Mott-Hubbard and Anderson Metal-Insulator Transitions

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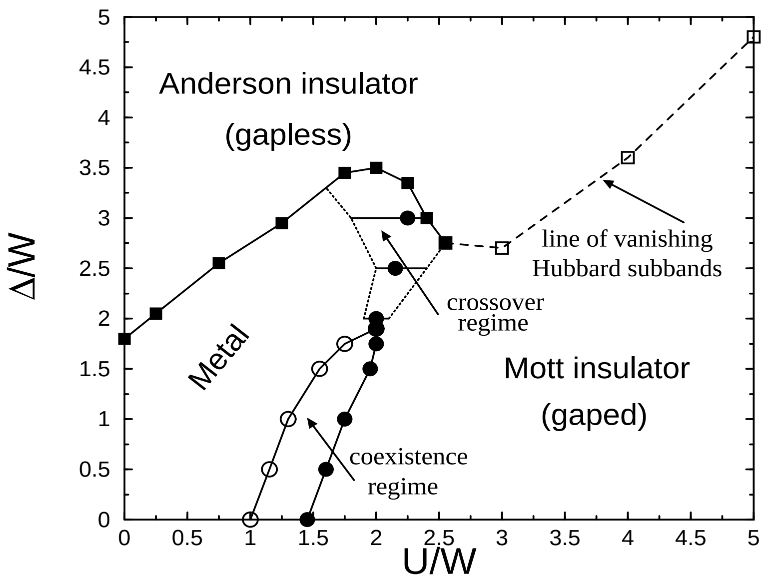
Main goal:

Some random events are better classified by geometric average

Main result:

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



U - interaction, Δ - disorder

Collaboration:

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

Plan of the talk:

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

Insulators:

$$\sigma^{DC}_{\alpha,\beta}(T=0) = \lim_{T\to 0^+} \lim_{\omega\to 0} \lim_{|\mathbf{q}|\to 0} \Re[\sigma_{\alpha,\beta}(\mathbf{q},\omega)] = 0$$

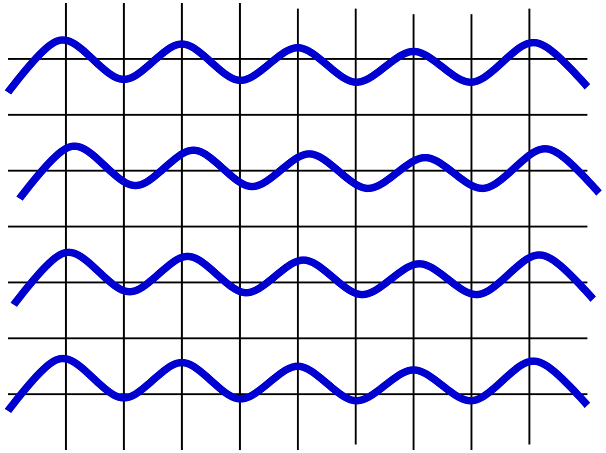
There is a gap $\Delta(\lambda) > 0$ in the single – particle spectrum

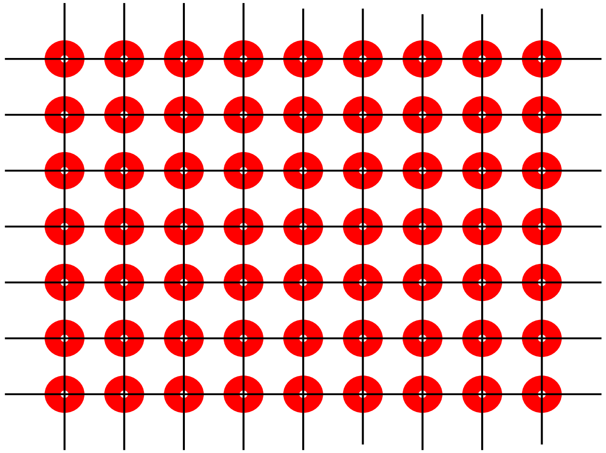
- robust gap – exists for all temperature
- soft gap – vanishes for $T > T_c$

- quantum phase transition – competition between E_{kin} and E_{pot}
- thermodynamic phase transitions – competition between U and S

- single – particle: due to electron – ion interactions
  - Bloch – Wilson (band) insulators
  - Peierls (lattice deformation) insulators
  - Anderson (lattice randomness) insulators (!)
- many – particle: due to electron – electron interactions
  - Slater (SDW) insulators
  - Mott – Hubbard (PM) insulators (!!)
  - Mott – Heisenberg (localized AF) insulators

Mott-Hubbard metal-insulator transition at $n = 1$

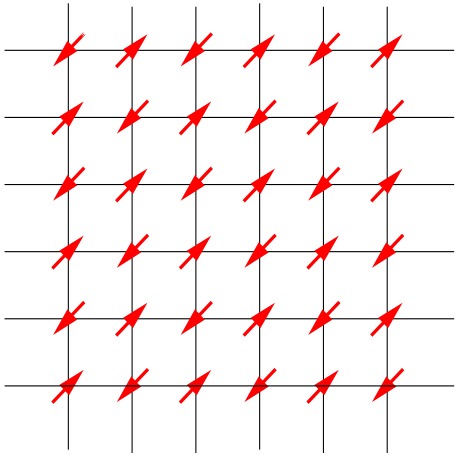




$U \ll |t_{ij}|$, $\Delta\mathbf{p} = 0$

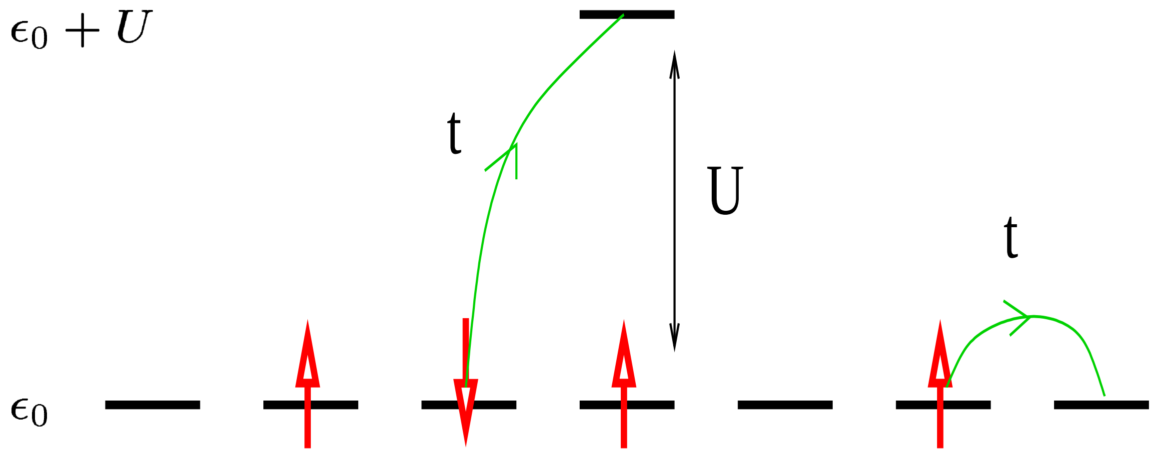
$U \gg |t_{ij}|$, $\Delta\mathbf{r} = 0$

Antiferromagnetic Mott insulator



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

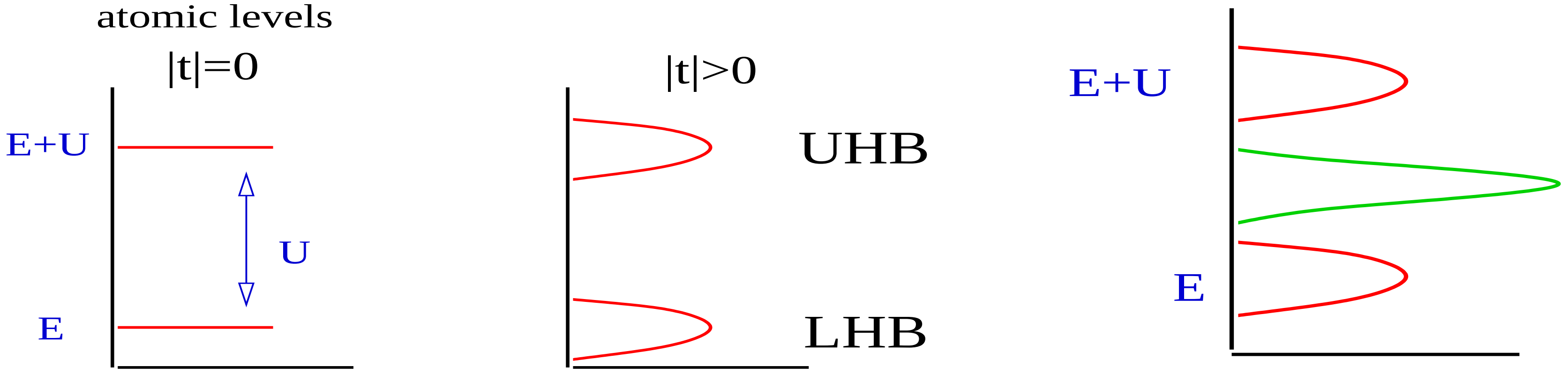
Hubbard model to capture right physics

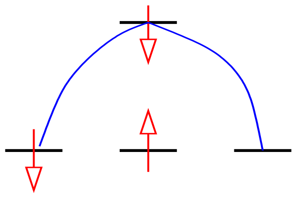


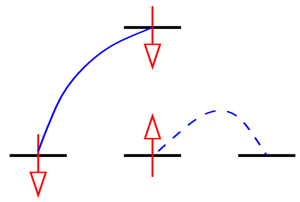
$$H = \sum_{i\sigma} \epsilon_0 n_{i\sigma} + \sum_{ij\sigma} t_{ij}\, a^\dagger_{i\sigma} a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

- long history, many contradictions
- exactly solvable in $d = 1$
- exactly solvable in $d = \infty$ (DMFT)
- how to approximate in $1 < d < \infty$?

Physical picture, $n = 1$







spin flip on central site

at $U = U_c$ resonance disapears
gaped insulator

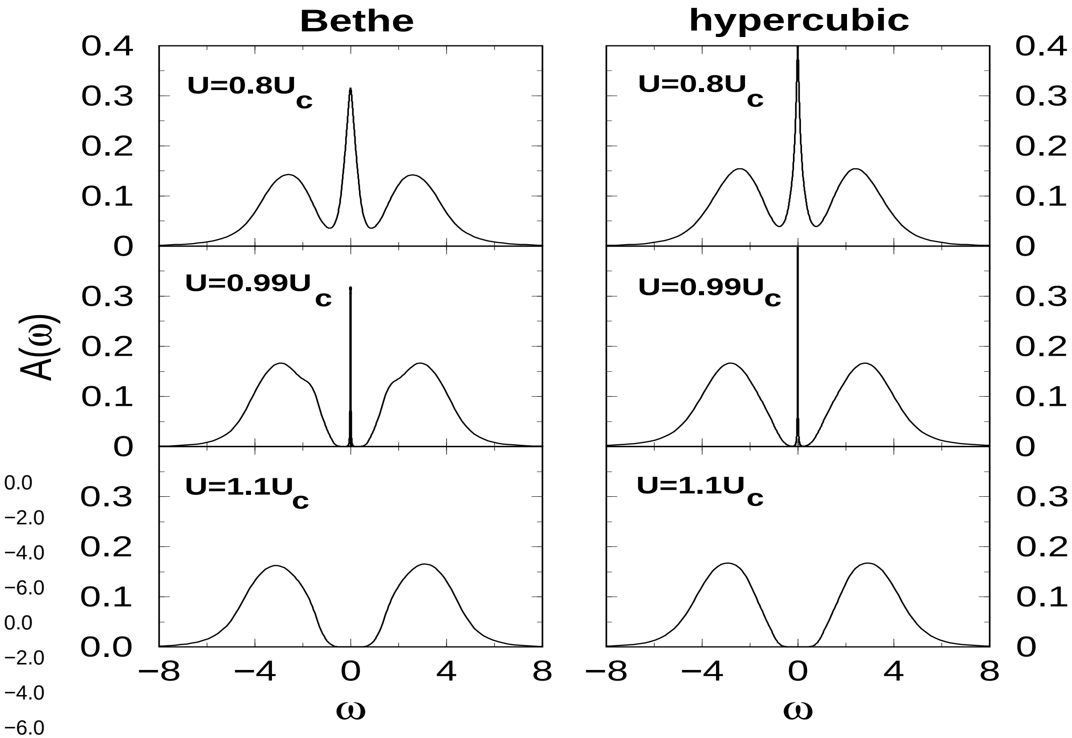
dynamical processes with spin-flips inject states into correlation gap giving a quasiparticle resonance

T=0 Mott transition according to DMFT

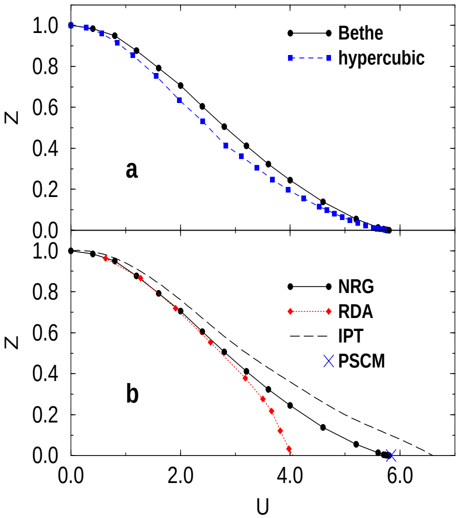
Kotliar et al. 92-96, Bulla, 99

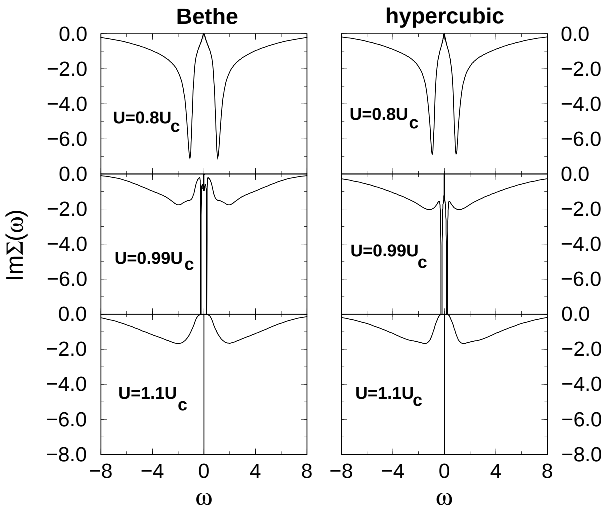
quantity to be determined

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



spectral density function

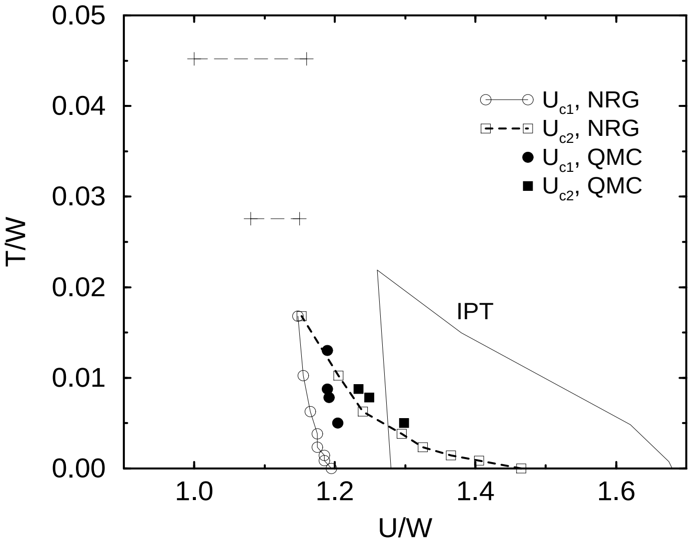


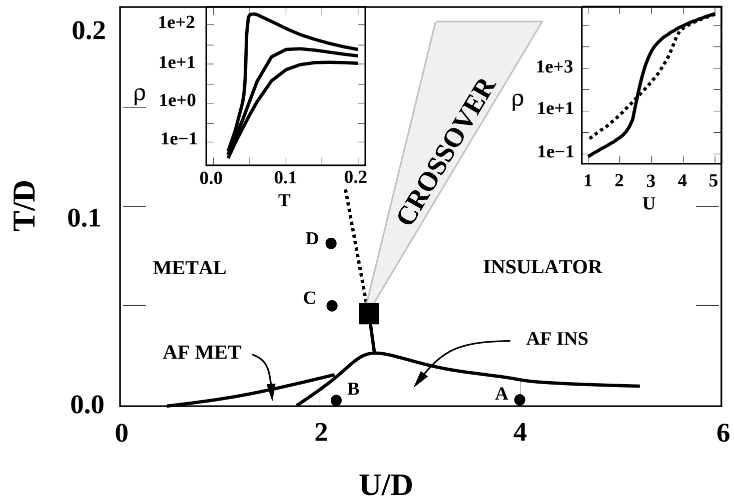


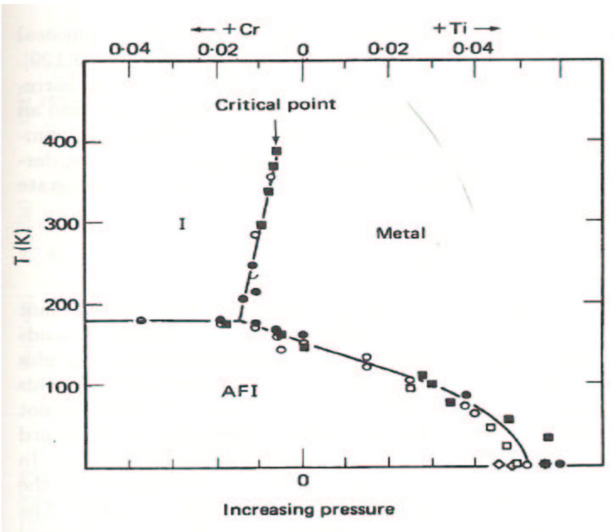
$$G(k,\omega) \sim \frac{Z}{\omega - \tilde{\epsilon}_k - i\alpha\ \omega^2} + G_{inc}$$

Mott transition at $T > 0$

Kotliar et al. 92-96, Bulla et al. 01, also Spalek 87



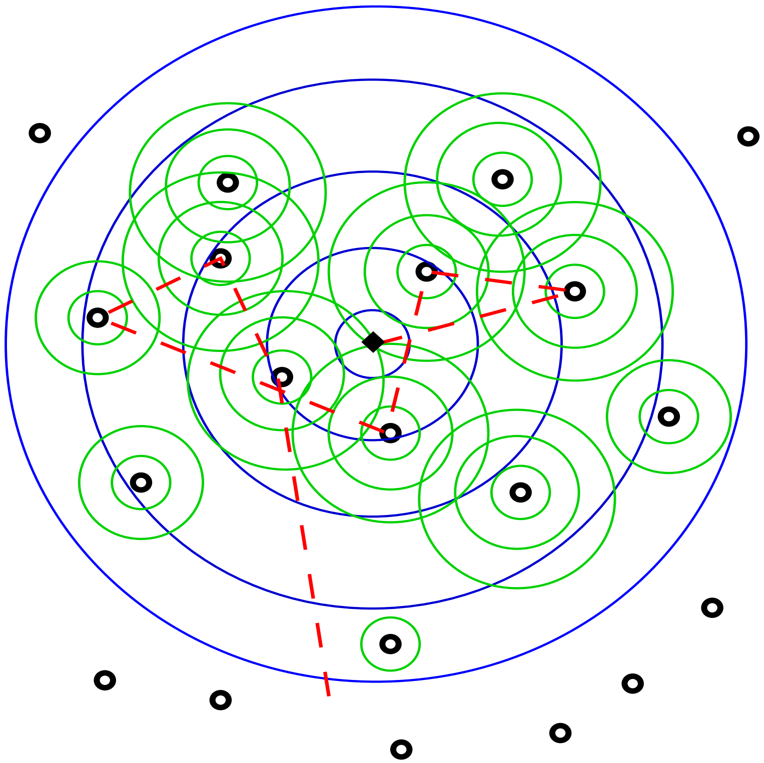




1^{st}-order transition

Anderson localization:

propagation of waves in a randomly inhomogeneous medium



random conservative linear wave equation

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

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

diffusive motion, memory of $\vec{V}(0)$ lost, "random walk" over long distances, friction imposed by averaging

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

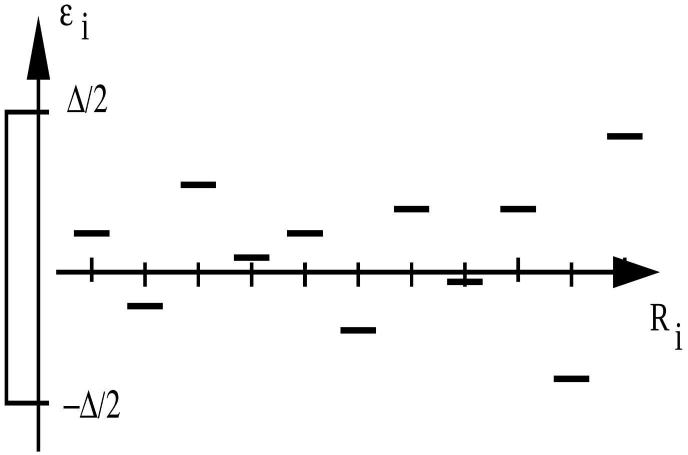
Localization is a destruction of coherent superposition of spatially separated states

Anderson model:

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

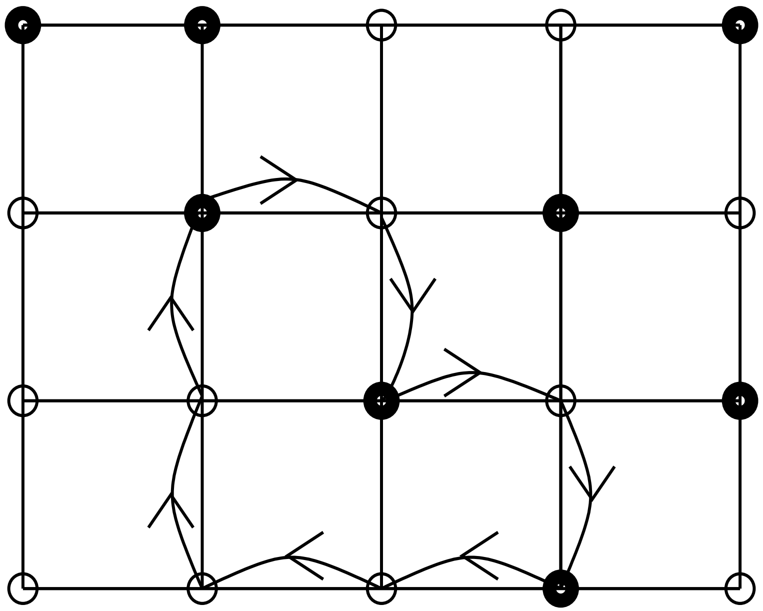
Probability distribution function

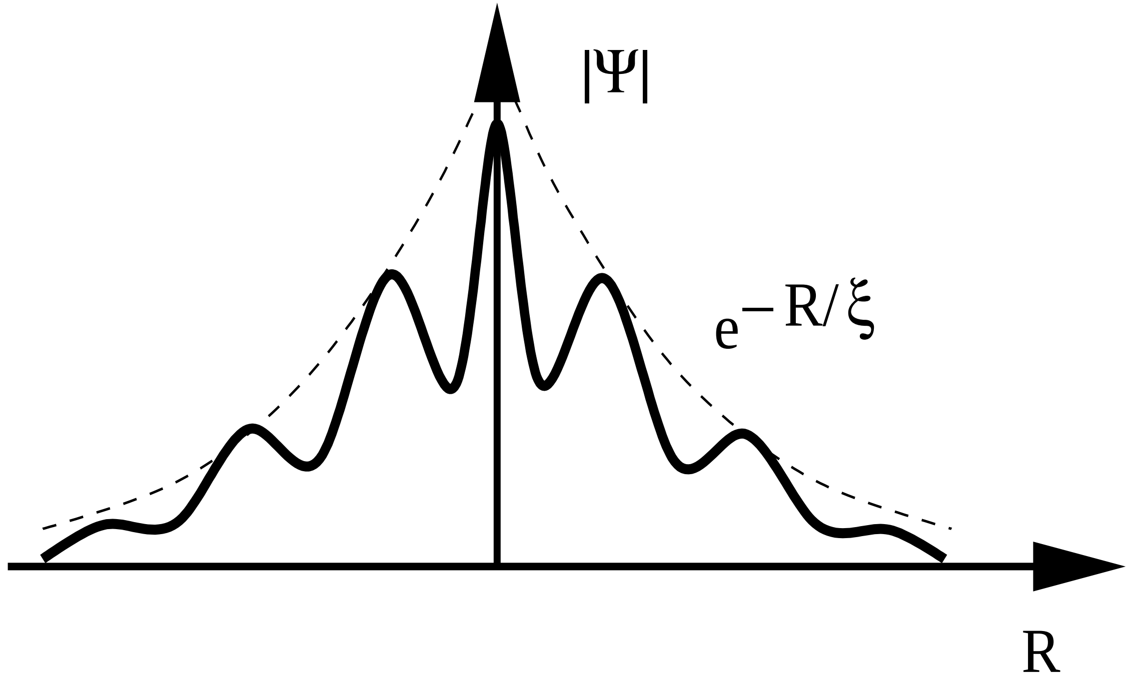
$$\mathcal{P}(\epsilon_i) = \frac{1}{\Delta}\Theta\left(\frac{\Delta}{2} - |\epsilon_i|\right)$$



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**

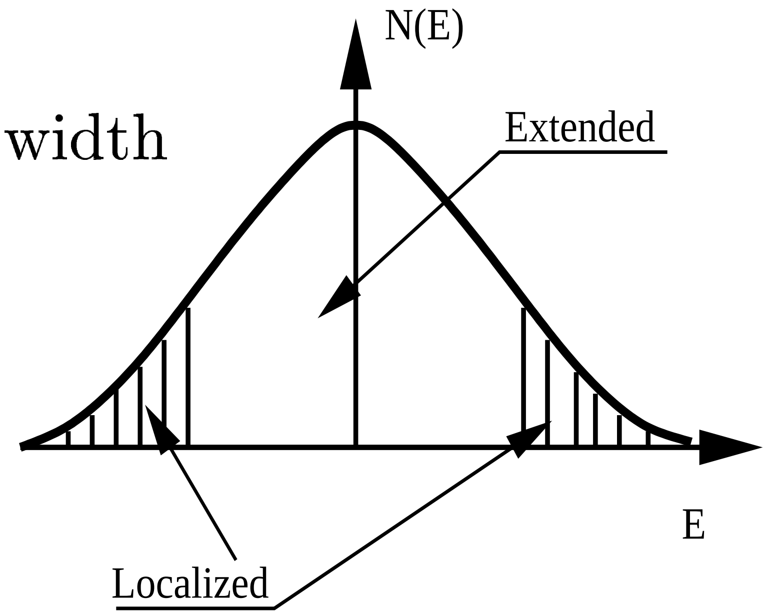
$P_{j \to j}(t \to \infty; V \to \infty) > 0$ **for localized states**

Anderson MIT - cont.:

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**

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



Characterization of Anderson localization:

- **Decaying of wavefunction**
  $|\Psi_n(r_i)| \sim e^{-|r-r_i|/\xi(E_n)}$
  - **metal** $\xi \to \infty$
  - **insulator** $\xi < \infty$

- **Inverse participation ratio** P^{-1} **[inverse number of sites that contribute to** $\Psi_n(r_i)$**]**
  - **metal** $P^{-1} \sim 1/N$
  - **insulator** $P^{-1} \sim \mathrm{const}$

Characterization of Anderson localization:

- **Conductance** G
  - **metal** $G > 0$
  - **insulator** $G = 0$
- **Local Density of States (LDOS)**

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

Local DOS in DMFT

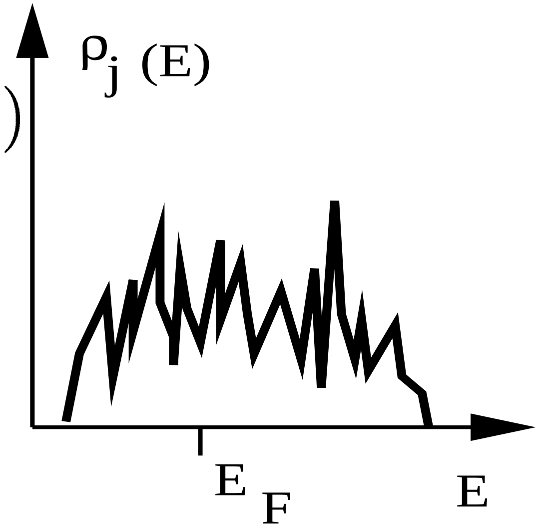
Heuristic arguments:

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

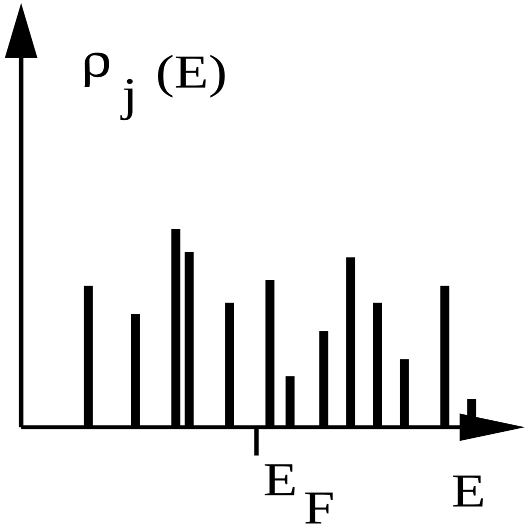
$$G_j(t) \sim e^{i(\epsilon_j+\Sigma'_j)t-|\Sigma''_j|t} \sim e^{-\frac{t}{\tau_{\rm esc}}}$$

Fermi Golden Rule

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



metal



insulator

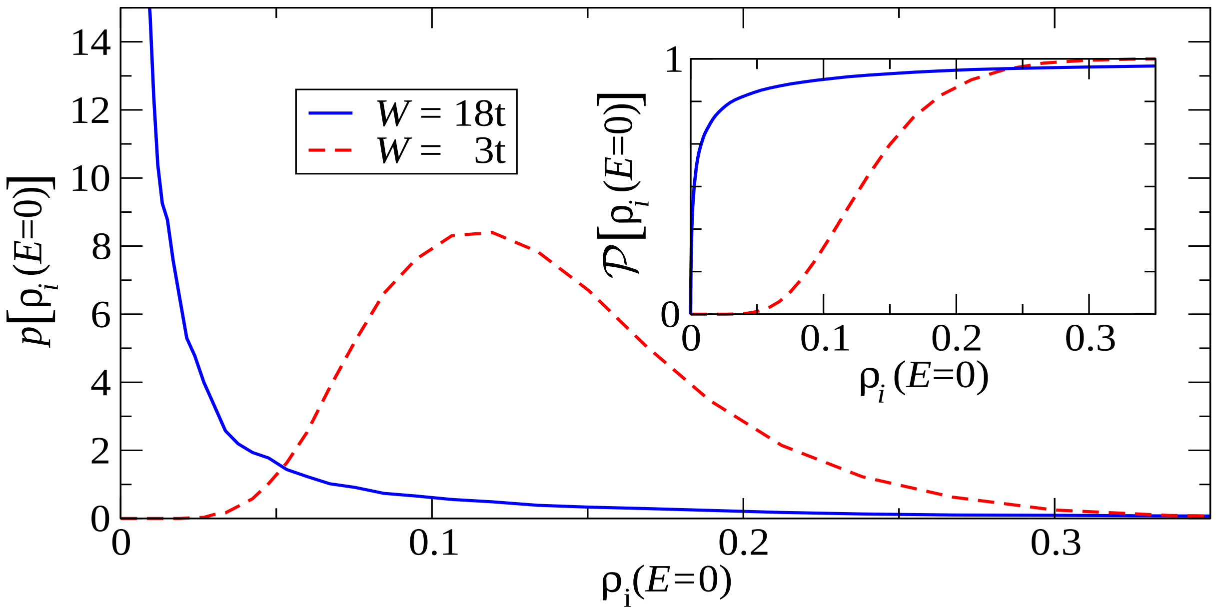
Statistics of LDOS:

$\rho_j(E)$ **is different at different** R_j**!**

Random quantity!

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

Exact diagonalization – Schubert et al. cond-mat/0309015



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

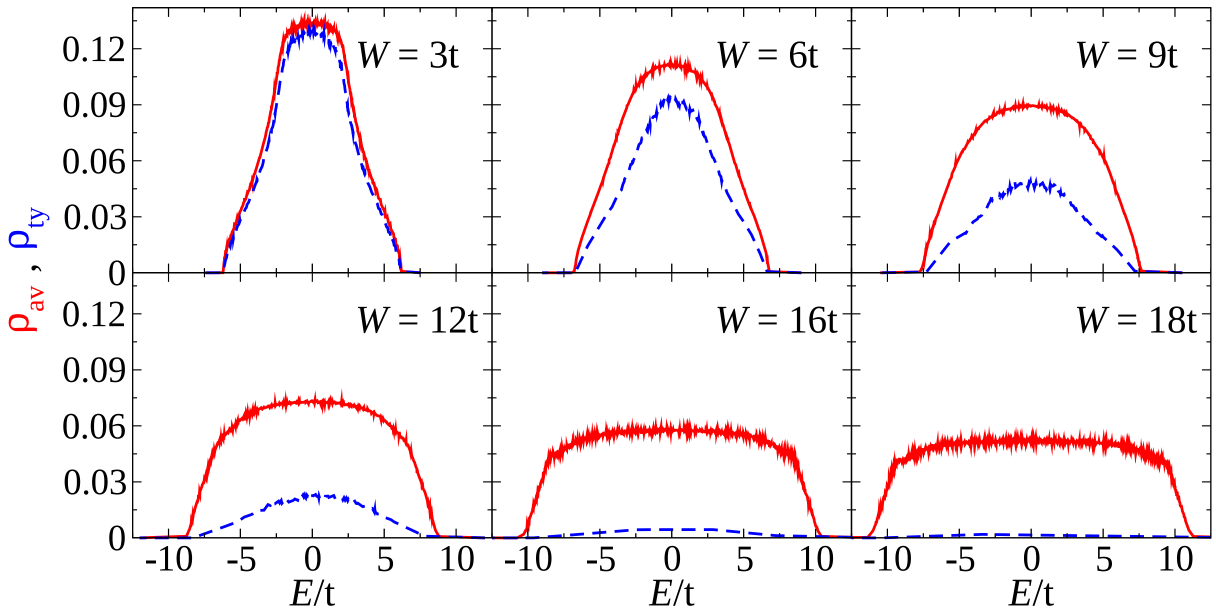
Multifractality - $\langle M^{(k)}\rangle \sim L^{-f(k)}$

Typical escape rate is determined by the typical LDOS

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

Anderson MIT - cont.:

Why should it work at all?

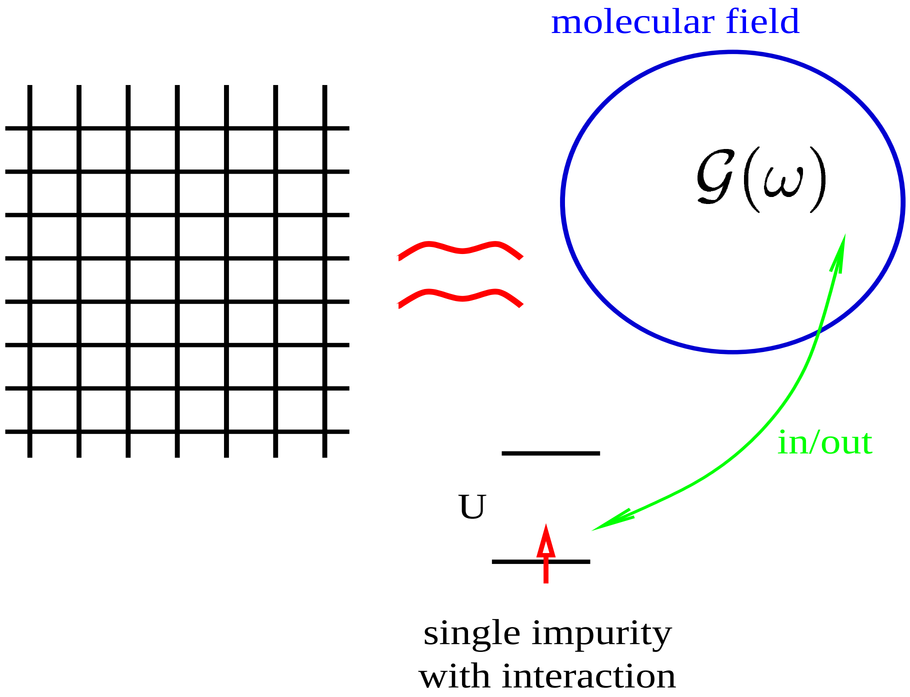
$$
\begin{aligned}
\rho_{geom}(E) &= e^{\langle \ln \rho_i(E) \rangle} = \\
& e^{\frac{1}{\Delta}\sum_{i=1}^{N} \ln \rho_i(E)} = \\
& \prod_{i=1}^{N} \rho_i(E)^{\frac{1}{\Delta}}
\end{aligned}
$$

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

Dynamical mean-field theory for U

Kotliar et al., Vollhardt et al.

Lattice problem of interacting particles is mapped onto a single impurity (single atom) coupled to the molecular bath



Molecular (Weiss) function $\mathcal{G}(\omega)$ is a dynamical quantity, determined self-consistently

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

DMFT with Anderson MIT:

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

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

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

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

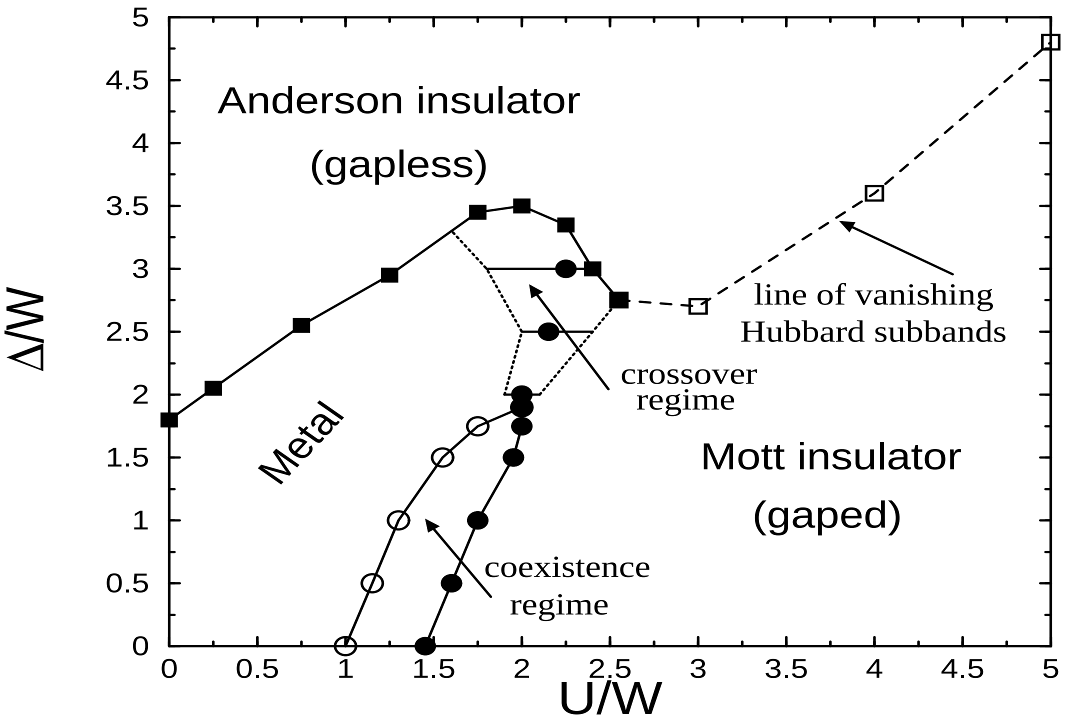
$$G^{-1}(\omega) = \omega - \eta(\omega) - \Sigma(\omega), \qquad \eta(\omega) = \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{\omega - \epsilon_{\mathbf{k}}}$$

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

Phase diagram for disordered Hubbard model:

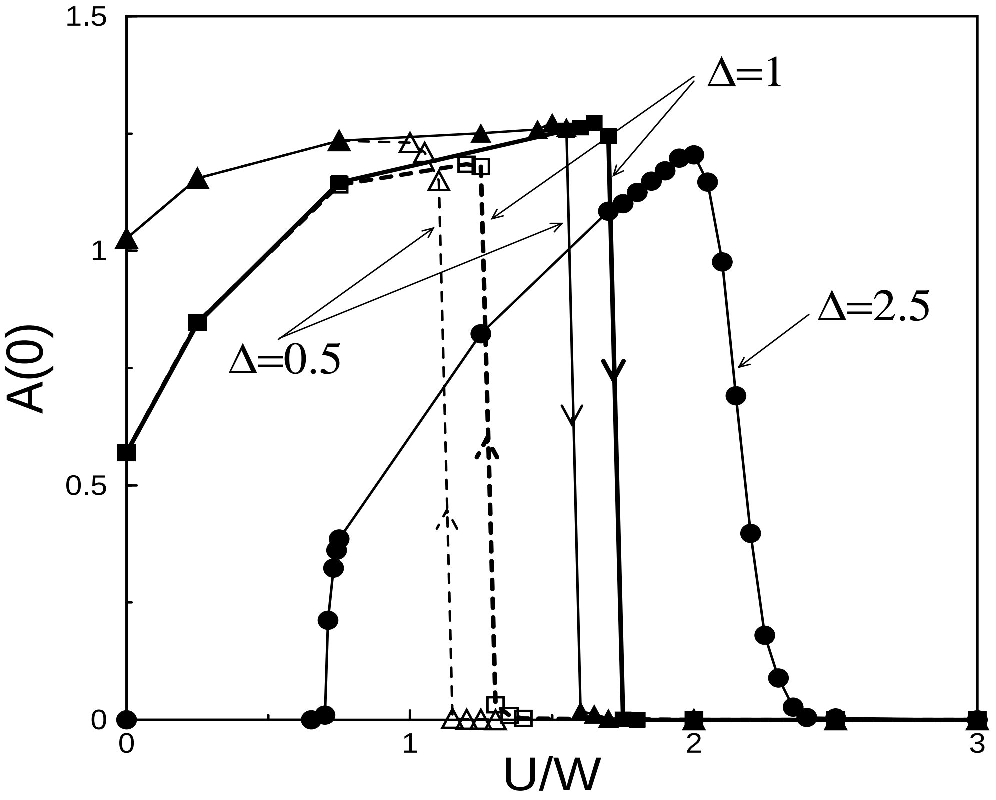
$$N_0(\epsilon) = \frac{2}{\pi D}\sqrt{D^2 - \epsilon^2}; \quad \eta(\omega) = \frac{D^2}{4} G(\omega)$$

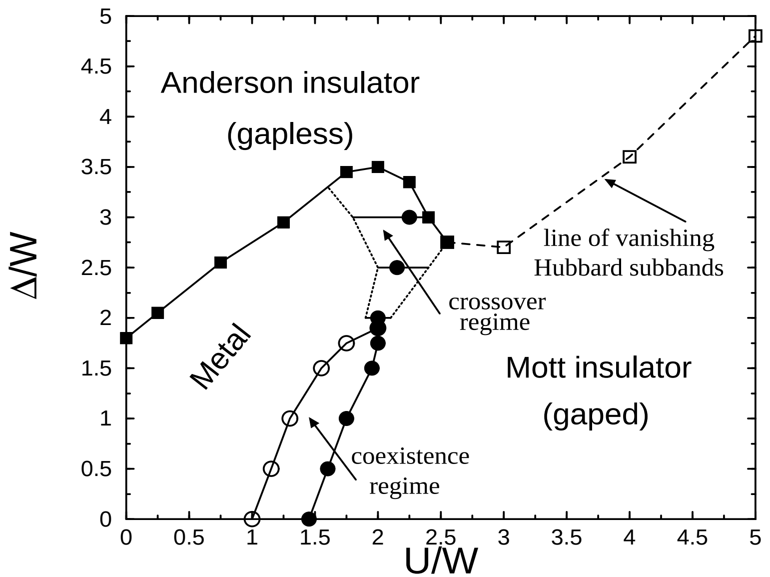
$T = 0$, $n = 1$, $W = 2D = 1$



U - **interaction,** Δ - **disorder**

Mott-Hubbard transition in disordered Hubbard model:





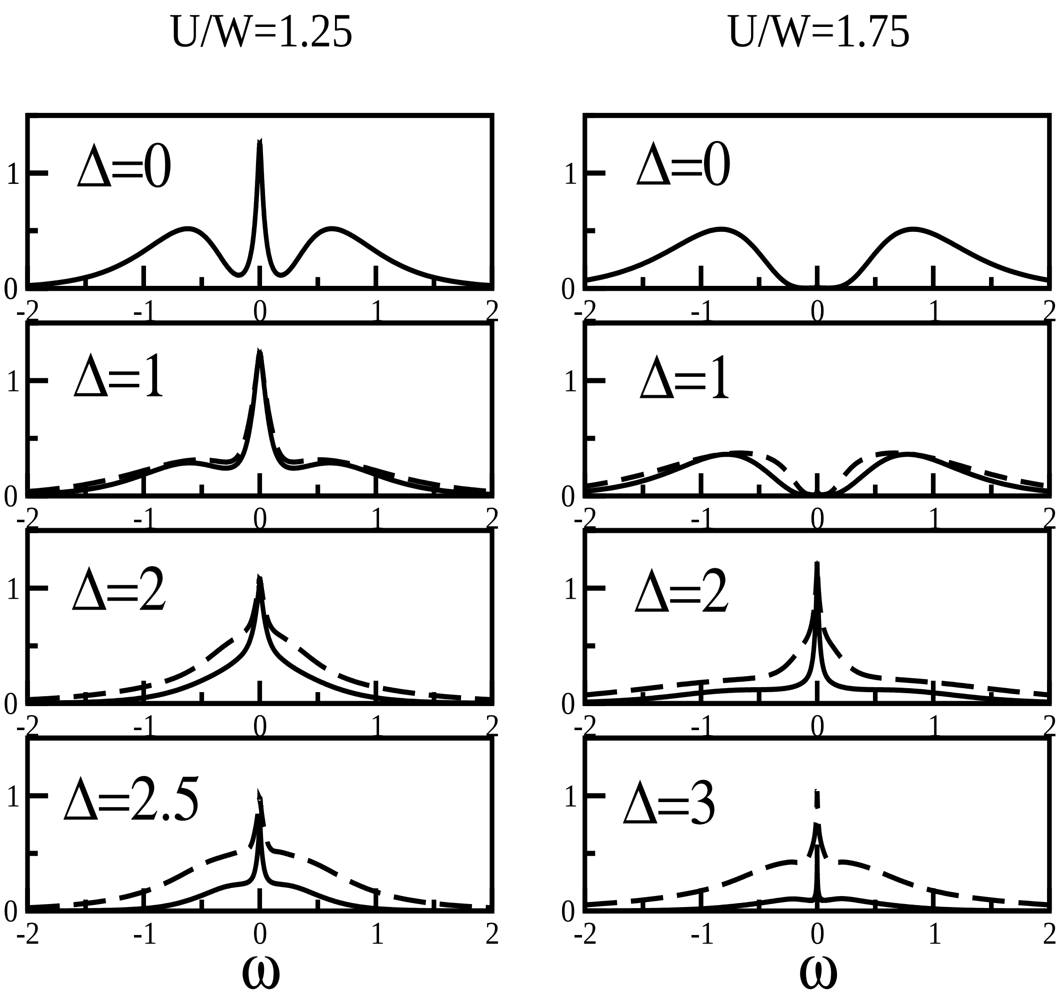
* **Friedel rule (FL due to U)**

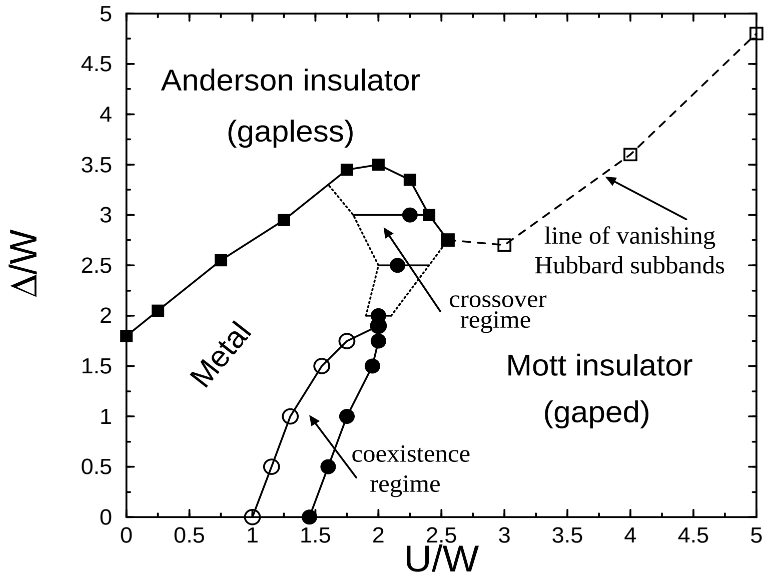
* **Hysterisis $\Delta_{c1}(U)$, $\Delta_{c2}(U)$**

* **Crossover**

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

Spectral functions in disordered Hubbard model:



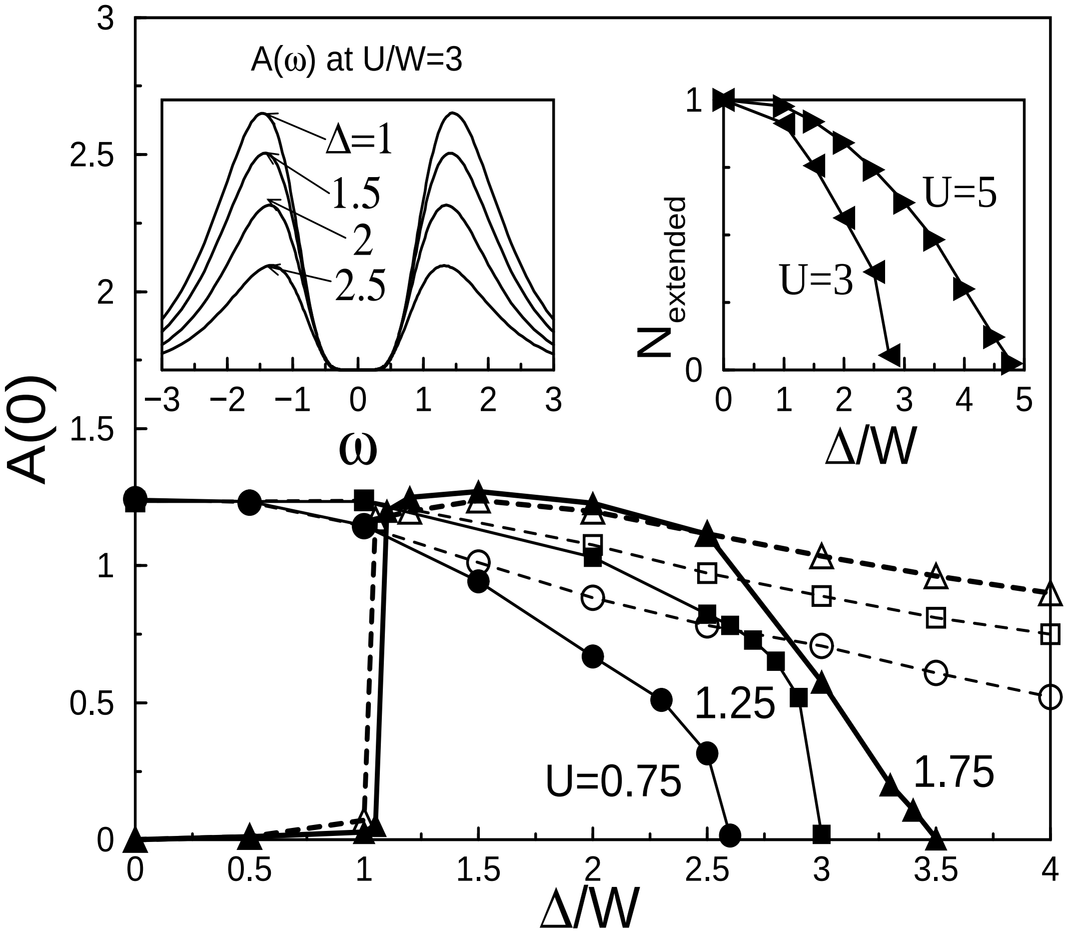


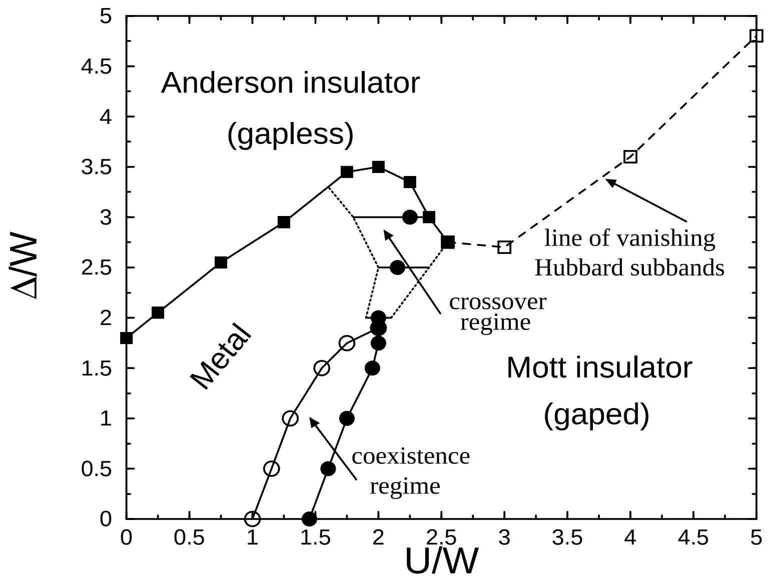
* **Redistribution of spectral weight**

* **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**

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

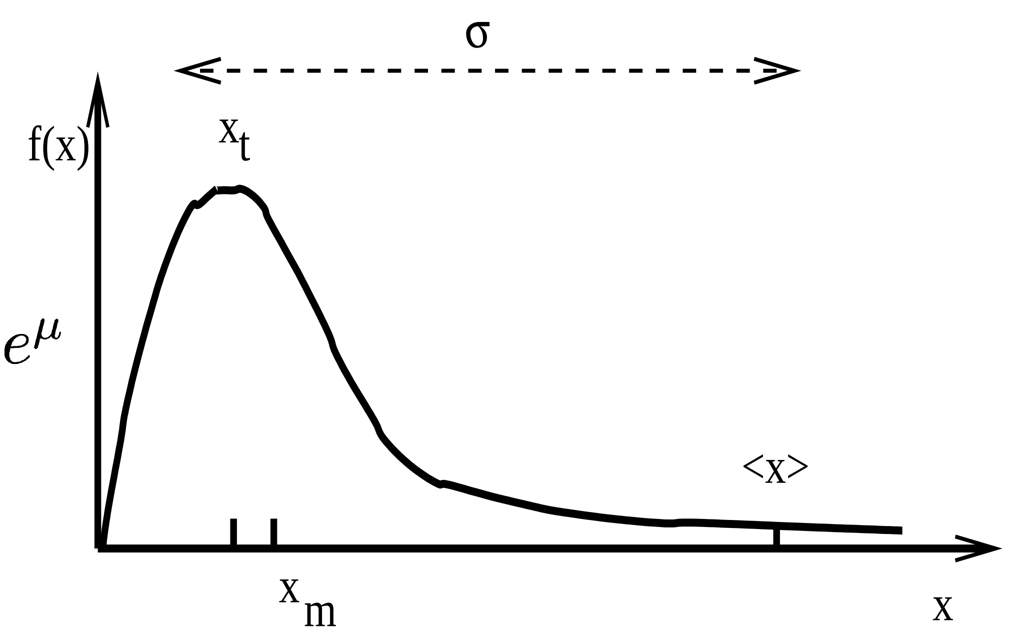
Conclusions:

- 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

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.