Introduction to DMFT

Lecture 3 : Introduction to cluster methods

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1. Cluster DMFT methods.
2. Application to high-Tc superconductors.

General references for Cluster DMFTs

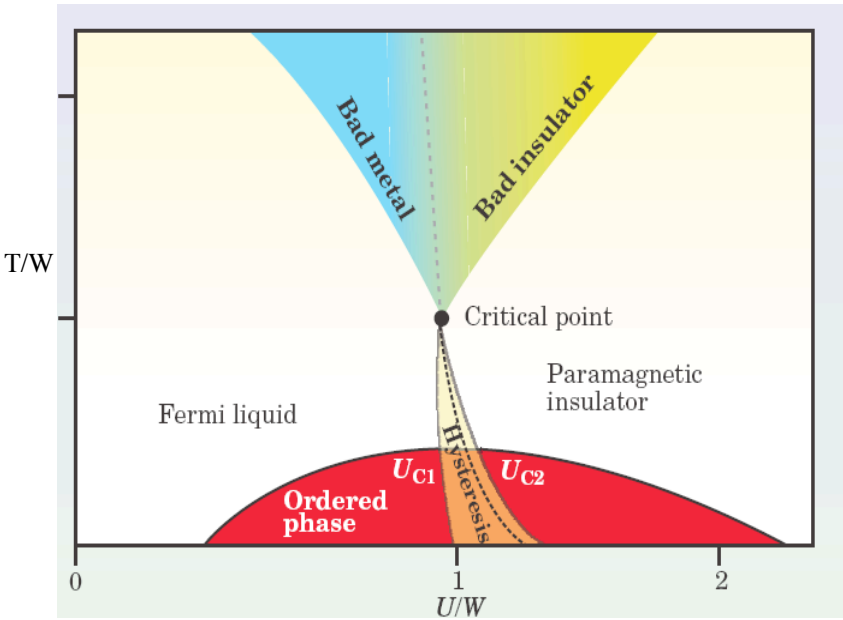
- G. Kotliar, S.Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, C.A. Marianetti, Rev. Mod. Phys. 78, 865 (2006)
- A. Georges, G. Kotliar, W. Krauth and M. Rozenberg, Rev. Mod. Phys. 68, 13, (1996).
- G. Biroli, O. Parcollet, G. Kotliar, PRB, 69,205108 (2004)
- T. Maier et al, Rev. Mod. Phys. 77,1027 (2005)

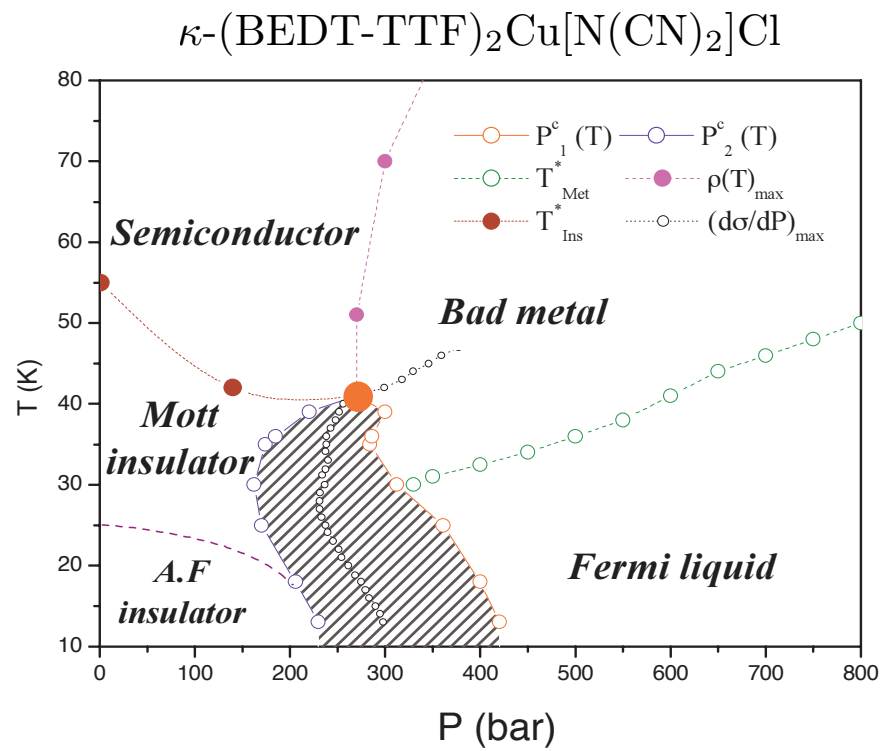
DMFT is a good starting point to study Mott physics.

But it has many limitations ...

Is the Mean Field picture correct ?

- Favorable comparisons (See lecture 1), but :
  - Stability with 1/d corrections.
  - Shape of the transition line. Description of the insulator.
  - Uc1,Uc2,Tc beyond mean field.





Clusters : an interpolation between mean field and d=2,3

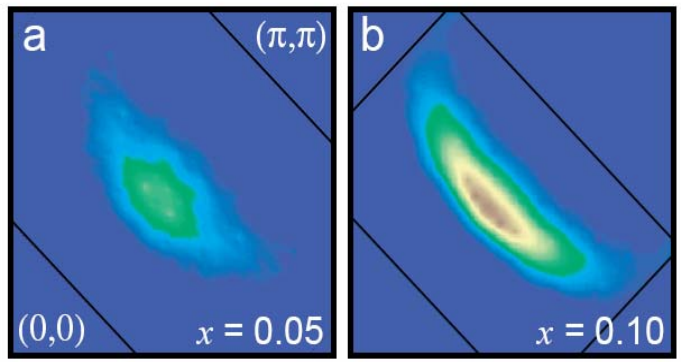
The self-energy in not local !

- In DMFT, no k-dependence of the self-energy.
- Consequences :
  - Effective mass and Z are linked $Z = \frac{m}{m^*}$
  - Finite temperature lifetime, Z are constant along the FS. Not sufficient for high-Tc.

$$G_{\mathrm{latt}}(k,\omega) = \frac{1}{\omega + \mu - \epsilon_k - \Sigma_{\mathrm{latt}}(k,\omega)}$$

$$\Sigma_{\mathrm{latt}}(k,\omega) = \Sigma_{\mathrm{impurity}}(\omega) \equiv G_0^{-1} - G_c^{-1}$$

$A(k, \omega = 0^+)$

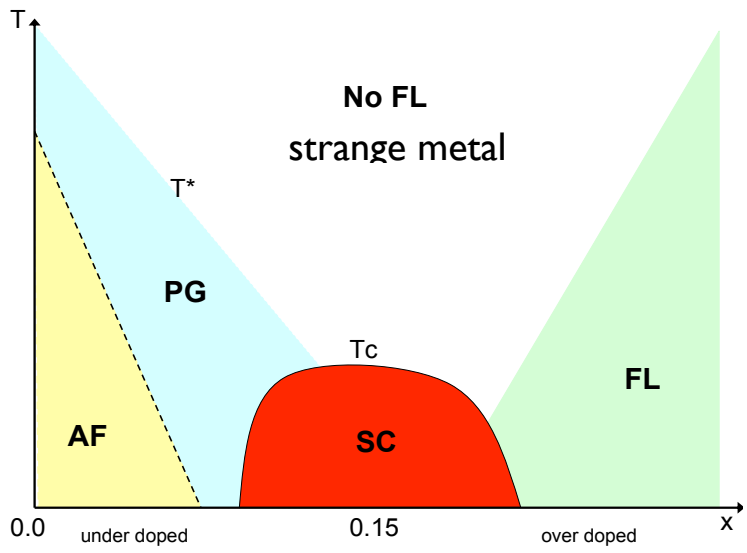


Shen et al. Science 307, 901 (2005)

Clusters reintroduce some k-dependence in Σ

DMFT is only 1 site in a bath....

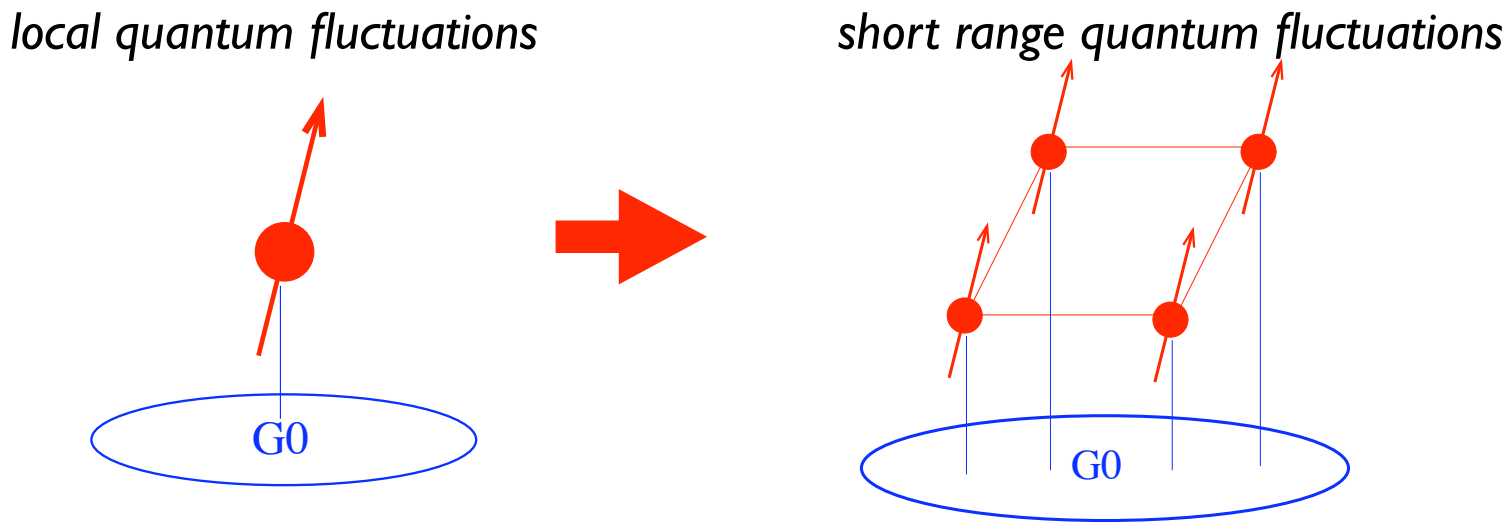
- d-wave superconductivity ? or DDW ? (need at least a link)
- Competition AF-SC ?
- Non trivial insulator a la RVB ? (need at least a singlet ?)
- Effect of J in the paramagnet not in DMFT
  e.g. cut divergence of the effective mass
  (See slave-bosons or large N,
  e.g. G. Kotliar, Les Houches 1988).



Clusters fix these problems (to some extent)

Cluster extensions of DMFT

- *Principle* : a finite number of sites in a self consistent bath.



- Interpolate between DMFT and finite dimensions
- Finite size systems BUT with "boundary conditions" G0.
- Many choices :
  - Type of clusters (e.g. shape, size)
  - Self-consistency condition : $G_0(i\omega_n) = \mathcal{F}_{\text{lattice}}[G_c](i\omega_n)$
  - How to approximate lattice quantities from cluster quantities ?

Cluster DMFT is not unique

How to build cluster methods ?

- 3 points of view on DMFT :
  - DMFT is 1 site in a self-consistent bath.
    - ➡ Real space cluster : *CDMFT* *(G. Kotliar et al. PRL 87 186401 2001)*
  - DMFT is about neglecting the k-dependence of Σ
    - ➡ Σ piecewise constant in the Brillouin zone: *DCA*
      M.H. Hettler, A.N. Tahvildar-Zadeh, M. Jarrell, T. Pruschke, H.R. Krishnamurthy PRB 98
  - DMFT is an approximation of the Luttinger-Ward functional

$$\Phi \approx \phi_{AIM}(G_{ii})$$

    - ➡ Higher approximation on phi.
      (A. Georges, G. Kotliar, W. Krauth and M. Rozenberg, Rev. Mod. Phys. 68, 13, (1996))
- There are other methods (more later) !

Equivalent for 1 site but lead to different cluster methods.

Reminder : DMFT equations (1 site, 1 orbital)

$$H = -J \sum_{ij} \sigma_i \sigma_j \qquad H = -\sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U n_{i\uparrow} n_{i\downarrow}$$

$$m = \langle \sigma \rangle \qquad G_c(\tau) = -\langle T c(\tau) c^\dagger(0) \rangle_{S_{eff}}$$

$$H_{\text{eff}} = -J h_{\text{eff}} \sigma \qquad S_{\text{eff}} = -\int_0^\beta c^\dagger_\sigma(\tau) G_0^{-1}(\tau - \tau') c_\sigma(\tau') + \int_0^\beta d\tau U n_\uparrow(\tau) n_\downarrow(\tau)$$

$$m = \tanh(\beta h_{\text{eff}})$$

$$\Sigma = G_0^{-1} - G_c^{-1}$$

$$h_{\text{eff}} = zJm \qquad G_0^{-1}(i\omega_n) = \left(\sum_k \frac{1}{i\omega_n + \mu - t(k) - \Sigma(i\omega_n)} \right)^{-1} + \Sigma(i\omega_n)$$

- Evaluation of lattice quantities.

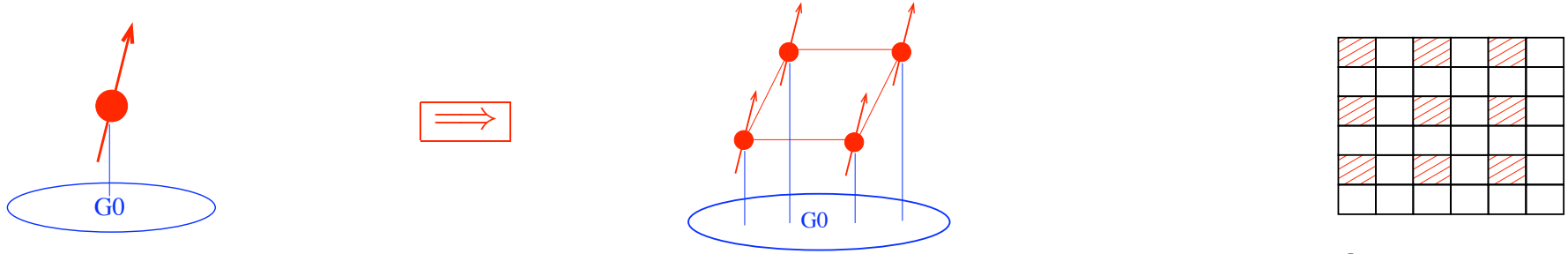
$$G_{\text{latt}}(k, \omega) = \frac{1}{\omega + \mu - \epsilon_k - \Sigma_{\text{latt}}(k, \omega)}$$

$$\Sigma_{\text{latt}}(k, \omega) = \Sigma_{\text{impurity}}(\omega) \equiv G_0^{-1} - G_c^{-1}$$

C-DMFT

- 4 Anderson impurities coupled to an effective bath

DMFT **Cluster DMFT**



Superlattice

$$S_{\text{eff}} = -\int\int_0^\beta d\tau d\tau' c_\mu^\dagger(\tau) G_{0,\mu\nu}^{-1}(\tau,\tau') c_\nu(\tau') + \int_0^\beta d\tau U(n_{i\uparrow} n_{i\downarrow})(\tau)$$

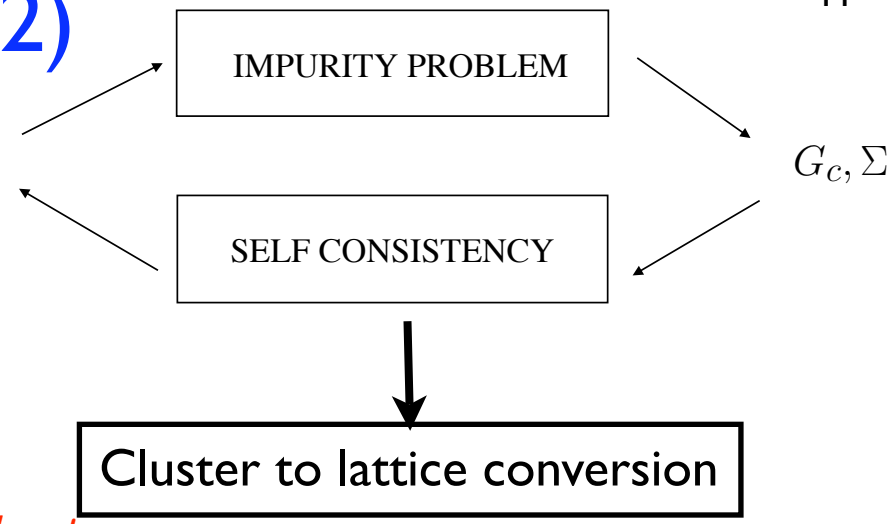
$$G_{c\mu\nu}(\tau) = -\langle T c_\mu(\tau) c_\nu^\dagger(0)\rangle_{S_{\text{eff}}} \qquad 1 \le \mu,\nu \le 4$$

$$\Sigma_c = G_0^{-1} - G_c^{-1}$$

$$G_0^{-1}(i\omega_n) = \left[\sum_{K\in R.B.Z.}{}' \left(i\omega_n + \mu - \hat{t}(K) - \Sigma_c(i\omega_n)\right)^{-1}\right]^{-1} + \Sigma_c(i\omega_n)$$

CDMFT equations

C-DMFT (2)



- How to evaluate lattice quantities ?
- Need to restore the translation invariance by periodization :

$$\mathcal{A}_{ij}^{Lattice} = \sum_{\alpha,\beta:\alpha-\beta=i-j} w_{\alpha,\beta}\mathcal{A}_{\alpha\beta}^{Cluster}$$

$$\text{with } w > 0 \text{ and } \sum_{\alpha\beta;\alpha-\beta=x} w_{\alpha,\beta} \to 1 \quad \forall x \text{ as } L_c \to \infty$$

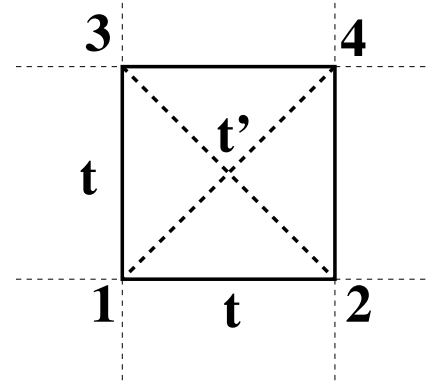
Simplest case : $w = 1/L^2$

- Which quantity should we periodize ?
  - Most irreducible (Σ rather than G !)
  - Σ-periodisation versus M-periodization (cumulant)
  - That choice is part of the cluster method.

C-DMFT : Σ-Periodization

- The original proposal *(G. Kotliar et al. PRL 87 186401 2001)*
- Example : 2x2 cluster on a square lattice, w= const

Cluster site labeling



$$\Sigma^{Lattice}(k) = \frac{1}{4}\sum_{i=1}^{4}\Sigma_{ii}^{Cluster} + \frac{1}{2}\Big[\left(\Sigma_{12}^{Cluster} + \Sigma_{34}^{Cluster}\right)\cos(k_x) +$$

$$\left(\Sigma_{24}^{Cluster} + \Sigma_{13}^{Cluster}\right)\cos(k_y) + \Sigma_{14}^{Cluster}\cos(k_x + k_y) + \Sigma_{23}^{Cluster}\cos(k_x - k_y)\Big]$$

Cluster quantities ⇔ harmonics on the lattice

Size of cluster = resolution in k space

C-DMFT : M-Periodization (1)

- Σ- periodization generates spurious mid-gap states in Mott insulator
  (B. Kyung, A.M. Tremblay et al)
- Definition of the irreducible cumulant :
  Sum of all diagrams 1-particle irreducible in an expansion around the atomic limit (i.e. in t, not in U).
- For a presentation of this diagrammatics : *(W. Metzner, PRB 43, 8549 1991)*
- Relation with the self-energy :

$$M^{-1}(k,\omega) = \omega + \mu - \Sigma(k,\omega)$$

- The Green function is :

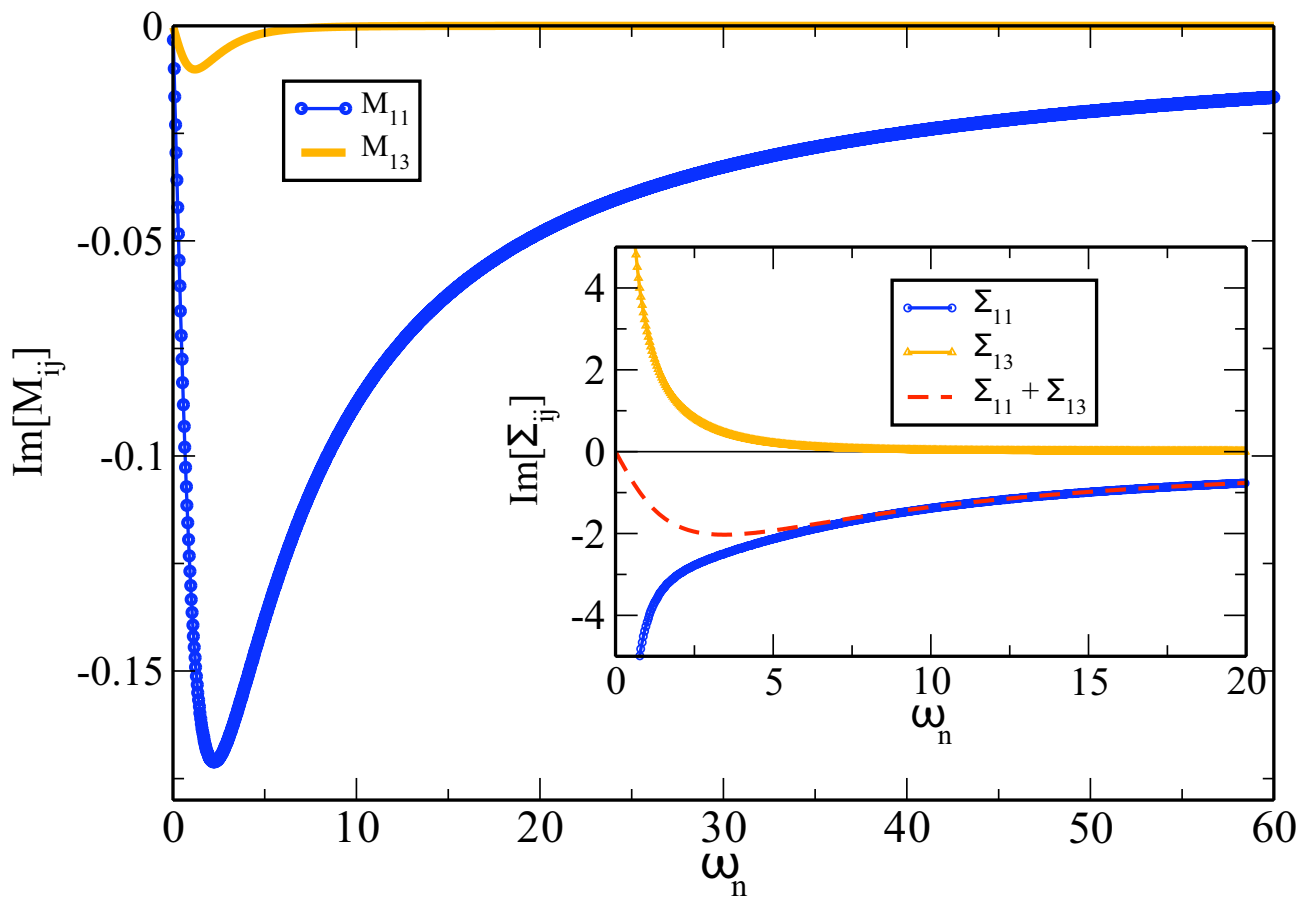
$$G(k,\omega) = \left(t(k) - M^{-1}(k,\omega)\right)^{-1}$$

C-DMFT : M-Periodization (2)

(T. Stanescu, G. Kotliar PRB 74, 125110, 2006)

- In DMFT, Σ and M are local.
- Hubbard, 1/2 filled,2x2 CDMFT, U/D = 2, ED solver, cluster quantities

M is more localized than Σ.



C-DMFT : M-Periodization (3)

(T. Stanescu, G. Kotliar PRB 74, 125110, 2006)

➡ Periodize the irreducible cumulant

- Same formula as for the self-energy :

$$M^{Lattice}(k) = \frac{1}{4}\sum_{i=1}^{4} M_{ii}^{Cluster} + \frac{1}{2}\Big[\left(M_{12}^{Cluster} + M_{34}^{Cluster}\right)\cos(k_x) + \left(M_{24}^{Cluster} + M_{13}^{Cluster}\right)\cos(k_y) + M_{14}^{Cluster}\cos(k_x + k_y) + M_{23}^{Cluster}\cos(k_x - k_y)\Big]$$

- A non-linear relation $\Rightarrow$ $\Sigma_{\text{lattice}}(k,0)$ can have singularity !

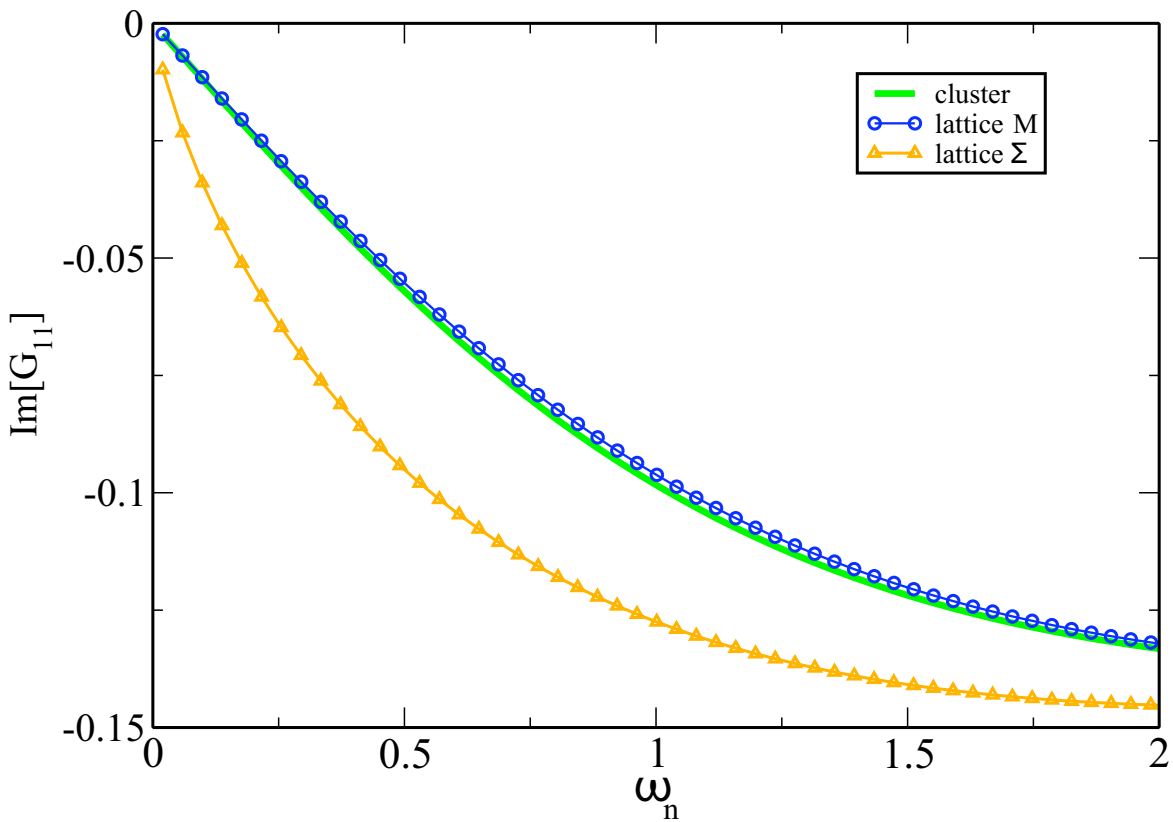
Some results (pockets) will rely on this periodization

C-DMFT : test of periodization procedure

- Consistency check :

$$G_{\mathrm{Cluster}}(\omega) = \sum_{k} G_{\mathrm{Lattice}}(k, \omega)$$

- Example of 1/2 filled Hubbard :



(T. Stanescu, G. Kotliar PRB 74, 125110, 2006)

DCA

- Cluster method in k-space : Σ piecewise constant on B.Z.
  M.H. Hettler, A.N. Tahvildar-Zadeh, M. Jarrell, T. Pruschke, H.R. Krishnamurthy PRB (1998)

- Example for 2x2 cluster on square lattice.

$$G(k_c, i\omega_n) = \sum_{\tilde{k}} \frac{1}{i\omega_n + \mu - t(\tilde{k}) - \Sigma(k_c, i\omega_n)}$$

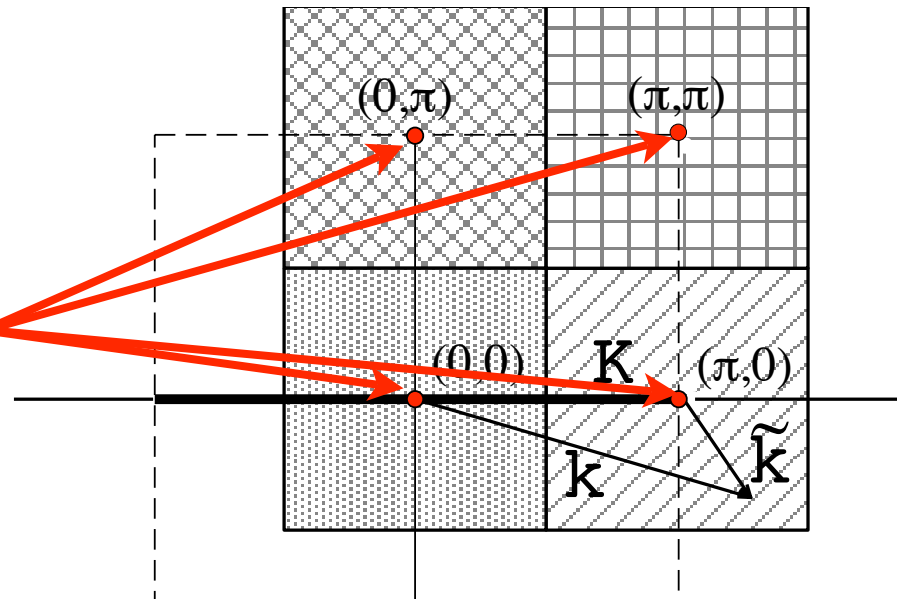
$$\Sigma(k, i\omega_n) \approx \Sigma_c(k_c(k), i\omega_n)$$

$$G_0^{-1}(k_c, i\omega_n) = G^{-1}(k_c, i\omega_n) + \Sigma_c(k_c, i\omega_n)$$

- Impurity model : same as for CDMFT.

- G, Σ cyclic on the cluster

Cluster momenta k_c



DCA (2)

- A real space formulation :
  CDMFT self-consistency condition with a modified hopping
  Also valid in the AF phase.
  (G. Biroli, O. Parcollet, G. Kotliar, PRB, 69,205108 (2004))

$$S_{\text{eff}} = -\int\int_0^\beta d\tau d\tau' c_\mu^\dagger(\tau) G^{-1}_{0,\mu\nu}(\tau,\tau') c_\nu(\tau') + \int_0^\beta d\tau U n_{\mu\downarrow} n_{\mu\uparrow}(\tau)$$

$$G_{c\mu\nu}(\tau) = -\left\langle T c_\mu(\tau) c_\nu^\dagger(0)\right\rangle_{S_{\text{eff}}}$$

$$\Sigma_c = G_0^{-1} - G_c^{-1}$$

$$G_0^{-1}(i\omega_n) = \left[\sum_{K\in R.B.Z.}{}' \left(i\omega_n + \mu - \hat{t}_{\text{DCA}}(K) - \Sigma_c(i\omega_n)\right)^{-1}\right]^{-1} + \Sigma_c(i\omega_n)$$

$$t^{DCA}_{\alpha\beta}(K) = \sum_{k_c} e^{ik_c(\alpha-\beta)} t(K+k_c)$$

DCA (3)

- Lattice quantities :
  - In DCA, translation invariance is preserved by construction
  - But there is still a need for cluster to lattice conversion
  - Use spline interpolation to get a smooth $\Sigma(k,\omega)$ on the lattice *(M. Jarrell et al.)*.

Functional point of view

- Functional formulation of DMFT

$$\Gamma_{BK}[G_{ij}] = \mathrm{Tr}\ln G_{ij} - \mathrm{Tr}(g_{0ij}^{-1}G_{ij}) + \Phi_{BKLW}[G_{ij}]$$

$$G_{ij}(t) \equiv -\left\langle Tc_i(t)c_j^\dagger(0)\right\rangle \qquad \Sigma_{ij} = \frac{\delta\Phi_{BKLW}}{\delta G_{ij}}$$

- DMFT as an approximation of the Baym-Kadanoff functional.

$$\Phi \approx \phi_{AIM}(G_{ii})$$

- Exact in large dimension *(Metzner-Vollhardt, 1989)*
- Anderson impurity model = machinery to solve this approximation *(Kotliar-Georges 1992)*

Φ-derivability

- CDMFT : the impurity problem is Φ-derivable :

$$\Phi_{CDMFT}(G) = \sum_R \Phi(G_{\mu,R;\nu,R} | G_{\rho,R;\lambda R'} = 0)$$

but the lattice conversion breaks the Φ-derivability.

- DCA is also Φ-derivable (but not the lattice conversion !).

$$\Phi_{DCA}(G) = N_{sites}\ \Phi(G(k))|_{U(k_1,k_2,k_3,k_4)=U_{DCA}(k_1,k_2,k_3,k_4)}$$

$$U_{DCA}(k_1,k_2,k_3,k_4) = \delta_{K_c(k_1)+K_c(k_2),K_c(k_3)+K_c(k_4)}/N_{sites}$$

Coarse-graining of the momentum conservation at the vertex.

T. Maier et al, Rev. Mod. Phys. 77,1027 (2005)

- Φ-derivability ⇒ conservative approximation (Baym-Kadanoff)

In particular, Luttinger Theorem ....

Luttinger Theorem

- In Fermi liquid, volume of the Fermi surface is conserved.
- Derivation is based on the existence of the Φ functional
  (See e.g. Abrikosov-Gorkov-Dzyaloshinky, sect 19.4)
- When Σ becomes singular : problem !
- Fermi surface : location of poles of G(k,0)
  Luttinger surface : location of zeros of G(k,0)
- BUT when Σ has a singularity, volume enclosed by both surfaces not necessarily conserved !
  (A. Georges, O. Parcollet and S.Sachdev, PRB 63 134406, (2001))

$$\int G \partial_\omega \Sigma \neq 0$$

Nested Schemes

- Take a higher approximation of the Luttinger Ward functional.

$$\Phi = \sum_i \tilde{\phi}_1(G_{ii}) + \sum_{<ij>} \tilde{\phi}_2(G_{ii}, G_{jj}, G_{ij}) + \cdots$$

- Apply it to a 1 site and a 2 site problem :

$$\begin{aligned} \phi_{1\text{site}}(G_{ii}) &= \tilde{\phi}_1(G_{ii}) \\ \phi_{2\text{sites}}(G_{ii}, G_{jj}, G_{ij}) &= \tilde{\phi}_2(G_{ii}, G_{jj}, G_{ij}) + \tilde{\phi}_1(G_{ii}) + \tilde{\phi}_1(G_{jj}) \end{aligned}$$

- Introducing z, the connectivity of the lattice :

$$\Phi_{\text{Nested}} \approx (1-z) \sum_i \phi_{1\text{site}}(G_{ii}) + \sum_{<ij>} \phi_{2\text{sites}}(G_{ii}, G_{jj}, G_{ij})$$

Nested Schemes (2)

- Complete equations :

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

$$\Sigma_{loc} = \frac{\delta\Phi}{\delta G_{ii}} = \frac{\delta\Phi_{1\text{site}}}{\delta G_{ii}} + z\left(\frac{\delta\Phi_{2\text{sites}}}{\delta G_{ii}} - \frac{\delta\Phi_{1\text{site}}}{\delta G_{ii}}\right)$$

$$\Sigma_{nn} = \frac{\delta\Phi_{2\text{sites}}}{\delta G_{ij}}$$

$$\Sigma^{latt} = \Sigma_{loc}(i\omega_n) + t(k)\Sigma_{nn}(i\omega_n)$$

$$G_{loc} = \sum_k \frac{1}{i\omega_n - t(k) - \Sigma_{loc}(i\omega_n) - t(k)\Sigma_{nn}(i\omega_n)}$$

$$G_{nn} = \sum_k \frac{e^{ik.\vec{\delta}}}{i\omega_n - t(k) - \Sigma_{loc}(i\omega_n) - t(k)\Sigma_{nn}(i\omega_n)}$$

$$G = \sum_{K \in R.B.Z.} \left(i\omega_n - t(K) - \Sigma^{\text{latt}}(K)\right)^{-1}$$

Many other possible schemes !

- For a review of some methods : *T. Maier et al, Rev. Mod. Phys. 77,1027 (2005)*
- Chain DMFT : a chain in a self-consistent bath (see below)
  (S. Biermann et al)
- Extended DMFT and Extended cluster DMFT. *(Q. Si et al., see e.g. K. Haule)*
- Cluster perturbation theory. Not self-consistent clusters
  A.M. Tremblay, D. Sénéchal et al., T. Maier et al, Rev. Mod. Phys. 77,1027 (2005)
- Self-energy functional *(M. Potthof et al.)*
- PCDMFT : use $\Sigma(k,\omega)$ in the self-consistency
  (G. Biroli, O. Parcollet, G. Kotliar, PRB, 69,205108 (2004))
- ...

So what is the best cluster method ?

Classical limit

- A large body of work in classical statistical mechanics
  (Bethe, Kikuchi, Cf Domb-Green series)

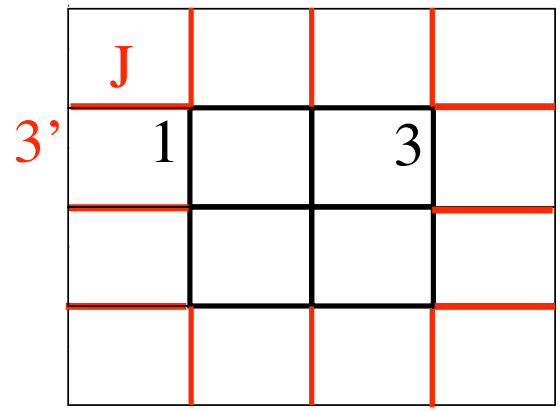
- How do our cluster methods connect to this ?
  For example large U limit of Falikov-Kimball model = Ising model
  (G. Biroli, O. Parcollet, G. Kotliar, PRB, 69,205108 (2004))

$$H = -\sum_{ij\sigma} t_{ij\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U n_{i\uparrow} n_{i\downarrow} \ \text{,with } t_{\downarrow} = 0$$

- CDMFT reduces to Ising cluster with a bath at the boundary.

$$H = H_{\text{Ising}} + J\sigma_1 \langle \sigma_3 \rangle$$

- *Exercise* : show that at large U,
  one finds the Ising Weiss theory.



Example of 2x2 cluster

Classical limit (2)

- DCA :
  Cluster is cyclic, no boundary. An effective J on ALL links.
  (G. Biroli, O. Parcollet, G. Kotliar, PRB, 69,205108 (2004))

- Nested scheme (2 sites) leads to Bethe-Kikuchi method.
  Solve 1 site and 2 sites problems and fix the field h so that local magnetization is the same in the 2 problems :

$$H^{(1)} = zhS^{(1)}$$

$$H^{(2)} = (z-1)h(S_1^{(2)} - S_2^{(2)}) + JS_1^{(2)}S_2^{(2)}$$

$$< S^{(1)} > = < S_1^{(2)} > = - < S_2^{(2)} >$$

- Convergence of Tc vs size much faster than CDMFT or DCA.

BUT ....

Causality issue

- Causality = Im Σ <0 (definite negative matrix)
- Strong Causality property : guarantee that Im Σ <0 for any bath G0
  Hence there will not be any causality violation at any step in the DMFT iterative loop.
- Quantum impurity problem is causal by construction :
  the problem lies in the self-consistency.
- It is not obvious to have a causal scheme :

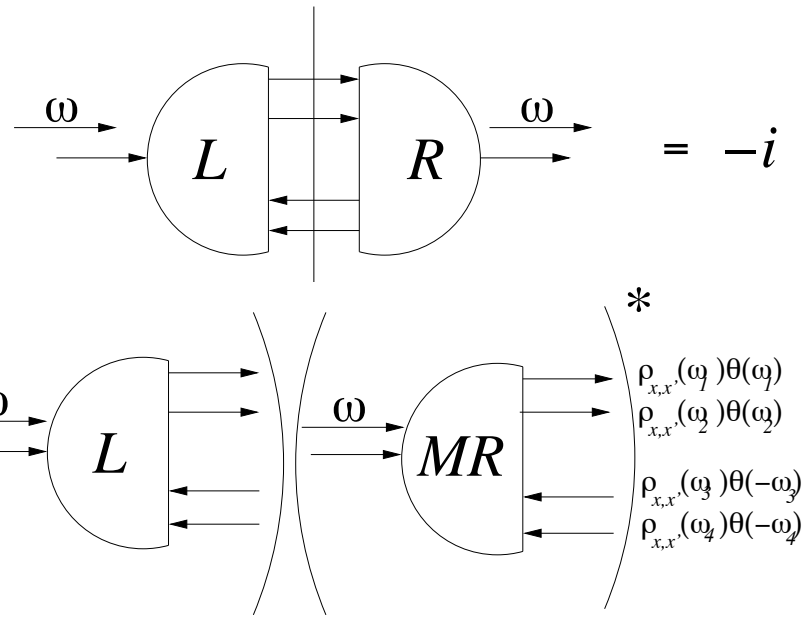
Nested schemes show causality violations

- CDMFT, DCA are proven to be causal *(See original papers)*

What is the origin of this problem ?

Origin of the causality problem

- Using Cutkovsky-t'Hooft-Veltmann cutting technique.
  (G. Biroli, O. Parcollet, G. Kotliar, PRB, 69,205108 (2004))
- Diagrammatic expansion of $Im\Sigma_R(\omega)$
- Use Keldysh technique



- $Im\Sigma_R(\omega)$ is a quadratic form in "half-diagrams" R and L
  Can we form a square ?
- Nested scheme is not causal (was known empirically before).
- Roughly speaking, problem arises when self-energy not local enough

See also A. Fuhrmann, S. Okamoto, H. Monien, and A. J. Millis PRB 75, 205118 (2007)

Convergence properties

- Debate in the literature about CDMFT and DCA convergence
  (See controversy by Biroli et al. vs Jarrell et al., 2002)
- DCA (cluster of linear size L) :

$$\delta m \equiv m - m_{L=\infty} \sim 1/L^2$$

- CDMFT :
  - A priori : $\delta m \sim 1/L$
  - But : $\delta m_{\text{center}} \sim e^{-L/\xi}$
  - Cavity construction is not exact : error of order 1 at the boundary.
  - Spurious transition in one dimension.
- Large sizes : Clusters DMFT are not better than finite systems !

Convergence properties (2)

- For large clusters, one has to improve CDMFT by using more the result at the center : *See G. Kotliar, S.Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, C.A. Marianetti, Rev. Mod. Phys. 78, 865 (2006)*

- Reweigh the self-energy in the self-consistency condition.

$$\Sigma^{\text{Cluster}}_{\alpha\beta} \rightarrow \Sigma^{\text{w-CDMFT}}_{\alpha'\beta'} = \sum_{\alpha'\beta'} w^{\alpha'\beta'}_{\alpha\beta} \Sigma^{\text{Cluster}}_{\alpha\beta}$$

$$w^{\alpha\beta}_{\gamma\delta} = \delta_{\alpha-\beta,\gamma-\delta} f_c(\alpha) f_c(\beta)$$

$$\sum_{\alpha} f_c(\alpha)^2 = 1$$

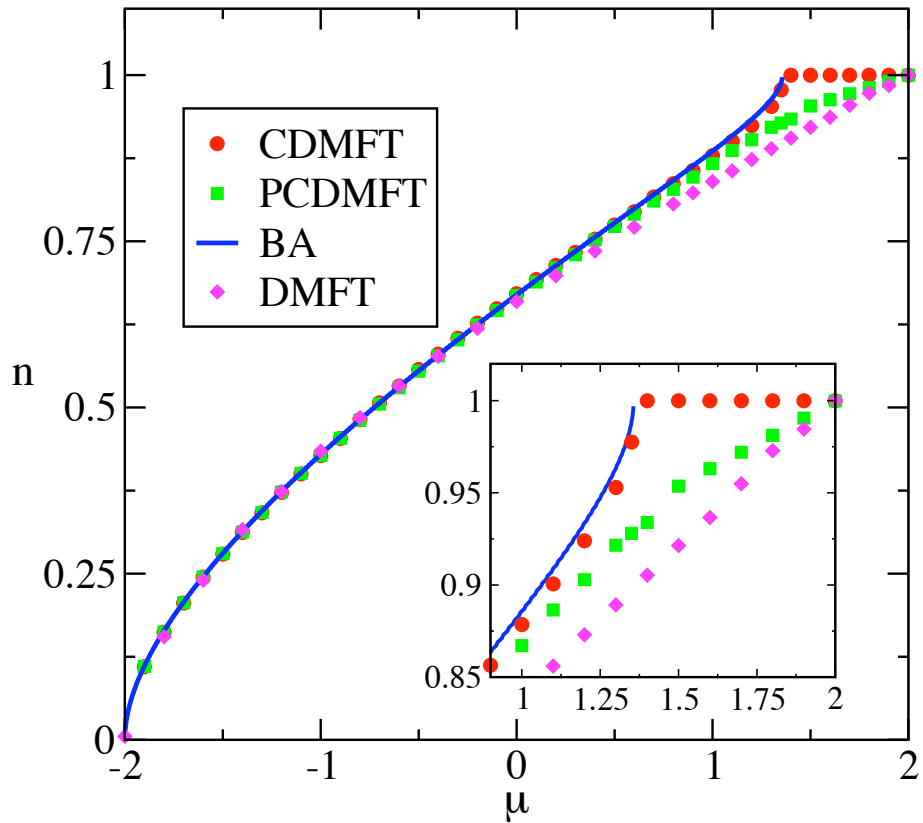
- Remove spurious transition in 1d.Tc convergence close to DCA.

- *This debate is interesting only if one can solve large clusters at large U !*

Test the cluster method in one dimension

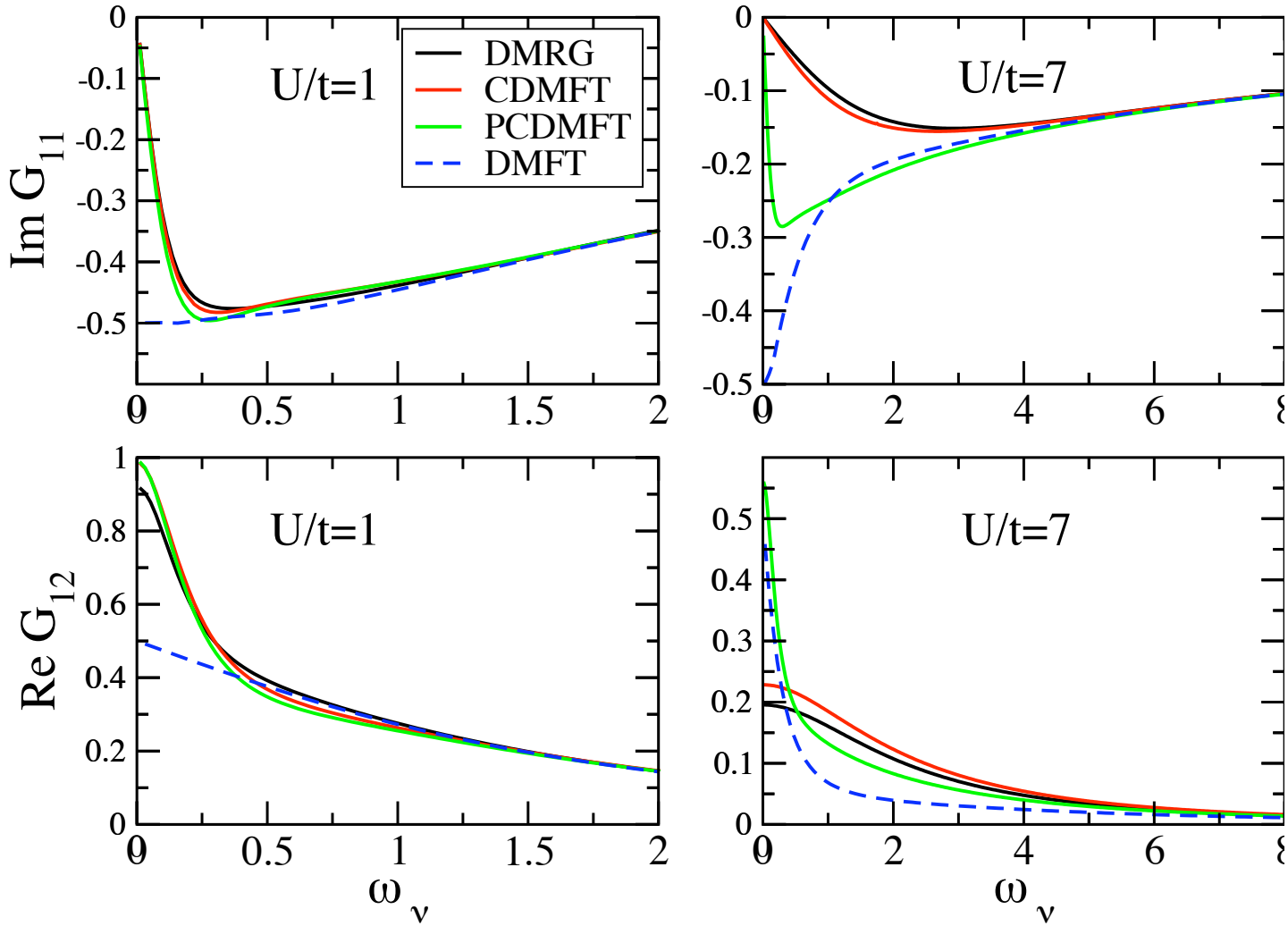
- A priori the worst case for a mean field methods
- Computation of short range physics, thermodynamics.
- DMFT can NOT capture Luttinger liquid large distance physics.
- e.g. : occupation vs chemical potential
  (M. Capone, M. Civelli, S.S. Kancharla, C. Castellani, G. Kotliar, PRB 69 195105 2004)

BA = Bethe Ansatz



Test the cluster method in one dimension (2)

- What about dynamical quantities ?
- Comparison to DMRG (in Matsubara, with Hallberg's algorithm)
  (M. Capone, M. Civelli, S.S. Kancharla, C. Castellani, G. Kotliar, PRB 69 195105 2004)

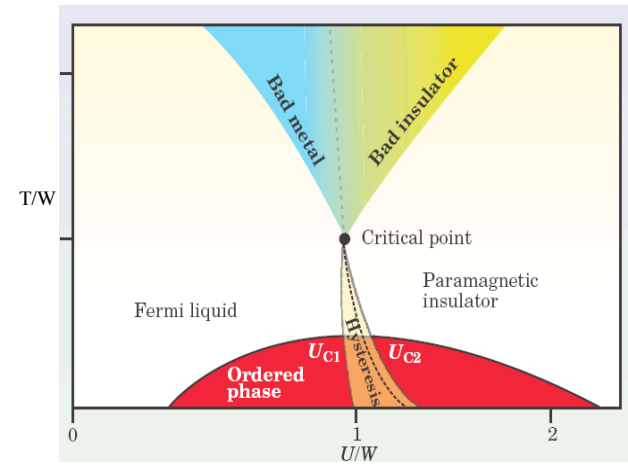


1. Cluster methods.
2. Application to high-Tc superconductors.

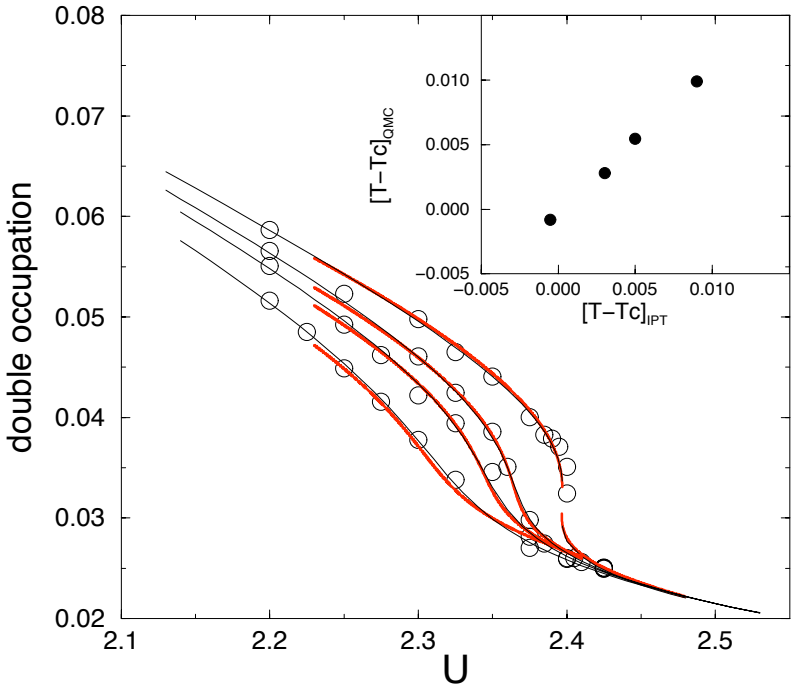
Is the DMFT scenario for Mott transition confirmed by clusters ?

U-driven Mott transition

- Frustrated model: signature of Mott transition in double occupancy, as in 1 site DMFT.
- Frustration is essential ! (hard for QMC)

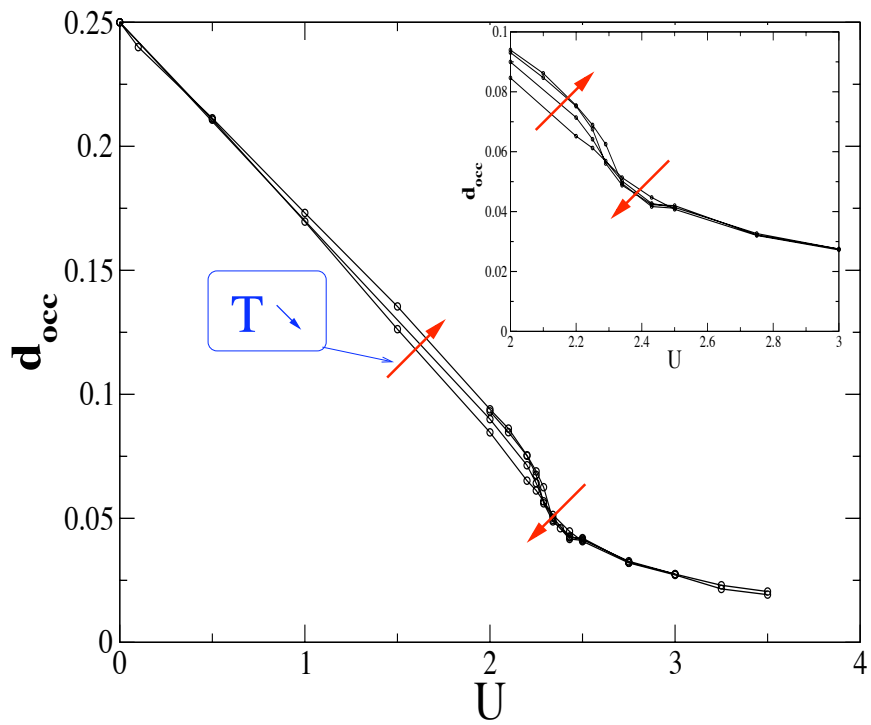


DMFT



(Kotliar et al. condmat/0003016)

C-DMFT (2x2)

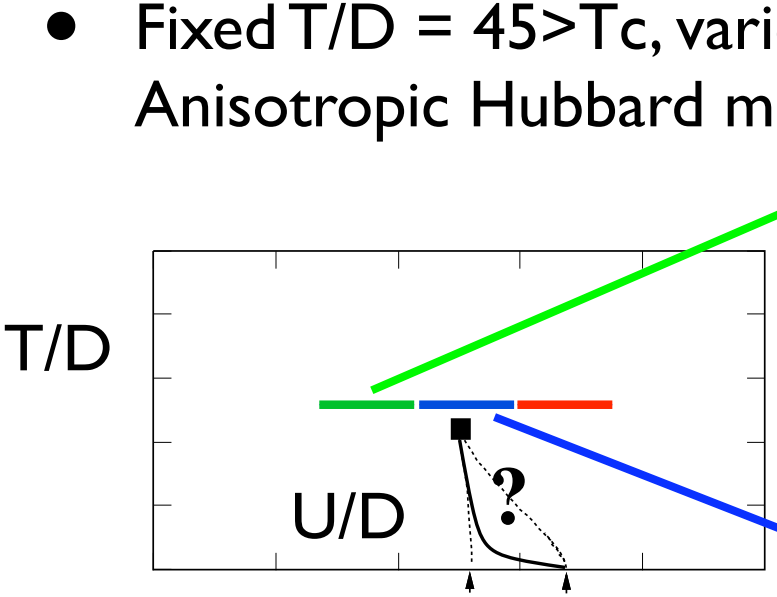


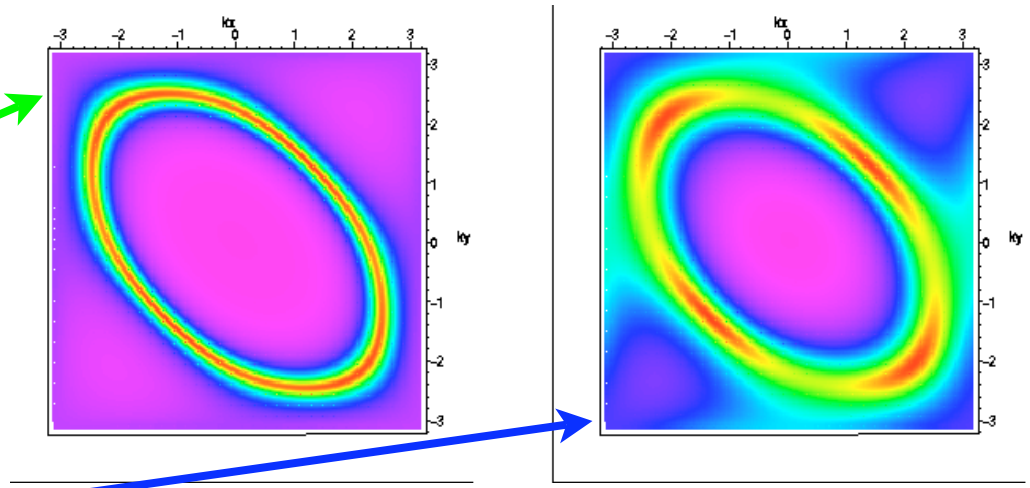
O. Parcollet et al. PRL 2003

But....

Cluster corrections close to Mott transition

- Fixed T/D = 45>Tc, various U.
  Anisotropic Hubbard model





$A(k, \omega = 0^+)$

DMFT metal	Metal. Hot-Cold spots	Finite T insulator
$U/D \leq 2.2$	$2.25 \leq U/D \leq 2.3$	$2.35 \leq U/D$
$\Sigma''_{11} \sim c_1 + \left(1 - \frac{1}{Z}\right) i\omega_n$	$\Sigma''_{11} \sim c_2 + \left(1 - \frac{1}{Z}\right) i\omega_n$	$\Sigma''_{11} \sim c_3$
$\Sigma''_{12}, \Sigma''_{14} \approx 0$	$\Sigma''_{14} \neq 0$	
$\partial_k \Sigma_{\text{lattice}} \approx 0$	Modulation of the finite T lifetime	

DMFT metal : a generic feature at small U, large doping.

Hot Cold regions due to local Mott physics

DMFT metal

Anisotropic metal

Metal

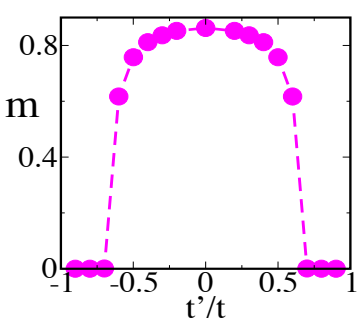
n=1 : Mott

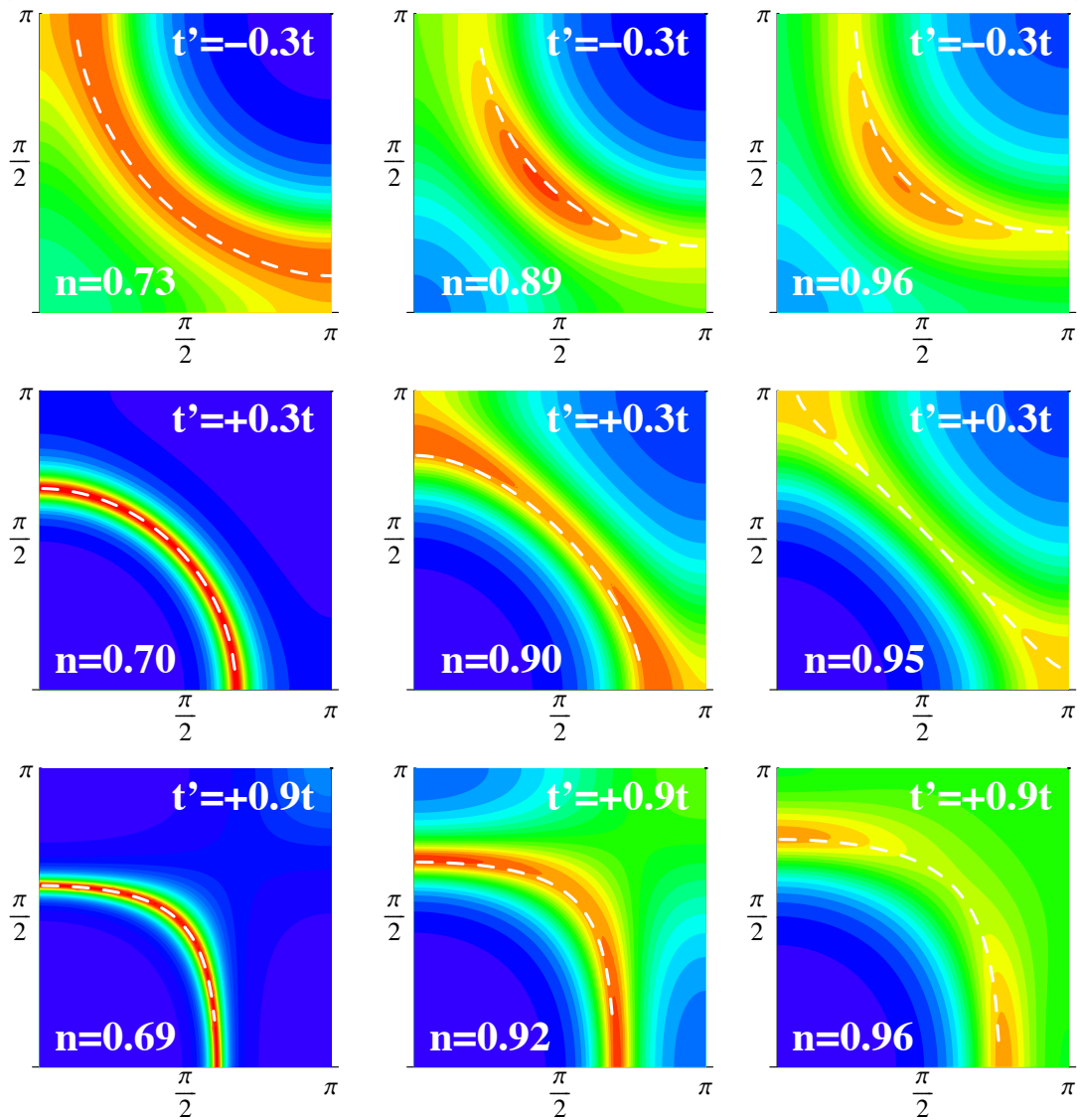
$A(k, \omega = 0^+)$

Teff= D/128, U=16t

t,t' isotropic
Hubbard model
2x2 CDMFT,ED

AF order vs t'/t





Hole doped

Electron doped

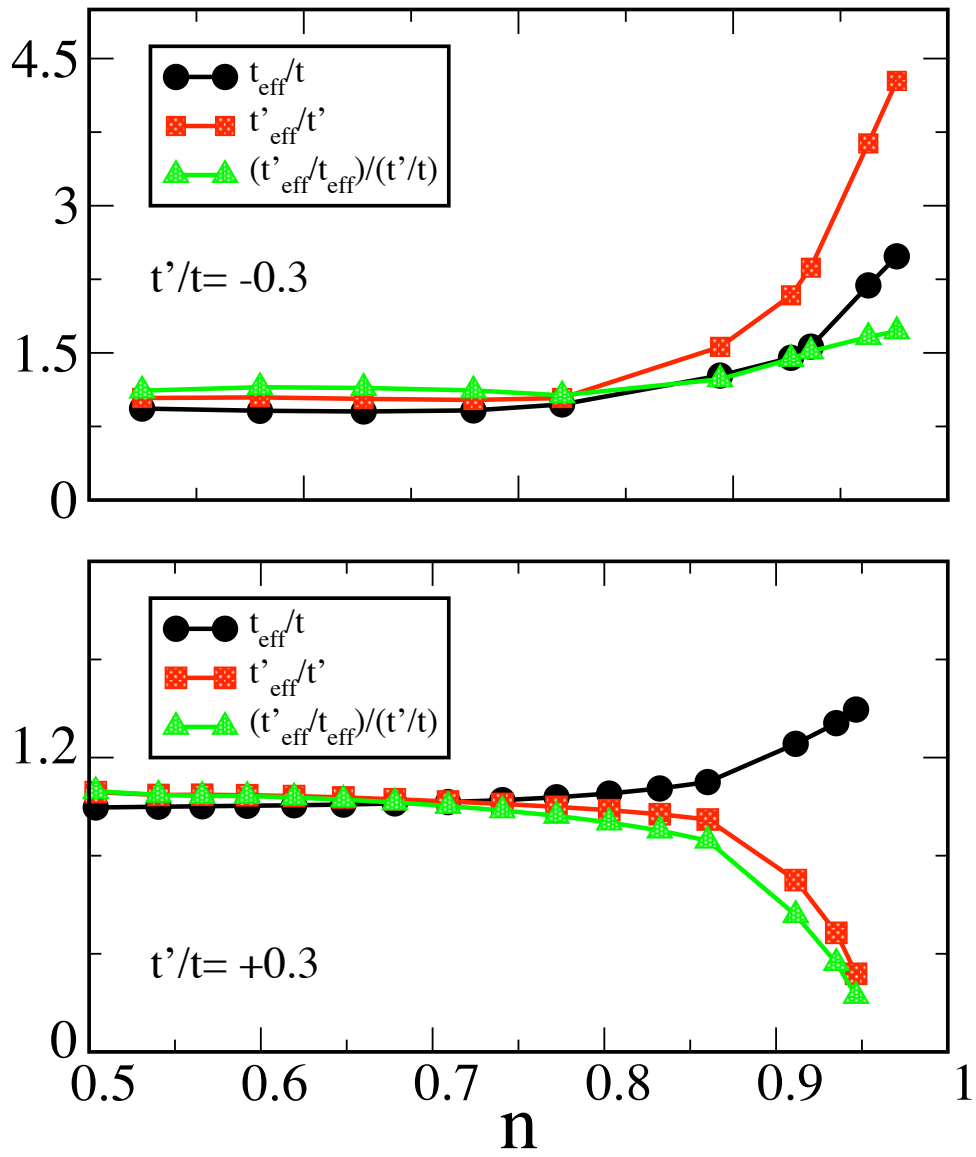
Highly frustrated

M. Civelli, M. Capone, S. S. Kancharla, O.P and G. Kotliar Phys. Rev. Lett. 95, 106402 (2005)

Renormalization of the Fermi surface

$$t_{\rm eff}(k) = t(k) - {\rm Re}\Sigma_{\rm lattice}(k,0)$$

- Fermi Surface can be strongly renormalized by interactions close to the Mott transition.
- Model dependent effect !
- Position of cold regions for hole/electrons doped similar to ARPES

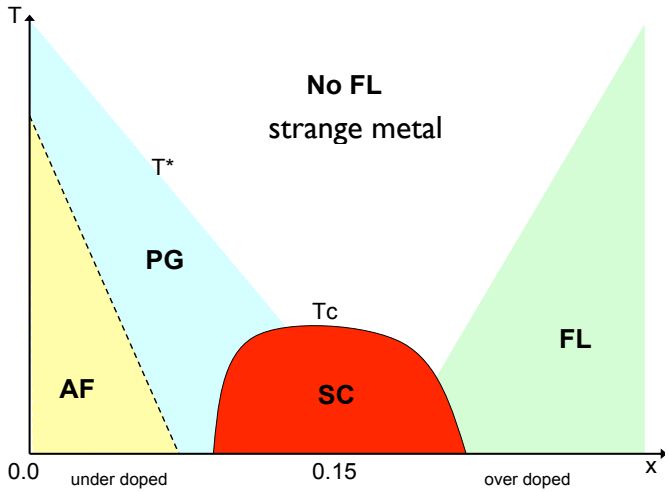


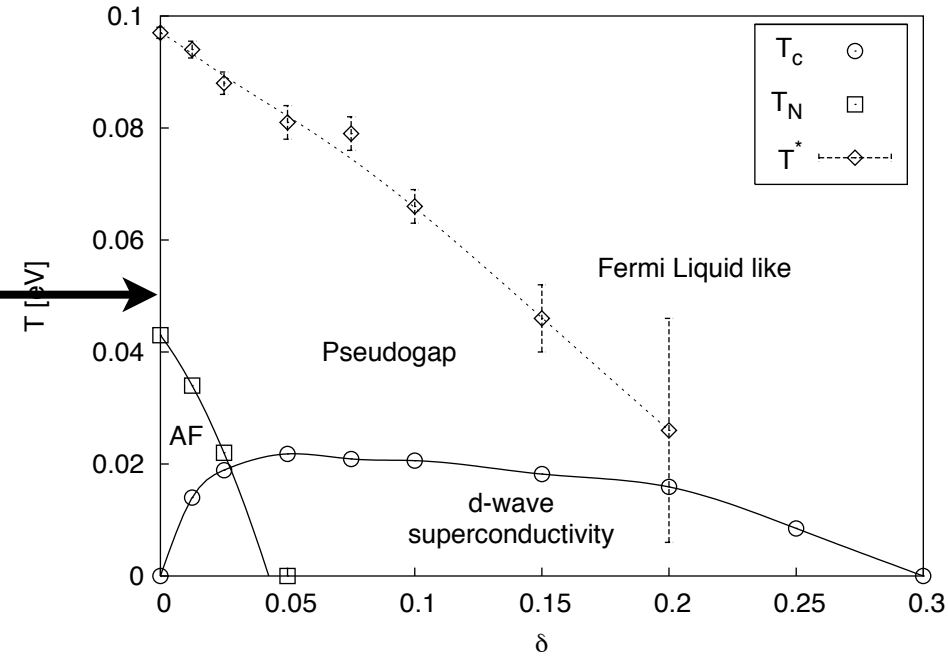
M. Civelli, M. Capone, S. S. Kancharla, O.P and G. Kotliar Phys. Rev. Lett. 95, 106402 (2005)

Phase diagram of the Hubbard model ?

Does the Hubbard model have d-SC ?

- Previous works with clusters :
  - *A. Lichtenstein et al. PRB 62, R9283 (2000)*
  - *DCA : M. Jarrell et al, PRL 85,1524 (2001)*





U/D=2

- Large Clusters at U/D=1 (DCA), up to 26 sites : *Tc ≈ 0.02t*
  T. Maier et al., PRL 95, 237001 (2005)

- 2x2 CDMFT also has d-SC phase, but at lower T *(M. Civelli, K. Haule)*.

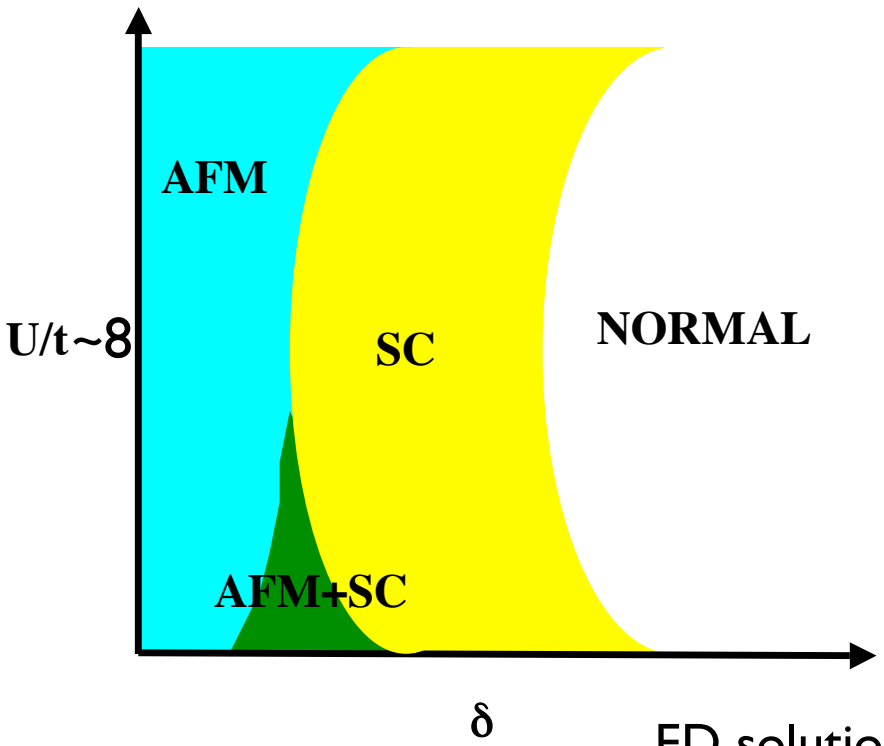
$$T_c \approx t/100 \ll T_c^{\mathrm{DCA\ 2x2}}$$

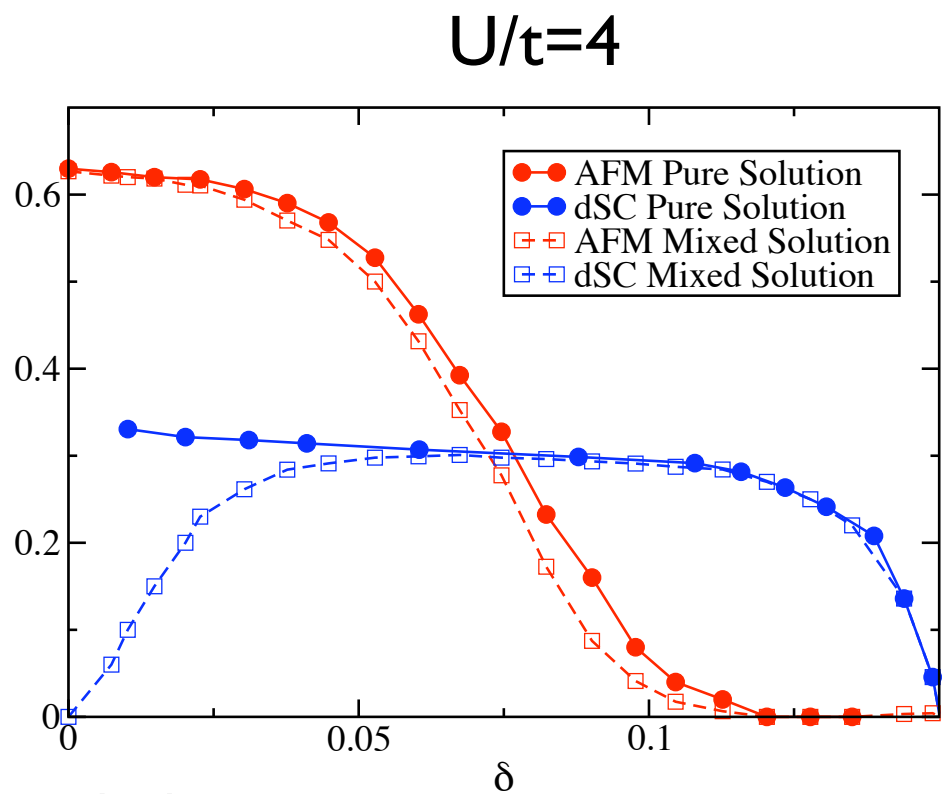
All cluster methods consistently predicts d-SC, AF, with different Tc

AF, d-SC : coexistence or competition ?

M. Capone, G. Kotliar Phys. Rev. B 74, 054513 (2006)

- Qualitative difference between large and small U.
  - Small U : coexistence between AF + d-SC
  - Higher U, first order transition.

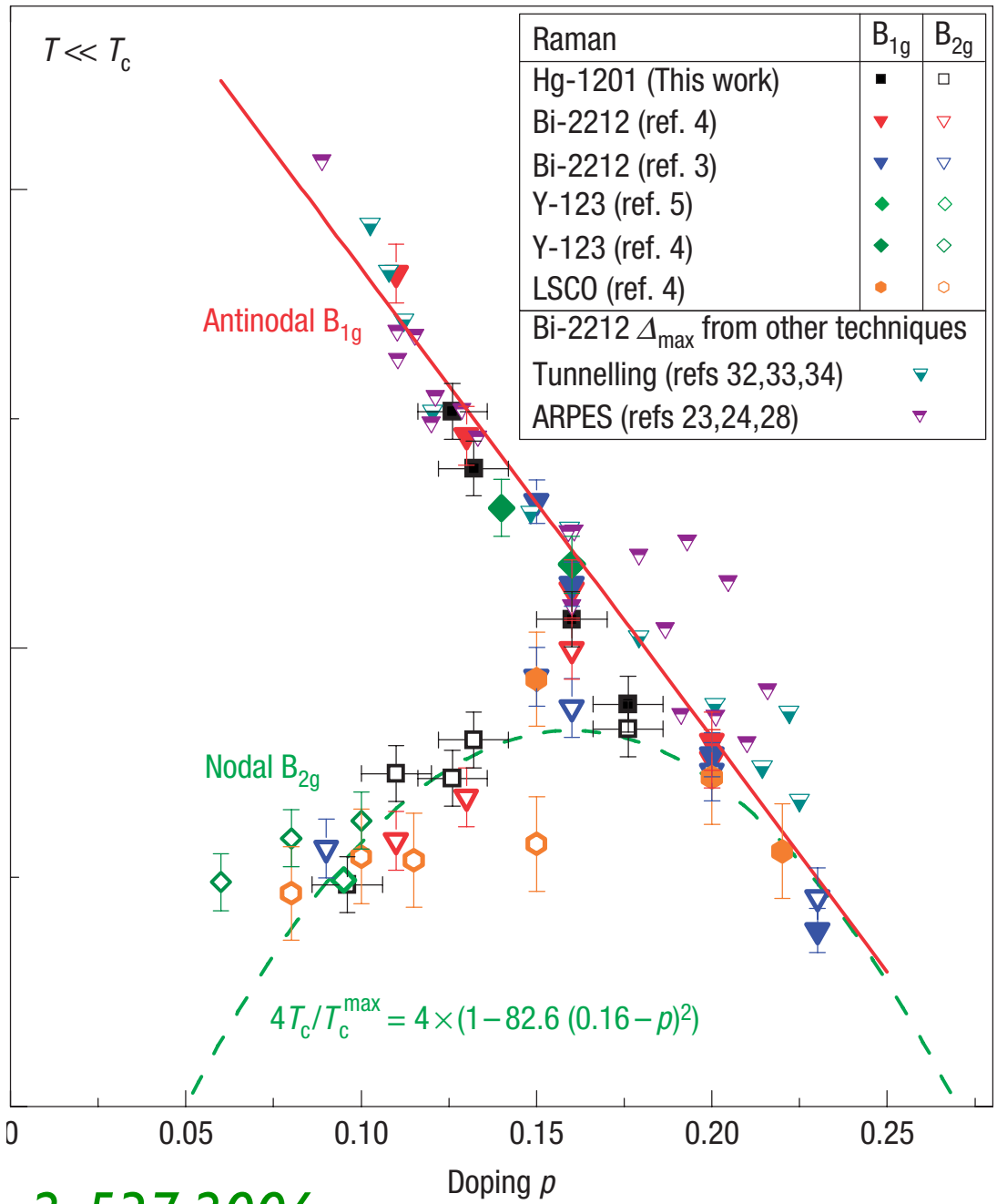




ED solution, 8 sites in bath

Two energy scales in SC phase

- Raman experiments.
- Mesure the gap around the node and at the antinode.

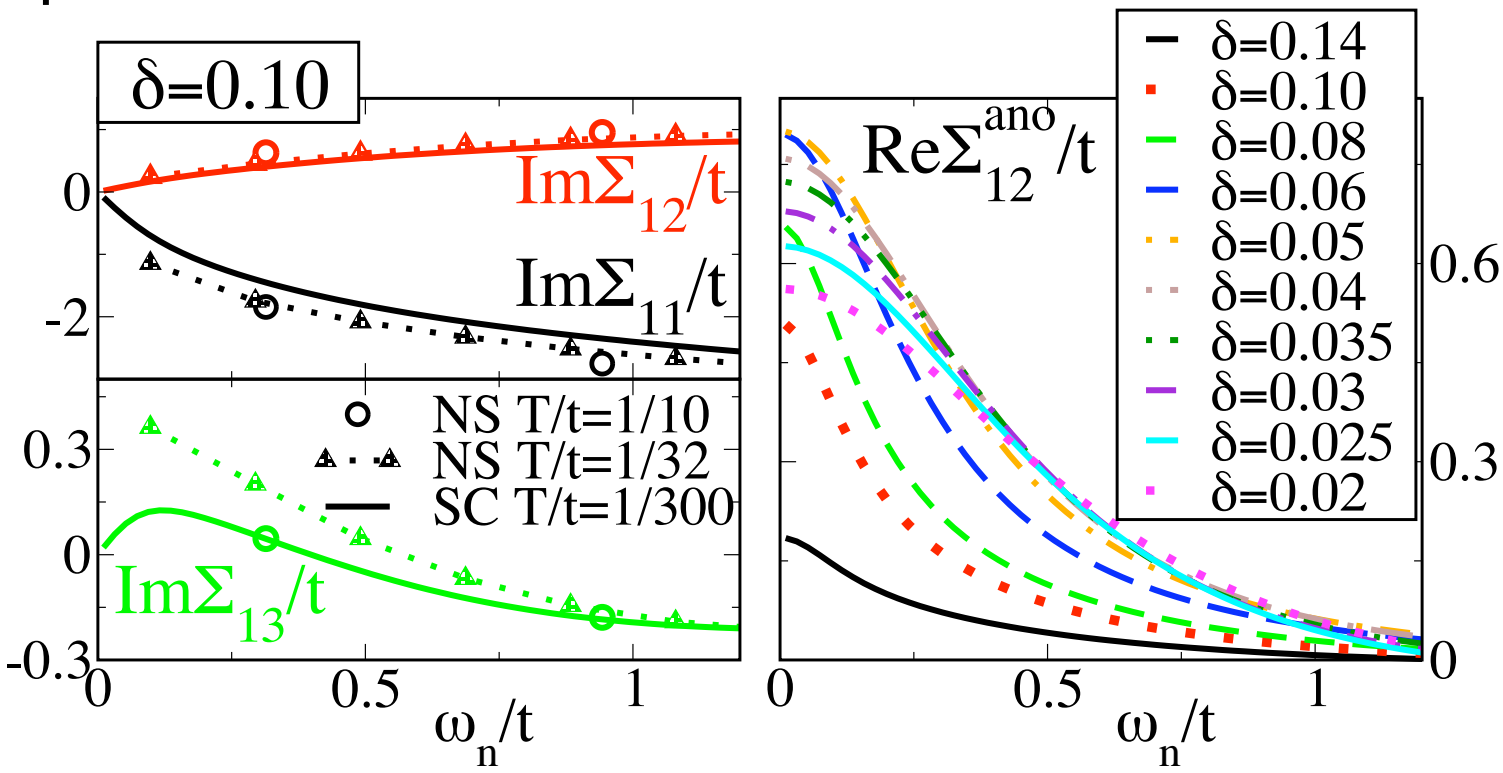


M. LeTacon et al., Nature Physics, 2, 537,2006

2 gaps in high-Tc superconductors

M. Civelli, M.Capone, A. Georges, K. Haule, O. Parcollet, T Stanescu, G. Kotliar, arXiv:0704.1486

- Solution of Hubbard model, 2x2 cluster, ED solver, SC phase
- Cluster quantities :



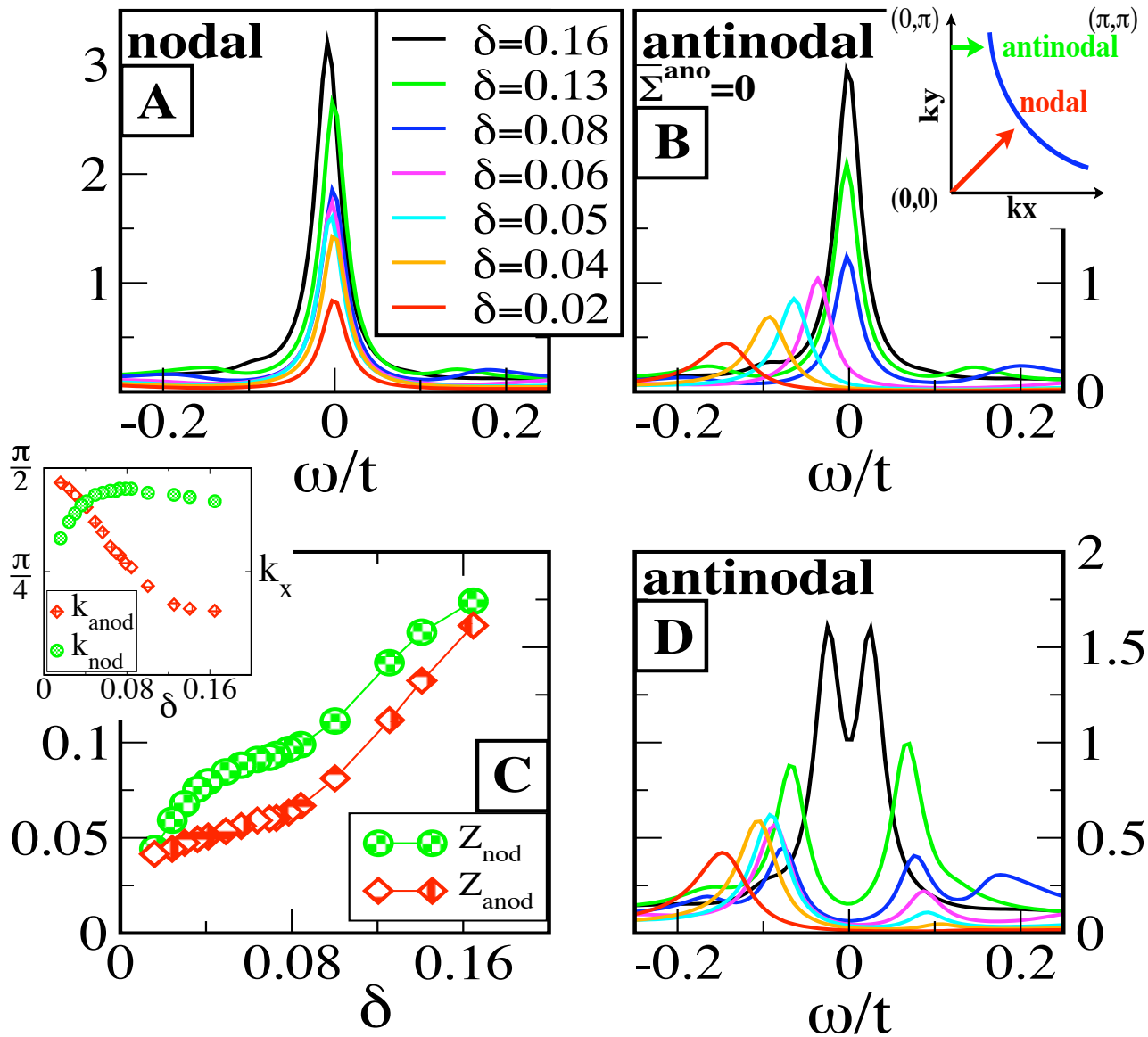
- Anomalous part non-monotonic in δ
- No FL at δ≈0.1 : $\mathrm{Im}\Sigma_{13}(0)$ not zero, does not scale like T^2

2 gaps in high-Tc superconductors

M. Civelli, M.Capone, A. Georges, K. Haule, O. Parcollet, T Stanescu, G. Kotliar, arXiv:0704.1486

- Analyze one particle spectrum, with/without anomalous Σ

- FL in the nodes
- Pseudo-gap at antinodes *(seen previously in normal phase, see below)*
- Asymmetric spectra close to δ=0 in SC



2 gaps in high-Tc superconductors

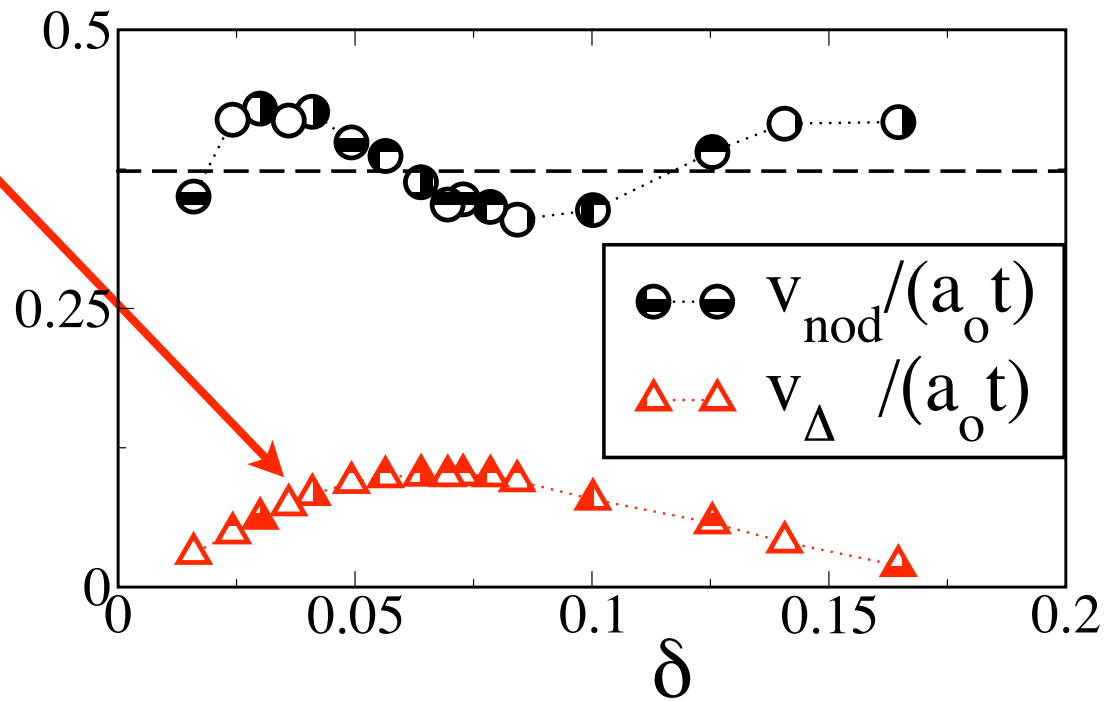
M. Civelli, M.Capone, A. Georges, K. Haule, O. Parcollet, T Stanescu, G. Kotliar, arXiv:0704.1486

- Low frequency analysis close to the node :

$$A(k,\omega) \simeq \mathcal{Z}_{nod}\,\delta\left(\omega - \sqrt{v_{nod}^2 k_\perp^2 + v_\Delta^2 k_\parallel^2}\right)$$

QP velocity ⊥ to FS → $v_{nod} = \mathcal{Z}_{nod}|\nabla_k \xi_k^0|$

Anomalous velocity // to FS
Slope of the gap to the node → $v_\Delta = \mathcal{Z}_{nod}|\nabla_k \Sigma^{\rm ano}(k)|$



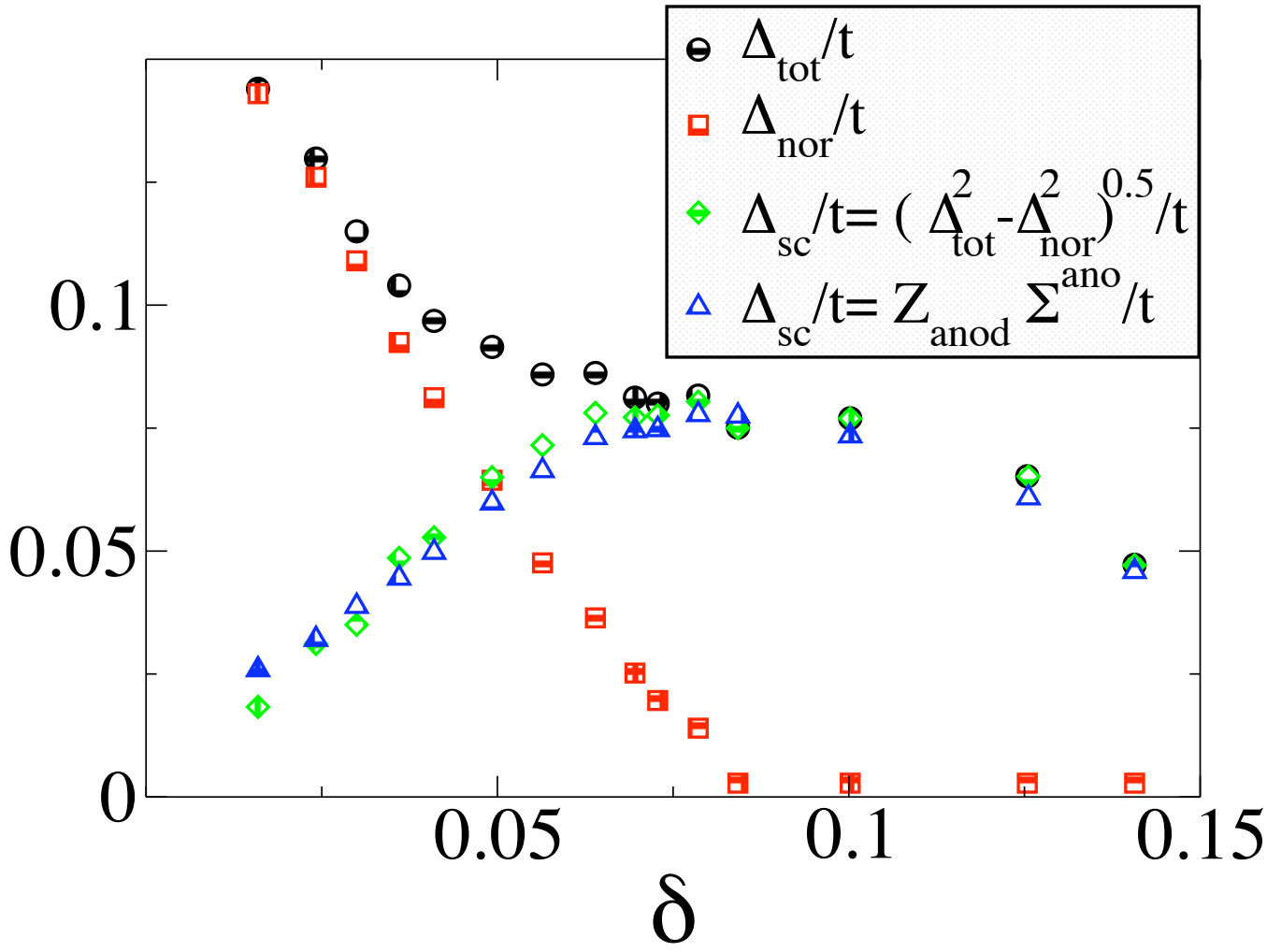
2 gaps in high-Tc superconductors

M. Civelli, M.Capone, A. Georges, K. Haule, O. Parcollet, T Stanescu, G. Kotliar, arXiv:0704.1486

- Decompose the gap in the 1 particle spectrum.

$$\Delta_{sc} = \sqrt{\Delta_{tot}^2 - \Delta_{nor}^2}$$

$$\Delta_{sc}(k) \sim \mathcal{Z}_{anod} |\Sigma^{\rm ano}(k,0)|$$



Two gaps picture similar to experiments

Fermi surface in normal phase ?

1d-2d transition

C. Berthod, T. Giamarchi, S. Biermann, A. Georges, PRL 97, 136401 (2006)

- Chain of spinless fermions with next-neighbor repulsion V, t=1 coupled by inter-chain hopping $t_\perp$.
- 1d + RPA approach : *F.H.L. Essler, A.M. Tsvelik, PRB 65, 115117, (2002)*
- Chain-DMFT : a periodic chain (32 sites) + DMFT in the transverse direction. Keep k resolution within the chain. Well controlled at small $t_\perp$.
- Solve with Hirsch-Fye QMC.

$$\mathcal{S}^0_{\text{eff}} = -\sum_{rr'} \int_0^\beta d\tau d\tau' c_r^\dagger(\tau) \mathcal{G}_0^{-1}(r - r', \tau - \tau') c_{r'}(\tau').$$

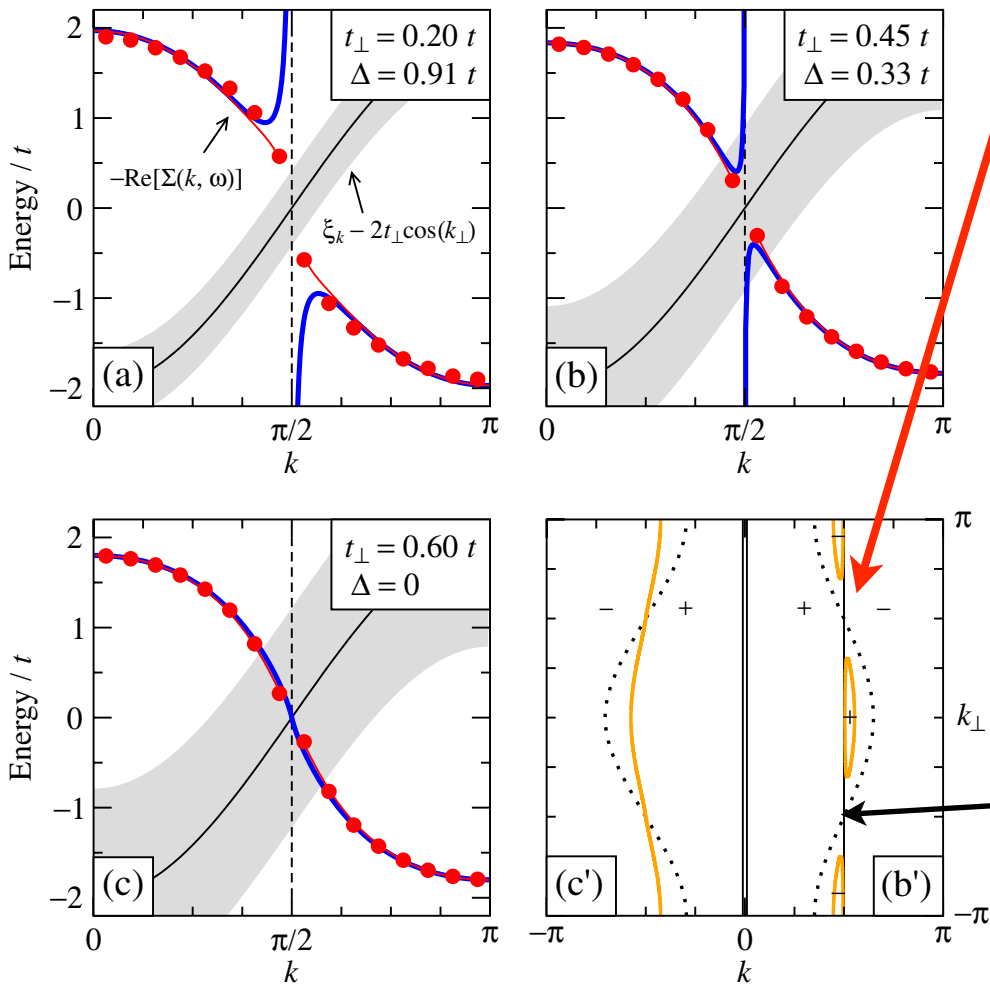
$$\mathcal{G}_0^{-1}(k, \omega) = \omega - \xi_k + \mathcal{G}^{-1}(k, \omega) - R[\mathcal{G}(k, \omega)],$$

$$\Sigma(k, \omega) = \mathcal{G}_0^{-1}(k, \omega) - \mathcal{G}^{-1}(k, \omega).$$

1d-2d transition

C. Berthod, T. Giamarchi, S. Biermann, A. Georges, PRL 97, 136401 (2006)

- 3 regimes in $t_\perp$: insulator, metal with pocket FS, metal with simple FS.



Fit of the self-energy

$$\Sigma(k,\omega) = \frac{(\Delta/2)^2}{\omega + \lambda\xi_k} + (1-\lambda)\xi_k + \Sigma_{int}$$

Red term : simple harmonics expansion in cumulant, not in Σ

Divergence of Σ, line of 0

Finite temperature fit

Zero temperature extrapolation

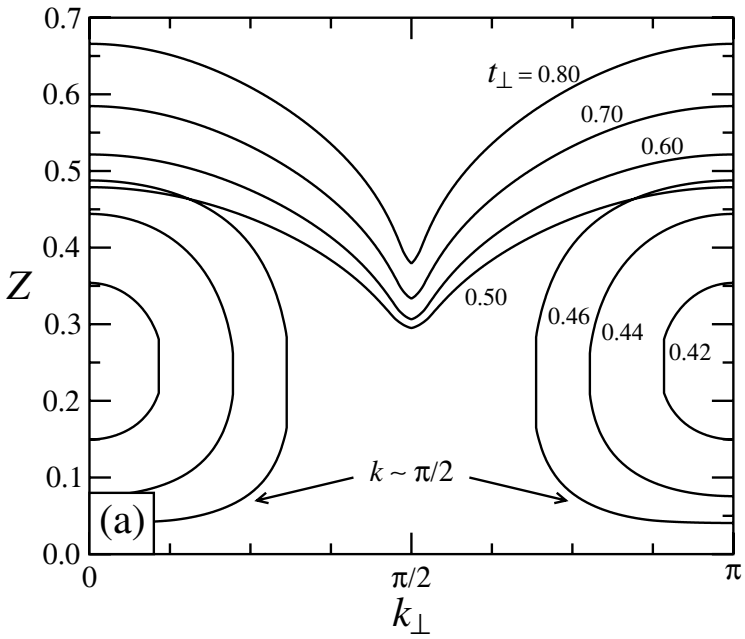
Shaded area : domain covered by the free dispersion

$$\xi_k - 2t_\perp \cos(k_\perp)$$

1d-2d transition

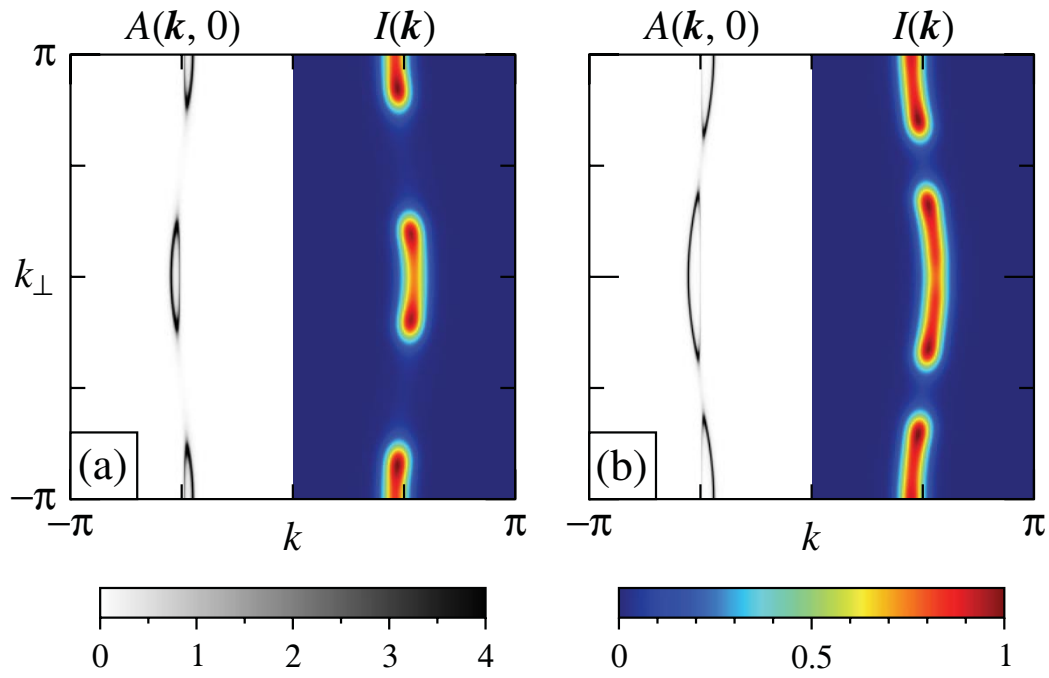
C. Berthod, T. Giamarchi, S. Biermann, A. Georges, PRL 97, 136401 (2006)

Z along the Fermi surface



- Large variation of Z along FS
- Hot spot remains in the metal

ARPES curves



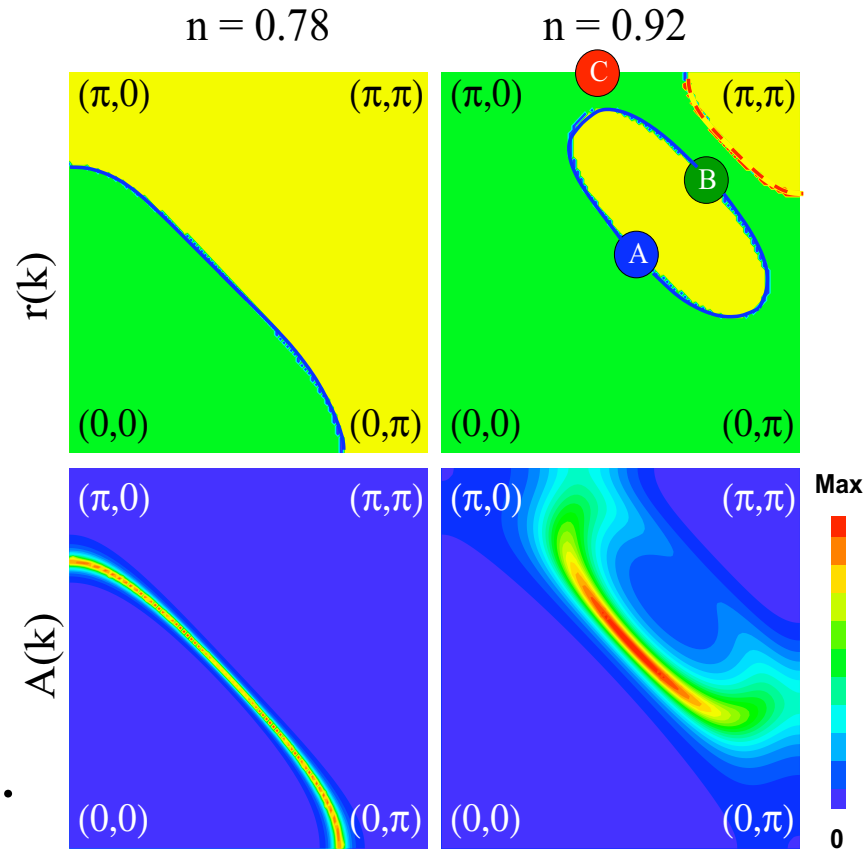
- I(k) : with some k resolution.
- The "rear" part of the FS can not be seen in experiments.

Pocket Fermi surface in 2d ?

(T. Stanescu, G. Kotliar PRB 74, 125110, 2006)

- CDMFT, Hubbard model, U/D = 2, vs δ, ED solver.
- At low δ, a line of zeros of G appears and the topology of the FS changes.
- At finite temperature/resolution, ARPES does not see the second part of the FS.
- ≠ 1d : Luttinger surface appears at low δ and evolve with δ
- Cumulant periodization is necessary here.
- Discussion : resolution ?
- Experiments on YBCO in high field : pocket Fermi surface.

N. Doiron-Leyraud at al, Nature, 2007



Self-energy plot/ ARPES

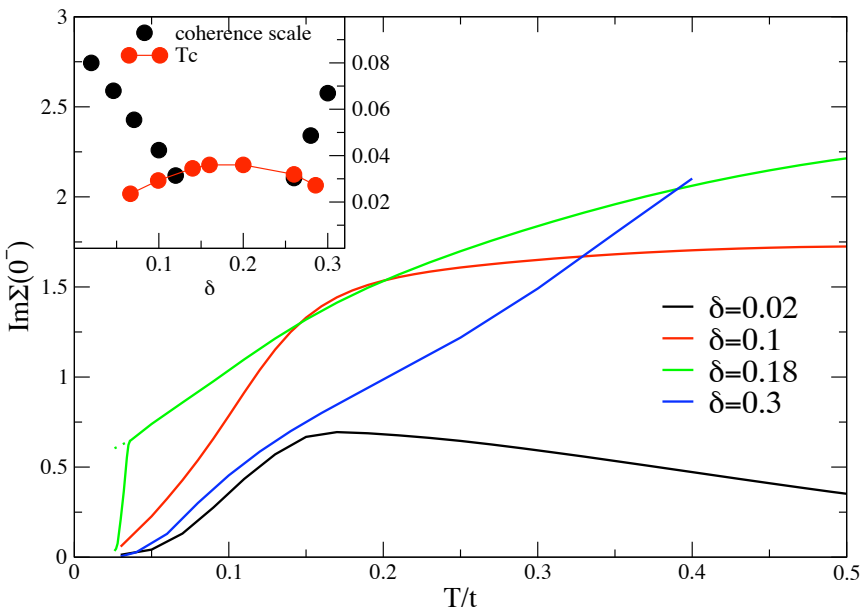
$$r(k,\omega) = t(k) - \mu - \Sigma(k,\omega)$$

Hidden quantum critical point ?

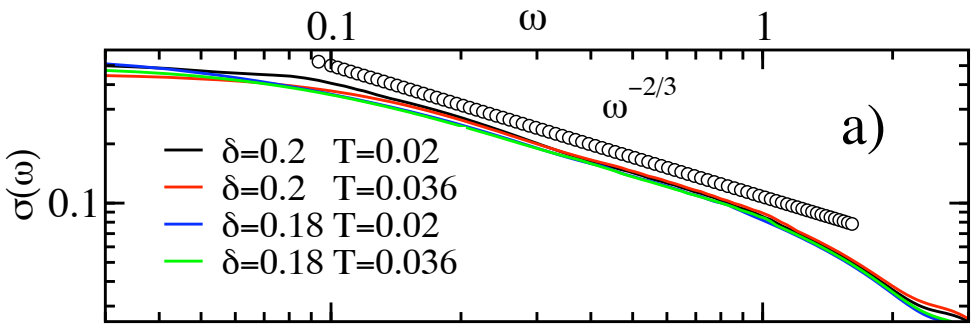
K. Haule, G. Kotliar, condmat/0605149

- Signatures of a critical point in the normal phase at δ≈0.1 (t-J model, NCA solver)

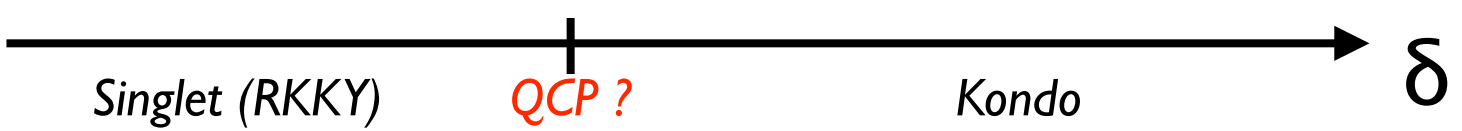
Large scattering rate in the (0,π) component of the cluster Σ.



Power law in optics at optimal doping

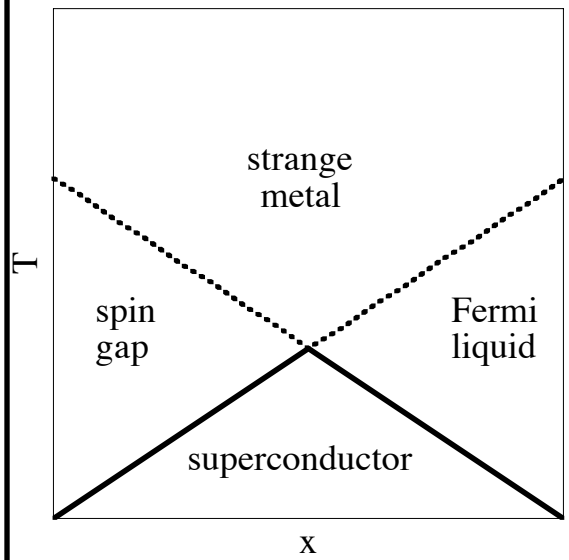


- NCA solution : hint towards a RKKY/Kondo QCP.

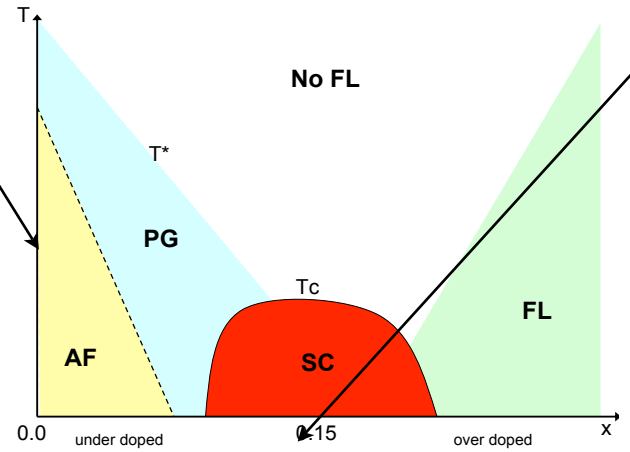


Will CDMFT unify high-Tc theory ??

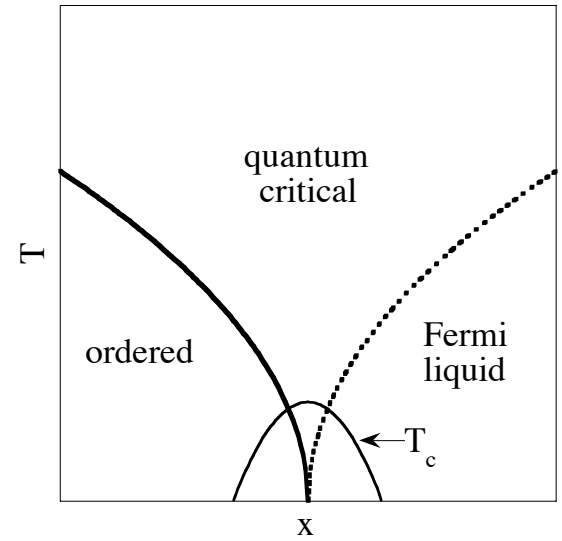
Doped Mott insulator



- RVB (Anderson 87)
- Kotliar-Liu (88)
  Prediction of d-SC !



Quantum phase transition hidden below the SC.



Low energy theory ?

RVB in slave bosons picture

G. Kotliar, J. Liu Phys. Rev. B 38, 5142 (1988)

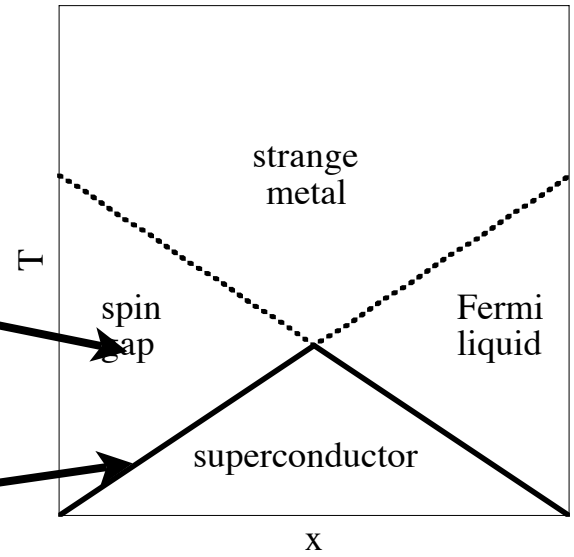
- t-J model in slave boson, no AF order, d-wave superconductivity

$$H = -t\sum_{\langle ij\rangle,\sigma}(f_{i,\sigma}^{\dagger}b_i b_j^{\dagger}f_{j,\sigma}+f_{j,\sigma}^{\dagger}b_j b_i^{\dagger}f_{i,\sigma})-\mu_0\sum_{i,\sigma}f_{i,\sigma}^{\dagger}f_{i,\sigma}$$
$$+J\sum_{\langle ij\rangle}(\sigma_i\cdot\sigma_j)-(1-b_i^{\dagger}b_i)(1-b_j^{\dagger}b_j)+\sum_i\lambda_i\left[\sum_{\sigma}f_{i,\sigma}^{\dagger}f_{i,\sigma}+b_i^{\dagger}b_i-1\right].$$

Schematic phase diagram

Pseudo-gap

Boson condenses



Low energy solution of Cluster DMFT ?

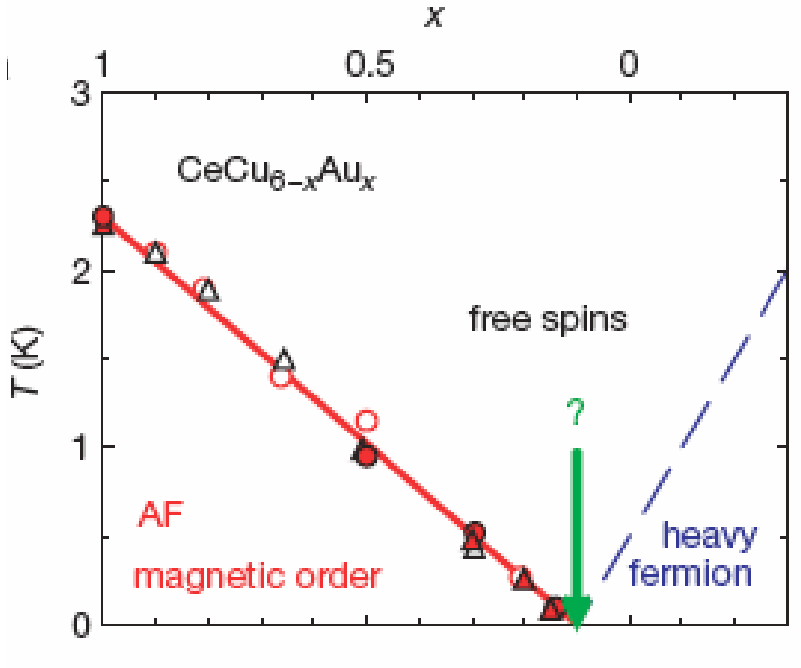
- Slave boson = 1 low energy theory of 1 site DMFT.
  - Σ is independant of k

$$\Sigma(k,\omega) = const + \omega\left(1 - \frac{1}{Z}\right), \quad Z = \delta$$

- Generalization : rotationally-invariant slave-boson
  F. Lechermann, A. Georges, G. Kotliar, O.Parcollet, arXiv:0704.1434
  - Describe multiplets (for realistic systems)
  - Describe Z(k) (variation along the Fermi surface)
  - Tested against CDMFT at low energy (Hot/cold region e.g.)

Heavy fermions

- Another class of strongly correlated materials
- Quantum critical points : scenario under debate...



- Theoretical model : Periodic Anderson Model.

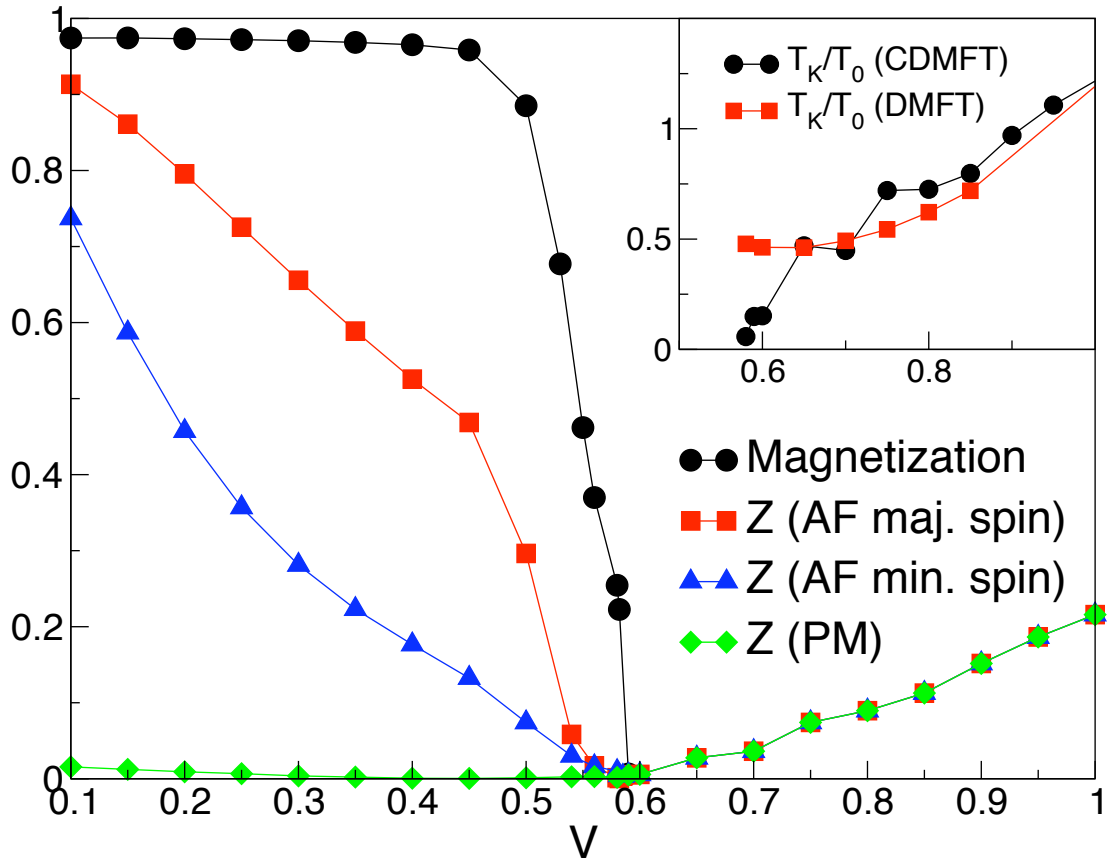
$$H = -t\sum_{\langle ij\rangle} c^{\dagger}_{i\sigma}c_{j\sigma} - \mu\sum_{i} c^{\dagger}_{i\sigma}c_{i\sigma} + V\sum_{i}\left(f^{\dagger}_{i\sigma}c_{i\sigma} + h.c.\right)$$
$$+(E_f-\mu)\sum_{i} f^{\dagger}_{i\sigma}f_{i\sigma} + U\sum_{i} n^{f}_{i\uparrow}n^{f}_{i\downarrow} \qquad (1)$$

Cluster for Anderson lattice

- Cluster DMFT solution of the Anderson lattice model (2 sites, ED solvers)

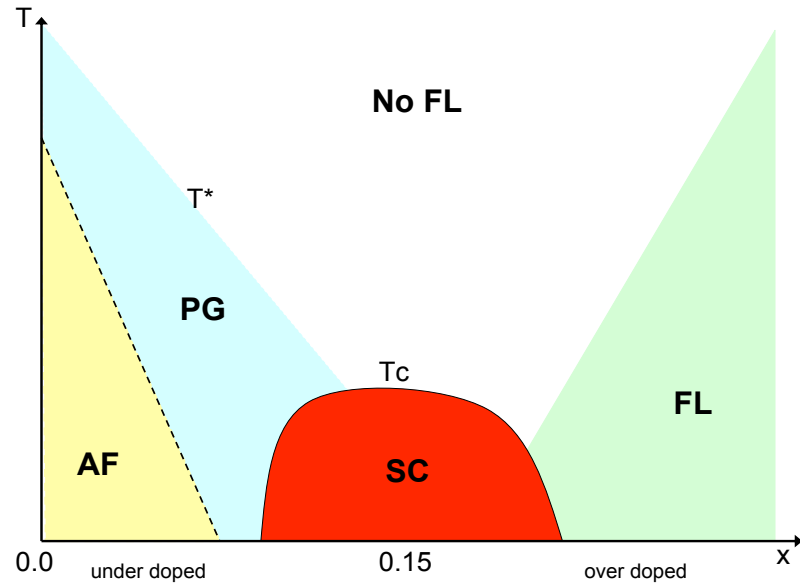
  L. De Leo, M. Civelli, G. Kotliar, condmat/0702559;
  see also work by Q. Si (extended DMFT), P. Sun et al...

- Work in progress : test various scenarios...



Summary

- CDMFT : a "dynamical" RVB ? Not only !
- Various phases (AF, PG, d-SC)
- SC phase : 2 gaps
- Normal phase : strong dichotomy node/antinodes. Pocket FS.



- Hidden quantum critical point ?
  Towards a unified theory with RVB and QCP ?
- Work still in progress :
  - Low energy solution : build a simple picture out of DMFT results.
  - Vertex calculation/ Real ω exact solution ?
  - Improve k resolution (patch basis)

Tomorrow

S. Biermann : DMFT and realistic calculations !