Magnetism, electronic properties and disorder in high-dimensional strongly correlated materials

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1. Disordered local moments formation in high dimensional strongly correlated materials (DMFT + IPT)

We have investigated the electronic properties of strongly correlated materials including the possibility of disordered local moments formation in the framework of the dynamical mean field theory (DMFT).
We used a self-consistent generalization of the iterated perturbation theory (IPT) and calculate the value of local moment amplitudes. Low energy behavior and temperature dependence of local moments are also examined.

Hubbard Model

$$H = -t \sum_{<i,j>\sigma} c^+_{i,\sigma} c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

- 2 types of site A (+μ) and B (-μ)
- 2 corresponding local Anderson models
- disorder : same effective medium

Iterated Perturbation Theory

$$\Sigma_{A\sigma}(\omega) = -\frac{\sigma}{2}U|\mu| + \Sigma^{(2)}_{A\sigma}(\omega)$$
$$\Sigma_{B\sigma}(\omega) = +\frac{\sigma}{2}U|\mu| + \Sigma^{(2)}_{B\sigma}(\omega)$$
$$\Sigma_{A\sigma}(\tau) = U^2 \left(G_{A\sigma}(\tau)\right)^2 G_{A\sigma}(-\tau)$$
$$\Sigma_{B\sigma}(\tau) = U^2 \left(G_{B\sigma}(\tau)\right)^2 G_{B\sigma}(-\tau)$$

DMFT →

Local AM on a Bethe lattice

$$G_{A\sigma}(\omega) = \left(\omega + \frac{\sigma}{2}U|\mu| - S_{A\sigma}(\omega) - \Sigma^{(2)}_{A\sigma}(\omega)\right)^{-1}$$
$$G_{B\sigma}(\omega) = \left(\omega - \frac{\sigma}{2}U|\mu| - S_{B\sigma}(\omega) - \Sigma^{(2)}_{B\sigma}(\omega)\right)^{-1}$$
$$S_{A\sigma}(\omega) = S_{B\sigma}(\omega) = \frac{1}{2}(t^*)^2 G(\omega)$$

↓ CPA

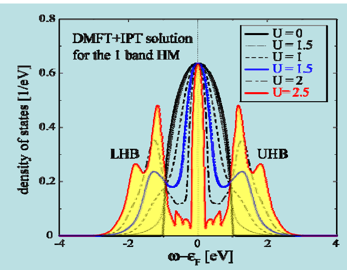
Disorder averaged GF

$$G(\omega) = \frac{1}{2}\left(G_{A\sigma}(\omega) + G_{B\sigma}(\omega)\right)$$

← Self-consistency

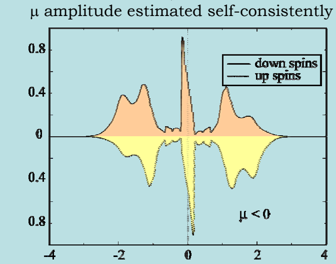
Local moment calculation

$$|\mu| = \int_{-\infty}^{+\infty} d\omega \left(\varrho_{A,\uparrow}(\omega) - \varrho_{A,\downarrow}(\omega)\right) f_{FD}(\omega)$$
$$\varrho_{A,\sigma}(\omega) = -\frac{1}{\pi}\mathrm{Im}\left(G_{A\sigma}(\omega)\right)$$



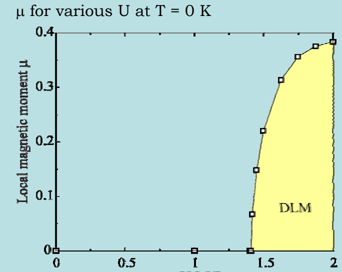
- various U in the moment-less Pauli paramagnetic (enforced by the model)
- Both low energy and high energy structures are present AND quasiparticle
- Mott MIT driven by correlations is reproduced

formation of local μ allowed
μ amplitude estimated self-consistently

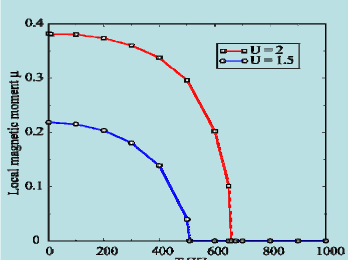


- for U large enough, μ non zero
- asymmetry between spin polarized DOS.
- QP peak is symmetrically shifted
- huge difference between spin polarized DOS at the Fermi level

μ for various U at T = 0 K



- critical U for the stability of the DLM phase U_c = 1.42
- DLM state relevant for intermediate correlation strength 1.42 < U < U_c[Mott] (2.15 by ED and 2.6 by IPT)



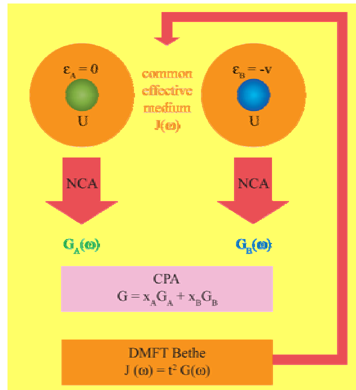
- For a fixed U, an increasing T destroys μ
- T_c decreases for decreasing U
- T_c = 508K for U=1.5, T_c = 650K for U=2

Conclusion :
- We have proposed a self-consistent approach in the framework of the dynamical mean field theory which is able to describe the disordered local moment phase.
- This intermediate phase is of primary importance since it is precursive to long range order magnetic phases.
- Low energy excitations persist in the DLM state. The presence of these excitations is confirmed by spin resolved photoemission experiments.

Perspectives :
- Possible short range ordering for the DLM state.
- Effect of orbital degeneracy of the d-band.

Ref : [1] A. Georges, G. Kotliar, W. Krauth, M.J. Rozenberg, *Rev. Mod. Phys.* **68** (1996) 13
[2] P. Lombardo, M. Avignon, *Physica B* **337** (2003) 186-192

2. Metal Insulator transition induced by disorder in strongly correlated materials (DMFT + NCA + CPA)



- NCA: hybridization expansion [4]
- exact in the large U/t limit

$$H_{\rm eff} = H_{\rm loc} + H_{\rm med}$$
$$H_{\rm loc} = \sum_{a\sigma} \varepsilon_a n_{a\sigma} + \frac{U}{2}\left(\sum_{a\sigma} n_{a\sigma} n_{a-\sigma} + \sum_{(a\neq b)} n_{\sigma a} n_{\sigma b}\right)$$
$$H_{\rm med} = \sum_{\vec{k}a\sigma}\left(W^a_{\vec{k}} b^+_{a\vec{k}\sigma} c_{\sigma a\sigma} + H.c.\right) + \sum_{\vec{k}a\sigma} \varepsilon^a_{\vec{k}} b^+_{a\vec{k}\sigma} b_{a\vec{k}\sigma}.$$

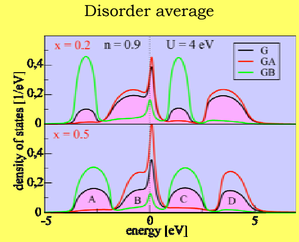
Equation of motion of the local Hamiltonian :

$$G_{a\sigma}(\omega)^{-1} = \omega - \varepsilon_a - \Sigma_{a\sigma}(\omega) - \mathcal{J}^a(\omega).$$
$$\mathcal{J}^a(\omega) = \sum_{\vec{k}} \frac{|W^a_{\vec{k}}|^2}{\omega + i0^+ - \varepsilon^a_{\vec{k}}}.$$

Bethe lattice : $G_{a\sigma}(\omega)^{-1} = \omega - \varepsilon_a - \Sigma_{a\sigma}(\omega) - t^2 G_{a\sigma}(\omega)$

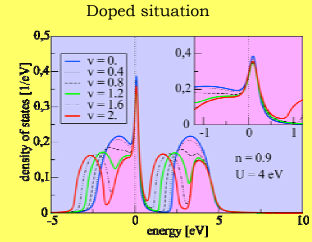
Self − consistent equation : $\mathcal{J}^a(\omega) = t^2 G_{a\sigma}(\omega)$.

Disorder average



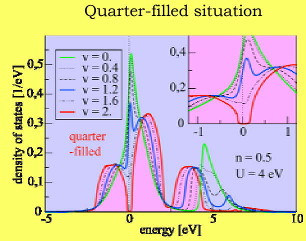
- Site specific and averaged DOS
- New states for increasing x mainly on B sites
- 2 Hubbard bands for each type of site
- B close to half filling

Doped situation



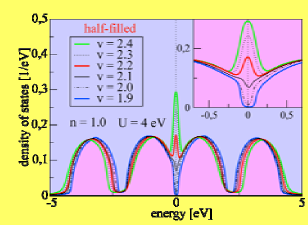
- no MIT for increasing v (for x=0.5) (diff [3])
- Hubbard band splitting
- Resonant quasiparticle weakly affected by disorder

Quarter-filled situation



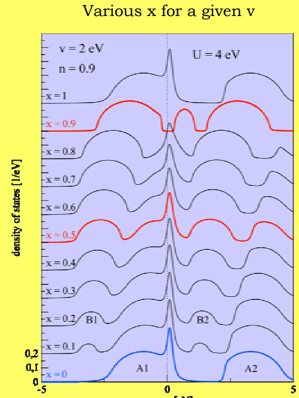
- MIT driven by disorder
- vanishing A sites occupation and A UHB
- half-filled B sites
- Kondo resonance destroyed by disorder

Half-filled situation



- MIT driven by *reducing* disorder
- Gap between A LHB and B UHB
- half-filled A and B sites
- v=0 situation : regular MOTT insulator

Various x for a given v



- identical x=0 and x=1 (except ε_F value)
- new states B1 on B sites
- Transfer of spectral weight from A bands
- MIT obtained for a particular x
- Charge transfer gap

- Equations NCA (1 orbitale, U fini) :

$$\Sigma_0(\omega) = 2\int d\varepsilon \tilde{\rho}(\varepsilon) f(\varepsilon) P_1(\omega+\varepsilon)$$
$$\Sigma_1(\omega) = \int d\varepsilon \tilde{\rho}(\varepsilon) f(-\varepsilon) P_0(\omega-\varepsilon) + \int d\varepsilon \tilde{\rho}(\varepsilon) f(\varepsilon) P_2(\omega+\varepsilon)$$
$$\Sigma_2(\omega) = 2\int d\varepsilon \tilde{\rho}(\varepsilon) f(-\varepsilon) P_1(\omega-\varepsilon)$$

where $P_\alpha(\omega) = \dfrac{1}{\omega + i0^+ - E_\alpha - \Sigma_\alpha(\omega)}$

and $\tilde{\rho}(\varepsilon) = -\dfrac{1}{\pi}\mathrm{Im}\left(\mathcal{J}(\omega)\right)$

Single part. GF :

$$G(\omega) = \frac{1}{Z_0}\int d\epsilon\, e^{-\beta\epsilon}[p_0(\varepsilon)P_1(\omega+\varepsilon) + p_1(\varepsilon)P_2(\omega+\varepsilon) - p_1(\varepsilon)P_0(\varepsilon-\omega)^* - p_2(\varepsilon)P_1(\varepsilon-\omega)^*]$$

where $p_\alpha(\varepsilon) = -\dfrac{1}{\pi}\mathrm{Im}(P_\alpha(\varepsilon))$

and $Z_0 = \int d\epsilon\, e^{-\beta\epsilon}[p_0(\varepsilon) + 2p_1(\varepsilon) + p_2(\varepsilon)]$

Conclusion :
- New type of MIT combining disorder and strong correlations
- Semiconductor doped with transition metals

[3] M. S. Laad, L. Craco, and E. Müller-Hartmann *Phys. Rev. B* **64** (2001)195114
[4] T. Pruschke, D.L. Cox, M. Jarrell, *Phys. Rev. B* **47**, 3553 (1993)

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