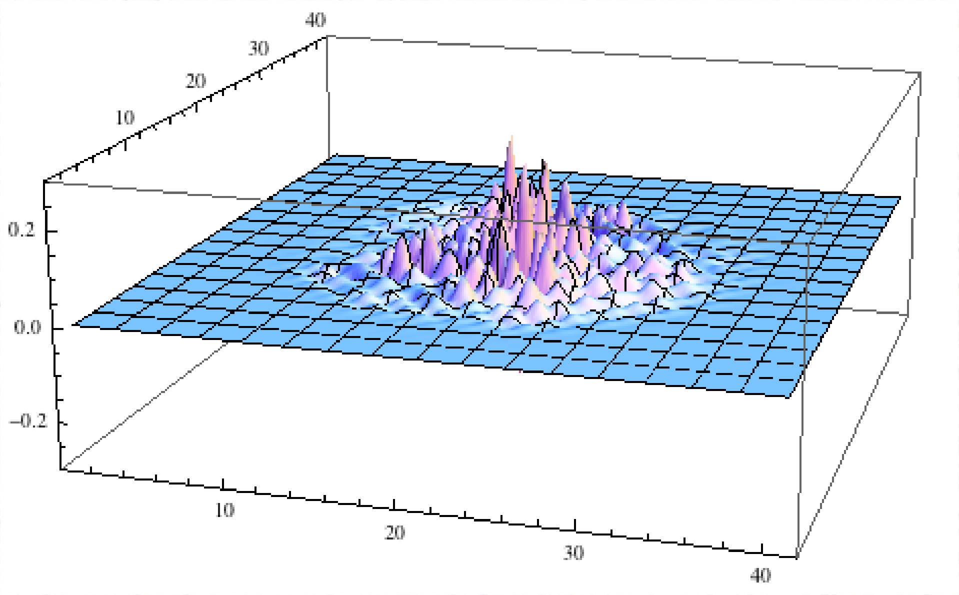
# Application of the Lanczos Algorithm to Anderson Localization





Adam Anderson
The University of Chicago
UW REU 2009

Advisor: David Thouless

# Effect of Impurities in Materials

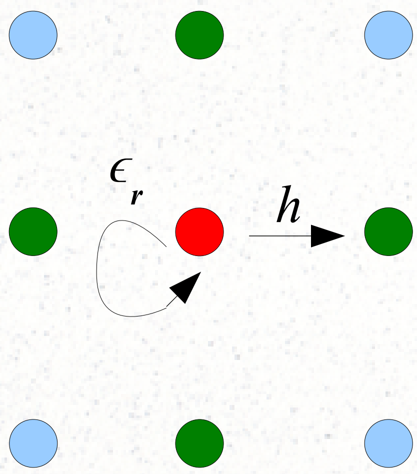
• Naively, one might expect that gradually increasing the number of impurities (i.e. disorder) in a material would cause a proportional decrease in conductivity.

• 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]



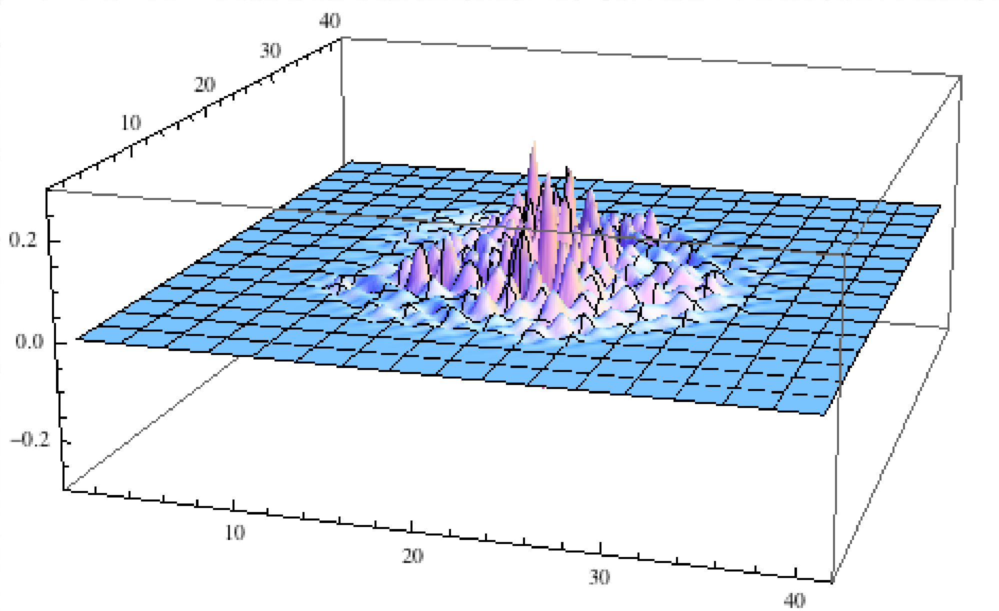

$$H = h \sum_{\substack{\mathbf{r}\in\mathbb{Z}^d \\ \mathbf{r}'\in \mathbf{N}(\mathbf{r})}} |\mathbf{r}\rangle\langle\mathbf{r}'| + \sum_{\mathbf{r}\in\mathbb{Z}^d} \epsilon_{\mathbf{r}} |\mathbf{r}\rangle\langle\mathbf{r}|$$

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

$$\psi(\mathbf{r}) = \sum_{\mathbf{r}\in\mathbb{Z}^d} e^{i\mathbf{k}\cdot\mathbf{r}} |\mathbf{r}\rangle$$

# 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

$$\begin{aligned}\lambda^{-1}(E_\beta) &= \lim_{N\to\infty}\frac{1}{N}\overline{\ln|G_{1N}(E_\beta)|}\\ &= \lim_{N\to\infty}\frac{1}{N}\overline{\left[\sum_{i=1}^{N-1}\ln|V_{i,i+1}| - \sum_{\alpha\neq\beta}\ln|E_\beta - E_\alpha|\right]}\end{aligned}$$

# 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>

$$H|0\rangle = a_0|0\rangle - b_0|1\rangle$$

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

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

$$\begin{aligned} a_n &= \langle n|H|n\rangle \\ b_n &= \left| b_{n-1}|n-1\rangle - a_n|n\rangle + H|n\rangle \right| \\ |n+1\rangle &= -\frac{1}{b_n}\left(-b_{n-1}|n-1\rangle + a_n|n\rangle - H|n\rangle\right) \end{aligned}$$

# 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.

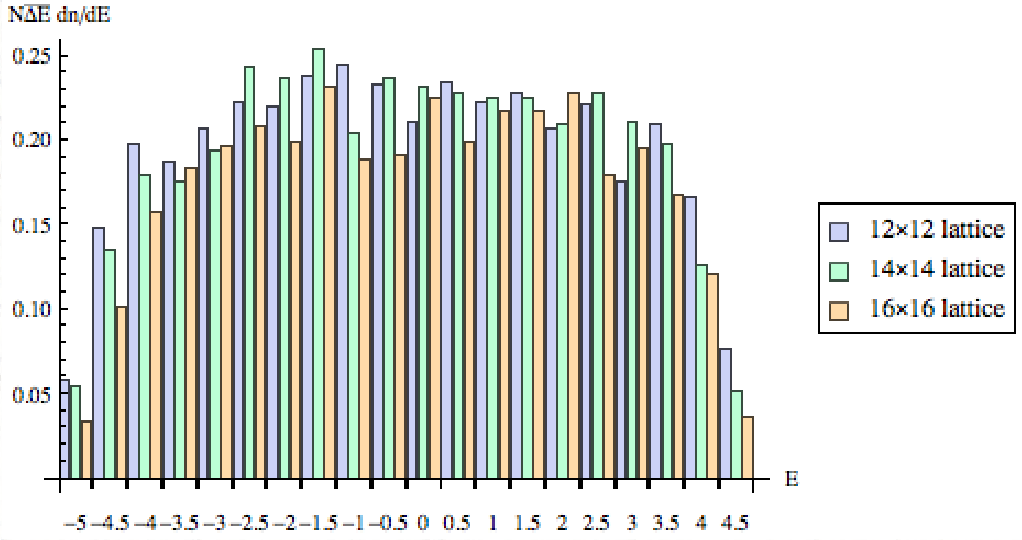
- **Form:** Brings a matrix to tridiagonal form:

$$\begin{bmatrix} a_0 & -b_0 & & & \\ -b_0 & a_1 & -b_1 & & \\ & -b_1 & a_2 & \ddots & \\ & & \ddots & \ddots & -b_{n-1} \\ & & & -b_{n-1} & a_n \end{bmatrix}$$

# Finite Lattices

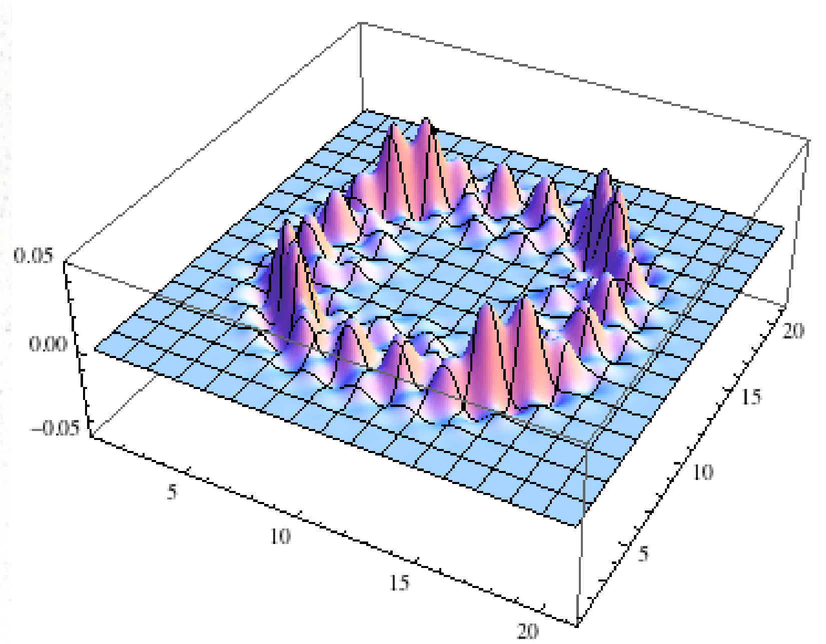
- **No disorder:**
  - Lanczos is useless
  - Tight-binding spectrum is degenerate, but Lanczos ignores degeneracy

- **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
  - $a_n = 0$
  - $b_n \to d$
  - Localization length tends to infinity, as expected
  - Basis vectors take form of random walk



# Infinite Lattices

- **Disorder:**
  - *Single-site disorder:*
    - $a_n \rightarrow 0$ (after initial increase)
    - $b_n \rightarrow d$ (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?

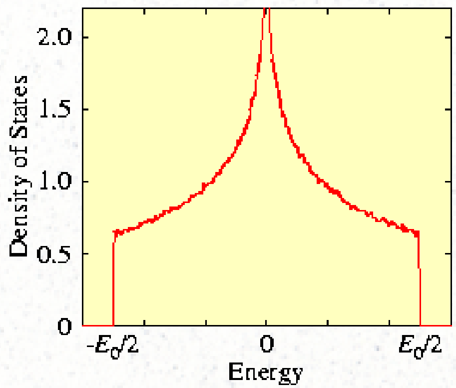
# Problems

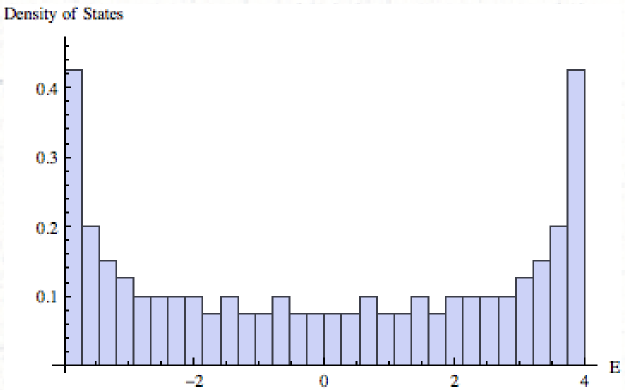
- *Density of States:* Numerical calculation suggests that the density of states of the original system is different than the Lanczos-transformed one.

Correct:

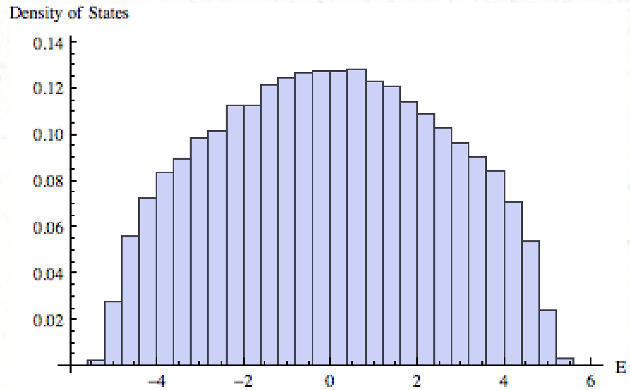
Lanczos:

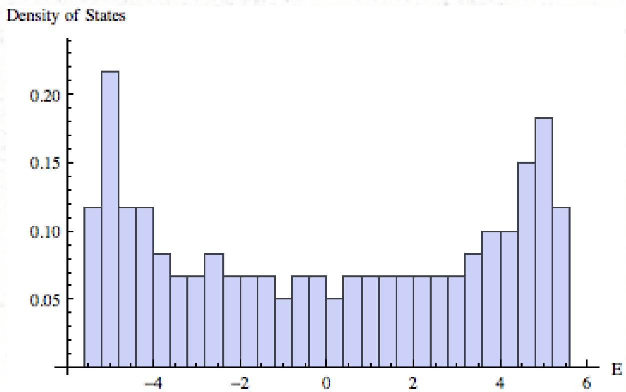
No disorder:




W/h=6:



# References

Goldenfeld and Hadock, Phys. Rev. B **73**, 045118 (2006).
Licciardello and Thouless, J. Phys. C **11**, 925 (1978).
Thouless, *Diffusion and localization in weak disorder*, (2009). Unpublished.

# Acknowledgments

Many thanks to David Thouless for supervising this work and for many interesting discussion, to the Institute for Nuclear Theory for hosting me, and to the NSF for paying me.