Dynamical Mean-Field Theory of Strongly Correlated Electron Systems

Krzysztof Byczuk

Institute of Theoretical Physics

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Collaboration

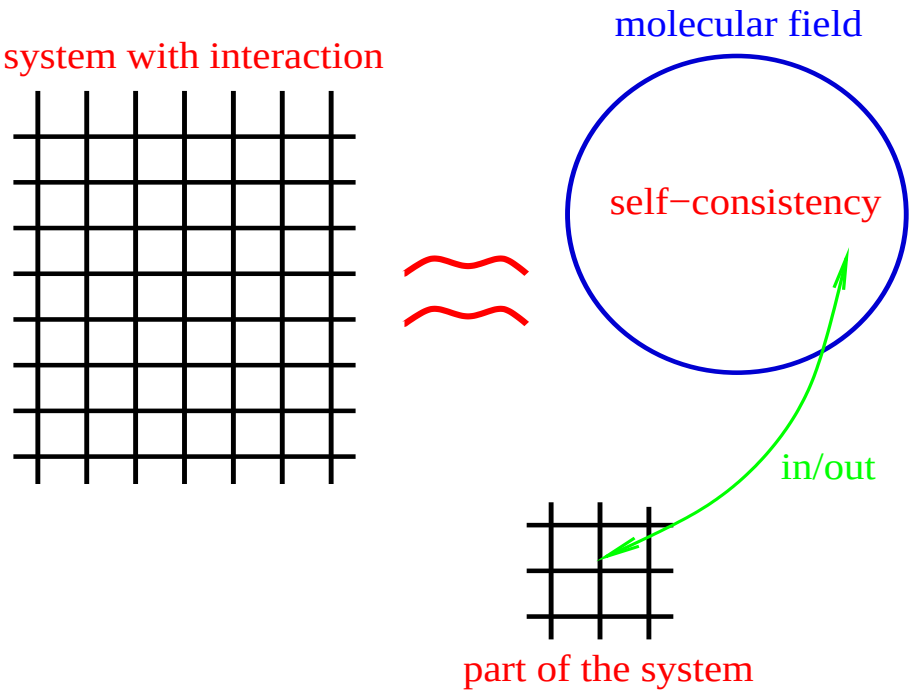
- Martin Ulmke - FGAN - FKIE, Wachtberg, Germany
- Walter Hofstetter - Harvard University, USA
- Dieter Vollhardt - Augsburg University, Germany

Outline of the talk

1. Strongly correlated systems
2. Experimental examples
3. Hubbard model
4. Dynamical mean-field theory
5. Metal-insulator transition
6. Paramagnet-ferromagnet transition
7. Perspectives

Goal of the lecture

In a mean-field theory we approximate the interacting system by introducing an effective (molecular, Weiss) field, determined self-consistently, and allowing the constituent of the system to interact with this field



e.g.

$$\hat{\mathcal{H}} = J \sum \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \approx \sum \mathbf{H}_{\text{eff}} \cdot \hat{\mathbf{S}}_i$$
$$\mathbf{H}_{\text{eff}} = J \sum \langle \hat{\mathbf{S}}_j \rangle$$

In the Dynamical Mean-Field Theory (DMFT) the effective field is a dynamical quantity (time dependent)

Standard view on electrons in crystals

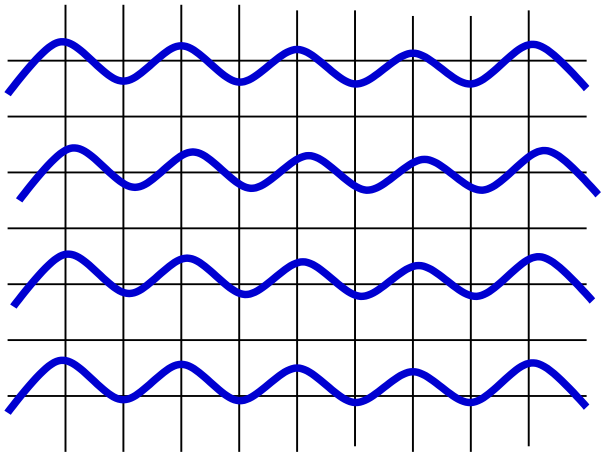
Bloch theorem: electrons in a periodic potential

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \mathbf{u}_{\mathbf{k}}(\mathbf{r})\mathbf{e}^{\mathbf{ik}\cdot\mathbf{r}}$$

with

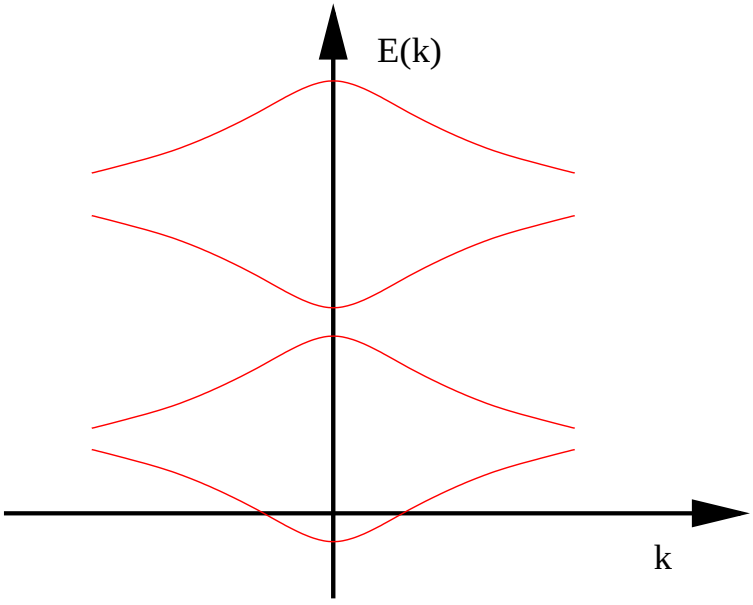
$$u_{\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{\mathbf{k}}(\mathbf{r})$$

There are bands of allowed energies $E(\mathbf{k})$



$\Delta\mathbf{p} = 0$

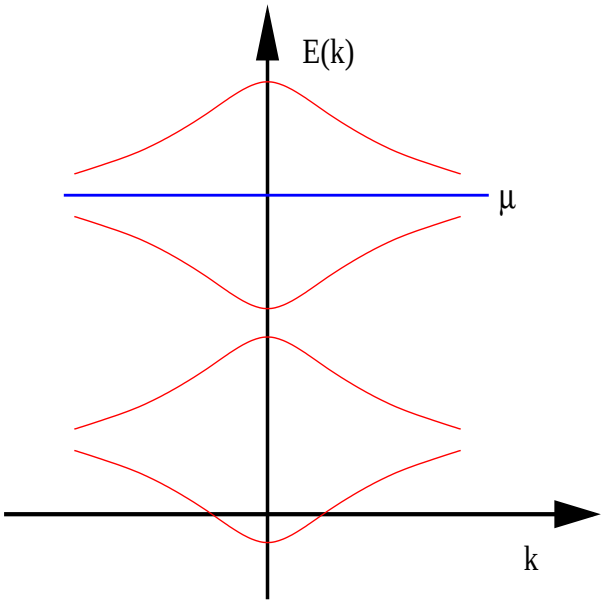
good quantum number



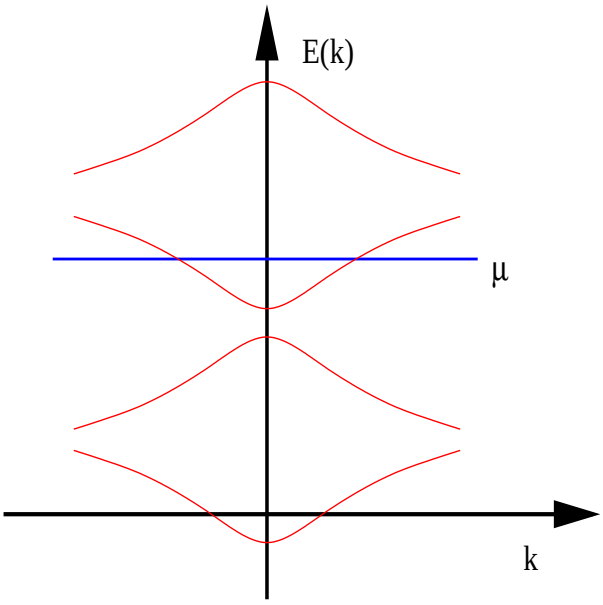
Metals and insulators

Band filling: $n = \frac{N_e}{N_a}$

- Band insulator (gaped) if $n = 0,\ 2,\ 4,\ \ldots$ (is even) closed shells
- Metal (gapless) if $n \neq 0,\ 2,\ 4,\ \ldots$ (is not even) open shells



insulator $T = 0$



metal $T = 0$

Coulomb interaction

- Long range part of Coulomb interaction always present
- In metals it is screened
- It leads to renormalization of the electrons
- Instead of the electrons the theory contains weakly interacting quasiparticles
- Landau Fermi liquid theory

It is not the end of the physics!

When interaction becomes important

Compare the kinetic energy

$$t_{ij} = \int d_3r\ \Phi_i(\mathbf{r})^* \left[-\frac{\nabla^2}{2m} + V(\mathbf{r}) \right] \Phi_j(\mathbf{r})$$

with the potential energy

$$U = \int d_3r d_3r'\ \Phi_i^*(\mathbf{r}) \Phi_i^*(\mathbf{r}') \frac{e}{|\mathbf{r} - \mathbf{r}'|} \Phi_i(\mathbf{r}') \Phi_i(\mathbf{r})$$

on a lattice of ions labeled by $i (\equiv \mathbf{R}_i)$ and j.

When

$$\frac{U}{|t_{ij}|} \gtrsim 1 \quad ?$$

Material ingredient

s and p valence orbitals have large effective radius

d and f valence orbitals have small effective radius

$$\frac{U}{|t_{ij}|} \ll 1$$

$$\frac{U}{|t_{ij}|} \gtrsim 1$$

Compounds with transition metal or rare earth elements are strongly correlated electron systems

Canonical example: V_2O_3

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

Phase diagram

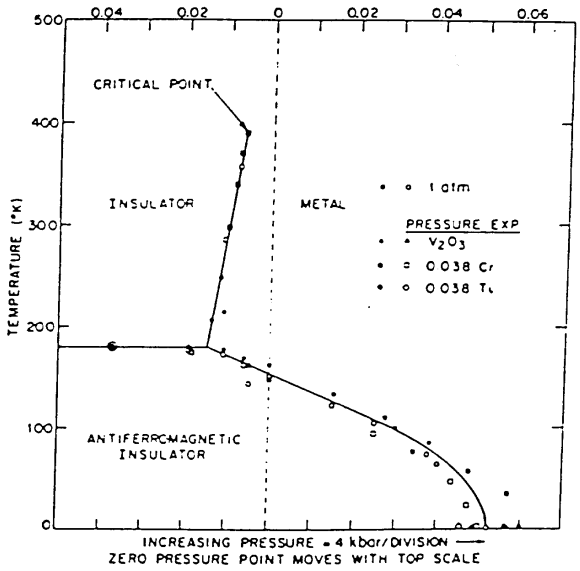
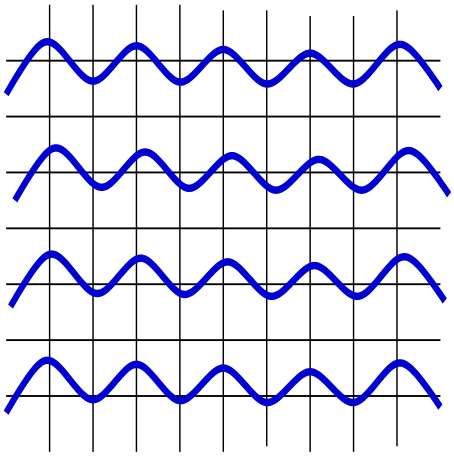


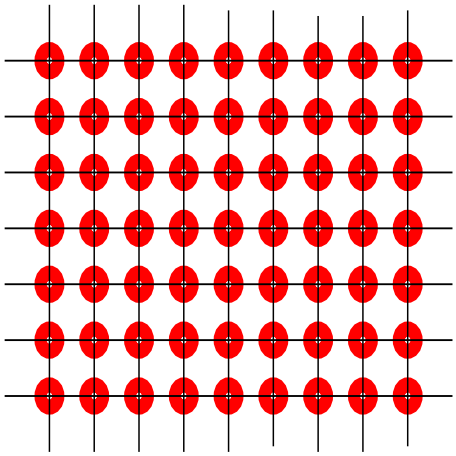
Fig. 23

Metal-insulator transition seen in experiment

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

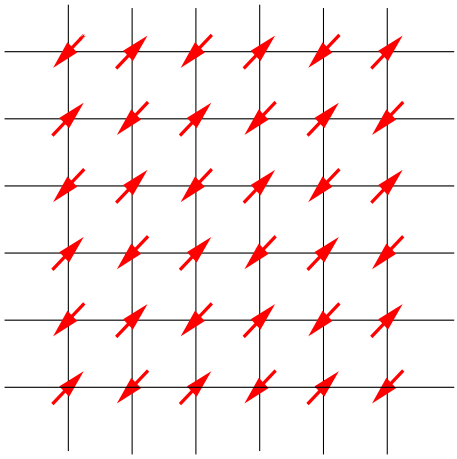


$U \ll |t_{ij}|,\ \Delta \mathbf{p} = 0$



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

Antiferromagnetic Mott insulator

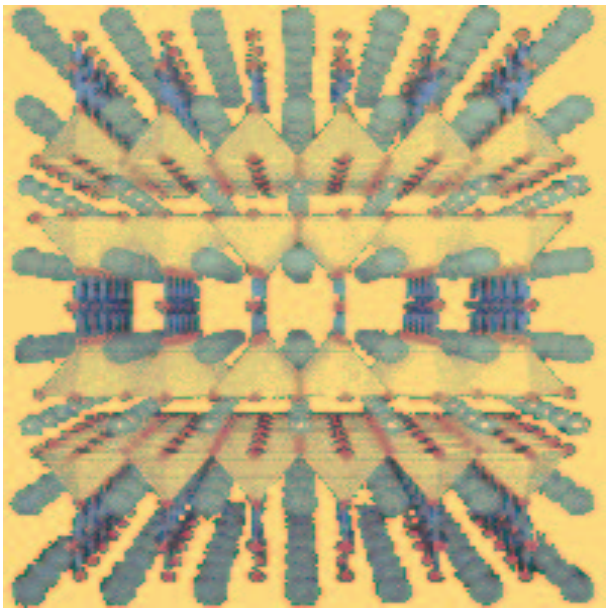


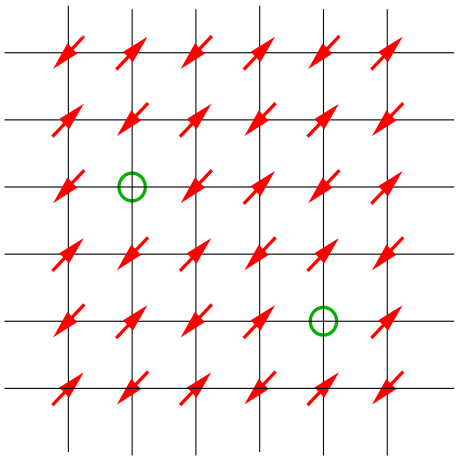
Mott-Hubbard metal-insulator transition is a typical intermediate coupling problem

$$U_c \approx |t_{ij}|$$

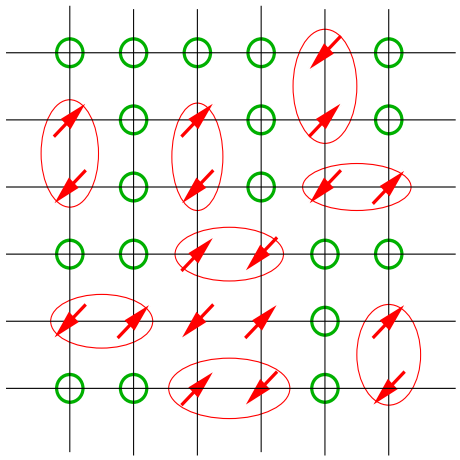
High-temperature superconductors as doped Mott insulators[1]

e.g. $La_{1-x}Sr_xCuO_4$, (La^{+3}, Sr^{+2})





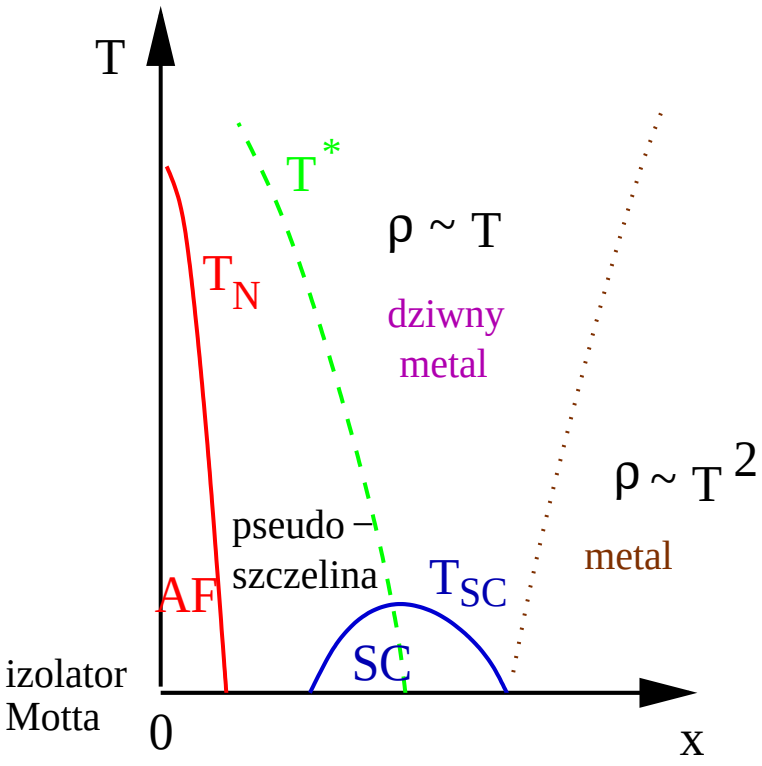
Doped insulator



RVB singlet state

[1] Bednorz, Müller 86

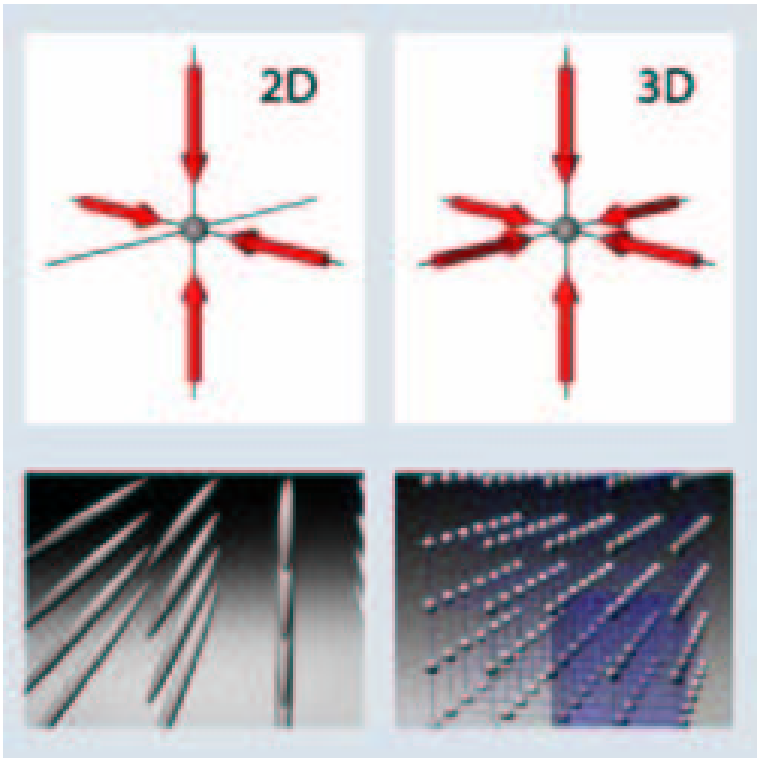
Phase diagram of high-temperature superconductors



Both U and t_{ij} are important but dimensionality $(d = 2)$ is crucial as well

Mott transition in a Bose system[2]

Using an atomic trap and standing waves of light one can create an optical lattice filled with bosonic (fermionic, not yet) atoms

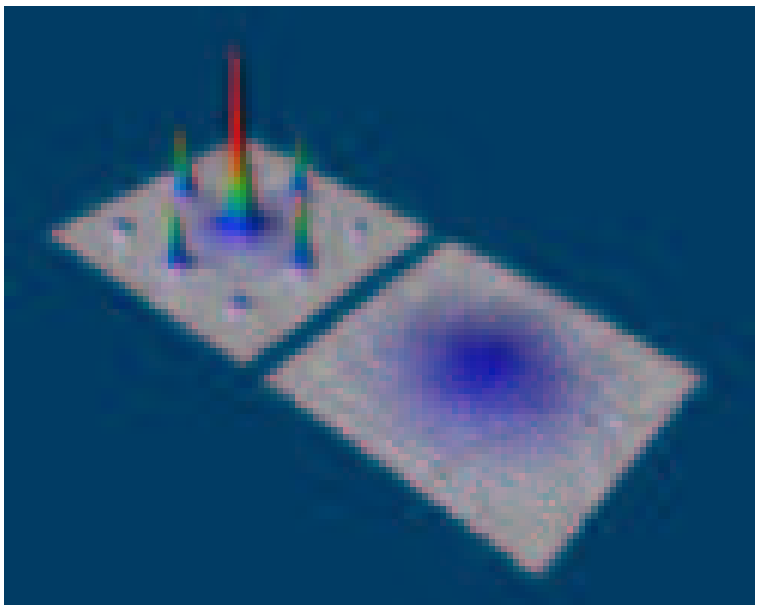


[2] Greiner et al. 02

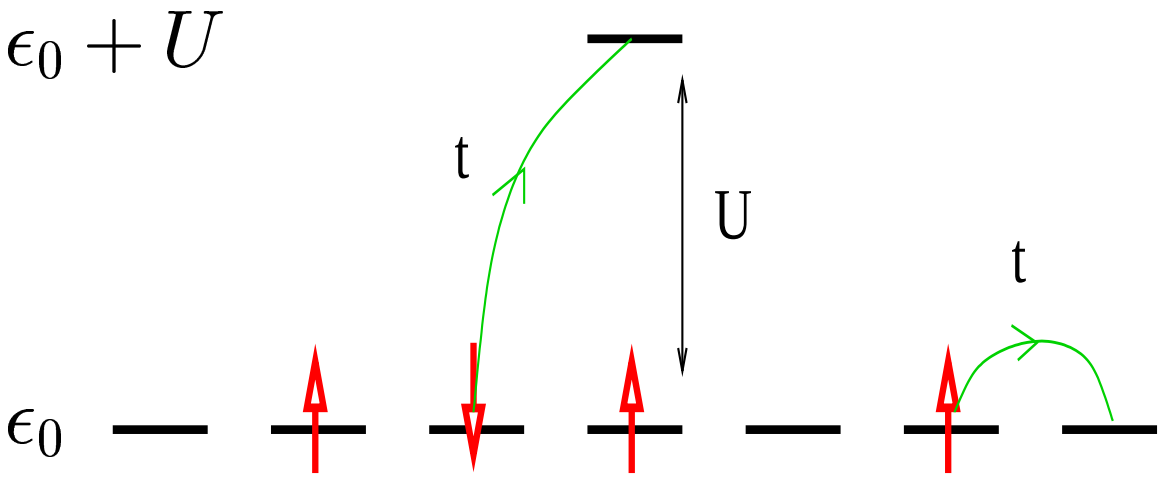
Two possible ground states

- Bose-Einstein condensate if $U \ll |t_{ij}|$
- Mott insulator if $U \gg |t_{ij}|$

Tuning t_{ij} or U a superfluid - Mott - insulator transition observed



Hubbard model to capture right physics[3]



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

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

[3] Hubbard 63

From $d = \infty$ to DMFT[4]

To have well defined limit $d = \infty$ we have to rescale

$$t \to \frac{t^*}{\sqrt{2d}}$$

$$t' \to \frac{t'^*}{2d}$$

etc., BUT

$$U \to U$$

Then the propagator (Green function)

$$G^0_{ij} \sim O\left(\frac{1}{d^{\frac{||R_i - R_j||}{2}}}\right)$$

[4] Mezner, Vollhardt 89

- simplification in $d = \infty$ because all connected, irreducible perturbation theory diagrams in position space collapse

- self-energy

$$\Sigma_{ij}(\omega) = \delta_{ij}\Sigma_{ii}(\omega)$$

  local quantity depending only on time (frequency)

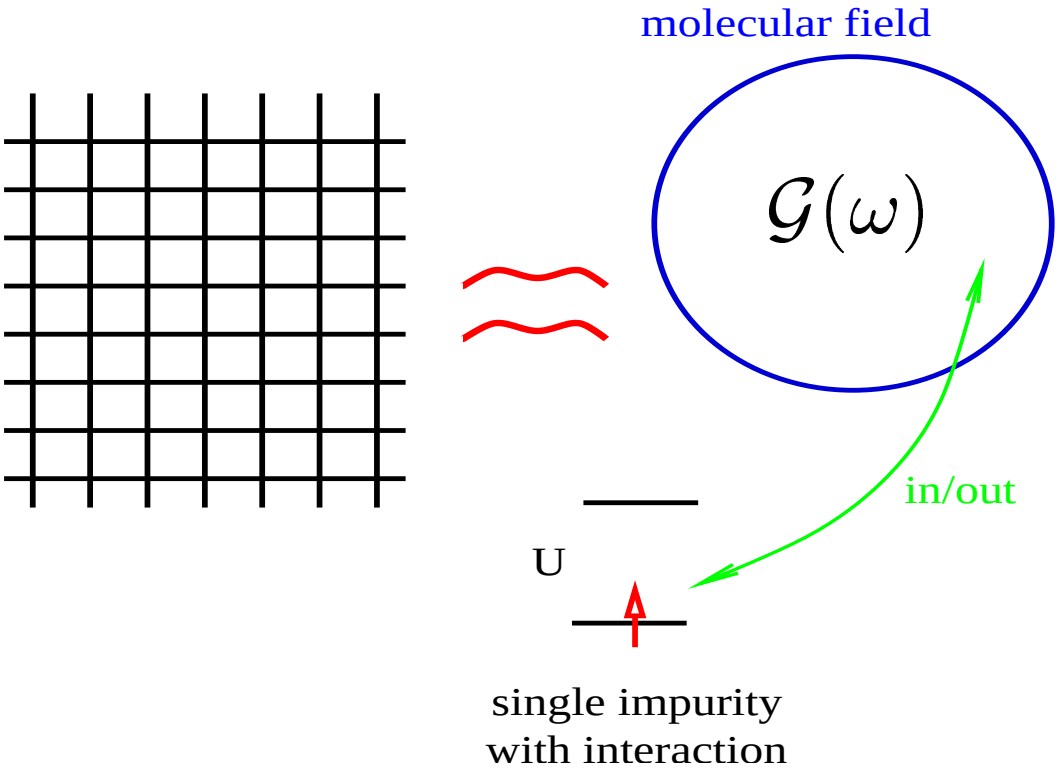
- in momentum space

$$\Sigma(\mathbf{k}, \omega) = \Sigma(\omega)$$

- quantum (local) dynamics survives

Dynamical mean-field theory[5]

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

[5] Kotliar et al., Vollhardt et al.

Dynamical mean-field equations

$$G_\sigma(\tau) = -\int D[c^*, c] c(\tau) c^*(0) e^{-S_{\rm eff}[c^*, c]}$$

where

$$S_{\rm eff}[c^*, c] = \\ -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c^*_\sigma(\tau) \mathcal{G}(\tau - \tau') c_\sigma(\tau') \\ +U \int_0^\beta d\tau n_\uparrow(\tau) n_\downarrow(\tau)$$

and

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

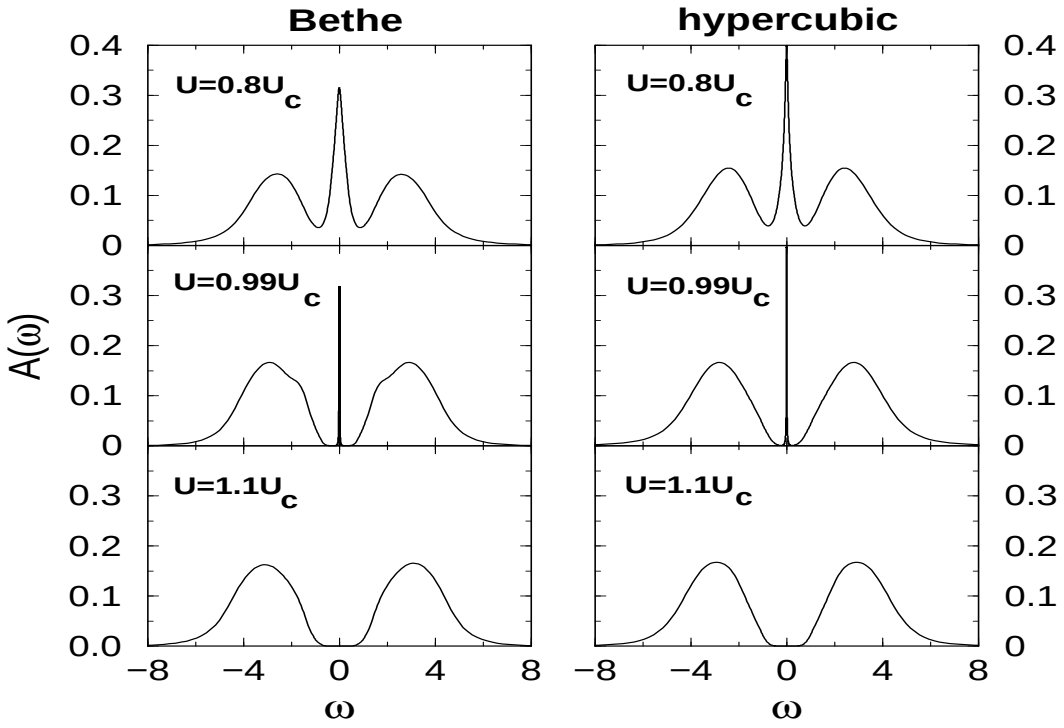
$$G_\sigma(i\omega_n) = \sum_{\mathbf{k}} \frac{1}{i\omega_n + \mu - E(\mathbf{k}) - \Sigma_\sigma(i\omega_n)}$$

Mott transition according to DMFT[6]

quantity to be determined

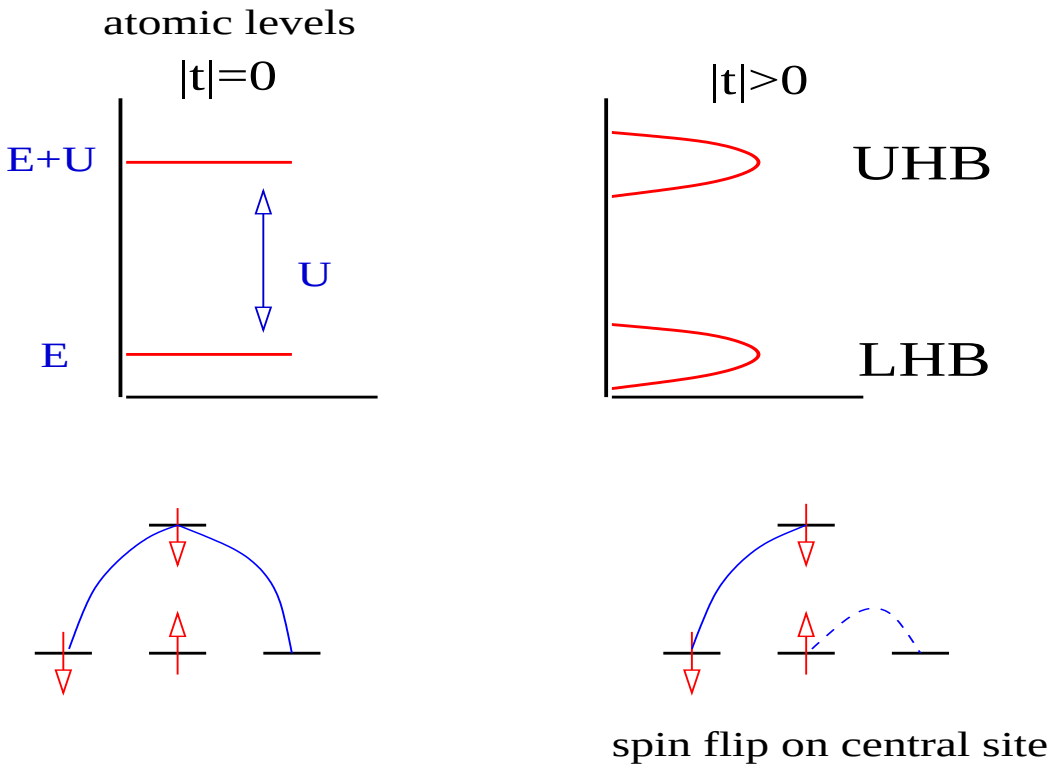
$$A(\omega) = -\frac{1}{\pi}\Im G(\omega)$$

spectral density function
(for $U = 0$ equals to the density of states)



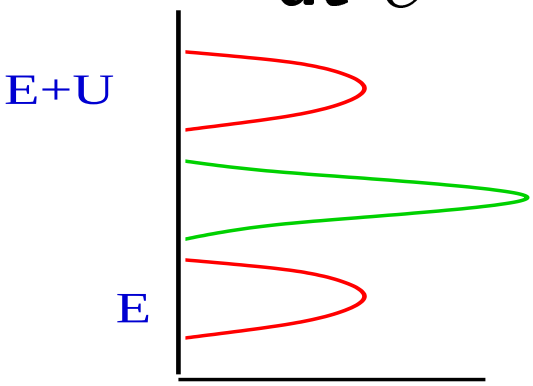
[6] Kotliar et al. 92-96, Bulla, 99

Physical picture, $n = 1$

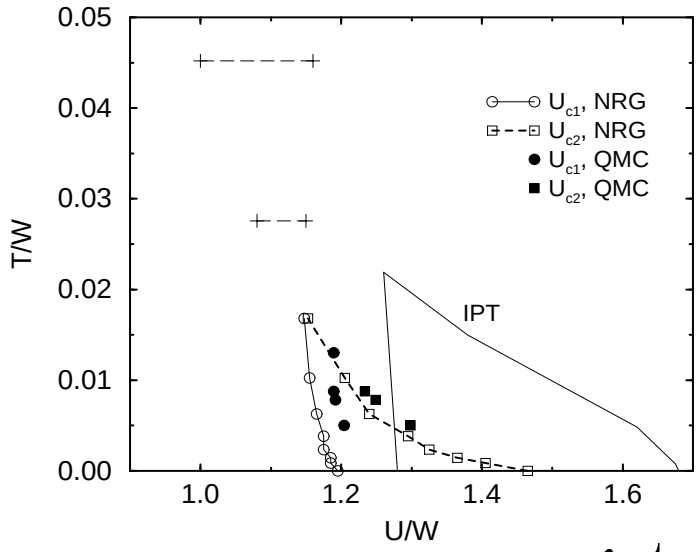


dynamical processes with spin-flips inject states into correlation gap giving a quasiparticle resonance

at $U = U_c$ resonance disapears gaped insulator



Mott transition at $T > 0$[7]



1st-order transition

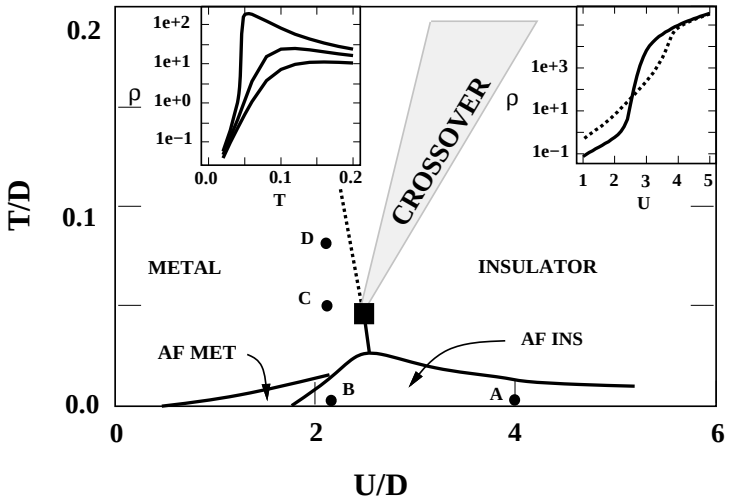


Fig.43

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

Mott transition in disordered systems[8]

Disordered alloy A_xB_{1-x}

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

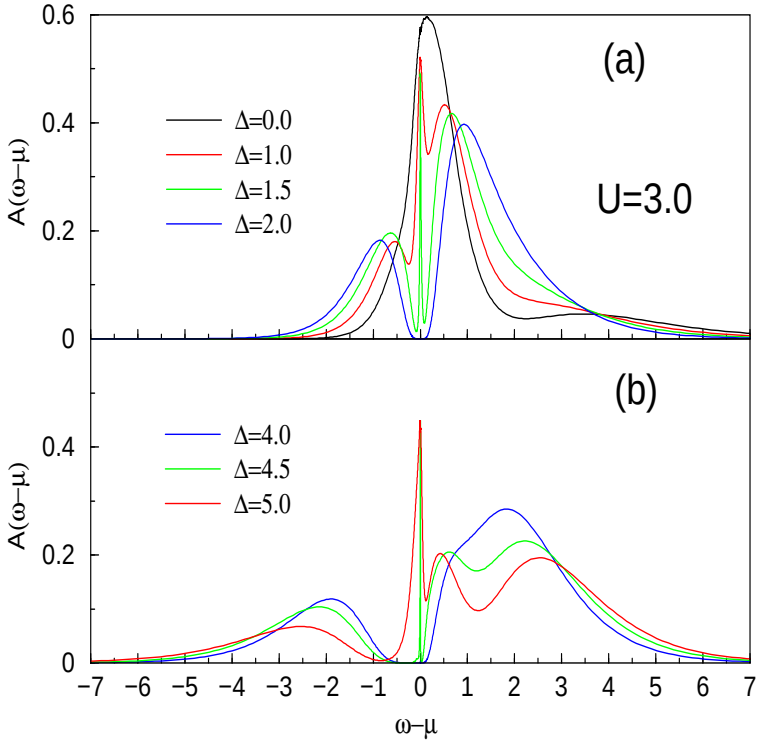
When $\Delta \gg |t_{ij}|$ **the spectral function splits into lower and upper alloy subbands**

Mott transition occurs if U **is strong enough and either lower alloy subband is half-filled** $n = x$ **or upper alloy subband is half-filled** $n = 1 + x$

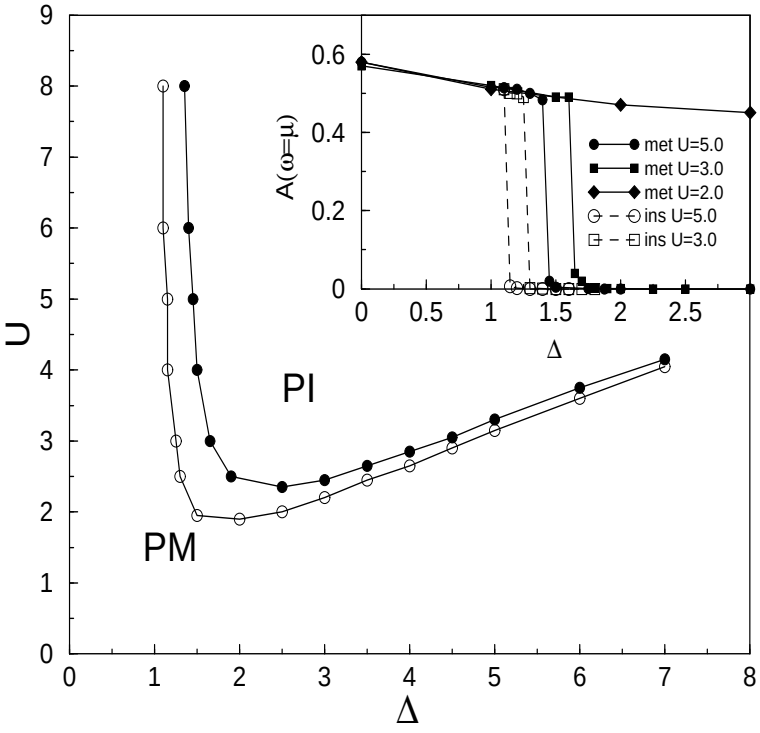
Mott insulator possible for arbitrary filling

[8] Byczuk et al. 02

$n = x = 1/2$



$T = 0$ **DMFT-NRG**

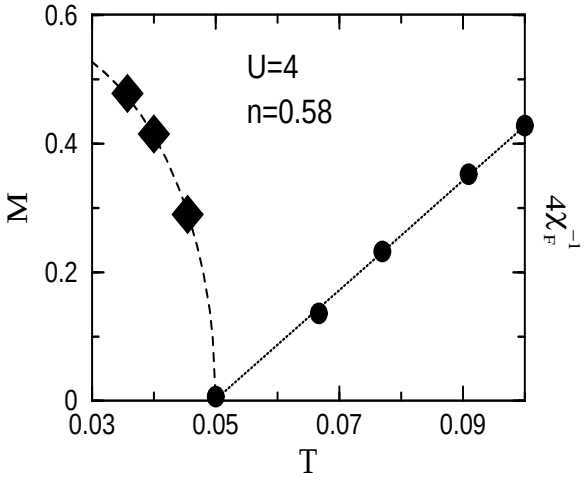


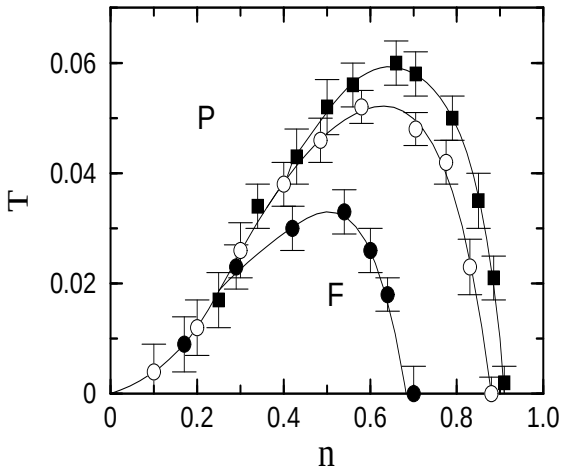
hysteresis, reentrant behavior

Itinerant ferromagnetism[9]

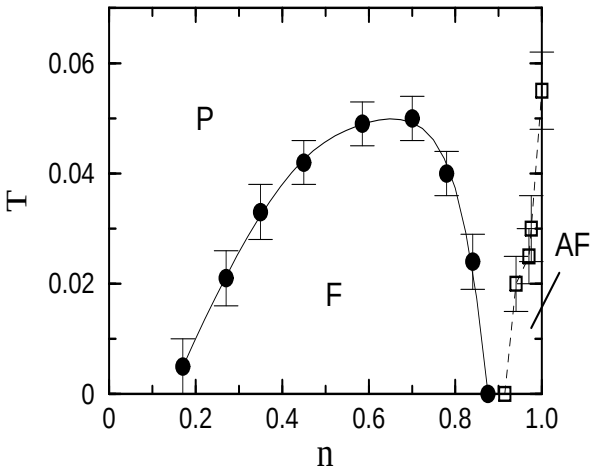
intermediate coupling problem !

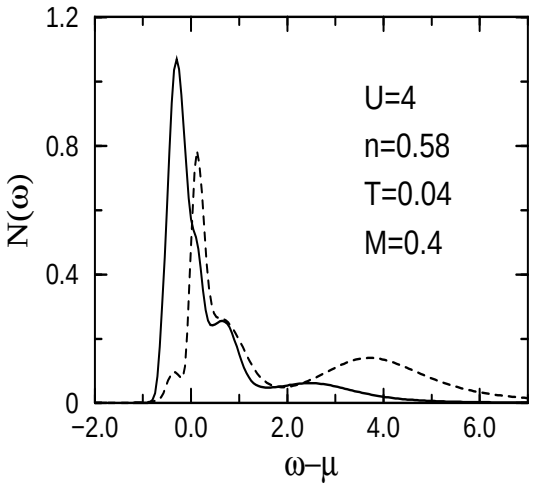
FCC lattice, DMFT-QMC





Curie-Weiss law

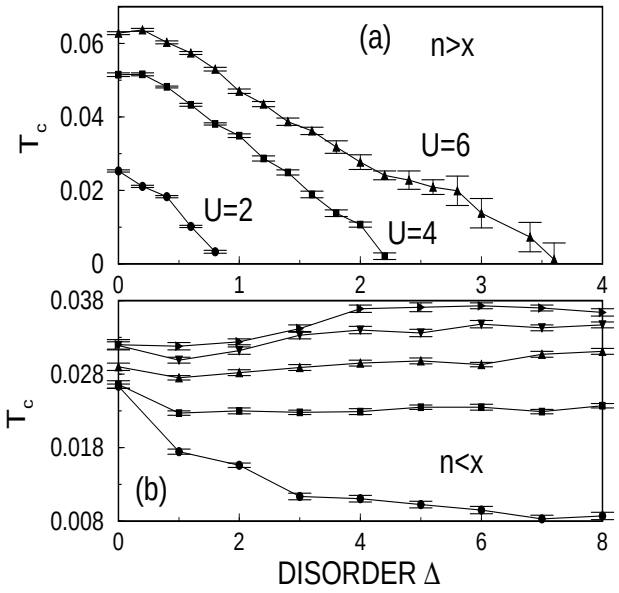




not DFT-SLDA!

[9] Ulmke 98, Byczuk, Vollhardt 02

Itinerant FM in disordered system[10]



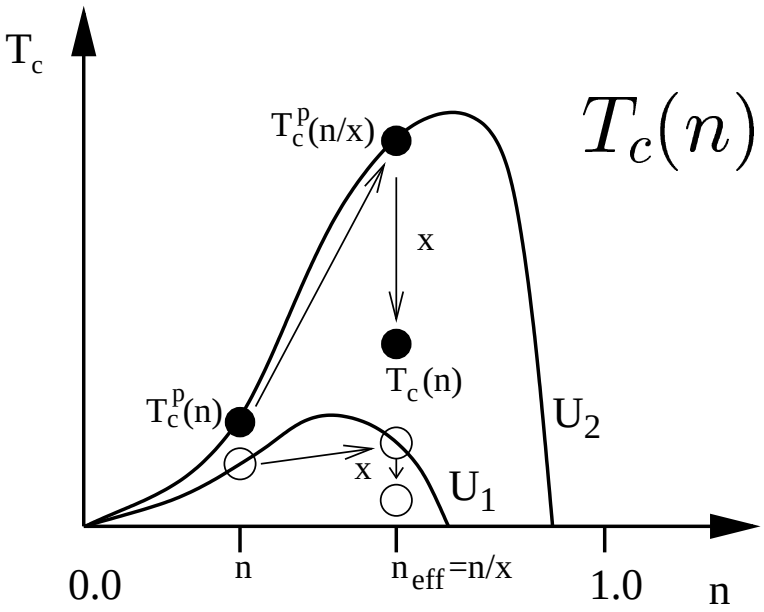
DMFT-QMC

FCC - DOS

$$n = x = 1/2$$

$$U = 2, 3, 4, 5, 6$$

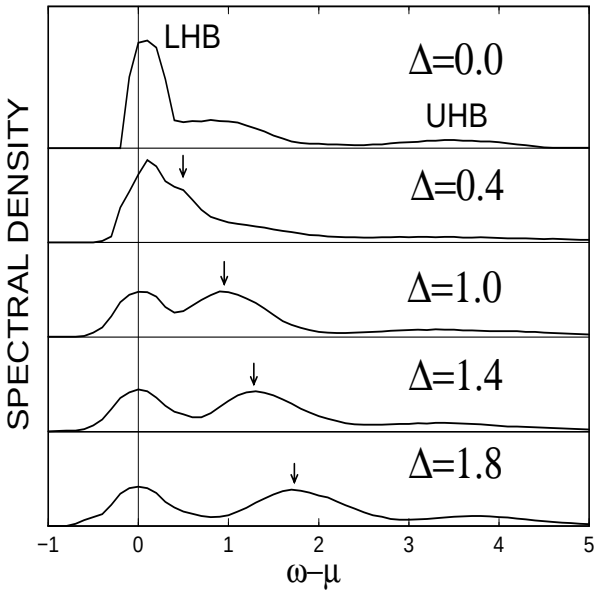
Effective filling $n_{\text{eff}} = \frac{n}{x}$



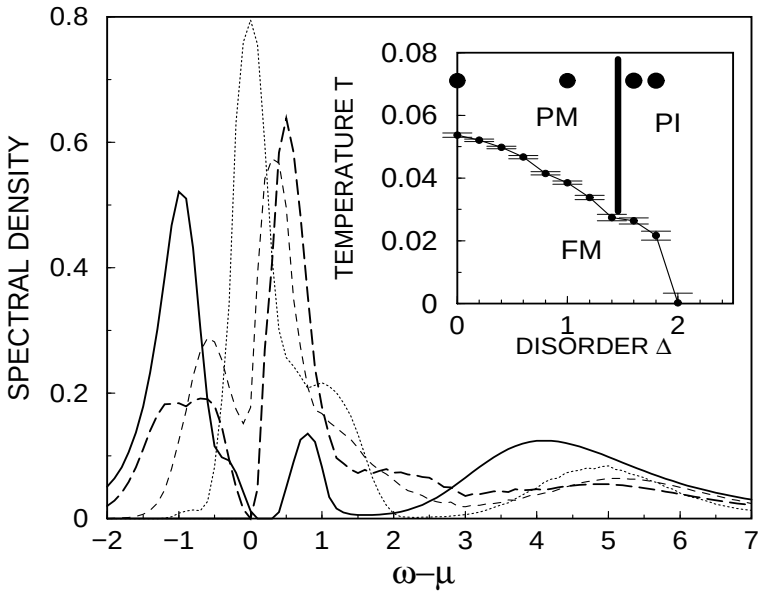
$$T_c(n) \approx x T_c^{\mathrm{p}}\left(\frac{n}{x}\right)$$

[10] Byczuk et al., 02

alloy band splitting



MIT at $n = x$



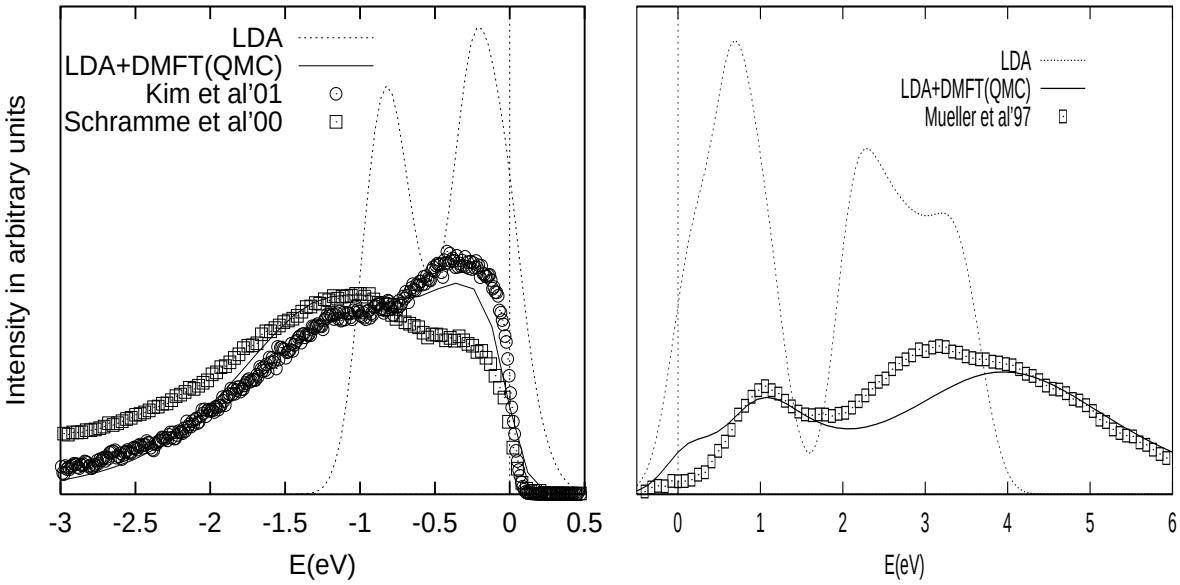
Perspectives

"ab initio" calculations, LDA+DMFT[11]

- **solve LDA for a given material:** $E(\mathbf{k})$ **and** $\phi_{\mathbf{k}}(\mathbf{r})$
- $H(\mathbf{k})$ **from LDA**
- U_{ij} **and** J_{ij} **from LDA**
- **build multiorbital "Hubbard" model**
- **solve within DMFT**

[11] Anisimov, Vollhardt et al., Kotliar et al., ...

V_2O_3 - comparison with photoemission[12]



[12] Held et al. 01

- **Broken symmetries DMFT**
- **Extended DMFT**
- **Cluster DMFT**
- **Chain DMFT**
- **non-equilibrium DMFT**
- **....**

Good for lots of many-body quantum problems