Application of the Lanczos Algorithm to Anderson Localization

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Effect of Impurities in Materials

- Naively, one might expect that gradually increasing the number of impurities (i.e. disorder) in a material would cause a proportional decrease in conductivity.

- But there is no a priori reason that phase transitions will not occur.

- P. W. Anderson argued in a famous 1958 paper, for which he won the 1977 Nobel prize, that a transition to zero conductivity occurs at a critical disorder at which all electron wavefunctions become localized.
Tight-Binding Model

- **Setting:** $d$-dimensional lattice (finite or infinite)
- **Hamiltonian:**
  - *Dynamics:* Constant hopping probability $h$ to nearest neighbor sites
  - *Disorder:* Random onsite potential $\epsilon_r$ chosen from uniform distribution $[-W/2, W/2]$

$$H = h \sum_{r \in \mathbb{Z}^d} |r\rangle \langle r'| + \sum_{r \in \mathbb{Z}^d} \epsilon_r |r\rangle \langle r'|$$

- **Solutions:**
  - *Case of no disorder:* Solutions are given by Bloch's theorem

$$\psi(r) = \sum_{r \in \mathbb{Z}^d} e^{ik \cdot r} |r\rangle$$
With Disorder: Localization

“Sufficient” disorder causes eigenstates to become exponentially localized in space:

Questions:
- What does “sufficient” mean?
- Dependence on hamiltonian?
- Experimentally detectable?

Approaches to Study of Localization:
- Green's functions
- Field theory
- Numerical simulations
- Rigorous mathematics (random matrix theory, decay estimates on Green's functions)
Quantities of Interest

- **Green's function**
  - In coordinate basis, gives the probability amplitude for a particle to move between two positions

- **Localization length**
  - A characteristic length scale for the spatial decay of the wavefunction

\[
\lambda^{-1}(E_\beta) = \lim_{N \to \infty} \frac{1}{N} \ln |G_{1N}(E_\beta)| \\
= \lim_{N \to \infty} \frac{1}{N} \left[ \sum_{i=1}^{N-1} \ln |V_{i,i+1}| - \sum_{\alpha \neq \beta} \ln |E_\beta - E_\alpha| \right]
\]
Lanczos Algorithm

- Goldenfeld and Haydock, 2006 change to a basis of distorted extended waves.

- We can change to another basis by application of Lanczos algorithm:
  - Iterative procedure for bringing a matrix to tridiagonal form
  - Start with arbitrary vector (we choose the vector that has amplitude 1 at the origin) $|0\rangle$

  \[
  H |0\rangle = a_0 |0\rangle - b_0 |1\rangle
  \]

  \[
  H |n\rangle = -b_{n-1} |n - 1\rangle + a_n |n\rangle - b_n |n + 1\rangle
  \]

- Iteratively calculate vectors $|n\rangle$ and matrix elements $a_n$, $b_n$ for the tridiagonal representation of the matrix or operator $H$

  \[
  a_n = \langle n|H|n\rangle
  \]

  \[
  b_n = |b_{n-1} |n - 1\rangle - a_n |n\rangle + H |n\rangle|
  \]

  \[
  |n + 1\rangle = -\frac{1}{b_n} ( -b_{n-1} |n - 1\rangle + a_n |n\rangle - H |n\rangle)
  \]
Properties of Lanczos

- **Termination**: If operator has \( N \) distinct eigenvalues, then algorithm truncates after \( N \) iterations in exact arithmetic (i.e. tridiagonal representation is insensitive to degeneracy in the original spectrum).

- **Rounding errors**: Accumulation of rounding errors prevents truncation and can produce spurious eigenvalues of the tridiagonal matrix.

- **Eigenvalues**: Even in presence of rounding errors, eigenvalues “converge” to some of the correct values.

- **Form**: Brings a matrix to tridiagonal form:

\[
\begin{bmatrix}
    a_0 & -b_0 \\
    -b_0 & a_1 & -b_1 \\
    & -b_1 & a_2 & \ddots \\
    & & \ddots & \ddots & -b_{n-1} \\
    & & & -b_{n-1} & a_n
\end{bmatrix}
\]
Finite Lattices

• No disorder:
  • Lanczos is useless
  • Tight-binding spectrum is degenerate, but Lanczos ignores degeneracy

• Disorder:
  • Any nonzero disorder breaks all degeneracy
  • Useful as computation aid
  • Can be used to calculate “mobility edge” as in Licciardello and Thouless, 1978
Infinite Lattices

- No disorder:
  - Lanczos never terminates anyway
  - $a_n = 0$
  - $b_n \rightarrow d$
  - Localization length tends to infinity, as expected
  - Basis vectors take form of random walk
Infinite Lattices

• Disorder:
  • Single-site disorder:
    • $a_n \to 0$ (after initial increase)
    • $b_n \to d$ (after initial perturbation)
  • Disorder at all sites:
    • Appears to localize all states when strong
    • Weak regime is difficult to calculate since lattice size requirements grow
    • Analytic extension of single-site disorder case?
Problems

- Density of States: Numerical calculation suggests that the density of states of the original system is different than the Lanczos-transformed one.

Correct:

![Graph showing no disorder with W/h=6](image)

Lanczos:

![Graph showing disorder with W/h=6](image)
References


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