# Long-range order and metal-insulator transitions in correlated electron systems with local disorder

Krzysztof Byczuk

Institute of Theoretical Physics
Department of Physics, University of Warsaw
and
Center for Electronic Correlations and Magnetism
Augsburg University

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# Collaboration

- Dieter Vollhardt - Augsburg University, Germany
- Walter Hofstetter - Frankfurt, Germany
- Martin Ulmke - FGAN - FKIE, Wachtberg, Germany
- Unjong Yu - Louisiana, US

**Binary alloy disorder and ferromagnetism in the Hubbard model**

Phys. Rev. Lett. **90**, 196403 (2003)
Phys. Rev. B **69**, 045112 (2004)
Eur. Phys. J. B **45**, 449 (2005)

**Binary alloy disorder and ferromagnetism in the periodic Anderson model**

Phys. Rev. Lett. **100**, 246401 (2008)
Phys. Rev. B **78**, 205118 (2008)

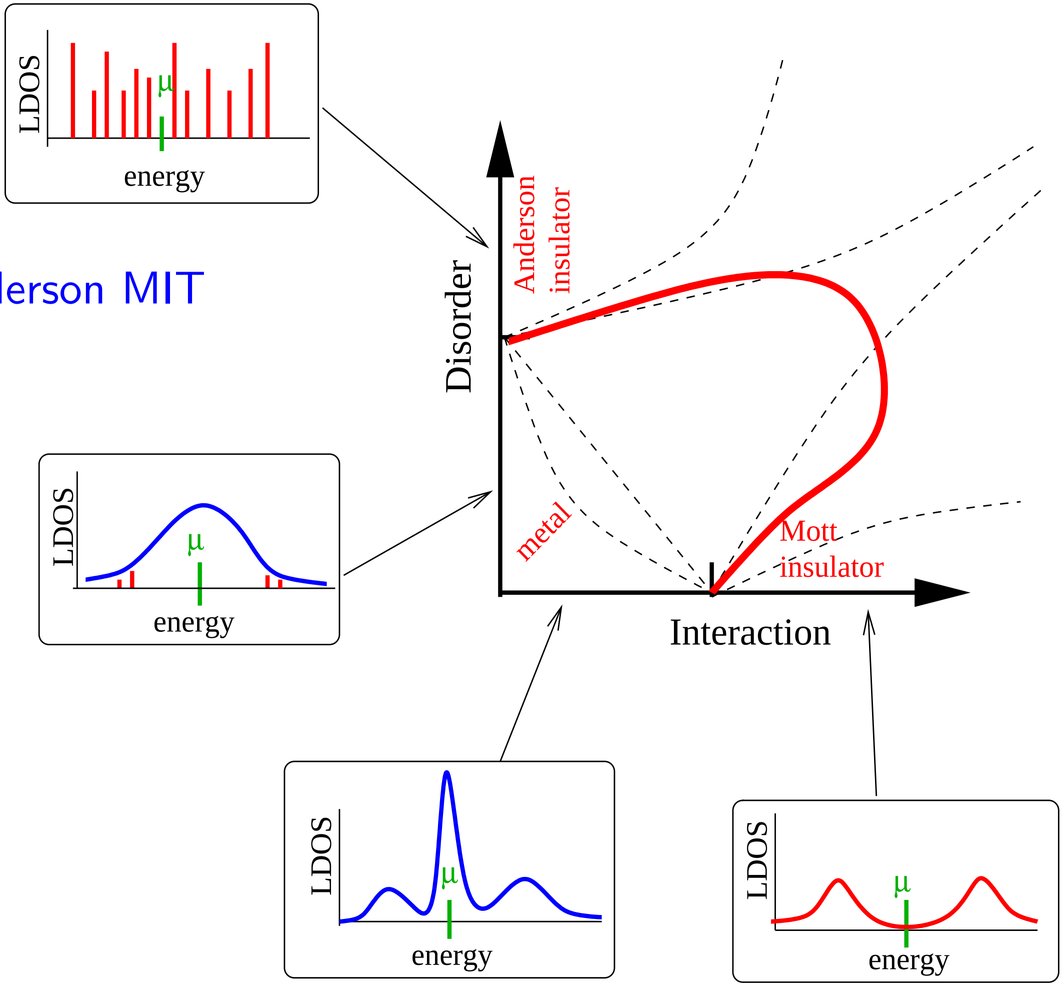
**Continuous disorder and antiferromagnetism in the Hubbard model**

Phys. Rev. Lett. **94**, 056404 (2005)
Physica B **359-361**, 651 (2005)
Phys. Rev. B **71**, 205105 (2005)
Phys. Rev. Lett. **102**, 146403 (2009)

Support from SFB 484

# Continuous disorder as a probe of correlations

Disorder ↔ Anderson MIT




Two insulators are

continuously connected

BUT

Interaction ↔ Mott-Hubbard MIT

i) Interaction and disorder compete with each other

ii) Protects metallic phase against insulators

# Hubbard model with disorder

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

- Interaction $U$
- Randomness $\epsilon_i$ with box PDF

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

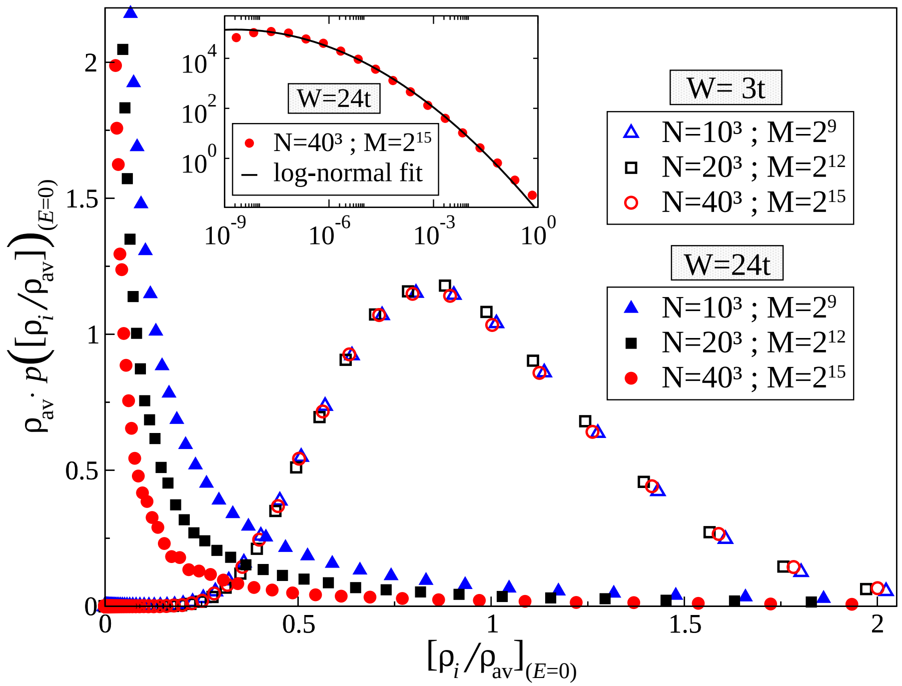
  and zero otherwise
- $t_{ij}$ hopping on a lattice, semielliptic bare DOS with $W = 1$
- DMFT treats the interaction $U$ accurately
- CPA arithmetic averaging over $\epsilon_i$ does not describe Anderson localization

# Typical vs. averaged behavior

Large disorder:

- PDF of DOS is very broad with long tails
- Typical DOS differs from its arithmetic average

Typical LDOS is approximated by geometrical mean $\rho_{typ}(E) \approx \rho_{geom}(E) = e^{\langle \ln \rho_i(E) \rangle}$



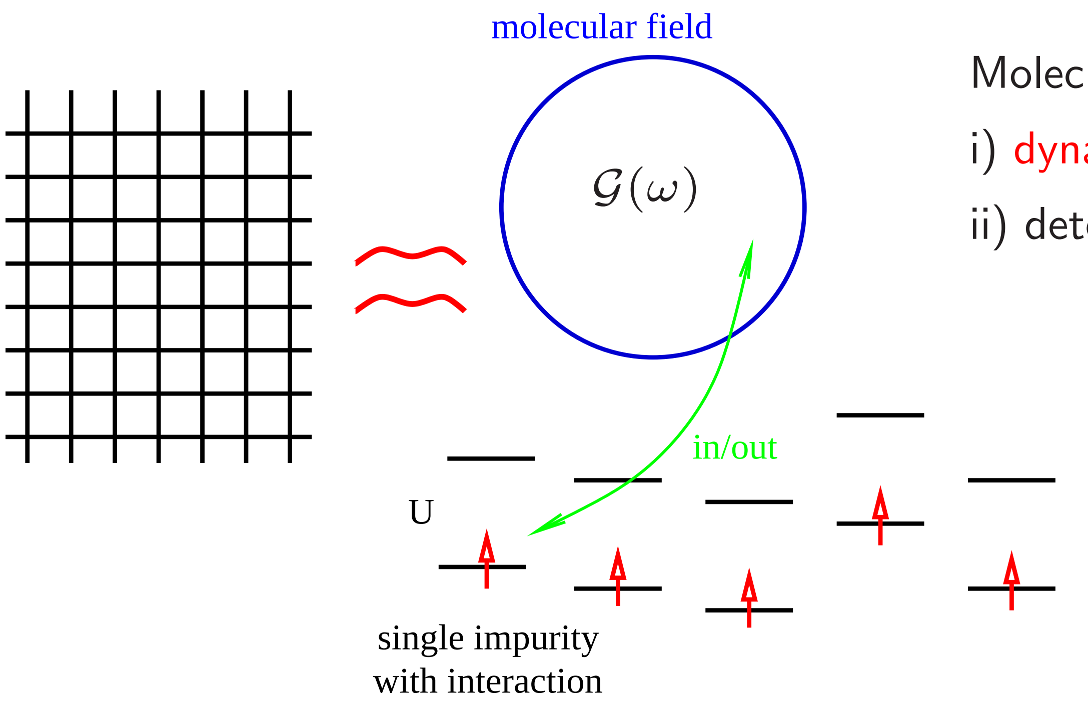

*Schubert, Weisse, Wellein, Fehske, cond-mat/0309015*

# Correlations ($U$) and disorder ($\Delta$): Dynamical mean-field theory

*KB, Hofstetter, Vollhardt, Phys. Rev. Lett. 94, 056404 (2005)*
after idea from: *Dobrosavljevic, Pastor, Nikolic, Europhys. Lett. 62, 76 (2003)*

Lattice problem of interacting particles is mapped onto

an ensemble of single impurities (single atoms)




Molecular (Weiss) function $\mathcal{G}(\omega)$:

i) dynamical quantity,

ii) determined self-consistently

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

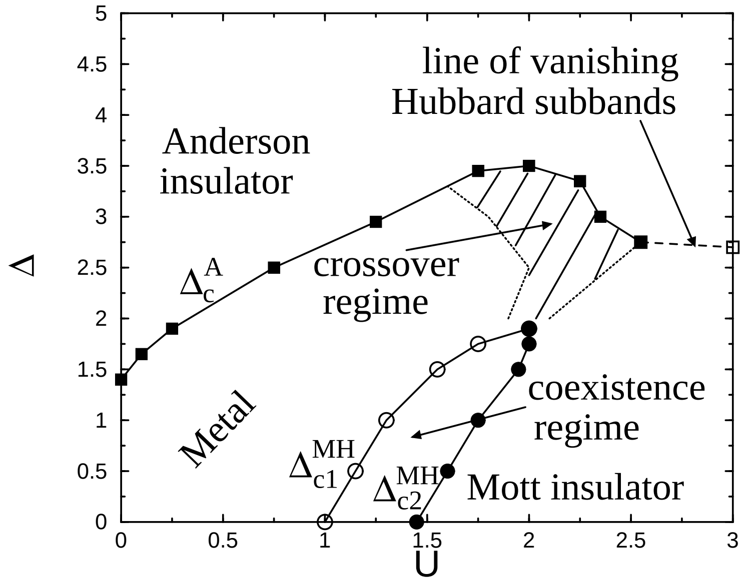
$$H = \sum_{i\sigma} \epsilon_i n_{i\sigma} + \sum_{ij\sigma} t_{ij}\, a^{\dagger}_{i\sigma} a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

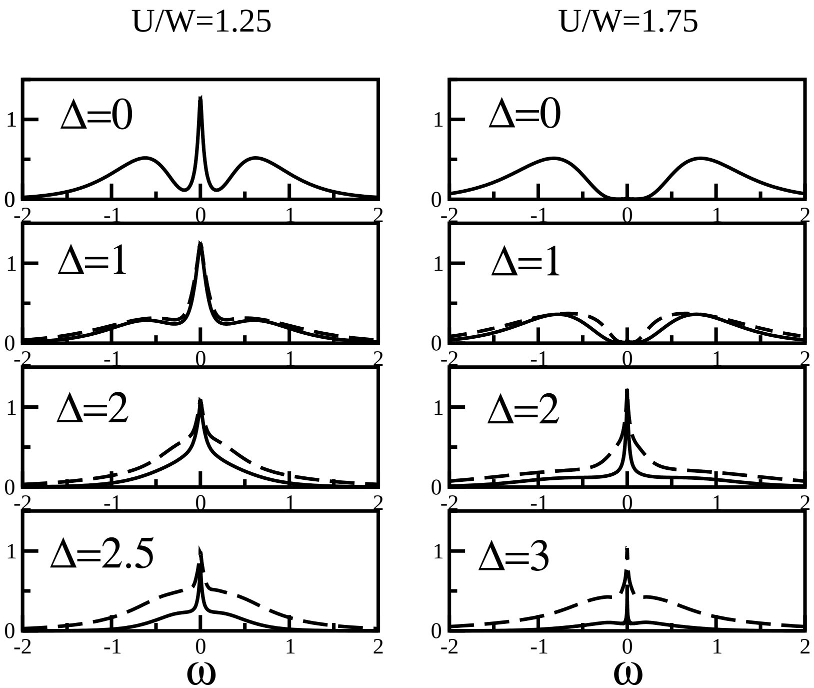
Cf. *Aguiar, Dobrosavljevic, Abrahams, Kotliar, Phys. Rev. Lett. 102 156402 (2009); Song, Wortis, Atkinson, Phys. Rev. B 77 054202 (2008); Alvermann, Fehske, Eur. Phys. J. B 48, 295 (2005)*

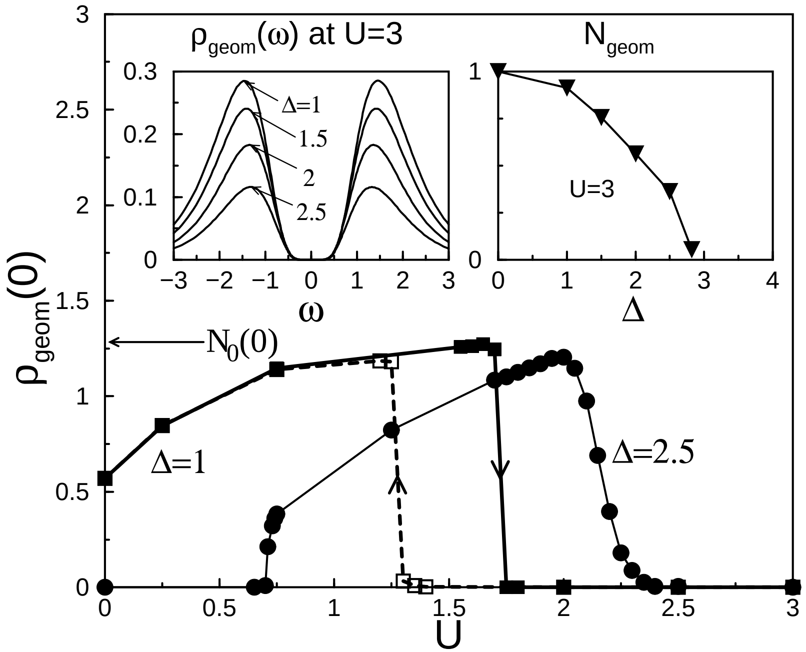
# Paramagnetic phase diagram for disordered Hubbard model

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

- Metallicity stabilized by $U$ and $\Delta$
- Mott gap closed by disorder, reentrant Mott-Hubbard MIT
- Anderson localization $U$-dependent (effective band-width)
- Luttinger theorem
- Hysteresis and crossover
- Insulators adiabatically connected



# Antiferromagnetic phase diagram for disordered Hubbard model

*KB, Hofstetter, Vollhardt, Phys. Rev. Lett. 102, 146403 (2009)*

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

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

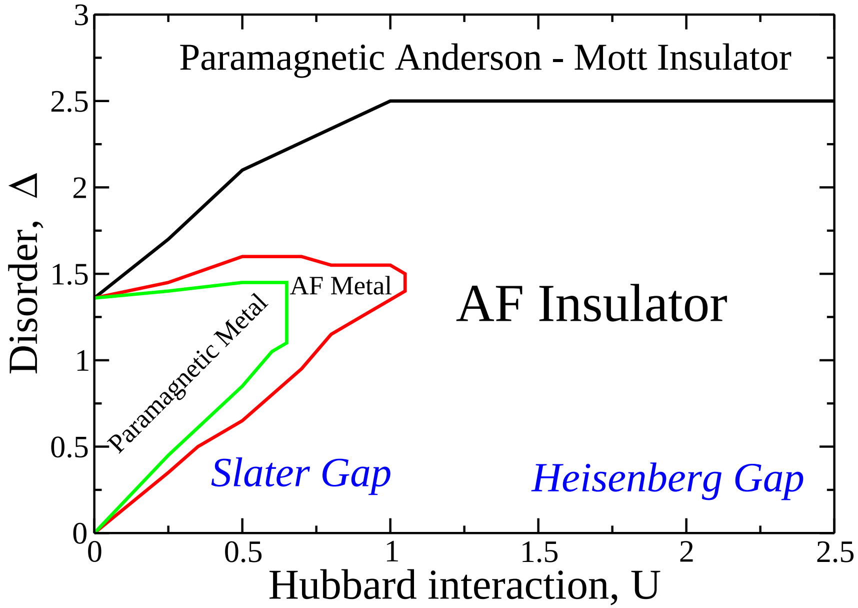
  $\xi^{A/B}_\sigma(\omega) = \omega + \mu - \Sigma^{A/B}_\sigma(\omega)$
- for Bethe DOS: $\eta_\sigma(\omega) = t^2 G_{-\sigma}(\omega)$

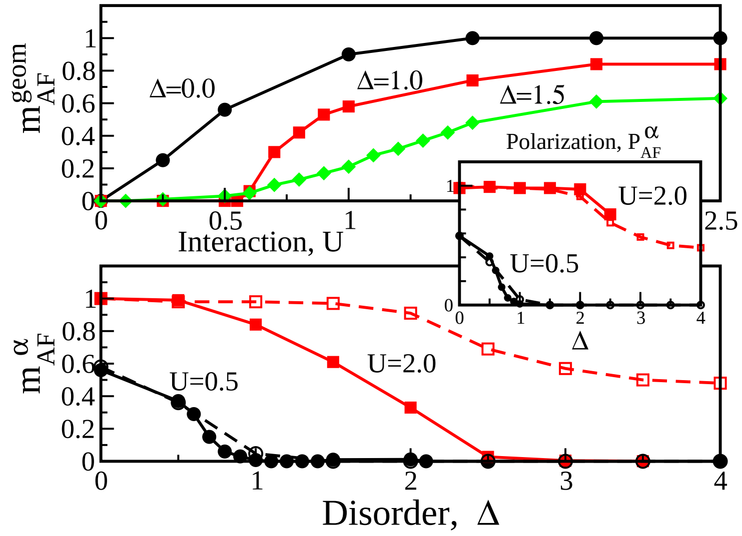
We calculate:

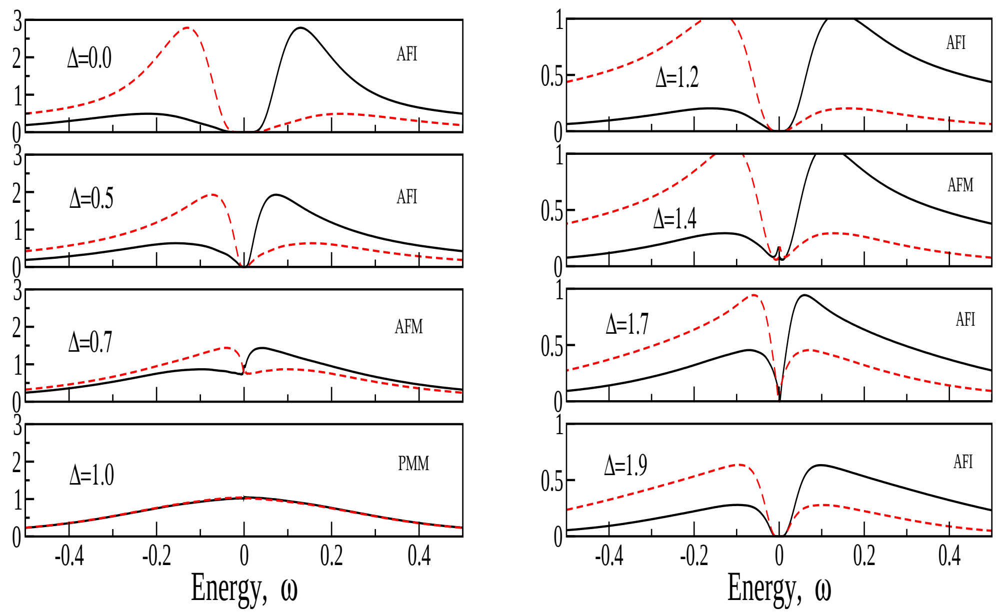
- spectral function $A^{A/B}(\omega) = \rho^{A/B}_g(\omega)$
- total DOS at Fermi level $N(0)$
- staggered magnetization $m_{\mathrm{st}} = |n_{A\uparrow} - n_{B\downarrow}|$

# Mott-Anderson MIT with AF long-range order

*K.B., Hofstetter, Vollhardt, Phys. Rev. Lett. 102, 146403 (2009)*




No phase transition between Slater and Heisenberg limits

**BUT**

AF and PM metals only in Slater limit with disorder

# Summary and outlook

- Disorder leads to a manifold of effects in correlated electron systems:
- Continuous disorder (this talk)
  - Enhances metallicity
  - Acts differently in Slater and Heisenberg AFs
- Binary alloy disorder (our other works)
  - Can enhance Curie temperature in itinerant ferromagnets
  - Can lead to MIT at non-integrer electron densities