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Workshop on
Novel States and Phase Transitions in Highly Correlated Matter

12 - 23 July 2004

Strongly correlated superconductivity from the Fullerenes to the Cuprates

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These are preliminary lecture notes, intended only for distribution to participants

Strongly Correlated Superconductivity from the Fullerenes to the Cuprates

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INFM SMC and Centro "Enrico Fermi", Roma

NOVEL STATES AND PHASE TRANSITIONS IN

HIGHLY CORRELATED MATTER (12 - 23 July 2004) (Miramare, Trieste, Italy)

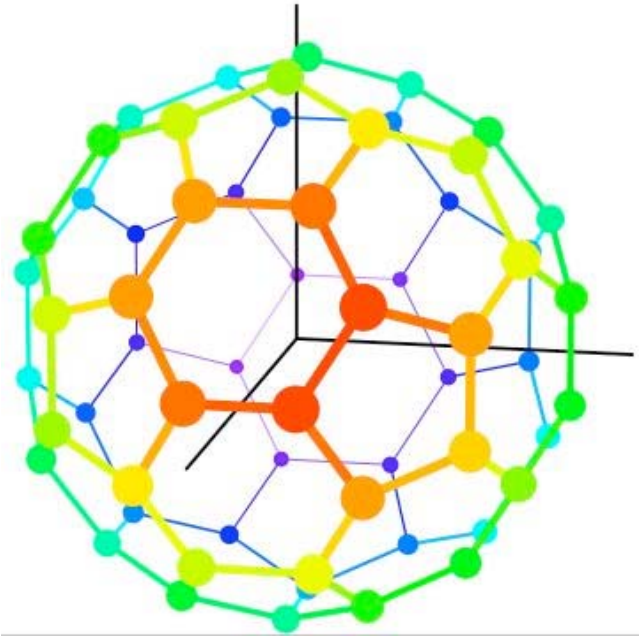
In collaboration with

- **M. Fabrizio, E. Tosatti** SISSA and ICTP
  (it all began here)
- **C. Castellani** University of Rome
- **L. De Leo** SISSA (the impury model guy)
- **G. Kotliar, M. Civelli** Rutgers,
  S. S. Kancharla Sherbrooke
  (CDMFT and d-wave)

Outline

- Strong Correlations in High-Temperature Superconductors: the case of Fullerene
- How can Correlation favor Superconductivity?
- DMFT study of the Mott transition in a model for C_{60}
- If the attraction does not couple to charge it survives close to the Mott transition and quasiparticle pairing is enhanced
- Doping a Singlet Mott Insulator: Pseudogap
- Insights from the single-impurity model
- Towards the Cuprates: d-wave Superconductivity

Fullerene C_{60}



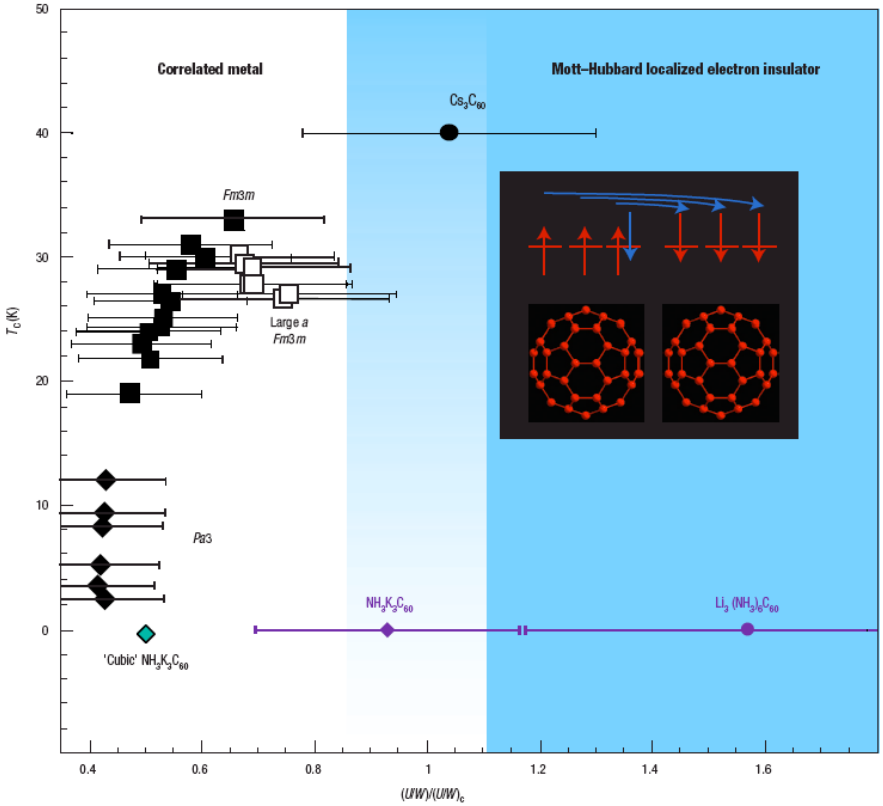
- Molecular Crystal with a Threefold Degenerate LUMO
- **A_nC_{60}**: alkali metal atoms donate electrons to the LUMO
- n=3 **Superconductor (Tc = 35K)**
- Phonon-mediated SC (Jahn-Teller distortions of the bucky-ball)

Electron-electron Correlations are Important

- A_4C_{60} are **Mott insulators**
- K_3C_{60} become **Mott insulators** expanding the lattice spacing [$NH_3K_3C_{60}$]
- **Strong Correlation** U/W> 1

"PRACTICAL" ADVANTAGES

- Isotropic **s-wave** Superconductors
- Less competing phases



Dynamical Mean-Field Theory (DMFT)

- **Simplify the Spatial Structure** of a problem in order to **exactly solve for the dynamics**
- Quantum Version of Mean-Field Theories
- We approximate the lattice model in the thermodynamic limit with an **effective single-site theory**
- The dynamics of each site may described as hybridization with a **bath** $G_0(i-_n)^{-1}$
- Becomes **exact in** in the limit d ∞ ∞

A. Georges, G. Kotliar, W. Krauth, M.J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996)

DMFT and Impurity Models

Dynamical Weiss Field ⇨ We can not write a Local Hamiltonian and introduce auxiliary fermions describing a **bath**

⇩

$$H = U n_{0\uparrow} n_{0\downarrow} - \mu n_0 + \sum_{k\varepsilon} V_k (c^{+}_{k\varepsilon} c_{0\varepsilon} + c^{+}_{0\varepsilon} c_{k\varepsilon}) + \sum_{k\varepsilon} \varepsilon_k c^{+}_{k\varepsilon} c_{k\varepsilon}$$

Anderson Impurity Model

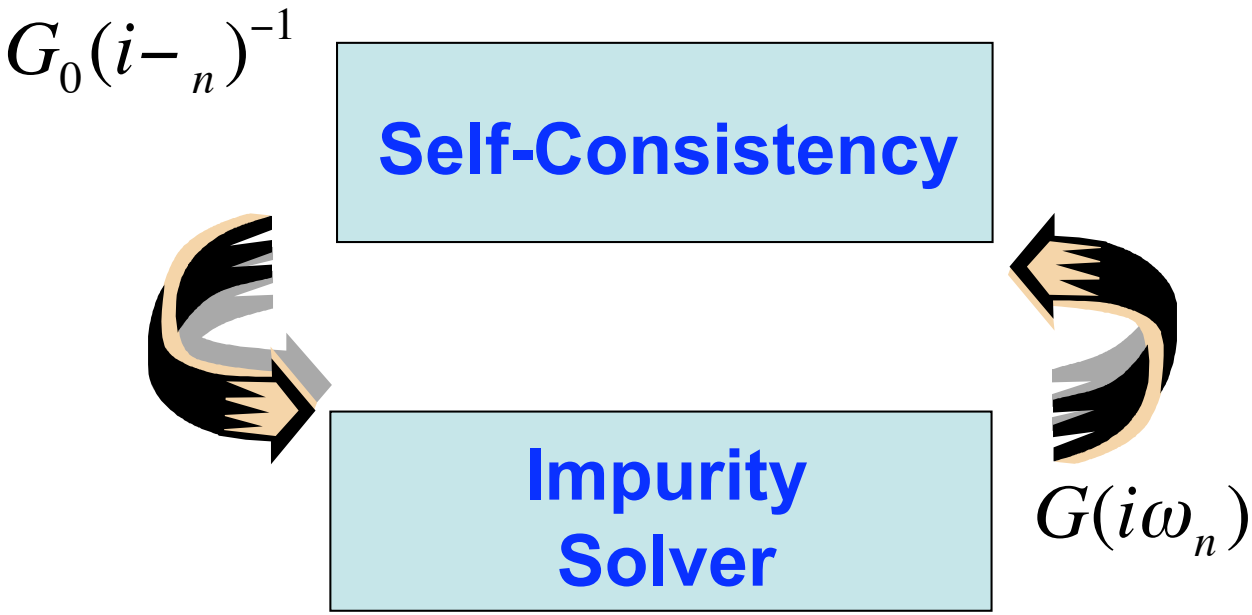
$$G_0(i\Sigma_n)^{\Sigma 1} = i\Sigma_n + \mu \Sigma \sum_k \frac{V_k^2}{i\Sigma_n \Sigma \Sigma_k}$$

+ Self-consistency

$$G_0(i__n)^{-1} = i__n + \mu - t^2 G(i__n)$$

I need to solve the model and **compute the Green's function**

Iterative Solution



Exact diagonalization to solve the Impurity model at T=0

$$G_0(i\Sigma_n)^{\Sigma 1} = i\Sigma_n + \mu \Sigma \sum_k \frac{V_k^2}{i\Sigma_n \Sigma\Sigma_k}$$

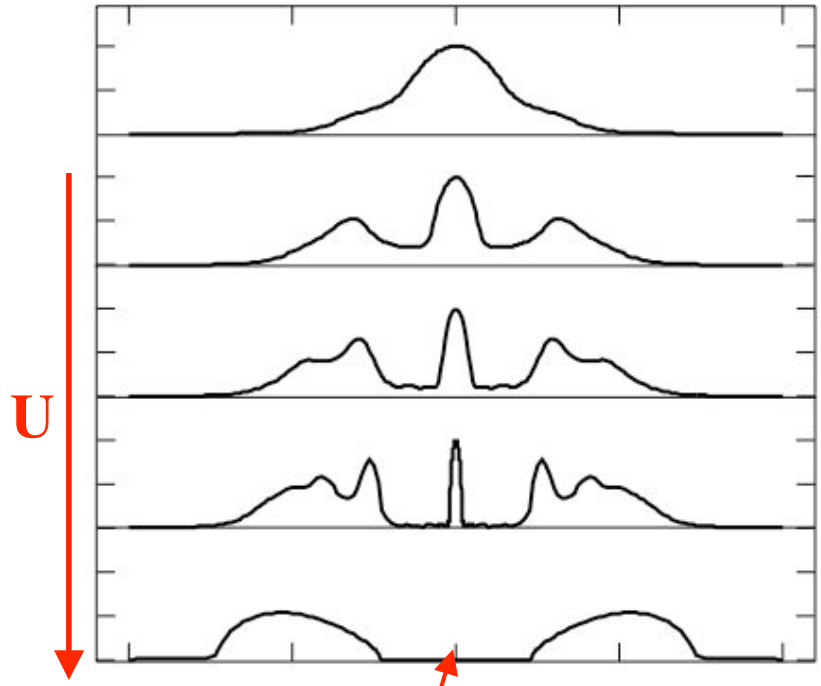
Is truncated to small number of levels

The Mott-Hubbard Transition

- Coexistence of **Metallic** e **Insulating** features
- **Metallic Peak (Kondo Resonance)** at the Fermi level of width **Z**, decreasing with **U**
- High-energy **Hubbard bands** at distance **U**
- MIT for

$$Z = \frac{1}{m^*} \infty \quad \infty$$

±



$$Z = \left| 1 \mid \frac{/ \mid (i/_n)}{/i/_n} \right|^{\mid 1}$$

How can Correlation favor Superconductivity?

$$T_c = \lambda_0 e^{\lambda \frac{1}{\lambda\lambda\mu^*}}$$

$\Delta = \Delta V$ → Attractive Potential

$\Delta = \Delta V$ → Density of States

Electron Correlation ⇒ Quasiparticles with Reduced Mobility

$W \longrightarrow ZW$ ⇒ $\propto\propto \frac{1}{W} \longrightarrow \Delta/Z >> \Delta$

$Z << 1$

⇓

Tc enhanced Repulsion?

How Can Correlation favor Superconductivity? (2)

Also the Attractive Potential is affected by correlation

$\Delta \longrightarrow \Delta / Z \qquad V \longrightarrow VZ^2$

$\Delta \longrightarrow \Delta\Delta << \Delta \Rightarrow T_c \downarrow$

To increase **Tc** through correlation I should

Gain in Δ without losing in V

Is it possible ?

Model for C_{60}

$$\sum_{\Sigma} t \sum_{<ija>} c^{+}_{ia\Sigma} c_{ja\Sigma}$$

Kinetic Term ⇨ 3 bands W~0.5 eV

$$+\frac{U}{2}\sum_{i} n_i^2$$

Coulomb Repulsion U~1/1.5 eV

$$+J(2S_i^2 + \frac{1}{2}L_i^2)$$

Attractive Term due to Phonons

J = 0 "Ordinary" Mott transition for **every integer n**

J > 0 favors **minimum S e L** (inverted Hund's rule)

Mott Transition

n=2 | We tune U/W | J = 0.02 U

U >> W → Mott Insulator J > 0 → S=0, L=0

A singlet on each site

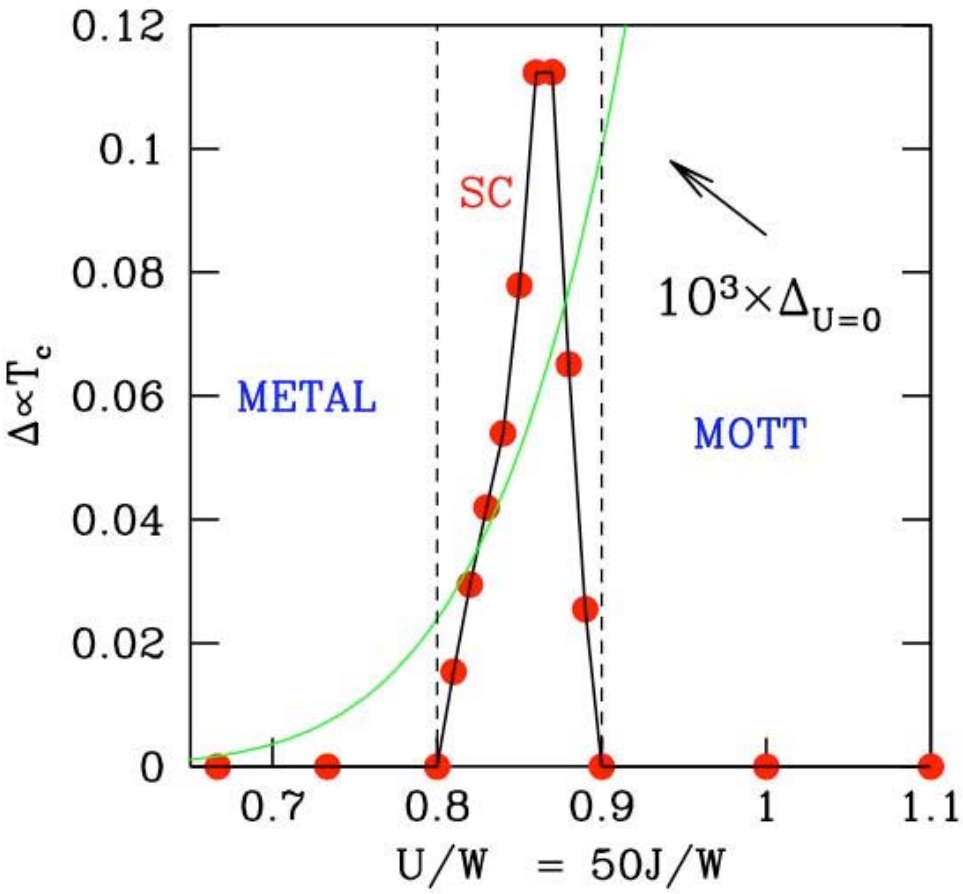
U <<W Metal + Attraction J + Repulsion U

S-wave SC $\Sigma = \sum_{ia} c^{+}_{ia\Sigma} c^{+}_{ia\Sigma}$

Who wins? → A = U - 10/3 J > 0 → Non-SC Metal

Effective Inteaction

Phase Diagram

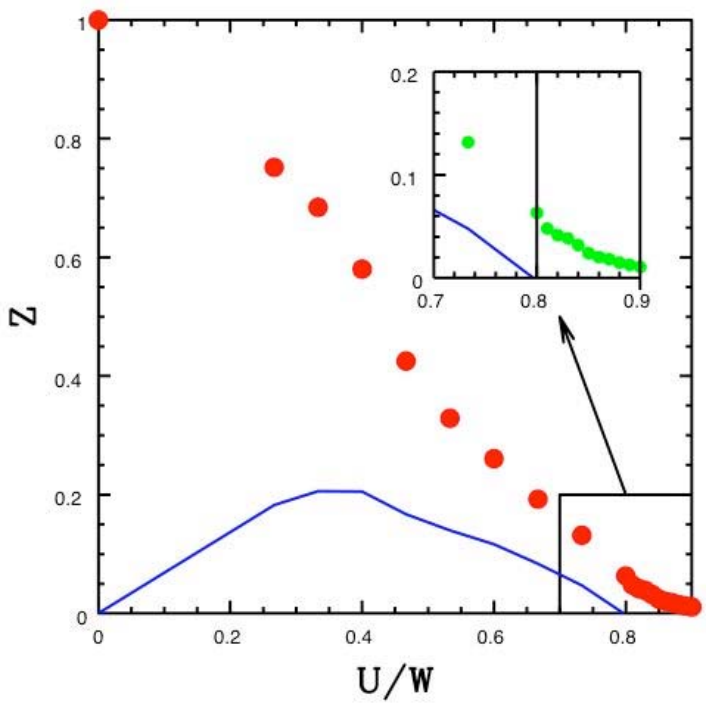


Superconductivity close to

The Mott Insulator

$\Delta(U) > 1000\ \Delta(U=0)$

Why is Superconductivity favored by repulsion?



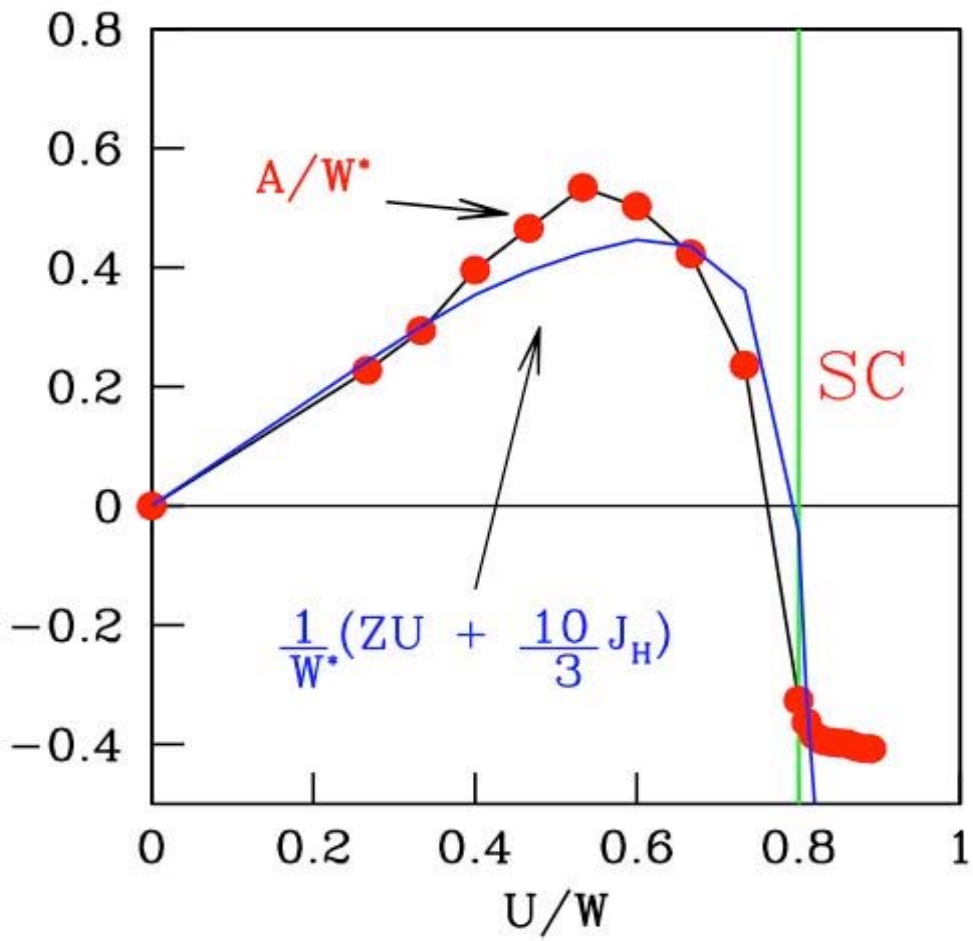
At the onset of SC $ZW \cong \frac{10}{3} J$

Quasiparticle Band

equal to the **bare attraction**

- In the attractive Hubbard model T_c maximum for **U** ~ **W**
- **Superconductivity only involves Quasiparticles?**

Quasiparticle Interactions



Response Functions

⇩

Effective Interactions

A = **Z**U -10/3 **J**

Perturbative Result

With **Renormalized U**

M.Capone, M. Fabrizio, C. Castellani, and E. Tosatti, Science 296, 2364 (2002).

The SCS Scenario

U renormalizes the Quasiparticles

Q.P. repulsion is strongly reduced

$$< H_U >= U < n_\alpha n_\alpha > \propto ZU$$

Attraction **J** unscreened **since it involves other degrees of freeedom**

$$A = ZU - 10/3\ J$$

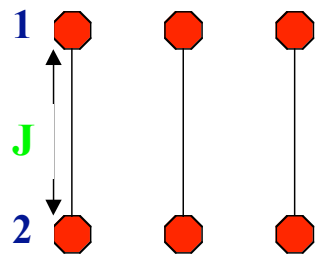
Strongly Correlated Superconductivity only involving

Quasiparticles with large effective mass

M.C., M. Fabrizio, C. Castellani, and E. Tosatti, Science 296, 2364 (2002).

A Simpler model for SCS: exE

Two-Orbital Hubbard model



Smaller Hilbert space ⇒ "Easier" Numerics

$$H = H_{hopping} + H_{Hubbard} \sum J \sum_i (l_x^2 + l_z^2)$$

$$l_x = \sum_{\Sigma} c_{1\Sigma}^{+} c_{2\Sigma} + c_{2\Sigma}^{+} c_{1\Sigma}$$

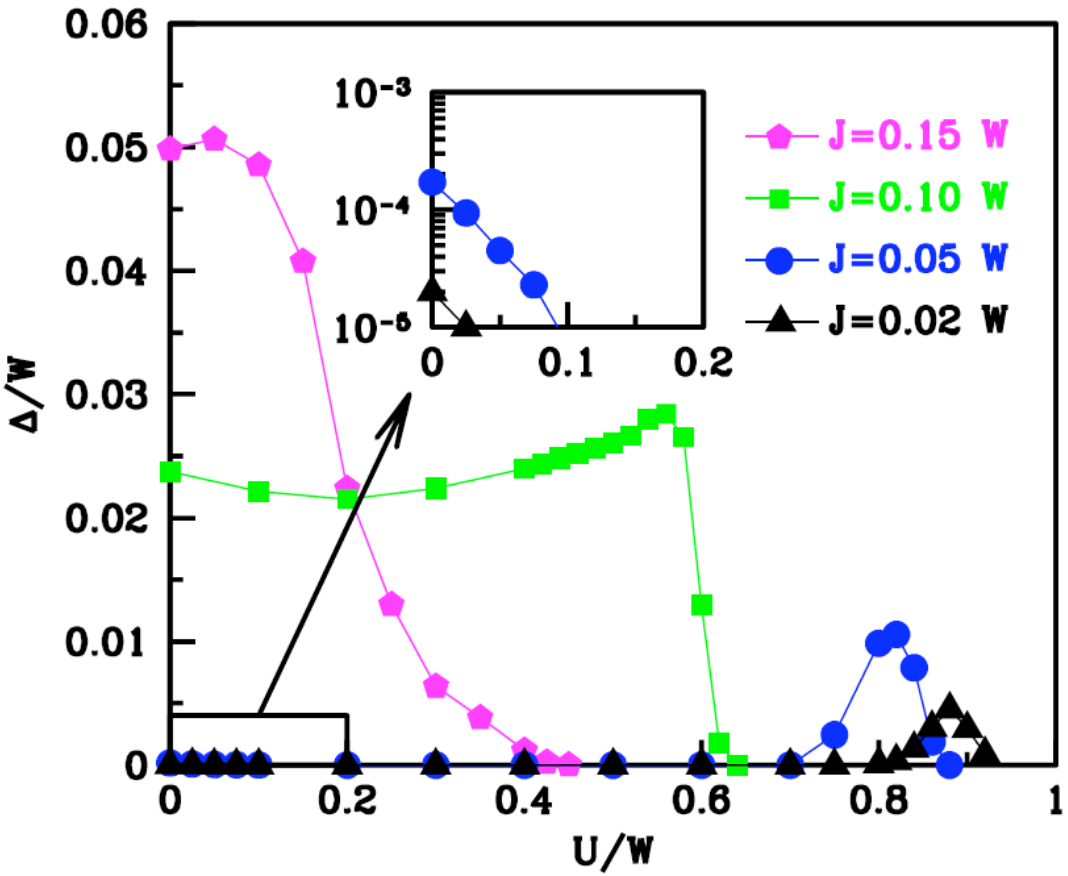
$$l_z = n_1 \cong n_2$$

⇓

The Molecular Groundstate is again
A non degenerate singlet

Bridge with the Cuprates: The pairs of molecular orbitals are local "bonds"

From Ordinar Superconductivity to SCS



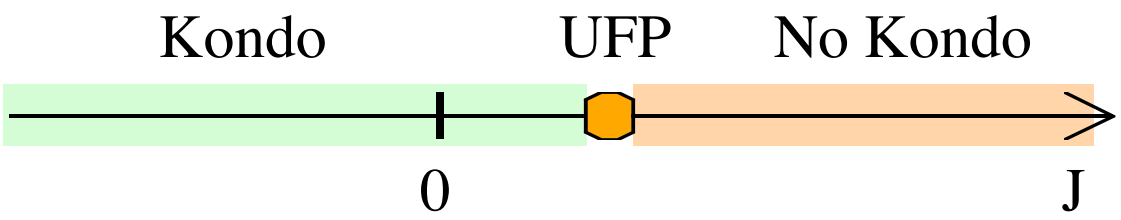
- **Large J:** usual reduction of Tc
- **Small J:** SCS - Tc enhanced by U

M.Capone, M. Fabrizio, C. Castellani, and E. Tosatti, cond-mat/0401090, PRL accepted

Insights from the Impurity Model

M. Fabrizio, A. F. Ho, L. De Leo, and G. E. Santoro, Phys. Rev. Lett. 91, 246402 (2003)

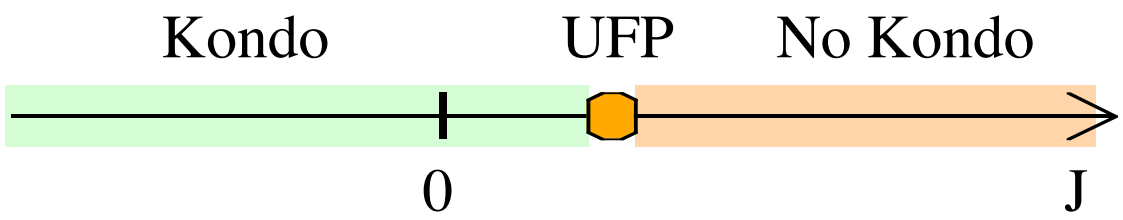
- Competition between ordinary Kondo screening leading to a local Fermi liquid and J which forms local singlets



- An unstable Fixed Point separates the Fermi-liquid Kondo phase and the unscreened phase

The Impurity Model Fixed Point

M. Fabrizio, A. F. Ho, L. De Leo, and G. E. Santoro, Phys. Rev. Lett. 91, 246402 (2003)



UFP ⇒ Divergent Susceptibilities in **s-wave in Cooper channel** with S=0, L=1, L_z=0 and L_x, L_z and SL_y in the particle-hole channel

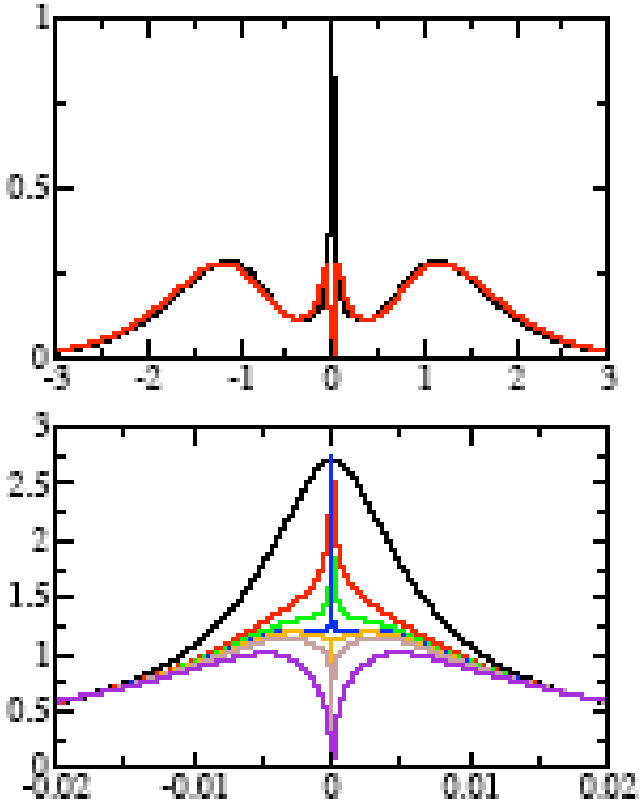
Two energy scales (T_K and J) ⇒ Two-stage quenching of the entropy

$$T_+ = \max(T_K, J)$$

$$T_\propto \propto |J \propto J^*|^2 / T_+$$

Spectral Functions close to the Unstable Fixed Point

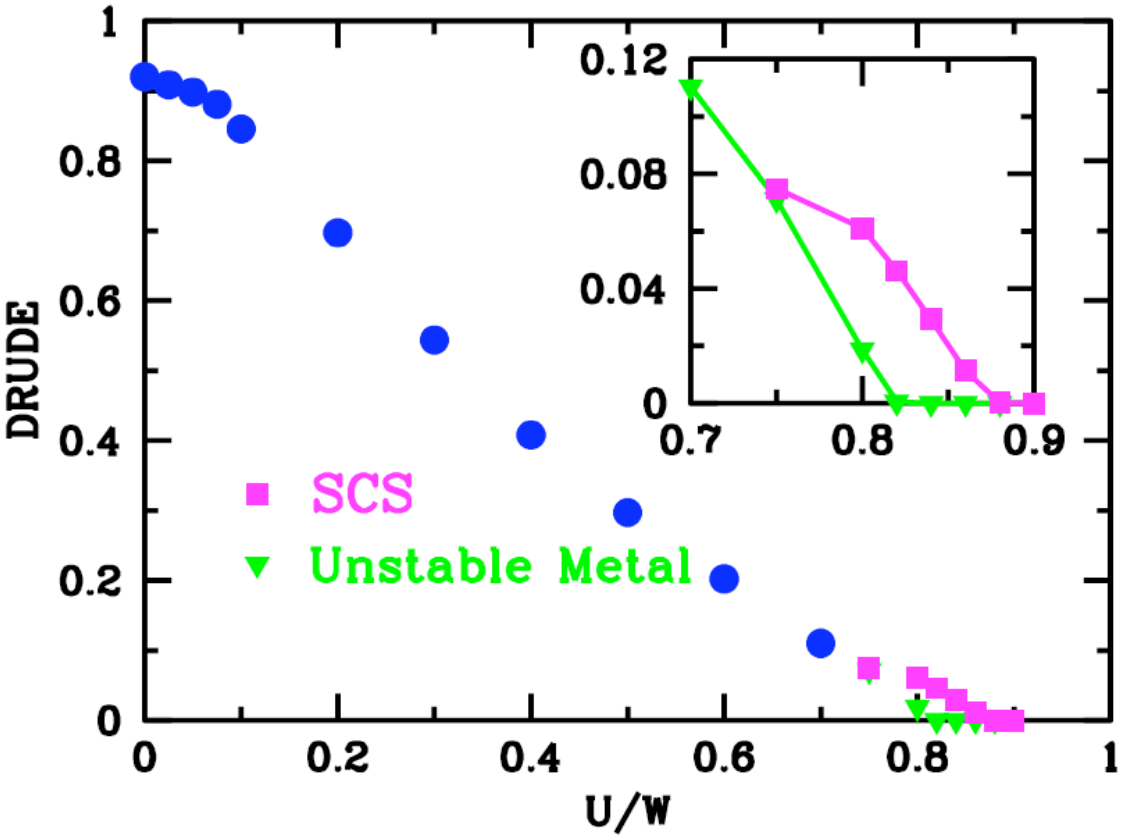
L. De Leo and M. Fabrizio, Phys. Rev. B. 69, 245114 (2004)



- In the Kondo-screened phase we obtain the Kondo resonance on top of a broader resonance and a Fermi-liquid self-energy
- In the unscreened phase the narrow peak becomes a **Pseudogap**
- At the Fixed Point only the broad resonance survives
- A model for the low-energy part of the spectrum

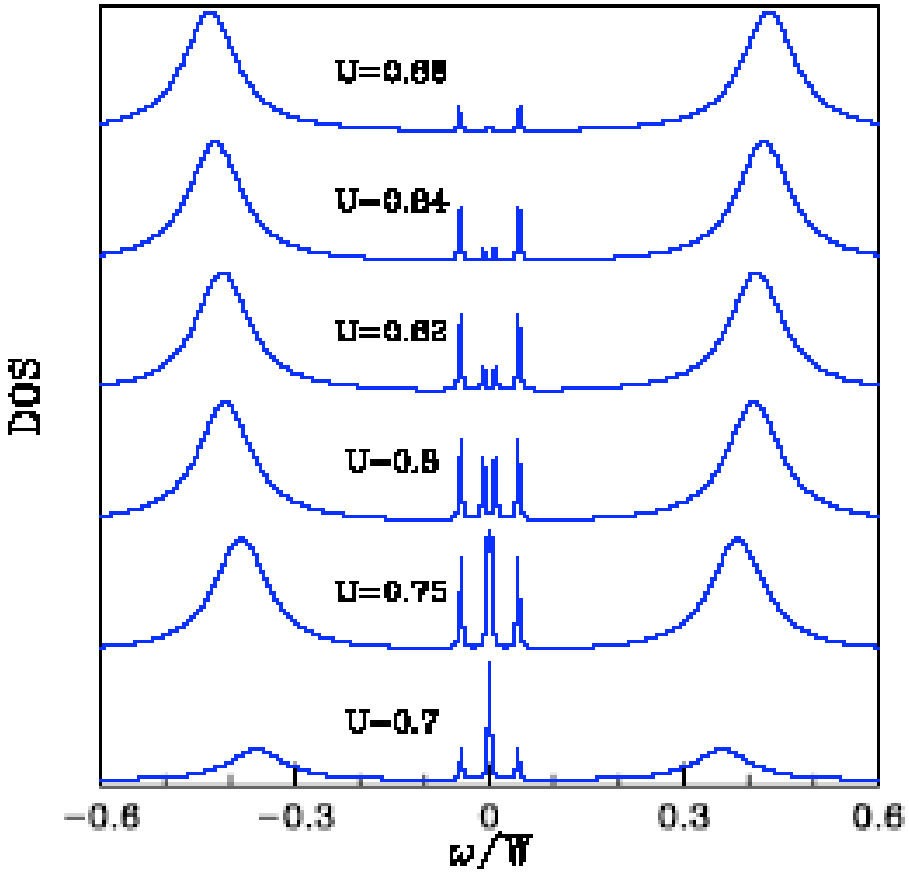
$$\rho_{\pm}(\omega) = \frac{\rho_0}{2}\left|\frac{T_+^2}{\omega^2 + T_+^2} \pm \frac{T_-^2}{\omega^2 + T_-^2}\right|$$

Drude Weight (Kinetic Energy) Gain in the Superconducting Phase



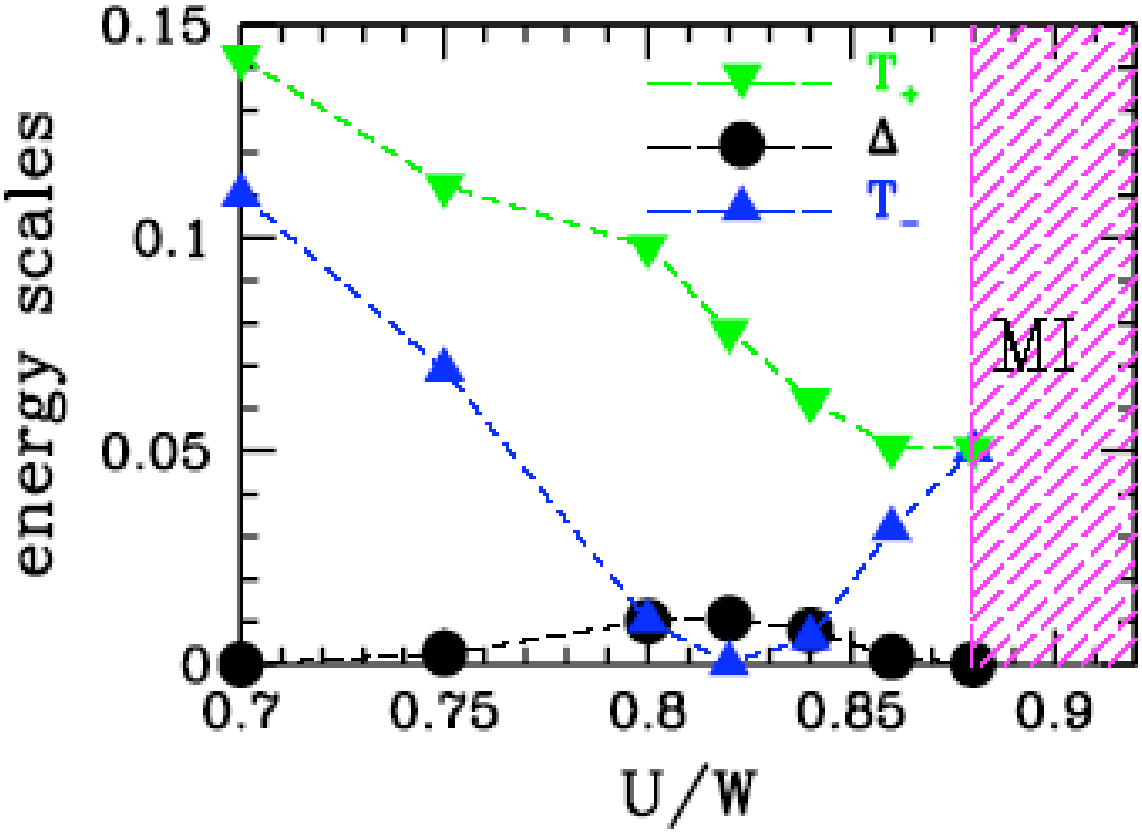
The Superconductor has a larger Drude weight

DMFT Spectral Function: The Pseudogap Phase



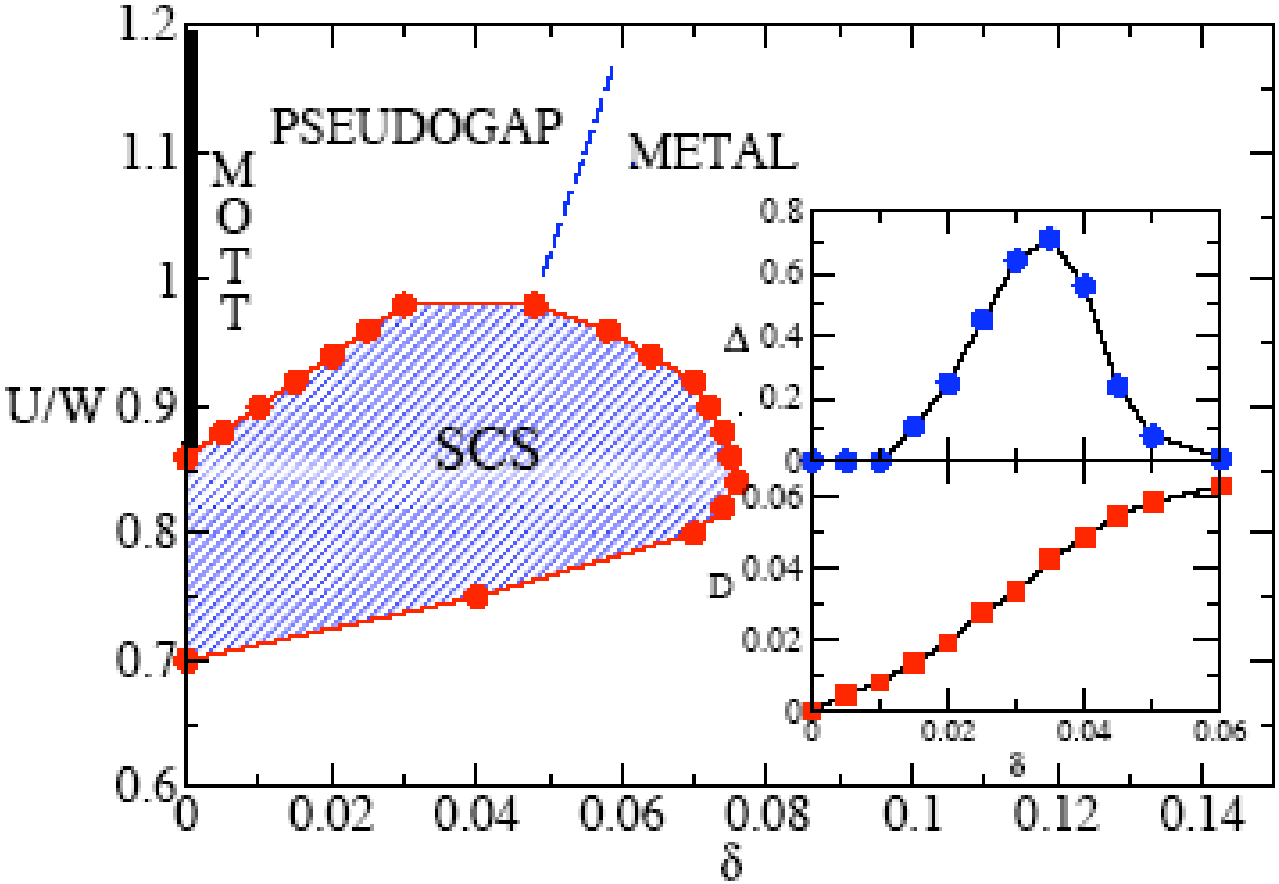
- **The unstable metallic phase** underlying the SCS phase shows the **pseudogap** within the quasiparticle peak
- A Structure exists at J (broad resonance of the AIM)
- Fit the low-energy part with the AIM formula (T_+ and T_-)

Energy Scales



- **SC phase around the AIM fixed point**
- Maximum Δ close to the AIM fixed point
- Two energy scales

Phase Diagram



Many features of the Cuprates!

M.Capone, M. Fabrizio, C. Castellani, and E. Tosatti, cond-mat/0401090, PRL to appear

Non-local Magnetic Interactions (Antiferromagnetism)

- If the interaction is not coupled to charge it
  Survives Correlations close to the Mott transition
- How about **Antiferromagnetic Interactions** in cuprates?

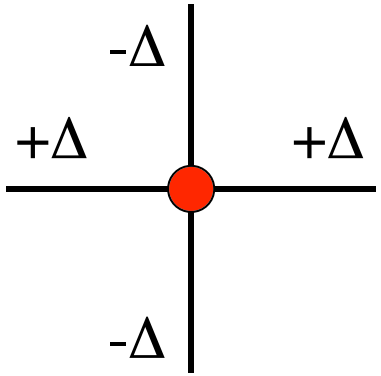
$$H_J = J \sum_{<ij>} \vec{S}_i \vec{S}_j$$

Within Slave Bosons J is not renormalized

Non-local J ⇒

- D-wave Superconductivity
- Competing Phases (Flux..)
- Unaccessible to DMFT

D-wave Superconductivity



$$\downarrow = < c^{+}_{i\downarrow} c^{+}_{j\downarrow} >$$

Order Parameter

- Non Local
- Space Structure
- Avoids Local Repulsion

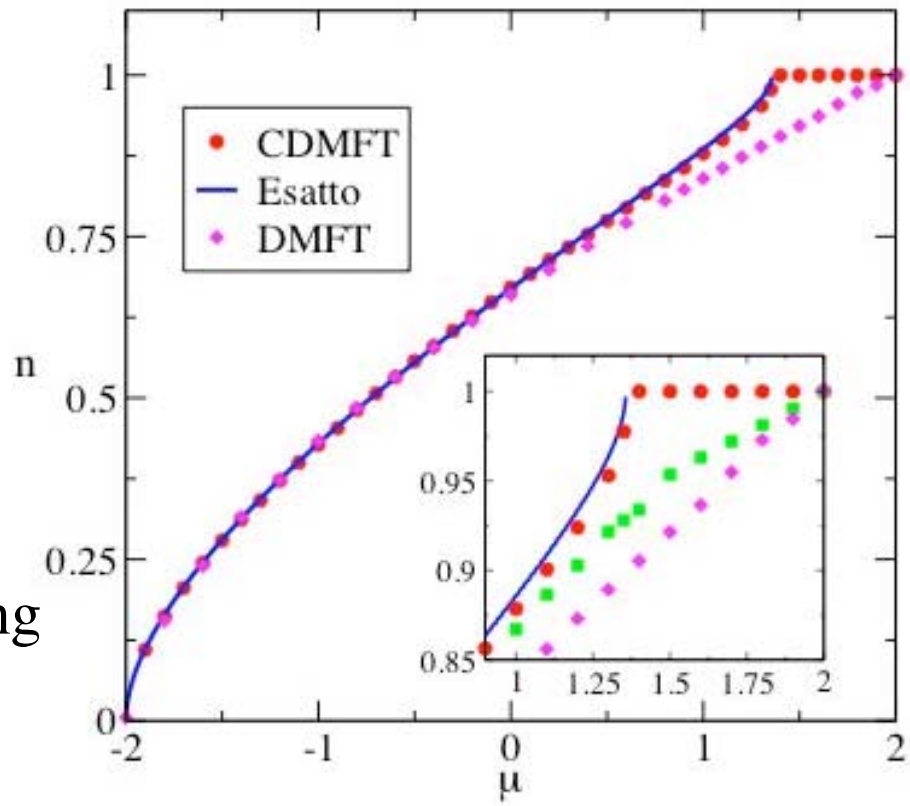
Unaccessible to DMFT

Need to introduce spatial Correlations beyond Mean-Field

O. Parcollet's talk

Cluster-DMFT: one-dimensional Hubbard model

- Extending DMFT to include **dynamical correlations within a cluster** of N_C sites
- Test in the **one-dimensional case** in which DMFT fails (worst case scenario for a mean-field theory)
- **Comparison with Exact Solution** is really encouraging



M.C.,M. Civelli, S.S. Kancharla, C. Castellani and G. Kotliar, Phys. Rev. B 69, 195105 (2004)

Conclusions

- Superconductivity **favored by strong correlation** if it involves spin/orbital degrees of freedom (**Strongly Correlated Superconductivity**)
- Lattices of Jahn-Teller centers (Fullerene models) are natural SCS systems
- SCS is associated to a Fixed Point of the Impurity Model, and it is accompanied by a **pseudogap phase**
- Doping dependence similar to the cuprates
- D-wave superconductivity in the pure Hubbard model is stable within CDMFT