Metal-insulator transitions of correlated lattice fermions with disorder

Disorder in Condensed Matter and Cold Atoms
Lorentz Center, Leiden; September 26, 2007

Dieter Vollhardt

Supported by Deutsche Forschungsgemeinschaft through SFB 484
• Metal-Insulator transitions: Examples

• Lattice models

• Dynamical Mean-Field Theory (DMFT) of correlated fermions & bosons

• Mott-Hubbard transition

• Disorder and averaging

• Binary alloy disorder: Mott-Hubbard transition at fractional filling

• Mott-Hubbard transition vs. Anderson localization

In collaboration with:

Krzysztof Byczuk
Walter Hofstetter
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** vs. **many-particle effects**

- Band filling (Bloch-Wilson)
- Lattice deformations (e.g., Peierls)
- Disorder/randomness (Anderson)
- Electronic correlations (Mott-Hubbard)
- Long-range order (Slater, Heisenberg, …)

Band insulator \[ \overset{\leftrightarrow}{\text{qualitatively different?}} \] 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. Mott transition in \((\text{TMTSF})_2\text{PF}_6\)

Dressel et al. (1996)

Giamarchi (1997)

\(d=1\)
3. 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)
4. Metal-Insulator transitions in La$_{1-x}$Sr$_x$MnO$_3$

Hemberger et al. (2002)
5. Anderson metal-insulator transition: (disorder induced)

6. Mott metal-insulator transition in $V_2O_3$ (interaction/correlation induced)

7. Superfluid-Mott transition of cold bosons in an optical lattice

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

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

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

**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

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

\[ = -t \sum_{\langle i,j \rangle} d_i^{\dagger} d_j + U \sum_i n_i^d n_i^f \]

d=2,3: 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

- $d=3$; coord. # $Z$
- fcc lattice: $Z=12$

- Hubbard model
- Metzner, DV (1989)
- Scaling of hopping $t = \frac{t^*}{\sqrt{Z}}$

- "single-impurity Anderson model" + self-consistency
  - Georges and Kotliar (1992)
Dynamical mean-field theory of correlated electrons

Proper time resolved treatment of local electronic interactions:

\[ \Sigma(k, \omega) \]

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

Reliable approximation in d=3

Kotliar, DV (2004)
DMFT self-consistency equations

(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 advance our understanding of, 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 filling
Single-particle spectral function $A(\omega) = -\frac{1}{\pi} \text{Im} G(\omega)$ in DMFT.

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

Hubbard model, n=1

Density of states

Quasiparticle renormalization $m^* \rightarrow \infty$
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 $t_2, t_3, \ldots$
- and/or non-bipartite lattices

$\Rightarrow$ magnetic "frustration"

Hartree theory, $d=3$

Hofstetter, DV (1998)
Strongly correlated electron materials: $V_2O_3$, $NiSe_{2-x}S_x$, $\kappa$-organics, ...

Metal-insulator transition in the one-band Hubbard model

Hubbard model (n=1)
Excursion: Dynamical Mean-Field Theory of Correlated Lattice Bosons (B-DMFT)
1. **Bose-Hubbard model**

\[ H = \sum_{ij} t_{ij} b_i^\dagger b_j + \frac{U}{2} \sum_i n_i(n_i - 1) \]

2. **Bose-Falicov-Kimball model**

\[ H = \sum_{ij} t_{ij} b_i^\dagger b_j + \epsilon_f \sum_i f_i^\dagger f_i + U_{bf} \sum_i n_{bi}n_{fi} + U_{ff} \sum_i n_{fi}n_{fi} \]

- mobile
- immobile

\(^7\text{Li}\)

\(^{87}\text{Rb}\)

*annealed disorder*
Scaling of hopping to derive B-DMFT

\[ \langle H_{\text{kin}} \rangle_0 = -t \sum_{i, \sigma} \sum_{j(\text{NN} \ i)} \frac{1}{Z} \langle b_{i \sigma}^\dagger b_{j \sigma} \rangle_0 \]

\[ t = \frac{t^*}{\sqrt{Z}} \]

Scaling not possible on Hamiltonian level, but in the action (cumulant expansion)
Bose-Hubbard model: B-DMFT

\[ S_{loc} = - \int_0^\beta \int_0^\beta d\tau d\tau' \tilde{b}(\tau) \tilde{G}^{-1}(\tau - \tau') \tilde{b}(\tau) + \kappa \int_0^\beta d\tau \tilde{\phi}^\dagger(\tau) \tilde{b}(\tau) + \frac{U}{2} \int_0^\beta n(\tau)(n(\tau) - 1) \]

\[ \kappa = \sum_{i \neq 0} t_{i0} \]

Condensate wave fct.

New: Coupling to generalized Gross-Pitaevskii eq. for condensate wave fct.

\[ \partial_\tau \tilde{\phi}(\tau) - \int_0^\beta d\tau' \hat{\Delta}(\tau - \tau') \tilde{\phi}(\tau') + \kappa \tilde{\phi}(\tau) + U |\tilde{\phi}(\tau)|^2 \tilde{\phi}(\tau) = \mu \tilde{\phi}(\tau) \]


Byczuk, DV (arXiv:0706.0839)
B-DMFT for Bose-Falicov-Kimball model  

Byczuk, DV (arXiv:0706.0839)

Hardcore f-bosons: \( n_f = 0, 1 \)  \( d=3 \), simple cubic lattice

- Correlation induced band splitting \( \rightarrow T_{\text{BEC}} \) increases
- Narrowing of lower subband \( \rightarrow T_{\text{BEC}} \) decreases

\( \rightarrow \) Enhancement of \( T_{\text{BEC}} \) due to interactions
Disorder (quenched)
Anderson disorder model on the lattice

\[ H = \sum_{\langle i,j \rangle, \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma} \epsilon_i n_{i\sigma} \]

Random hopping  Random local potential
Anderson disorder model on the lattice

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

Disorder \rightarrow Scattering of quantum particle

Scattering time \( \tau \rightarrow \)

\[ \Sigma(\omega = 0) \propto \frac{1}{\tau} \]

Weak scattering \((d=3)\)

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

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

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

e.g., local DOS \(\langle \rho(\varepsilon_i) \rangle_{\text{arith}}\)

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

\[
P(\varepsilon_i) = x \delta\left(\varepsilon_i + \frac{\Delta}{2}\right) + (1-x) \delta\left(\varepsilon_i - \frac{\Delta}{2}\right)
\]
Disorder affects wave fct. \( \psi(r) = |\psi(r)| e^{i\phi(r)} \)

Localization \( \sigma(0) = 0 \) 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 \( \langle \rho(\varepsilon_i) \rangle_{\text{arith}} \Leftrightarrow \text{CPA} \)

CPA: Coherent potential approximation

("best single-site approx.")

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

Vlaming, DV (1992)  
Janis, DV (1992)

Soven (1967)  
Taylor (1967)
Example: CPA results for phonon DOS for disordered cubic crystal

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)].

Elliot, Krumhansl, Leath (RMP, 1974)
Interactions + binary disorder:
Mott-Hubbard metal-insulator transition at fractional filling
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
  \[ P(\epsilon_i) = x \delta \left( \epsilon_i + \frac{\Delta}{2} \right) + (1-x) \delta \left( \epsilon_i - \frac{\Delta}{2} \right) \]
  \[ \Delta: \text{disorder strength} \]

# A,B-atoms: \( N_{A,B} \)  \( \rightarrow \) concentration \( x = \frac{N_A}{N_L}, 1-x = \frac{N_B}{N_L} \)

# lattice sites: \( N_L \)

# electrons: \( N \)  \( \rightarrow \) filling \( n = \frac{N}{N_L} \)

- Arithmetic averaging:
  \[ \langle O_i \rangle_{\text{arith}} = \int d\epsilon_i P(\epsilon_i) O_i \]

- DMFT(NRG)
Mott-Hubbard transition at fractional filling (binary alloy disorder)

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

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

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

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

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

Mott-Hubbard transition at fractional filling

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

Filling $n=x=0.5$

$x = N_A / N_L$, $1-x = N_B / N_L$

Ground-state phase diagram

Hysteresis

Effective theory for LHB for $\Delta \gg U, t$

$U_c = 6\sqrt{x} \bigg|_{x=0.5} = 3 / \sqrt{2}$

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. Can both transitions be characterized by the (average local) DOS?
2. Further destabilization of correlated metallic phase by disorder?
3. Are the Mott insulator and Anderson insulator separated by another (metallic) phase?

\( \Delta = 0: \) 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)
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

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

**Which average?**

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

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

**Why?**

Localized phase: Log-normal distribution

<table>
<thead>
<tr>
<th>Property</th>
<th>Normal distribution (Gaussian, or additive normal, distribution)</th>
<th>Log-normal distribution (Multiplicative normal distribution)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \frac{1}{\sqrt{2\pi \sigma^2}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma^2}\right)^2} )</td>
<td>( \frac{1}{\sqrt{2\pi \sigma^2 x}} e^{-\frac{1}{2}\left(\frac{\ln x-\mu}{\sigma^2}\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: \( \rho_i(E) \)\textsubscript{typical} = \( \langle \rho_i(E) \rangle \)\textsubscript{geometric} = \( e^{\langle \ln \rho_i(E) \rangle} \)

Anderson (1958)

Life is log-normal

Limpert, Stahel (2001)
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)

Better “typical” values of the local DOS by the Hölder mean?

\[ M_q(x) = \left( \frac{1}{n} \sum_{i=1}^{n} x_i^q \right)^{1/q} \quad x \in \mathbb{R}^+, q \in \mathbb{R} \]

q → 0 geometric mean
q = 1 arithmetic mean

q < 0.5: \[ \rho_q(\omega = 0) = 0 \text{ at } \Delta^c_q(U) \]

Souza, Maionchi, Herrmann; cond-mat/0702355
Mott-Hubbard Transition vs. Anderson Localization

Disorder ↔ Anderson MIT

Interaction ↔ Mott-Hubbard MIT
Anderson-Hubbard Hamiltonian

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

Solution by DMFT(NRG)

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

Non-magnetic phase diagram; n=1, T=0

Critical behavior at localization transition

Byczuk, Hofstetter, DV (2005)
Anderson-Hubbard Hamiltonian

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

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

- Disorder increases \( U_c \)
- Interaction in/decreases \( \Delta^A_c \)

\[ \rightarrow \text{Interactions may increase metallicity} \]

\( d=2: \)
Denteneer, Scalettar, Trivedi (1999)

Byczuk, Hofstetter, DV (2005)
Anderson-Hubbard Hamiltonian

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

\( \Delta \): disorder strength

DMRG for disordered bosons in \( d=1 \)

Anderson and Mott insulator neighboring

Rapsch, Schollwöck, Zwerger (1999)

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

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

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

Unrestricted Hartree-Fock, d=3

\( \Delta: \text{disorder strength} \)

Tusch, Logan (1993)
Anderson-Hubbard Hamiltonian

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

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

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

DMFT: Non-magnetic phase diagram

Magnetic phase diagram

No boundary between Slater- and Heisenberg AFI