Metal-Insulator Transitions in the Falicov-Kimball model with Disorder

Krzysztof Byczuk

Institute of Physics, Augsburg University

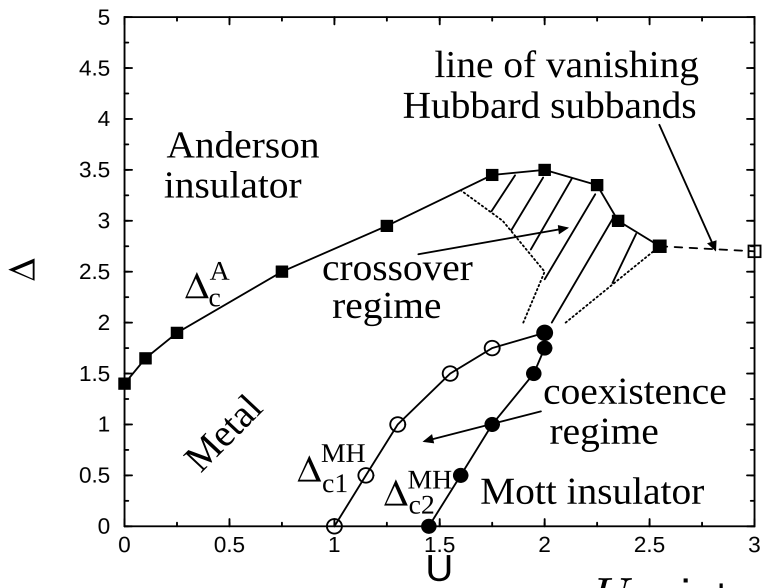
Institute of Theoretical Physics, Warsaw University

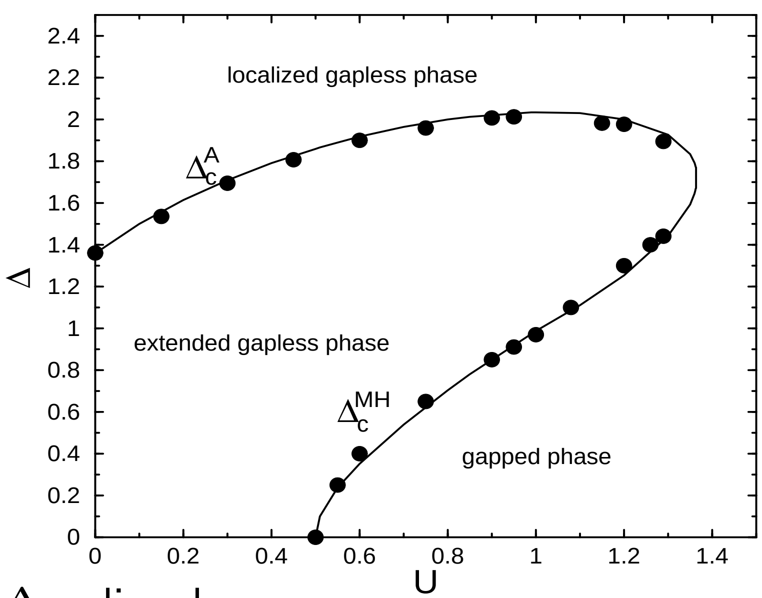
June 29th, 2005

Main goal:

- 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

Collaboration and discussions:

- Walter Hofstetter - Aachen, Germany
- Romek Lemański - Wrocław, Poland
- Dieter Vollhardt - Augsburg, Germany

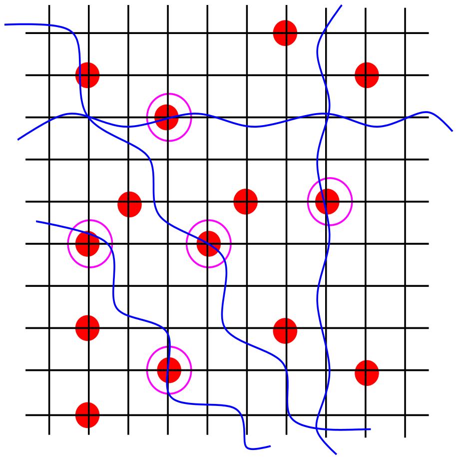
Phys. Rev. Lett.**94**, 056404 (2005); cond-mat/0403765
Physica B **359-361**, 651 (2005); cond-mat/0502257
Phys. Rev. B **71**, 205105 (2005); cond-mat/0412590

Plan of the talk:

1. Introduction
   - Falicov-Kimball model
   - Description of Mott – Hubbard localization – DMFT
   - Description of Anderson localization
   - Arithmetic vs. geometric means
2. FK model with disorder - phase diagram and MITs in details
3. Conclusions and outlook

Introduction:
Falicov-Kimball model and MIT

Falicov-Kimball model



poor brother/sister of Hubbard model

n_c and n_f independently fixed (canonical approach)

$n_c + n_f$ fixed (grant canonical approach)

– mobile particles on a lattice

– localized particles on a lattice

– local interaction

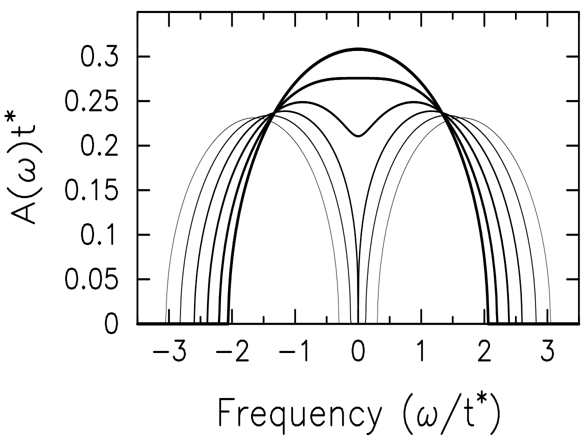
$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \epsilon_f \sum_i f_i^\dagger f_i + U \sum_i f_i^\dagger f_i c_i^\dagger c_i$$

Interest in Falicov-Kimball model

- 1969 - L.M. Falicov and J.C. Kimball introduced this model to study MITs in mixed valance compounds of rare earth and transition metal oxides (localized f-electrons interacting with itinerant d-electrons).
- ordering phenomena in mixed valance systems, binary alloys, magnets, ...
- approximate solution to Hubbard model.
- 1986 - T. Kennedy and E. Lieb reinterpreted FK model as a primitive model for matter to study crystallization: For $n_e = n_f = 1/2$ and a bipartite lattice there exists a long-range order (crystal) at low temperatures and for any coupling U and dimension $d \geq 2$. At higher temperatures the LRO is absent (fluid).
- LRO, phase separation, stripes, ...
- 2005 - C. Ates and K. Ziegler used FK model to study mixtures of cold atoms.
- DMFT - exact solution in $d = \infty$ limit: U. Brandt *et al.*, P.G.J van Dongen and D. Vollhardt, V. Janiš, J.K. Freericks *et al.*, A.M. Shvaika, and many others.
- ... many extentions: spins (CMR, DMS), phonons (Holstein), correlated hopping, ..., disorder (K. Byczuk).

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.



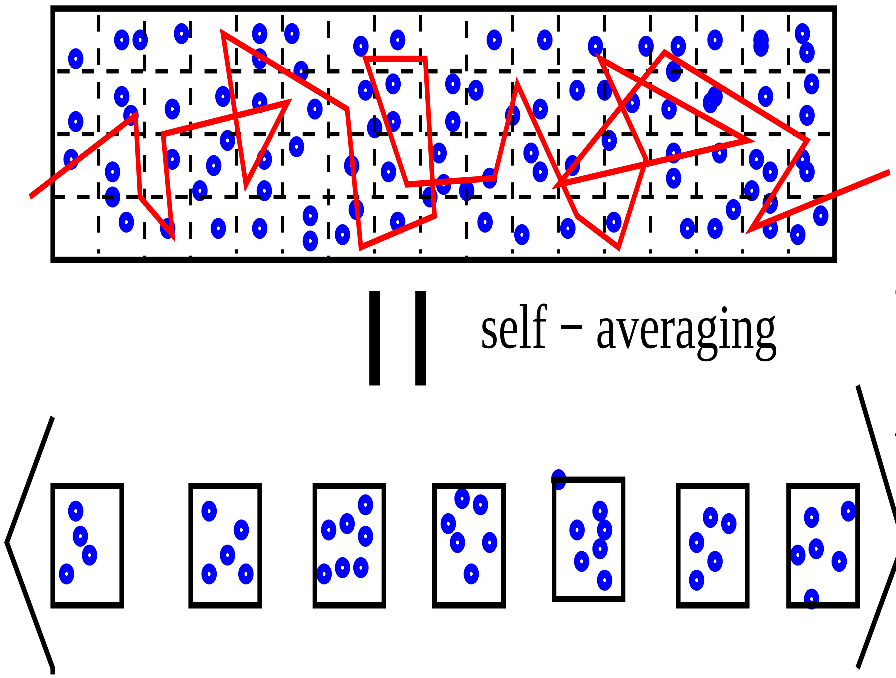
van Dongen and Lainung 1997, DMFT, Bethe, no CDW, $U = 0.5 - 3.0$

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

Introduction:
disorder systems and Anderson localization

Waves in random system

propagation of waves in a randomly inhomogeneous medium



random conservative linear wave equation

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

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

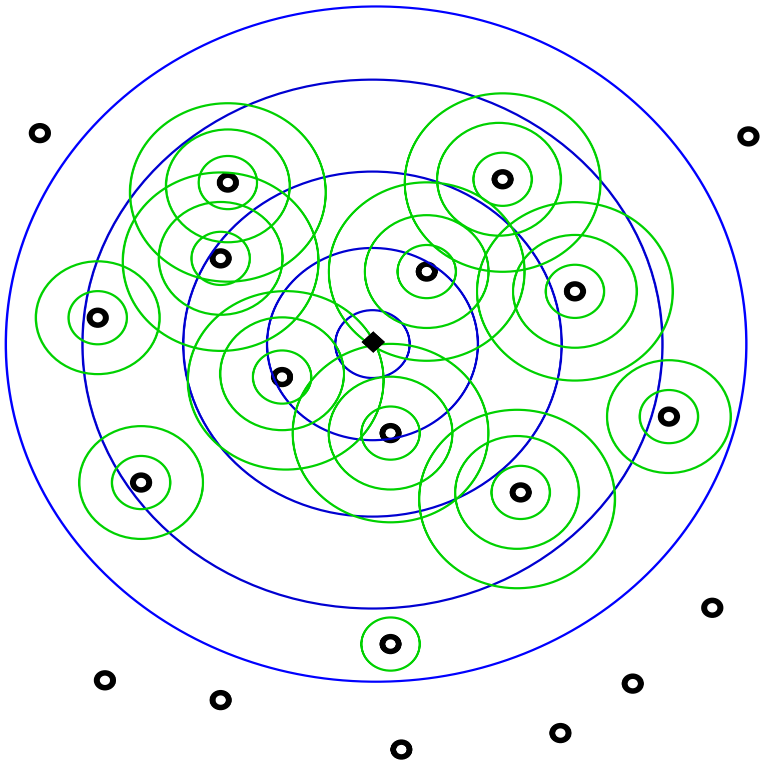
diffusive motion, memory of $\vec{V}(0)$ lost,

"random walk" over long distances,

friction imposed by averaging

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

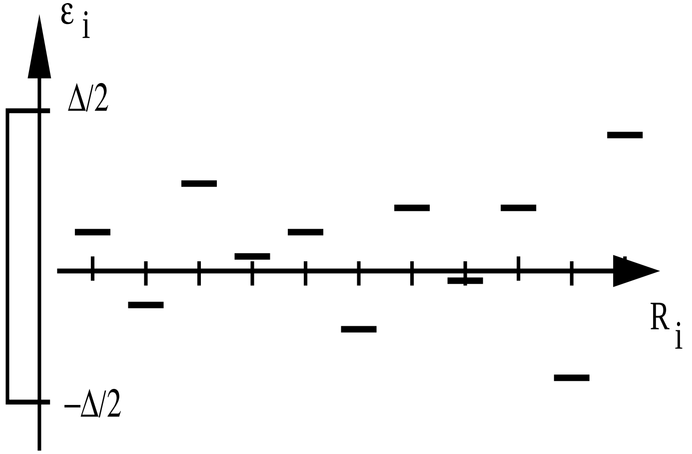
Localization is a destruction of coherent superposition of spatially separated states

Anderson model

$$H = \sum_{i\sigma} \epsilon_i n_{i\sigma} + \sum_{ij\sigma} t_{ij}\, c^\dagger_{i\sigma} c_{j\sigma}$$

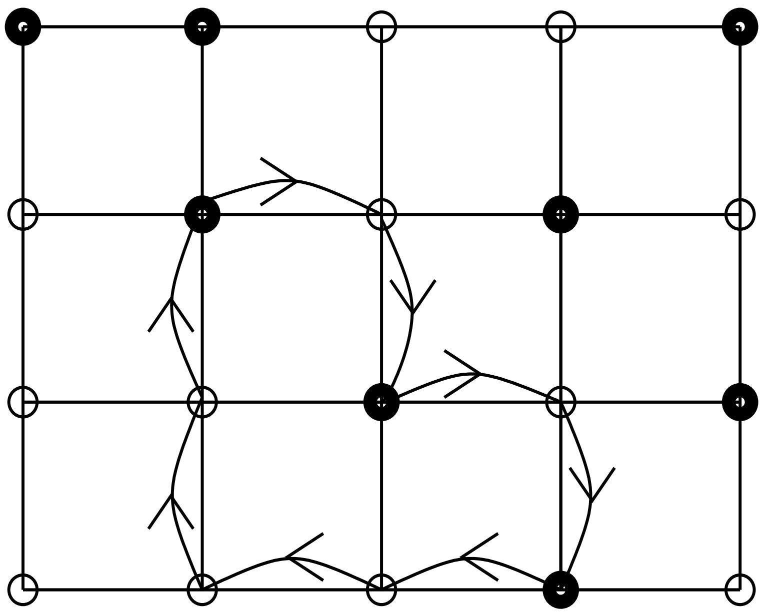
Probability distribution function

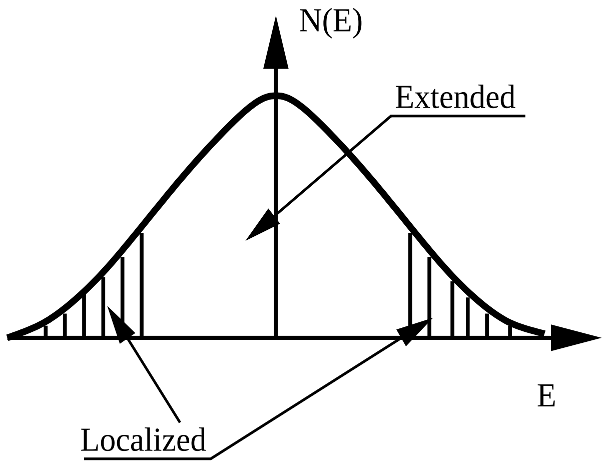
$$\mathcal{P}(\epsilon_i) = \frac{1}{\Delta}\Theta\left(\frac{\Delta}{2} - |\epsilon_i|\right)$$

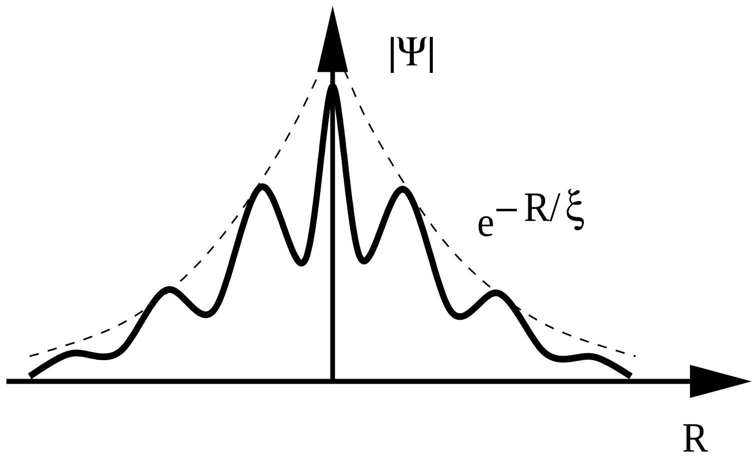


Anderson MIT - cont.

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)

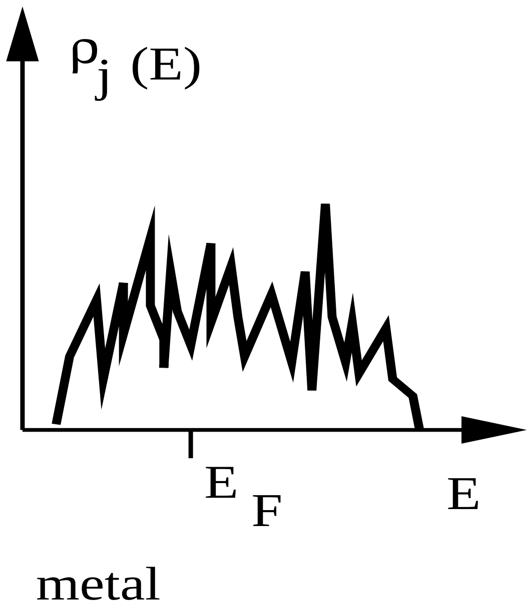
$\rho_i(E) = \sum_{n=1}^{N} |\Psi_n(r_i)|^2 \delta(E - E_n)$

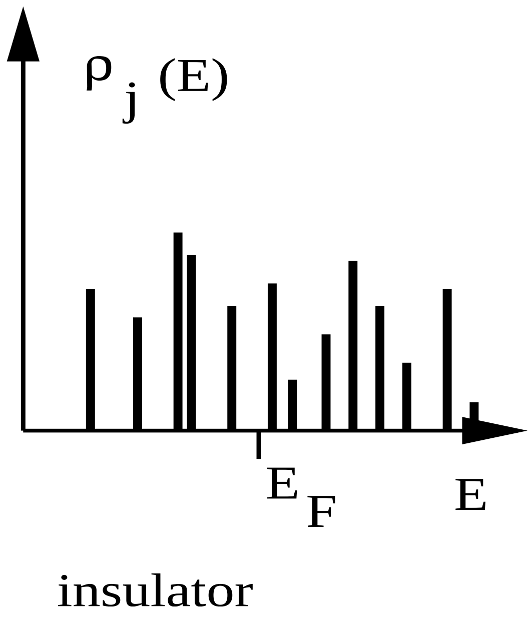
$P_{j\to j}(t) = |G_j(t)|^2$

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

Fermi Golden Rule

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

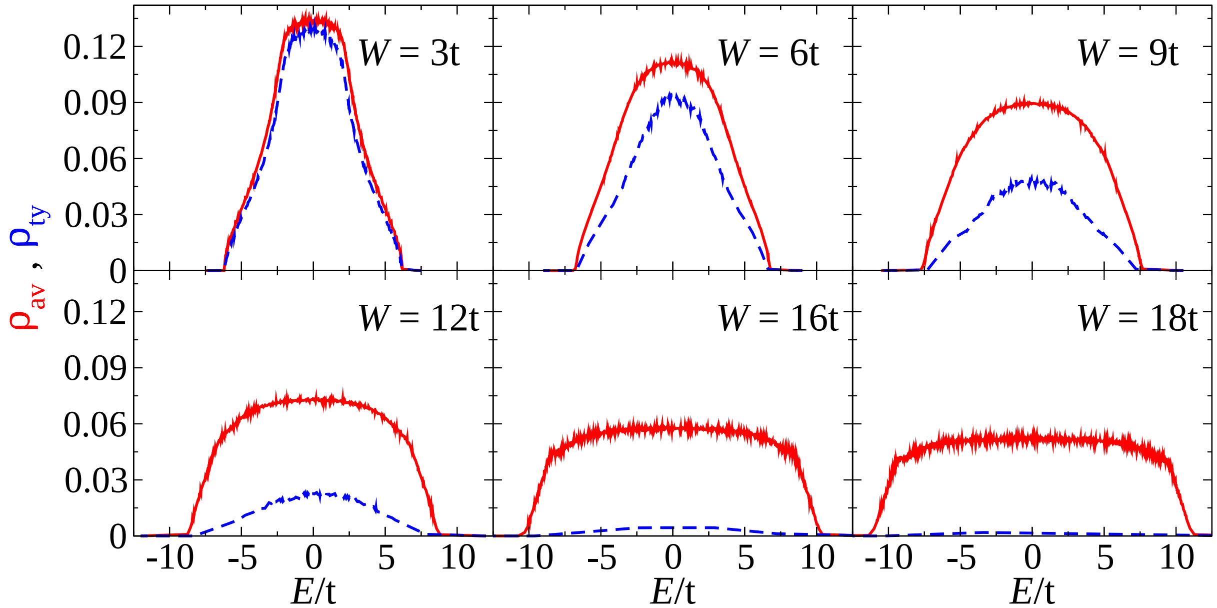




Anderson MIT - cont.

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

Main part:
FK model with disorder, our results

Falicov-Kimball model with disorder

Motivation: easier to solve, no high-tech numerics (QMC, NRG, ED), details on mobility and band edges

Our model (only mobile particles subjected to the structural disorder):

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

ϵ_i - random quantity with box PDF

DMFT for Falicov-Kimball model with disorder

$$G_{ii}(\omega) = \frac{1}{\omega + \mu - \epsilon_i - \eta(\omega) - \Sigma(\omega, \epsilon_i)} \equiv G(\omega, \epsilon_i)$$

$$\Sigma(\omega, \epsilon_i) = wU + \frac{w(1-w)U^2}{\omega + \mu - \epsilon_i - (1-w)U - \eta(\omega)}$$

$\langle f_i^\dagger f_i \rangle = n_f = w$

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

$$A_{\mathrm{geom}}(\omega) = \exp\left[\langle \ln A(\omega, \epsilon_i) \rangle_{\mathrm{dis}}\right]$$

$$A_{\mathrm{arith}}(\omega) = \langle A(\omega, \epsilon_i) \rangle_{\mathrm{dis}}$$

$$G(\omega) = \int d\omega' \frac{A_\alpha(\omega')}{\omega - \omega'}$$

On the Bethe lattice, no LRO

$$\eta(\omega) = W^2 G(\omega)/16$$

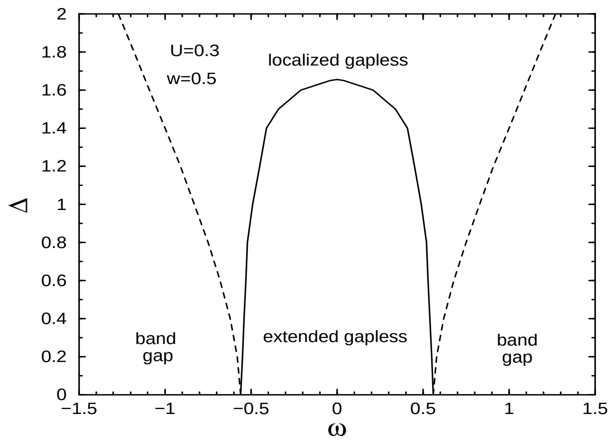
Here: $n_e = 1/2$, $n_f = w = 1/2$, $\mu = U/2$, $W = 1$

Criteria for Anderson and Mott MIT

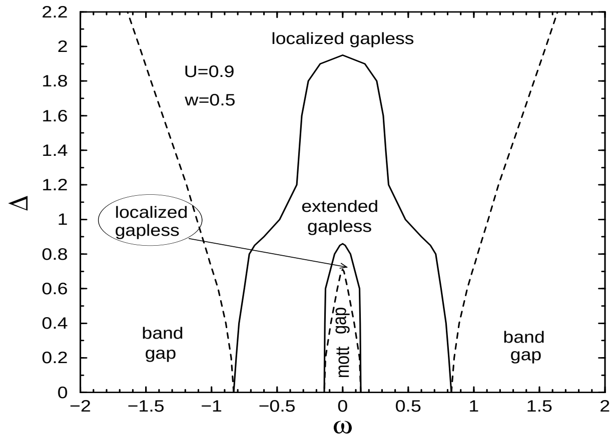
- $A_{\mathrm{geom}}(\omega) > 0$ and $A_{\mathrm{arith}}(\omega) > 0$ – extended gapless states at ω
- $A_{\mathrm{geom}}(\omega) = 0$ and $A_{\mathrm{arith}}(\omega) = 0$ – correlation or band gap at ω
- $A_{\mathrm{geom}}(\omega) = 0$ and $A_{\mathrm{arith}}(\omega) > 0$ – localized gapless states at ω

Spectral phase diagrams

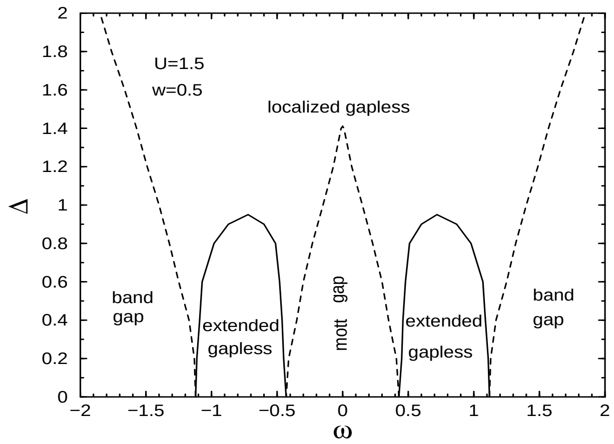
weak coupling $0 < U < W/2$



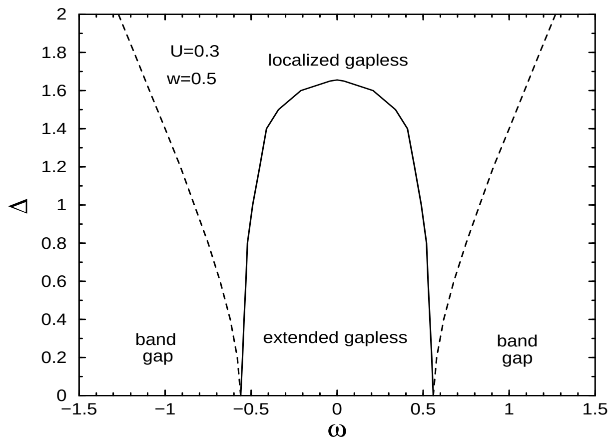
medium coupling $W/2 < U \lesssim 1.36W$

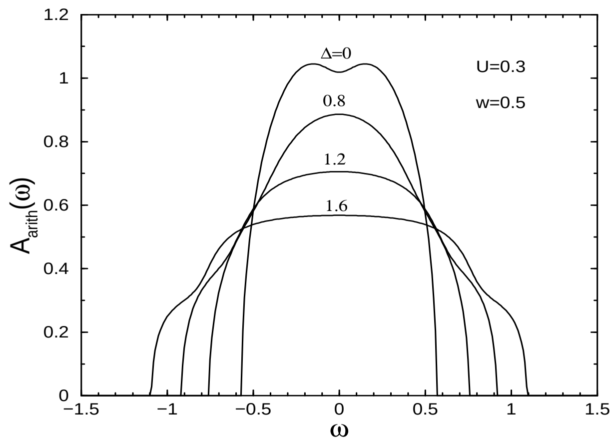


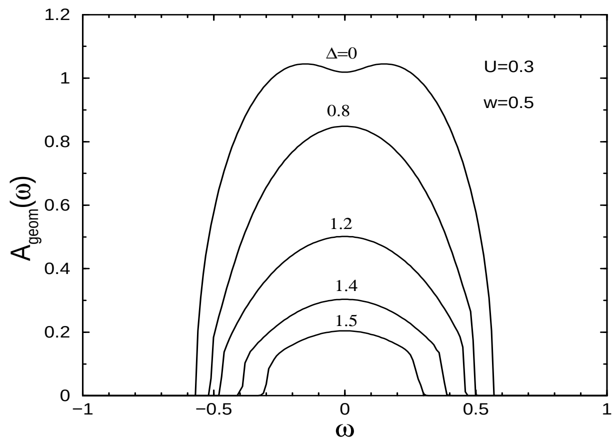
strong coupling $1.36W \lesssim U$



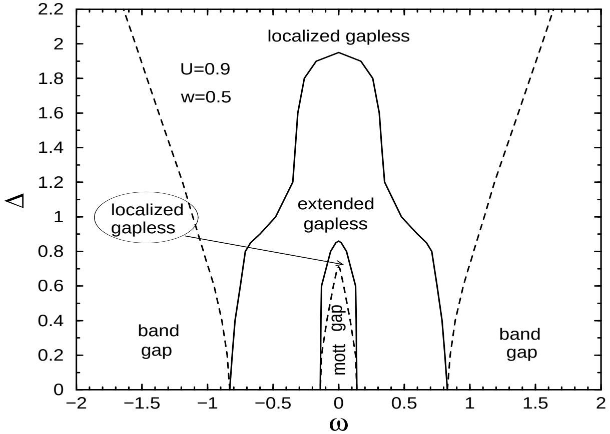
Spectral phase diagrams
- weak coupling $0 < U < W/2$

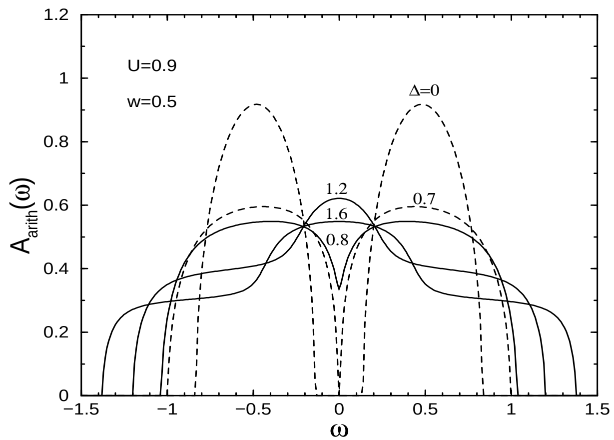


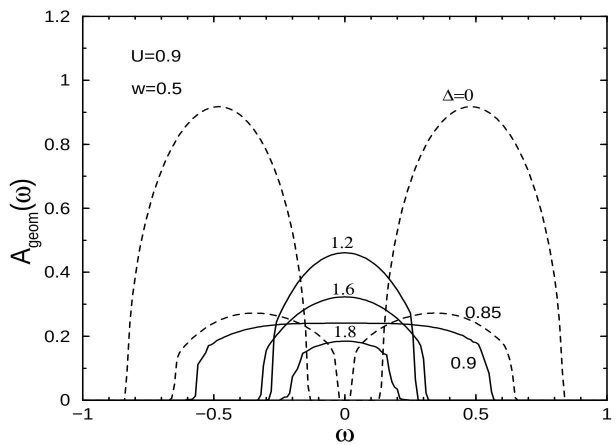




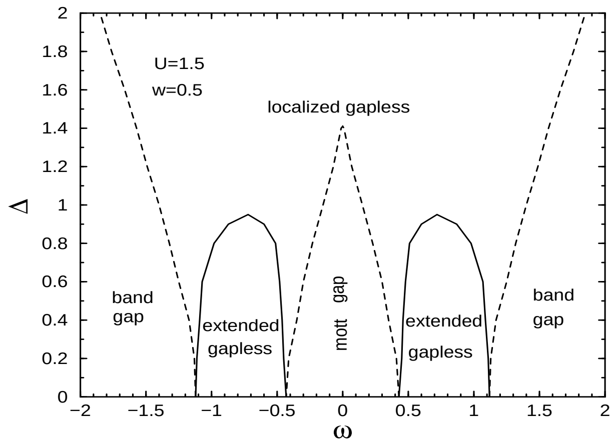
Spectral phase diagrams
- medium coupling $W/2 < U \lesssim 1.36W$

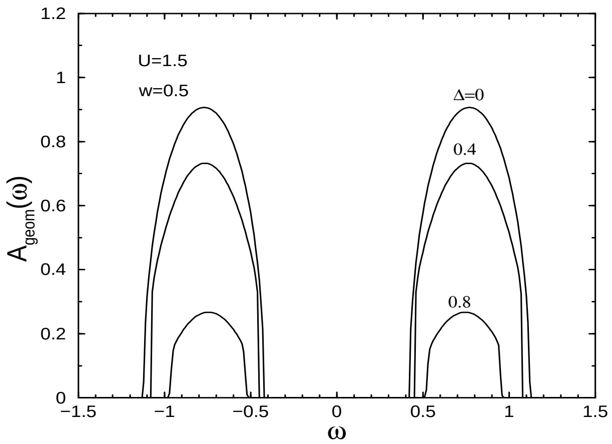




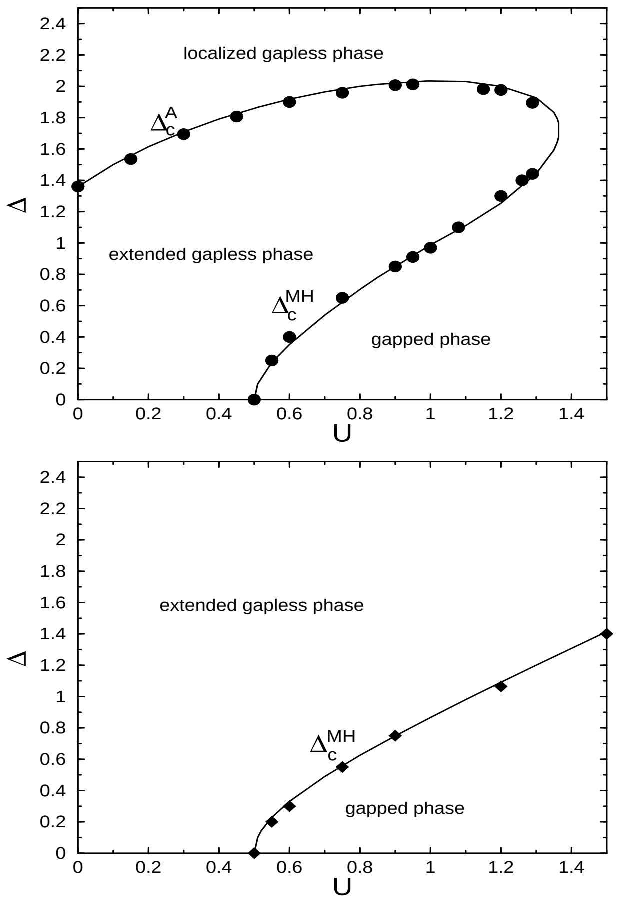


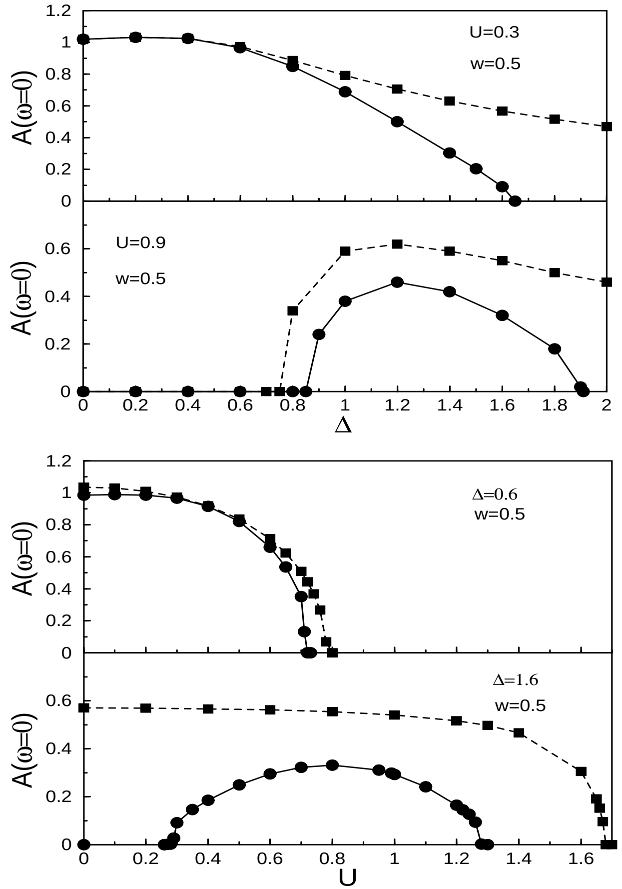
Spectral phase diagrams
- strong coupling $1.36W \lesssim U$





States in a band center





NFL

reentrant MIT

continuity between insulators

metallicity stabilized

Linearized DMFT

Geometric average

$$1 = \frac{W^2}{16} \exp\left[I_{\rm geom}(U,\Delta)\right]$$

where

$$I_{\rm geom}(U,\Delta) = 2 + \ln\left[\left(\frac{U}{2}\right)^2 + \left(\frac{\Delta}{2}\right)^2\right] - 2\ln\left[\left(\frac{U}{2}\right)^2 - \left(\frac{\Delta}{2}\right)^2\right] + \frac{2U}{\Delta}\left[\arctan\left(\frac{\Delta}{U}\right) - \ln\left|\frac{\Delta+U}{\Delta-U}\right|\right]$$

Arithmetic average

$$1 = \frac{W^2}{16} I_{\rm arith}(U,\Delta)$$

where

$$I_{\rm arith}(U,\Delta) = \frac{1}{\left(\frac{U}{2}\right)^2 - \left(\frac{\Delta}{2}\right)^2}$$

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