Mott-Hubbard and Anderson Metal-Insulator Transitions in Correlated and Disordered Electronic Systems

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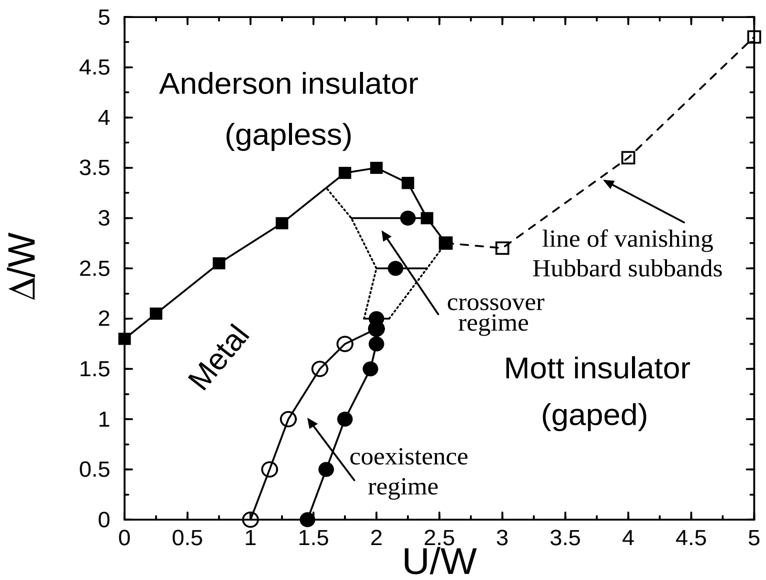
Main goal:

Some random events are better classified by means that are different than the arithmetic average

Main result:

Zero-temperature phase diagram of the disordered Hubbard model at half filling



Collaboration:

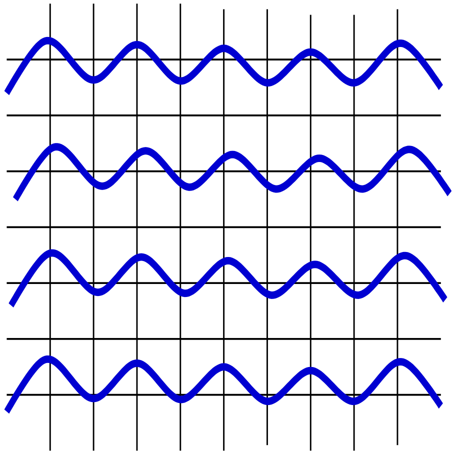
- Walter Hofstetter - Harvard University, USA
- Dieter Vollhardt - Augsburg University, Germany

Plan of the talk:

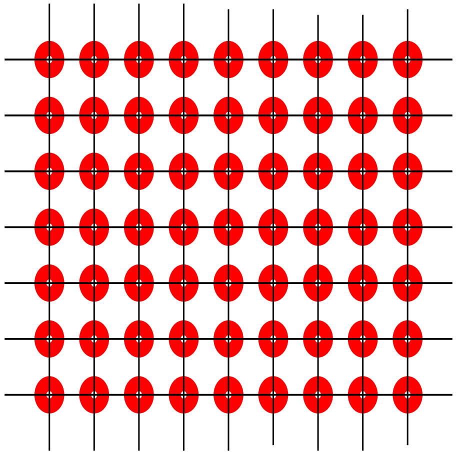
1. Introduction
   - Mott-Hubbard and Anderson metal-insulator transitions (MIT)
   - Anderson-Hubbard Hamiltonian
   - Description of Anderson localization
   - Widely distributed random quantities
   - Arithmetic vs. geometric means
   - Log-normal distribution
2. Modification within DMFT to include Anderson localization
3. Phase diagram and MITs in details
4. Conclusions

Mott-Hubbard MIT at $n = 1$:

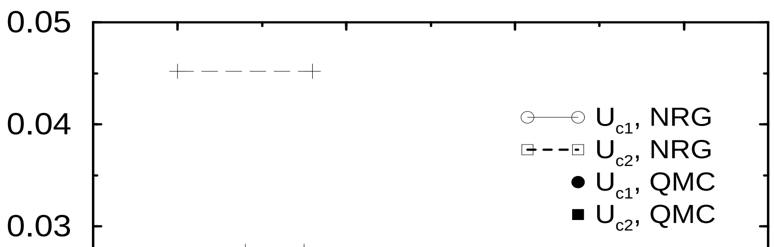
$$H = \epsilon_0 \sum_{i\sigma} n_{i\sigma} + \sum_{ij\sigma} t_{ij}\, a^{\dagger}_{i\sigma} a_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



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



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



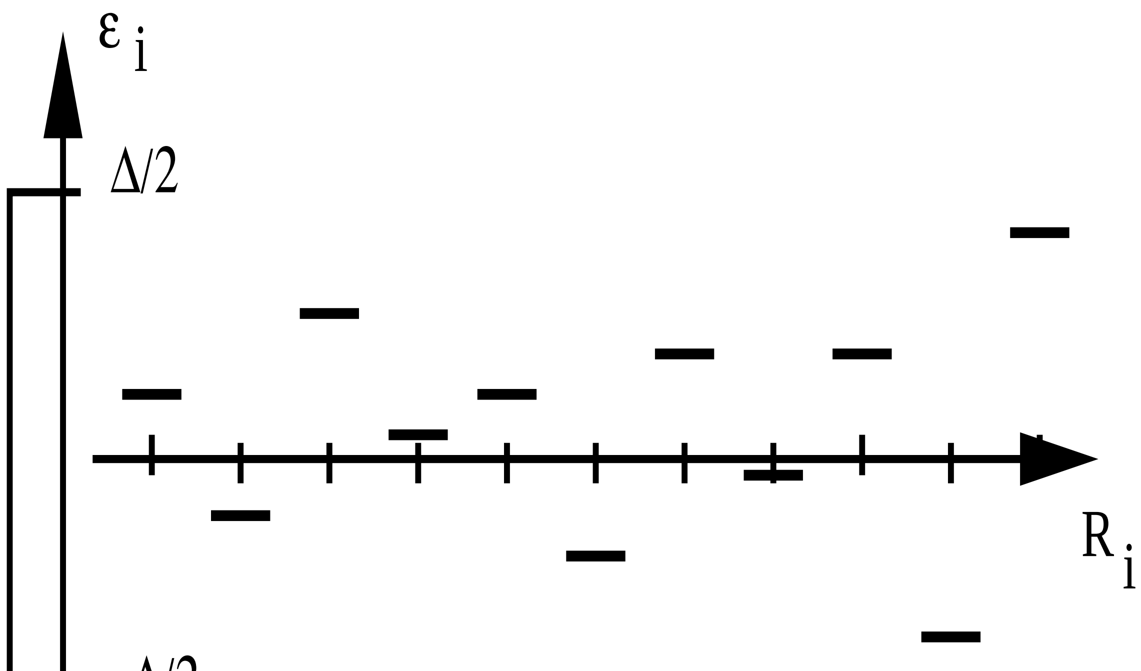
DMFT scenario

Anderson MIT:

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

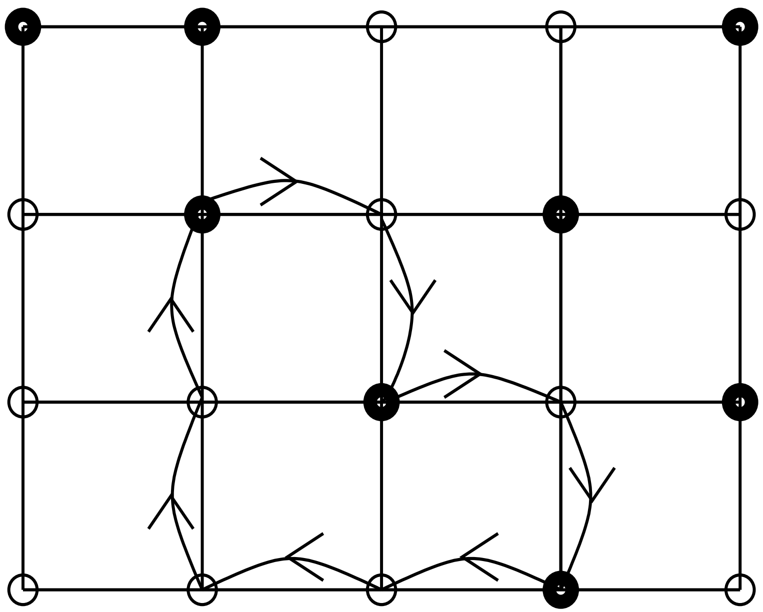
Probability distribution function

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



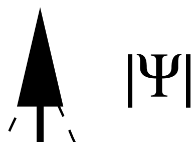
Anderson MIT - cont.:

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



Anderson MIT - cont.:

Anderson, PR 109, 1492 (1958) - At strong disorder the nature of electronic states at a given energy changes from extended to exponentially localized

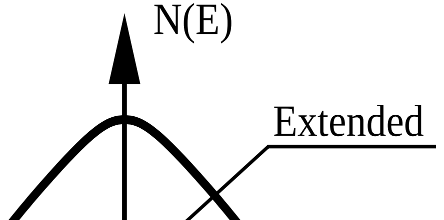
Accumulation of quantum interference corrections affects the transport

According to one-parameter scaling theory $[g = g(L)]$ (noninteracting system)

- If dim$= 1$ or 2 all states are localized
- If dim$=3$ there is a critical disorder above which the states are localized

Abrahams et al., PRL 42, 673 (1979)

$\Delta_c \sim \mathrm{band-width}$



Anderson MIT - cont.:

Which quantity characterizes Anderson MIT?

1. Decaying of wavefunction $|\Psi_n(r_i)| \sim e^{-|r-r_i|/\xi(E_n)}$
   - metal $\xi \to \infty$
   - insulator $\xi < \infty$
2. Inverse participation ratio P^{-1} [inverse number of sites that contribute to $\Psi_n(r_i)$]
   - metal $P^{-1} \sim 1/N$
   - insulator $P^{-1} \sim \mathrm{const}$
3. Conductance G
   - metal $G > 0$
   - insulator $G = 0$
4. Local Density of States (LDOS)

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

To match the Anderson localization theory with DMFT (strong correlations) the most useful is to use LDOS

Anderson MIT - cont.:

Why LDOS?

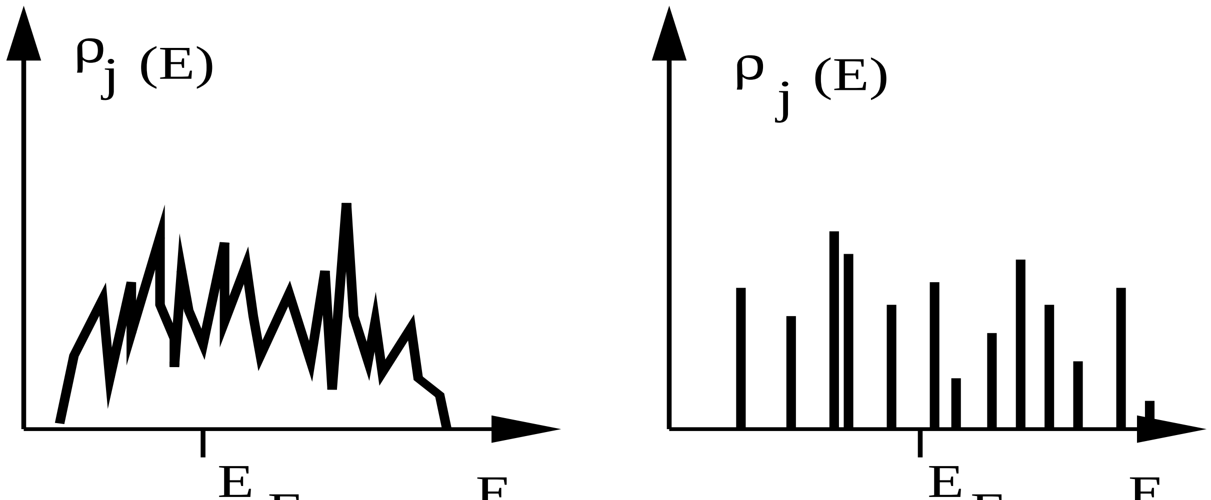
Heuristic arguments:

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

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

Fermi Golden Rule

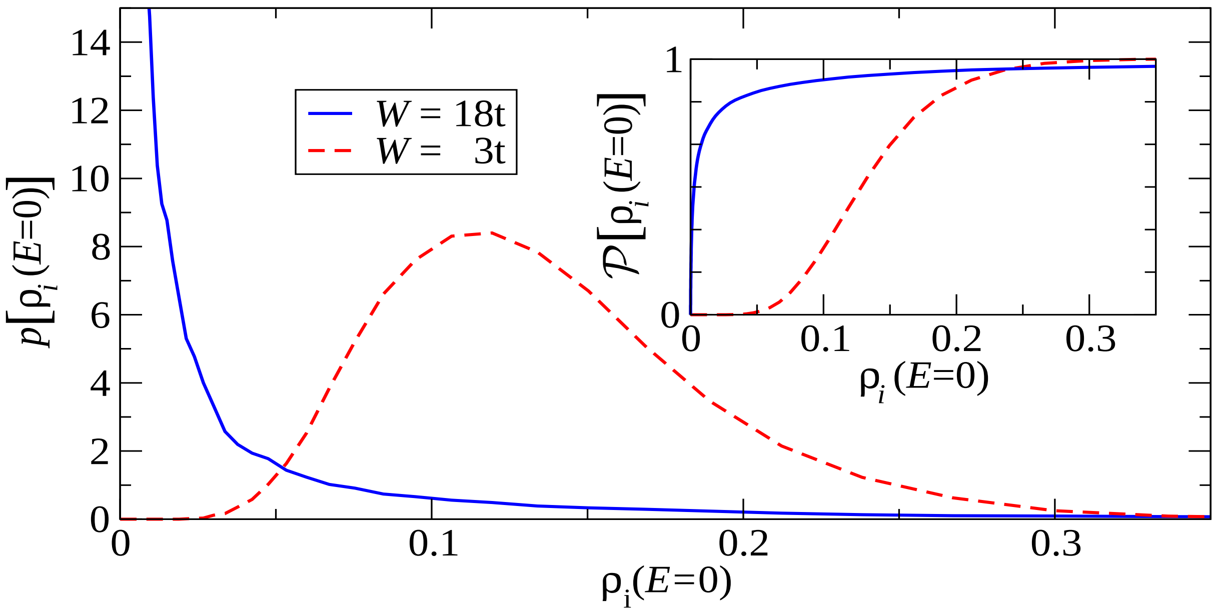
$$\frac{1}{\tau_{\rm esc}} \sim t^2 \rho_j(E_F)$$



Anderson MIT - cont.:

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

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



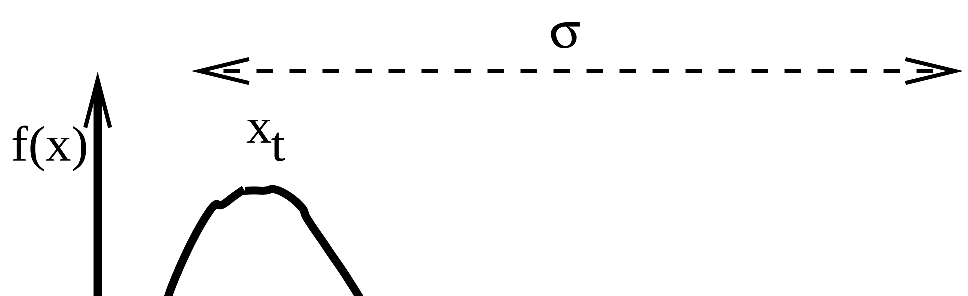
Schubert et al. cond-mat/0309015

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

Log-normal distribution - tutorial:

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \frac{1}{x} e^{-\frac{(\ln x - \mu)^2}{2\sigma^2}}$$

- It has both long tail and all moments
- Typical value $x_{typ} = e^{\mu - \sigma^2}$
- Median $x^{med} = e^{\mu}$
- Arithmetic mean $\langle x \rangle = e^{\mu + \frac{\sigma^2}{2}}$
- Geometric mean $x_{geom} = e^{\langle \ln x \rangle} = e^{\mu}$



Log-normal distribution - cont.:

Log-normal distribution serves as a prototype distribution which is characterized by infinitely many moments

F. Galton 1879; D. McAlister 1879

How to get log-normal?

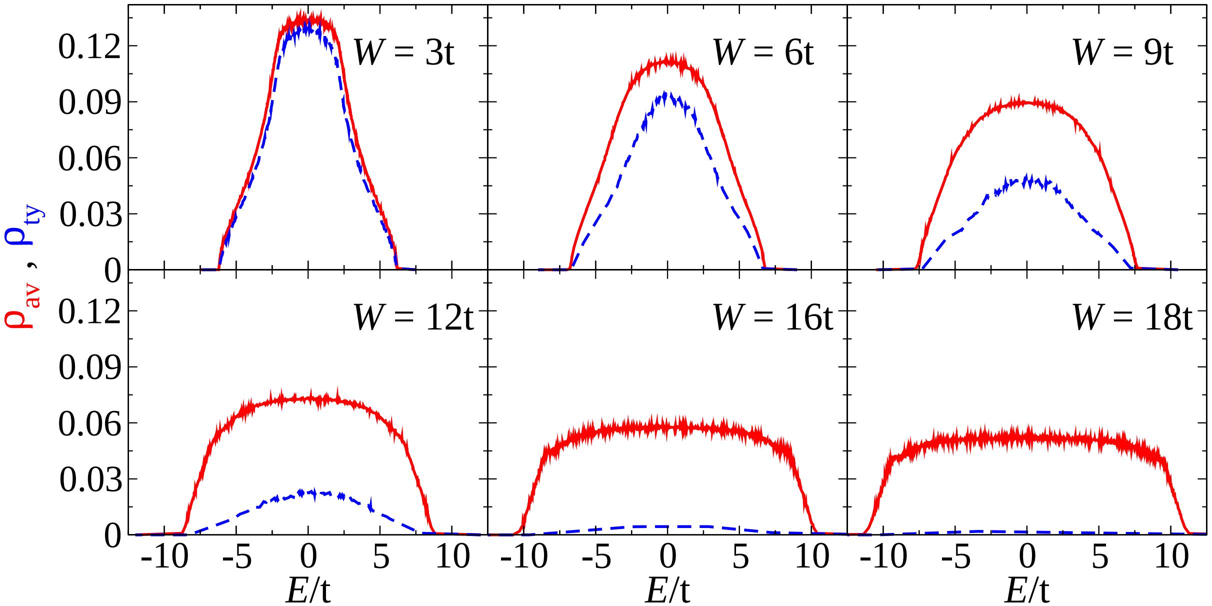
- $x = e^y$
- $x_n = \prod_{i=1}^{n} y_i$ with CLT

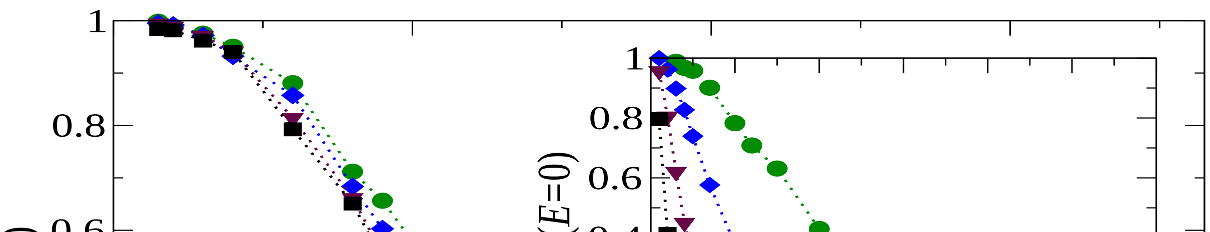
Applications:
astrophysics, physics (glass, polymers, networks), economy, sociology, biology, geology, etc.

Anderson MIT - cont.:

Near Anderson localization typical LDOS is approximated by geometrical mean

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





Anderson MIT - cont.:

Why should it work at all?

$$
\begin{aligned}
\rho_{geom}(E) &= e^{\langle \ln \rho_i(E) \rangle} = \\
& e^{\frac{1}{\Delta}\sum_{i=1}^{N} \ln \rho_i(E)} = \\
& \prod_{i=1}^{N} \rho_i(E)^{\frac{1}{\Delta}}
\end{aligned}
$$

$$\exists \;\; \rho_i(E) = 0 \Longrightarrow \rho_{geom}(E) = 0$$

Theorem (F.Wegner 1981):

$$\rho(E) = \langle \rho_i(E) \rangle > 0$$

DMFT with Anderson MIT:

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

$$H^{\mathrm{SIAM}} = \sum_{\sigma} (\epsilon_i - \mu) a^{\dagger}_{i\sigma} a_{i\sigma} + U n_{i\uparrow} n_{i\downarrow}$$

$$+ \sum_{\mathbf{k}\sigma} V_{\mathbf{k}} a^{\dagger}_{i\sigma} c_{\mathbf{k}\sigma} + hc + \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

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

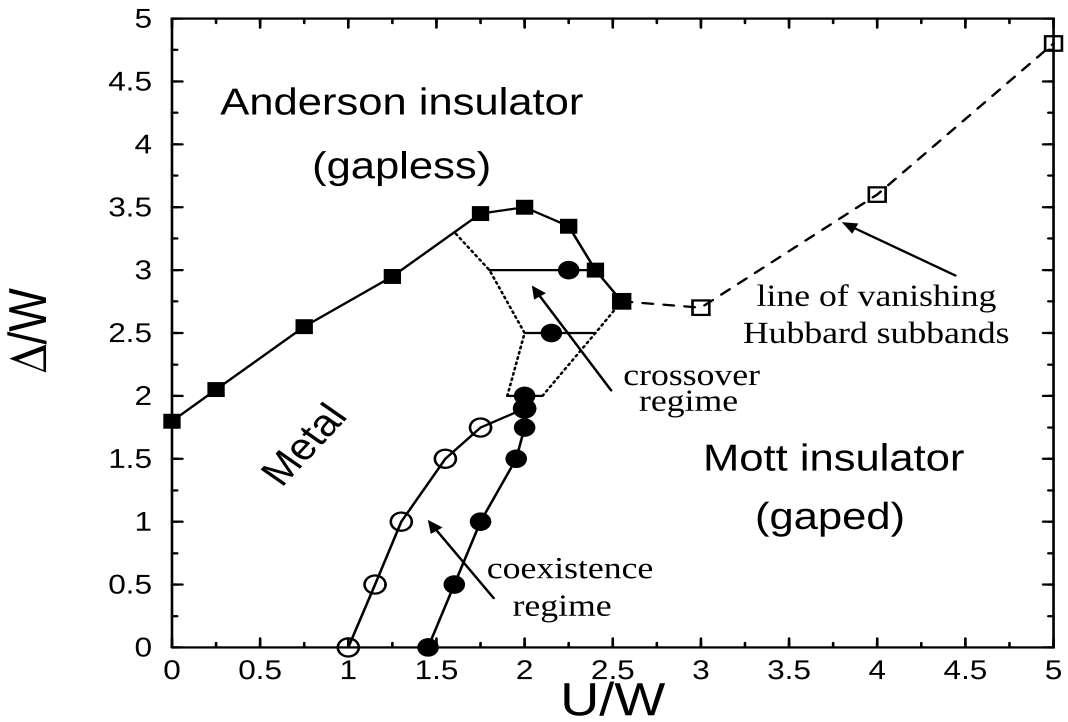
$$\rho_g(\omega) = e^{\langle \ln \rho_i(\omega) \rangle}; \quad G(\omega) = \int d\omega' \frac{\rho_g(\omega)}{\omega - \omega'}$$

$$G^{-1}(\omega) = \omega - \eta(\omega) - \Sigma(\omega)$$

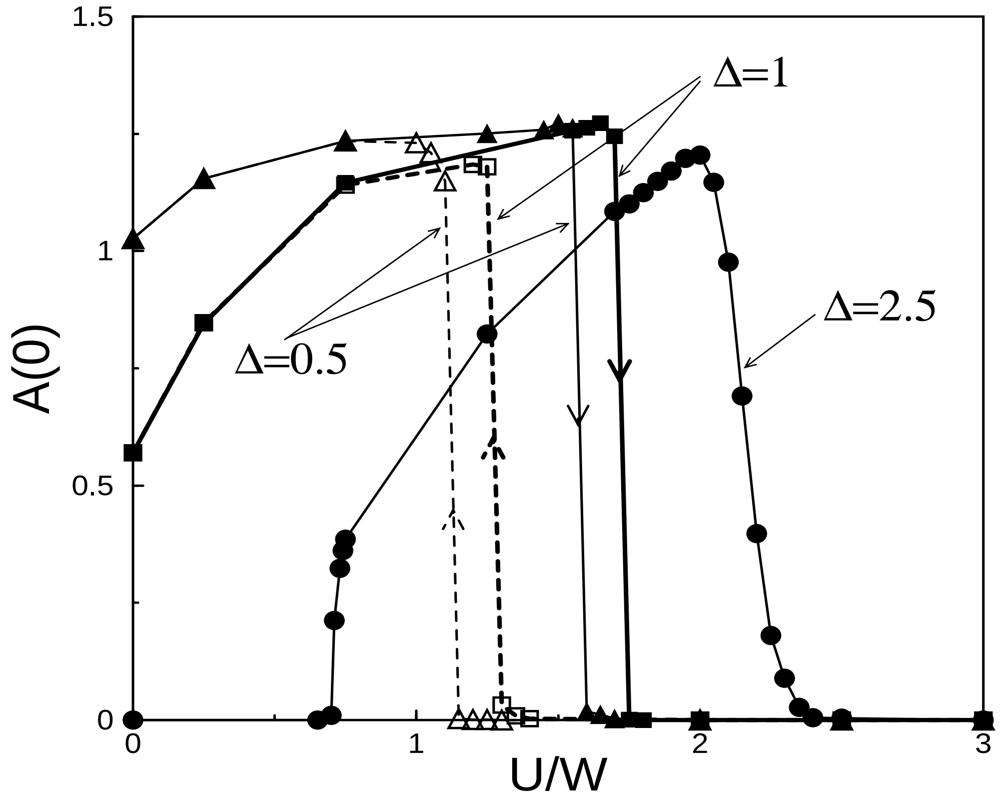
Phase diagram for disordered Hubbard model:

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

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



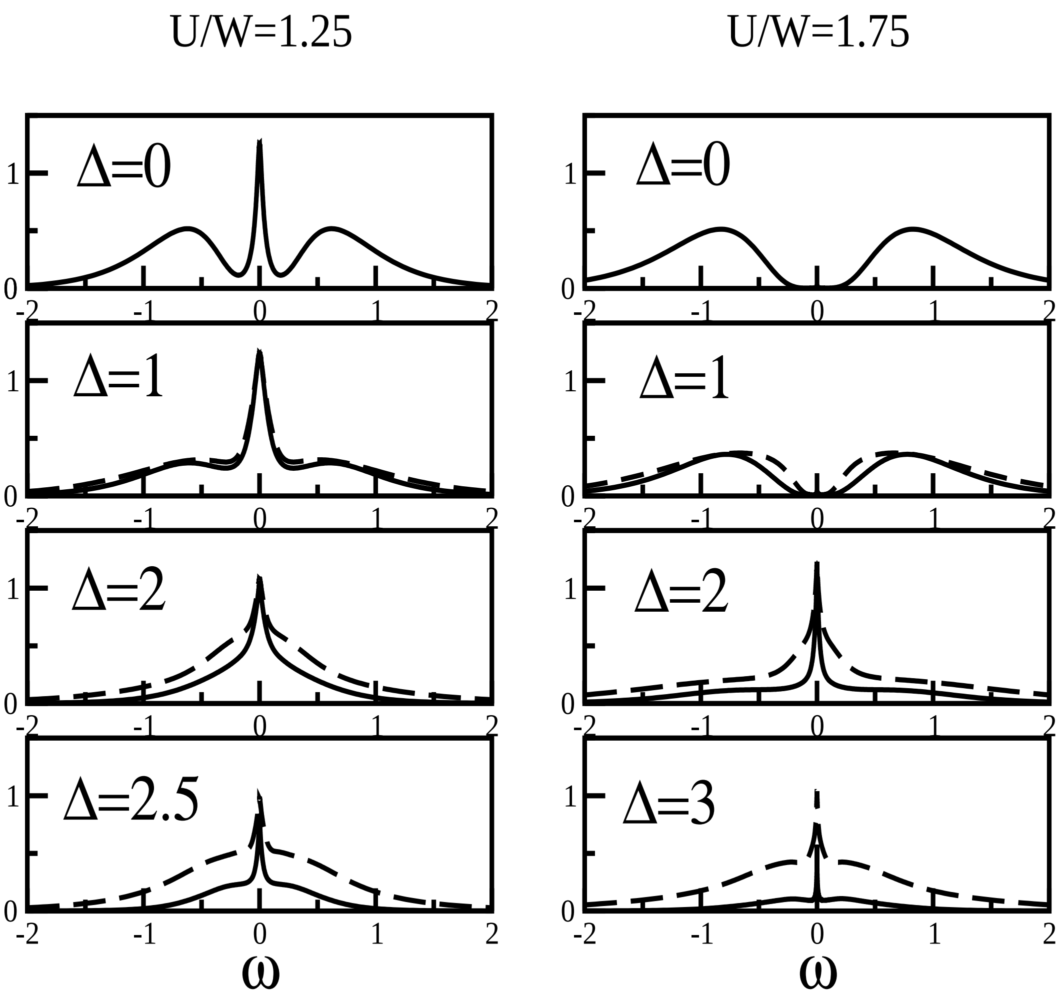
Mott-Hubbard transition in disordered Hubbard model:



* Friedel rule

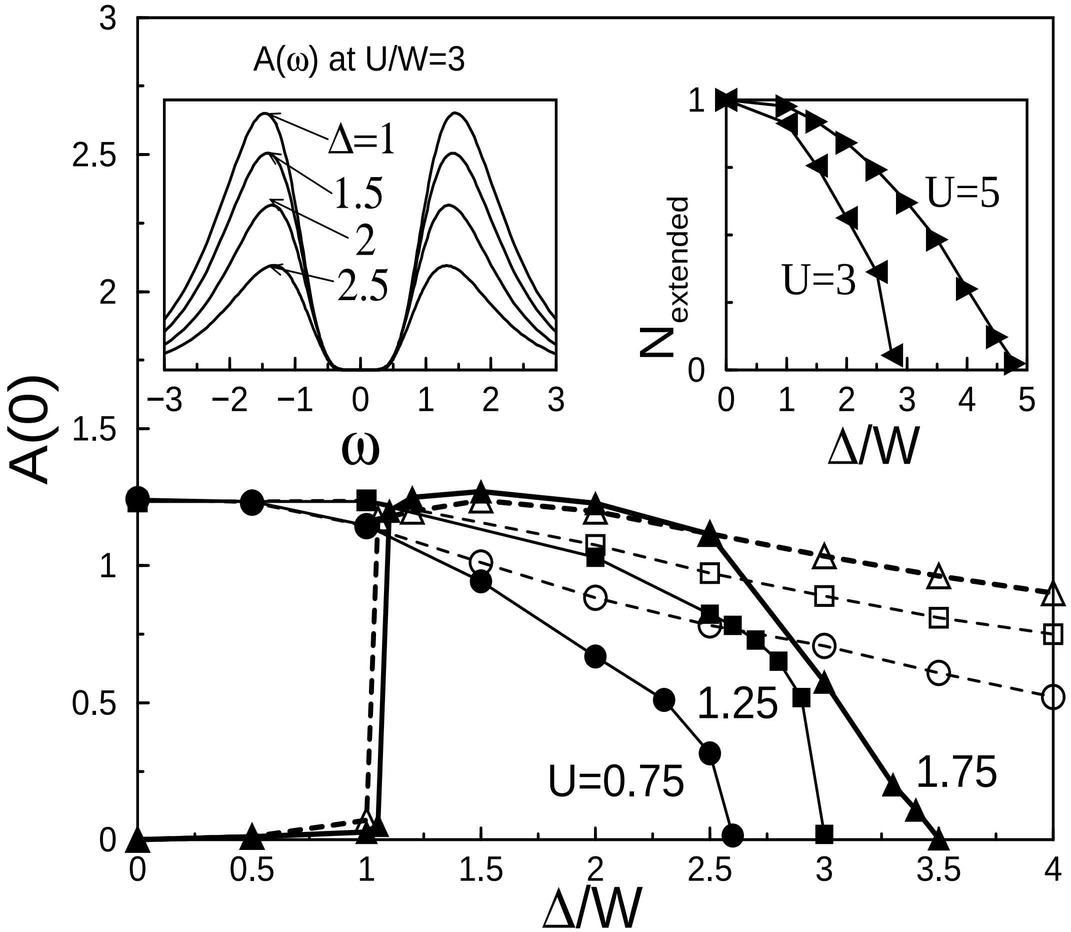
* Hysterisis $\Delta_{c1}(U)$, $\Delta_{c2}(U)$

Spectral functions in disordered Hubbard model:



* Redistribution of spectral weight

Anderson transition in Hubbard model:



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

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

Conclusions:

- Geometrical means used to study Anderson MIT in correlated electron system within DMFT

- Complete phase diagram

- Hysteresis and crossover in Mott-Hubbard MIT

- Nonmonotonic behavior of $\Delta_c(U)$ at Anderson MIT

- Two insulators connected adiabatically