Metal-insulator transitions of correlated lattice fermions with disorder

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• Lattice fermion models

• Mott-Hubbard metal-insulator transition

• Disorder and averaging

• Correlated electrons + binary alloy disorder

• Mott-Hubbard transition vs. Anderson localization

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Walter Hofstetter
**Insulator vs. Metal**

**Insulator:**
\[
\sigma_{\alpha,\beta}^{DC}(T = 0) = \lim_{T \to 0^+} \lim_{\omega \to 0^+} \lim_{|q| \to 0} \Re[\sigma_{\alpha,\beta}(q, \omega)] = 0
\]

Classification of insulators:

- **single-particle effects**
  - Band filling (Bloch-Wilson)
  - Lattice deformations (e.g., Peierls)
  - Disorder/randomness (Anderson)

- **many-particle effects**
  - Electronic correlations (Mott-Hubbard)
  - Long-range order (Slater, Heisenberg,...)

Band insulator \[\rightarrow\] Mott insulator

Need better understanding of insulators
Metal-Insulator Transitions: Examples
1. Squeezable nanocrystal film switching between metal and insulator

Compressed film: metal
(metallic sheen)

Uncompressed film: insulator
(shininess is gone)

Discontinuous transition

Collier, Saykally, Shiang, Henrichs, Heath (1997)
2. Metal-insulator transition in a dilute, low-disordered Si MOSFET

Kravchenko, Mason, Bowker, Furneaux, Pudalov, D’Iorio (1995)

Anissimova, Kravchenko, Punnoose, Finkel’stein, Klapwijk (2007)
3. Anderson metal-insulator transition: (disorder induced)

4. Mott metal-insulator transition in $V_2O_3$ (correlation induced)

McWhan et al. (1971)  
Kuwamoto, Honig, Appel (1980)
5. Metal-Insulator transitions in La$_{1-x}$Sr$_x$MnO$_3$
(electronic correlations + disorder)

Hemberger et al. (2002)
6. Superfluid-Mott transition of cold bosons in an optical lattice

Greiner, Mandel, Esslinger, Hänsch, Bloch (2002)
Correlated Lattice Fermions: Models

e^{-}, {}^{6}\text{Li}, {}^{40}\text{K}, {}^{171}\text{Yb},...
1. **Hubbard model:**
   Simplest lattice fermion model

\[ H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

**Local ("Hubbard") physics:**

\[ \langle n_{i\uparrow} n_{i\downarrow} \rangle \neq \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle \]

**Correlation phenomena:**
- Metal-insulator transition
- Ferromagnetisms,...
2. Falicov-Kimball model

\[ H_{FK} = -t \sum_{\langle i,j \rangle} c_{i \uparrow}^\dagger c_{j \uparrow} + U \sum_i n_{i \uparrow} n_{i \downarrow} \]

\[ = -t \sum_{\langle i,j \rangle} d_{i \uparrow}^\dagger d_{j \uparrow} + U \sum_i n_{i \uparrow} n_{i \downarrow} \]

\[ d=2,3: \text{unsolvable many-body problems} \]

mobile fermion ("d") \[ ^6\text{Li} \]
immobile fermion ("f") \[ ^{171}\text{Yb} \]

annealed disorder

Reliable approximations?
Dynamical Mean-Field Theory (DMFT) of Correlated Lattice Fermions
Dynamical mean-field theory of correlated electrons

Metzner, DV (1989)

Georges and Kotliar (1992)

"single-impurity Anderson model"
+ self-consistency

Georges and Kotliar (1992)

$\Sigma(\omega) \rightarrow \infty$
$Z \rightarrow \infty$

Scaling of hopping $t = \frac{t^*}{\sqrt{Z}}$

$\Sigma(k, \omega) \rightarrow \infty$
$Z \rightarrow \infty$

$\Sigma(\omega)$
Dynamical mean-field theory of correlated electrons

Proper time resolved treatment of local electronic interactions:

Kotliar, DV (Physics Today; March, 2004)

DMFT: “local” theory with full many-body dynamics

Research since 1992 shows: Reliable approximation for $d=3$
(i) Effective single impurity problem

\[ G = -\frac{1}{Z} \int \mathcal{D}[\psi \psi^*] \psi \psi^* e^{\psi^* [G^{-1} + \Sigma] \psi - U \psi^* \psi \psi^* \psi} \]

(ii) \( k \)-integrated Dyson equation (lattice enters)

\[ G(\omega) = \int d\varepsilon \frac{N^0(\varepsilon)}{\omega - \Sigma(\omega) - \varepsilon} \]

Solve with an „impurity solver“, e.g., QMC, NRG, ED,…
DMFT helped to understand, e.g.:

- Correlation phenomena at intermediate couplings
- Mott-Hubbard metal-insulator transition

Georges, Kotliar, Krauth, Rozenberg (1996)

Kotliar, DV (2004)
Mott-Hubbard metal-insulator transition at integer density
Single-particle spectral function $A(\omega) = -\frac{1}{\pi} \text{Im} G(\omega)$ in DMFT

Hubbard model, density $n=1$
Single-particle spectral function \( A(\omega) = -\frac{1}{\pi} \text{Im} G(\omega) \) in DMFT

Hubbard model, density \( n=1 \)

Density of states

Quasiparticle renormalization: \( \frac{m^*}{m} \rightarrow \infty \)
magnetically frustrated

Metal-insulator transition in the one-band Hubbard model

DMFT(IPT): Georges et al. (1996)

High precision phase diagram

One-band Hubbard model +
- next-neighbor hopping $t$
- bipartite lattice
- half-filling ($n=1$)
  $\Rightarrow$ „perfect nesting“
  $\Rightarrow$ antiferromagnetic (AF) order

- further-range hopping $t_2$, $t_3$, ...
- and/or non-bipartite lattices
  $\Rightarrow$ magnetic „frustration“
Strongly correlated electron materials: \( V_2O_3 \), \( NiSe_{2-x}S_x \), \( \kappa \)-organics, ... also Helium-3

Kotliar, DV (2004)

Universality due to Fermi statistics
Disorder
(quenched)
Anderson disorder model on the lattice

\[ H = \sum_{\langle i,j \rangle, \sigma} t_{ij} c_i^\dagger c_j + \sum_{i, \sigma} \varepsilon_i n_i \]

Random hopping  Random local potential

→ e.g., R. A. Römer, Habilitation Thesis (1999)
Anderson disorder model on the lattice

\[ H = -t \sum_{\langle i,j \rangle,\sigma} C_{i\sigma}^\dagger C_{j\sigma} + \sum_{i\sigma} \varepsilon_i n_{i\sigma} \]

Disorder due to non-stoichiometric composition, e.g., by

1. doping: \( \text{La}_{1-x}\text{Sr}_x\text{MnO}_3 \)
   \( \text{La}_{1-x}\text{Sr}_x\text{CuO}_4 \)
   Sr ion changes local potential → affects correlated \( d \)-electrons

2. alloying with different transition metal (TM) ions, e.g., \( \text{Co}_{1-x}\text{Fe}_x\text{S}_2 \)
   \( \text{Ni}_{1-x}\text{Co}_x\text{S}_2 \)
   TM ions located randomly → 2 different atomic levels created for correlated \( d \)-electrons
Anderson disorder model on the lattice

\[ H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma} \varepsilon_i n_{i\sigma} \]

Disorder \rightarrow \text{Scattering of quantum particle}

\text{Scattering time } \tau \rightarrow \Sigma(\omega = 0) \propto \frac{1}{\tau}

\text{Weak scattering (d=3)}

\[ \sigma(0) \equiv \sigma_0 = \frac{e^2 n}{m \tau} \]

Drude-Boltzmann conductivity
### Anderson disorder model on the lattice

\[ H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i\sigma} \varepsilon_i n_{i\sigma} \]

Random local potential

**Disorder distributions, e.g.,**:

**Box disorder**

\[ P(\varepsilon_i) = \frac{\Theta\left(\frac{\Delta}{2} - |\varepsilon_i|\right)}{\Delta} \]

\[ \langle O_i \rangle_{\text{arith}} = \int d\varepsilon_i P(\varepsilon_i) O_i(\varepsilon_i) \]

e.g., local DOS \( \rho_i(\varepsilon_i) \)

**Binary alloy disorder** (alloys \( A_{1-x}B_x \), e.g., \( \text{Fe}_{1-x}\text{Co}_x \))

\[ P(\varepsilon_i) = x\delta\left(\varepsilon_i + \frac{\Delta}{2}\right) + (1-x)\delta\left(\varepsilon_i - \frac{\Delta}{2}\right) \]

\( x \): alloy concentration

\( \Delta \): disorder strength
Effect of disorder

Disorder affects wave fct. \( \psi(r) = |\psi(r)| e^{i\phi(r)} \)

\( \sigma(0) = 0 \) ("localization") due to, e.g.,

Anderson localization

\[ \Delta \geq \Delta_c : \text{Anderson localization (1958)} \]

due to coherent back scattering

\[ \Delta_c \begin{cases} = 0, & d=1,2 \\ > 0, & d=3 \end{cases} \]

Alloy band splitting

Binary alloy disorder, bounded Hamiltonian

\[ \Delta > \Delta_c \gg \max(\{|t|,U\}), \text{ for } d \geq 1 \]
DMFT for disordered systems
Anderson disorder model on the lattice

\[ H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma} \varepsilon_i n_{i\sigma} \]

DMFT with \( \langle \rho_i(\varepsilon_i) \rangle_{\text{arith}} \leftrightarrow \text{CPA} \)

CPA: Coherent potential approximation
   ("best single-site approx.")

   - robust results for \( \langle \rho_i(\varepsilon_i) \rangle_{\text{arith}} \)
   - cannot describe Anderson localization

Vlamington, DV (1992)
Janis, DV (1992)

Sovent (1967)
Taylor (1967)
FIG. 20. The phonon density of states \( \rho(\omega^2) \) versus \( \omega^2/\omega_m^2 \) for disordered simple cubic lattices with \( M_B = 3M_A \) at four concentrations \( c \) of B atoms. A comparison between the CPA (solid line) and the machine calculations of Payton and Visscher (1967) [after Taylor (1967)].
Interactions + Binary Alloy Disorder:
Mott-Hubbard metal-insulator transition
at fractional densities
Anderson-Hubbard Hamiltonian

\[ H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \sum_{i\sigma} \epsilon_{i} n_{i\sigma} \]

- Binary alloy disorder
  \[ P(\epsilon_{i}) = x \delta \left( \epsilon_{i} + \frac{\Delta}{2} \right) + (1-x) \delta \left( \epsilon_{i} - \frac{\Delta}{2} \right) \]

\[ \Delta: \text{disorder strength} \]
\[ x: \text{alloy concentration} \]

# A,B-atoms: \( N_{A,B} \)
# lattice sites: \( N_{L} \)
\[ \Rightarrow x=N_{A}/N_{L}, \ 1-x=N_{B}/N_{L} \]

# electrons: \( N \) \( \rightarrow \) density \( n=N/N_{L} \)

- Arithmetic averaging:
  \[ \langle O_{i} \rangle_{\text{arith}} = \int d\epsilon_{i} P(\epsilon_{i}) O_{i}(\epsilon_{i}) \]
- DMFT(NRG): \( T=0 \)
Mott-Hubbard transition at fractional densities (binary alloy disorder)

Mott-Hubbard transition at fractional densities (binary alloy disorder)

\[ x = \frac{N_A}{N_L}, \quad 1-x = \frac{N_B}{N_L} \]

No interactions

Mott-Hubbard transition at fractional densities (binary alloy disorder)

\[ x = \frac{N_A}{N_L}, \ 1-x = \frac{N_B}{N_L} \]


Mott-Hubbard transition at fractional densities (binary alloy disorder)

\( x = N_A / N_L, \quad 1-x = N_B / N_L \)

Density \( n = x \): half filled LAB

Mott-Hubbard transition at fractional density

Mott-Hubbard Transition vs. Anderson Localization
**Anderson-Hubbard Hamiltonian**

\[ H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{i\sigma} \epsilon_i n_{i\sigma} \]

1. Box disorder
   \[ P(\epsilon_i) = \frac{\Theta(\frac{\Delta}{2} - |\epsilon_i|)}{\Delta} \]
   \( \Delta: \) disorder strength

- \( \Delta=0: \) Mott-Hubbard metal-insulator transition for \( U>U_c \)
- \( U=0: \) Anderson localization for \( \Delta > \Delta_c > 0 \) in \( d>2 \)

- \( d=2: \) QMC study Chakraborty, Denteneer, Scalettar (2007)

**Questions:**

1. Both transitions described by the (average local) DOS?
2. Further destabilization of correlated metallic phase by disorder?
3. Mott insulator and Anderson insulator separated by another (metallic) phase?
Anderson localization characterized by

local density of states (LDOS) $\rho_i(E)$

Anderson (1958)

Search for „typical“ value of $\rho_i(E)$

= most probable value
= maximum of probability distribution function (PDF)

Usually unknown
Approximation of PDF: calculate averages + moments

Which average?

\[ \langle \rho_i(E) \rangle_{\text{arith}} > 0 \] does not detect localization

Why?

PDF of disordered systems: very broad with long tails
→ system not self-averaging

Distribution of LDOS (d=3)

N: # sites

Localized phase: Log-normal distribution

<table>
<thead>
<tr>
<th>Property</th>
<th>Normal distribution</th>
<th>Log-normal distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(Gaussian, or additive normal distribution)</td>
<td>(Multiplicative normal distribution)</td>
</tr>
<tr>
<td></td>
<td>$\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2} \left( \frac{x-\mu}{\sigma} \right)^2}$</td>
<td>$\frac{1}{\sqrt{2\pi\sigma^2}} \frac{1}{x} e^{-\frac{1}{2} \left( \frac{\ln x-\mu}{\sigma} \right)^2}$</td>
</tr>
<tr>
<td>Effects (central limit theorem)</td>
<td>Additive</td>
<td>Multiplicative</td>
</tr>
<tr>
<td>Shape of distribution</td>
<td>Symmetrical</td>
<td>Skewed</td>
</tr>
<tr>
<td>Mean</td>
<td>$\bar{x}$, Arithmetic</td>
<td>$\bar{x}^*$ Geometric</td>
</tr>
</tbody>
</table>
Anderson localization: \( \rho_i(E) \big|_{\text{typical}} = \langle \rho_i(E) \rangle_{\text{geometric}} = e^{\langle \ln \rho_i(E) \rangle} \)
DMFT for Anderson-Hubbard model

\[ G(\omega, \epsilon_i) \rightarrow \rho_i(\omega) = -\frac{1}{\pi} \text{Im} G(\omega, \epsilon_i) \]

\[ \rho_g(\omega) = e^{\langle \ln \rho_i(\omega) \rangle}; \quad G(\omega) = \int d\omega' \frac{\rho_g(\omega)}{\omega - \omega'} \] : lattice Green function

Dobrosavljevic, Pastor, Nikolic (2003)
Mott-Hubbard Transition vs. Anderson Localization

 Disorder $\leftrightarrow$ Anderson MIT

 Anderson insulator
 $\Delta_c$

 metal

 Interaction $\leftrightarrow$ Mott-Hubbard MIT

 Disorder

 Interaction

 LDOS

 energy

 LDOS

 energy

 LDOS

 energy

 LDOS

 energy

 U_c

 Mott-Hubbard insulator
Anderson-Hubbard Hamiltonian

\[ H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{i\sigma} \varepsilon_i n_{i\sigma} \]

Solution by DMFT(NRG)

\[ \Delta: \text{disorder strength} \]
Anderson-Hubbard Hamiltonian

\[ H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_i \varepsilon_i n_{i\sigma} \]

\( \Delta \): disorder strength

- Disorder increases \( U_c \)
- Interaction in/decreases \( \Delta_c^A \)

\( \rightarrow \) Interactions may increase metallicity

Byczuk, Hofstetter, DV (2005)
Antiferromagnetism vs. Anderson Localization
Anderson-Hubbard Hamiltonian

\[ H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_i \epsilon_i n_{i\sigma} \]

NN hopping, bipartite lattice, n=1: Take into account antiferromagnetic order

\[ \Delta: \text{disorder strength} \]

DMFT: Non-magnetic phase diagram

Magnetic phase diagram

Byczuk, Hofstetter, DV (2008)
Conclusion

- Mott-Hubbard metal-insulator transition
- Arithmetic vs. geometric average over disorder
- Binary alloy disorder: Mott-Hubbard transition at fractional density
- Mott-Hubbard transition vs. Anderson localization
- Realizable by cold atoms in optical lattices