Dynamical mean-field theory for correlated and disordered electrons

Krzysztof Byczuk

Institute of Physics, EKM, Augsburg University, Germany

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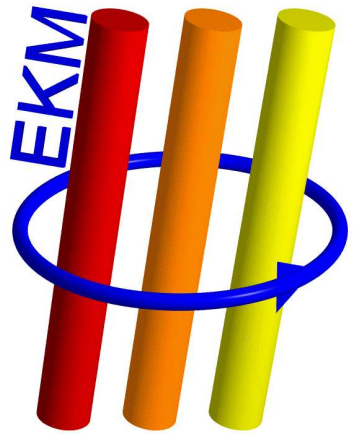


Plan of our 4 lectures

1. Correlated electrons and dynamical mean-field theory (DMFT) - 2X45min.
   - Correlated electrons and models
   - Needs for **the** mean-field theory
   - Limit of infinite dimension
   - Feynman diagrams simplification

2. Application of DMFT to pure systems - 2X45min.
   - Analytically solvable Falicov-Kimball model
   - MIT at half-filling in Hubbard model and experiment
   - Electronic kinks in correlated metals
   - Mott-Anderson MIT in correlated electron systems with disorder
   - Itinerant ferromagnetism
   - MIT in binary alloy systems
   - Itinerant ferromagnetism in binary alloy systems

Correlation

- Correlation [lat.]: con+relatio (“with relation”)

- Mathematics, Statistics, Natural Science:

$$\langle xy \rangle \neq \langle x \rangle \langle y \rangle$$

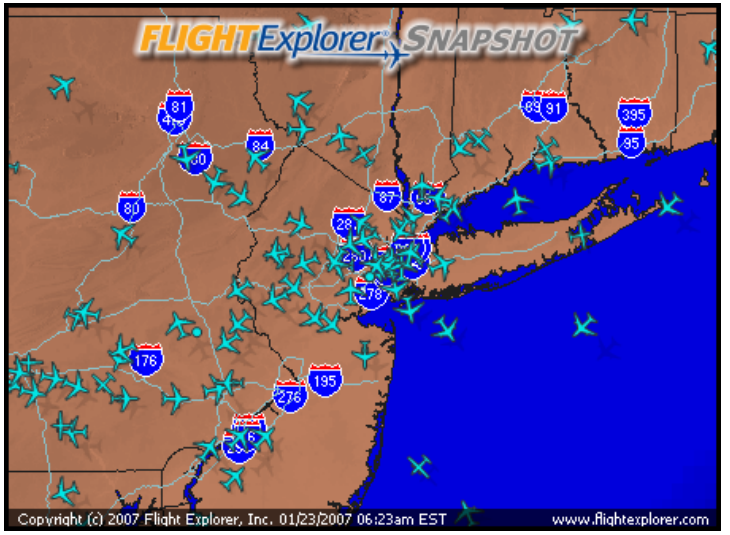
  The term correlation stems from mathematical statistics and means that two distribution functions, $f(x)$ and $g(y)$, are not independent of each other.

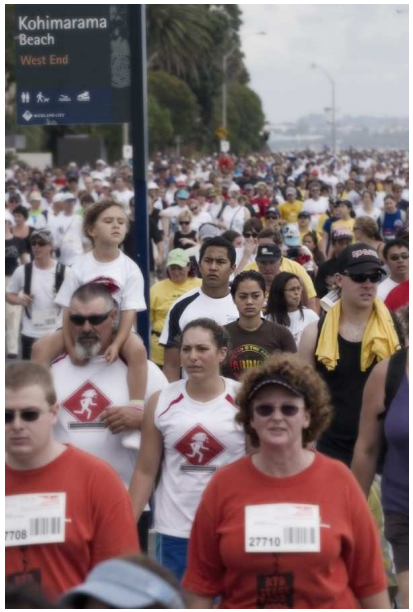
- In many body physics: correlations are effects beyond factorizing approximations

$$\langle \rho(r,t)\rho(r',t') \rangle \approx \langle \rho(r,t) \rangle \langle \rho(r',t') \rangle,$$

  as in Weiss or Hartree-Fock mean-field theories

Spatial and temporal correlations everywhere





car traffic

air traffic

human traffic

electron traffic

more .....

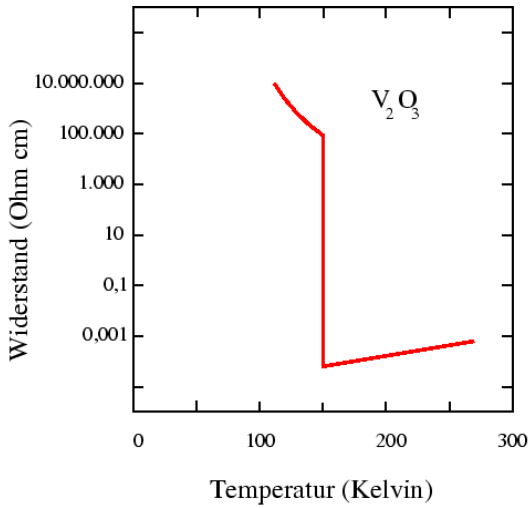


Abb. 3: Beispiel eines Metall-Isolator-Übergangs: Bei Abkühlung unter eine Temperatur von ca. 150 Kelvin erhöht sich der elektrische Widerstand von metallischem Vanadiumoxid (V_2O_3) schlagartig um das Einhundertmillionenfache (Faktor 10^8) – das System wird zum Isolator.

Spatial and temporal correlations neglected

time/space average insufficient

$$\langle \rho(r,t)\rho(r',t')\rangle \approx \langle \rho(r,t)\rangle\langle \rho(r',t')\rangle = \text{disaster!}$$

Boeing 757 and Tupolev 154 collided at 35,400ft. in 2001

Pilot of Tupolev received at the same time two conflicting (uncorrelated) instructions

Spatial and temporal correlations neglected

Local density approximation (LDA) disaster in HTC

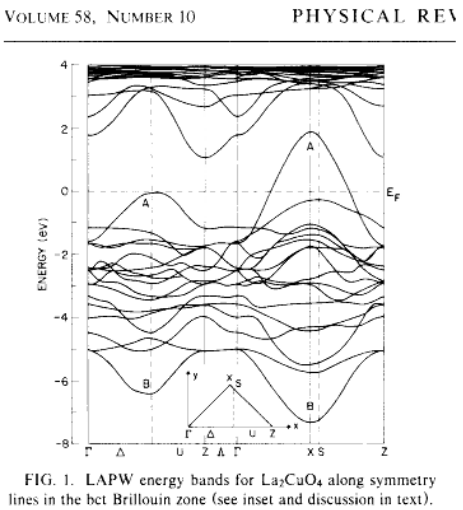
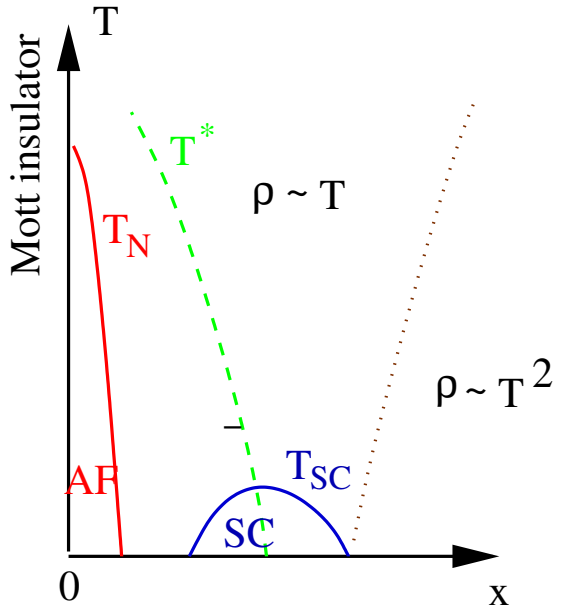


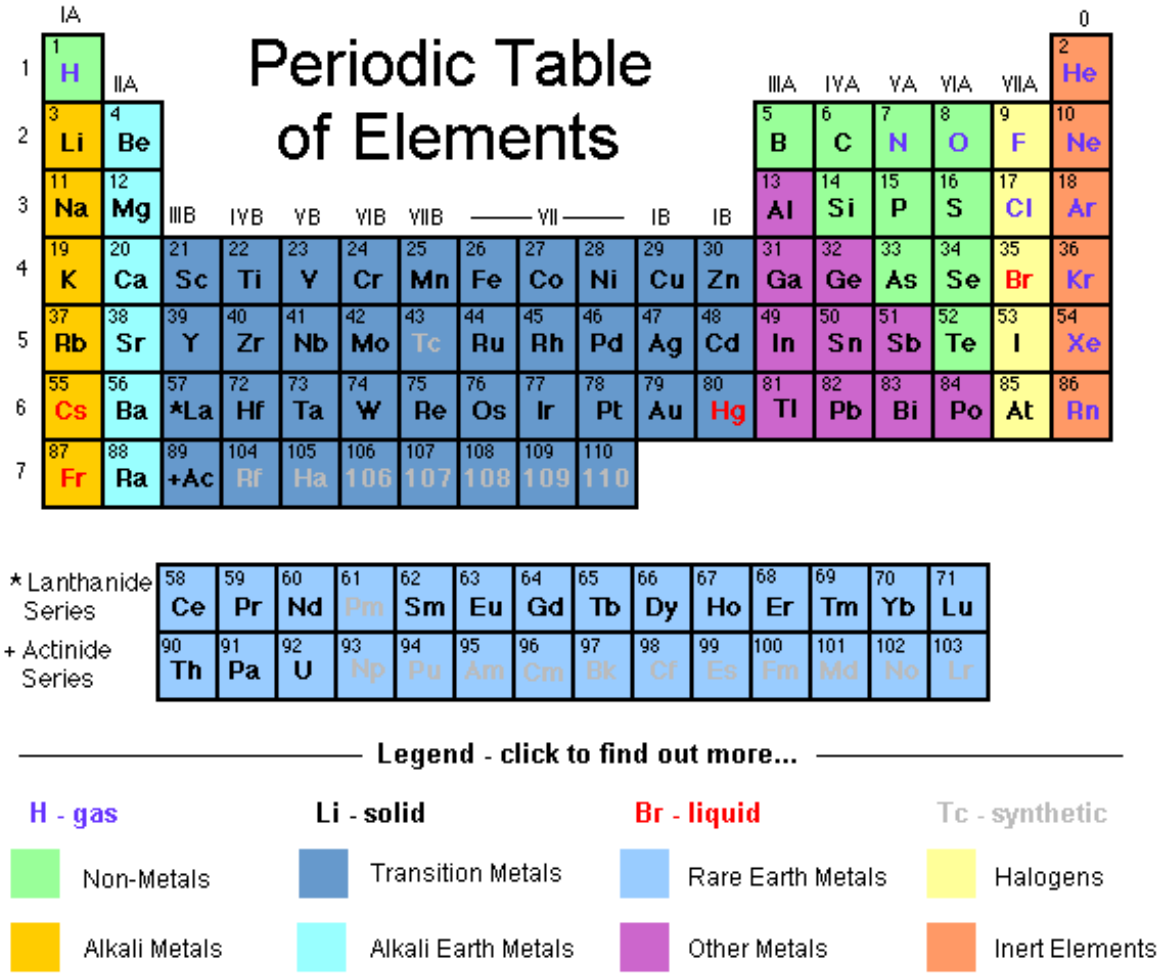
FIG. 1. LAPW energy bands for La_2CuO_4 along symmetry lines in the bct Brillouin zone (see inset and discussion in text).



$LaCuO_4$ Mott (correlated) insulator predicted to be a metal

Partially curred by (AF) long-range order ... but correlations are still missed

Correlated electrons

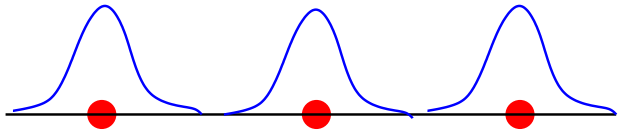


Narrow d,f-orbitals/bands → strong electronic correlations

Electronic bands in solids

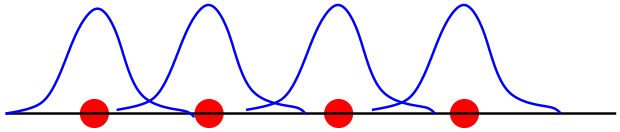
Wave function overlap $\sim t_{ij} = \langle i|\hat{T}|j\rangle \rightarrow |E_{\mathbf{k}}| \sim$ bandwidth W

Band insulators, e.g. NaCl



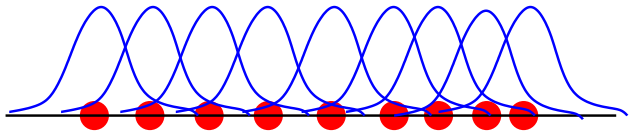
Atomic levels, localized electrons $|\mathbf{R}_i\sigma\rangle$

Correlated metals, e.g. Ni, V_2O_3, Ce



Narrow bands, $|\mathbf{R}_i\sigma\rangle \leftrightarrow |\mathbf{k}\sigma\rangle$

Simple metals, e.g. Na, Al



Broad bands, extended Bloch waves $|\mathbf{k}\sigma\rangle$

Electronic bands in solids

Mean time τ spent by the electron on an atom in a solid
depends on the band width W

$$\text{group velocity} \quad v_{\mathbf{k}} \approx \frac{\text{lattice spacing}}{\text{mean time}} = \frac{a}{\tau}$$

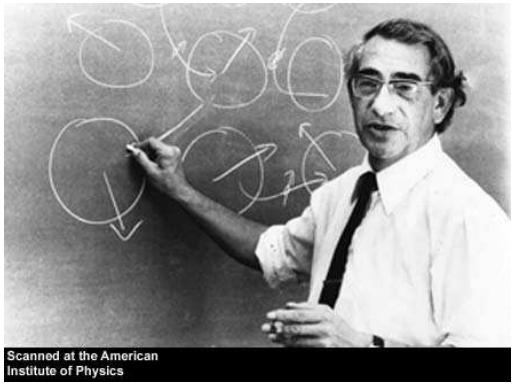
$$\text{Heisenberg principle} \quad W\tau \sim \hbar$$

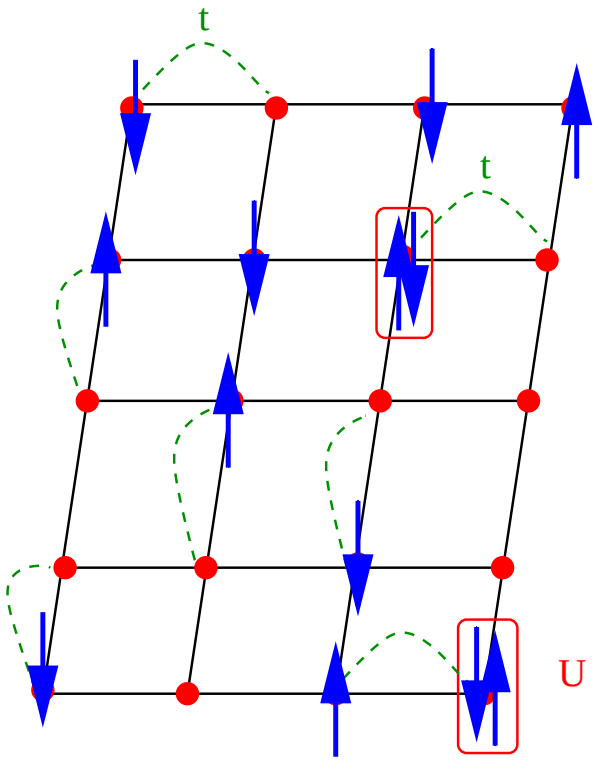
$$\frac{a}{\tau} \sim \frac{aW}{\hbar} \Longrightarrow \tau \sim \frac{\hbar}{W}$$

Small W longer interaction with another electron on the same atom
Strong electronic correlations

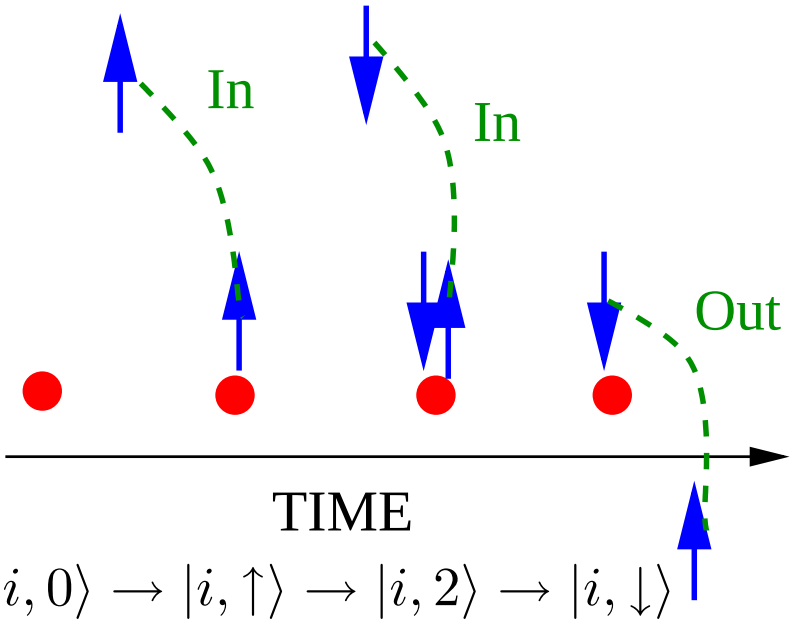
Hubbard model for strongly correlated electrons

$$H = -\sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$





Local Hubbard physics



The Holy Grail for correlated electrons

Fact: Hubbard model is not solved for arbitrary cases

Find the best comprehensive approximation

- valid for all values of parameters t, U, $n = N_e/N_L$, T
- thermodynamically consistent
- conserving
- possessing a small expansion (control) parameter and exact in some limit
- flexible to be applied to different systems and material specific calculations

What we need for Hubbard model

We need propagator (one-particle Green function)

$$G_{ij\sigma}(t) = -i\langle T_t c_{i\sigma}(t) c^\dagger_{j\sigma}(0)\rangle \underbrace{\longrightarrow}_{F.T.} G_\sigma(\mathbf{k},\omega) = \frac{1}{\omega + \mu - \epsilon_{\mathbf{k}} - \Sigma_\sigma(\mathbf{k},\omega)}$$

At finite temperatures $t \to -i\tau$

$$G_{ij\sigma}(\tau) = -\langle T_\tau c_{i\sigma}(\tau) c^\dagger_{j\sigma}(0)\rangle = -\frac{1}{Z}\int D[c^*,c] c_{i\sigma}(\tau) c^*_{j\sigma}(0) e^{-S[c^*,c]}$$

with the action (Lagrangian)

$$S[c^*,c] = -\int_0^{\beta=1/T} d\tau \sum_{i\sigma} c^*_{i\sigma}(\tau)(\partial_\tau - \mu) c_{i\sigma}(\tau) - H[c^*,c]$$

Later two-particle Green functions

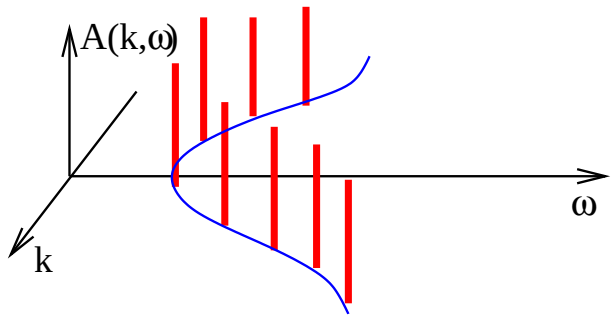
All what we know about Hubbard model

Solved in $U = 0$ limit (non-interacting limit)

$$G_\sigma(\mathbf{k}, \omega) = \frac{1}{\omega + \mu - \epsilon_\mathbf{k}}$$

Dispersion relation

$$\epsilon_\mathbf{k} = \sum_{j(i)} t_{ij} e^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)}$$

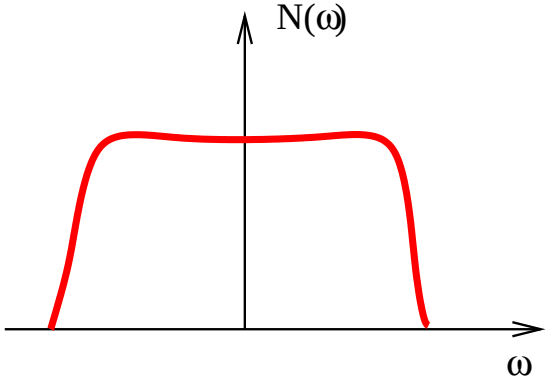


Spectral function - one-particle excitations

$$A_\sigma(\mathbf{k}, \omega) \equiv -\frac{1}{\pi} \mathrm{Im} G(\mathbf{k}, \omega) = \delta(\omega + \mu - \epsilon_\mathbf{k})$$

Density of states (DOS) - thermodynamics

$$N_\sigma(\omega) \equiv \sum_\mathbf{k} A(\mathbf{k}, \omega) = \sum_\mathbf{k} \delta(\omega + \mu - \epsilon_\mathbf{k})$$



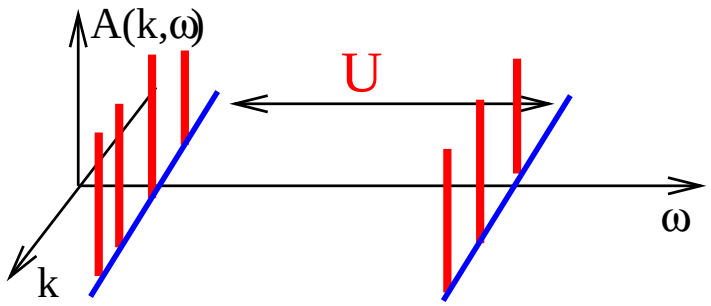
All what we know about Hubbard model

Solved in $t = 0$ limit (atomic limit)

$$G_\sigma(\mathbf{k},\omega) = \frac{1-n_{-\sigma}}{\omega+\mu} + \frac{n_{-\sigma}}{\omega+\mu-U} = \frac{1}{\omega+\mu-\Sigma_\sigma(\omega)}$$

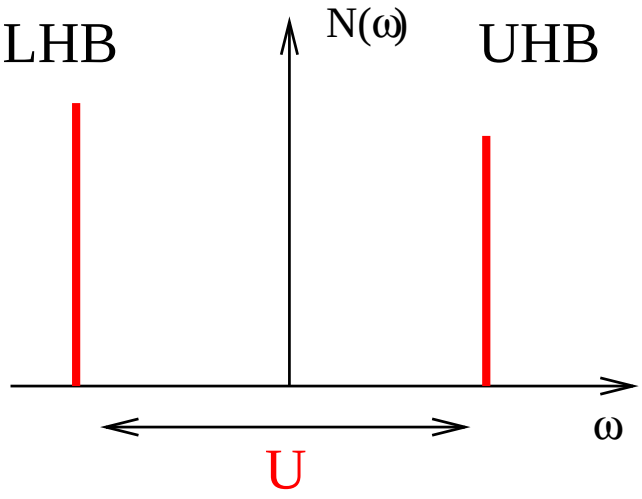
Real self-energy

$$\Sigma_\sigma(\omega) = n_\sigma U + \frac{n_{-\sigma}(1-n_{-\sigma})U^2}{\omega+\mu-(1-n_{-\sigma})U}$$



Spectral function

$$A_\sigma(\mathbf{k},\omega) = (1-n_{-\sigma})\delta(\omega+\mu) + n_{-\sigma}\delta(\omega+\mu-U)$$



Green function and self-energy are local,
i.e. $\mathbf{k}$ independent

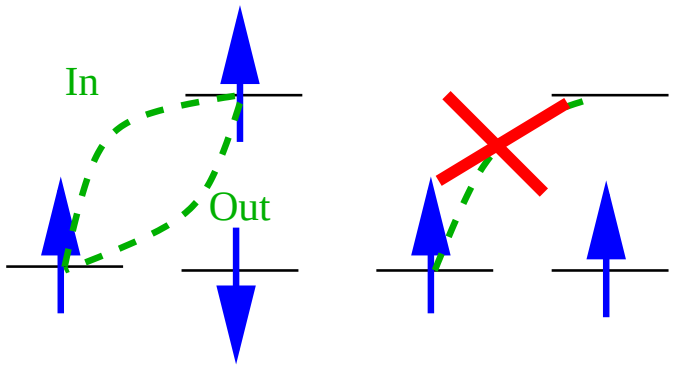
Summary - Correlations and models

- What is correlations and why they are important
- Correlated electrons
- Hubbard model (HM) for correlated electrons
- Quantities of interest
- Simple solvable limits of HM

Hubbard model at large U

Project onto the Hilbert subspace without double occupied sites, $t \ll U$

$$P = \prod_i (1 - n_{i\uparrow} n_{i\downarrow})$$



Effective tJ-Hamiltonian

$$H_{tJ} = P^\dagger H P = \sum_{ij\sigma} t_{ij} \tilde{c}^\dagger_{i\sigma} \tilde{c}_{j\sigma} - \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

when $n = 1$

$$H_{exch} = -\sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

where antiferromagnetic kinetic exchange coupling $J_{ij} = 4t_{ij}^2/U \ll t_{ij}$

Static mean-field for exchange Hamiltonian

Replace many-body Hamiltonian by one-body Hamiltonian with external (molecular or Weiss) field

$$Z = e^{-\beta F} = Tr_{\mathbf{S}_i} e^{-\beta H_{exch}} = Tr_{\mathbf{S}_i} e^{-\beta H_{MF}}$$

where

$$H_{MF} = \sum_i \mathbf{B}_{MF} \cdot \mathbf{S}_i + E_{shift}$$

Make mean-field (decoupling) approximation and determine $\mathbf{B}_{MF}$

$$\mathbf{B}_{MF} = \sum_{j(i)} J_{ij} \langle \mathbf{S}_j \rangle_{H_{MF}}$$

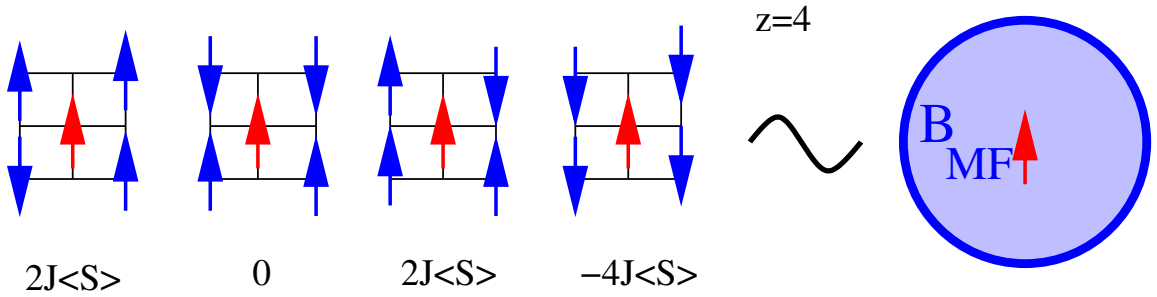
where $\langle \mathbf{S}_j \rangle = \langle S^z \rangle_{H_{MF}}$ is found self-consistently

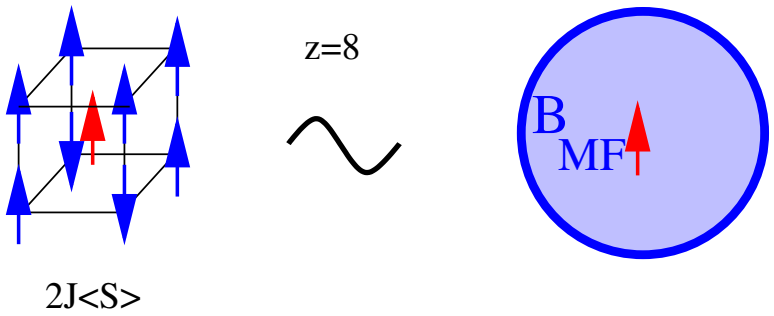
$$\langle S^z \rangle_{H_{MF}} = \tanh\left(\beta J \langle S^z \rangle_{H_{MF}}\right)$$

Static mean-field – principal approximation

Spin-spin correlations are neglected

$$\langle [\mathbf{S}_i - \langle \mathbf{S}_i \rangle] \cdot [\mathbf{S}_j - \langle \mathbf{S}_j \rangle] \rangle = 0 \Longrightarrow \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle = \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle$$





Quality of mean-field approximation improves when z is large

Static mean-field – exact when $z \to \infty$

$$\langle [\mathbf{S}_i - \langle \mathbf{S}_i \rangle] \cdot [\mathbf{S}_j - \langle \mathbf{S}_j \rangle] \rangle \to_{z\to\infty} 0 \Longrightarrow \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle \to_{z\to\infty} \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle$$

No spatial correlations in $z \to \infty$ limit

Rescaling for nearest neighbor (nn) exchange coupling

$$J \to \frac{J^*}{z}, \qquad J^* = \text{const}$$

then

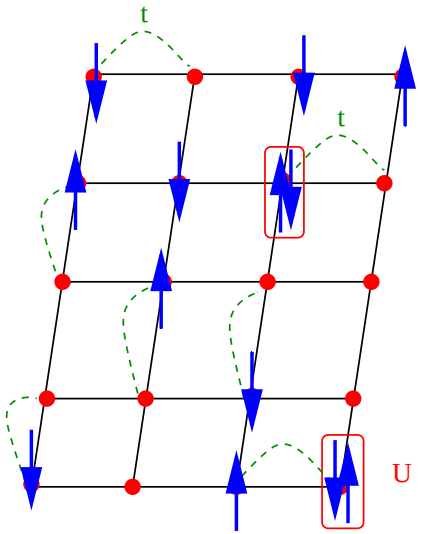
$$\mathbf{B}_{MF} = \sum_{j=1}^{z} J \langle \mathbf{S} \rangle_{H_{MF}} = \frac{J^*}{z} \sum_{j=1}^{z} \langle \mathbf{S} \rangle_{H_{MF}} = J^* \langle \mathbf{S} \rangle_{H_{MF}}$$

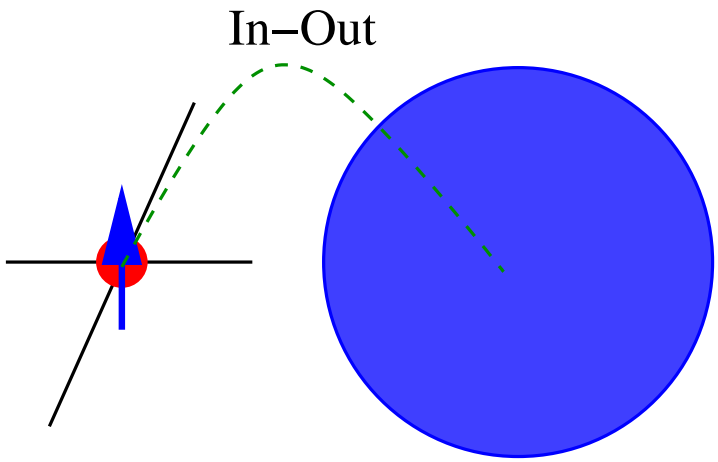
is bounded when $z \to \infty$

Static mean-field theory is exact and nontrivial when $z \to \infty$;
there exists a small (expansion) parameter $1/z$

Summary - Static mean-field

- Static mean field-theory, though exact in $z \to \infty$ limit,
  is not a comprehensive theory for Hubbard model
- It is valid only for large U
- But we learned potential usefulness of $z \to \infty$ limit
- We also understood general idea about mean-field (Weiss field, molecular field) approximation





Dynamical mean-field theory – heuristic approach

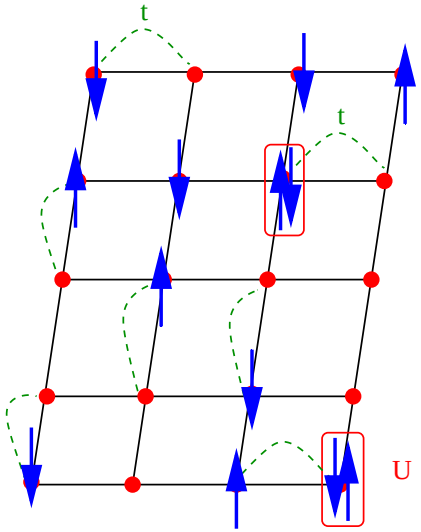
Find a comprehensive mean-field theory for Hubbard model

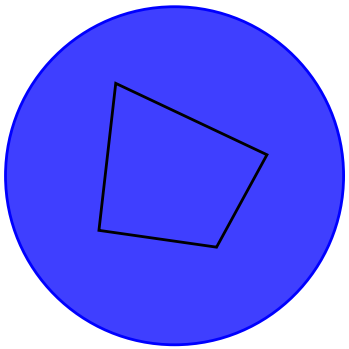
Exact free energy

$$F = -\frac{1}{\beta}\ln\int D[c^*,c]e^{-S[c^*,c]} = \frac{1}{\beta}\mathrm{Tr}\ln G_\sigma(\mathbf{k},\omega_n) = -\frac{1}{\beta}\mathrm{Tr}\ln[i\omega_n+\mu-\epsilon_{\mathbf{k}}-\Sigma_\sigma(\mathbf{k},\omega_n)]$$

Approximation $\Sigma_\sigma(\mathbf{k},\omega_n) = \Sigma_\sigma(\omega_n)$ - local approximation keeping full dynamics

$$F_{med}[\Sigma] = -\frac{1}{\beta}\mathrm{Tr}\ln[i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma_\sigma(\omega_n)]$$





$\Sigma(\omega)$

Dynamical mean-field theory – heuristic approach

Need a prescription to determine $\Sigma_\sigma(\omega_n)$

"Remove" a single site in the effective medium and replace it by the actual, bare interaction

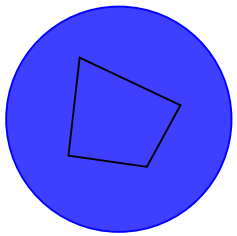
$$F = F_{med}[\Sigma] - F_i[\Sigma] + F_i^{bare}$$

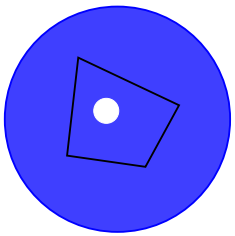
Local Green function ($i = j$ and index omitted)

$$G_\sigma(i\omega_n) = \sum_{\mathbf{k}} G_\sigma(\mathbf{k}, \omega_n) = \sum_{\mathbf{k}} \frac{1}{i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma_\sigma(\omega_n)} = G^0_\sigma(i\omega + \mu - \Sigma_\sigma(\omega_n))$$

and

$$F_i[\Sigma] = -\frac{1}{\beta} \mathrm{Tr} \ln[G^0_\sigma(i\omega + \mu - \Sigma_\sigma(\omega_n))]^{-1}$$





Dynamical mean-field theory – heuristic approach

Actual bare interaction

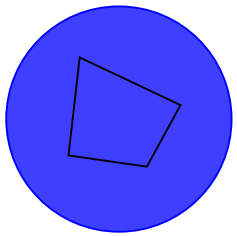
$$F_i^{bare}[\mathcal{G}] = -\frac{1}{\beta}\ln\int D[c^*,c]e^{-S_{loc}^{bare}[c^*,c]}$$

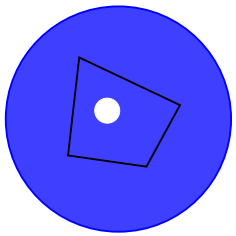
where

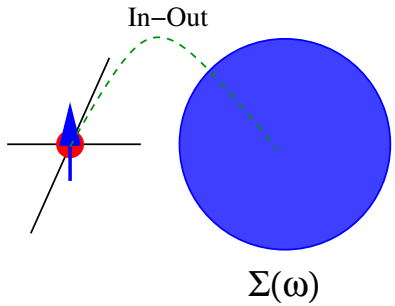
$$S_{loc}^{bare} = \sum_\sigma \int d\tau d\tau' c_\sigma^*(\tau)\mathcal{G}_\sigma^{-1}(\tau-\tau')c_\sigma(\tau') + U\int d\tau n_\uparrow(\tau)n_\downarrow(\tau)$$

and the local-Dyson equation defines

$$\mathcal{G}_\sigma^{-1}(\omega_n) = G_\sigma^{-1}(\omega_n) + \Sigma_\sigma(\omega_n)$$







Dynamical mean-field theory – heuristic approach

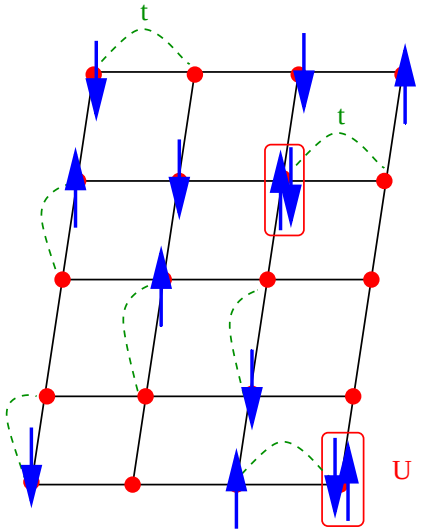
to close the set of equations use stationary condition

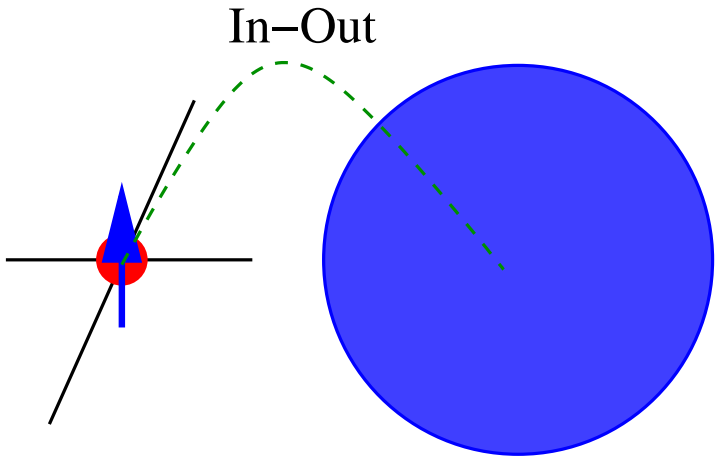
$$\frac{\delta F[\Sigma, \mathcal{G}^{-1}]}{\delta \mathcal{G}^{-1}} = 0$$

hence

$$G_\sigma(\tau) = -\langle T_\tau c_\sigma(\tau) c_\sigma^*(0) \rangle_{S_{loc}^{bare}}$$

and all three local but dynamical variables G, $\mathcal{G}$, and Σ are determined





Summary – DMFT - full glory

Local Green function

$$G_\sigma(\tau) = -\langle T_\tau c_\sigma(\tau) c_\sigma^*(0) \rangle_{S_{loc}^{bare}}$$

where

$$S_{loc}^{bare} = \sum_\sigma \int d\tau d\tau' c_\sigma^*(\tau) \mathcal{G}_\sigma^{-1}(\tau - \tau') c_\sigma(\tau') + U \int d\tau n_\uparrow(\tau) n_\downarrow(\tau)$$

Weiss (mean-field) function and self-energy

$$\mathcal{G}_\sigma^{-1}(\omega_n) = G_\sigma^{-1}(\omega_n) + \Sigma_\sigma(\omega_n)$$

Local Green function and lattice system self-consistency

$$G_\sigma(i\omega_n) = \sum_{\mathbf{k}} G_\sigma(\mathbf{k}, \omega_n) = \sum_{\mathbf{k}} \frac{1}{i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma_\sigma(\omega_n)} = G_\sigma^0(i\omega + \mu - \Sigma_\sigma(\omega_n))$$

DMFT – what is neglected, what is kept

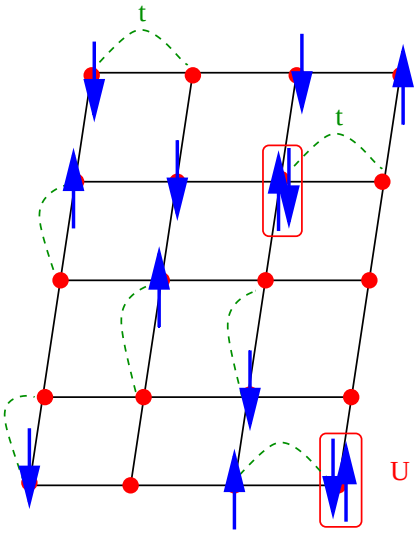
Spatial correlations are neglected (LRO is OK)

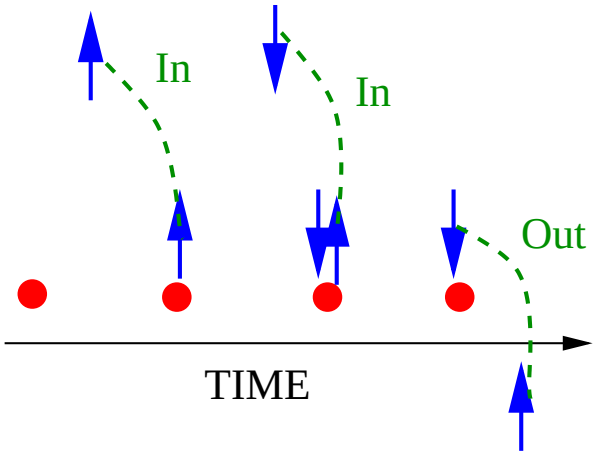
$$\langle [n_{i\sigma}(\tau) - \langle n_{i\sigma}(\tau)\rangle][n_{j\sigma'}(\tau') - \langle n_{j\sigma'}(\tau')\rangle]\rangle_{S_{loc}} = 0$$

Local temporal correlations are kept exactly

$$\langle [n_{i\sigma}(\tau) - \langle n_{i\sigma}(\tau)\rangle][n_{i\sigma'}(\tau') - \langle n_{i\sigma'}(\tau')\rangle]\rangle_{S_{loc}} = \text{“exact”}$$

Local dynamical Hubbard physics described well





DMFT – conserving theory

any reliable approximation should be conserving, i.e. all microscopic conservation laws should be preserved by an approximate theory

Φ-derivable theory (Baym, Kadanoff - 1962)

$$\Omega[\Sigma] = \Phi[\Sigma] - \mathrm{Tr}(\Sigma G) - \mathrm{Tr}(G_0^{-1} - \Sigma)$$

where

$$\Sigma = \frac{\delta \Phi}{\delta \Sigma}$$

is conserving because vertices

$$\Lambda = \frac{\delta^2 \Phi}{\delta \Sigma \delta \Sigma}$$

are approximated in the same way

dynamical mean-field theory is a conserving approximation due to construction

DMFT – consistent and comprehensive

DMFT is thermodynamically consistent, e.g.

$$n = -\frac{1}{\beta}\frac{\partial F}{\partial \mu} = -\frac{1}{\beta}\sum_{n\sigma} G_\sigma(\omega_n)$$

DMFT is valid for any value of the microscopic parameters,
no expansion wrt U, t, β, n or $1/n$

DMFT is comprehensive theory for correlated electrons

DMFT – flexibility; LDA+DMFT

Multi-band systems (Anisimov et al. 97; ... Nekrasov et al. 00, ...)

$$H = H_{LDA} + H_{int} - H^{U}_{LDA} = H^{0}_{LDA} + H_{int}$$

direct and exchange interaction

$$H_{int} = \frac{1}{2} \sum_{i=i_d, l=l_d} \sum_{m\sigma, m'\sigma'} U^{\sigma\sigma'}_{mm'} \, n_{ilm\sigma} n_{ilm'\sigma'}$$

$$-\frac{1}{2} \sum_{i=i_d, l=l_d} \sum_{m\sigma, m'} J_{mm'} \, c^{\dagger}_{ilm\sigma} c^{\dagger}_{ilm'-\sigma} c_{ilm'\sigma} c_{ilm-\sigma}$$

kinetic part, determined from DFT-LDA calculation (material specific)

$$H^{0}_{LDA} = \sum_{ilm, jl'm', \sigma} t^{0}_{ilm, jl'm'} c^{\dagger}_{ilm\sigma} c_{jl'm'\sigma}$$

LDA+DMFT - state of the art for realistic approach to correlated electron systems

DMFT scheme

S_{loc} - local interactions U or J from a model **TB** or a microscopic **LDA** Hamiltonian

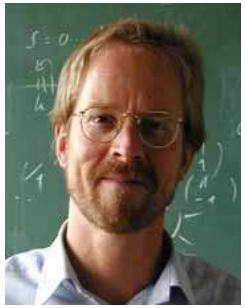
D. Vollhardt

$$\hat{G} = -\langle T\hat{C}(\tau)\hat{C}^*(0)\rangle_{S_{loc}}$$

DMFT

$$\hat{\mathcal{G}}^{-1} = \hat{G}^{-1} + \hat{\Sigma} \qquad \hat{\Sigma} \qquad \hat{\Sigma} = \hat{\mathcal{G}}^{-1} - \hat{G}^{-1}$$

$$\hat{G} = \sum[(\omega + \mu)\hat{1} - \hat{H}^0 - \hat{\Sigma}]^{-1}$$



W. Metzner

G. Kotliar

A. Georges

$\hat{H}^0$ is a model **TB** or a microscopic **LDA** Hamiltonian

DMFT – flexibility; disordered systems

Correlated electrons with local disorder

$$H = -\sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \sum_{i\sigma} \epsilon_i n_{i\sigma}$$

where ϵ_i is random (on-site) local energy with fixed probability distribution function (PDF) $P(\epsilon_i)$

In self-averaged systems, physical quantities are given by arithmetic average

$$G(\omega)_{av} = -\int d\epsilon_i P(\epsilon_i) \langle c(\omega) c^*(\omega) \rangle_{S_{loc}(\epsilon_i)} \equiv \langle \langle c(\omega) c^*(\omega) \rangle_{S_{loc}(\epsilon_i)} \rangle_{dis}$$

In non-self-averaged systems, physical quantities are given by typical ones - geometric average $O_{geom} = \exp[\langle \ln O \rangle]$

$$-\mathrm{Im} G(\omega)_{typ} = e^{\langle \ln[-\mathrm{Im} \langle c(\omega) c^*(\omega) \rangle_{S_{loc}(\epsilon_i)}] \rangle_{dis}}$$

Summary – DMFT - flexibility

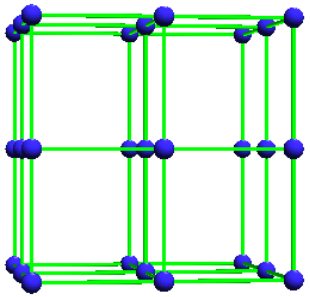
- Local temporal correlations exact
- Spatial correlations neglected
- Conserving and thermodynamically consistent
- Comprehensive mean-field theory
- LDA+DMFT
- DMFT for disordered electrons

DMFT – $d \to \infty$ limit, small parameter O$(1/z)$

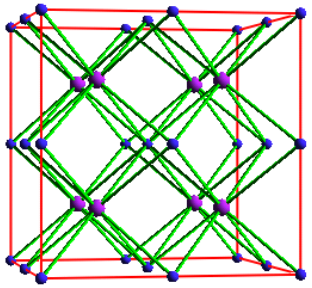
Idea: spatial correlations are absent when number of neighbors is large (infinite)

Crystal lattices in $d = 3$:

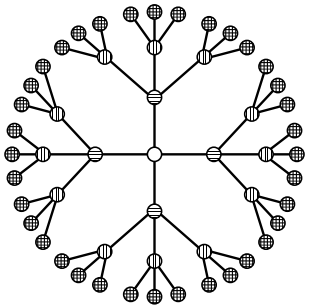
simple cubic (sc) - $z = 6$
body center cubic (bcc) - $z = 8$
face centered cubic (fcc) - $z = 12$

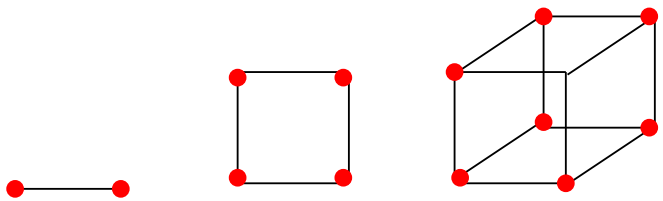


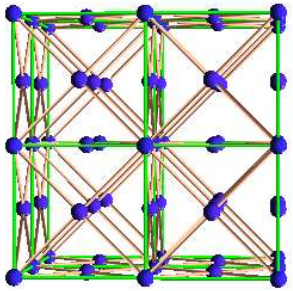
Hypercubic lattice in d-dimension - $z = 2d$



Bethe (Caley) tree - $z = K + 1$







Simple $d \to \infty$ limit

Kinetic energy

$$H_0 = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

NN hopping:

$$t_{ij} = t(\mathbf{R}_i - \mathbf{R}_j) = \begin{cases} -t & \text{if} \quad \mathbf{R}_i - \mathbf{R}_j = \pm \mathbf{e}_n \\ 0 & \text{otherwise} \end{cases}$$

Bare dispersion

$$\epsilon_{\mathbf{k}} = -2t \sum_{i=1}^{d} \cos k_i$$

Density of states

$$N_d(\epsilon) \sum_{\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k}}) \to_{d\to\infty} \frac{1}{2t\sqrt{\pi d}} e^{-\left(\frac{\epsilon}{2t\sqrt{d}}\right)^2}$$

arbitrary broad and featureless in $d \to \infty$ limit

Non-trivial $d \to \infty$ limit

Non-trivial DOS is obtained when hopping is rescaled

$$t \to \frac{t^*}{\sqrt{2d}}, \qquad t^* = \text{const}$$

$$N_\infty(\epsilon) = \frac{1}{\sqrt{2\pi}t^*} e^{-\left(\frac{\epsilon}{2t^*}\right)^2}$$

(Metzner, Vollhardt, 1989)

In general

$$t_{ij} \to \frac{t^*_{ij}}{\sqrt{d||\mathbf{R}_i - \mathbf{R}_j||}}$$

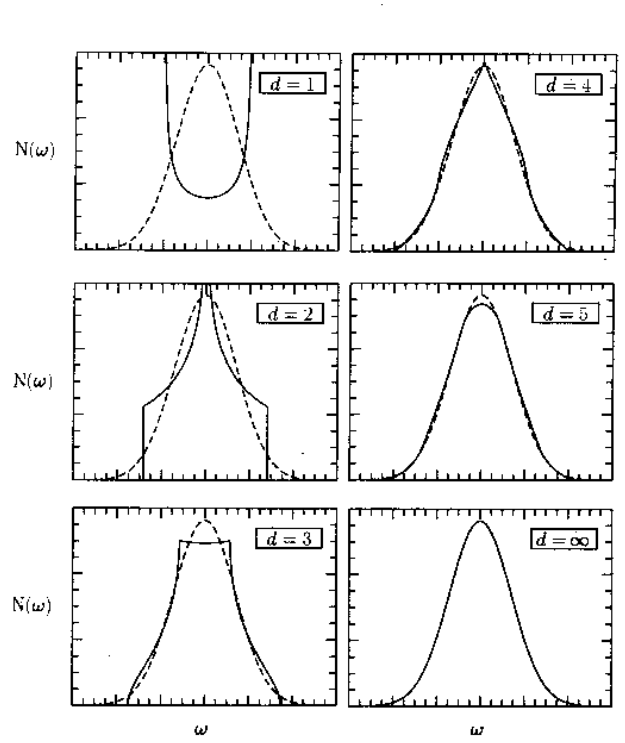
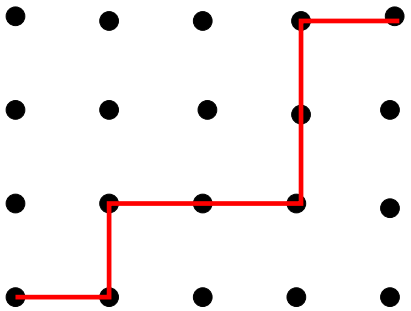


Fig. 1.2 Tight-binding density of states in $d = 1, 2, 3, 4, 5$ as compared with th
for $d = \infty$.



$||\mathbf{R}_i - \mathbf{R}_j||$ - taxi cab (Manhattan, New York) distance

Non-trivial $d \to \infty$ limit

Non-trivial (asymptotic) theory is well defined such that the energy density is generically finite and non-zero

$$\frac{1}{N_L} E_{kin} = \frac{1}{N_L} \sum_{ij\sigma} t_{ij} \langle c^\dagger_{i\sigma} c_{j\sigma} \rangle = \frac{1}{N_L} \sum_{i\sigma} \underbrace{\sum_{j(i)}}_{O(d^{||\mathbf{R}_i - \mathbf{R}_j||})} t_{ij} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} G_{ij\sigma}(\omega) \sim O(1)$$

Fact, since G_{ij} is probability amplitude for hopping,

$$G_{ij} \sim O(d^{-\frac{||\mathbf{R}_i - \mathbf{R}_j||}{2}})$$

with rescaling

$$t_{ij} \to \frac{t^*_{ij}}{\sqrt{d^{||\mathbf{R}_i - \mathbf{R}_j||}}}$$

sum $\sum_{j(i)}$ is compensated and energy is finite (Metzner, Vollhardt, 1989)

$d \to \infty$ limit – Feynman diagrams simplification

One proves, term by term, that skeleton expansion for the self-energy $\Sigma_{ij}[G]$ has only local contributions

$$\Sigma_{ij\sigma}(\omega_n) \to_{d\to\infty} \Sigma_{ii\sigma}(\omega_n)\delta_{ij}$$

Fourier transform is $\mathbf{k}$-independent

$$\Sigma_{\sigma}(\mathbf{k},\omega_n) \to_{d\to\infty} \Sigma_{\sigma}(\omega_n)$$

DMFT is an exact theory in infinite dimension (coordination number) and small control parameter is $1/d$ $(1/z)$

(Metzner, Vollhardt, 1989)

ansatz in heuristic derivation is then exact (Janis, Vollhrdt, 1992)

$$F = F_{med}[\Sigma] = -\frac{1}{\beta}\mathrm{Tr}\ln[i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma_{\sigma}(\omega_n)]$$

Summary – DMFT exact in large dimension

- Construction models nontrivial in $d \to \infty$ limit
- Rescaling of hoppings
- Simplifications for diagrams

DMFT in practice

The hardest part of DMFT is to solve local, many-body problem

$$G_\sigma(\tau) = -\langle T_\tau c_\sigma(\tau) c^*_\sigma(0) \rangle_{S^{bare}_{loc}}$$

where

$$S^{bare}_{loc} = \sum_\sigma \int d\tau d\tau' c^*_\sigma(\tau) \mathcal{G}^{-1}_\sigma(\tau - \tau') c_\sigma(\tau') + U \int d\tau n_\uparrow(\tau) n_\downarrow(\tau)$$

it is usually mapped onto the Single Impurity Anderson Model
(Kotliar, Georges, 1992; Jarrell, 1992)

$$H_{SIAM} = \epsilon_d \sum_\sigma n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_{\mathbf{k}\sigma} V_{\mathbf{k}} d^\dagger_\sigma c_{\mathbf{k}\sigma} + H.c. + \sum_{\mathbf{k}\sigma} \epsilon^{aux}_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

DMFT solvers in practice

- Analytical approaches (approximate, but fast)
  - (IPT) Iterative perturbation expansion
  - (NCA) Non-crossing approximation
  - (LMA) Local moment approach
  - (LDMFT) Linear DMFT
  - (Hubbard I or III) Strong coupling approach

- Numerical approaches (formally exact, but expensive)
  - (QMC) Quantum Monte Carlo - Trotter decomposition, large T, limited U
  - (QMC) Quantum Monte Carlo - continuum time, perturbative character (?)
  - (PQMC) Projected quantum Monte Carlo - only ground state
  - (ED) Exact diagonalization - small system, discrete spectrum
  - (NRG) Numerical renormalization group - logarithmic broadening
  - (DMRG) Dynamical matrix renormalization group - poor low energy

Find the best solver to you physical problem

DMFT – long-range orders and susceptibilities

Broken symmetry phases (infinite-long range orders) are described by generalized local problem and self-consistency condition

e.g., for AF we need to sites (A or B) which are coupled be opposite spins

Susceptibilities (two-particle correlation functions) are determined by the corresponding local quantities and non-interacting lattice parts

$$\hat{\chi}_{\mathbf{q}}^{-1} = \hat{\chi}_{loc}^{-1} + \hat{\chi}_{0,\mathbf{q}}^{-1} - \hat{\chi}_{0,loc}^{-1}$$

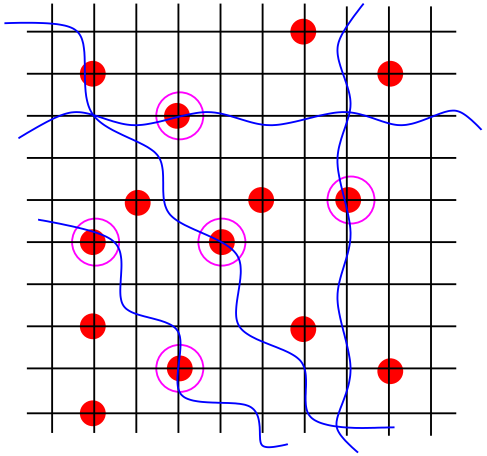
Summary – DMFT in practice

- Mapping onto impurity model
- Impurity solvers
- Long-range order
- Two-particle correlation functions

Examples

1. Analytically solvable Falicov-Kimball model
2. MIT at half-filling in Hubbard model and experiment
3. Electronic kinks in correlated metals
4. Mott-Anderson MIT in correlated electron systems with disorder
5. Itinerant ferromagnetism
6. MIT in binary alloy systems
7. Itinerant ferromagnetism in binary alloy systems

1. Falicov-Kimball model



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

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

1. Falicov-Kimball model

Self-consistency for f-electrons is simple: $\mathcal{G}_f^{-1} = \partial_\tau - \mu$

DMFT local action

$$S_{loc} = \int d\tau d\tau' c^*(\tau)\mathcal{G}_c^{-1}(\tau - \tau')c(\tau')$$

$$+ \int d\tau f^*(\tau)(\partial_\tau - \mu + \epsilon_f)f(\tau) + U \int d\tau f^*(\tau)f(\tau)c^*(\tau)c(\tau)$$

Integrate out f-electrons (atomic limit) analytically

$$G_d(i\omega_n) = \frac{n_f}{\mathcal{G}_d(i\omega_n)^{-1} - U} + \frac{1 - n_f}{\mathcal{G}_d(i\omega_n)^{-1}}$$

1. Falicov-Kimball model

Self-consistency equations:

$$G_d(i\omega_n) = \int d\epsilon \frac{N_0(\epsilon)}{i\omega_n + \mu - \Sigma_d(i\omega_n) - \epsilon}$$

and

$$G_d(i\omega_n)^{-1} = \mathcal{G}_d(i\omega_n)^{-1} - \Sigma_d(i\omega_n)$$

determines $G_d(i\omega_n)$ for any DOS

Skeleton functional $\Sigma_D[G_d]$

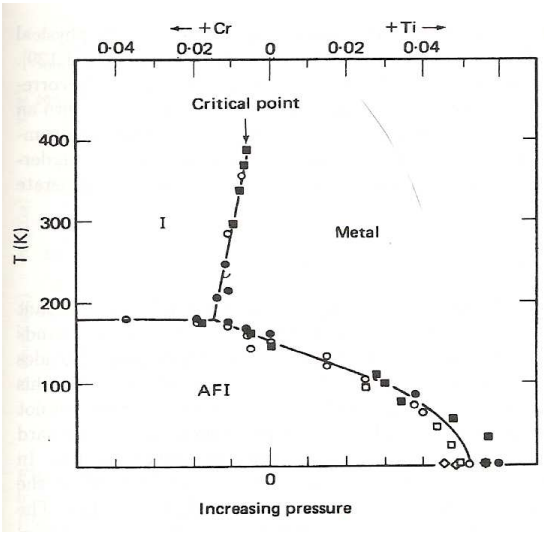
$$\Sigma_d(i\omega_n) = \frac{U}{2} - \frac{1}{2G_d(i\omega_n)} \pm \sqrt{\left(\frac{U}{2} - \frac{1}{2G_d(i\omega_n)}\right)^2 + U\frac{n_f}{G_d(i\omega_n)}}$$

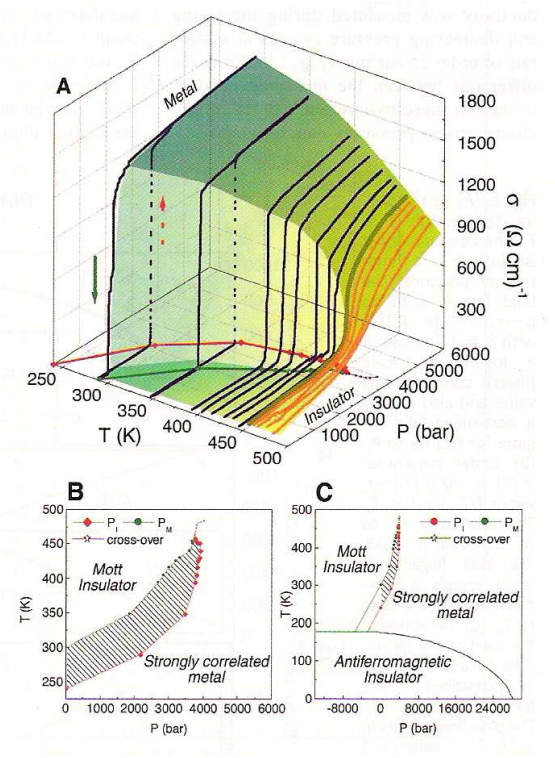
involves all orders in U

Brand and Mielsch 89, van Dongen and Vollhardt 90, Si et al. 92, Frireecks and Zlatic 03, Lemanski et al. 00-01

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

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



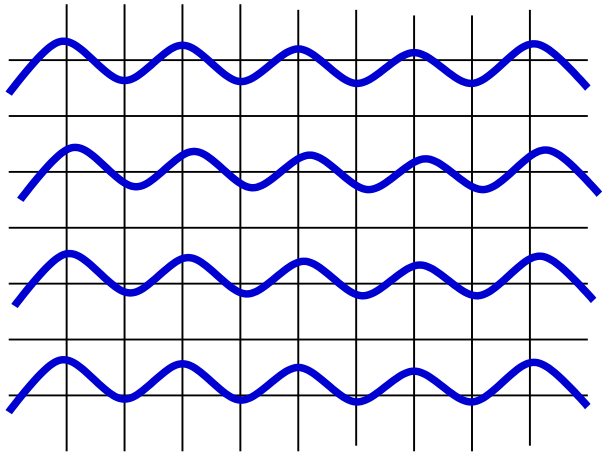


True Mott insulator

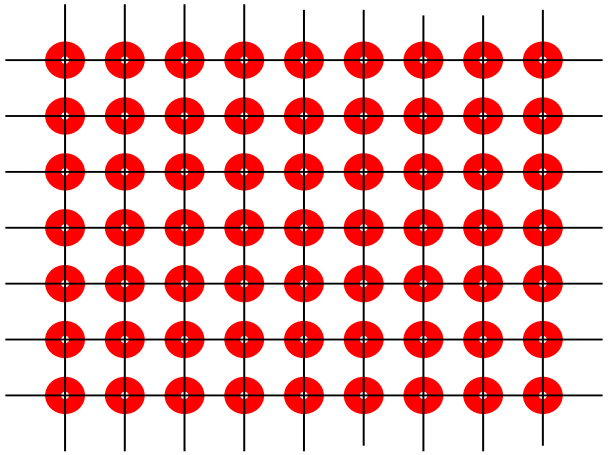
persists above T_N

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

2. MIT at half-filling

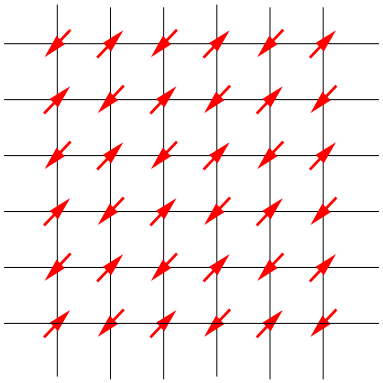


$U \ll |t_{ij}|$, $\Delta \mathbf{p} = 0$



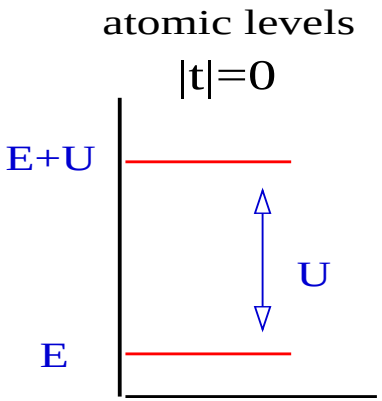
$U \gg |t_{ij}|$, $\Delta \mathbf{r} = 0$

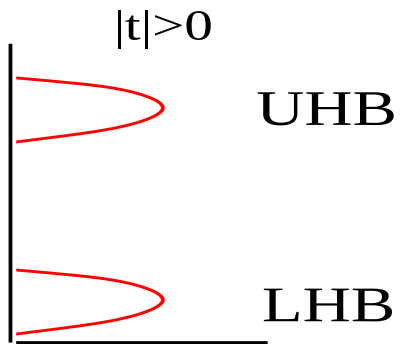
Antiferromagnetic Mott insulator

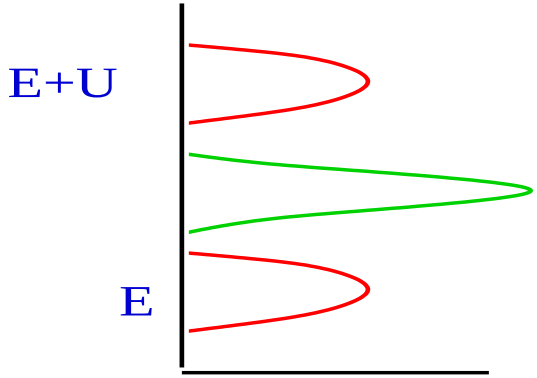


typical intermediate coupling problem $U_c \approx |t_{ij}|$

2. MIT at half-filling







spin flip on central site

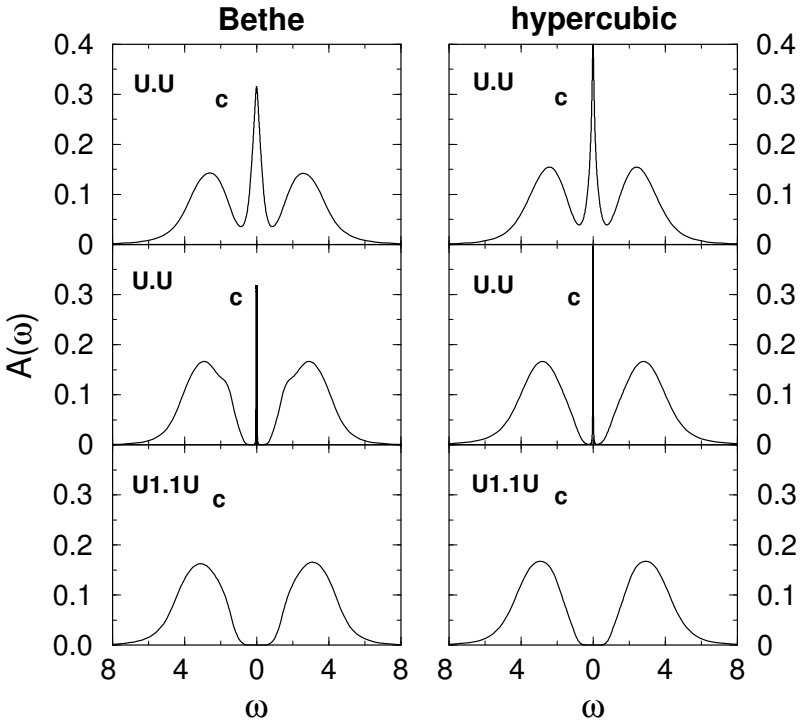
at $U = U_c$ resonance disapears

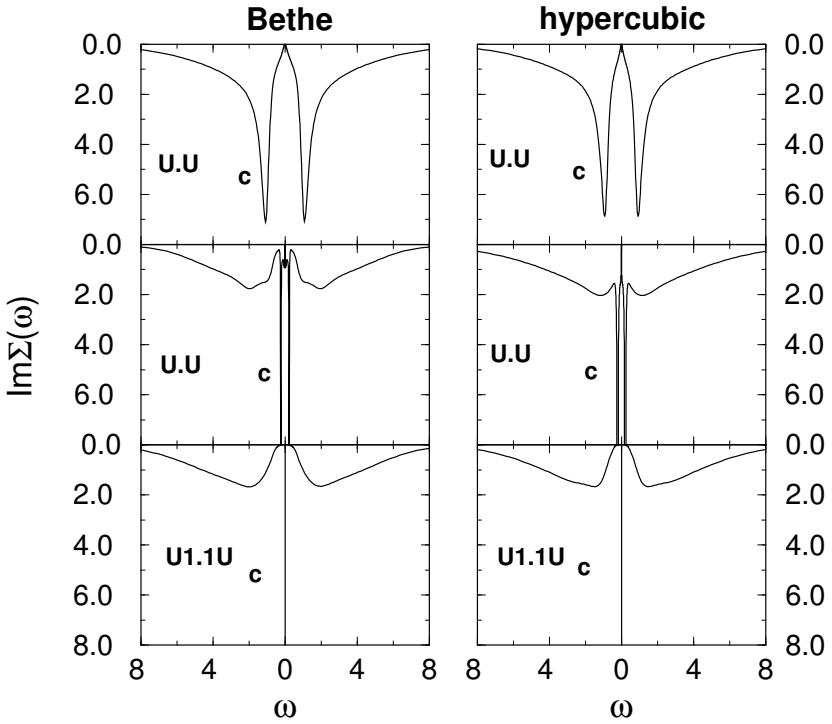
gaped insulator

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

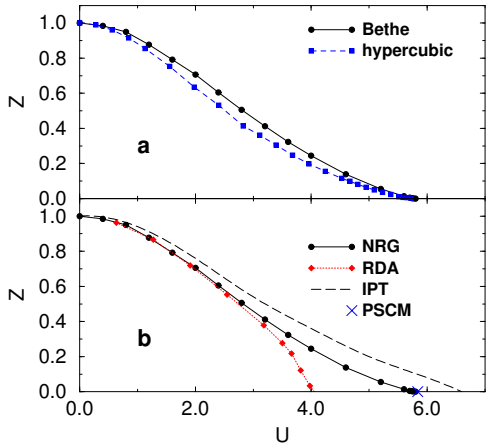
2. MIT at half-filling at $T = 0$ according to DMFT

Kotliar et al. 92-96, Bulla, 99





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



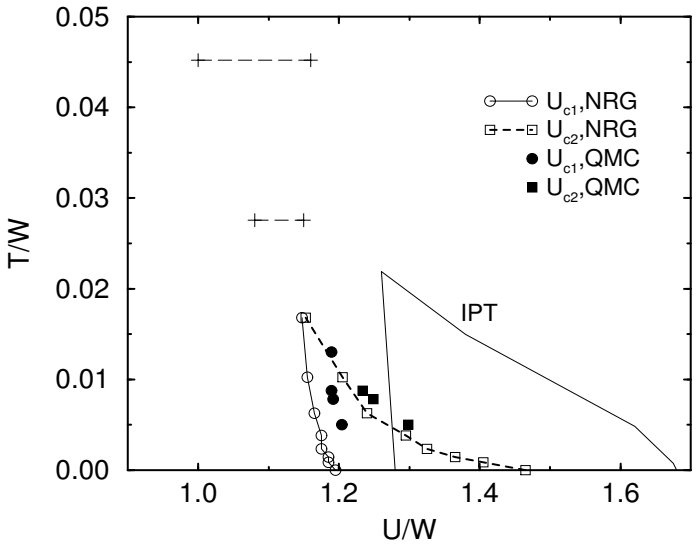
Luttinger pinning $A(0) = N_0(0)$

Fermi liquid

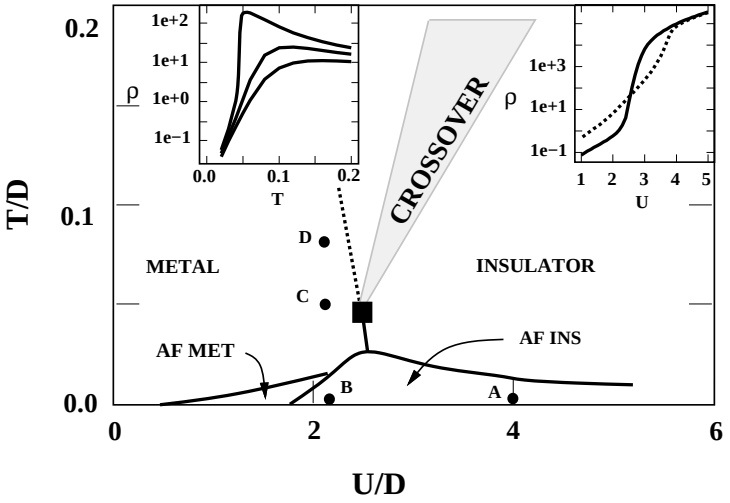
Muller-Hartmann 1989

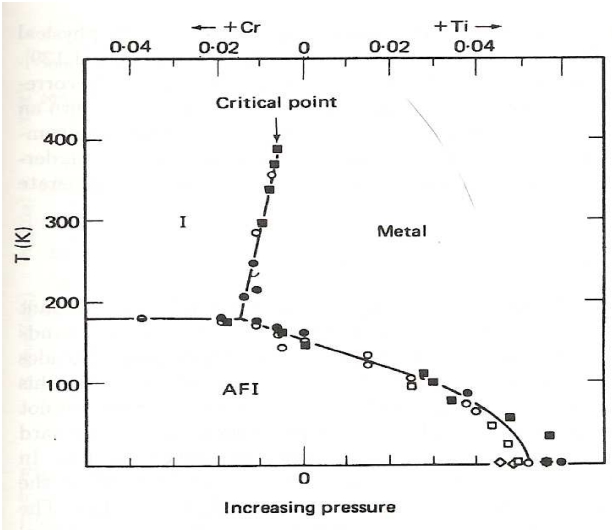
2. MIT at half-filling at $T > 0$ according to DMFT

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



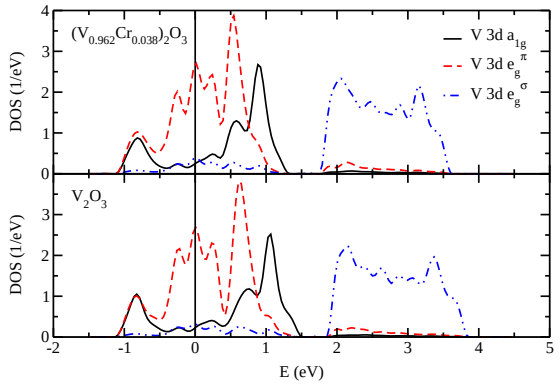
1st-order transition



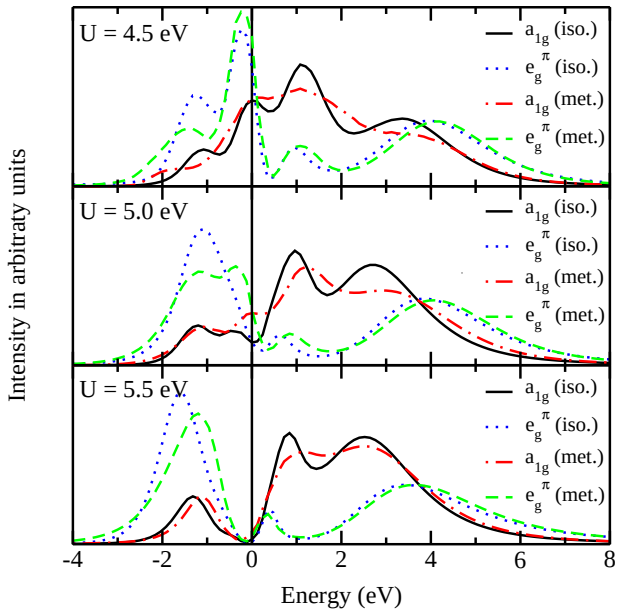


2. MIT in V_2O_3 according to DMFT+DMFT

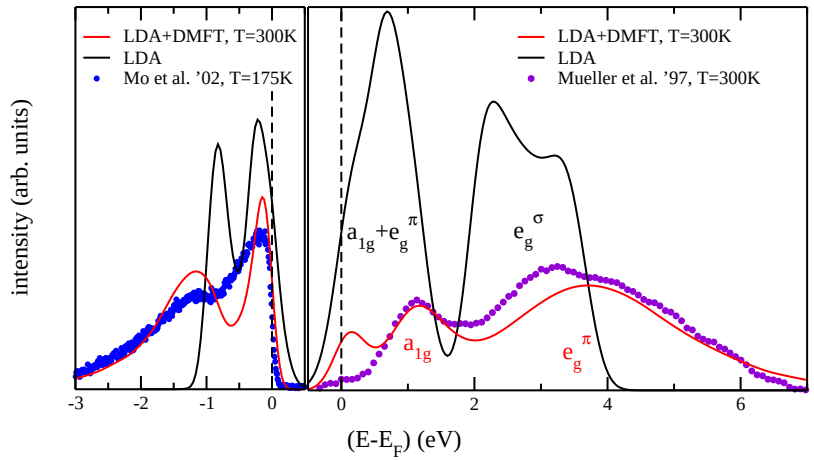
Held et al. 01, Keller et al. 04

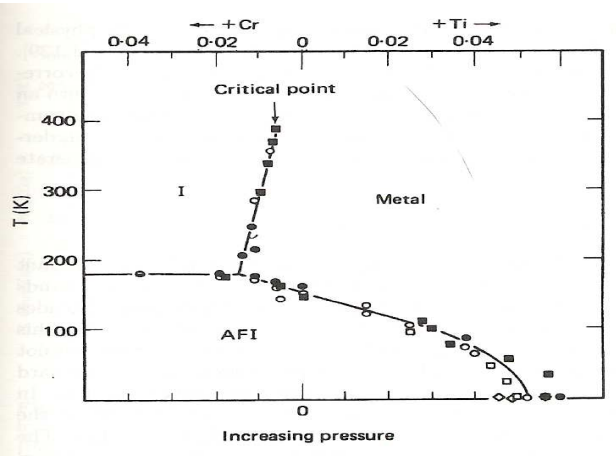


LDA



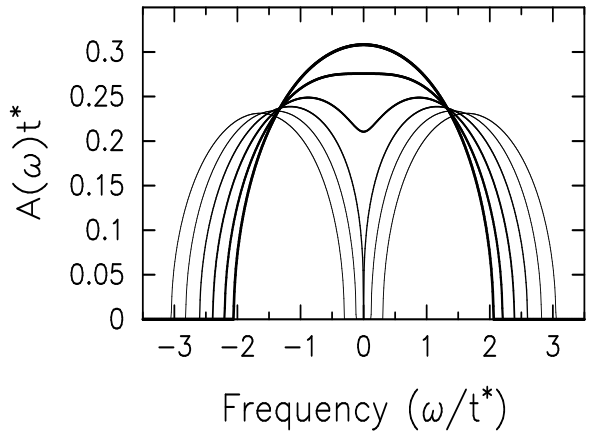
LDA+DMFT





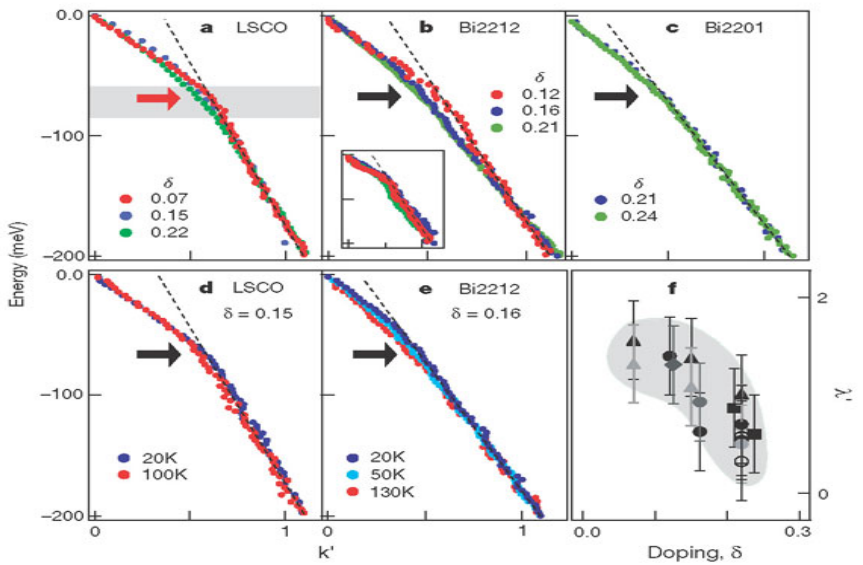
2. Mott MIT in Falicov-Kimball model - DMFT

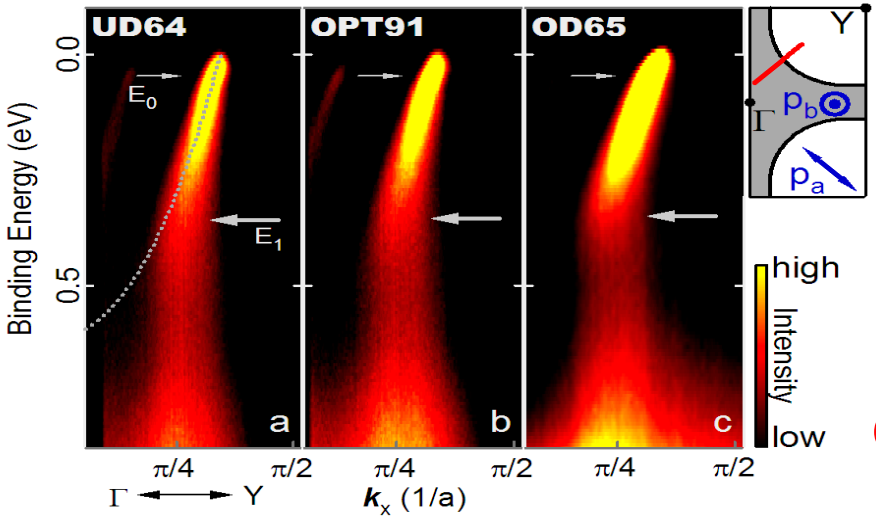
- f-particles appear as like disorder scatterers (with an annealed averaging).
- No Fermi liquid property of FK model if $n_f \neq 0$ or 1.
- Pseudo-gap regime.
- For $n_e = n_f = 0.5$ and $U = U_c \sim W$ continuous Mott like MIT.
- Correlation gap opened.

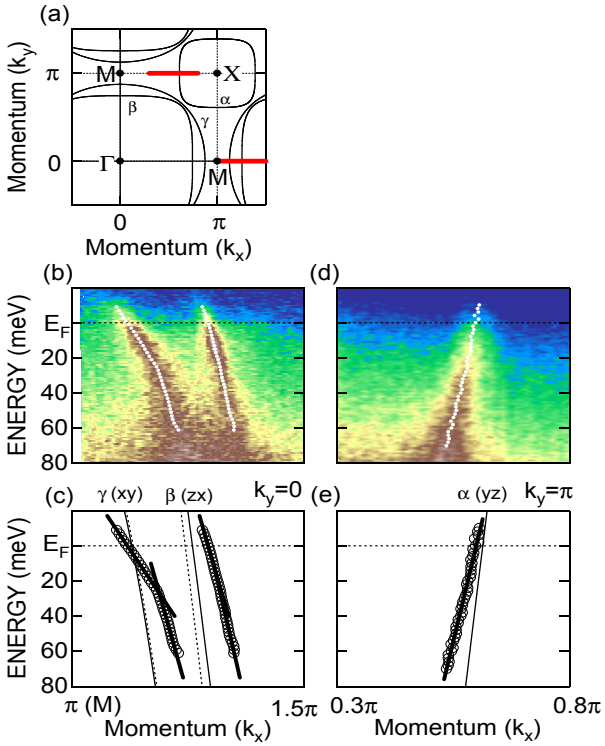


van Dongen and Lainung 1997, DMFT, Bethe, no CDW, $U = 0.5 - 3.0$

3. Electronic kinks in correlated metals







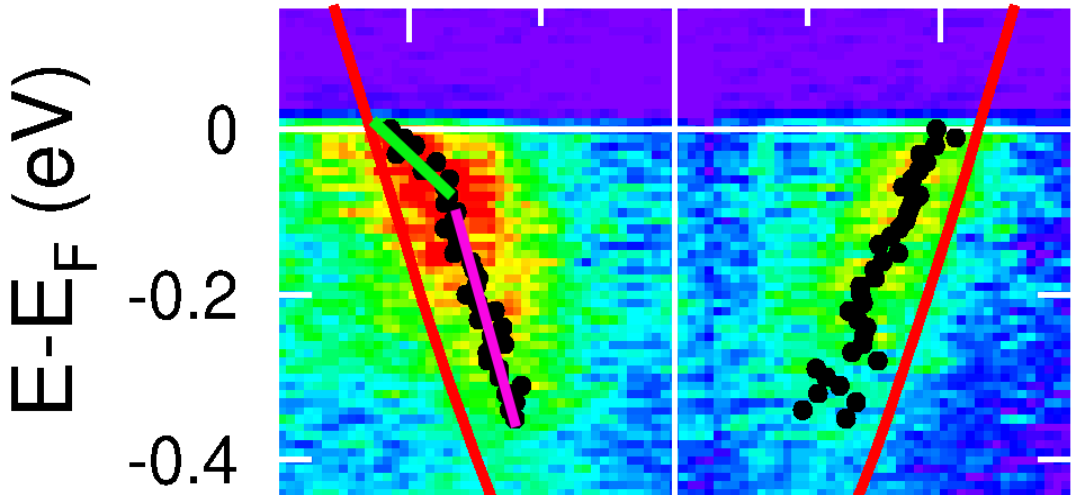
Sr_2RuO_4, cond-mat/0508312

Kinks seen experimentally between 20-800 meV

Origin: phonos, spin fluctuations, often not known

water falls in different HTC systems, cond-mat/0604284, cond-mat/0607319

3. Kinks - more examples of kinks in ARPES



$SrVO_3$, cond-mat/0504075

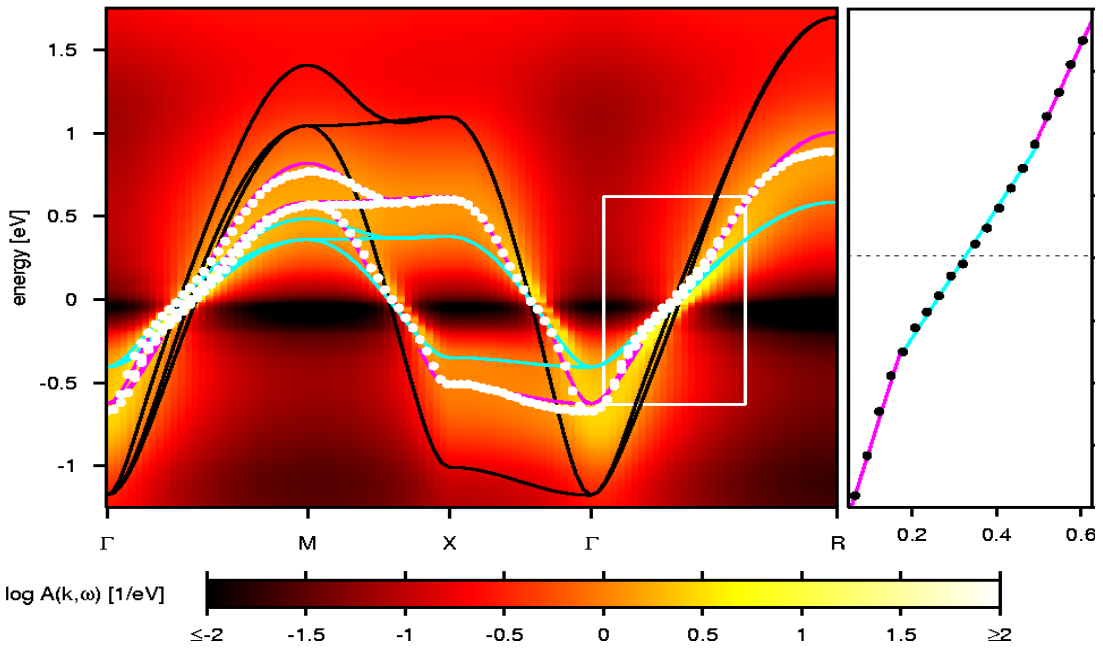
Kinks seen experimentally at 150 meV

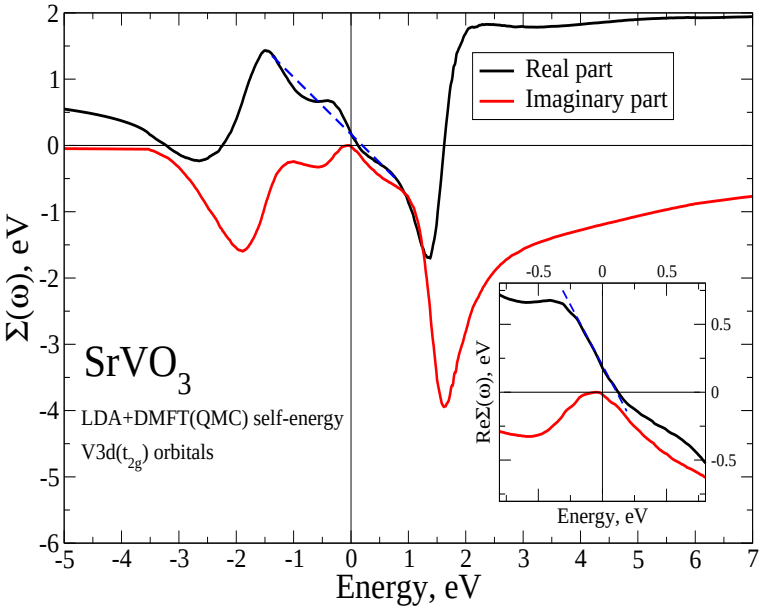
Pure electronic origin?

3. Kinks in LDA+DMFT study of $SrVO_3$

plain band model with local correlations, no other bosons, ... but kinks!

I.A. Nekrasov *et al.*, cond-mat/0508313, PRB (2006)



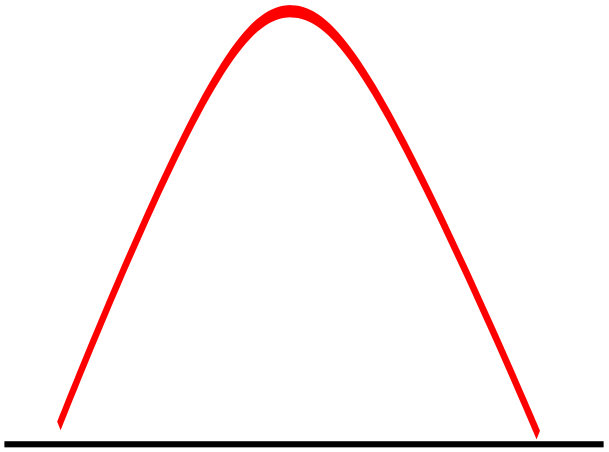


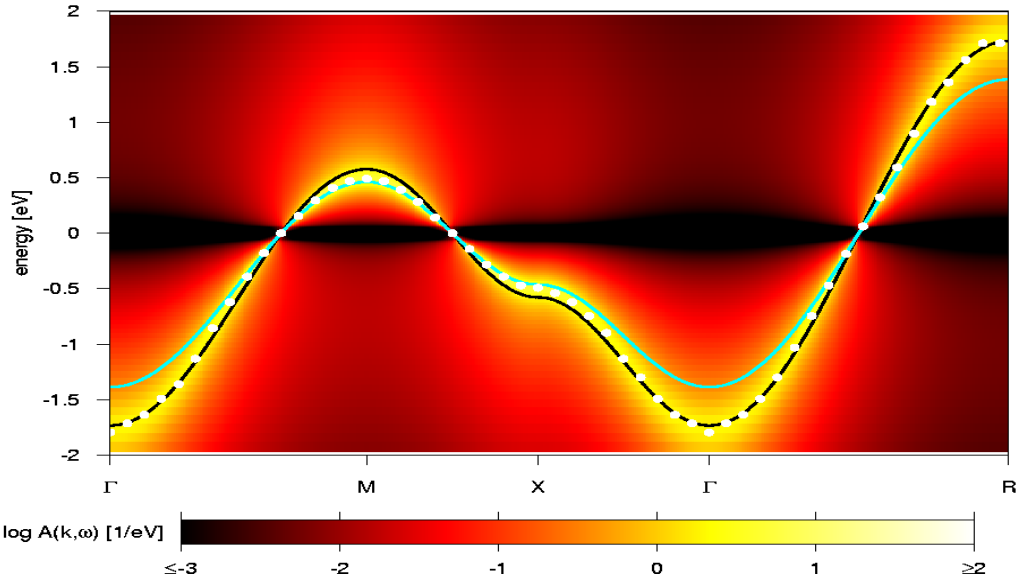
$$G_{\mathbf{k}}(\omega) = \frac{1}{\omega + \mu - \epsilon_{\mathbf{k}} - \Sigma(\omega)} \qquad \rightarrow E_{\mathbf{k}} + \mu - \epsilon_{\mathbf{k}} - \mathrm{Re}\Sigma(E_{\mathbf{k}}) = 0$$

Not found in SIAM with simple hybridization function! → DMFT self-consistency effect

3. Kinks - weakly correlated system

K. Byczuk, M. Kollar, K. Held, Y.-F. Yang, I. A. Nekrasov, Th. Pruschke, D. Vollhardt, cond-mat/0609594



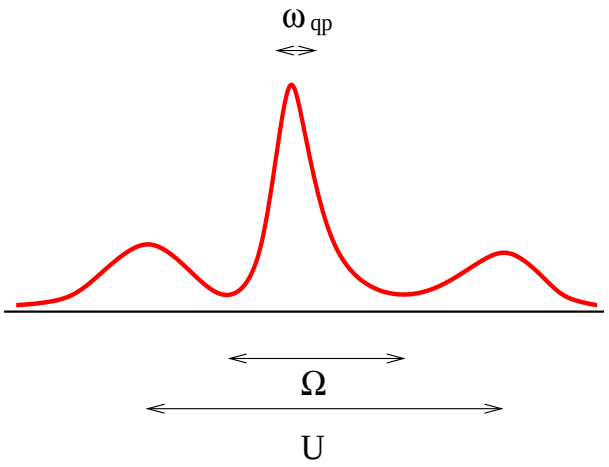


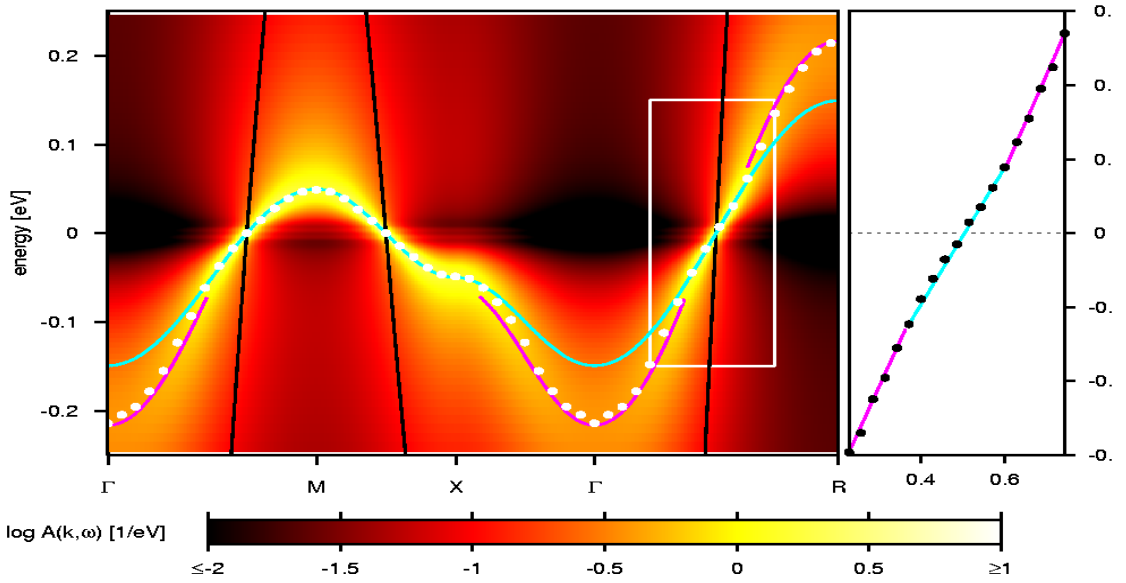
Fermi liquid $Z_{FL} \lesssim 1$: $E_{\mathbf{k}} = Z_{FL}\epsilon_{\mathbf{k}}$ for $|E_{\mathbf{k}}| < \omega_*$

$E_{\mathbf{k}} = \epsilon_{\mathbf{k}}$ for $|E_{\mathbf{k}}| > \omega_*$

3. Kinks due to strong correlations

K. Byczuk, M. Kollar, K. Held, Y.-F. Yang, I. A. Nekrasov, Th. Pruschke, D. Vollhardt, cond-mat/0609594





Fermi liquid $Z_{FL} \ll 1$: $E_{\mathbf{k}} = Z_{FL}\epsilon_{\mathbf{k}}$ for $|E_{\mathbf{k}}| < \omega_*$

Different renormalization $Z_{CP} \ll 1$: $E_{\mathbf{k}} = Z_{CP}\epsilon_{\mathbf{k}} \pm c$ for $|E_{\mathbf{k}}| > \omega_*$

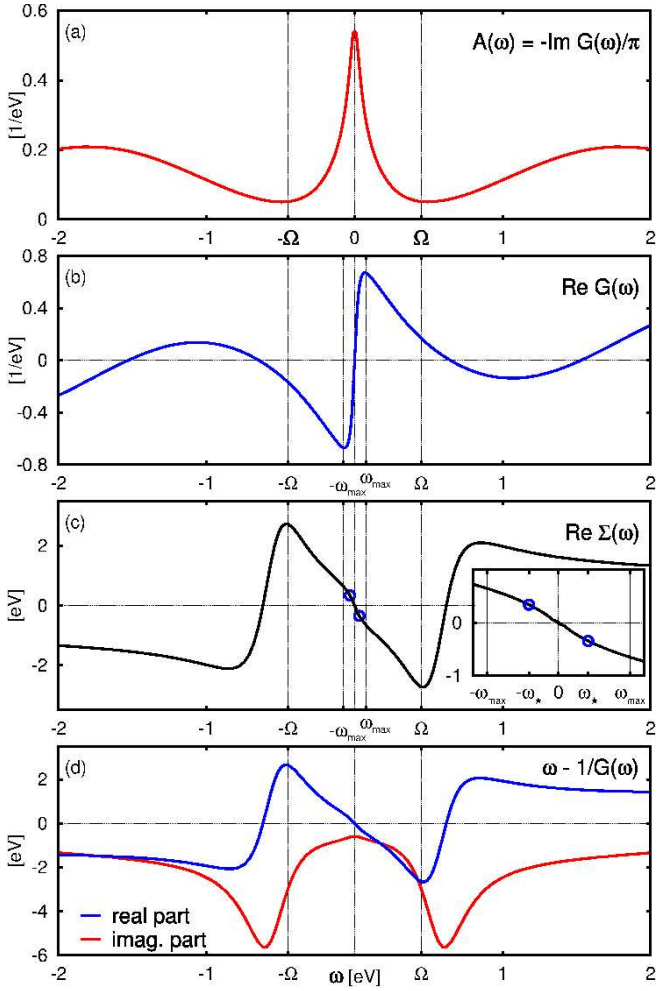
3. Kinks - microscopic explanation within DMFT

K. Byczuk, M. Kollar, K. Held, Y.-F. Yang, I. A. Nekrasov, Th. Pruschke, D. Vollhardt, cond-mat/0609594

DMFT self-consistency condition

$$\Sigma(\omega) = \omega - 1/G(\omega) - \Delta(G(\omega))$$

$$\Delta(G(\omega)) \approx (m_2 - m_1^2)G(\omega) + ...$$



3. Kinks- microscopic predictions

- Strong correlations (three peak spectral function) a sufficient condition for electronic kinks

- Energy scale for electronic kinks $\omega_* = Z_{FL} D$ determined by Fermi-liquid renormalization and bare (LDA) density of states

- ω_* sets the energy scale for Fermi-liquid regime where $E_{\mathbf{k}} = Z_{FL} \epsilon_{\mathbf{k}}$ for $|E_{\mathbf{k}}| < \omega_*$

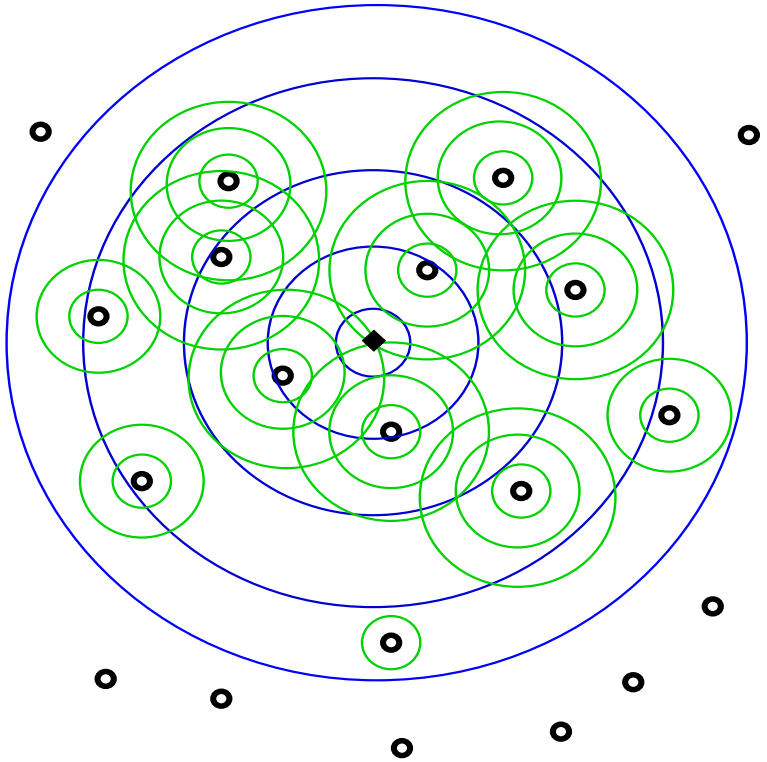
- Beyond Fermi-liquid regime the dispersion is still renormalized and useful $E_{\mathbf{k}} = Z_{CP} \epsilon_{\mathbf{k}} \pm c$ for $|E_{\mathbf{k}}| > \omega_*$ where the offset c and Z_{CP} determined by Z_{FL} and D

- Electronic kinks are within cluster extension of DMFT (DCA) $\Sigma_{\mathbf{K}}(\omega) = \omega - \frac{1}{G_{\mathbf{K}}(\omega)} - \Delta(G_{\mathbf{K}}(\omega))$

- Electronic kinks are generic feature of strongly correlated systems

4. 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

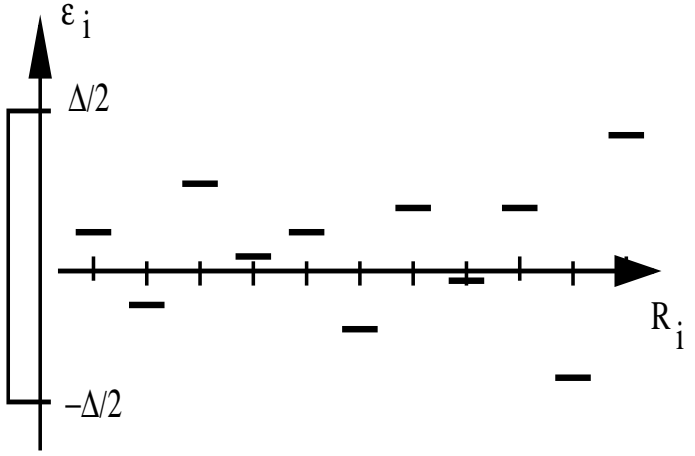
Localization is a destruction of coherent
superposition of spatially separated states

4. Anderson model

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

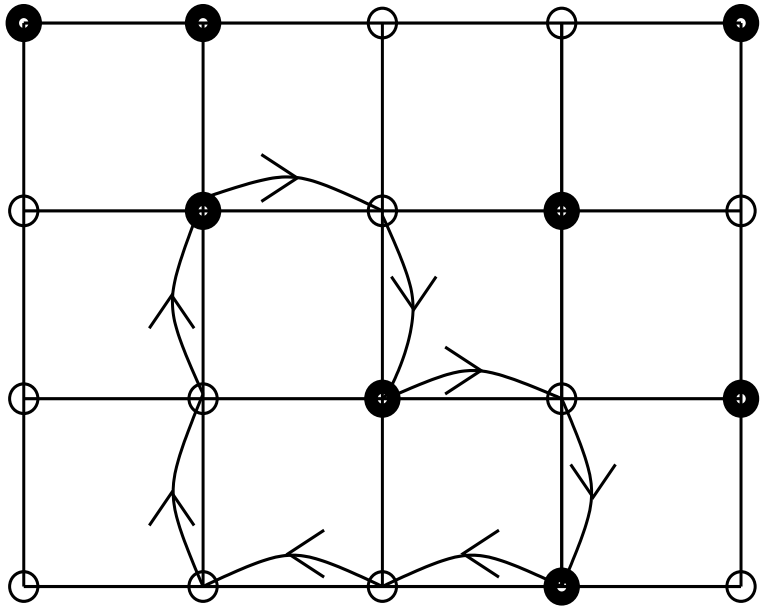
Probability distribution function

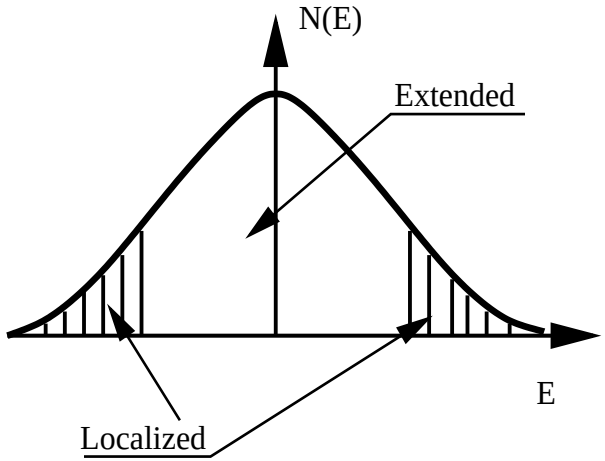
$$\mathcal{P}(\epsilon_i) = \frac{1}{\Delta}\Theta\left(\frac{\Delta}{2} - |\epsilon_i|\right)$$

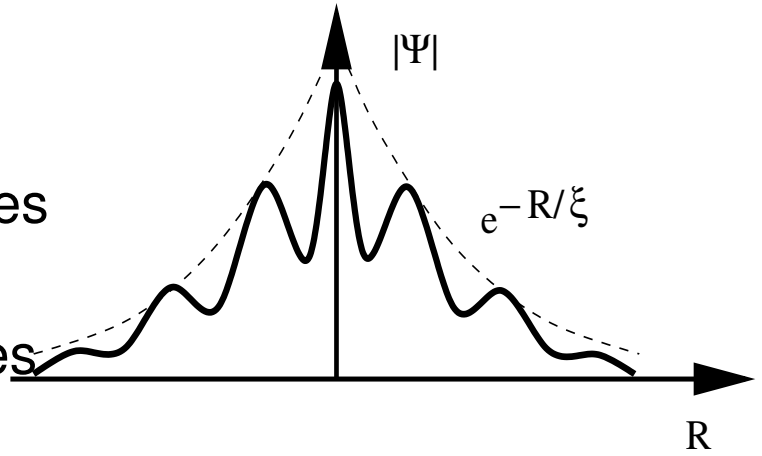


4. Anderson MIT - cont.

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

4. Characterization of Anderson localization

Local Density of States (LDOS)

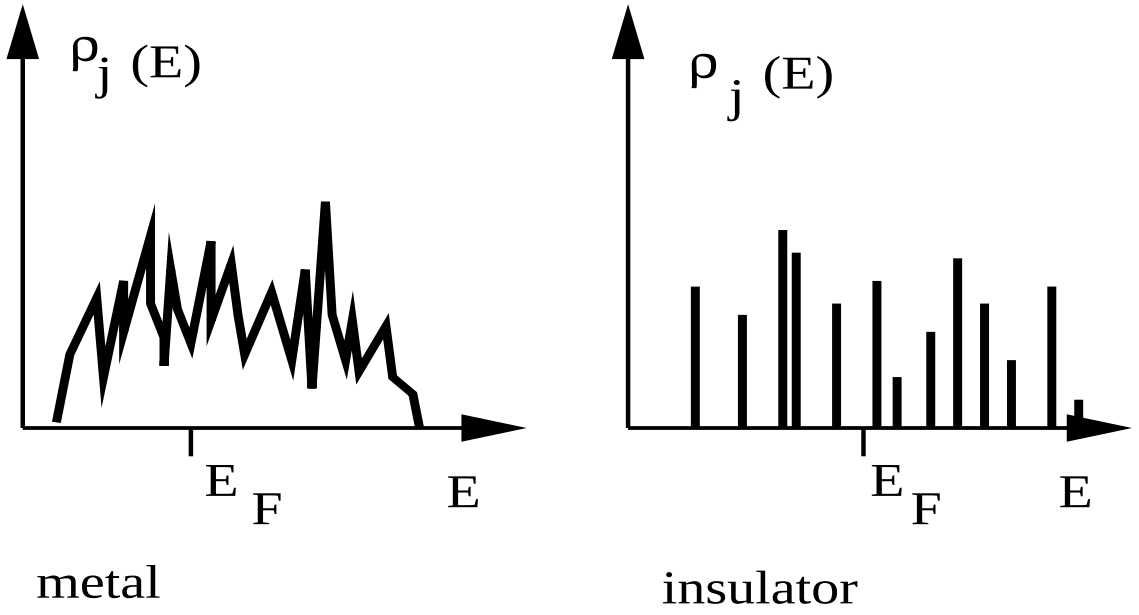
$$\rho_i(E) = \sum_{n=1}^{N} |\Psi_n(r_i)|^2 \delta(E - E_n)$$

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

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

Fermi Golden Rule

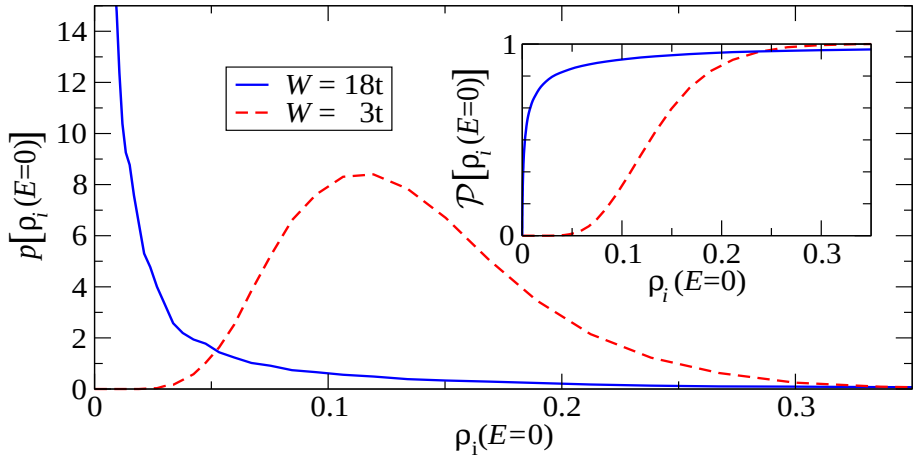
$$\frac{1}{\tau_{\rm esc}} \sim |t_{ji}|^2 \rho_j(E_F)$$



4. 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

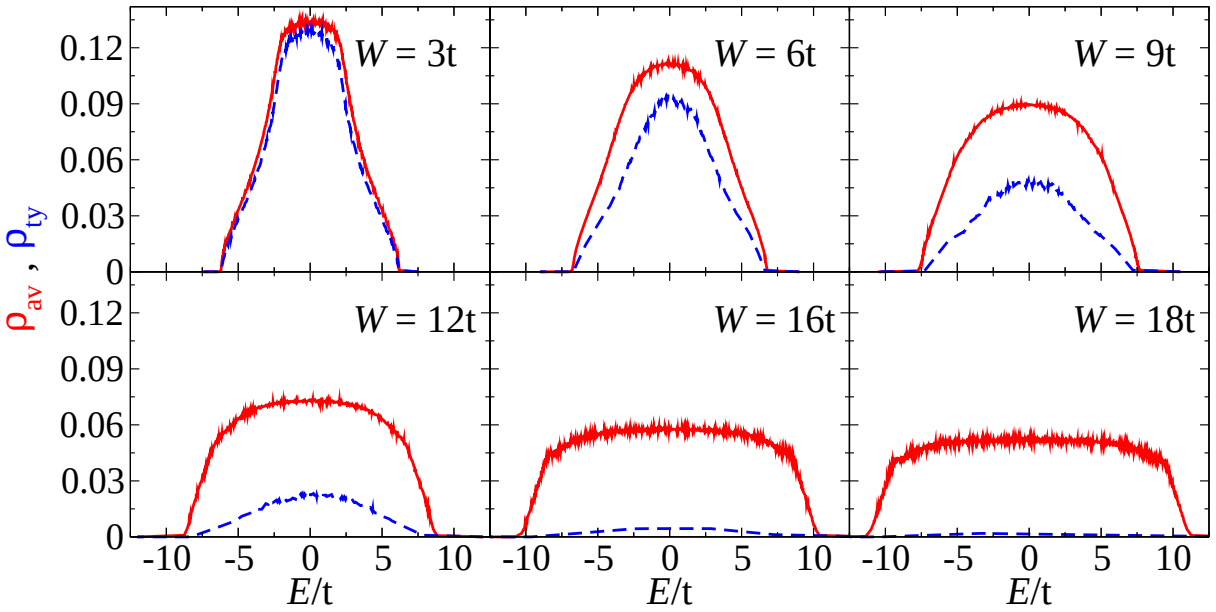
Multifractality - $\langle M^{(k)} \rangle \sim L^{-f(k)}$

Schubert et al. cond-mat/0309015

4. Anderson MIT - cont.

Near Anderson localization typical LDOS is approximated by geometrical mean

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



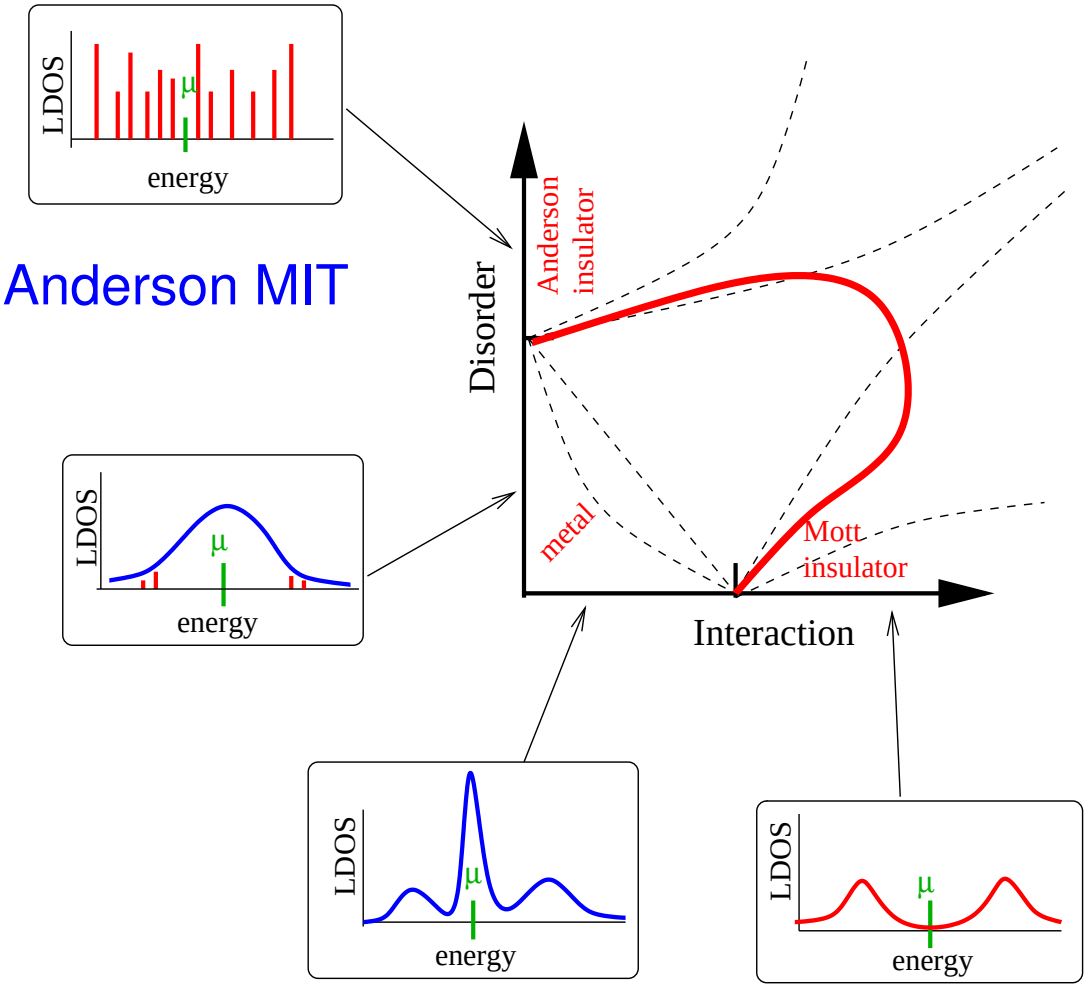
Theorem (F.Wegner 1981):

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

within a band for any finite Δ

Schubert et al. cond-mat/0309015

4. Mott-Anderson MIT

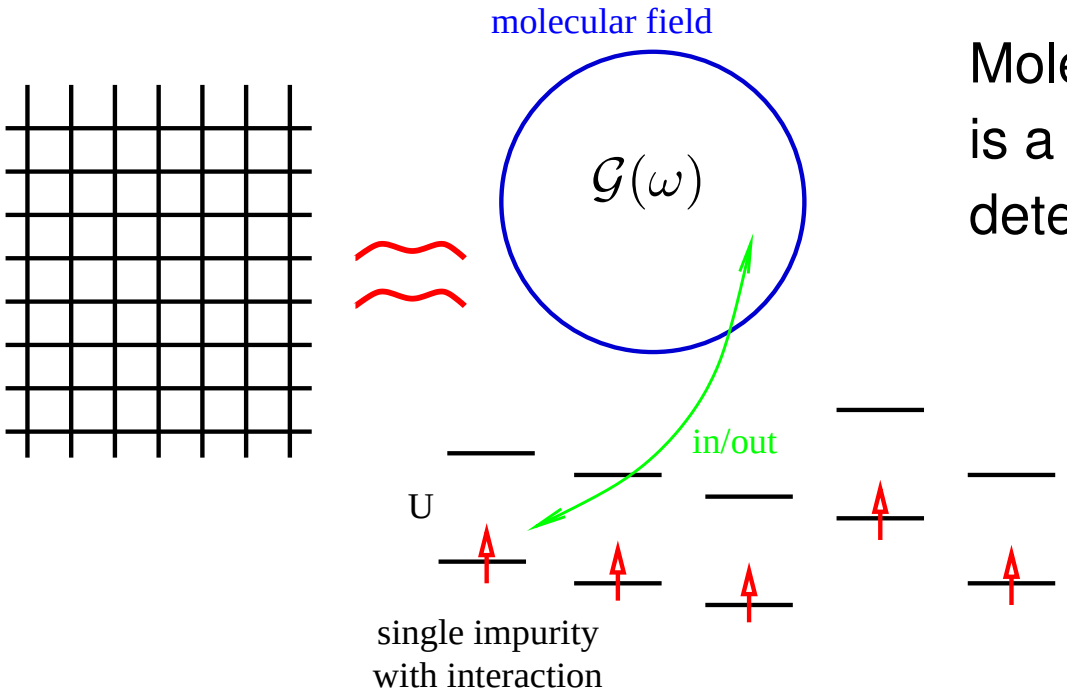


Interaction and disorder compete with each other stabilizing the metallic phase against the occurring one of the insulators

4. Dynamical mean-field theory for U and Δ

Byczuk, Hofstetter, Vollhardt 05

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)

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

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

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

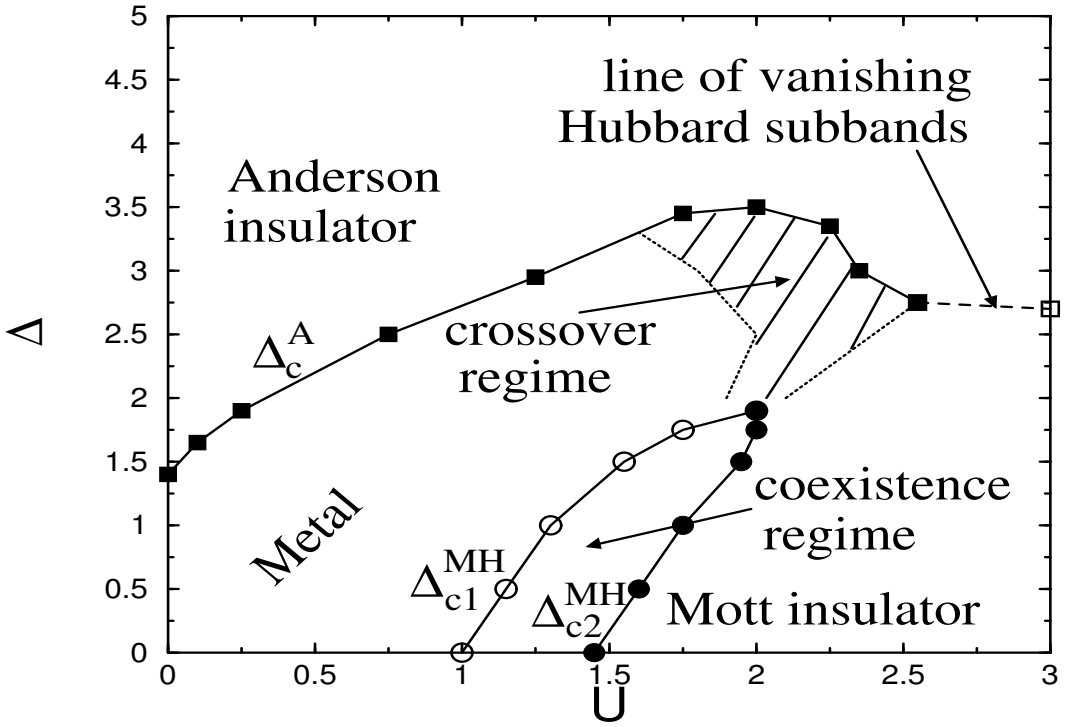
$$G^{-1}(\omega) = \omega - \eta(\omega) - \Sigma(\omega), \quad \eta(\omega) = \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{\omega - \epsilon_{\mathbf{k}}}$$

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

4. Phase diagram for disordered Hubbard model

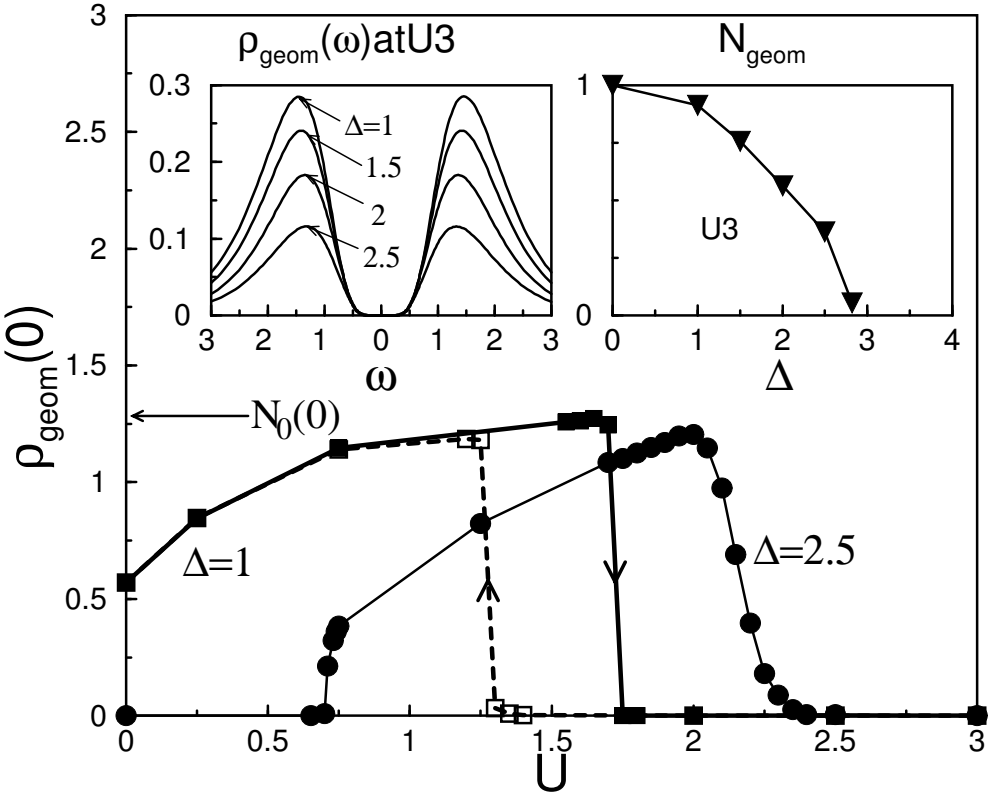
$$N_0(\epsilon) = \frac{2}{\pi D}\sqrt{D^2 - \epsilon^2}; \quad \eta(\omega) = \frac{D^2}{4} G(\omega)$$

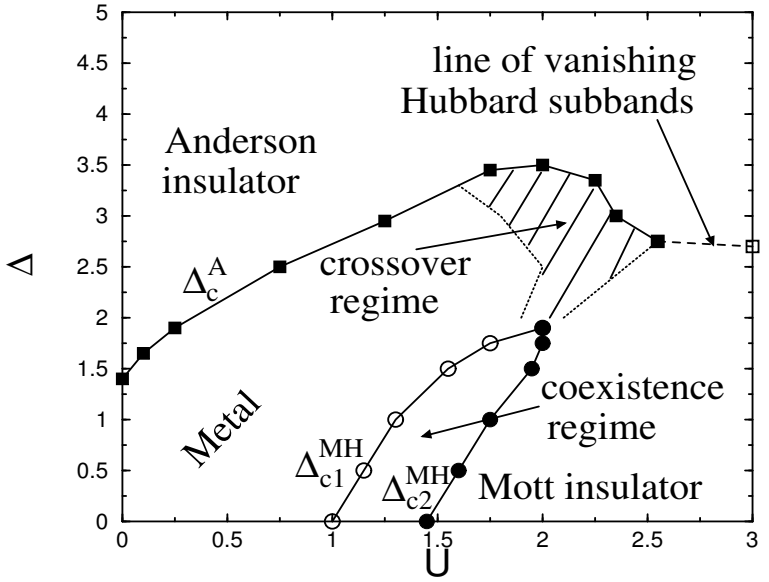
$T = 0$, $n = 1$, $W = 2D = 1$, NRG solver



U - interaction, Δ - disorder

4. Mott-Hubbard MIT in disordered Hubbard model





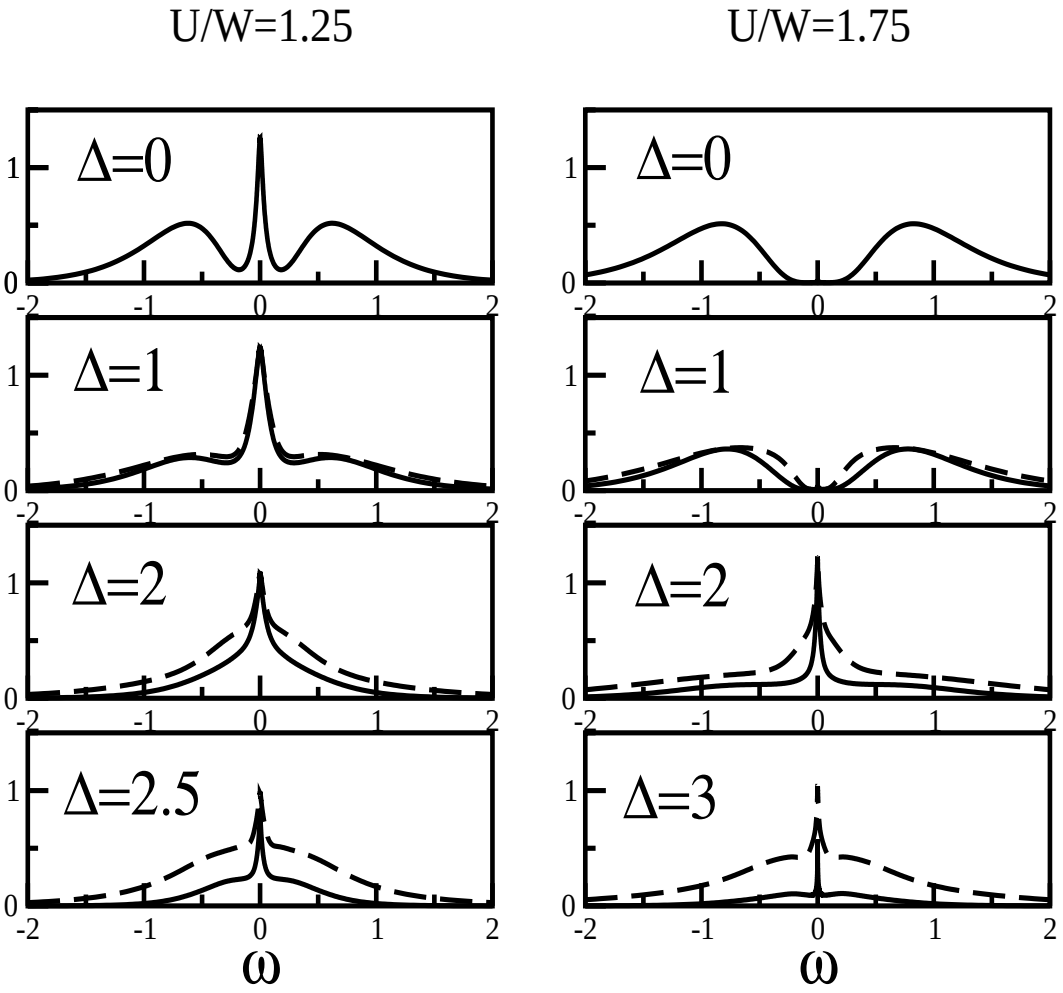
* Luttinger (FL due to U)

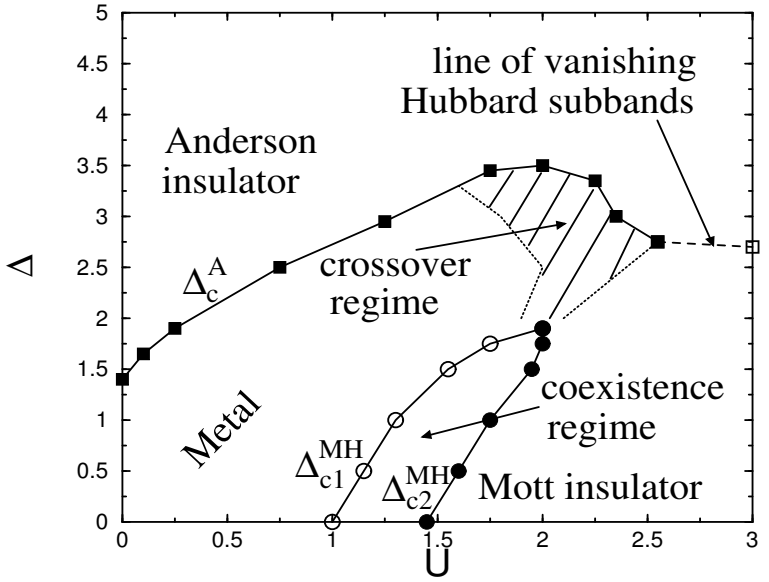
* Hysterisis $\Delta_{c1}(U)$, $\Delta_{c2}(U)$

* Crossover

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

4. Spectral functions in disordered Hubbard model



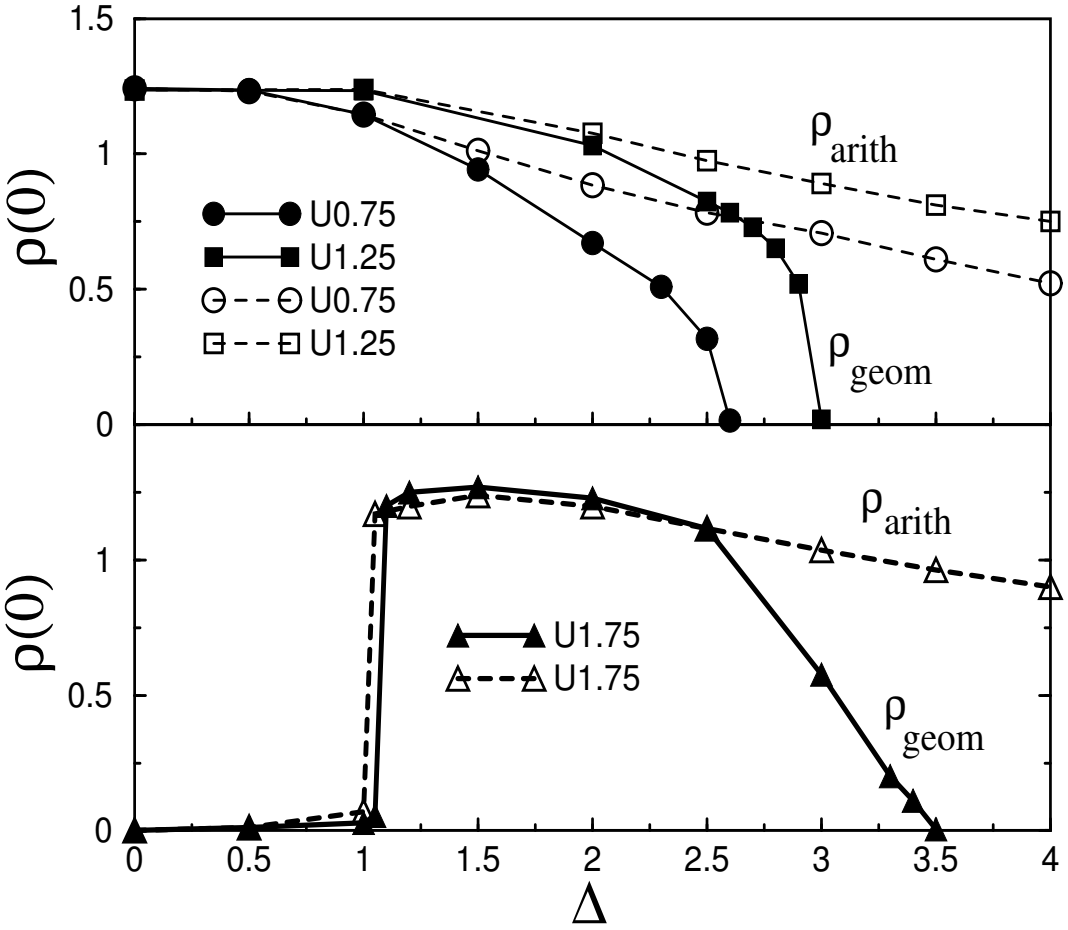


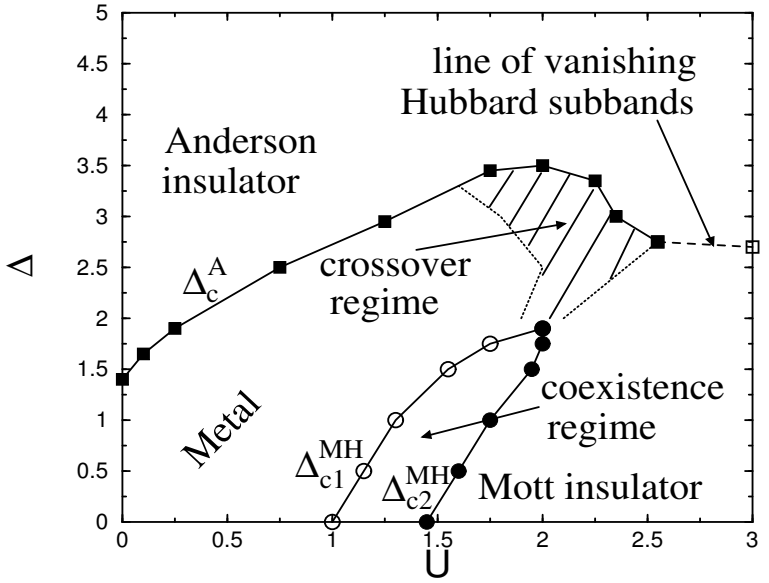
* Redistribution of spectral weight

* 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

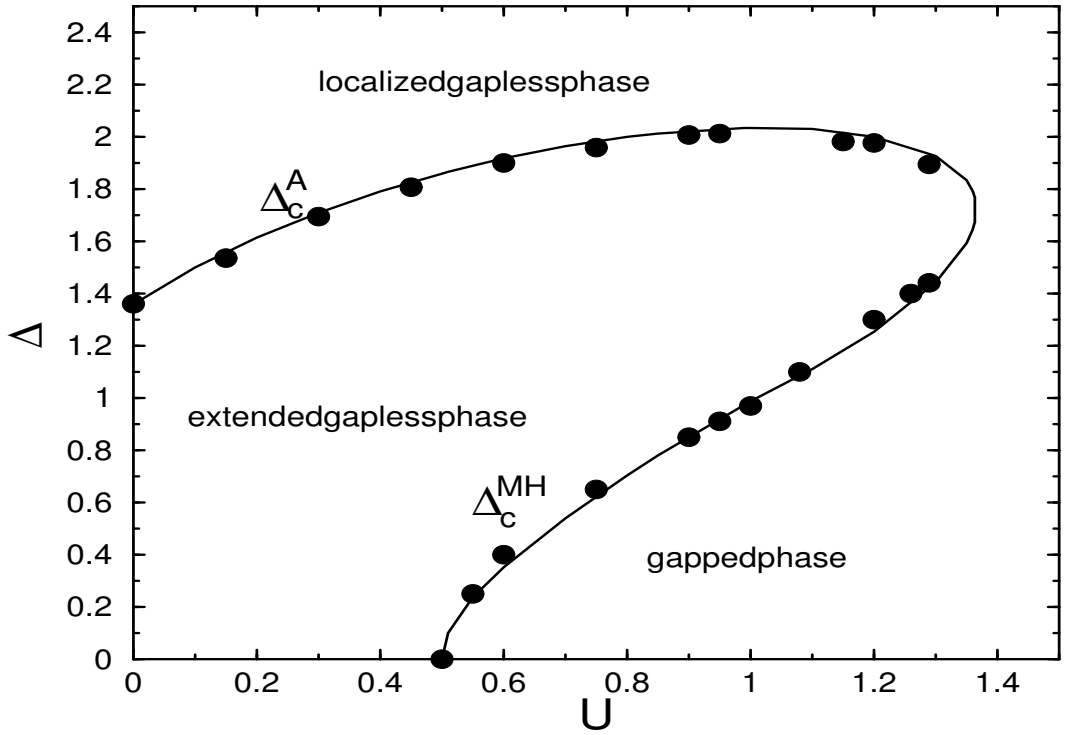
* Adiabatic continuity

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

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

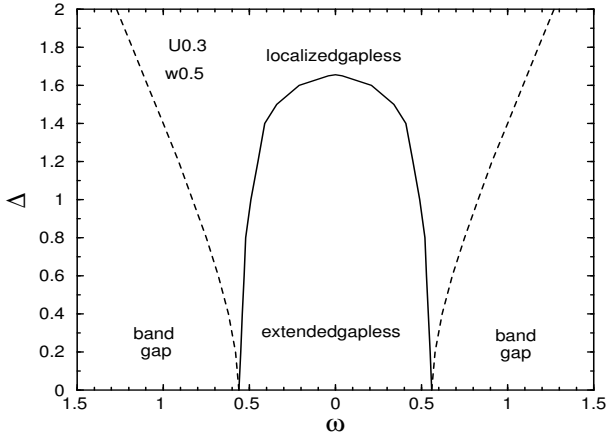


U - interaction, Δ - disorder

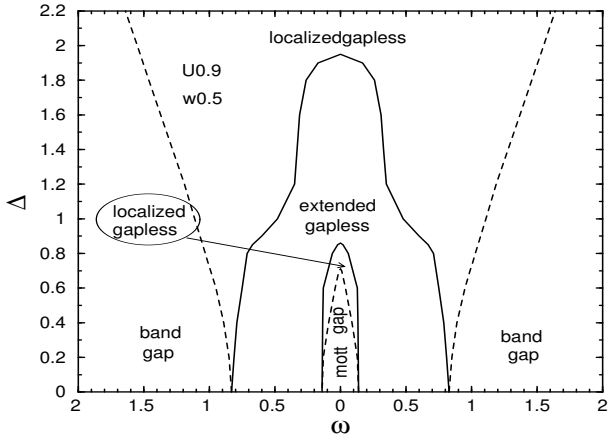
Byczuk 05

4. Spectral phase diagrams

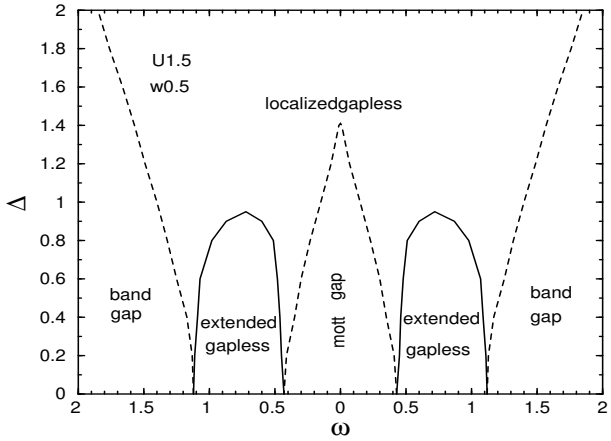
weak coupling $0 < U < W/2$



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



strong coupling $1.36W \lesssim U$



4. 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

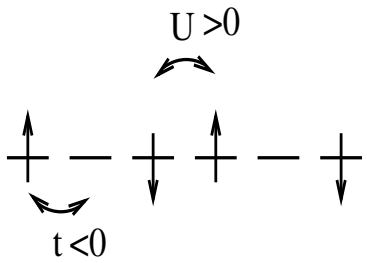
Further projects: AF, CDW phases and Anderson localization in Hubbard and FK models

5. Itinerant Ferromagnetism

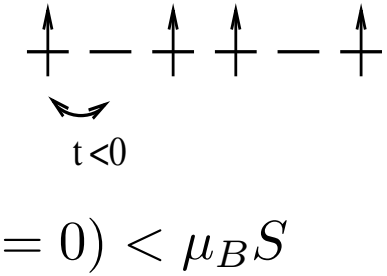
Dynamical way to make FM

To reduce interaction energy electrons prefer FM state

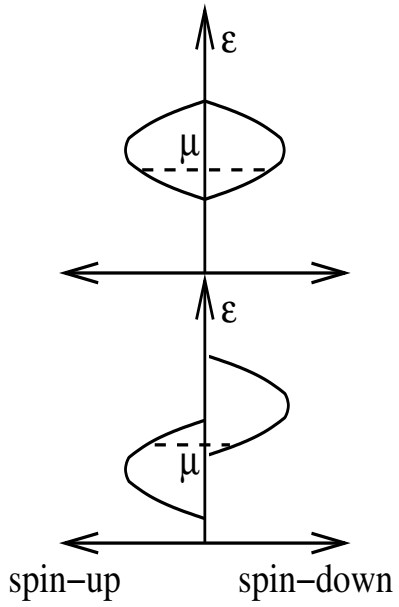
due to Pauli principle $E_{\rm int}^{\rm FM} = 0$



However, $|E_{\rm kin}^{\rm FM}| < |E_{\rm kin}^{\rm PM}|$!



Saturated magnetization $M(T=0) < \mu_B S$



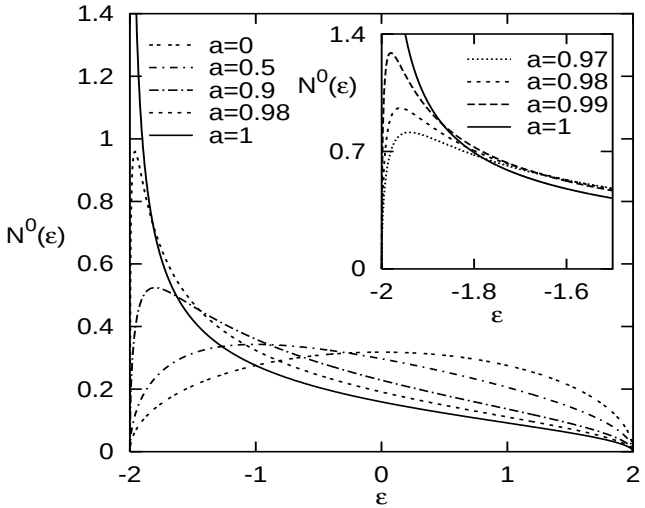
FM stable if $U \gtrsim |t|$ - **intermediate coupling problem !!!**

Many itinerant FM are alloys

5. Route to FM in one-band Hubbard (DMFT)

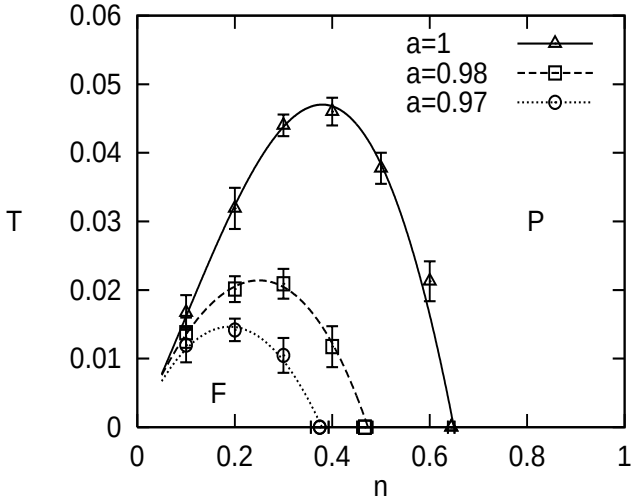
$$H = \sum t a^{\dagger}_{i\sigma} a_{j\sigma} + U \sum n_{i\uparrow} n_{i\downarrow}$$

DOS asymmetry - a

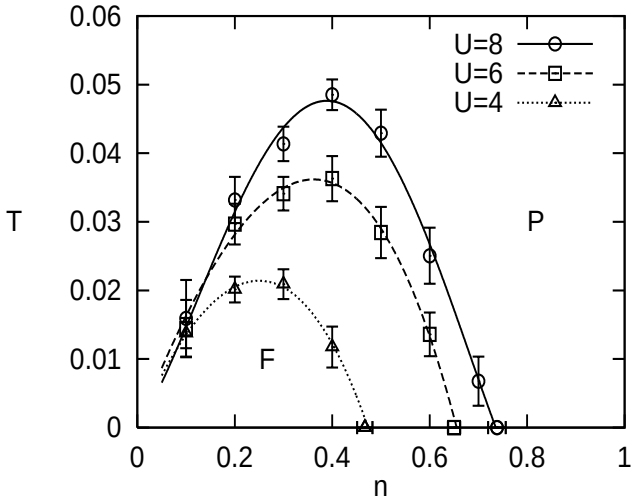


Interaction - U

Wahle et al. 1998



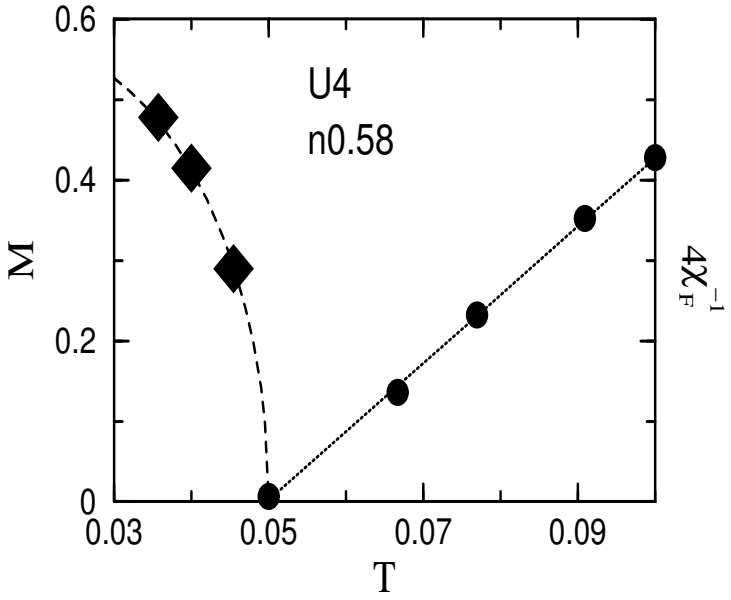
$U = 4$



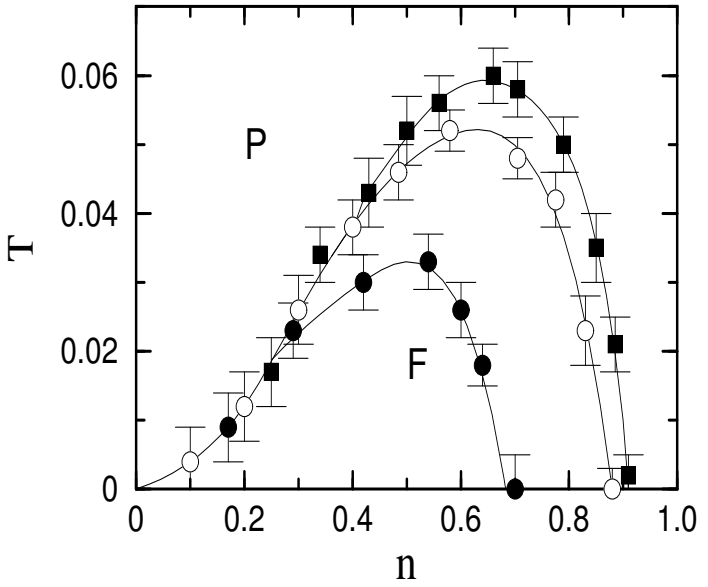
$a = 0.98$

5. FCC $d = \infty$ FM in one-band Hubbard

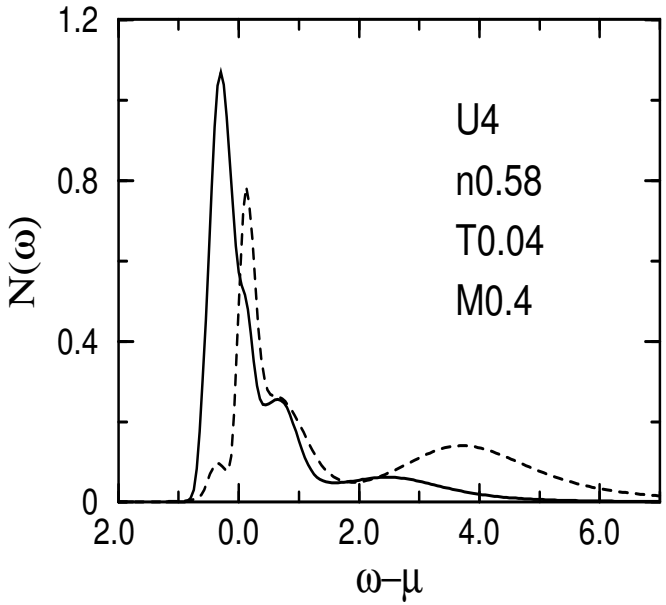
$$N^0(\epsilon) = \frac{\exp[-\frac{1+\sqrt{2}\epsilon}{2}]}{\sqrt{\pi(1+\sqrt{2}\epsilon)}}$$



Ulmke et al. 1998



$U = 2, 4, 5$

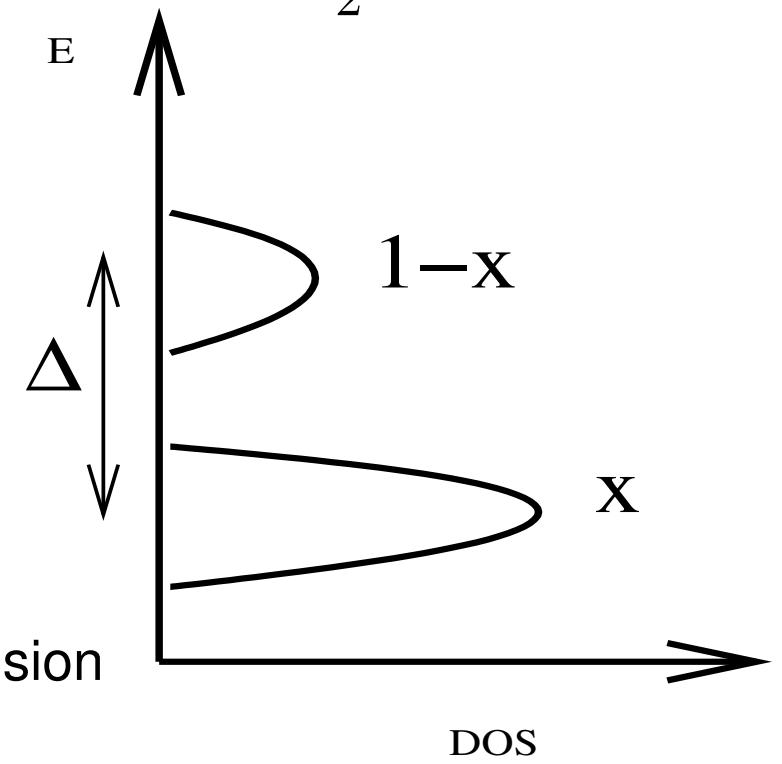


6. Alloy disorder and Band Splitting

Binary alloy disorder (alloys $A_{1-x}B_x$, e.g $Fe_{1-x}Co_x$)

$$\mathcal{P}(\epsilon_i) = x\delta(\epsilon_i + \frac{\Delta}{2}) + (1-x)\delta(\epsilon_i - \frac{\Delta}{2})$$

$$H = \sum_i \epsilon_i + t \sum_{ij} a_i^\dagger a_j$$

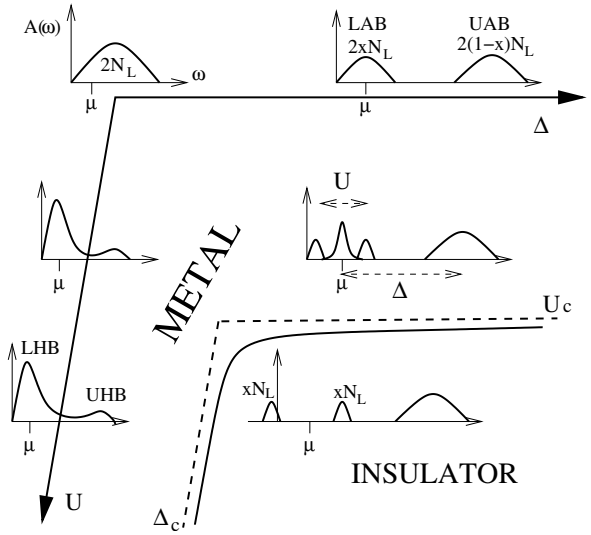


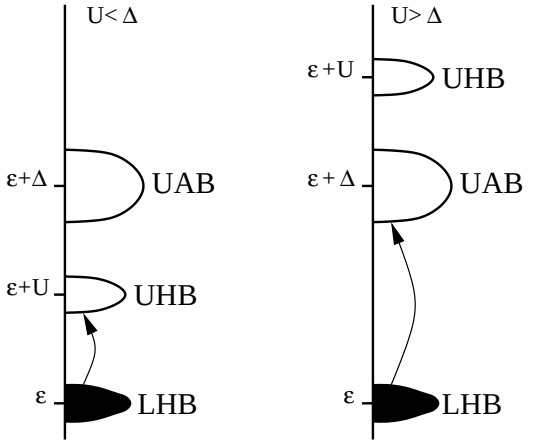
alloy band splitting for $\Delta \gtrsim W$ in any dimension

intermediate "coupling" problem !!!

physical quantity: $O = \int d\epsilon \mathcal{P}(\epsilon) < \hat{O}(\epsilon) >$

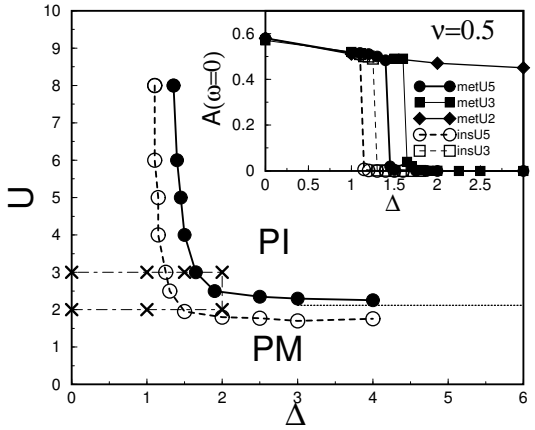
6. Mott–Hubbard at fractional filling

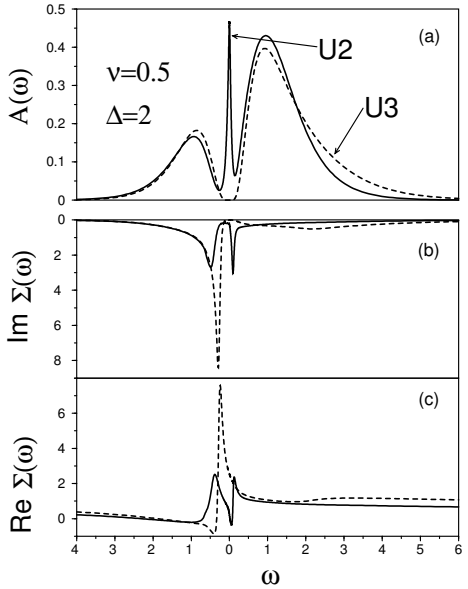




alloy Mott insulator

alloy charge transfer insulator





Byczuk, Hofstetter, Vollhardt 04

7. FM in binary alloy itinerant electrons

Anderson–Hubbard Hamiltonian

$$H = \sum_{ij,\sigma} t_{ij} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \sum_{i\sigma} \epsilon_i \hat{n}_{i\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

where ϵ is random variable with bimodal PDF

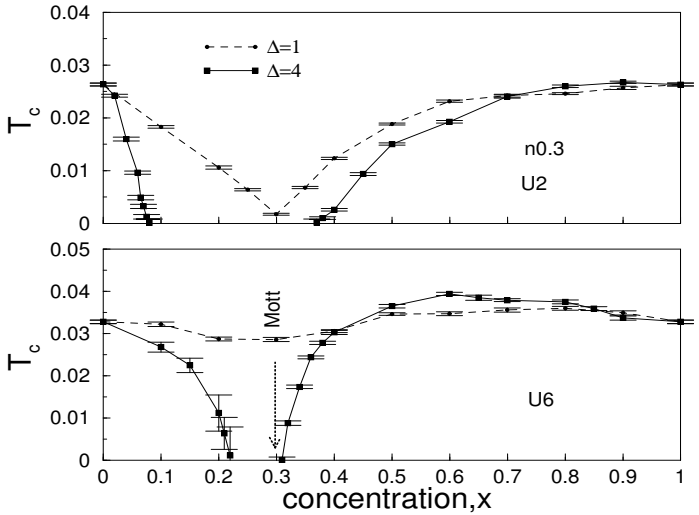
$$P(\epsilon) = x\delta\left(\epsilon + \frac{\Delta}{2}\right) + (1-x)\delta\left(\epsilon - \frac{\Delta}{2}\right)$$

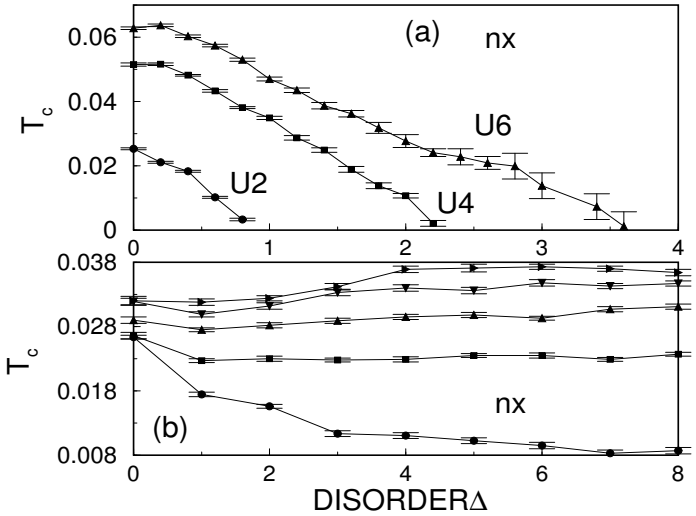
Physical observable averaged arithmetically

$$\langle \cdots \rangle_{\mathrm{dis}} = \int d\epsilon P(\epsilon)(\cdots)$$

$d = \infty$ FCC DOS $N^0(\omega) = \frac{\exp[-\frac{1+\sqrt{2}\omega}{2}]}{\sqrt{\pi(1+\sqrt{2}\omega)}}$ stabilizes FM

7. Curie temperature

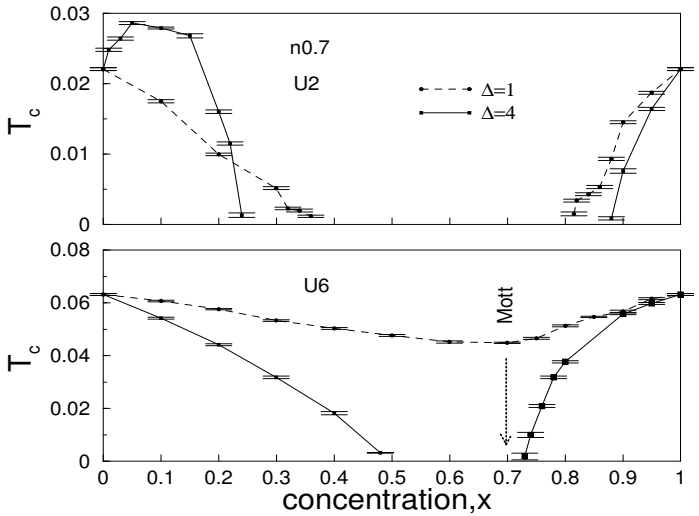


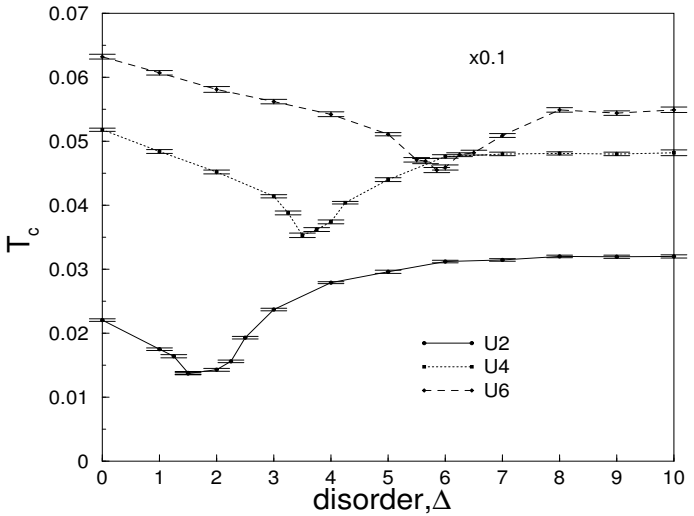


$n = 0.7\ x = 0.5$

$n = 0.3\ x = 0.5$

$T_c(x)$ increases !!! at some cases



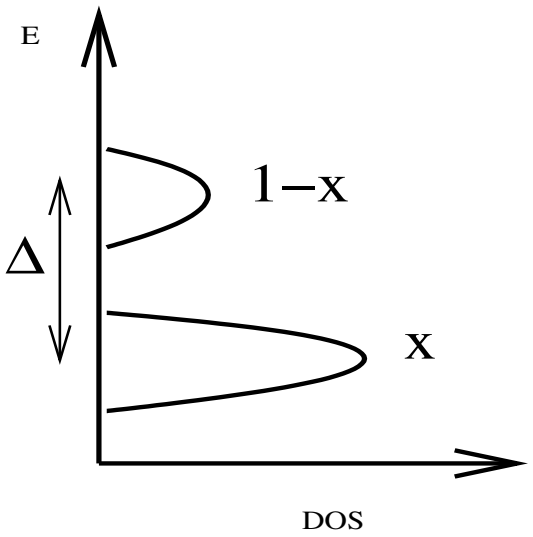


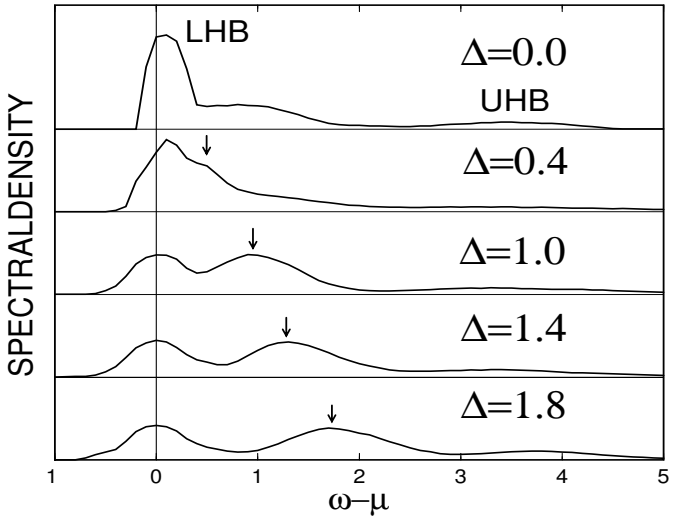
$n = 0.7$

Byczuk, Ulmke, Vollhardt 03; Byczuk, Ulmke 05

7. Is there an alloy band splitting at $U > 0$?

$U = 4,\ n = 0.3,\ n = 0.5,\ T = 0.071$, MEM

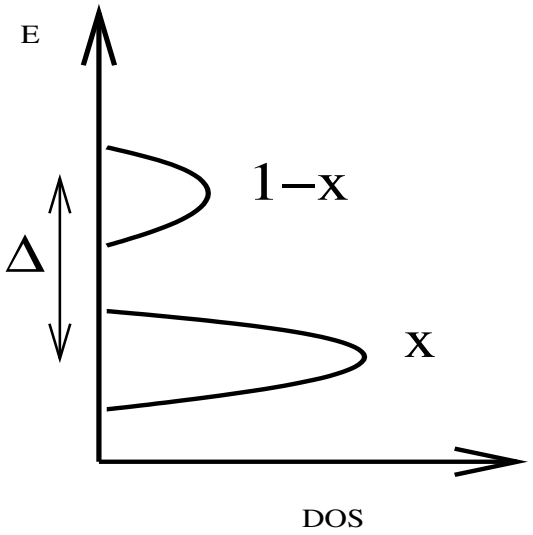


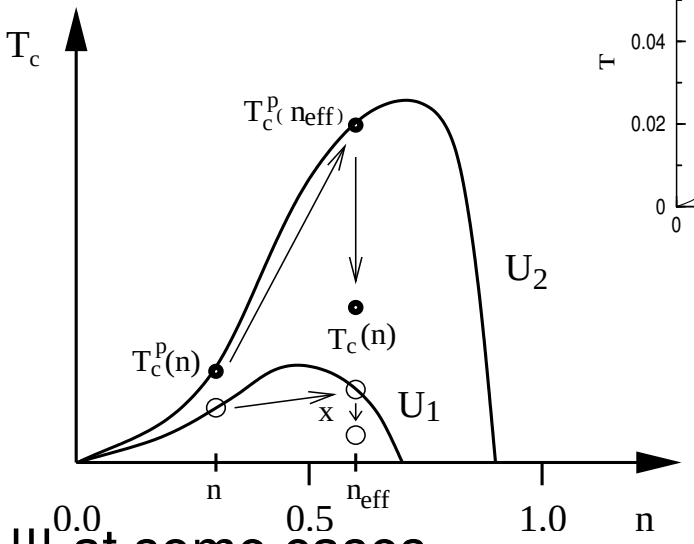


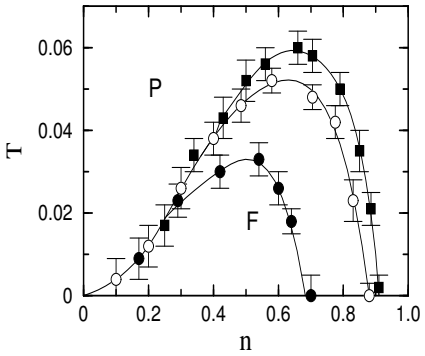
Subtle interplay between Δ and U increases T_c!

7. Why is Curie temperature enhanced?

$$n < 2x \rightarrow n_{\text{eff}} = \frac{n}{x}$$
$$T_c = xT_c^p$$



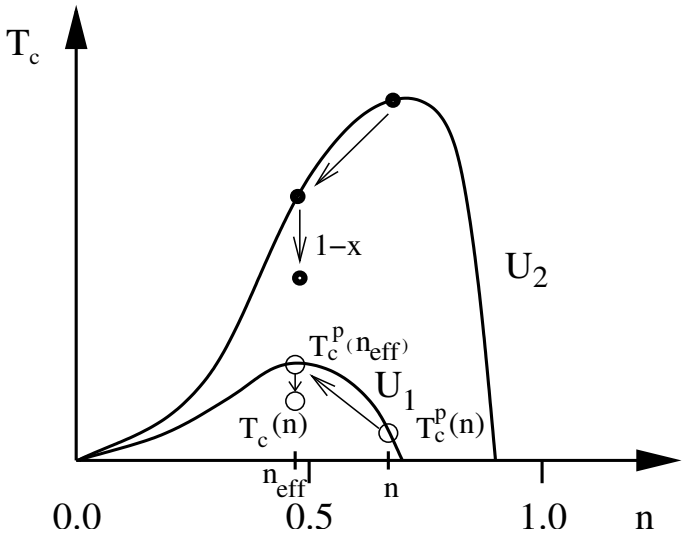




$T_c(x)$ increases !!! at some cases

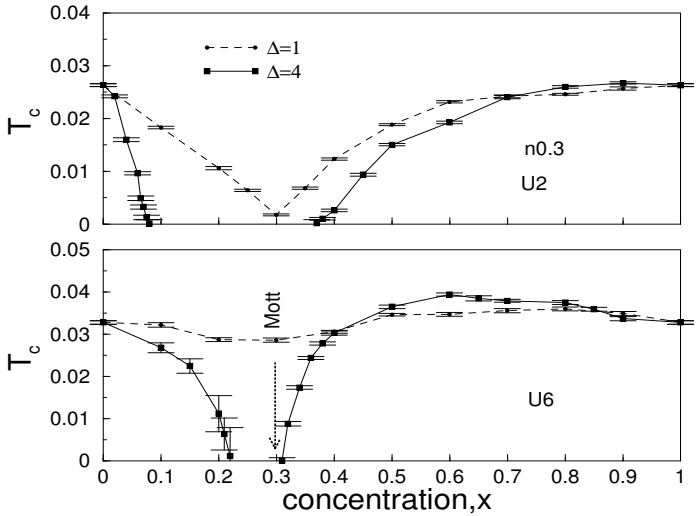
Good for large U

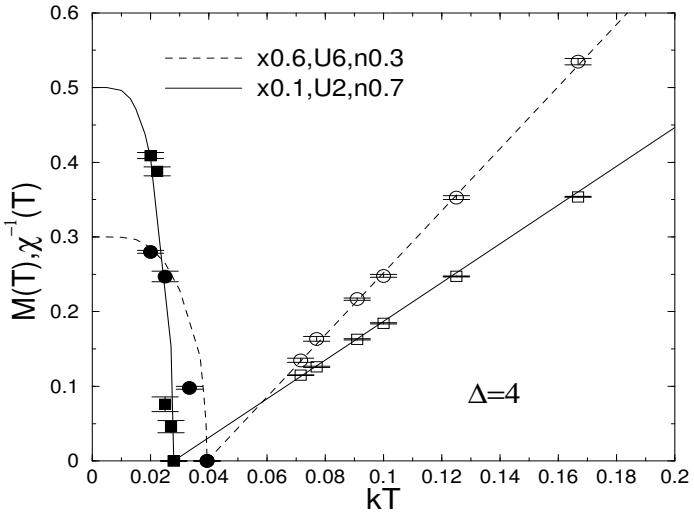
$$n > 2x \rightarrow n_{\text{eff}} = \frac{n-2x}{1-x}$$
$$T_c = (1-x)T_c^p$$



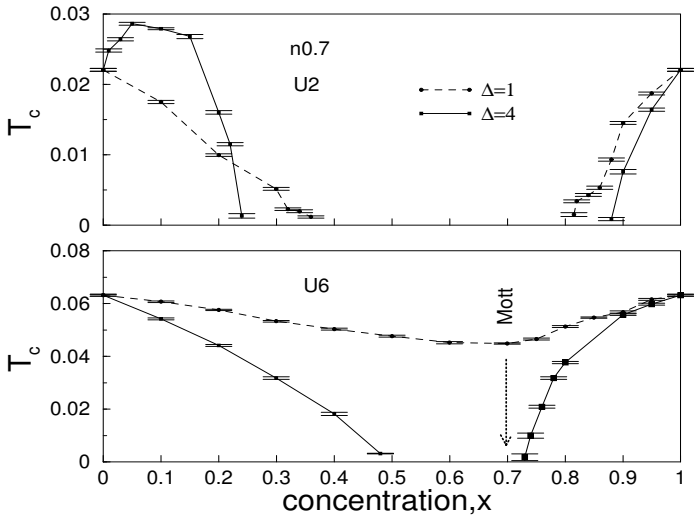
Good for small U

7. Magnetization and Curie-Weiss law





If $\Delta \gg W$ and $n < 2x \rightarrow M_s = n$ but $n > 2x \rightarrow M_s = n - 2x$



$$\frac{M(T)}{M_s} = \tanh[\frac{T_c M(T)}{T M_s}]$$

$\chi(T) = \frac{C}{T - T_c}$, where $C \approx M_s$

$\frac{C_1}{C_2} = 0.623$ close to $\frac{3}{5}$

7. Summary of MIT and FM in binary alloy systems

- New collective effects induced by correlation and disorder
- Possibilities of T_c increase in binary alloy ferromagnet
- New Mott–Hubbard metal–insulator transition at $n \neq 1$
- Alloy Mott insulator vs. Alloy charge transfer insulator
- Alloy concentration controlled Mott MIT

Outlook

- $T_c(x)$ - QPT ? 2nd vs 1st order PT ?
- Multi-band Hubbard model, role of Hund and exchange coupling, which from our findings are generic for many orbitals ?
- Material specific models ?? LDA+DMFT+disorder ???