Competing Phases in Correlated Lattice Fermions with Disorder

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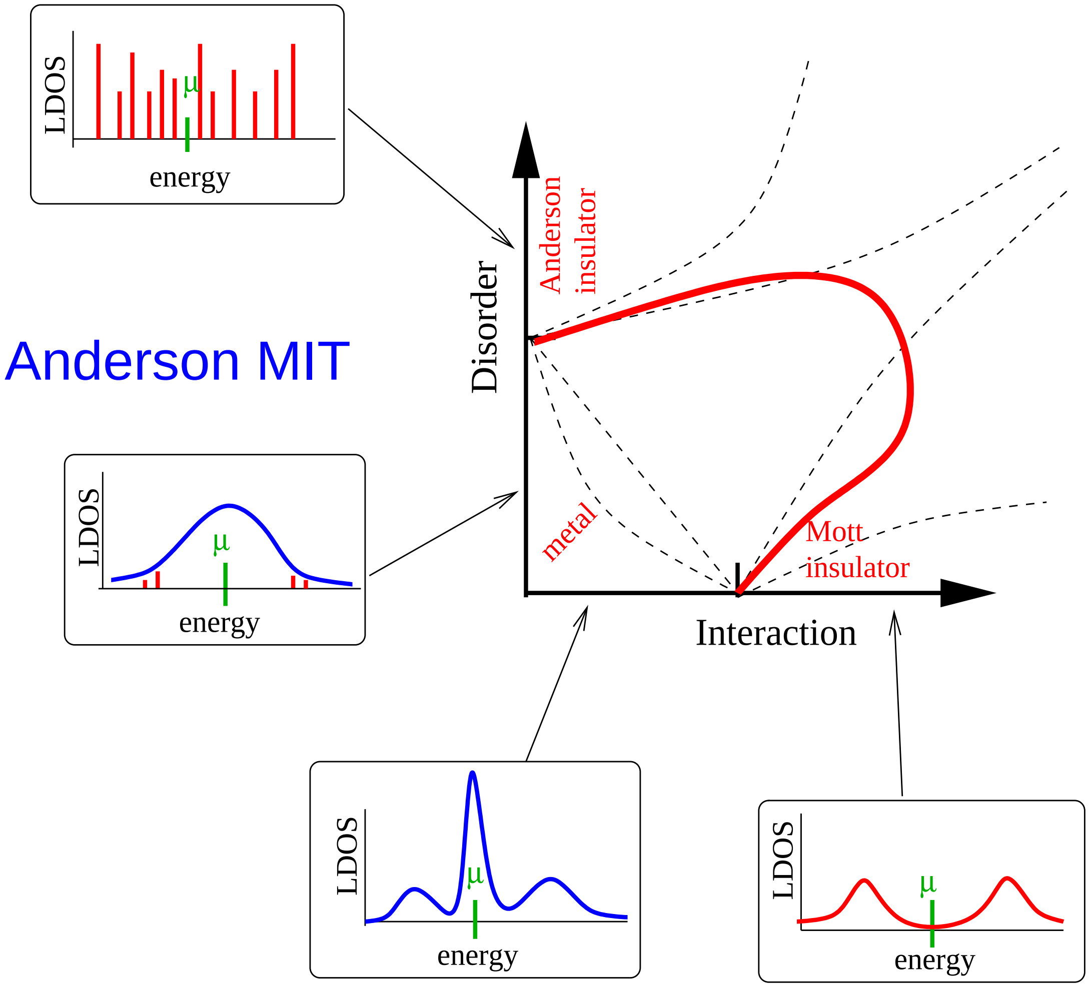
1. Main results

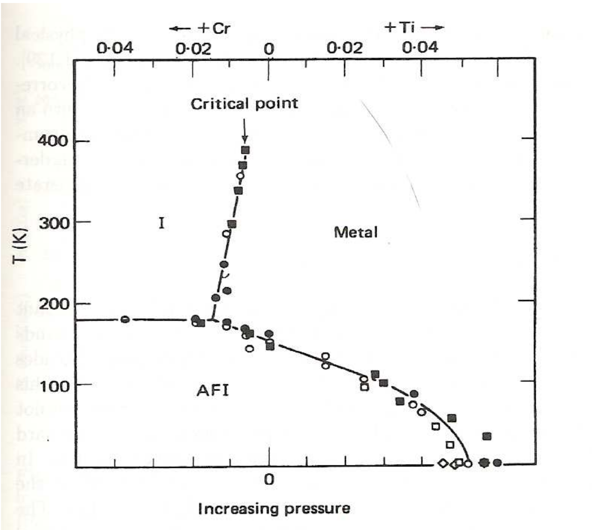
Disorder ↔ Anderson MIT

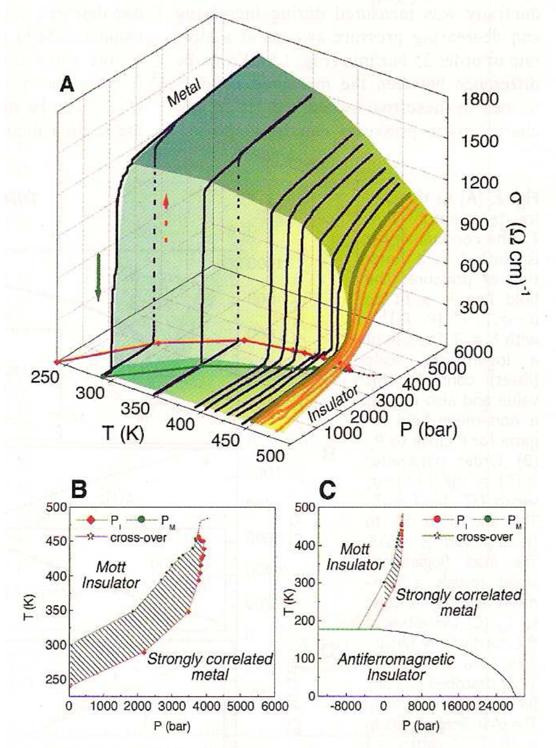


Interaction ↔ Mott-Hubbard MIT

2. MIT at half-filling – canonical example: V_2O_3

$V \quad ([Ar]3d^2 4s^2)$ gives V^{+3} valence band partially filled (metallic?)



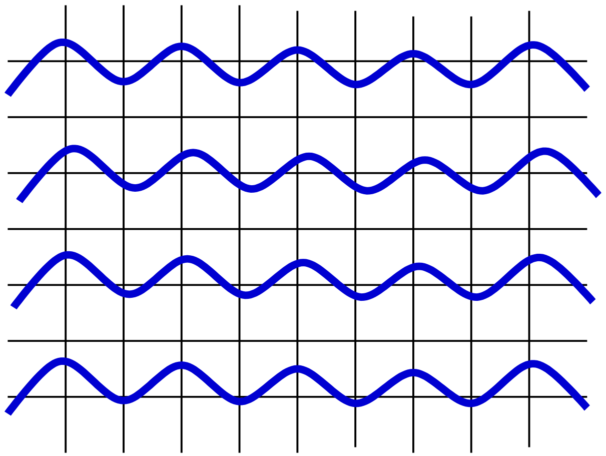


True Mott insulator

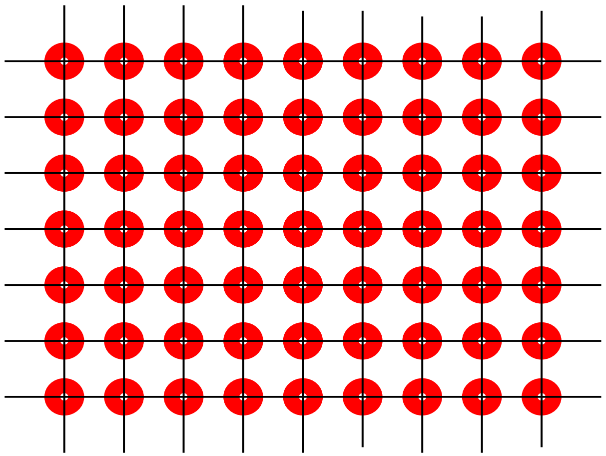
persists above T_N

Mott – Hubbard Insulator, Mott – Heisenberg Insulator, and Slater Insulator

2. MIT at half-filling

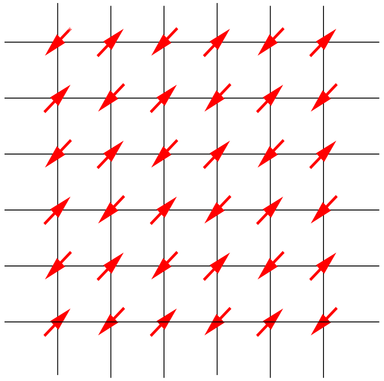


$U \ll |t_{ij}|$, $\Delta\mathbf{p} = 0$



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

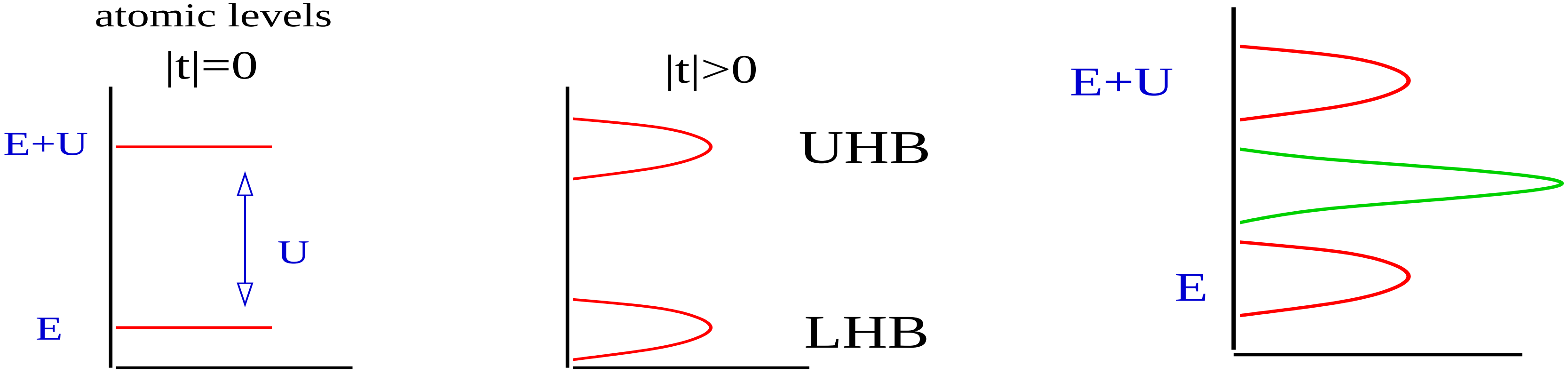
Antiferromagnetic Mott insulator



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

2. MIT at half-filling in Hubbard model

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



spin flip on central site

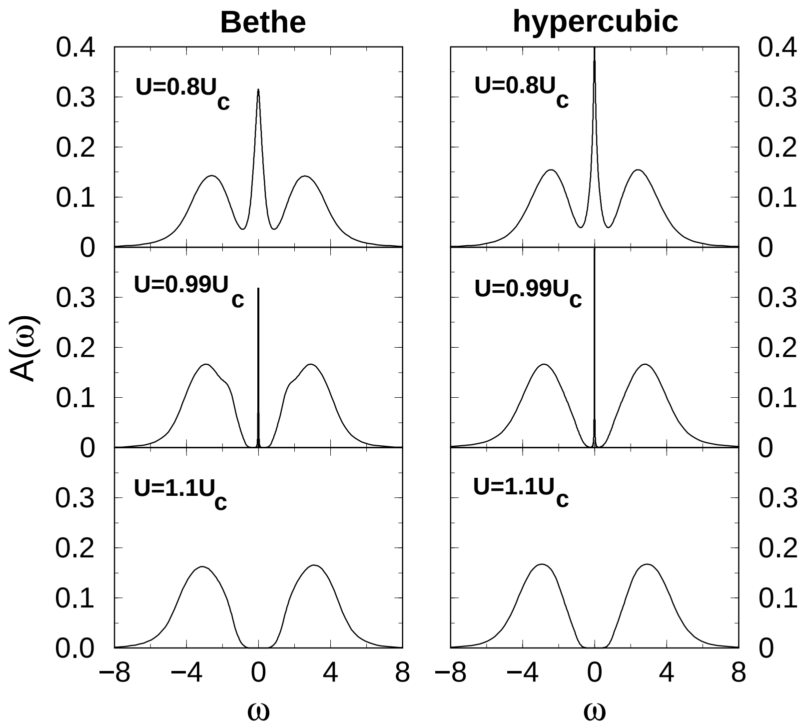
at $U = U_c$ resonance disapears

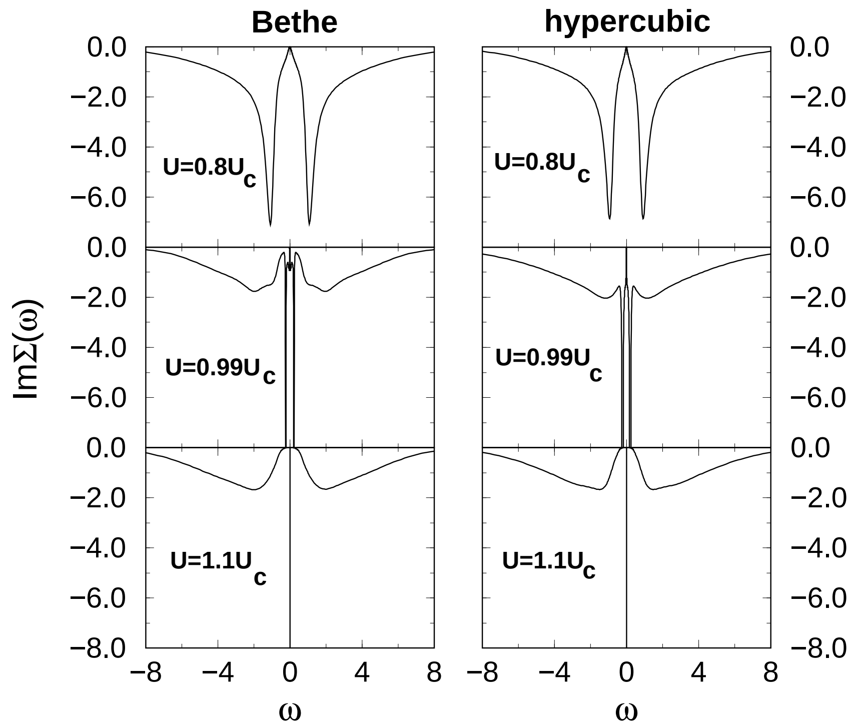
gaped insulator

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

2. MIT at half-filling at $T = 0$ according to DMFT

Kotliar et al. 92-96, Bulla, 99





Luttinger pinning $A(0) = N_0(0)$

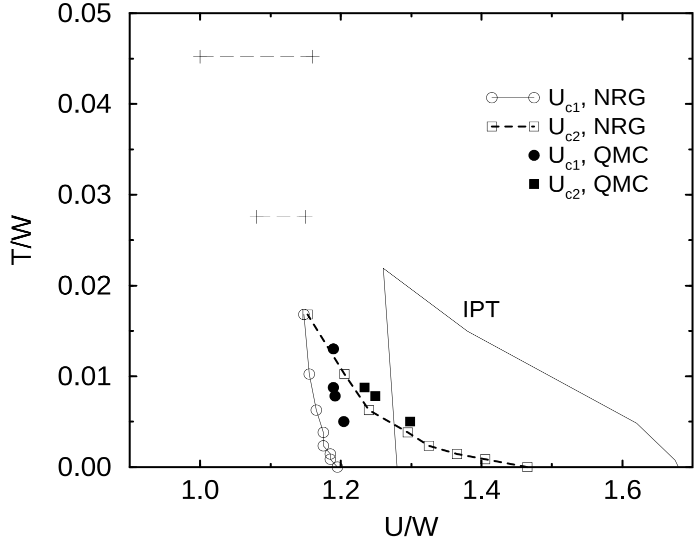
Fermi liquid

Muller-Hartmann 1989

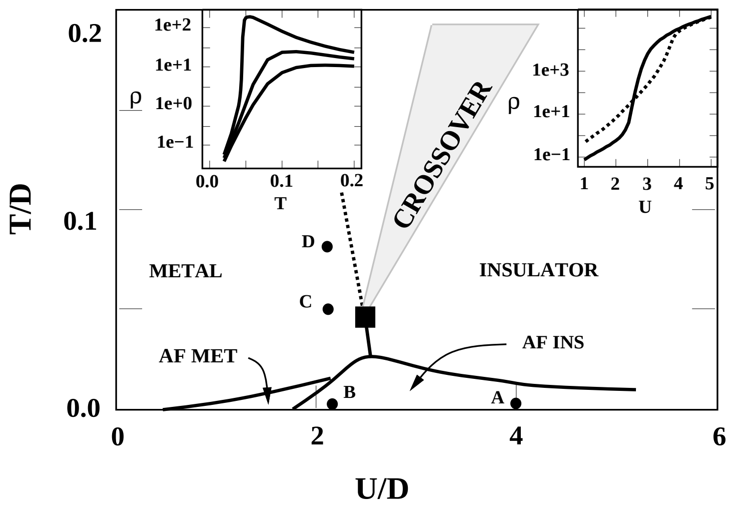
$$G(k,\omega) \sim \frac{Z}{\omega - \tilde{\epsilon}_k - i\alpha\ \omega^2} + G_{inc}$$

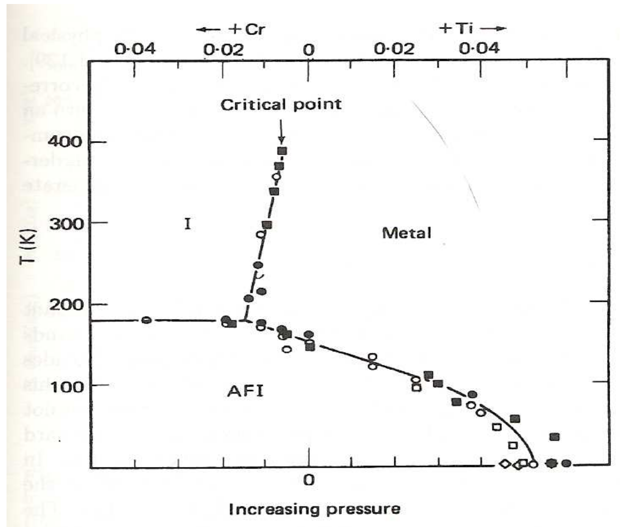
2. MIT at half-filling at $T > 0$ according to DMFT

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



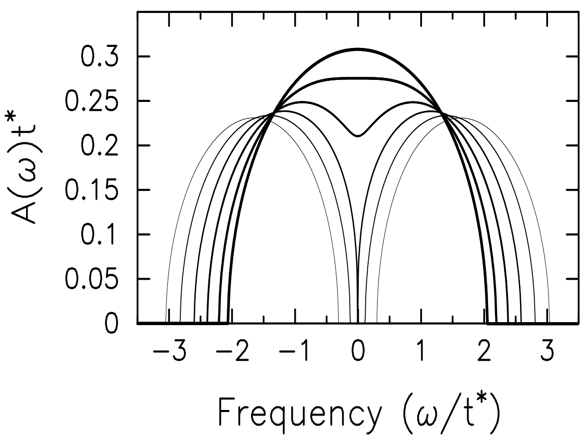
1$^{\mathrm{st}}$-order transition





2. Mott MIT in Falicov-Kimball model - DMFT

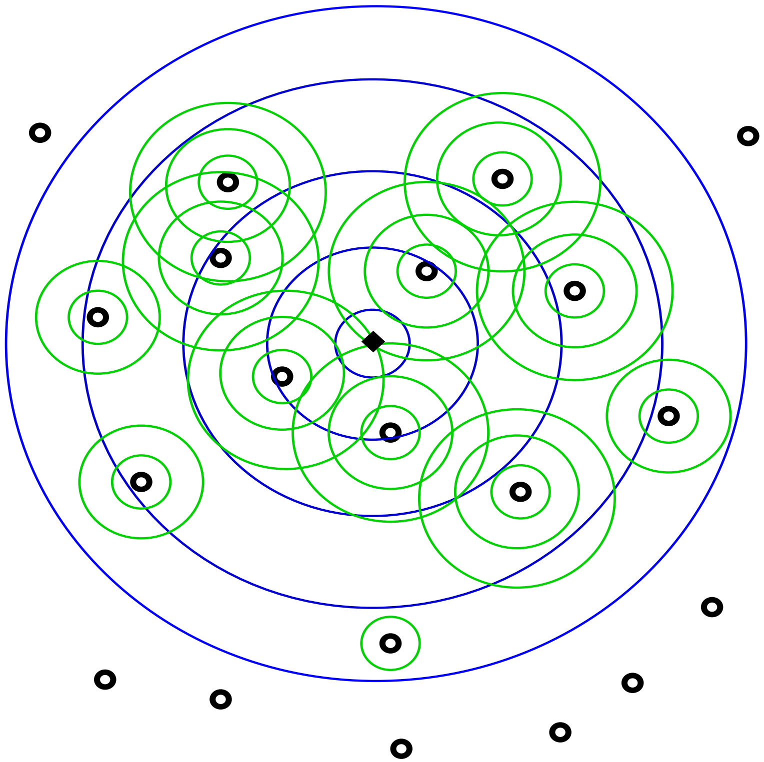
- f-particles appear as like disorder scatterers (with an annealed averaging).
- No Fermi liquid property of FK model if $n_f \neq 0 \text{ or } 1$.
- Pseudo-gap regime.
- For $n_e = n_f = 0.5$ and $U = U_c \sim W$ continuous Mott like MIT.
- Correlation gap opened.



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

3. 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

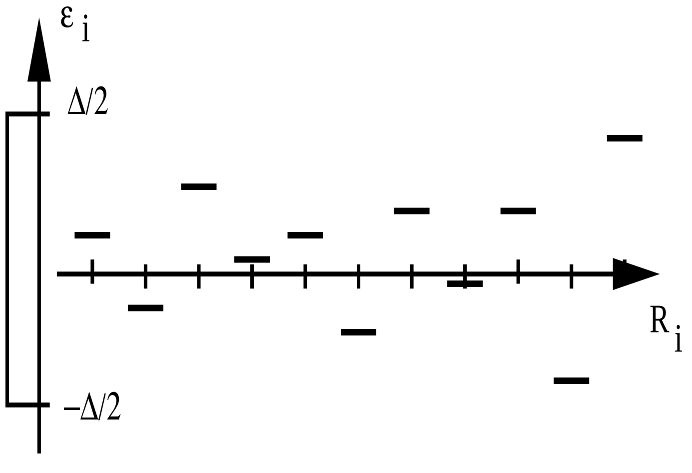
Localization is a destruction of coherent superposition of spatially separated states

3. Anderson model

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

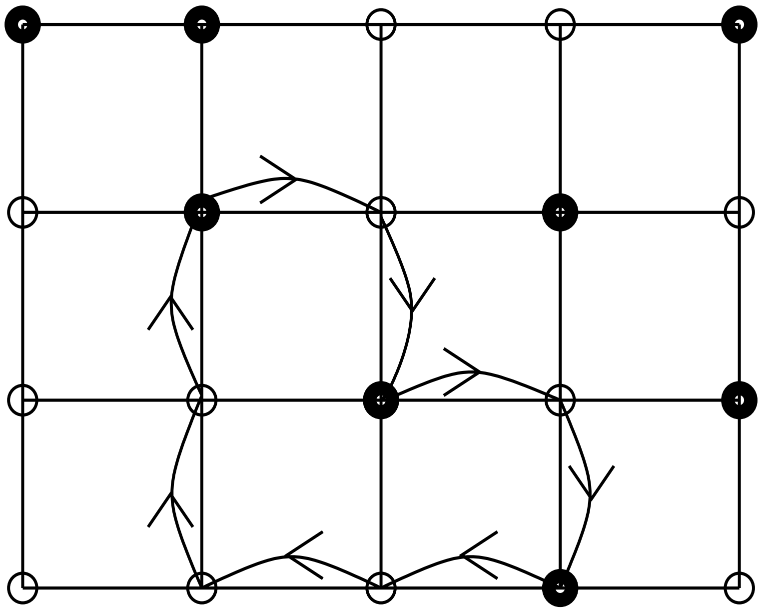
Probability distribution function

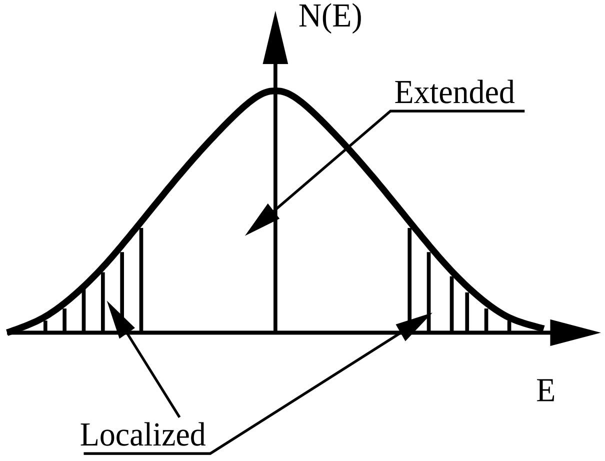
$$\mathcal{P}(\epsilon_i) = \frac{1}{\Delta}\Theta\left(\frac{\Delta}{2} - |\epsilon_i|\right)$$

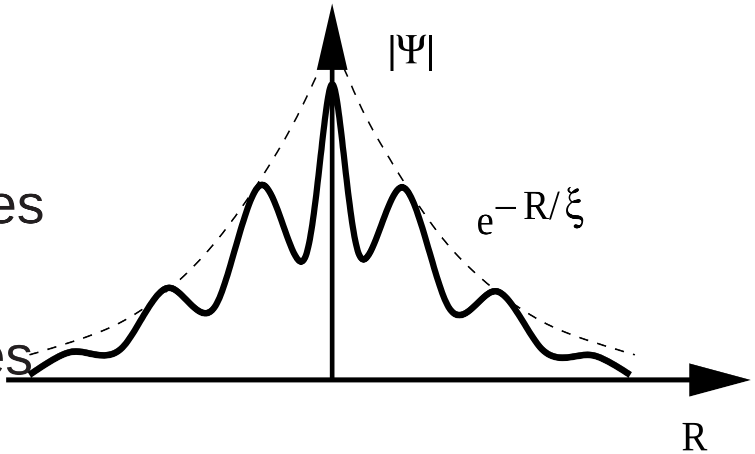


3. Anderson MIT - cont.

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

3. Characterization of Anderson localization

Local Density of States (LDOS)

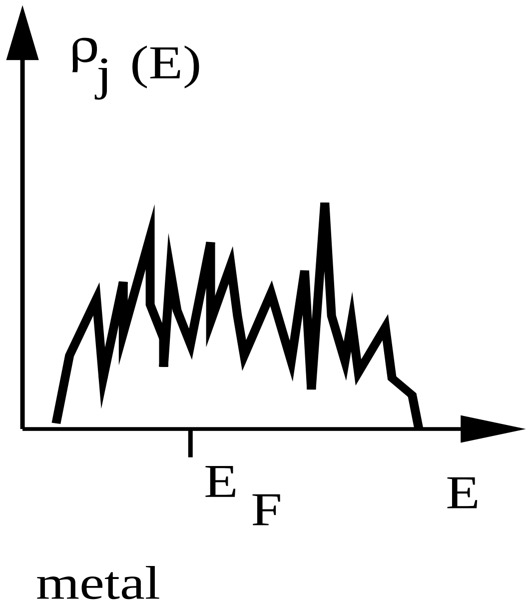
$$\rho_i(E) = \sum_{n=1}^{N} |\Psi_n(r_i)|^2 \delta(E - E_n)$$

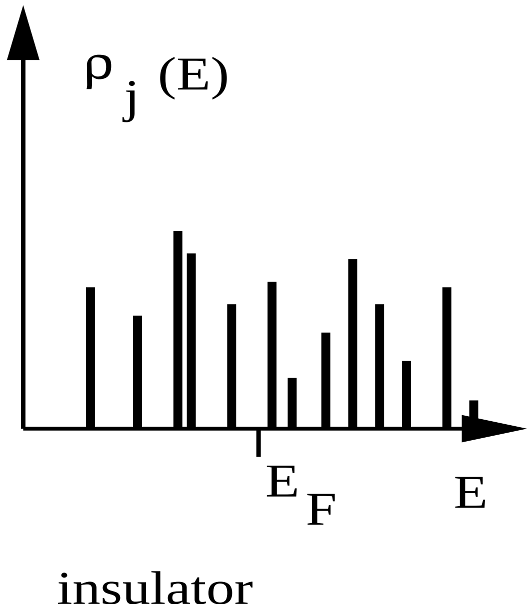
$$P_{j\to j}(t) = |G_j(t)|^2$$

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

Fermi Golden Rule

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

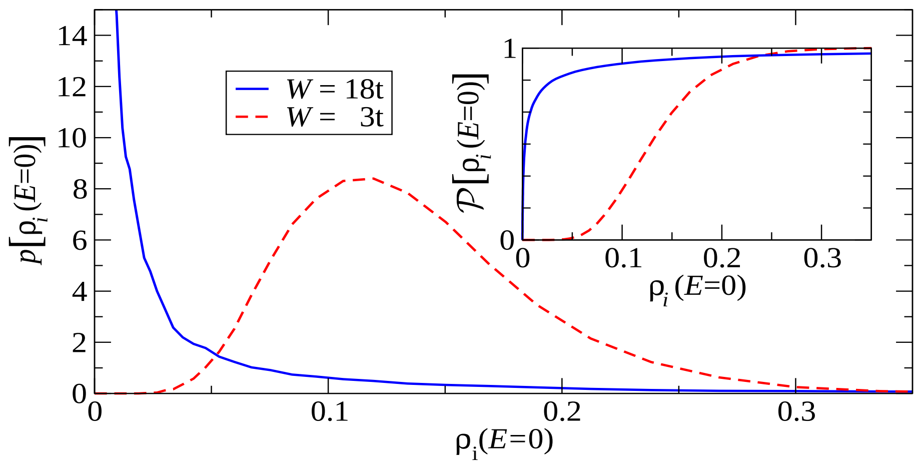




3. Anderson MIT - cont.

$\rho_j(E)$ 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

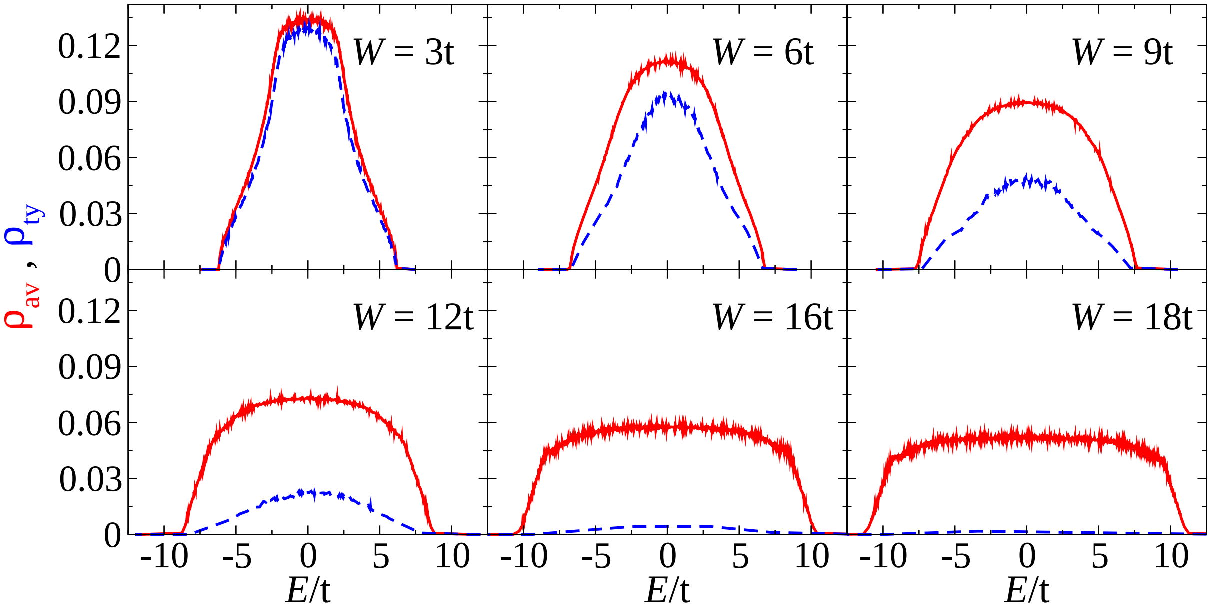
Multifractality - $\langle M^{(k)} \rangle \sim L^{-f(k)}$

Schubert et al. cond-mat/0309015

3. Anderson MIT - cont.

Near Anderson localization typical LDOS is approximated by geometrical mean

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



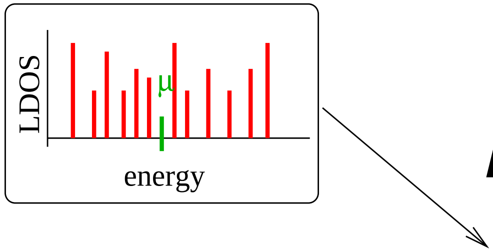
Theorem (F.Wegner 1981):

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

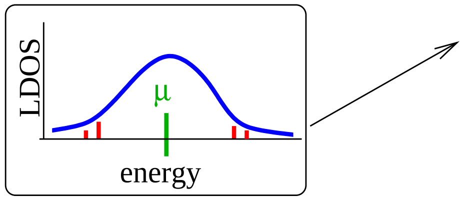
within a band for any finite Δ

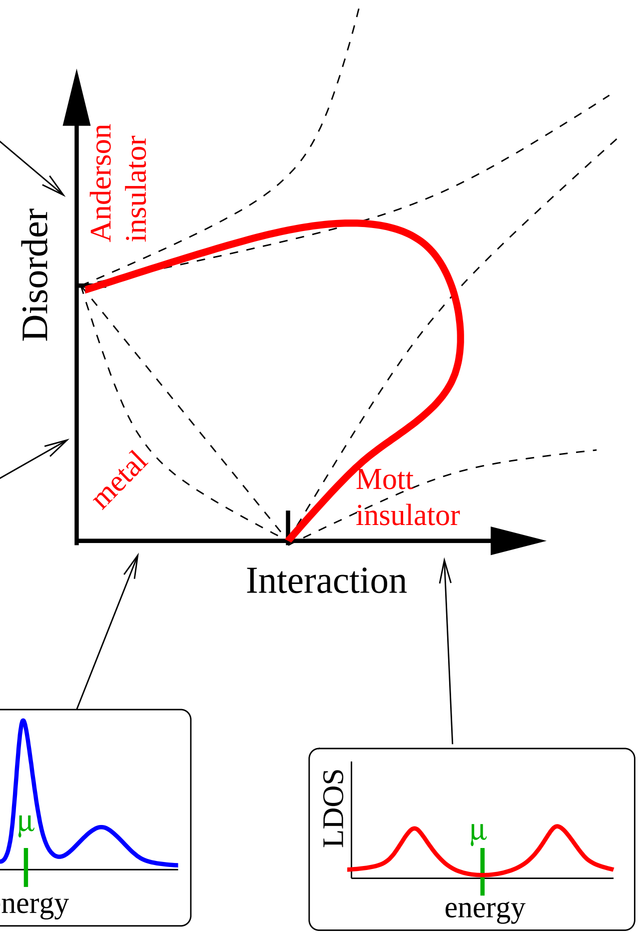
Schubert et al. cond-mat/0309015

4. Mott-Anderson MIT



Disorder ↔ Anderson MIT





Two insulators are
continously connected

BUT

Interaction ↔ Mott-Hubbard MIT

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

4. Dynamical mean-field theory for U and Δ

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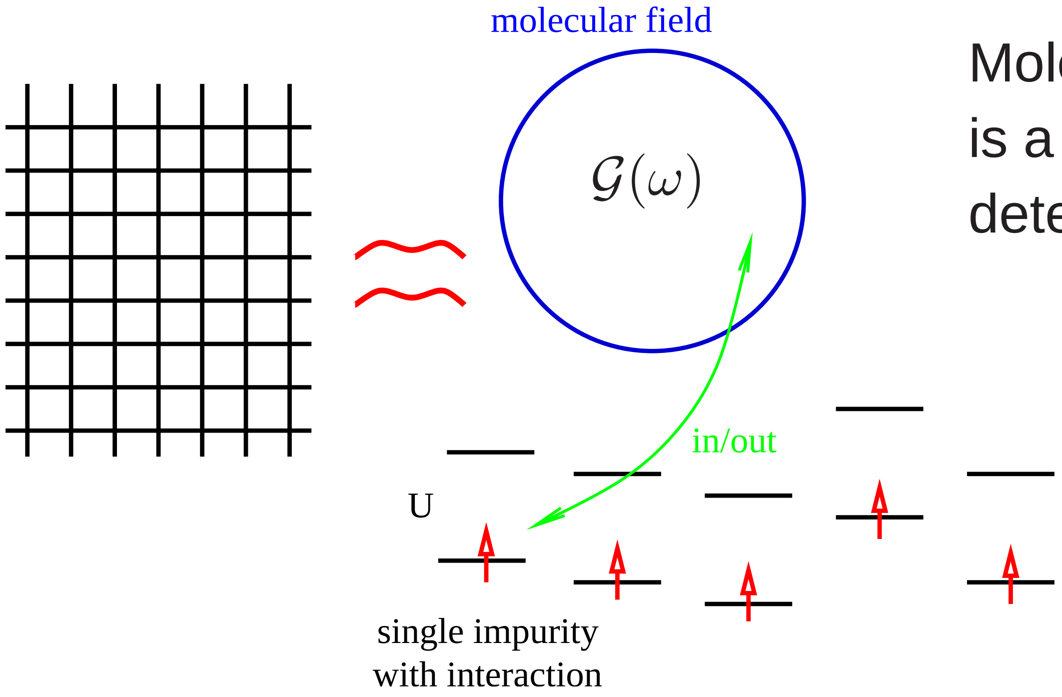
Lattice problem of interacting particles is mapped onto an ensamble of single impurities (single atoms)



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

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

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

4. DMFT with Anderson MIT

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

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

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

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

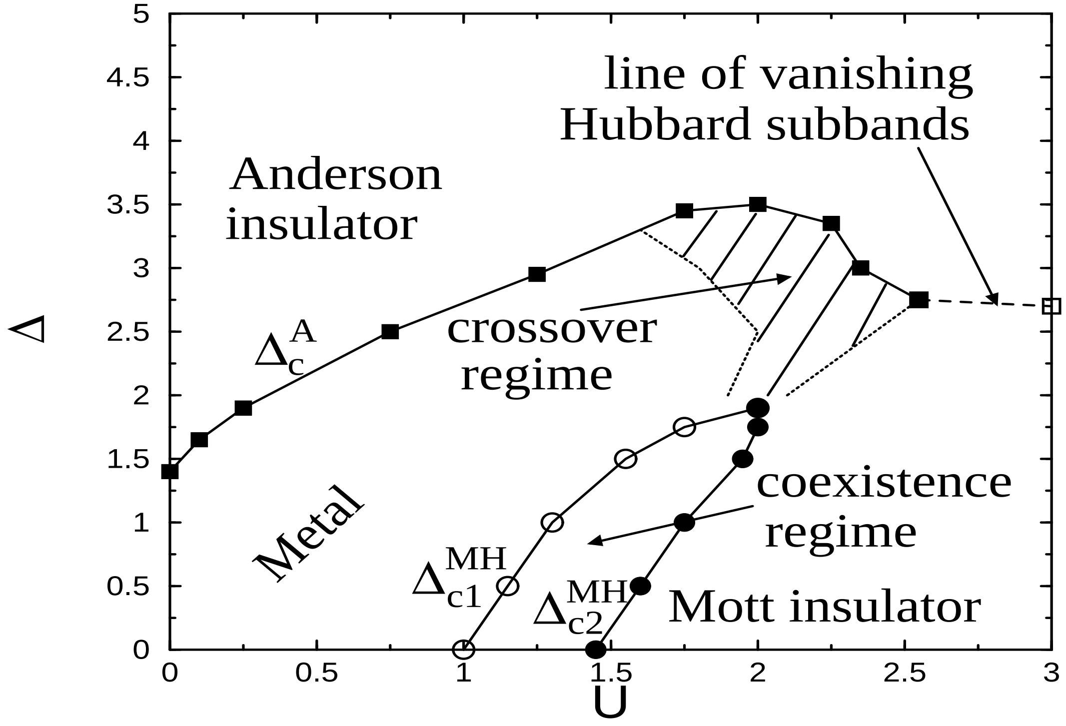
$$G^{-1}(\omega) = \omega - \eta(\omega) - \Sigma(\omega), \qquad \eta(\omega) = \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{\omega - \epsilon_{\mathbf{k}}}$$

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

4. Phase diagram for disordered Hubbard model

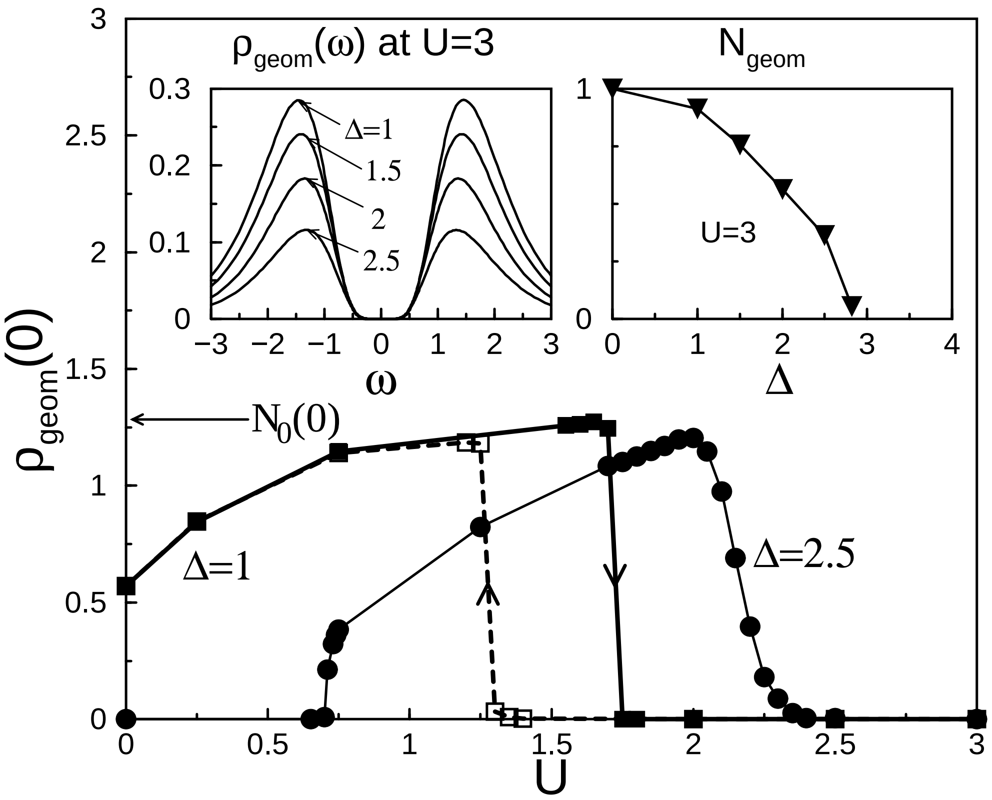
$$N_0(\epsilon) = \frac{2}{\pi D}\sqrt{D^2 - \epsilon^2}; \quad \eta(\omega) = \frac{D^2}{4} G(\omega)$$

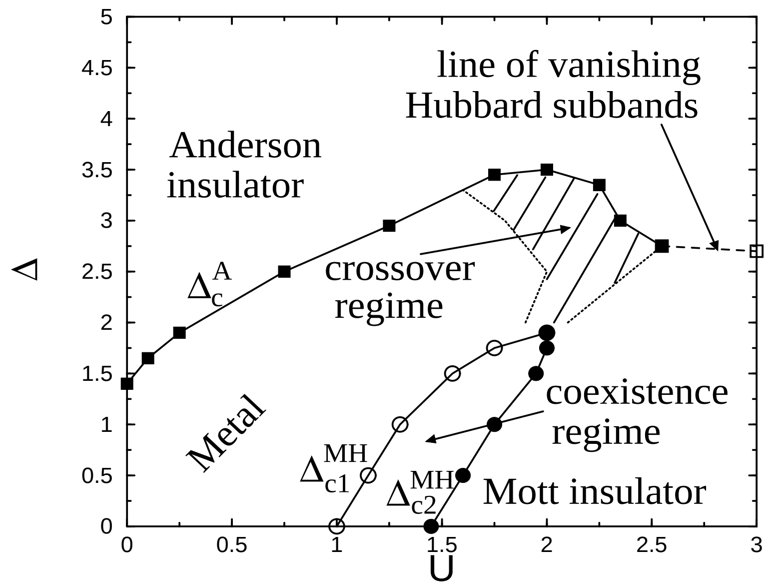
$T = 0$, $n = 1$, $W = 2D = 1$, NRG solver



U - interaction, Δ - disorder

4. Mott-Hubbard MIT in disordered Hubbard model





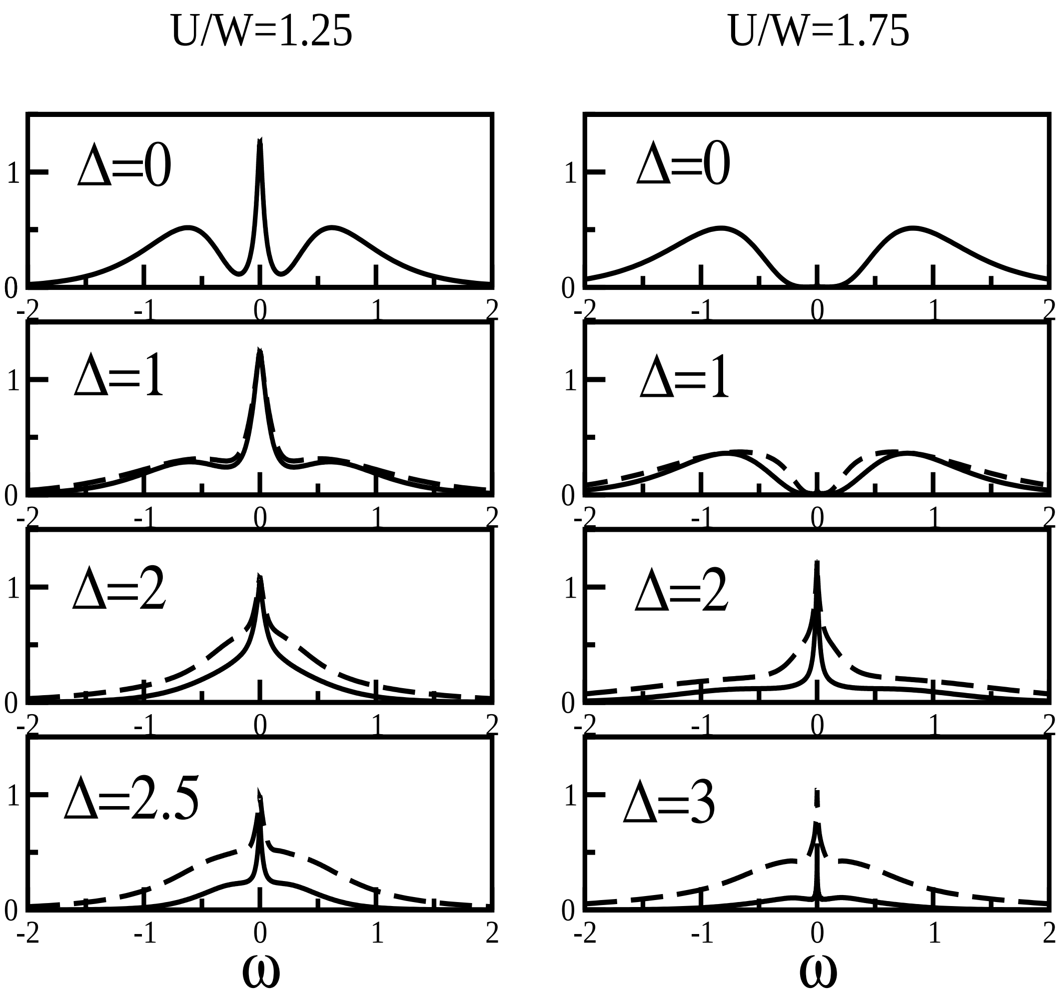
* Luttinger (FL due to U)

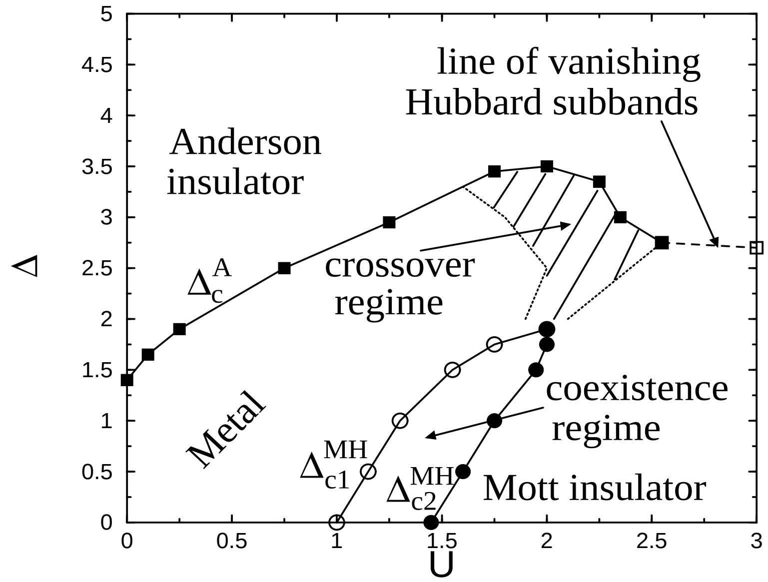
* Hysterisis $\Delta_{c1}(U)$, $\Delta_{c2}(U)$

* Crossover

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

4. Spectral functions in disordered Hubbard model



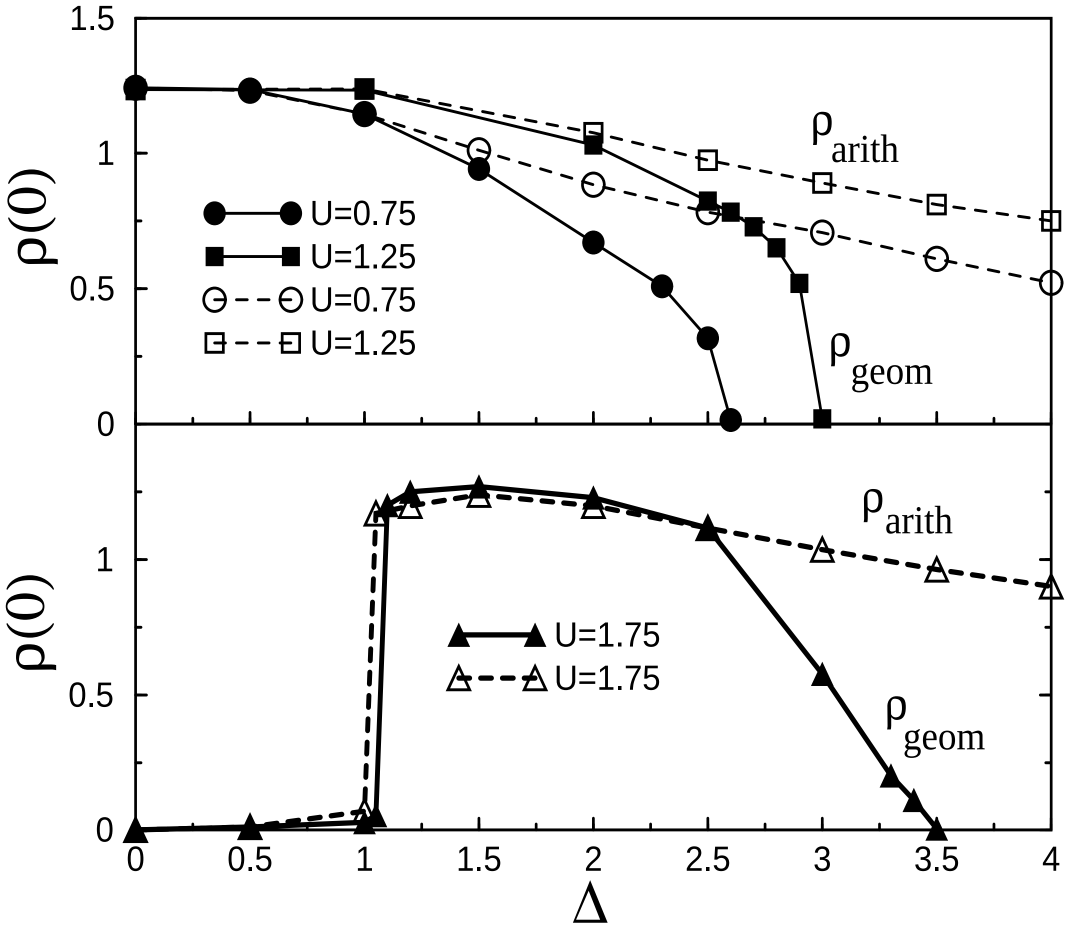


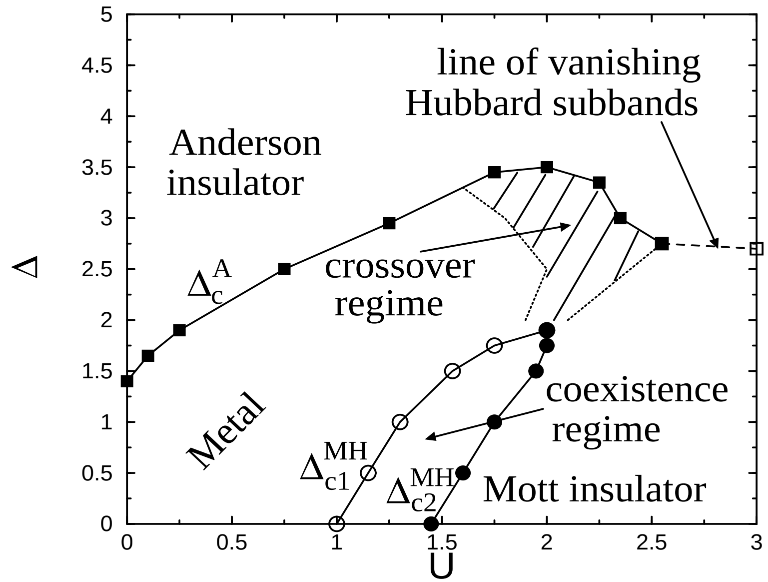
* Redistribution of spectral weight

* Reentrant Mott-Hubbard MIT

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

4. 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

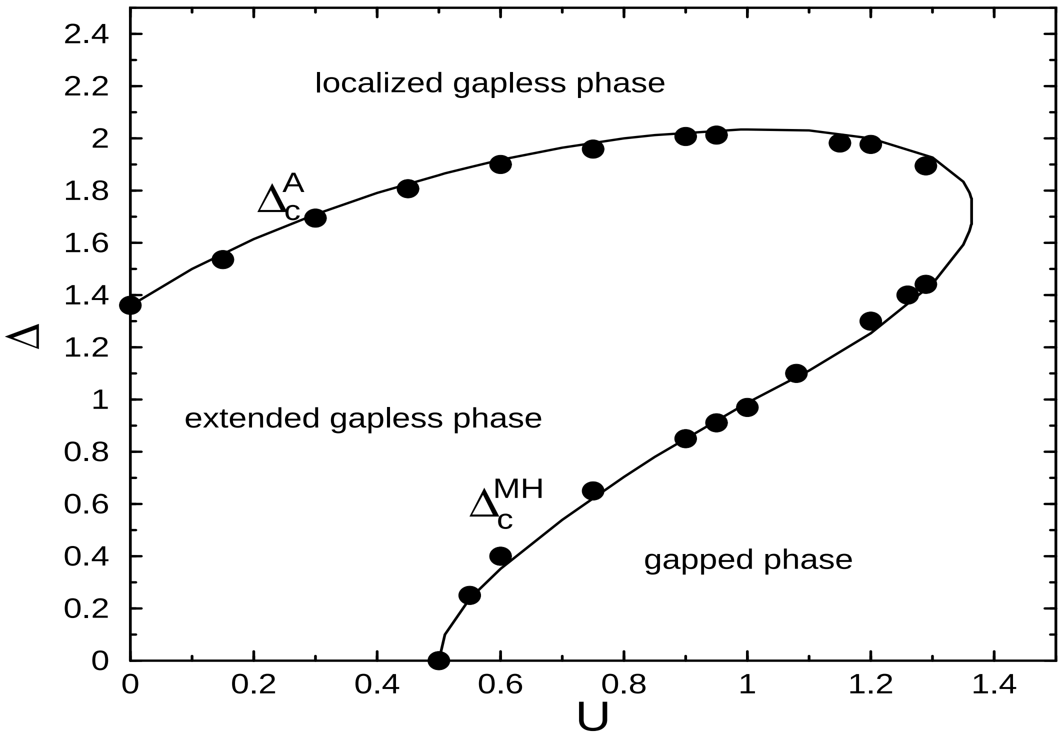
* Adiabatic continuity

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

4. Phase diagram for disordered FK 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

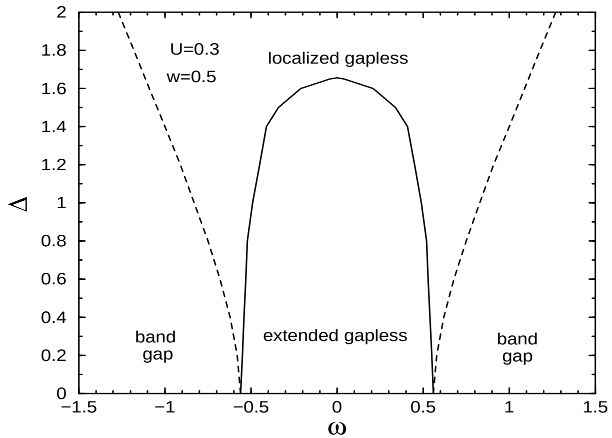


U - interaction, Δ - disorder

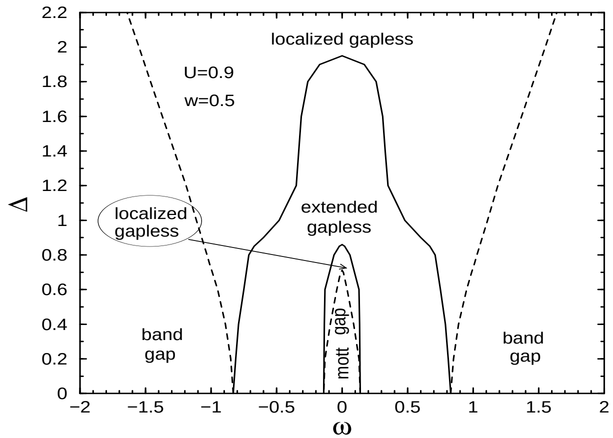
Byczuk 05

4. Spectral phase diagrams

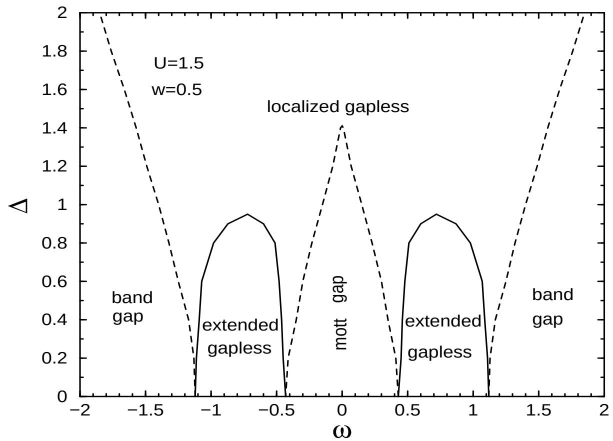
weak coupling $0 < U < W/2$



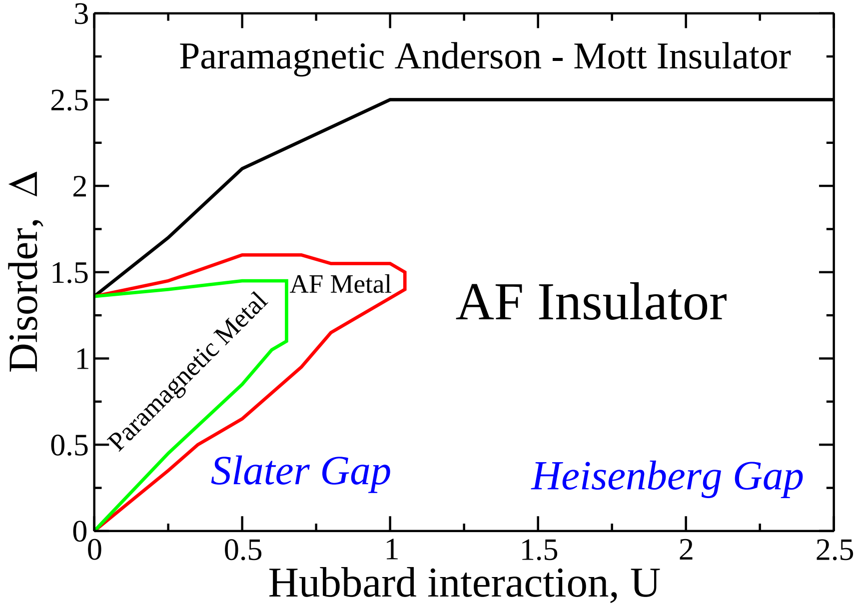
medium coupling $W/2 < U \lesssim 1.36W$

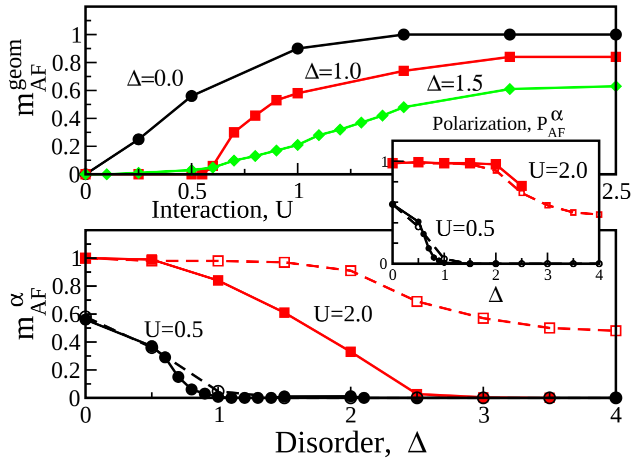


strong coupling $1.36W \lesssim U$



5. Mott-Anderson MIT with AF long-range order





No phase transition between Slater and Heisenberg limits

BUT

AF and PM metal only in Slater limit with disorder

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6. Mott-Anderson MIT – conclusions

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
- AF-LRO destabilized in Slater limit, PM and AF metals with disorder
- AF-LRO stable in Heisenberg limit until Anderson-like transition