Metal insulator transition in correlated electrons with long-range order and disorder

Krzysztof Byczuk

Institute of Physics, EKM, Augsburg University

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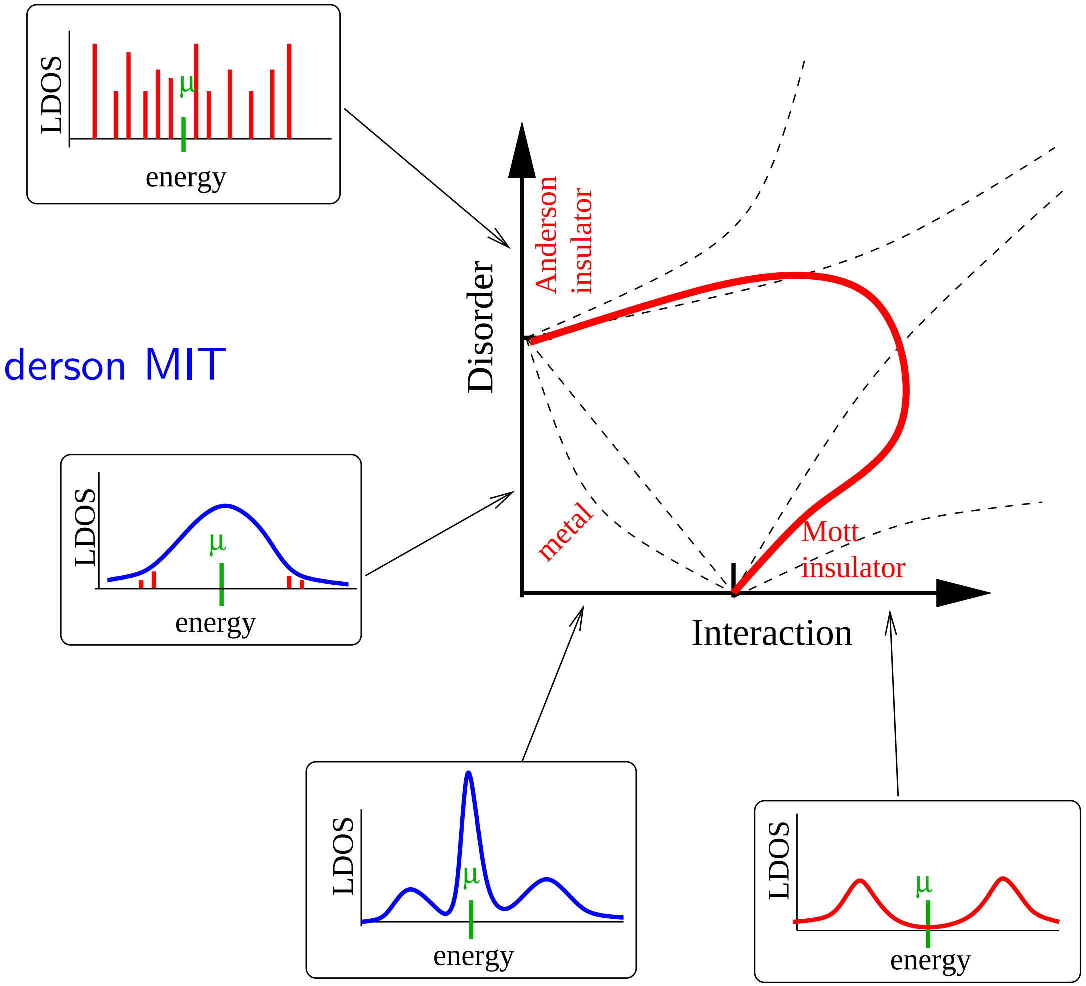
Collaboration

- Walter Hofstetter - Frankfurt, Germany
- Dieter Vollhardt - Augsburg, Germany

Phys. Rev. Lett. **94**, 056404 (2005); cond-mat/0403765
Physica B **359-361**, 651 (2005); cond-mat/0502257
Phys. Rev. B **71**, 205105 (2005); cond-mat/0412590

Support from SFB 484

Paramagnetic phase



Disorder ↔ Anderson MIT

Interaction ↔ Mott-Hubbard MIT

Two insulators are continously connected

BUT

Interaction and disorder compete with each other stabilizing the metallic phase against the occurring one of the insulators

Antiferromagnetic phase

Many works on AF within DMFT:
e.g. from Augsburg
i) with disorder - Ulmke, Janis, Vollhardt (1995); Singh, Ulmke, Vollhardt (1998)
enhancement of T_N

$$J_{ij} = \frac{t^2}{U - (\epsilon_i - \epsilon_j)} + \frac{t^2}{U - (\epsilon_j - \epsilon_i)} \approx \frac{2t^2}{U} \left[1 + \frac{(\epsilon_i - \epsilon_j)^2}{U^2} \right]$$

hence $J_{eff} = \langle J_{ij} \rangle = J_0 \left[1 + \lambda \frac{\Delta^2}{U^2} \right]$
closing charge gap by increasing disorder (CPA)
ii) with frustration - Zitzler, Tong, Pruschke, Bulla (2004); Eckstein (2006)
suppression and first order transition

How does full phase diagram look like?

How good is disorder to destroy AF LRO?

What is role of Anderson localization vs. AF LRO?

Hubbard model with disorder

$$H = \sum_{i\sigma} \epsilon_i n_{i\sigma} + \sum_{ij\sigma} t_{ij}\ a^{\dagger}_{i\sigma} a_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

- Interaction U.
- Randomness ϵ_i with box PDF

$$\mathcal{P}(\epsilon_i) = \frac{1}{\Delta} \quad \text{for} \quad |\epsilon_{\rm i}| < \frac{\Delta}{2}$$

  and zero otherwise.
- t_{ij} hopping on a lattice, used semielliptic bare DOS with $W = 1$.

- DMFT deals well with the interaction U
- CPA arithmetic averaging over ϵ_i does not describe Anderson localization

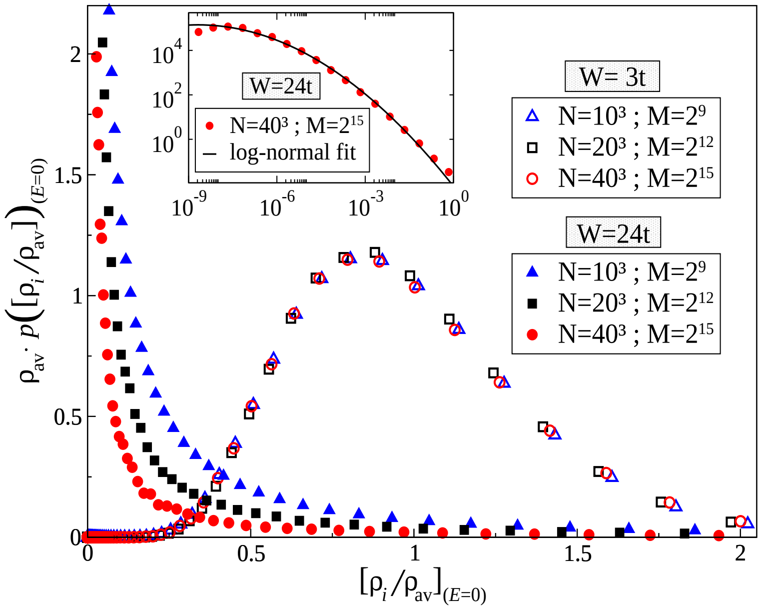
Typical behavior vs. geometric averaging

At large disorder:

- PDF of DOS is very broad with long tails
- Typical DOS is different from arithmetically averaged one
- PDF well fitted by log-normal distribution

Typical LDOS is approximated by geometrical mean

$$\rho_{typ}(E) \approx \rho_{geom}(E) = e^{\langle \ln \rho_i(E) \rangle}$$

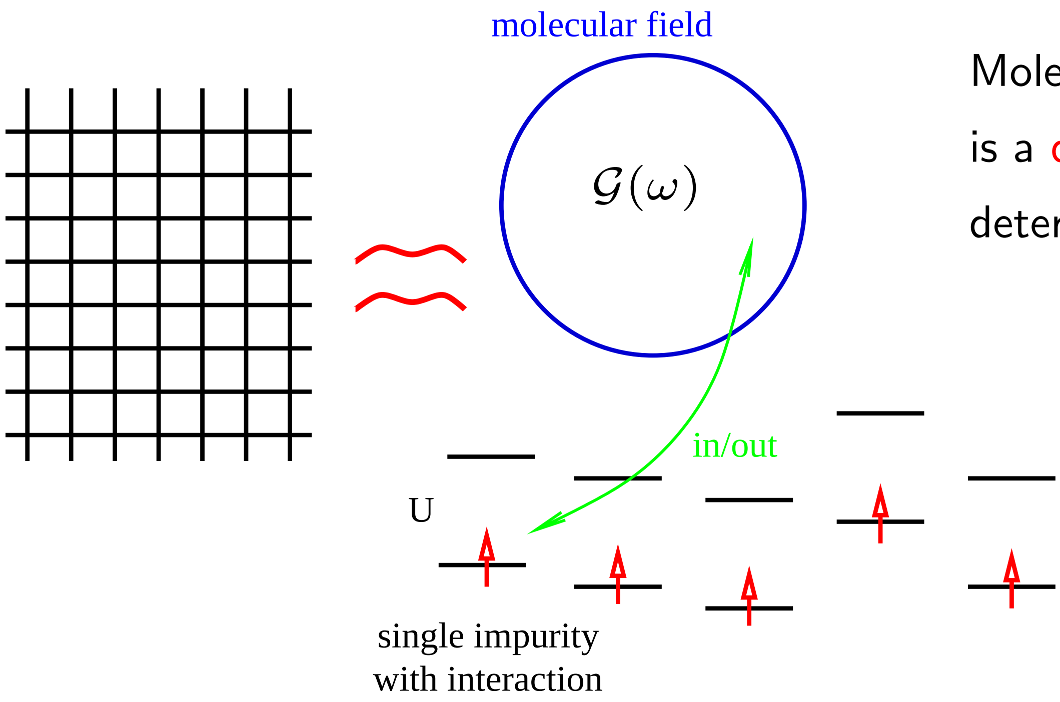


Schubert et al., cond-mat/0309015

Dynamical mean-field theory for U and Δ

Byczuk, Hofstetter, Vollhardt, Phys. Rev. Lett. **94**, 056404 (2005)
after idea from: Dobrosavljevic et al., Europhys. Lett. **62**, 76 (2003)

Lattice problem of interacting particles is mapped onto
an ensamble of single impurities (single atoms)



Molecular (Weiss) function $\mathcal{G}(\omega)$
is a dynamical quantity,
determined self-consistently

$$\rho_{typ}(E) = e^{\langle \ln \rho_i(E) \rangle}$$

$$H = \sum_{i\sigma} \epsilon_i n_{i\sigma} + \sum_{ij\sigma} t_{ij}\, a^\dagger_{i\sigma} a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

DMFT with Anderson MIT

$$H^{\rm SIAM} = \sum_\sigma (\epsilon_i - \mu) a^\dagger_{i\sigma} a_{i\sigma} + U n_{i\uparrow} n_{i\downarrow} + \sum_{\mathbf{k}\sigma} V_{\mathbf{k}} a^\dagger_{i\sigma} c_{\mathbf{k}\sigma} + hc + \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

$$G(\omega, \epsilon_i) \longrightarrow \rho_i(\omega) = -\frac{1}{\pi} \mathrm{ImG}(\omega, \epsilon_{\mathrm{i}})$$

$$\rho_g(\omega) = e^{\langle \ln \rho_i(\omega) \rangle}; \quad G(\omega) = \int d\omega' \frac{\rho_g(\omega)}{\omega - \omega'}$$

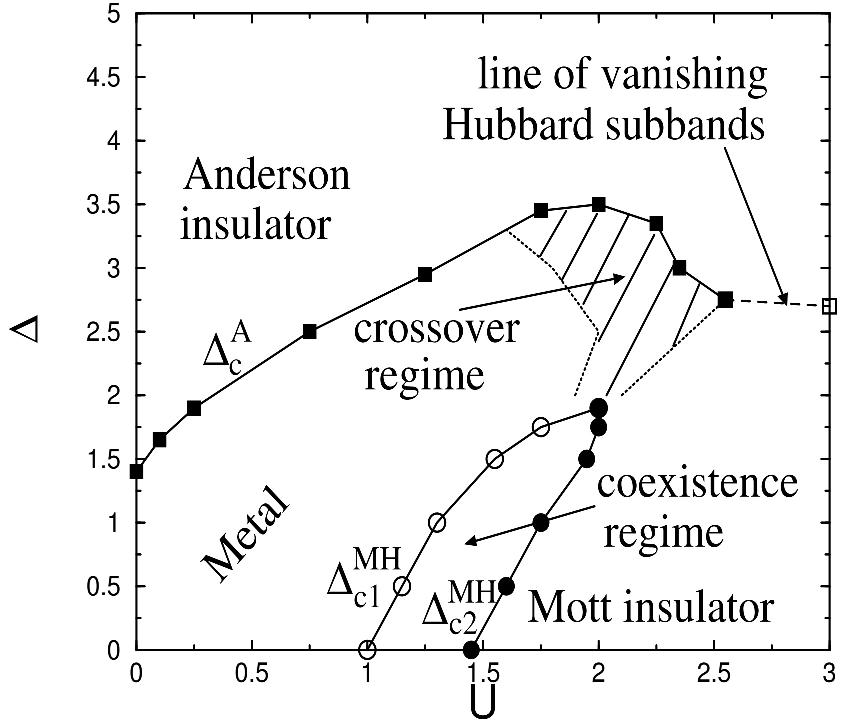
$$G^{-1}(\omega) = \omega - \eta(\omega) - \Sigma(\omega), \qquad \eta(\omega) = \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{\omega - \epsilon_{\mathbf{k}}}$$

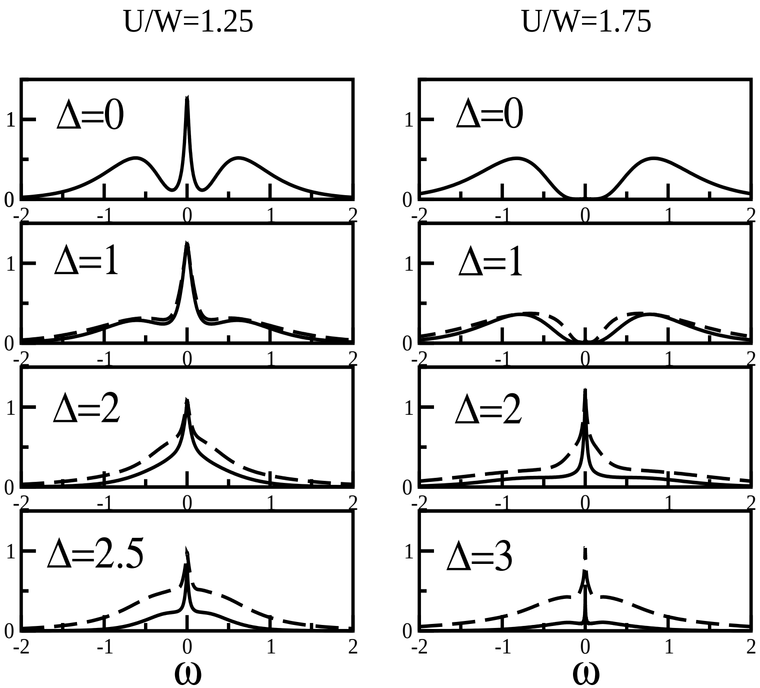
$$G(\omega) = \int d\epsilon \frac{N_0(\epsilon)}{\omega - \epsilon - \Sigma(\omega)}$$

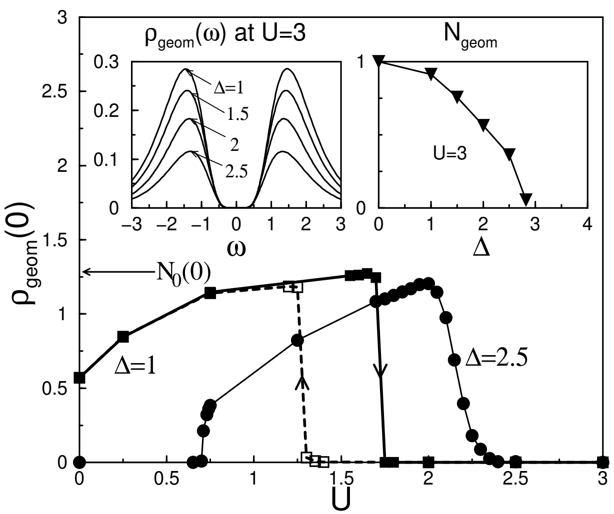
Paramagnetic phase diagram for disordered Hubbard model

(NRG solver, PM phase, $n = 1$, $T = 0$, Bethe DOS)

- Metallicity stabilized by U and Δ
- Mott gap closed by disorder, reentrant Mott-Hubbard MIT
- Anderson localization U-dependent (effective band-width)
- Luttinger (FL) due to U
- Hysteresis and crossover
- Insulators adiabatically connected







Antiferromagnetic phase of disordered Hubbard model

- Neel order: bipartite lattice (A,B)
- Due to symmetry $G^B_{-\sigma}(\omega) = G^A_\sigma(\omega) \equiv G_\sigma(\omega)$
- Lattice Green function

$$G_{\mathbf{k}\sigma}(\omega) = \begin{pmatrix} \xi^A_\sigma(\omega) & -\epsilon_{\mathbf{k}} \\ -\epsilon_{\mathbf{k}} & \xi^B_\sigma(\omega) \end{pmatrix}^{-1}$$

$\xi^{A/B}_\sigma(\omega) = \omega + \mu - \Sigma^{A/B}_\sigma(\omega)$

- for Bethe DOS: $\eta_\sigma(\omega) = t^2 G_{-\sigma}(\omega)$

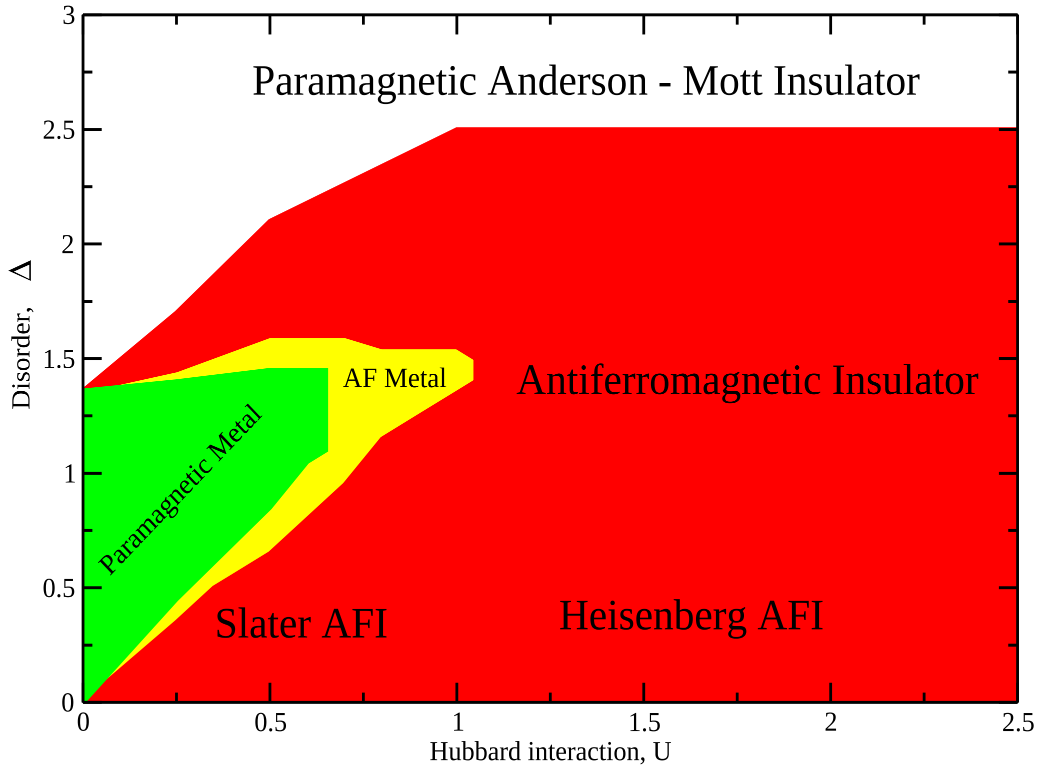
We calculate:

- spectral function $A^{A/B}(\omega) = \rho_g^{A/B}(\omega)$
- total DOS at Fermi level $N(0)$
- staggered magnetization $m_{\text{st}} = |n_{A\uparrow} - n_{B\downarrow}|$

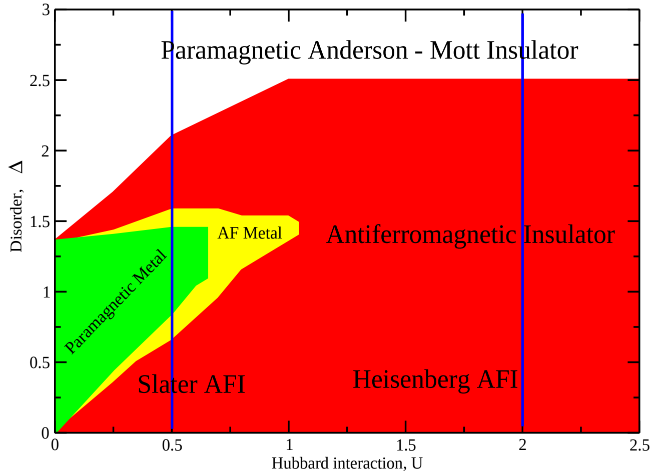
Antiferromagnetic phase diagram for disordered Hubbard model

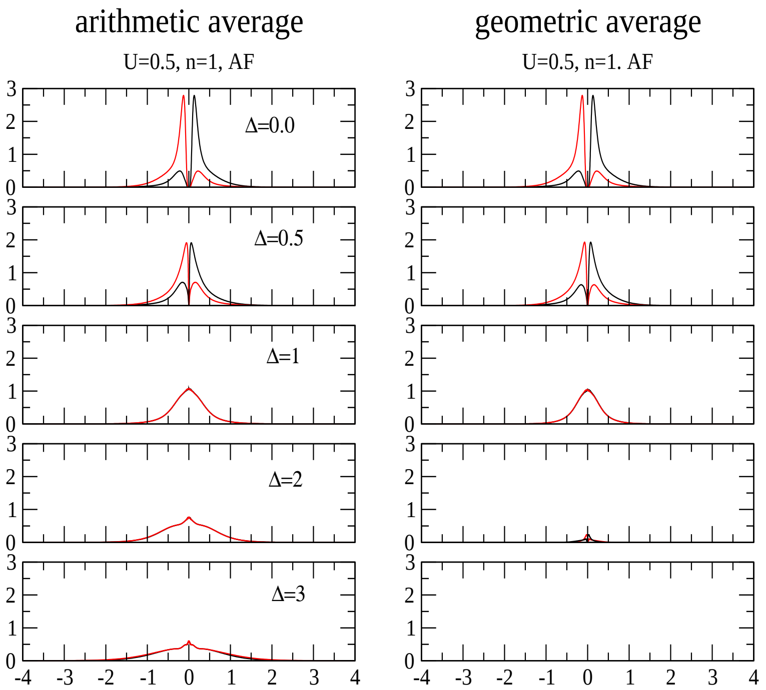
(NRG solver, AF phase, $n = 1$, $T = 0$, Bethe DOS)

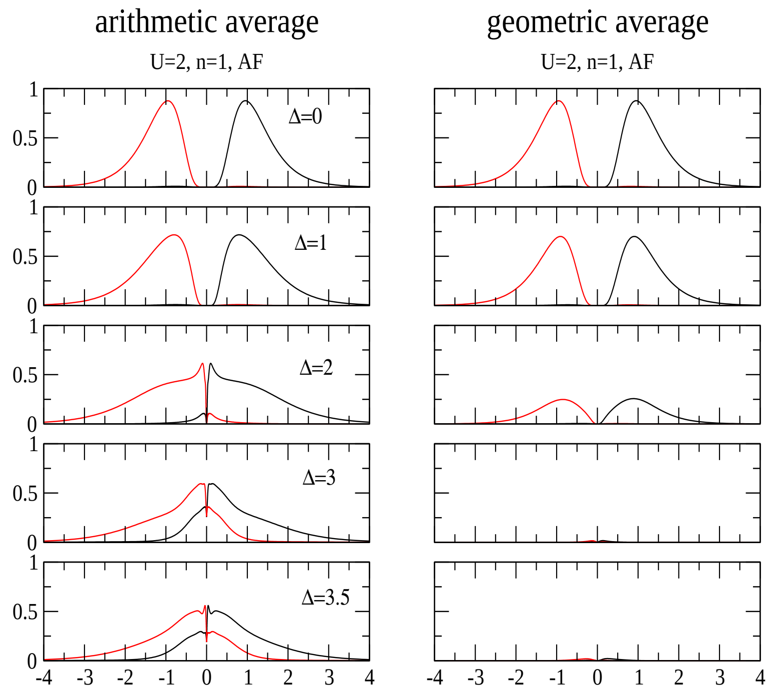
- Metallicity stabilized by U and Δ
- Slater AF insulator - AF metal transition (small U)
- Heisenberg AF insulator stable (large U)



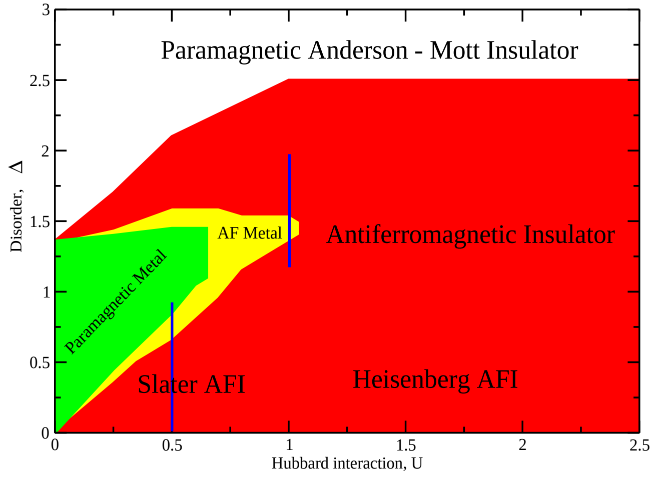
AF - spectral functions

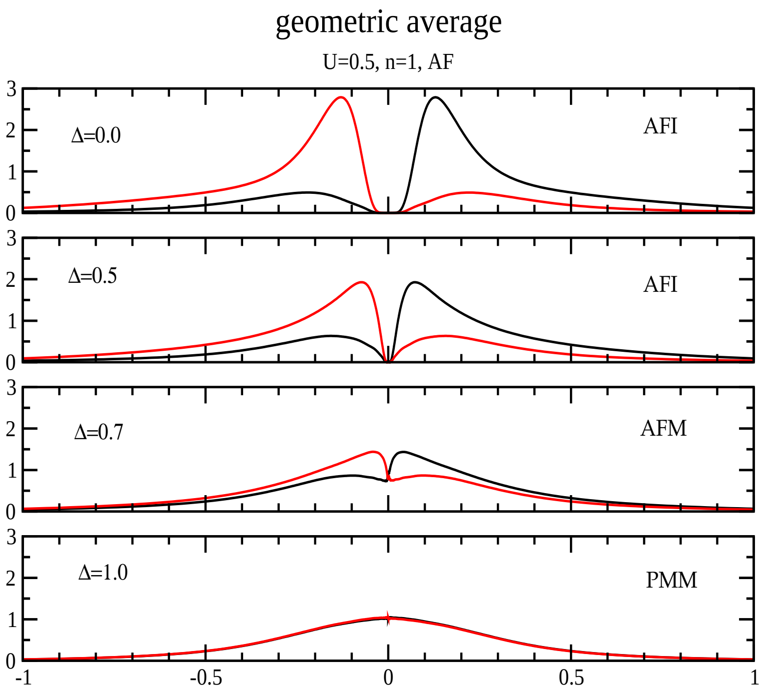


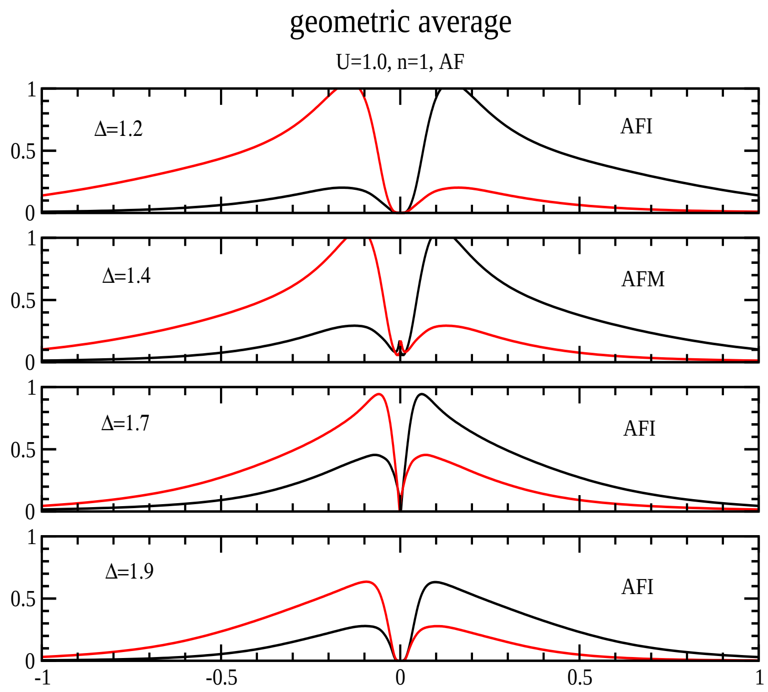




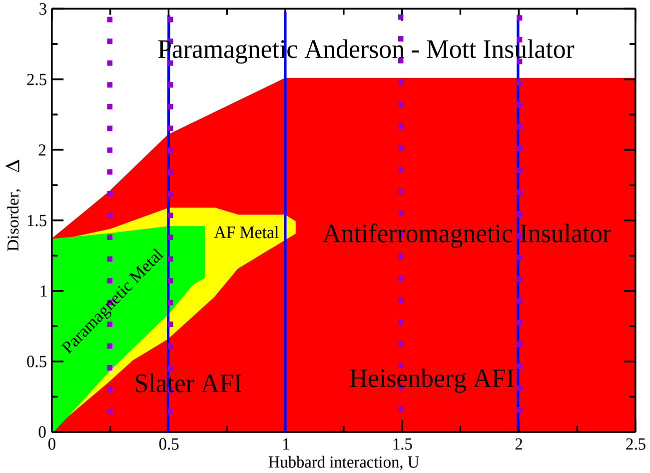
AF - spectral functions

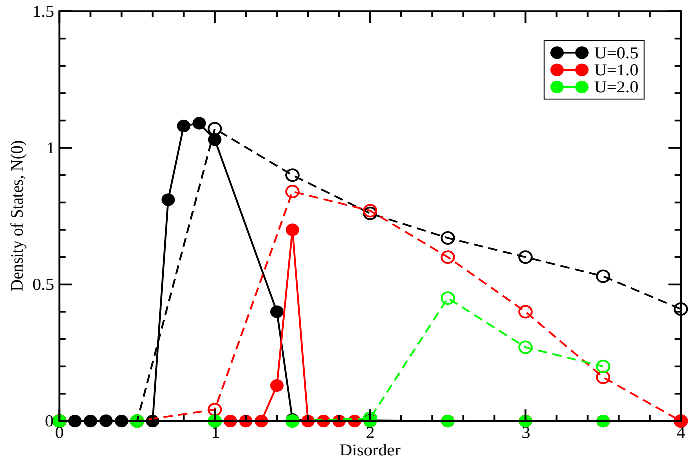




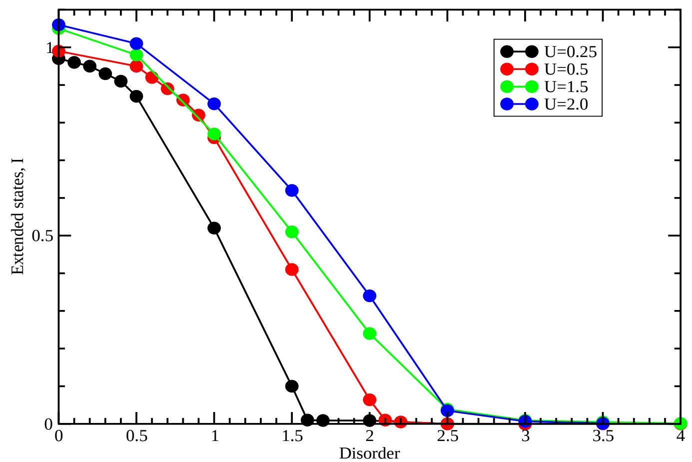


AF - Metal - insulator transition and Anderson localization

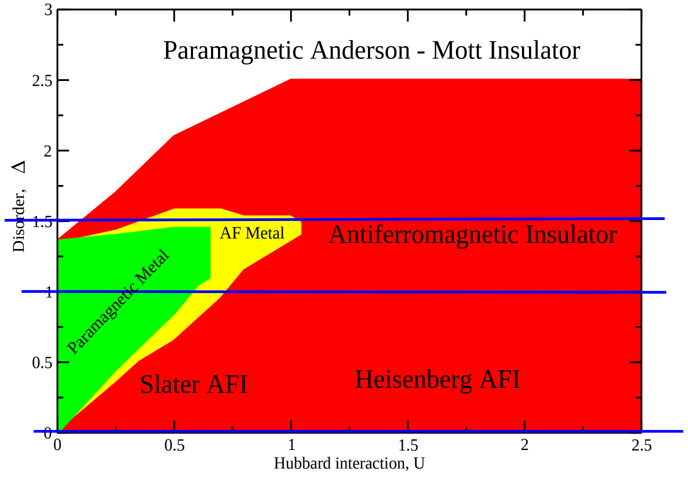


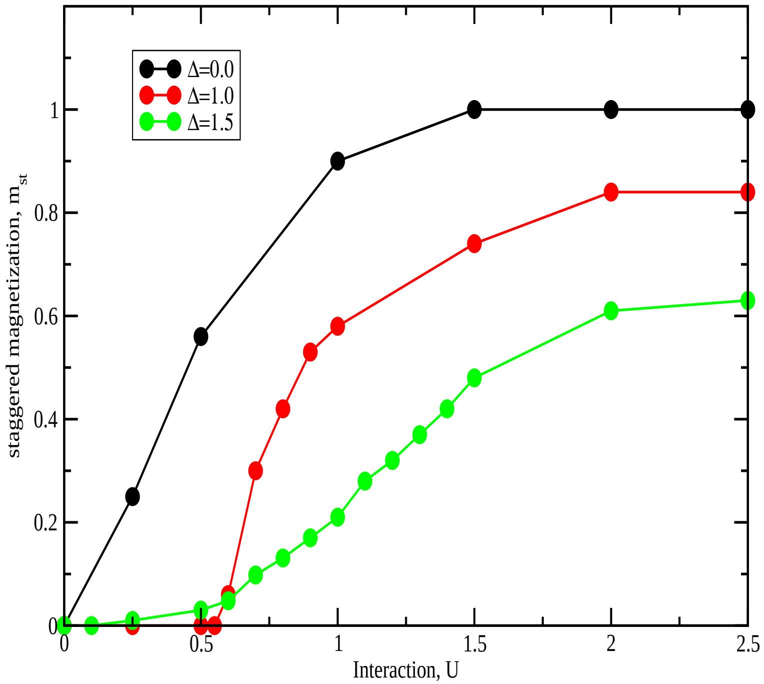


$$I = \int_{-\infty}^{\infty} d\omega \rho_g(\omega)$$

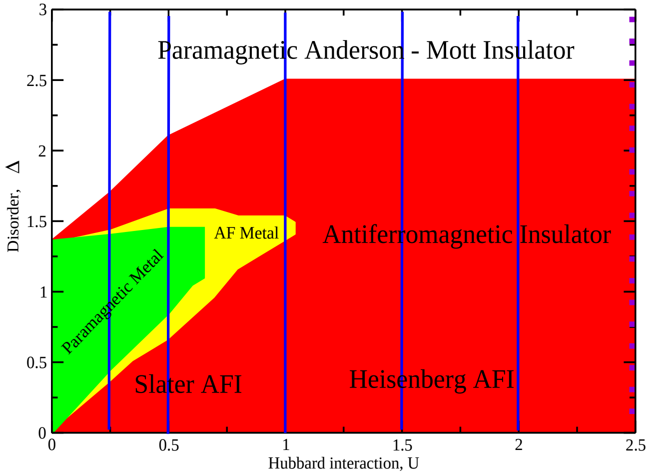


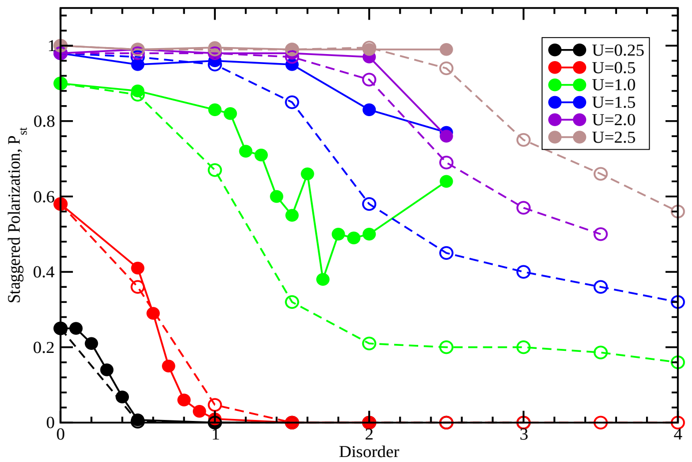
AF - staggered magnetization vs. U

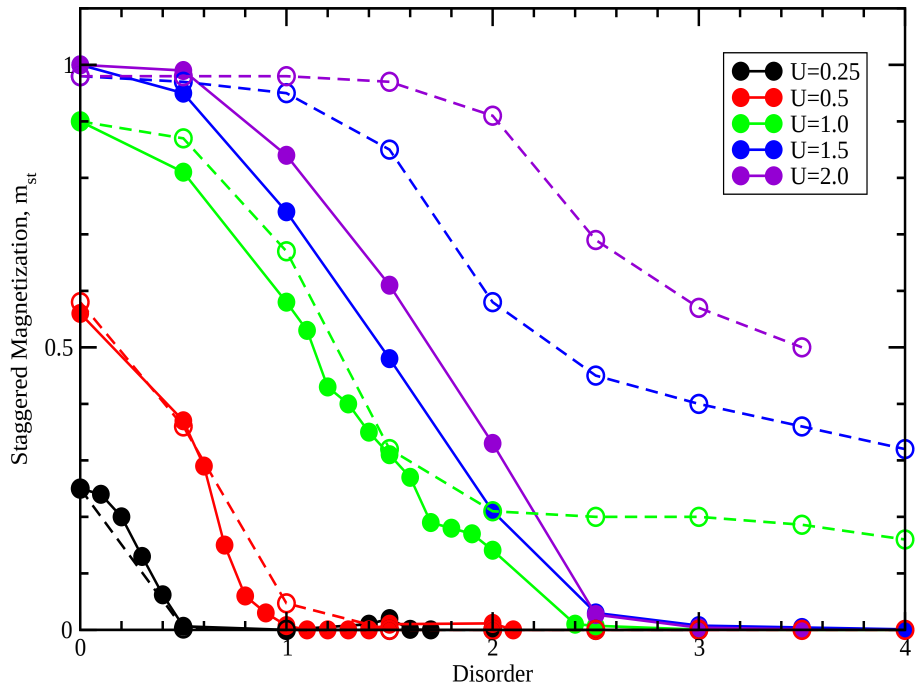




AF - staggered magnetization vs. Δ







$$P_{\rm st} = \frac{m_{\rm st}}{I}$$

Where to look for?

Most of Mott insulators are antiferromagnetically ordered, e.g. V_2O_3 or NiS_2
Disorder induced by doping $(V,Cr)_2O_3$, $(V,Ti)_2O_3$ or stechiometry $Ni(S,Se)_2$

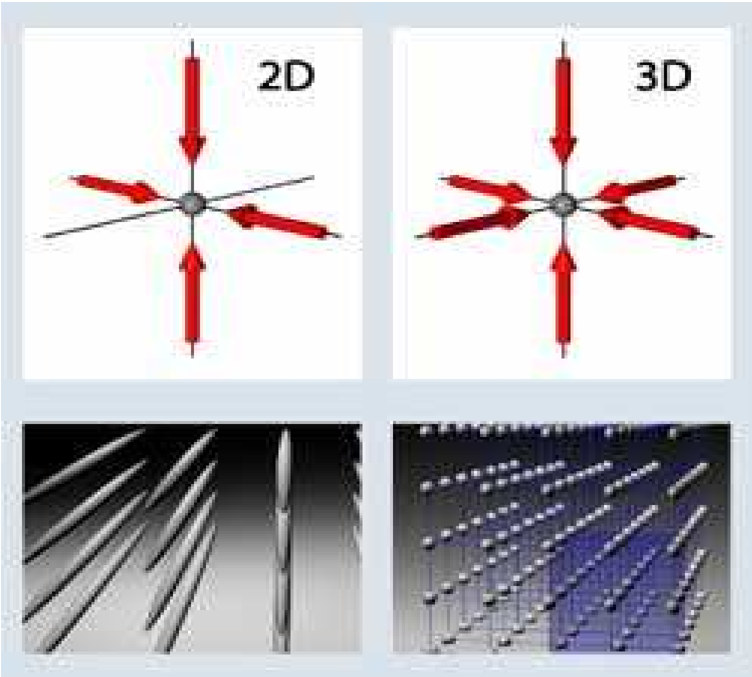
but this is never under full control over wide range of parameters as we would wish

Is there our idealistic model somewhere in Nature?

Optical lattices filled with bosons or fermions

Greiner et al. 02, and other works

atomic trap and standing waves of light create optical lattices $a \sim 400 - 500nm$

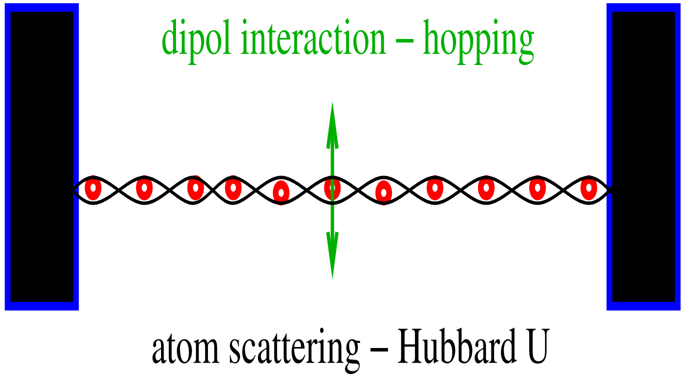


alkali atoms with ns^1 electronic state $J = S = 1/2$

$$\mathbf{F} = \mathbf{J} + \mathbf{I}$$

^{87}Rb, ^{23}Na, ^{7}Li - $I = 3/2$: effective bosons

^{6}Li - $I = 1$, ^{40}K - $I = 4$: effective fermions

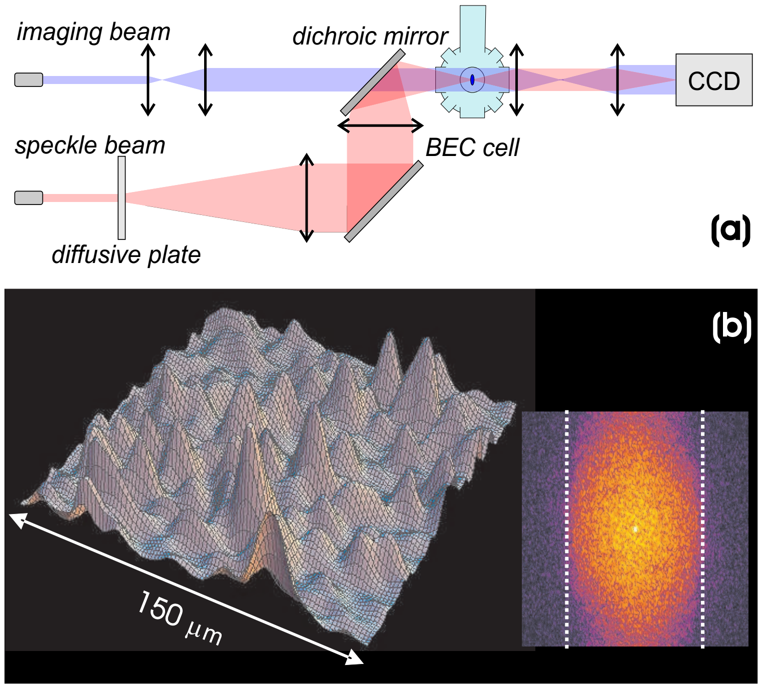


$$H = J \sum_{ij} a^{\dagger}_{i\sigma} a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Optical lattices with random disorder

Lye et al. 05', and other works

- impurity atoms
- superposition of waves with different amplitudes (pseudo-random)
- speckle laser field on top of lattice (good random distribution)
- atom chips



$$H = J \sum_{ij} a^{\dagger}_{i\sigma} a_{j\sigma} + \sum_i \epsilon_i n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Conclusions and outlook

- Geometrical means used to study Anderson MIT in correlated electron system within DMFT
- Complete phase diagrams
- PM case: Two insulators connected continuously
- PM and AF cases: Interaction and disorder compete with each other stabilizing the metallic phase against the occurring one of the insulators
- AF case: AFI-AFM-PMM-PMAI transitions
- AF case: at strong coupling $(U > 1)$ AF LRO robust against disorder
- Optical lattices seem promising to test out theory