Anderson Localization: Localization by Disorder

Tobias Binninger

Seminar: Quantendynamik in mesoskopischen Systemen
Albert-Ludwigs-Universität Freiburg

June 8, 2010
Outline

1. Delocalization in perfect crystals
2. Disorder induced localization: Intuitive explanations
   - Amorphous Si
   - Randomly scattered water waves
3. Disorder induced localization: Theoretical concepts
   - Basic definitions
   - Localization in 1 dimension: Transfer matrix
   - Green’s Functions
4. Disorder and Transport
   - Anderson transition
   - Hopping Transport
   - Weak Localization
5. Summary
Delocalization in perfect crystals:

Electronic states
Electronic states in perfect crystals

Translation operator:

\[(T_R \psi)(r) = \psi(r + R)\]

**Perfect crystal:** Translational symmetry of the potential

\[\Rightarrow [H, T_R] = 0 \quad \forall R \in \text{Lattice}\]

**Bloch Theorem**

There exists a basis of Hamiltonian eigenstates of the form:

\[\psi_{n,k}(r) = e^{ik \cdot r} u_{n,k}(r)\]

\[u_{n,k}(r + R) = u_{n,k}(r)\]

**Bloch states are delocalized**
Bloch states are extended

Density of states: \[ D(E) = \frac{dN}{dE} \]
Disorder induced localization:

Intuitive explanations
Localization in amorphous Si

Tight binding model:

- Electronic states of the crystal: linear combination of atomic orbitals (LCAO) located at each lattice site
- Sharp atomic energy levels are broadened ⇒ energy bands
- Band width \( \propto \) overlap integral of neighboring atomic orbitals
- **Crystalline Si:** interatomic distance \( r_0 \) ⇒ sharp band gap
Amorphous Si: interatomic distance statistically distributed around average value:

- band gap is softened
- spectral density of states (DOS) forms tails reaching into band gap
- value of DOS reflects the probability of having the corresponding binding length
- small DOS in tail region: seldomly realized binding configurations  
  ⇒ corresponding states are largely separated and don’t overlap
  ⇒ localized states in band tails
Randomly scattered water waves

- regularly distributed scatterers: waves are spreading all over the surface
- randomly distributed scatterers: waves remain localized in some areas
Disorder induced localization:

Theoretical concepts
Types of disorder:

- **Structural disorder:**
  disorder in lattice structure
  (e.g. glassy and amorphous systems)

- **Compositional disorder:**
  different kinds of atoms
  randomly distributed on
  lattice sites
  (e.g. impurities, doped semiconductors, alloys)

**Note:** statistical nature of disorder \(\Rightarrow\) statistical ensembles of systems
Tight binding Hamiltonian for electrons:

\[
H = \sum_{j\nu} E_{j\nu} |j\nu\rangle \langle j\nu| + \sum_{j\nu,k\mu} V_{j\nu,k\mu} |j\nu\rangle \langle k\mu|
\]

- \(|j\nu\rangle\): Atomic orbital with quantum number \(\nu\) located at lattice site \(j\)
- diagonal elements \(E_{j\nu}\): Energy of state \(|j\nu\rangle\) (expectation value)
- nondiagonal elements \(V_{j\nu,k\mu}\):
  matrix elements responsible for “hopping” between different sites

**Anderson model**:

- statistically distributed site energies \(E_{j\nu}\)
- statistically independent site energies:

\[
P(\{E_{j\nu}\}) = \prod_{j\nu} p(E_{j\nu})
\]
Compositional disorder: Anderson model

Tight binding Hamiltonian:

\[ H = \sum_{j,\nu} E_{j,\nu} |j,\nu\rangle \langle j,\nu| + \sum_{j,\nu,k,\mu} V_{j,\nu,k,\mu} |j,\nu\rangle \langle k,\mu| \]

Distribution functions for site energies

1. binary alloy made up of two-components \( A_x B_{1-x} \):

\[ p(E_{j,\nu}) = x \delta(E_{j,\nu} - E_A) + (1-x) \delta(E_{j,\nu} - E_B) \]

2. Anderson model: continuous distribution of site energies:

\[ p(E_{j,\nu}) = \frac{1}{W} \Theta\left(\frac{1}{2}W - |E_{j,\nu}|\right) \]

width \( W \): magnitude of disorder
1. **Asymptotic behaviour of wavefunction**: Localization length $\lambda$:

$$\psi(r) = f(r) e^{-r/\lambda}$$

2. **“Diameter” $R$ of wavefunction**:

![Wavefunction depiction]

3. **Transport related quantities**: Transmission probability from $r$ to $r'$:

$$t(r, r'; E) = \langle |\langle r | G(E) | r' \rangle|^2 \rangle$$

$$G(E) = (E - H)^{-1}$$

Localization length $\lambda$: exponential decay length of transmission probability:

$$\frac{2}{\lambda} = - \lim_{|r - r'| \to \infty} \frac{\log t(r, r'; E)}{|r - r'|}$$
Localization in 1 dimension:
Transfer matrix formalism

All eigenstates in a one-dimensional disordered lattice are localized!
Localization in 1 dimension

Schrödinger equation for 1 dimensional tight-binding model:

\[
\left( \sum_{j\nu} E_{j\nu} |j\nu\rangle \langle j\nu| + \sum_{j\nu, k\mu} V_{j\nu, k\mu} |j\nu\rangle \langle k\mu| \right) |\psi\rangle = E |\psi\rangle
\]

ansatz: \( |\psi\rangle = \sum_{j\nu} a_{j\nu} |j\nu\rangle \)

\[
\langle n\nu|H|\psi\rangle = E \langle n\nu|\psi\rangle
\]

\[
\Rightarrow \quad E_{n\nu} a_{n\nu} + \sum_{k\mu} V_{n\nu, k\mu} a_{k\mu} = E a_{n\nu}
\]

consider only one atomic orbital, only next neighbor coupling \( V = 1 \)

\[
\Rightarrow \quad E_n a_n + a_{n+1} + a_{n-1} = E a_n
\]
Transfer matrix

\[ E_n a_n + a_{n+1} + a_{n-1} = E a_n \]

Solution for initial values \( a_0, a_1 \) (semi-infinite lattice):

\[
\begin{pmatrix} a_{n+1} \\ a_n \end{pmatrix} = T_n T_{n-1} \cdots T_1 \begin{pmatrix} a_1 \\ a_0 \end{pmatrix}
\]

Transfer matrices \( T_n \):

\[
T_n = \begin{pmatrix} E - E_n & -1 \\ 1 & 0 \end{pmatrix}
\]

\( E_n \) random variables \( \Rightarrow \) \( T_n \) random matrices!
Fürstenberg’s theorem for products of random matrices:

\[
\lim_{n \to \infty} \frac{1}{n} \log \| T_n \cdots T_1 \vec{a}_0 \| = \gamma > 0
\]

Consider finite system with \( N \) lattice sites:
localization length (exponential decay length) of solution with energy \( E \):

\[
\lambda(E, N) := -\frac{1}{N} \log |a_0(E, N)a_N(E, N)|
\]

for \( N \to \infty \):
\( \lambda \) can be related with \( \gamma \) (no rigorous proof!):

\[
0 < \gamma = \lambda < \infty
\]

All eigenstates in a one-dimensional disordered lattice are localized!
Green’s functions:

Disordered systems of arbitrary dimension
Green’s functions

Hamiltonian $H$ with discrete eigenvalues \( \{E_1, E_2, \ldots\} \) and eigenbasis \( \{|\phi_n\rangle\}_{n \in \mathbb{N}} \)

Green’s Operator:

$$
G(z) := \frac{1}{z - H} = \sum_n \frac{|\phi_n\rangle\langle\phi_n|}{z - E_n} \quad \text{for } z \in \mathbb{C} \setminus \{E_1, E_2, \ldots\}
$$

Green’s function:

$$
G(r, r'; z) := \langle r | G(z) | r' \rangle
$$

Green’s function contains information about the system and its Hamiltonian:

- eigenvalues $E_n$ are poles of Green’s function
- eigenfunctions can be deduced from the residues at the corresponding poles
From Green’s function for a disordered system we can calculate:

- **Density of states** $D(E)$
  
  (for Hamiltonian with continuous spectrum $\text{spec}(H) \subseteq \mathbb{C}$):
  
  $$D(E) = -\frac{1}{2\pi i} \text{Tr}[G^+(E) - G^-(E)]$$

  $$G^{\pm}(E) := \lim_{\eta \to 0^+} G(E \pm i\eta)$$

- **Localization length** $\lambda$:
  
  $$\frac{1}{\lambda} = -\lim_{|r-r'| \to \infty} \frac{\langle \log |G(r, r'; E)| \rangle}{|r-r'|}$$

- **DC electrical conductivity** $\sigma$:
  
  $$\sigma = \frac{2e^2}{h} \lim_{\eta \to 0^+} 4\eta^2 \int dr \ r^2 \langle |G^+(r; E)|^2 \rangle$$
Calculating Green’s Functions

- Consider disorder as perturbation:

\[ H = H_0 + H_1 \]

\[ G_0(z) = (z - H_0)^{-1} \]

\[
G(z) = (z - H)^{-1} = (z - H_0 - H_1)^{-1} = (1 - G_0(z)H_1)^{-1} G_0(z) \\
= G_0 + G_0 H_1 G_0 + G_0 H_1 G_0 H_1 G_0 + \cdots \\
= G_0 + G_0 H_1 G \\
= G_0 + G H_1 G_0
\]

- Different methods to evaluate the ensemble average of the perturbation series: \( < G(z) > \)
Anderson Model: Theoretical Results

Dimensionality of the system $d \leq 2$

All eigenstates are localized, no matter how weak the disorder!

Dimensionality of the system $d = 3$

- DOS forms tails of the band consisting of localized states
- Interior of the band corresponds to extended states
- Critical energies $E_c$ separating localized from extended states: Mobility edges

Note: No rigorous proof of these results!
Disorder and Transport
Anderson transition

- Only extended states contribute to transport/conductivity significantly.
- Position of mobility edge depends on magnitude of disorder.
- At critical magnitude of disorder:
  **Metal-Insulator Phase Transition**
Hopping transport

- Current transport by electrons with energy \( E \approx E_F \)
- for \( E_F < E_c \): Current transport by localized electrons:
  Electrons tunnel/hop from one localized state to the other
- Tunnel probability \( i \rightarrow j \) :
  \[ p(r_{ij}, E_j, E_i) \propto e^{-\alpha r_{ij}} e^{-(E_j - E_i)/kT} \]
- Mott’s \( T^{-\frac{1}{4}} \)-law for conductivity:
  \[ \sigma(T) \propto e^{-(T_0/T)^{1/4}} \]
Weak Localization

- for $E_F > E_c$: Fermi-energy within region of extended states: Metallic regime
- disorder leads to positive interference of certain terms in perturbation expansion of conductivity: enhanced backscattering (weak localization) $\Rightarrow$ reduced conductivity
- Magnetic field destroys positive interference and weak localization
Perfect crystal: Delocalized electronic eigenstates

1-D and 2-D disordered systems: All eigenstates are localized!

3-D disordered systems:
Energy band forms tails of localized states: Mobility edges

Anderson transition:
Metal-Insulator phase transition at critical disorder

Hopping transport by localized electrons:
Mott’s $T^{-\frac{1}{4}}$-law for conductivity

$$\sigma(T) \propto e^{-(T_0/T)^{1/4}}$$

Weak localization:
Reduced conductivity in metallic regime due to disorder enhanced backscattering
Ibach/Lüth: Festkörperphysik, Springer
Ziman: Models of disorder, Cambridge Univ. Press
Economou: Green’s Functions in Quantum Physics, Springer