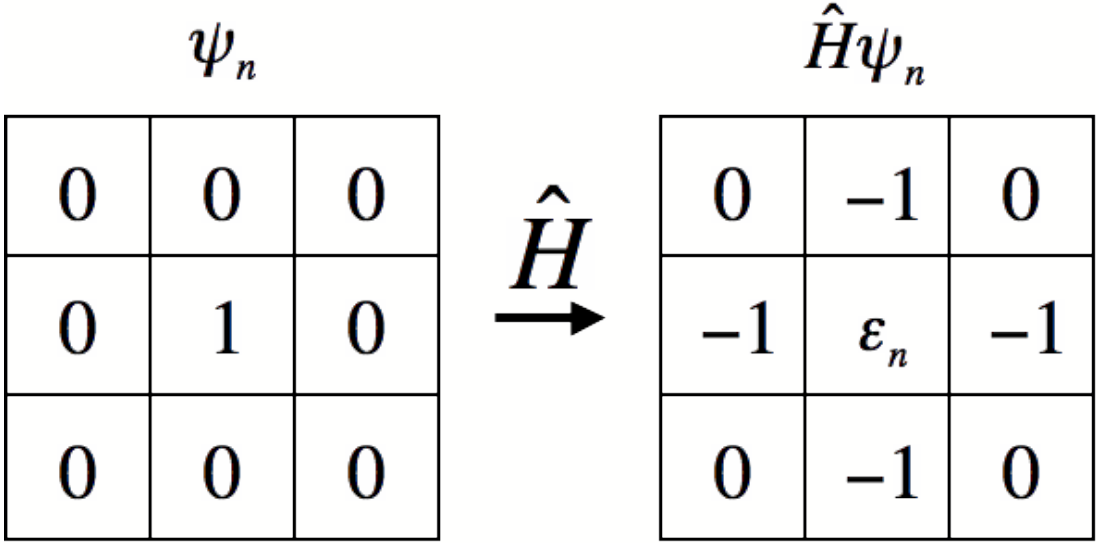
- In 1958, P. W. Anderson showed that for a lattice with strong disorder there is an absence of diffusion. (localized states)
- In a one dimensional chain, any amount of disorder produces localized states.
- The behavior of electrons in 2D without strong disorder is unclear.

Motivation

- Semiconductor is like a weakly disordered lattice.
- Localized states correspond to less conduction.
  - Conductors have extended electron states, and go to finite conductivity at low temperature.
  - Insulators have localized states, and go to zero conductivity at low temperatures.
- Scaling theory suggests that all disordered states in a 2D lattice are localized, but we have found 2D conductors.
- Does any amount of disorder result in localized states?

The Model

- We have a single electron and a 2D square lattice, with the wavefunction of the electron defined at every site of the lattice.
- Our Hamiltonian is a hopping matrix.



- How do electron's behave in this system?

Strategy

- The space we are considering is infinite, and we have infinitely many eigenstates, so we cannot use the standard method of analysis.
- Instead, we try to calculate the tridiagonal matrix representation of the Hamiltonian, using the Lanczos Algorithm.
  - Tridiagonal matrix has many useful properties, including the fact that it's eigenvalues approach eigenvalues of the Hamiltonian.
- Lanczos Algorithm only requires the original matrix and an initial state to produce an orthonormal basis and approximate eigenvalues.

Lanczos Algorithm Pt. 1

- In order to generate an orthonormal set of wavefunctions $(\psi_0, \psi_1, \psi_2, ..., \psi_N)$, we use the recursive relation:

$$\hat{H}\psi_n = -b_{n-1}\psi_{n-1} + a_n\psi_n - b_n\psi_{n+1}. \tag{1}$$

- Thus, $a_n = \psi_n \hat{H} \psi_n$, and $b_{n-1} = -\psi_{n-1}\hat{H}\psi_n$.
- This provides us with an algorithm, where we can determine the tridiagonal matrix for the Hamiltonian.

Lanczos Algorithm Pt. 2

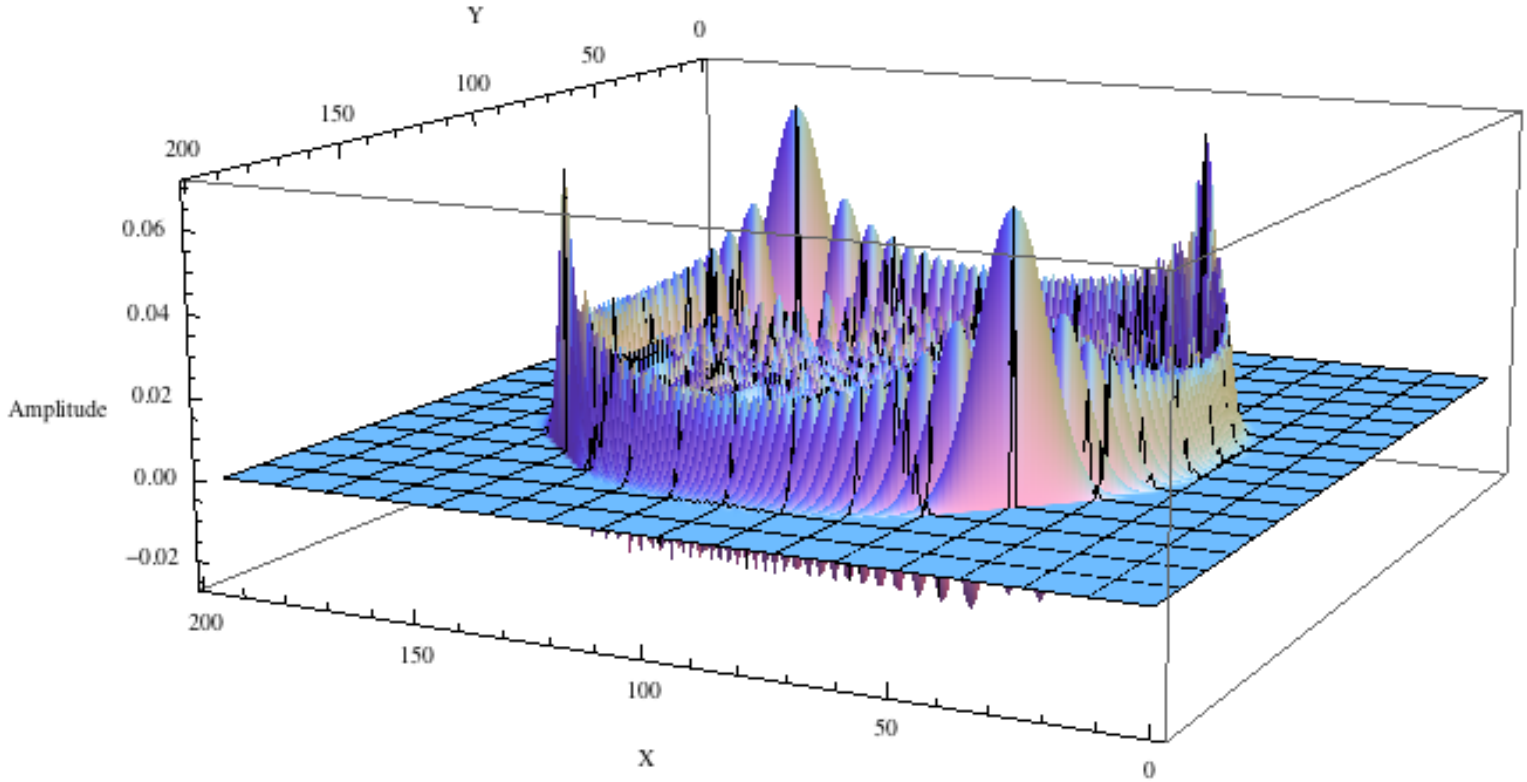
- We start with an initial state ψ_0 for which the wavefunction is zero everywhere, representing no electron, and ψ_1, where the wavefunction is all located at the origin of the lattice.
- With the a_n and b_n generated from these initial states, we get the tridiagonal matrix.

$$\begin{pmatrix} a_1 & b_1 & \cdots & 0 & 0 \\ b_1 & a_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & a_{N-1} & b_{N-1} \\ 0 & 0 & \cdots & b_{N-1} & a_N \end{pmatrix} \tag{2}$$

Simple Case Pt. 1

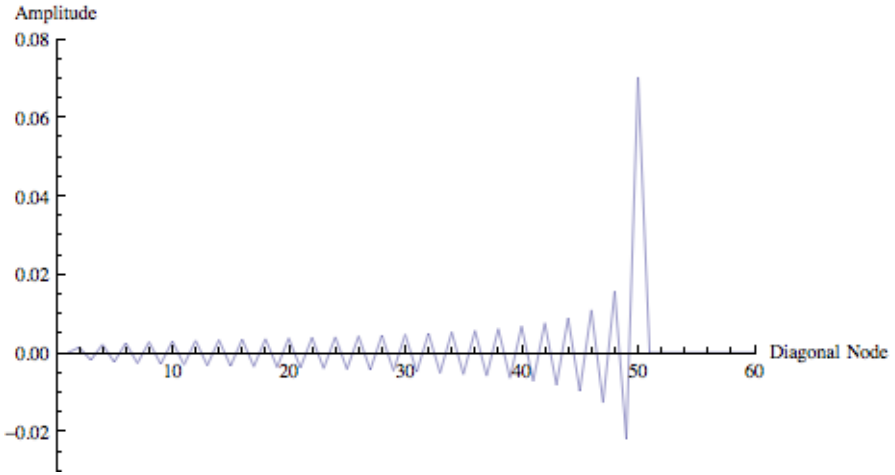
What if we consider the case of no disorder?

- The sequential ψ_n have the following behavior:

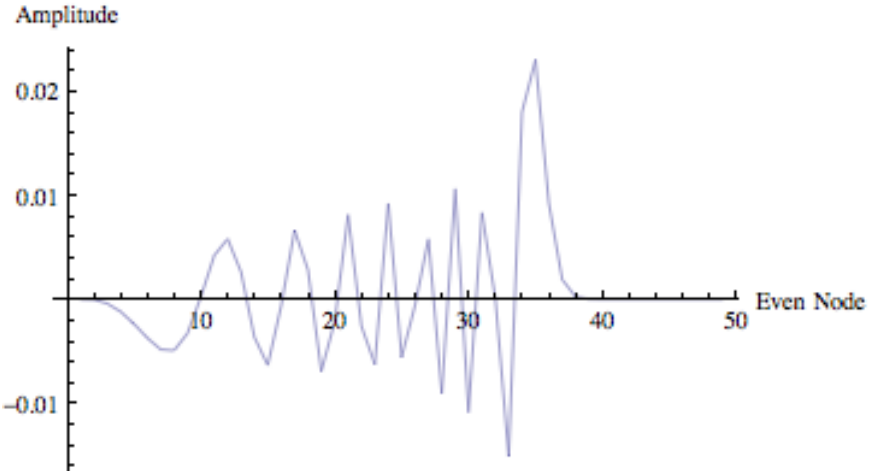


Simple Case Pt. 2

- The amplitude along the diagonal is an analytically derivable oscillating function, with a maximum at the edge of the support.



- The amplitude along the axes peaks at approximately $\frac{1}{\sqrt{2}}$ the way to the edge of the support.



Simple Case Pt. 3

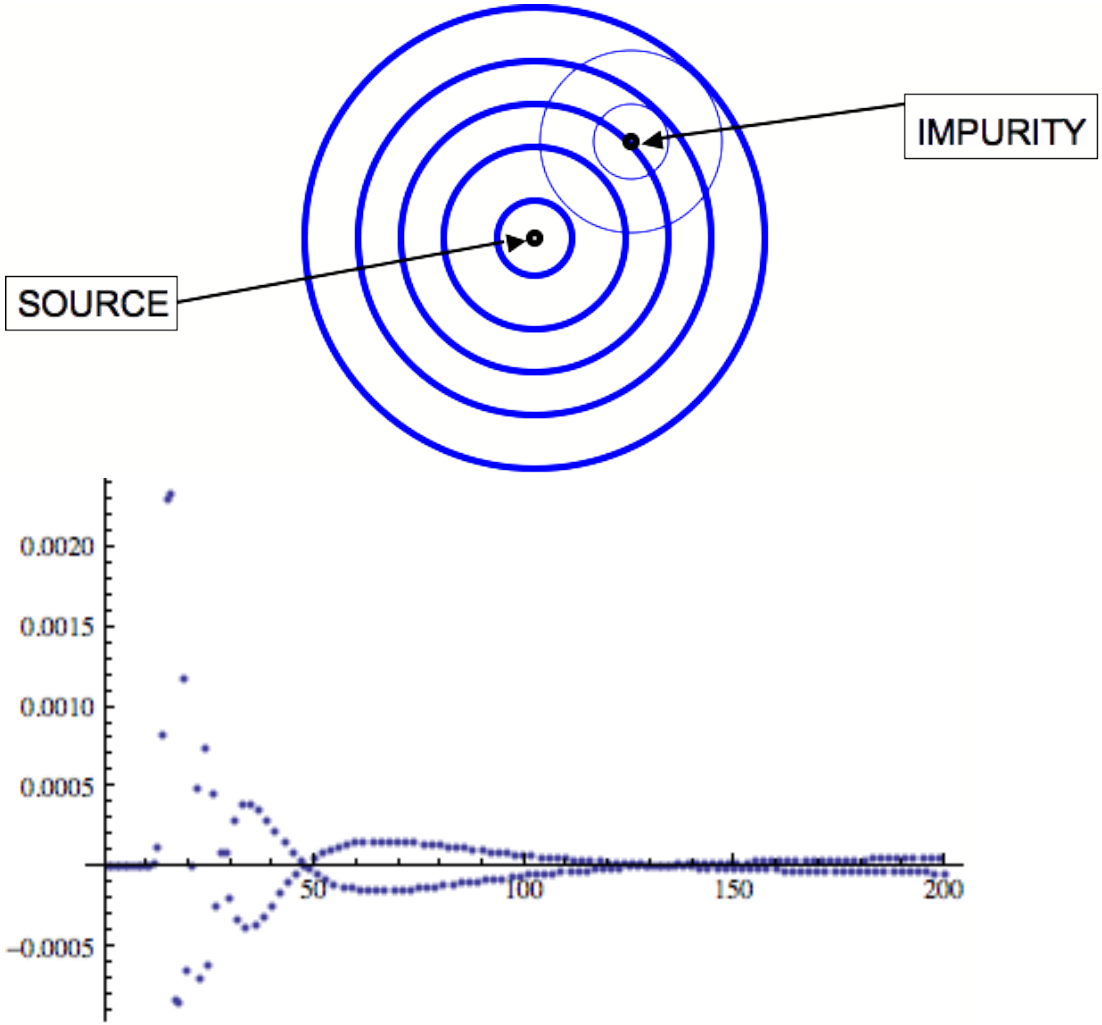
The tridiagonal becomes simple.

- $b_n = 2$ and $a_n = 0$ for all n.

$$\begin{pmatrix} 0 & 2 & \cdots & 0 & 0 \\ 2 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 2 \\ 0 & 0 & \cdots & 2 & 0 \end{pmatrix} \tag{3}$$

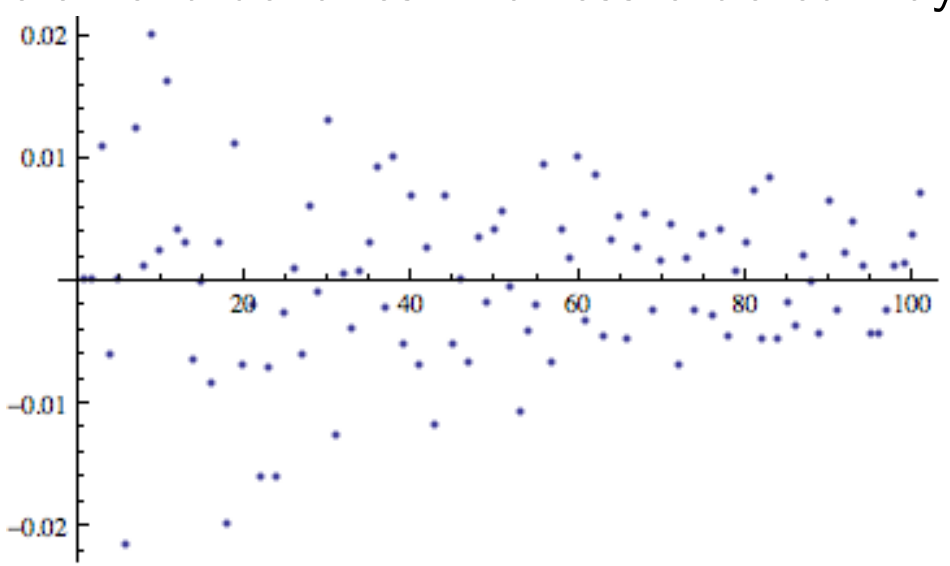
A Single Impurity

- Introduce an energy ϵ_i at the a single site.
- You can view the resulting disorder as scattering of the wave-front off of that impurity.
- The disorder from the impurity manifests as a spike in the diagonal element of the tridiagonal matrix, which decreases over sequential iterations.



Uniform Random Disorder

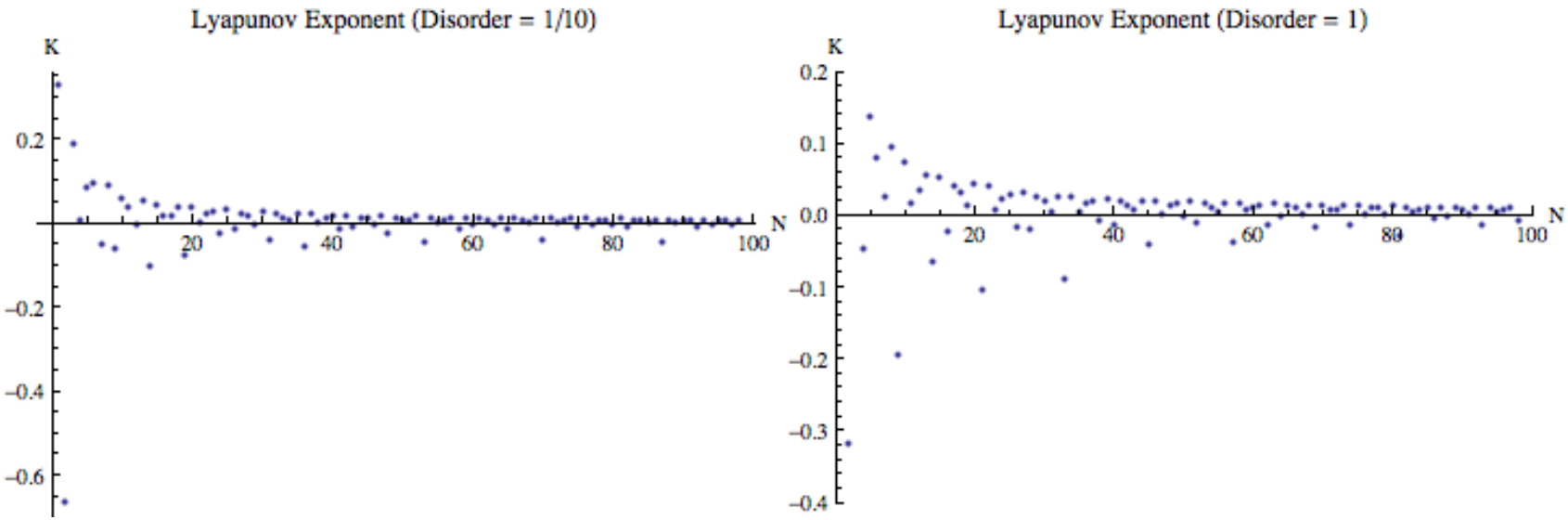
- We introduce a bounded random disorder ϵ_n at every point.
- Can be viewed as a sum of the effects caused by individual sites if considering small disorder.
- If we select ϵ_n within the region $(-\frac{1}{10}, \frac{1}{10})$, the diagonal element behaves in a less ordered way.



Lyapunov Exponent

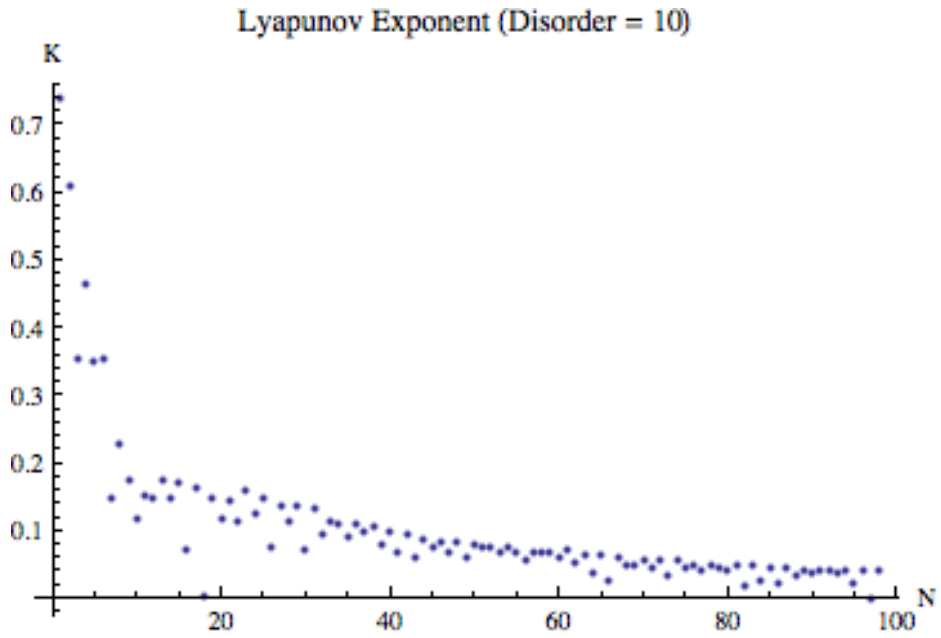
- $R_{1,N}(E) = \frac{\prod_{i=1}^{N-1} b_i}{det(EI - T^N)}$ is the upper right corner element of the Green matrix, which is the inverse of $(EI - T^N)$.
- $R_{1,N}(E)$ represents the probability amplitude of an electron with energy E tunneling across the support.
- $\kappa = -\frac{1}{N} ln|\frac{\prod_{i=1}^{N-1} b_i}{det(T^N - E*I)}|$ is the Lyapunov exponent.
- For extended states, $\kappa \longrightarrow 0$ as $N \longrightarrow \infty$.
- For localized states, κ trends to a number greater than zero as $N \longrightarrow \infty$.

Interim Results



Interim Results

- Localization is only obvious for relatively high disorder.



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