Metal-Insulator Transitions in Correlated Electron Systems with Disorder

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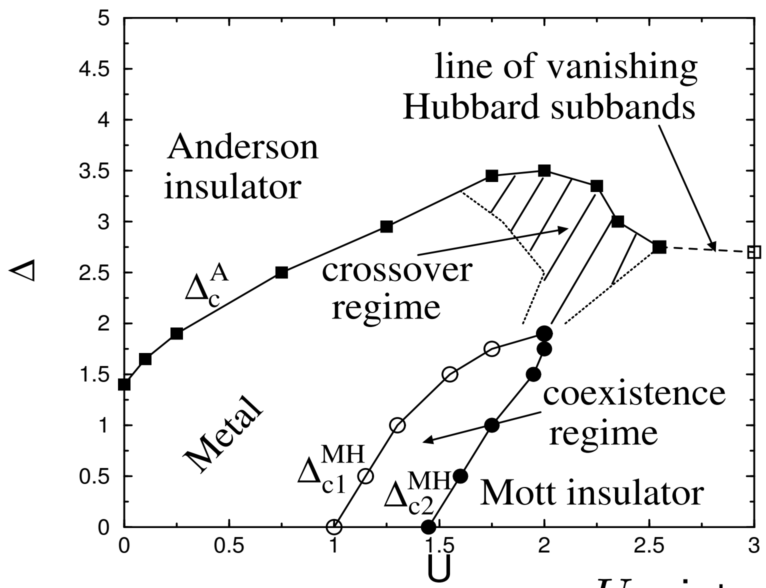
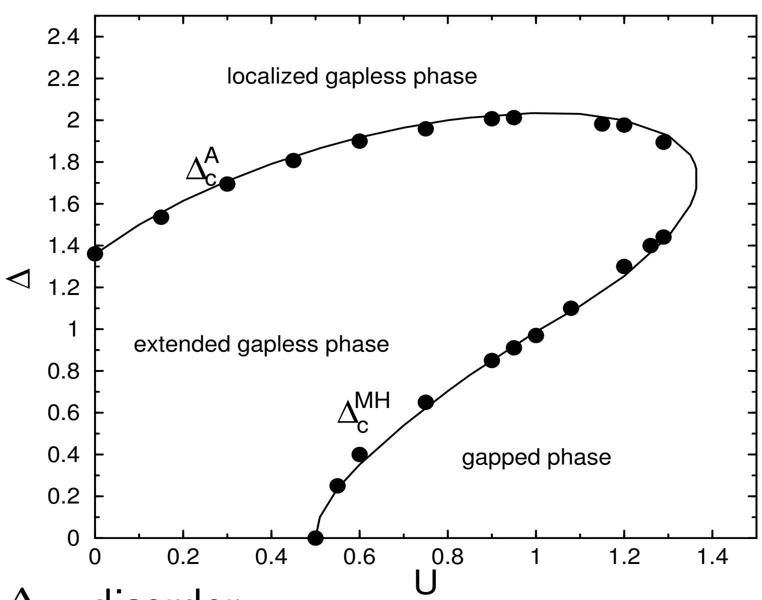
Main goal I

- Interaction $\leftrightarrow$ Mott – Hubbard MIT
- Disorder $\leftrightarrow$ Anderson MIT

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





U - interaction, Δ - disorder

Hubbard model

Falicov-Kimball model

Main goal II

Geometric average

$$O_{\text{geom}} = e^{\langle \ln O_i \rangle_{\text{arith}}}$$

Collaboration

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

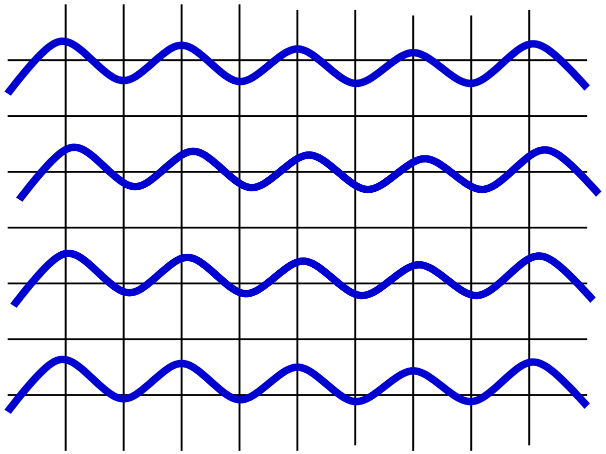
Phys. Rev. Lett.**94**, 056404 (2005); cond-mat/0403765
Physica B **359-361**, 651 (2005); cond-mat/0502257
Phys. Rev. B **71**, 205105 (2005); cond-mat/0412590

Plan of the talk:

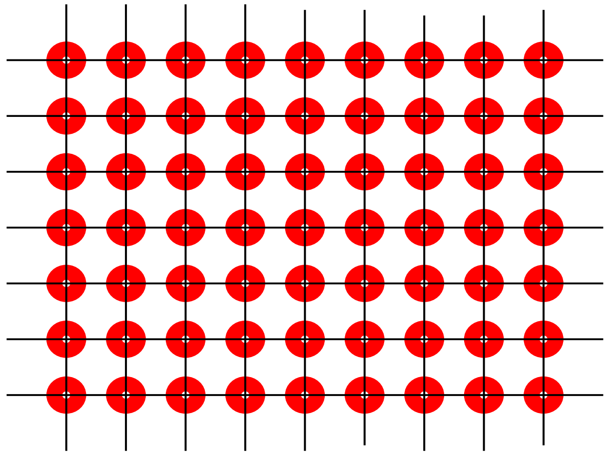
1. Introduction
   - Mott-Hubbard MIT
   - Anderson localization
   - Arithmetic vs. geometric means
2. Model with correlated electrons with disorder - phase diagram and MITs in details
3. Conclusions and outlook

Mott-Hubbard MIT at $n = 1$

$$H = \sum_{i\sigma} \epsilon_0 n_{i\sigma} + \sum_{ij\sigma} t_{ij}\; a^\dagger_{i\sigma} a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



$U \ll |t_{ij}|$, $\mathbf{\Delta p} = 0$



$U \gg |t_{ij}|$, $\mathbf{\Delta r} = 0$

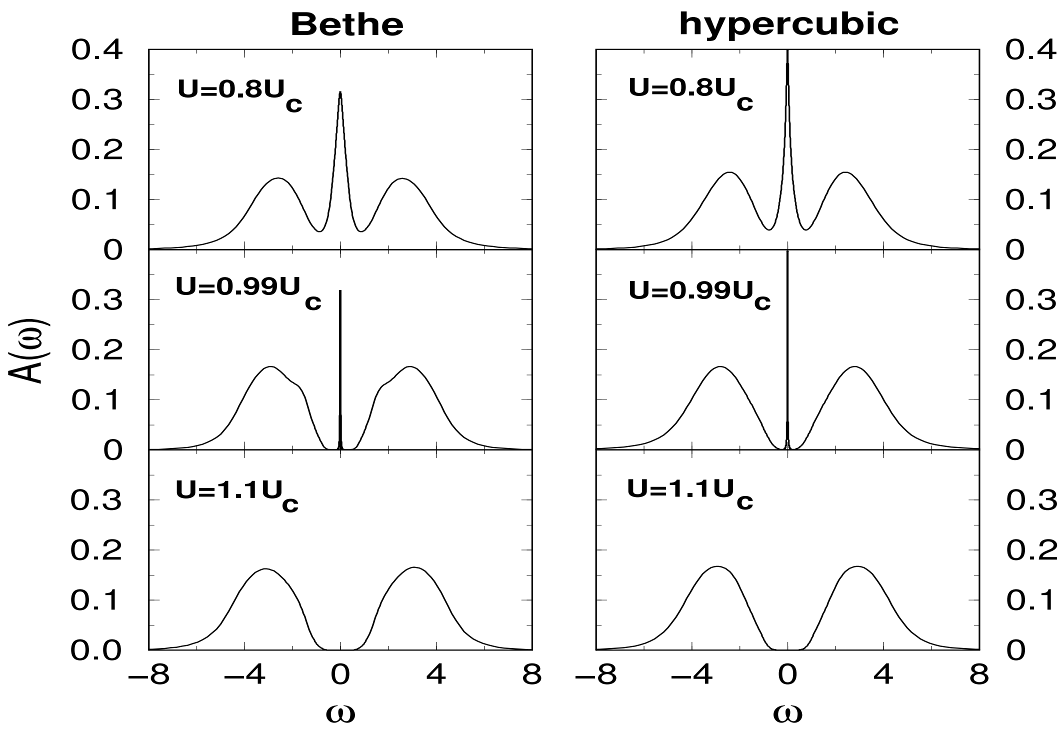
typical intermediate coupling problem $U_c \approx |t_{ij}|$

T=0 Mott transition according to DMFT

quantity to be determined

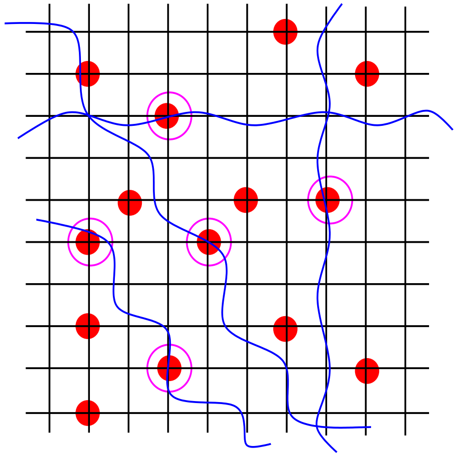
$$A(\omega) = -\frac{1}{\pi}\Im G(\omega)$$

spectral density function



R. Bulla'99 - NRG

Falicov-Kimball model



poor brother/sister of Hubbard model

n_c and n_f independently fixed

$n_c + n_f$ fixed

– mobile particles on a lattice

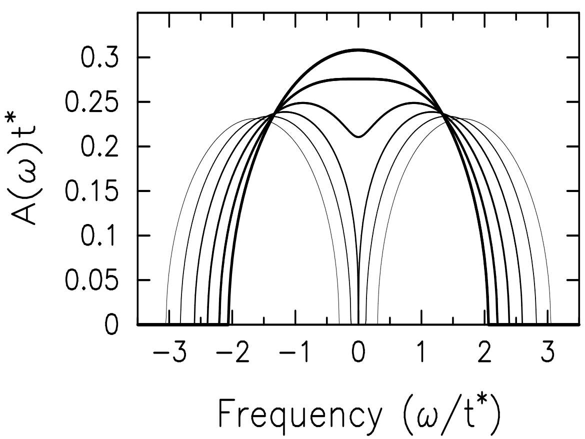
– localized particles on a lattice

– local interaction

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

Mott MIT in Falicov-Kimball model

- f-particles appear as like disorder scatterers (with an annealed averaging).
- No Fermi liquid property of FK model if $n_f \neq 0$ or 1.
- Pseudo-gap regime.
- For $n_e = n_f = 0.5$ and $U = U_c \sim W$ continuous Mott like MIT.
- Correlation gap opened.

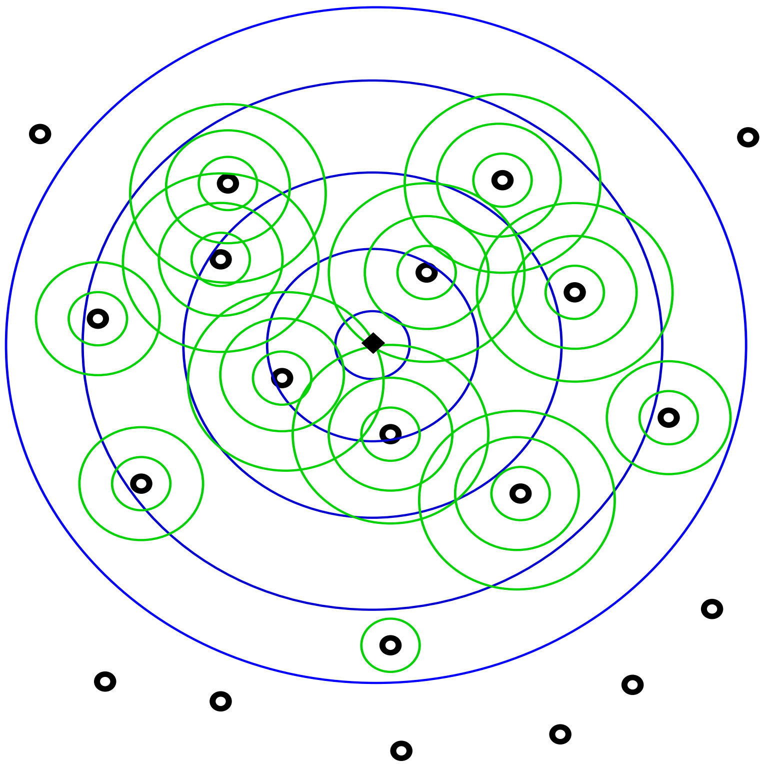


van Dongen and Lainung 1997, DMFT, Bethe, no CDW, $U = 0.5 - 3.0$

Note: Falicov-Kimball (CT) like MIT is when $n_e(T) + n_f(T) = \mathrm{const.}$

Anderson localization

propagation of waves in a randomly inhomogeneous medium



random conservative linear wave equation

$$\frac{\partial^2 w}{\partial t^2} = c(x)^2 \frac{\partial^2 w}{\partial x^2}$$

$$i\frac{\partial w}{\partial t} = -\frac{\partial^2 w}{\partial x^2} + \nu(x) w$$

$$\Psi_{k(E)}(r) \sim \sum_i \sin(kr + \delta_i)$$

Anderson 1958: (no averaging) – strong scattering forms "standing" waves, sloshing back and forth in a bounded region of space

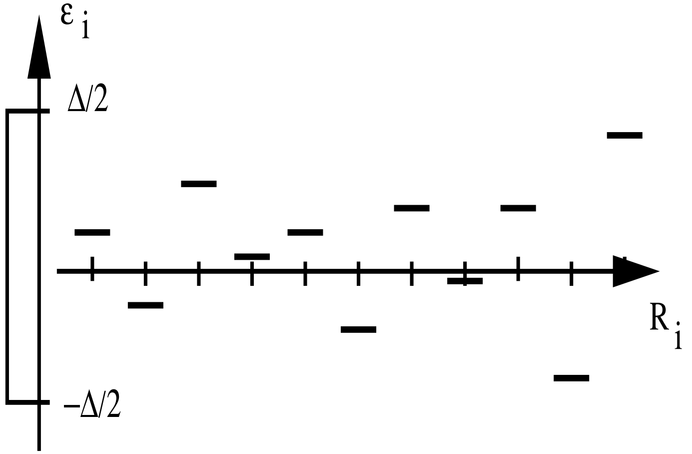
Localization is a destruction of coherent superposition of spatially separated states

Anderson model

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

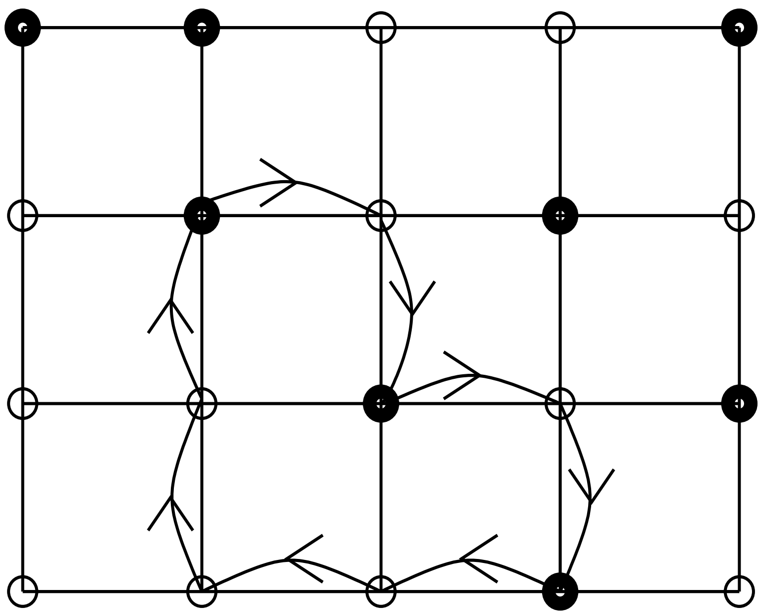
Probability distribution function

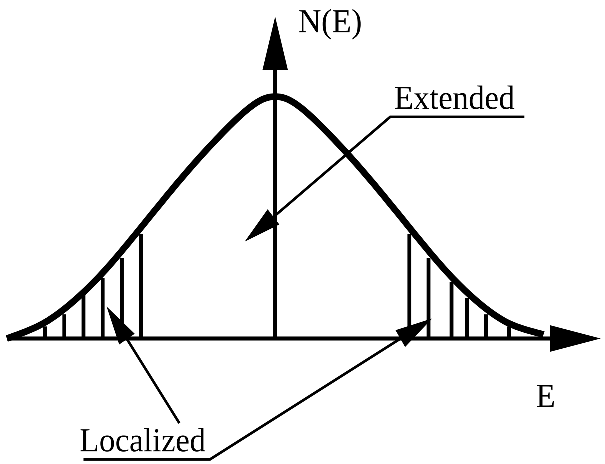
$$\mathcal{P}(\epsilon_i) = \frac{1}{\Delta} \Theta \left(\frac{\Delta}{2} - |\epsilon_i| \right)$$

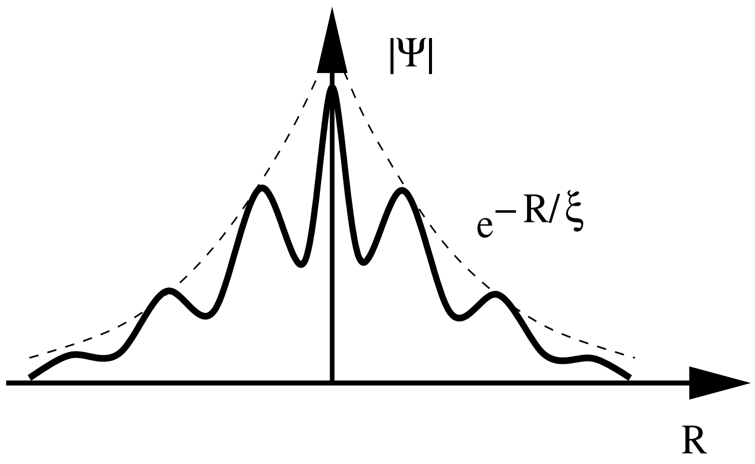


Anderson MIT - cont.

Returning probability $P_{j \to j}(t \to \infty; V \to \infty)$?







$P_{j \to j}(t \to \infty; V \to \infty) = 0$ for extended states

$P_{j \to j}(t \to \infty; V \to \infty) > 0$ for localized states

Characterization of Anderson localization

Local Density of States (LDOS)

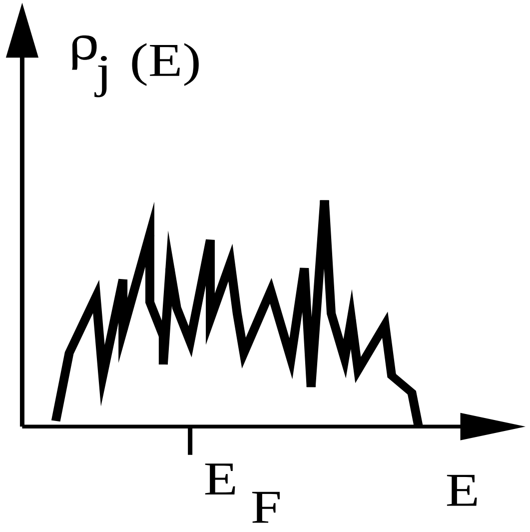
$\rho_i(E) = \sum_{n=1}^{N} |\Psi_n(r_i)|^2 \delta(E - E_n)$

$P_{j\to j}(t) = |G_j(t)|^2$

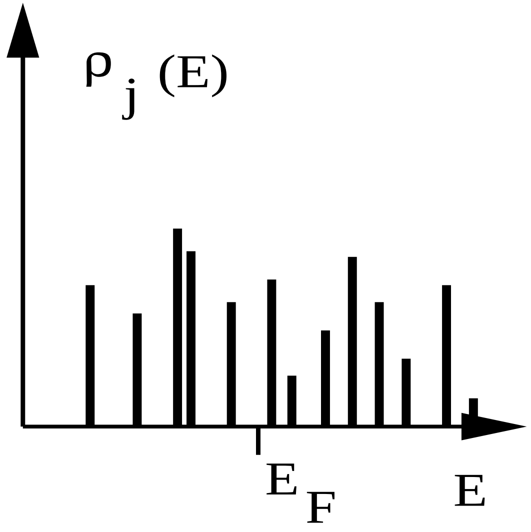
$G_j(t) \sim e^{i(\epsilon_j + \Sigma'_j)t - |\Sigma''_j|t} \sim e^{-\frac{t}{\tau_{\rm esc}}}$

Fermi Golden Rule

$$\frac{1}{\tau_{\rm esc}} \sim |t_{ji}|^2 \rho_j(E_F)$$



metal

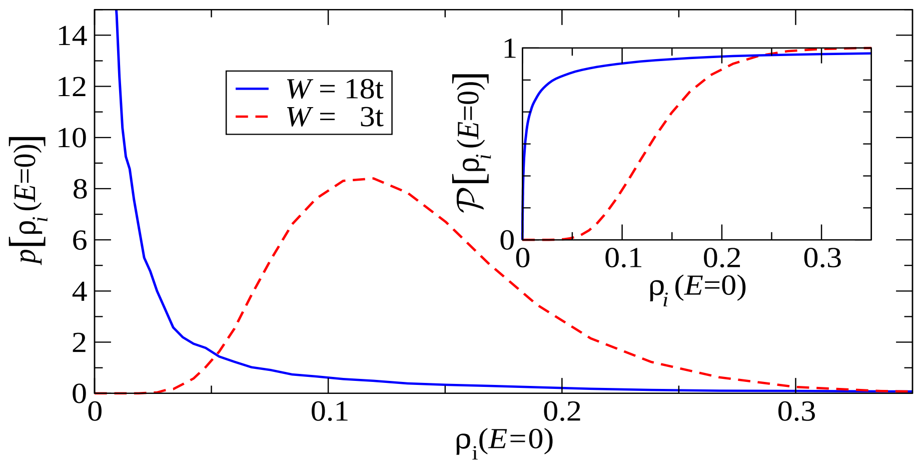


insulator

Anderson MIT - cont.

$\rho_j(E)$ is different at different R_j! Random quantity!

Statistical description $P[\rho_j(E)]$!



Broadly distributed $P[\rho_j(E_F)]$

Typical escape rate is determined

by the typical LDOS

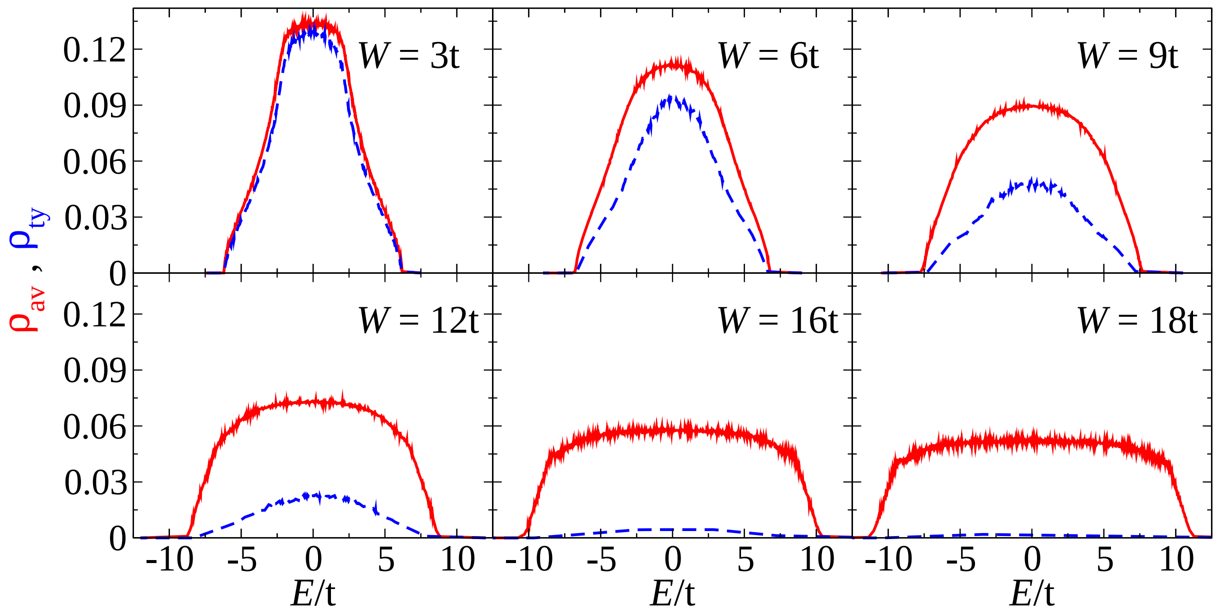
Multifractality - $\langle M^{(k)} \rangle \sim L^{-f(k)}$

Schubert et al. cond-mat/0309015

Anderson MIT - cont.

Near Anderson localization typical LDOS is approximated by geometrical mean

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



Theorem (F.Wegner 1981):

$$\rho(E)_{av} = \langle \rho_i(E) \rangle > 0$$

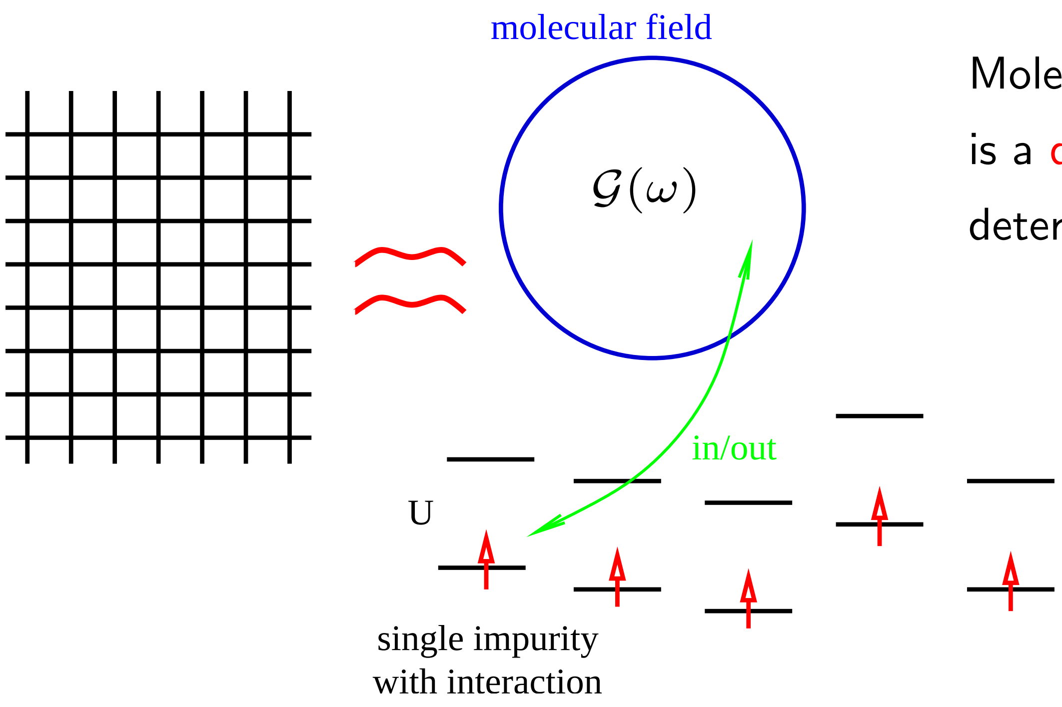
within a band for any finite Δ

Schubert et al. cond-mat/0309015

Dynamical mean-field theory for U and Δ

Byczuk, Hofstetter, Vollhardt

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

after idea from: Dobrosavljevic et al., Europhys. Lett. 62, 76 (2003)

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

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

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

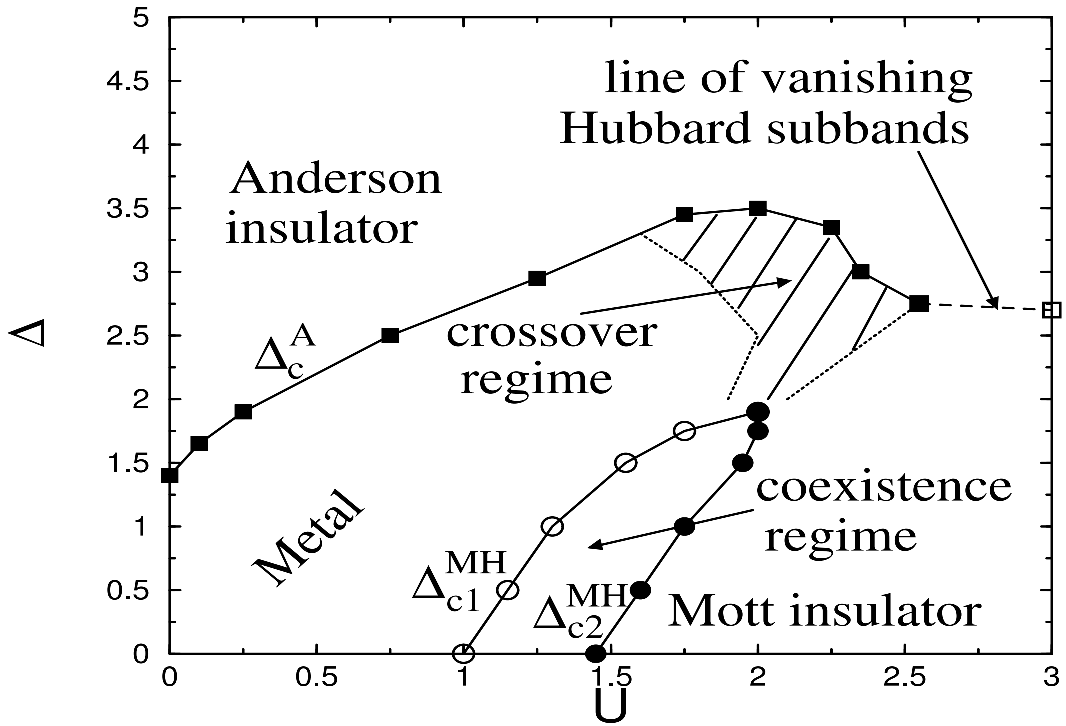
$$G^{-1}(\omega) = \omega - \eta(\omega) - \Sigma(\omega), \qquad \eta(\omega) = \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{\omega - \epsilon_{\mathbf{k}}}$$

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

Phase diagram for disordered Hubbard model

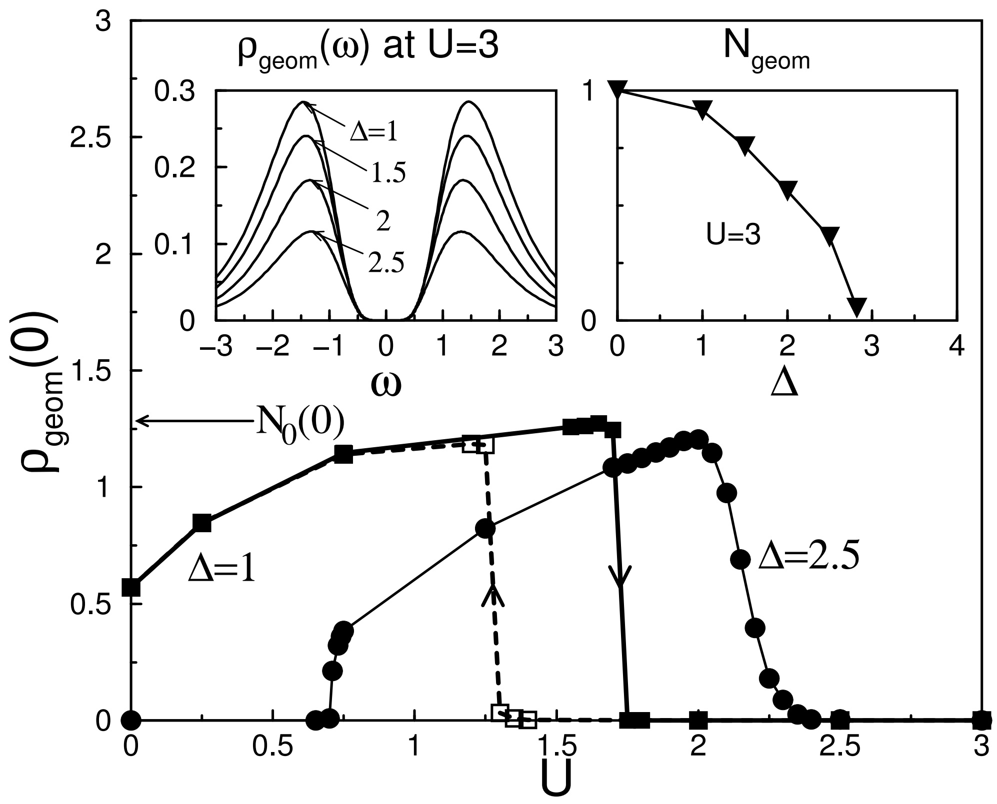
$$N_0(\epsilon) = \frac{2}{\pi D}\sqrt{D^2 - \epsilon^2}; \quad \eta(\omega) = \frac{D^2}{4} G(\omega)$$

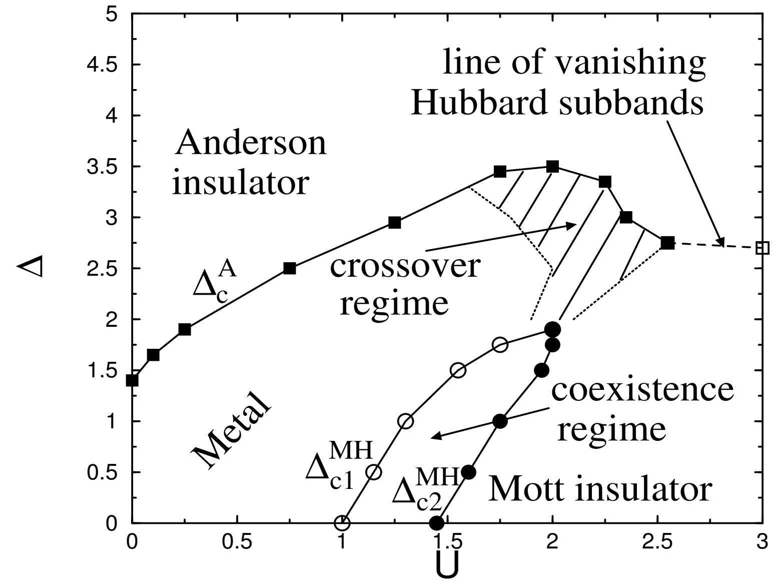
$T = 0$, $n = 1$, $W = 2D = 1$, NRG solver



U - interaction, Δ - disorder

Mott-Hubbard transition in disordered Hubbard model





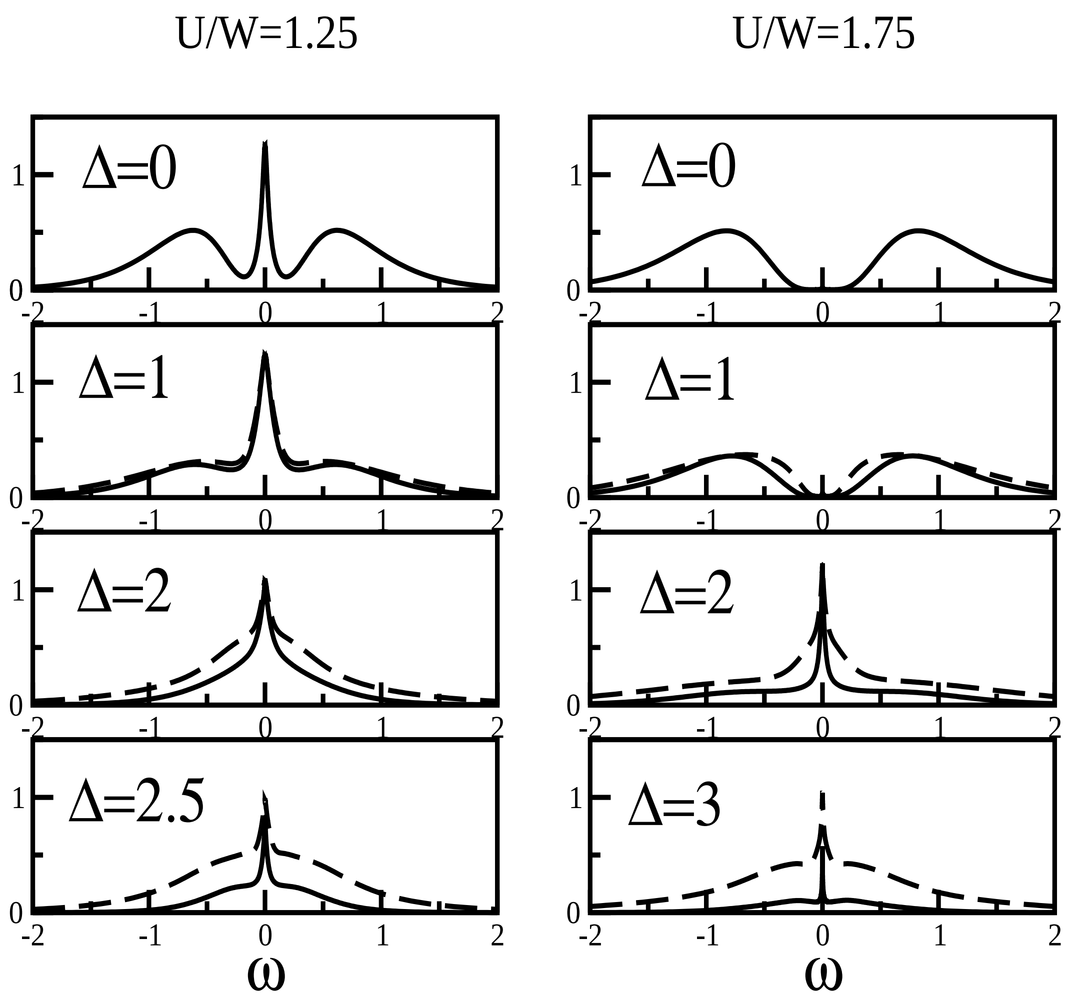
* Luttinger (FL due to U)

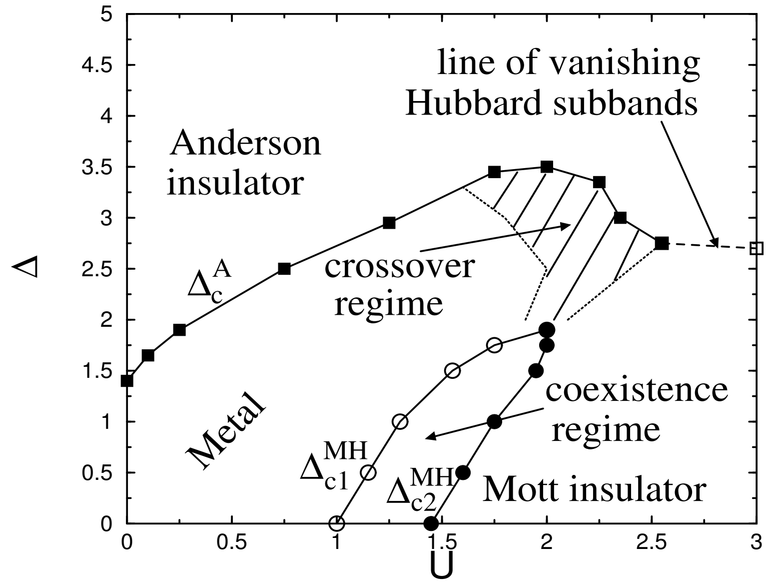
* Hysterisis $\Delta_{c1}(U)$, $\Delta_{c2}(U)$

* Crossover

* Similar conclusions with $\langle \rho_j \rangle$ schme

Spectral functions in disordered Hubbard model



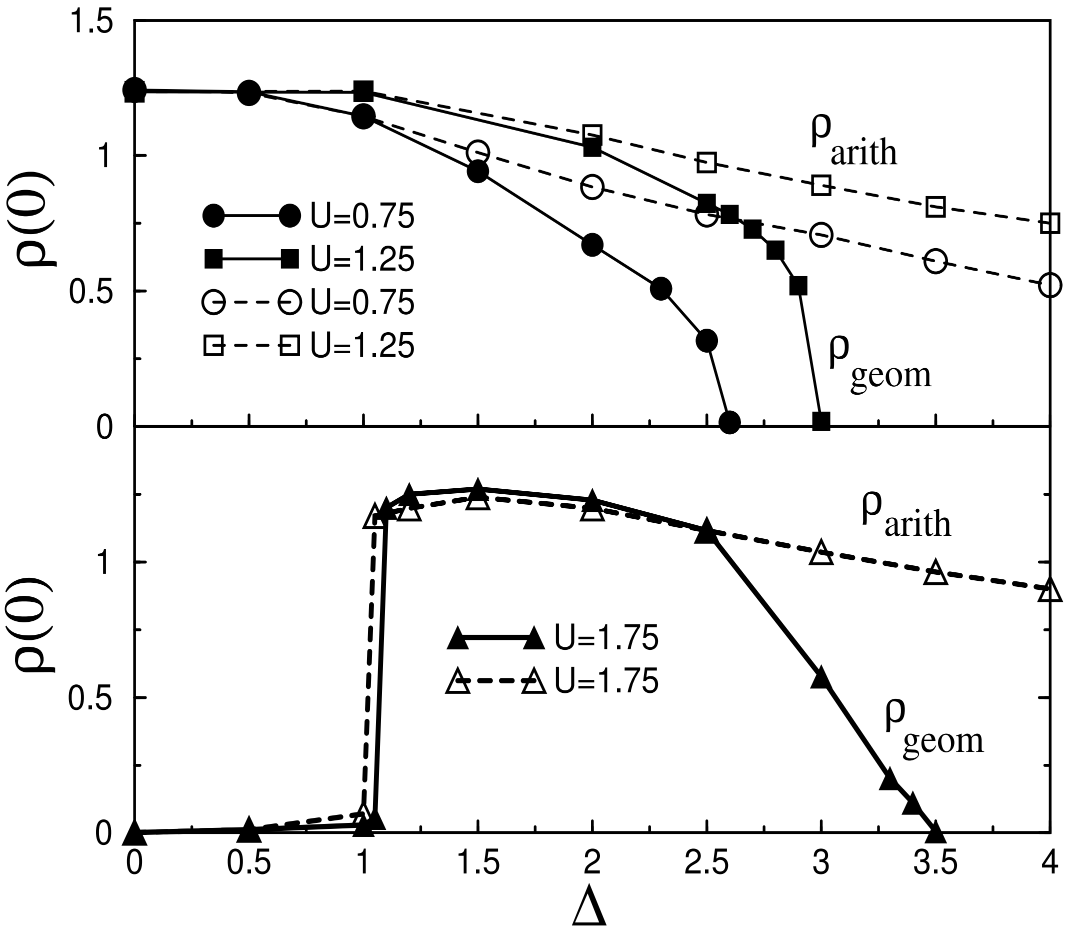


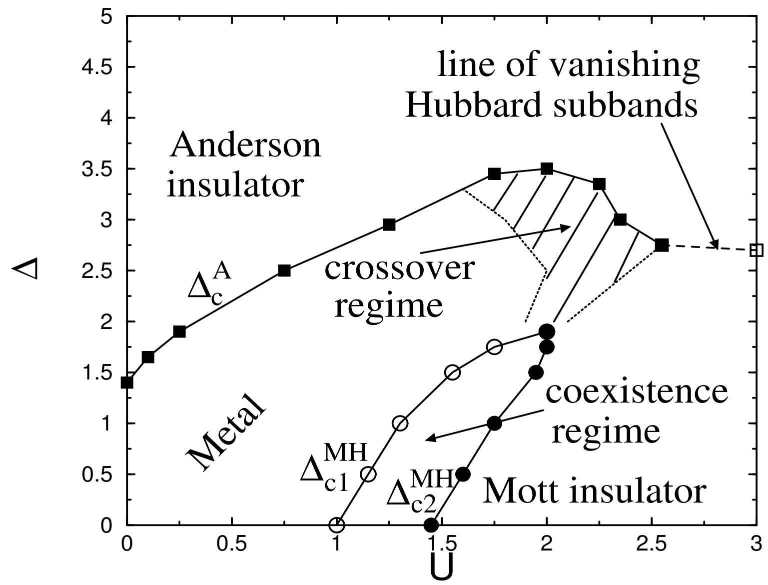
* Redistribution of spectral weight

* Reentrant Mott-Hubbard MIT

* Anderson MIT - $\rho_{geom}(\omega) \rightarrow 0$

Anderson transition in Hubbard model





* $A(0) \sim [\Delta_c(U) - \Delta(U)]^\beta$

with $\beta = 1$ or $\beta < 1$

* Two insulators: Mott and Anderson

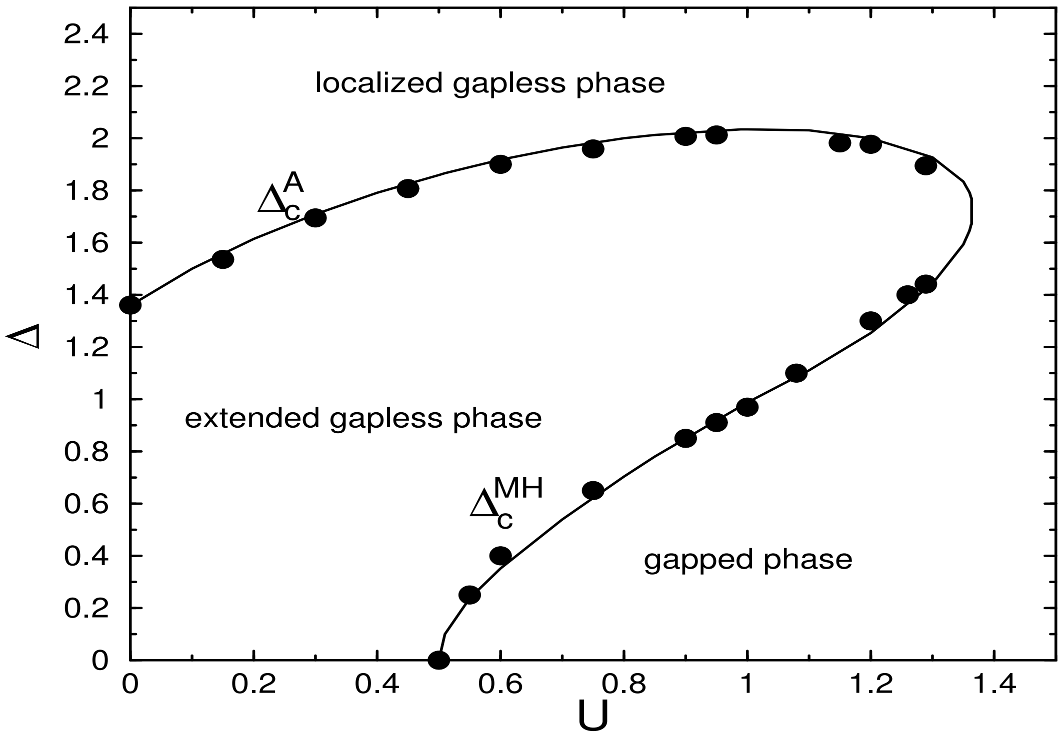
* Adiabatic continuity

$$(U > 0, \Delta = 0) \rightarrow (U = 0, \Delta > 0)$$

Phase diagram for disordered Falicov-Kimball model

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

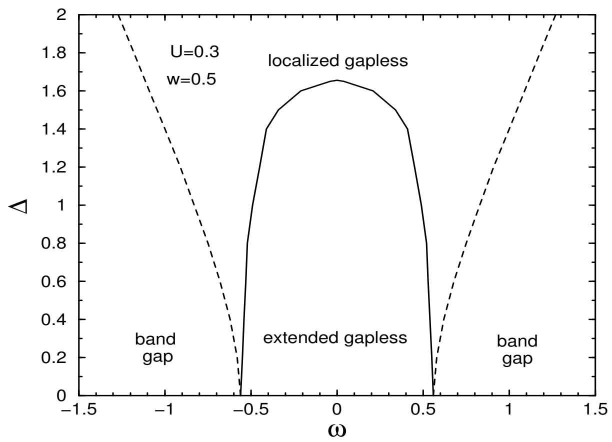
$T = 0$, $n = 1$, $W = 2D = 1$, analytical solver



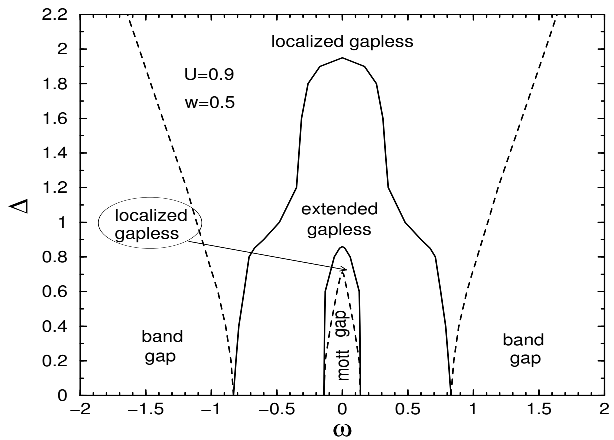
U - interaction, Δ - disorder

Spectral phase diagrams

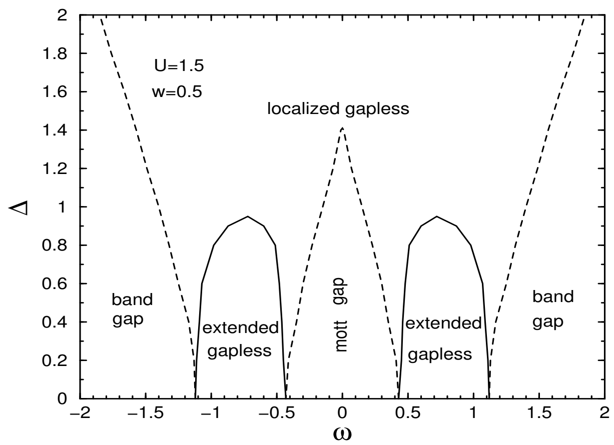
weak coupling $0 < U < W/2$



medium coupling $W/2 < U \lesssim 1.36W$



strong coupling $1.36W \lesssim U$

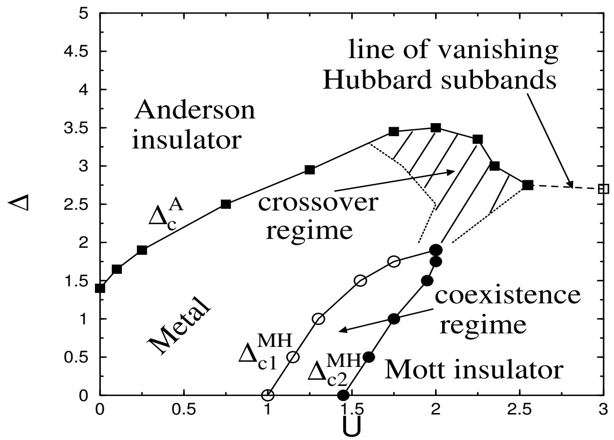


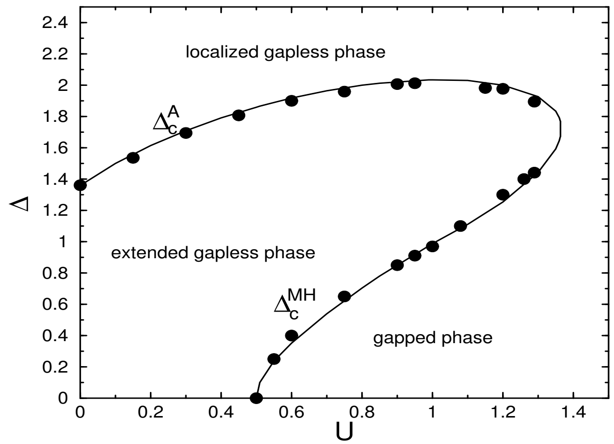
Conclusions and outlook

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

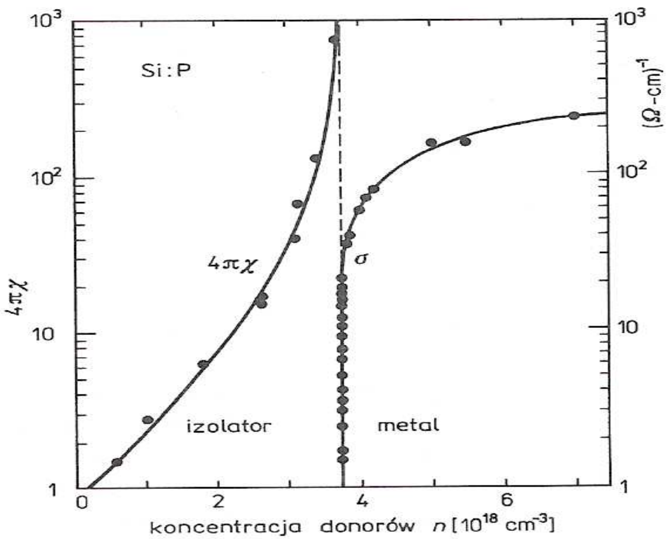
- Geometrical means used to study Anderson MIT in correlated electron system within DMFT
- Complete phase diagrams
- Nonmonotonic behavior of $\Delta_c(U)$ at Anderson MIT
- Two insulators connected continously
- Certain similarity/differences between Hubbard and FK models

Further projects: AF, CDW phases and Anderson localization in Hubbard and FK models





Physical systems



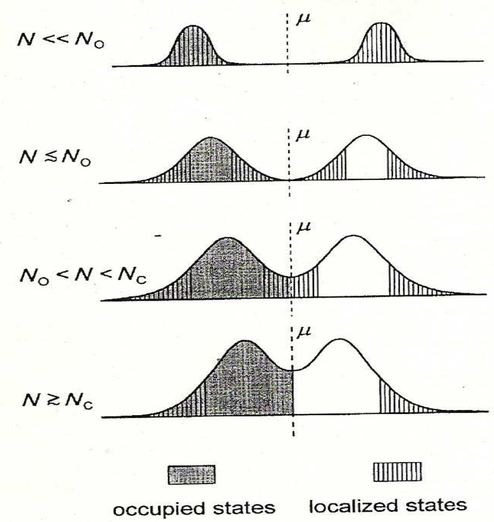


Figure 9 Qualitative sketch of the density of states of the impurity band of uncompensated Si:P for several P concentrations N, indicating the splitting into lower and upper Hubbard band around the chemical potential μ. See text for details.

KIM *et al.*

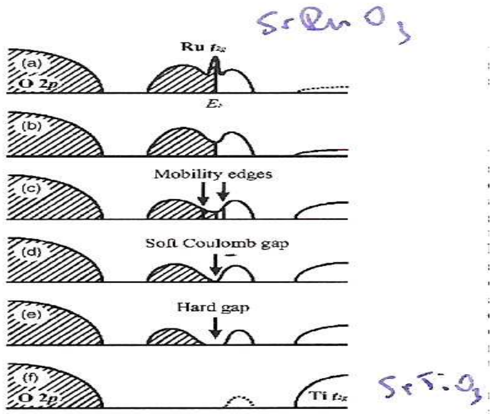


FIG. 9. A schematic diagram for $SrTi_{1-x}Ru_xO_3$. As x decreases, (a) DOS of a correlated metal ($x \sim 1$) shows (b) suppression in the correlated quasiparticle peak first due to disorder (a disordered metal, $x \sim 0.7$). With further decrease of x, (c) mobility edges are formed near E_F (an Anderson insulator, $x \sim 0.5$) and (d) the increased Coulomb interaction results in a soft Coulomb gap at E_F (a soft Coulomb gap insulator, $x \sim 0.4$). (e) Finally the disorder induced correlation opens a hard gap (a disordered correlation insulator, $x \sim 0.2$). And further decrease of x makes the system (f) a band insulator with a wide optical gap ($x \sim 0$).