Mott-Hubbard and Anderson Metal-Insulator Transitions

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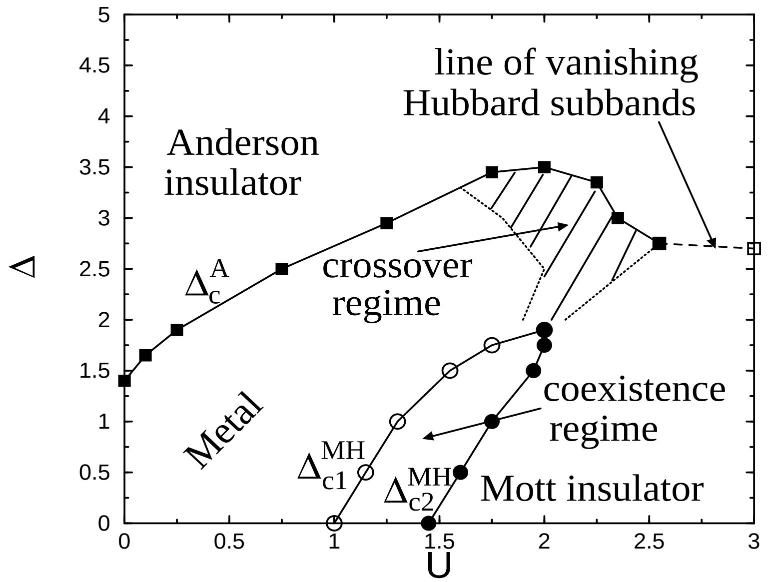
Main goal:

Mott – Hubbard MIT ↔ Interaction
Anderson MIT ↔ Disorder
Some random events are better classified by geometric average

Main result:

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

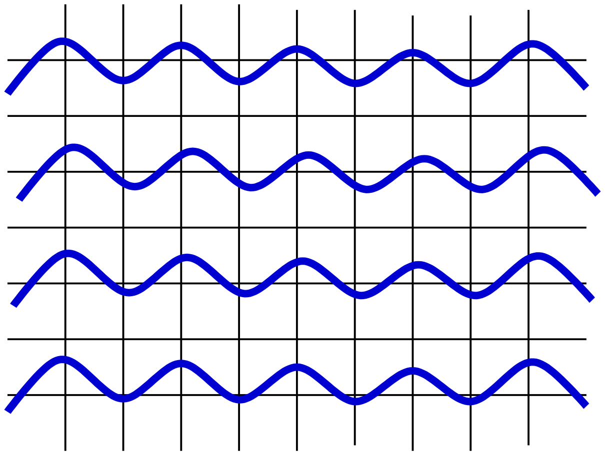


U - interaction, Δ - disorder

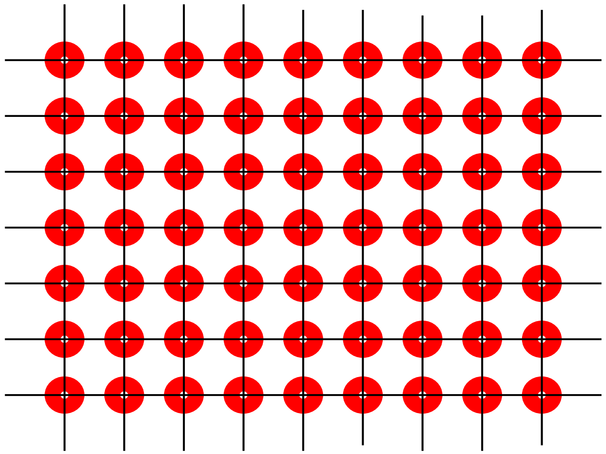
Collaboration:

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

Mott-Hubbard MIT at $n = 1$

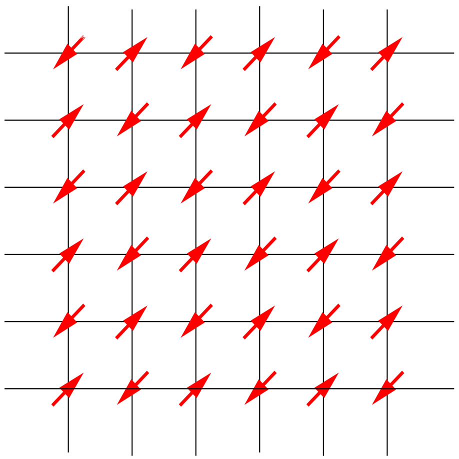


$U \ll |t_{ij}|$, $\Delta\mathbf{p} = 0$



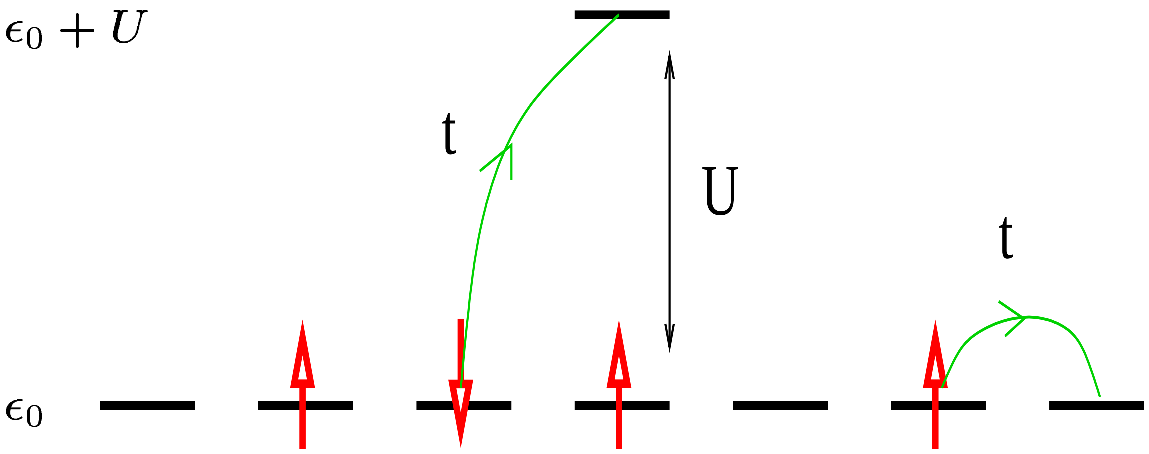
$U \gg |t_{ij}|$, $\Delta\mathbf{r} = 0$

Antiferromagnetic Mott insulator



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

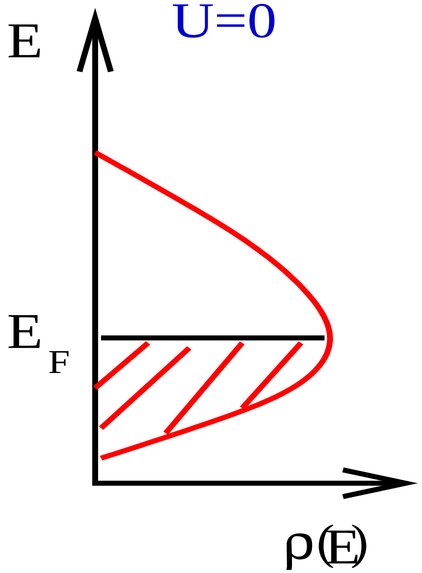
Hubbard model to capture right physics

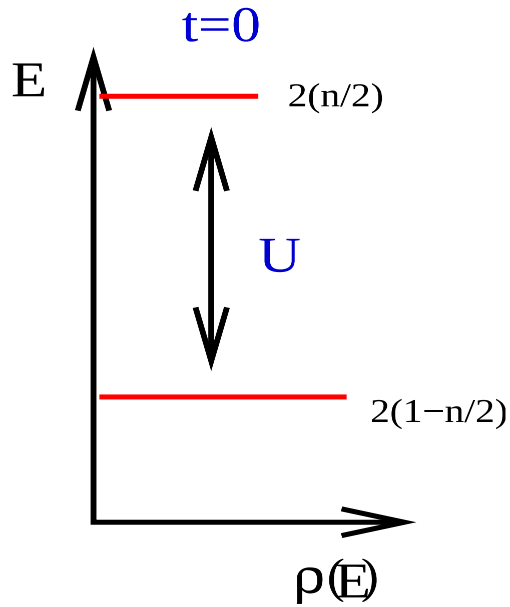


DOS: $\rho(E) = \sum_n \int dx |\psi_n(x)| \delta(E - \epsilon_n)$

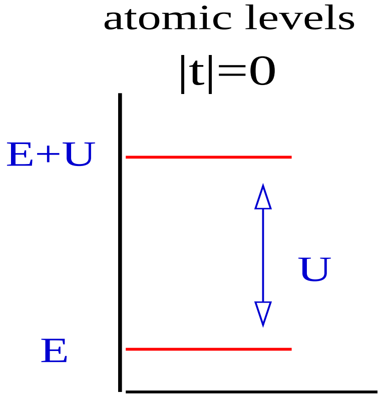
$$H = \sum_{i\sigma} \epsilon_0 n_{i\sigma} + \sum_{ij\sigma} t_{ij}\, a^\dagger_{i\sigma} a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

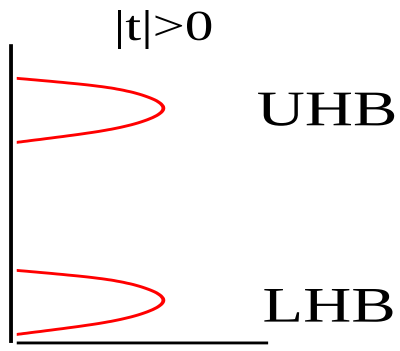
- long history, many contradictions
- exactly solvable in $d = 1$
- exactly solvable in $d = \infty$ (DMFT)
- how to approximate in $1 < d < \infty$?

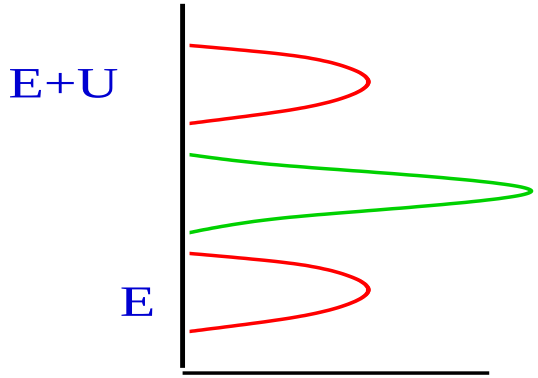


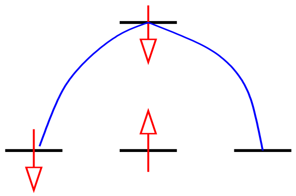


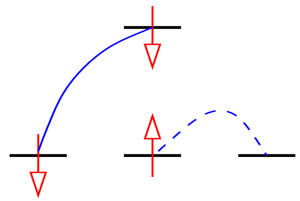
Physical picture, $n = 1$











spin flip on central site

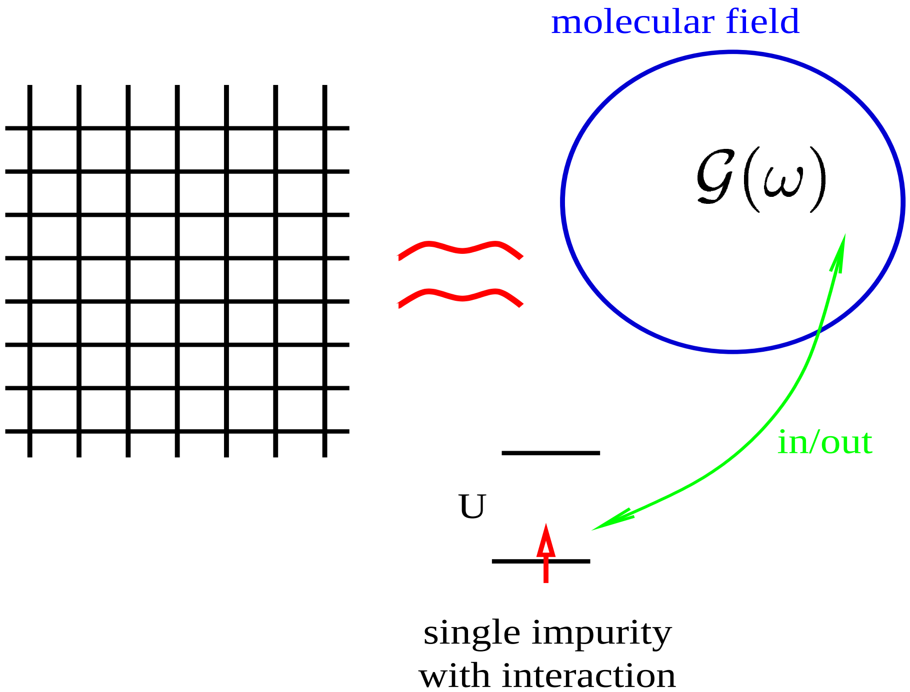
at $U = U_c$ resonance disapears
gaped insulator

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

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

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

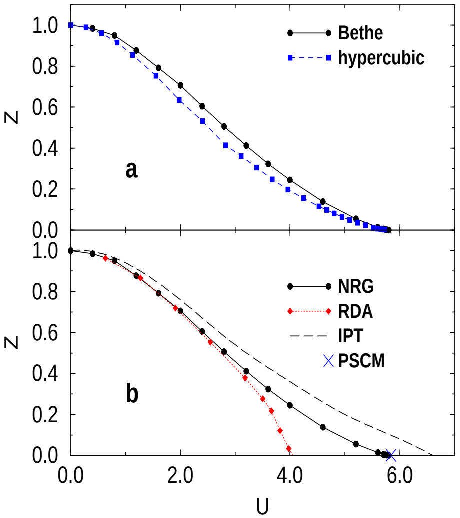
T=0 Mott transition according to DMFT

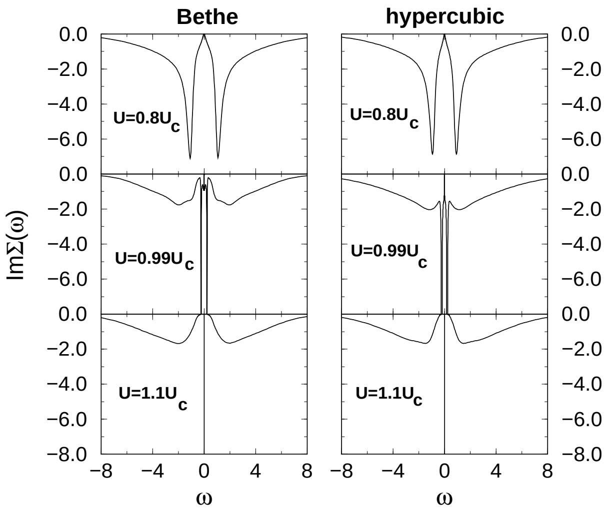
Kotliar et al. 92-96, Bulla, 99

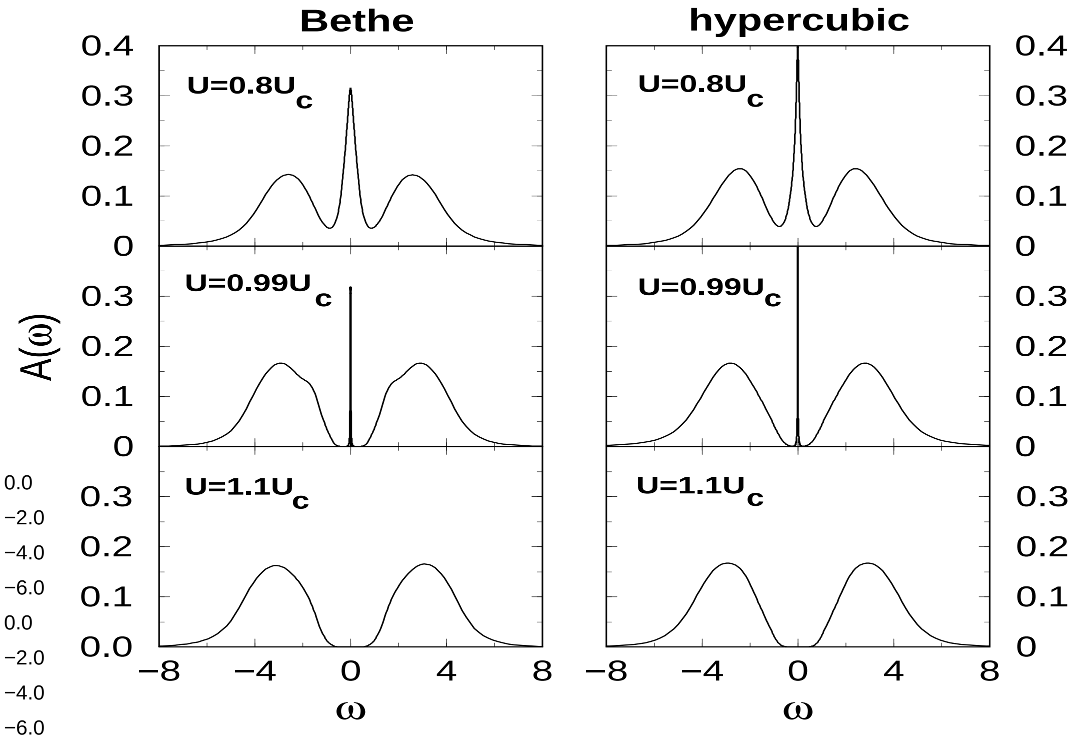
quantity to be determined

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

spectral density function



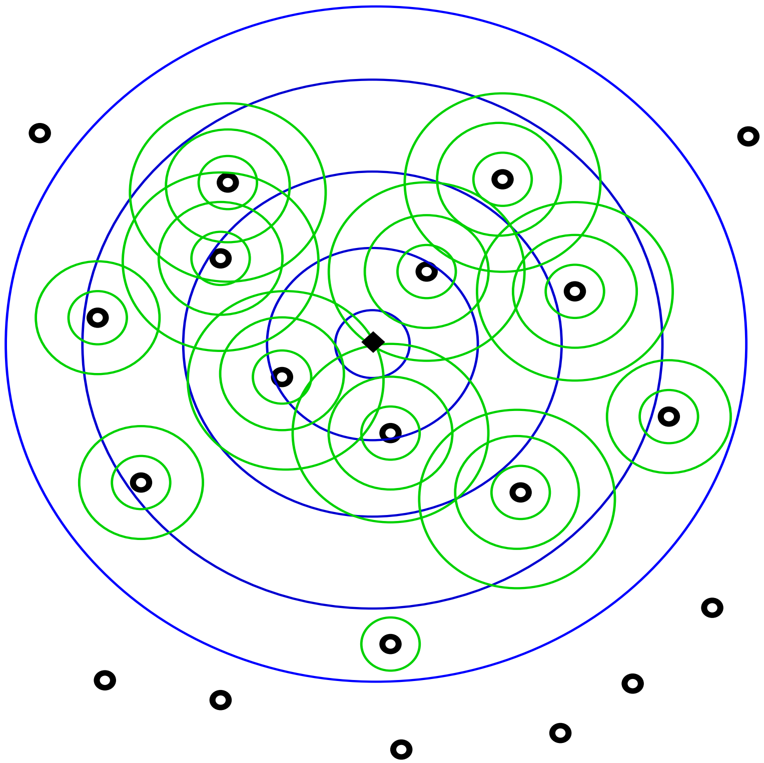




$$G(k,\omega) \sim \frac{Z}{\omega - \tilde{\epsilon}_k - i\alpha\ \omega^2} + G_{inc}$$

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

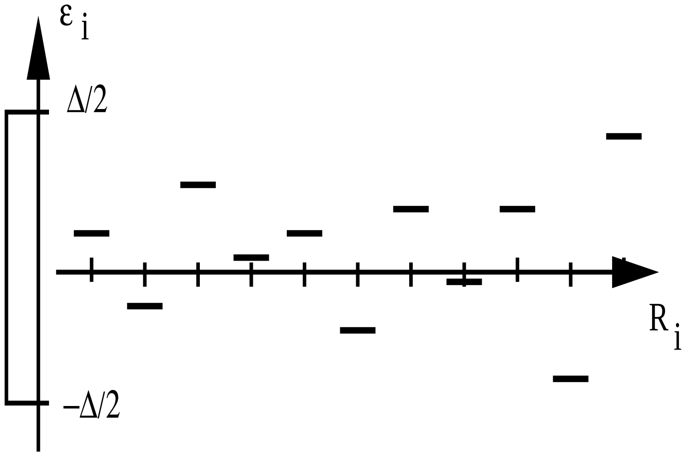
Localization is a destruction of coherent superposition of spatially separated states

Anderson model:

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

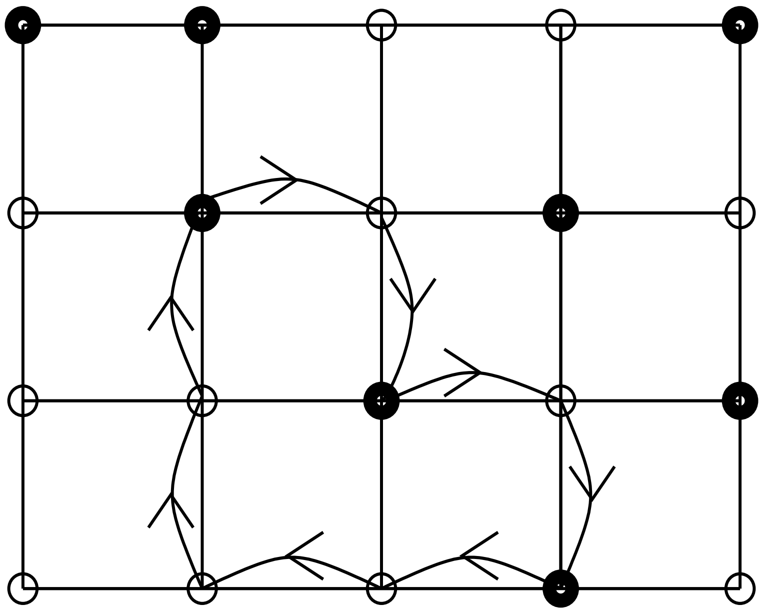
Probability distribution function

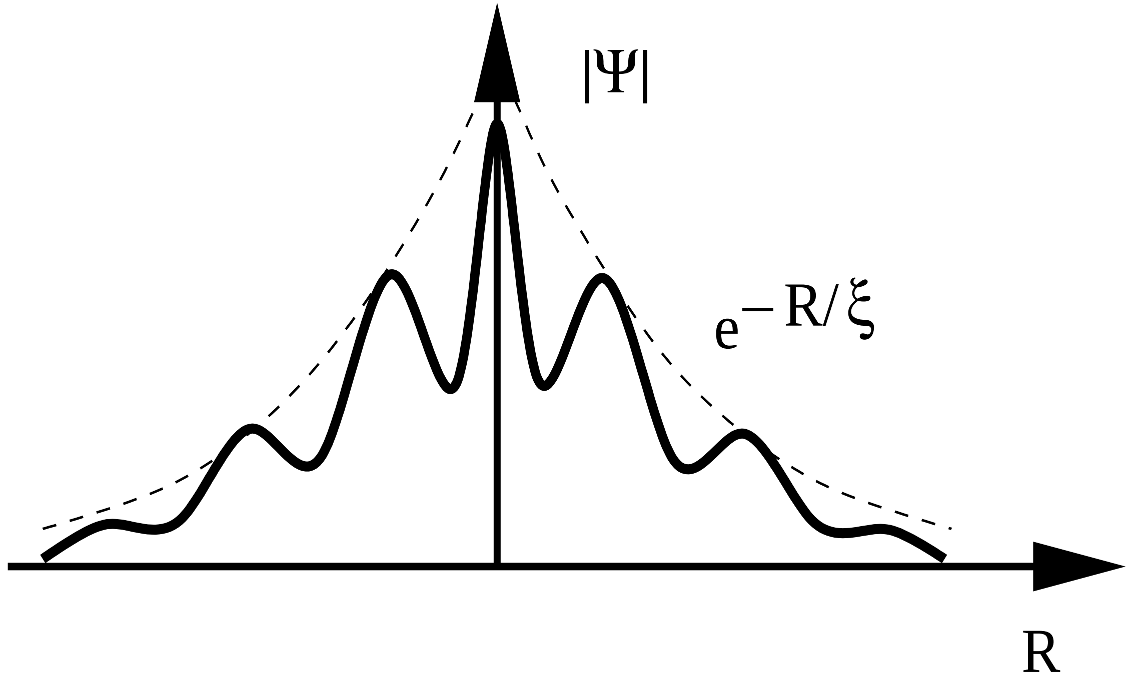
$$\mathcal{P}(\epsilon_i) = \frac{1}{\Delta}\Theta\left(\frac{\Delta}{2} - |\epsilon_i|\right)$$



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)

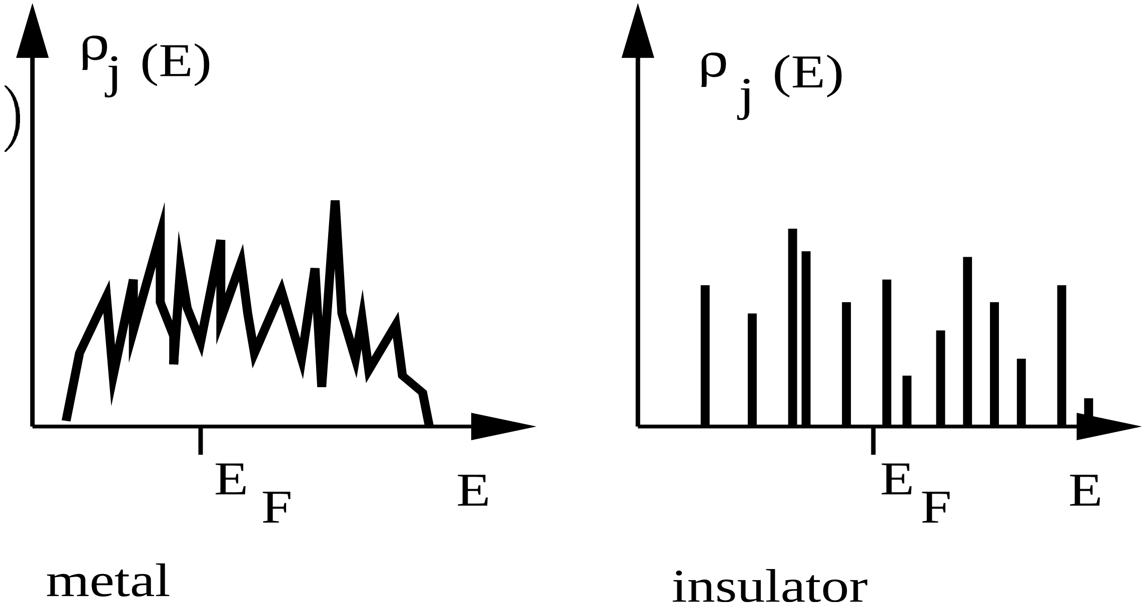
$$\rho_i(E) = \sum_{n=1}^{N} |\Psi_n(r_i)|^2 \delta(E - E_n)$$

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

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

Fermi Golden Rule

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

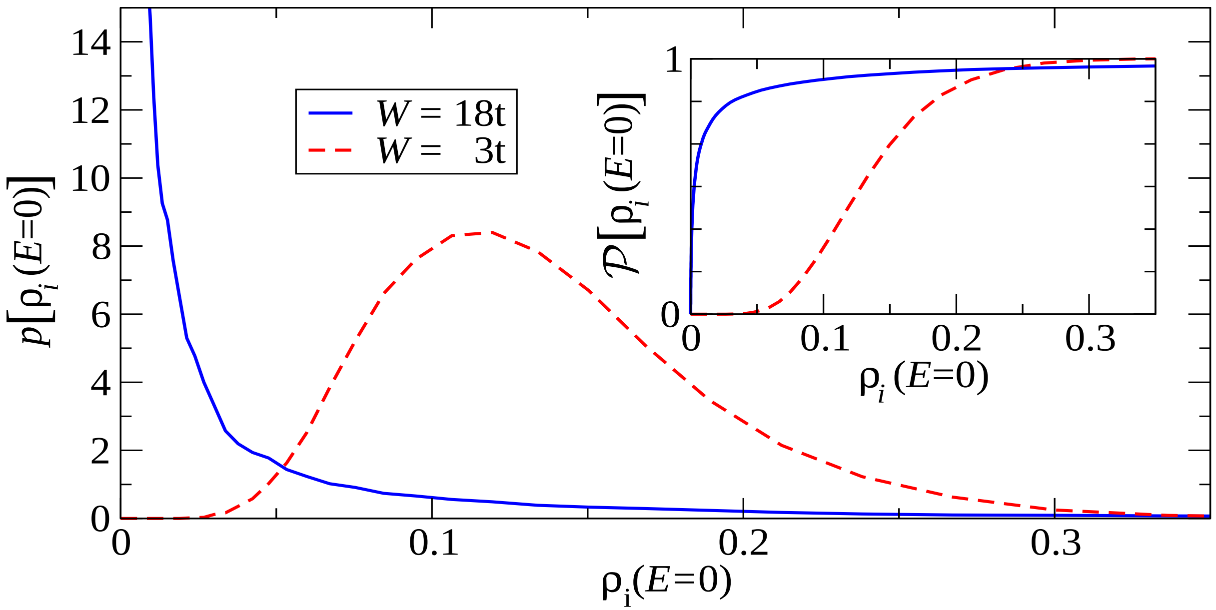


Statistics of LDOS:

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

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

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



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

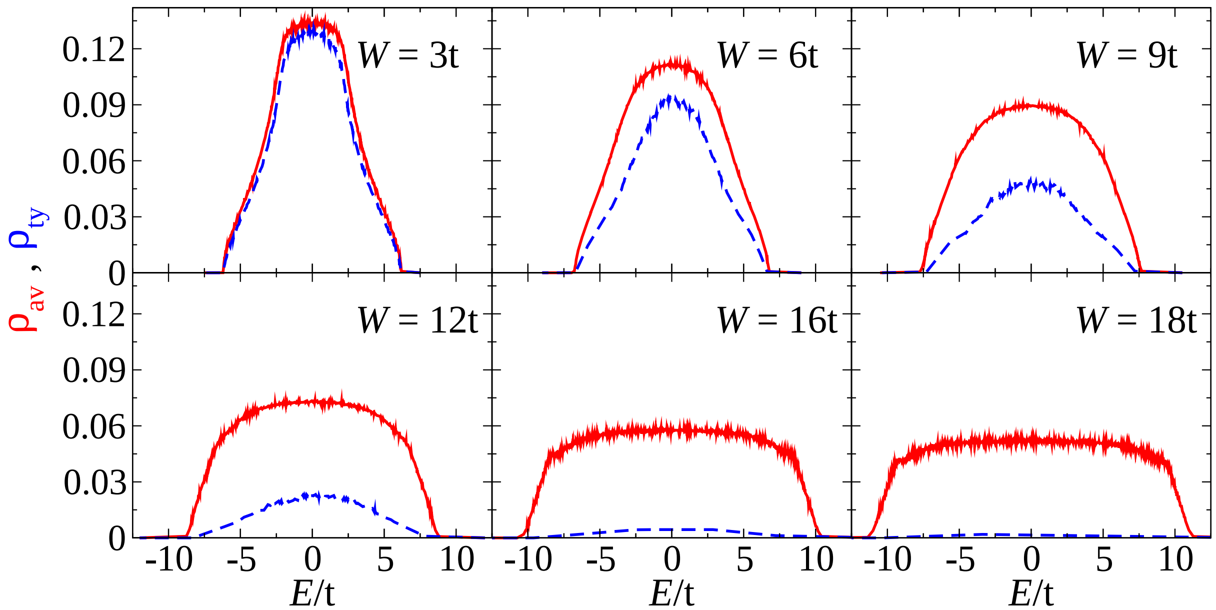
Multifractality - $\langle M^{(k)} \rangle \sim L^{-f(k)}$

Typical escape rate is determined by the typical LDOS

Anderson MIT - cont.:

Near Anderson localization typical LDOS is approximated by geometrical mean

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



Schubert et al. cond-mat/0309015

Theorem (F.Wegner 1981):

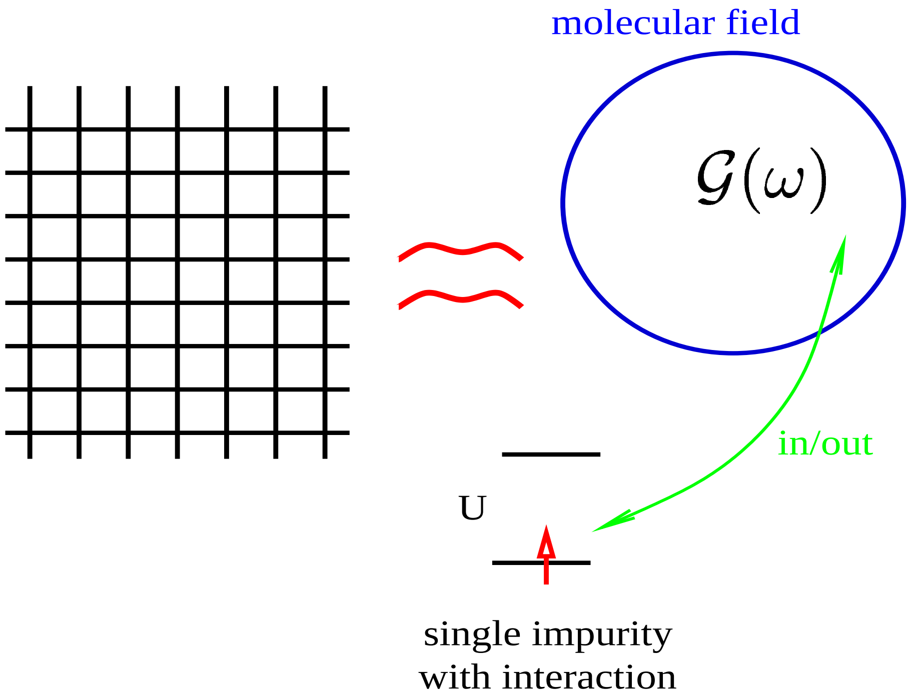
$$\rho(E)_{av} = \langle \rho_i(E) \rangle > 0$$

within a band for any finite Δ

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)

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

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

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

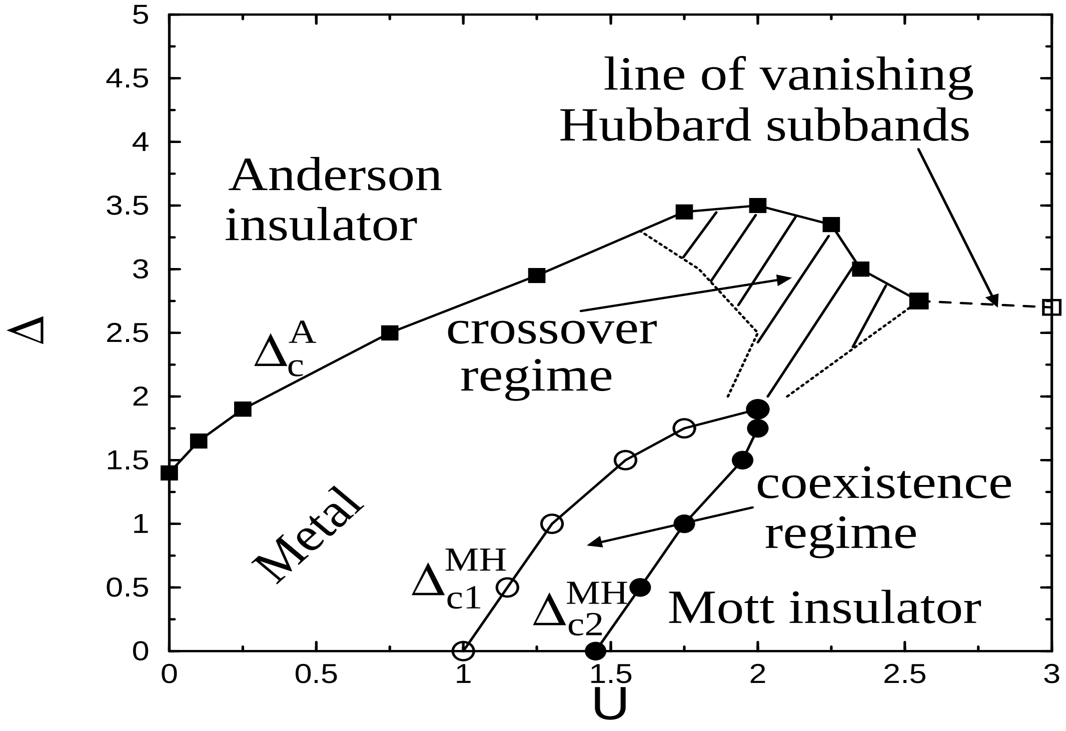
$$G^{-1}(\omega) = \omega - \eta(\omega) - \Sigma(\omega), \qquad \eta(\omega) = \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{\omega - \epsilon_{\mathbf{k}}}$$

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

Phase diagram for disordered Hubbard model:

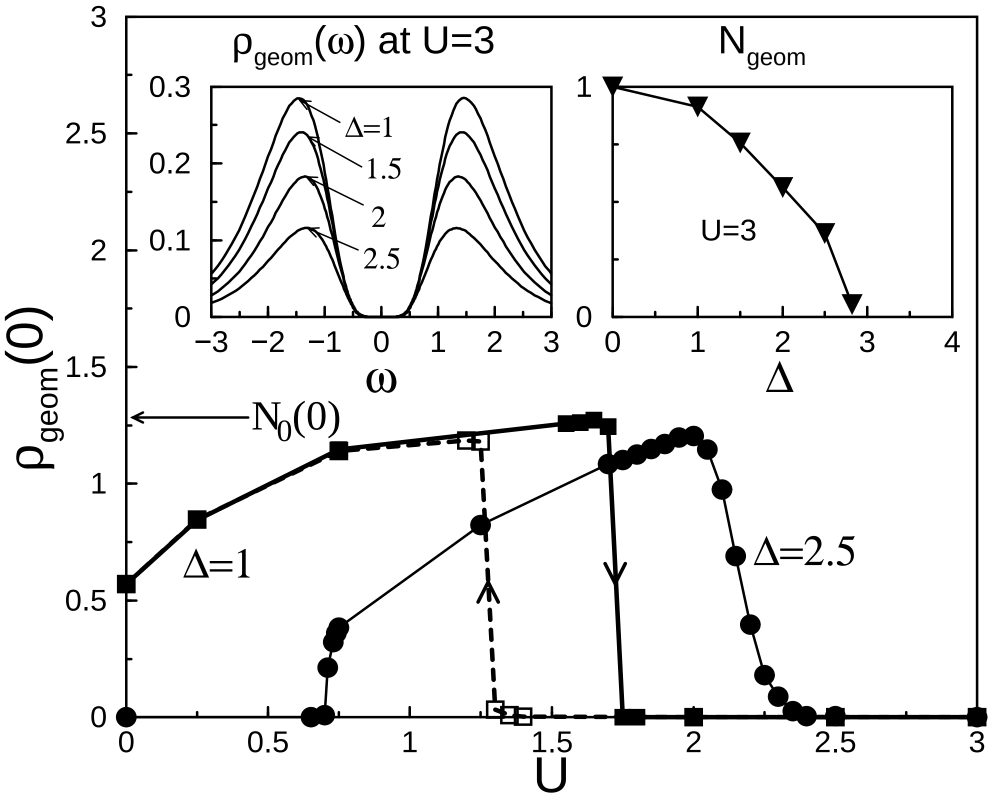
$$N_0(\epsilon) = \frac{2}{\pi D}\sqrt{D^2 - \epsilon^2}; \quad \eta(\omega) = \frac{D^2}{4}G(\omega)$$

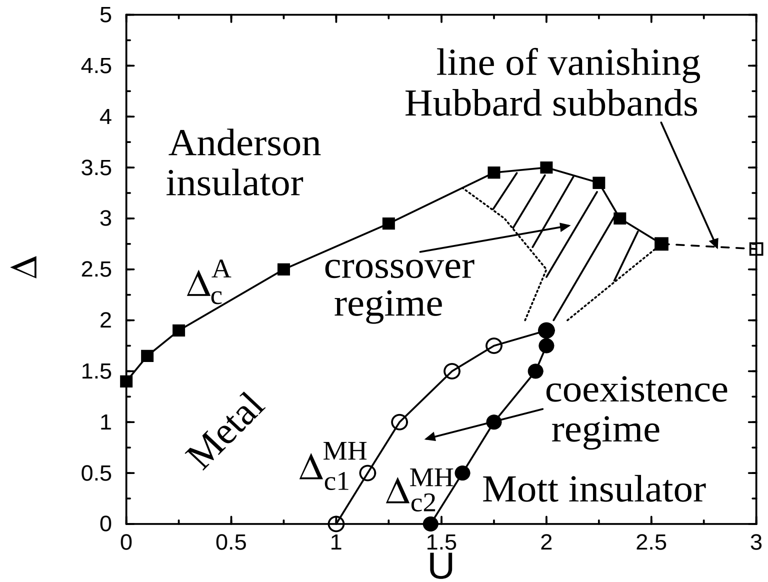
$T = 0$, $n = 1$, $W = 2D = 1$



U - **interaction,** Δ - **disorder**

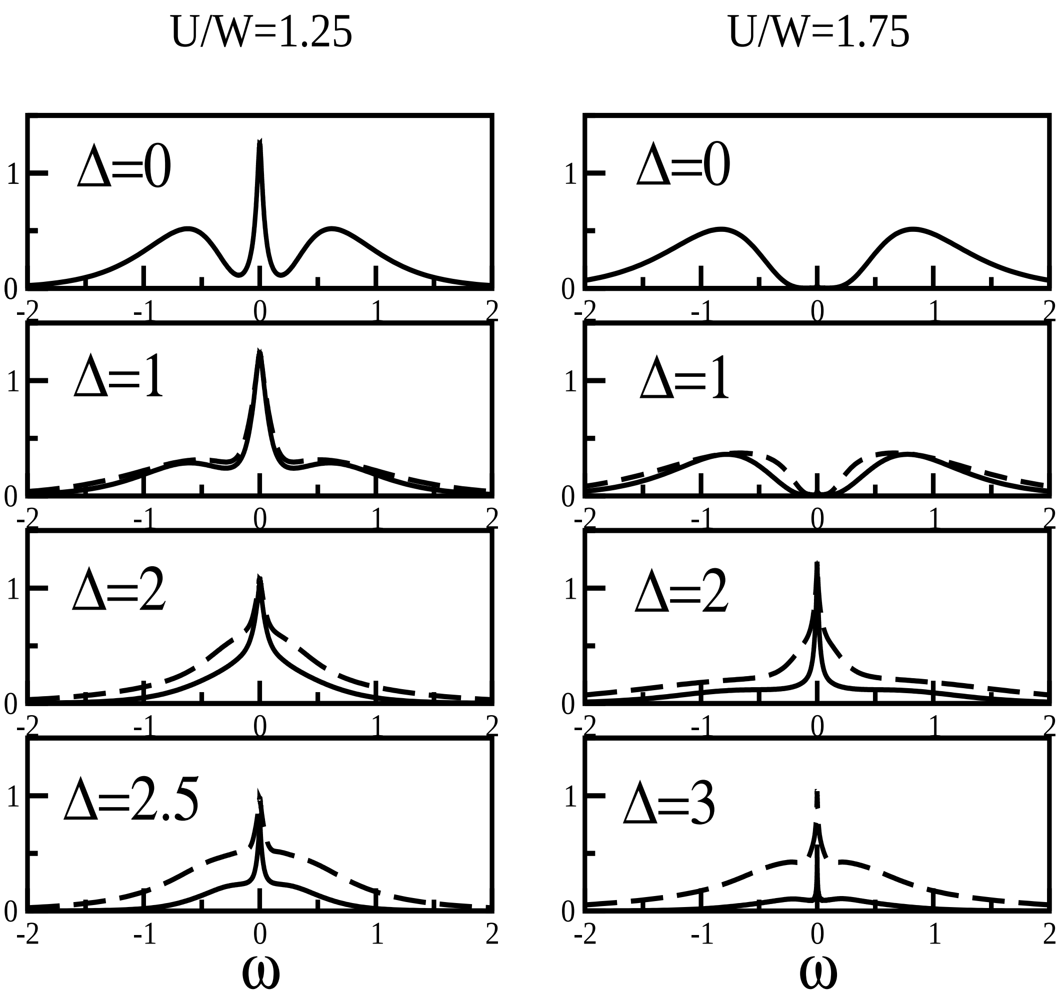
Mott-Hubbard transition in disordered Hubbard model:

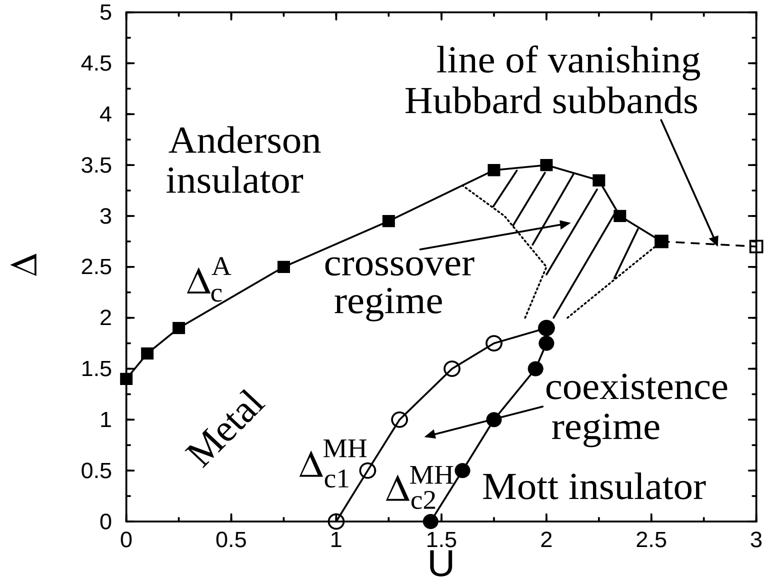




* **Luttinger (FL due to U)**
* **Hysterisis $\Delta_{c1}(U)$, $\Delta_{c2}(U)$**
* **Crossover**
* **Similar conclusions with $\langle\rho_j\rangle$ schme**

Spectral functions in disordered Hubbard model:



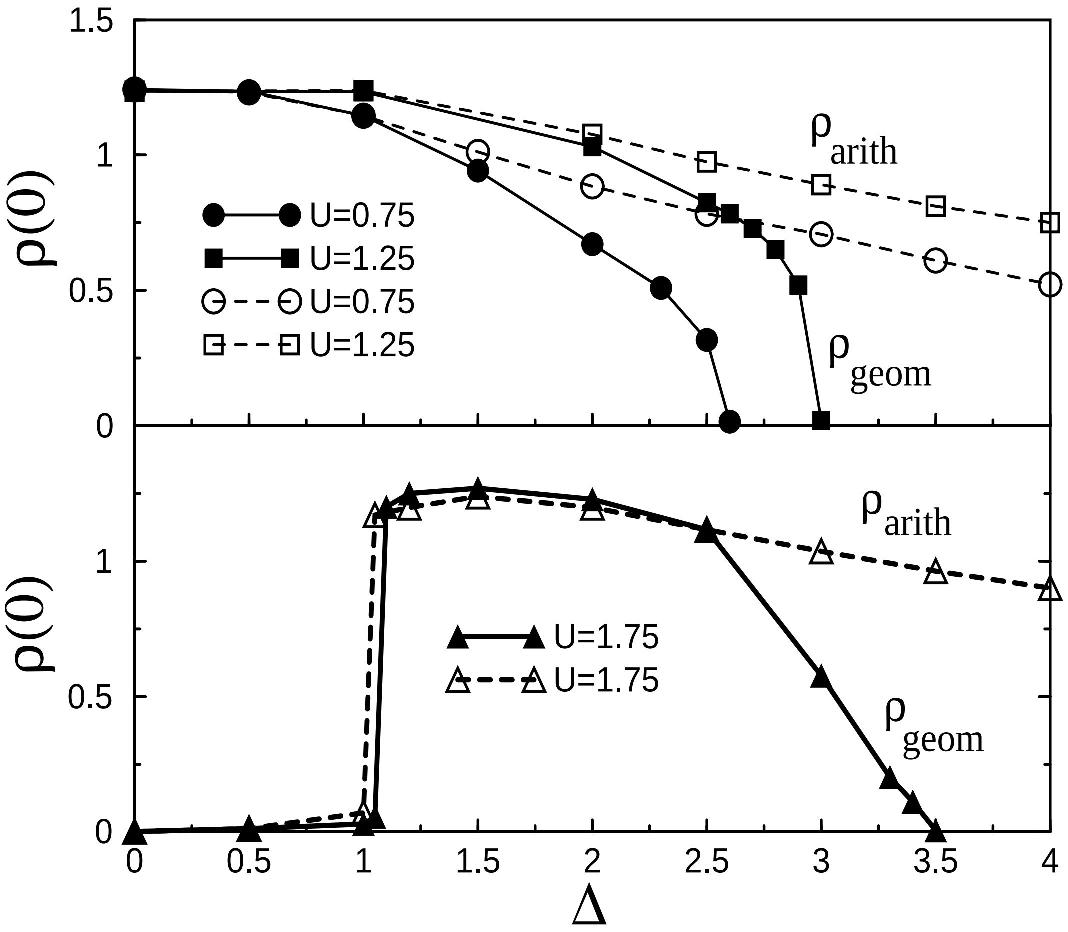


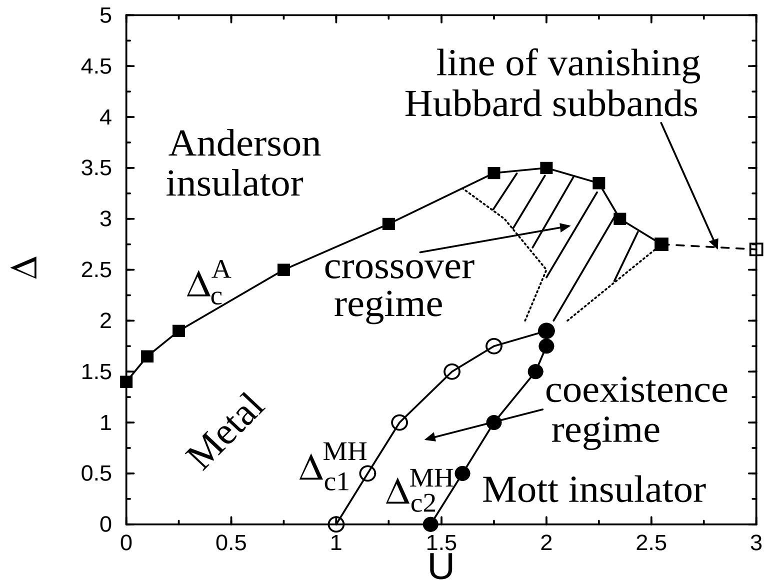
* **Redistribution of spectral weight**

* **Reentrant Mott-Hubbard MIT**

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

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**

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

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**