Quantifying correlation and effects of disorder in the Hubbard model

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Collaboration

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- Walter Hofstetter - Frankfurt, Germany
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- 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)

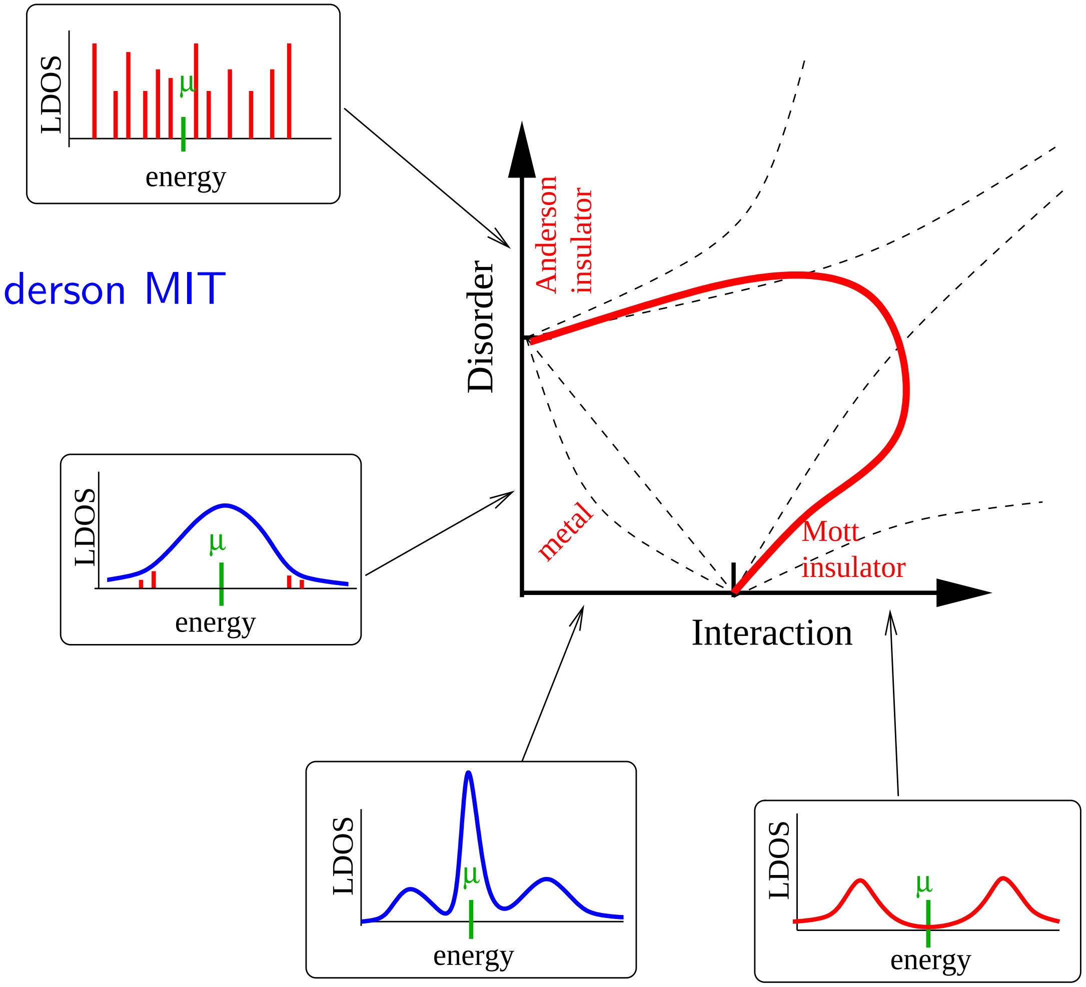
Continuous disorder and antiferromagnetism in the Hubbard model

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

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

- Interaction U
- Randomness ϵ_i with box PDF

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

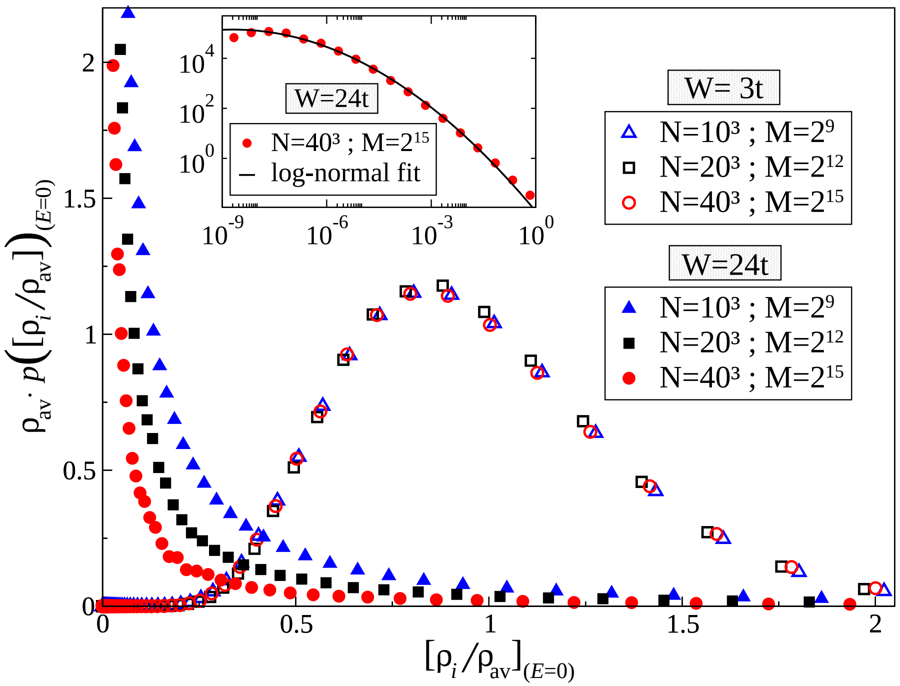
  and zero otherwise
- t_{ij} hopping on a lattice, semielliptic bare DOS with $W = 1$
- DMFT treats the interaction U accurately
- CPA arithmetic averaging over ϵ_i does not describe Anderson localization

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

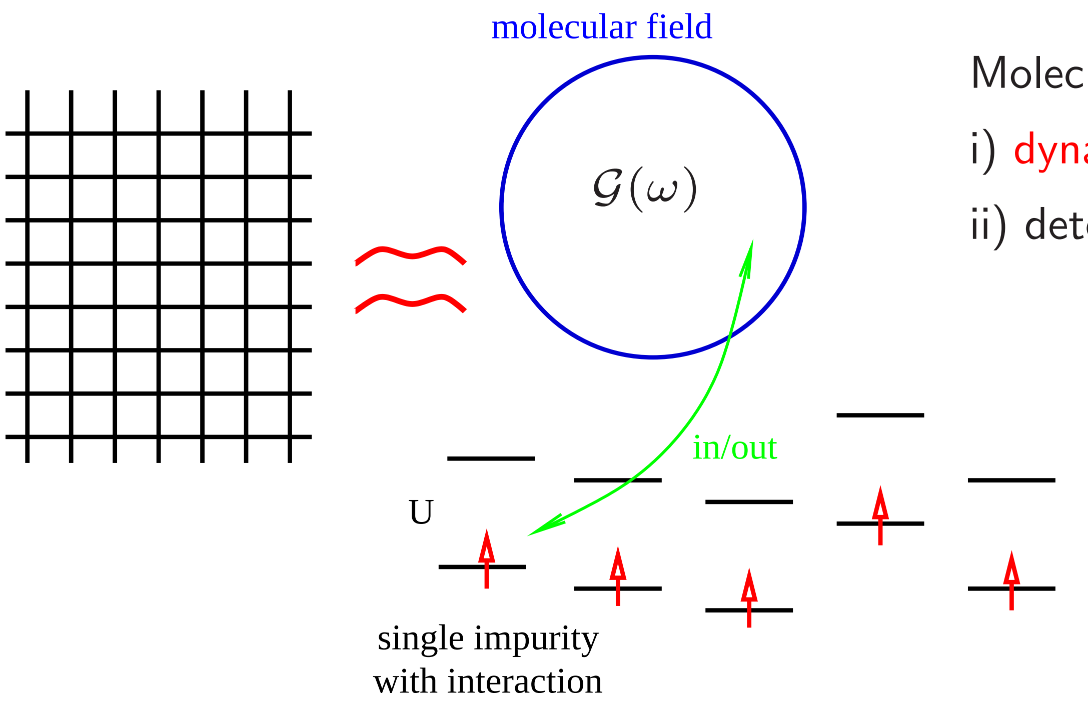


Schubert, Weisse, Wellein, Fehske, cond-mat/0309015

Correlations (U) and disorder (Δ): 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)*

DMFT with Anderson MIT

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

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

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

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

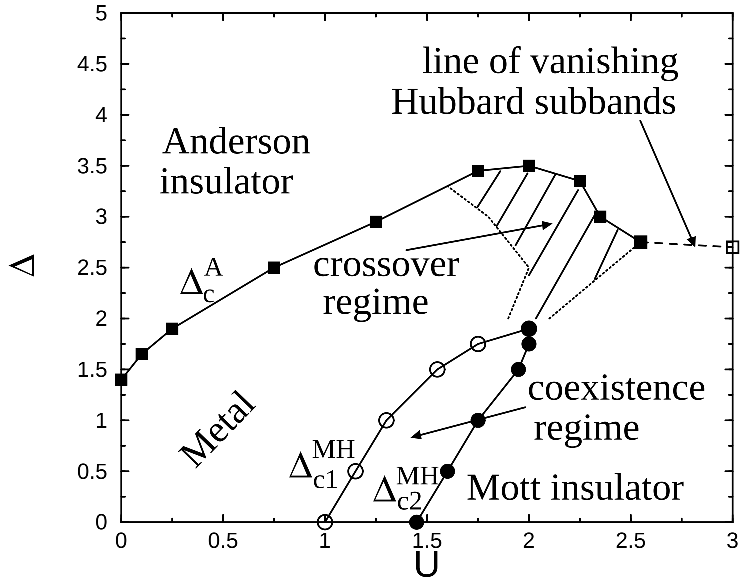
$$G(\omega) = \int d\epsilon \frac{N_0(\epsilon)}{\omega - \epsilon - \Sigma(\omega)}$$

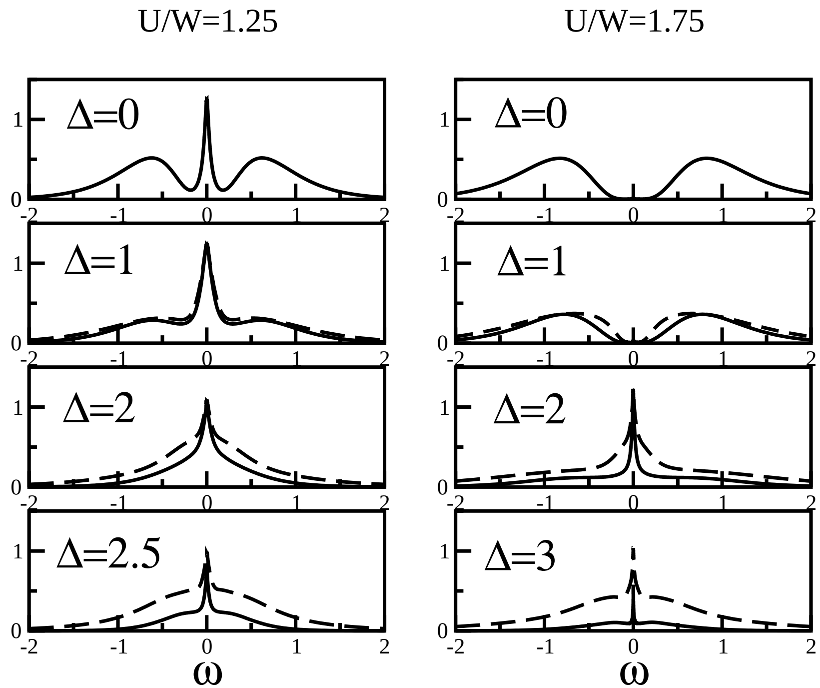
- Method, in spirit of CPA, works with one-particle many-body correlation functions
- Possible extension in the direction KKR-CPA$_{\mathrm{typ}}$-DMFT
  cf. *J. Minar, L. Chioncel, A. Perlov, H. Ebert, M. I. Katsnelson, and A. I. Lichtenstein, Phys. Rev. B 72, 045125 (2005)*

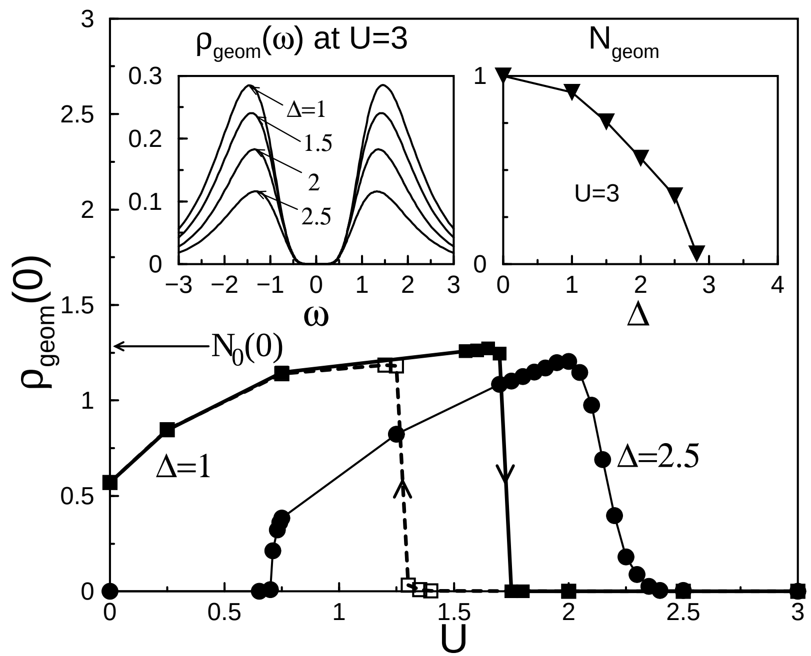
Paramagnetic phase diagram for disordered Hubbard model

(NRG solver, $n = 1$, $T = 0$, 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 theorem
- Hysteresis and crossover
- Insulators adiabatically connected





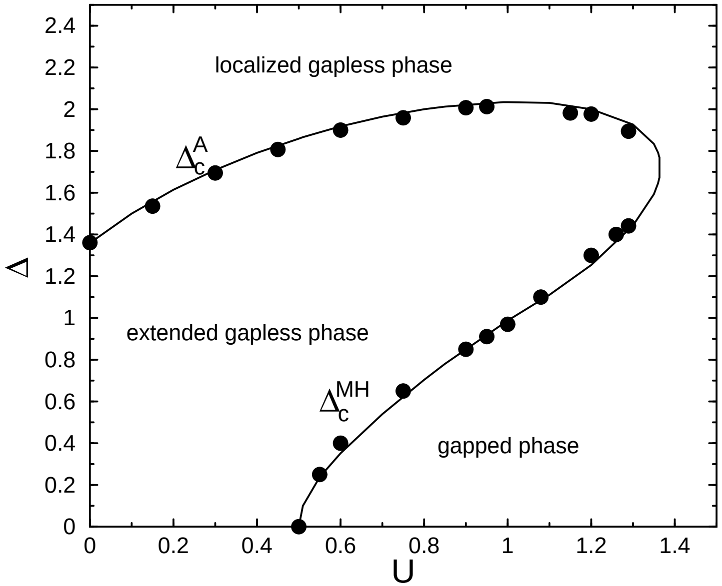


PM phase diagram for disordered Falicov-Kimball model

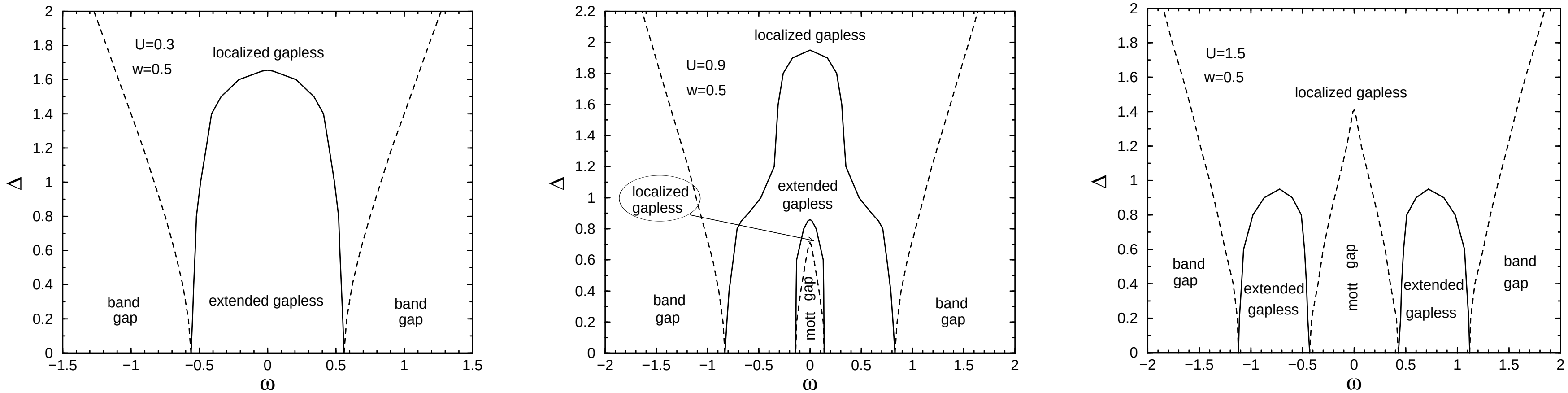
$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_i \epsilon_i c_i^\dagger c_i + U \sum_i f_i^\dagger f_i c_i^\dagger c_i$$

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

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



KB, Phys. Rev. B 71, 205105 (2005)



Also: M.-H. Tran, PR B 76, 245122 (2007), M. A. Gusmao, PR B 77, 245116 (2008)

Antiferromagnetic phase

Many works on AF within DMFT, e.g.:
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
Chitra, Kotliar (1999); Zitzler, Tong, Pruschke, Bulla (2004); Eckstein, Kollar, Potthoff, Vollhardt (2006)
suppression and first order transition

- **How does a full magnetic phase diagram look like?**
- **How does disorder cope with AF LRO?**
- **Anderson localization vs. AF LRO?**

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

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

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

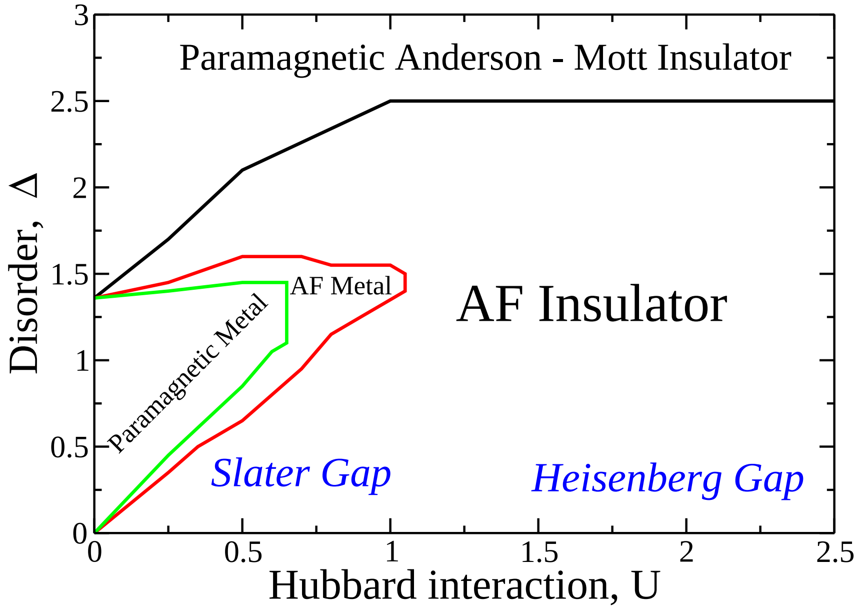
- for Bethe DOS: $\eta_\sigma(\omega) = t^2 G_{-\sigma}(\omega)$

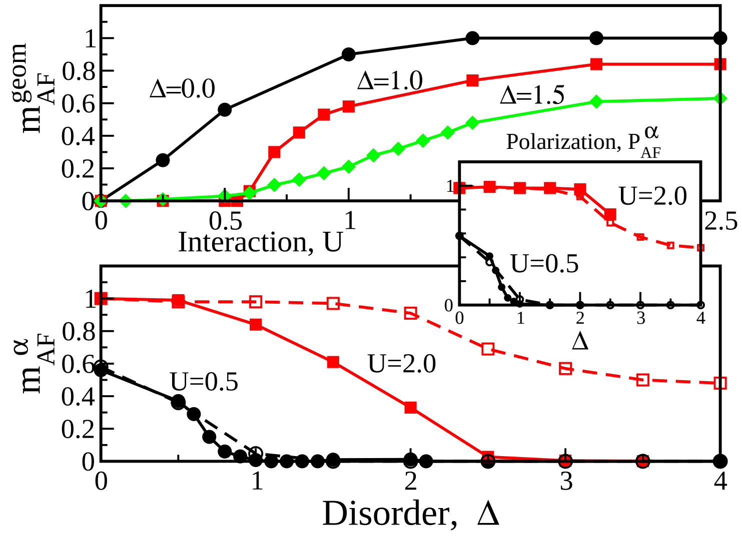
We calculate:

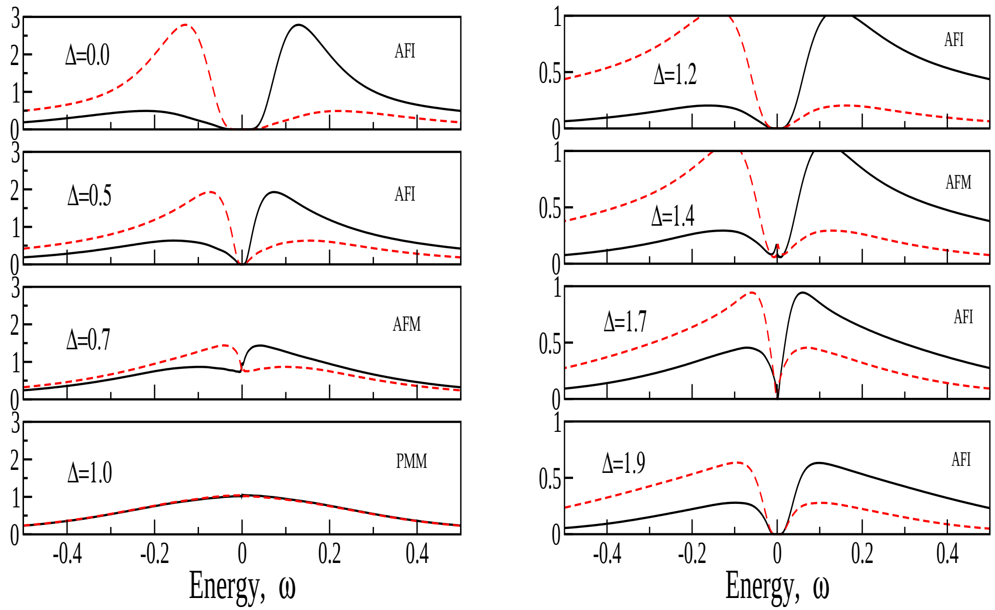
- spectral function $A^{A/B}(\omega) = \rho^{A/B}_g(\omega)$
- total DOS at Fermi level $N(0)$
- staggered magnetization $m_{\mathrm{st}} = |n_{A\uparrow} - n_{B\downarrow}|$

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

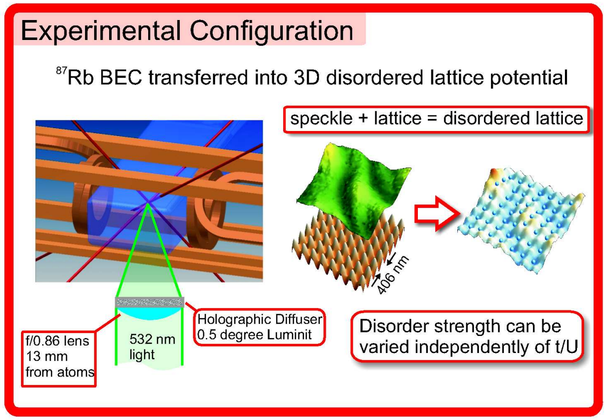
Summary and outlook

- 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

Investigating correlation by controlling disorder in experimental systems

Quantum Simulator with ultra-cold atoms

M. White et al., Phys. Rev. Lett. 102, 055301 (2009)



Efficient cooling problem, cf.

F.Werner, O.Parcollet, A.Georges, S.R.Hassan, Phys. Rev. Lett. 95, 056401 (2005)

A.-M. Dar, L. Raymond, G. Albinet, A.-M.S. Tremblay, Phys. Rev. B 76, 064402 (2007)