DMFT and beyond :

From quantum impurities to high temperature superconductors

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Outline

1. Physical motivations
2. DMFT and clusters
3. Selective Mott transition in k space
4. Two gaps in the SC phase

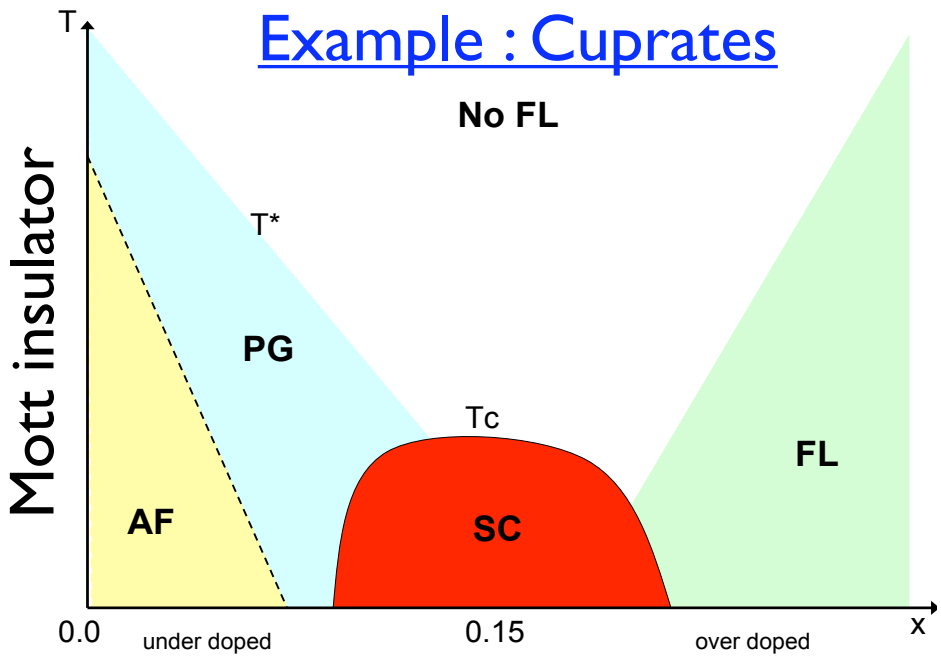
Mott physics

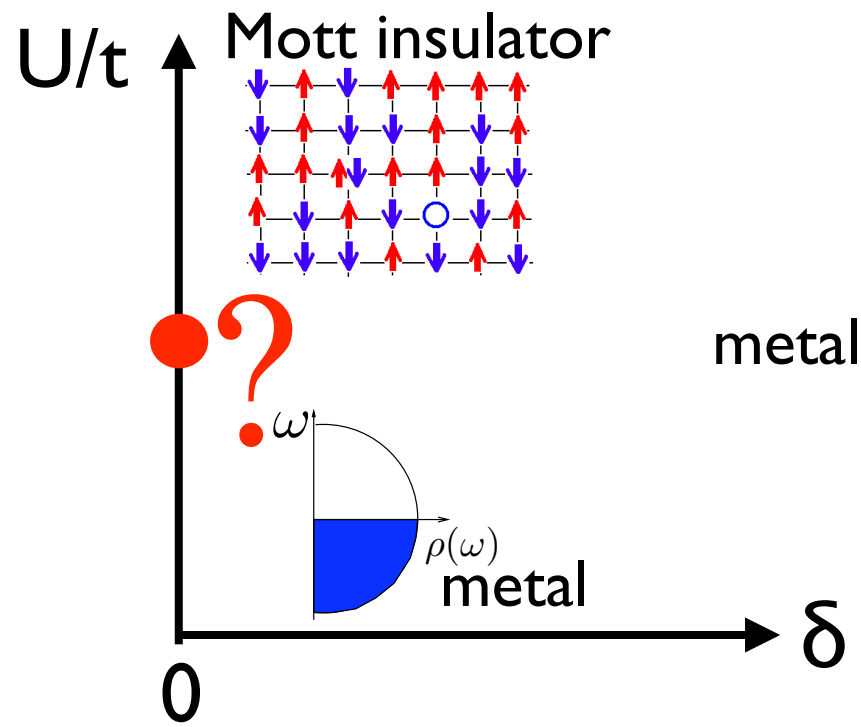
- Mott transition = Metal-Insulator transition due to interactions
- Hubbard model, a minimal model for theorists.

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

$$\delta = 1 - \langle n_{\uparrow} + n_{\downarrow} \rangle$$

How is a metal(superconductor) destroyed close to a Mott transition ?





Doped Mott insulators Anderson (1987), ...

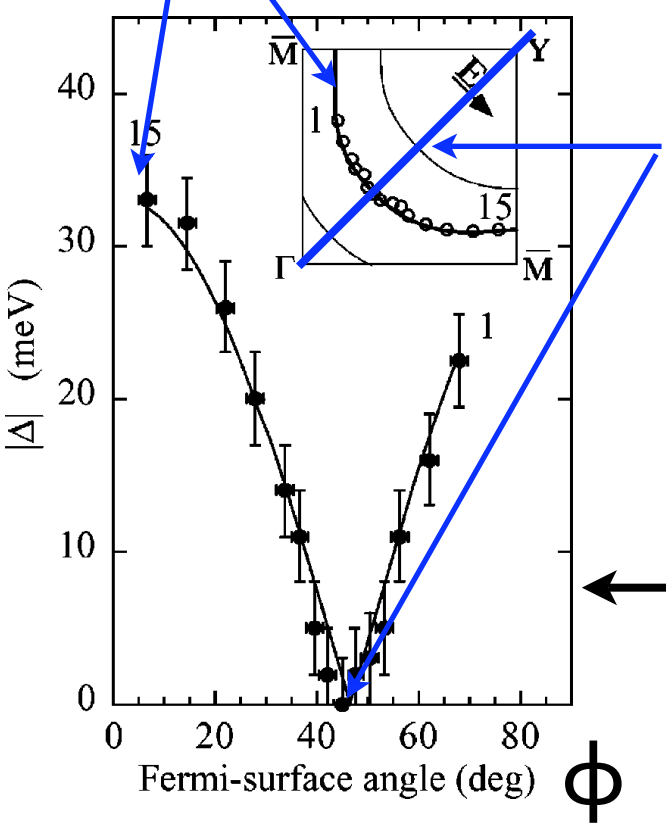
Nodes and Antinodes

d-wave gap and order parameter (with nodes)

$$\Delta(k) \propto \Delta_0\left(cos(k_x) - cos(k_y)\right) + \ldots$$

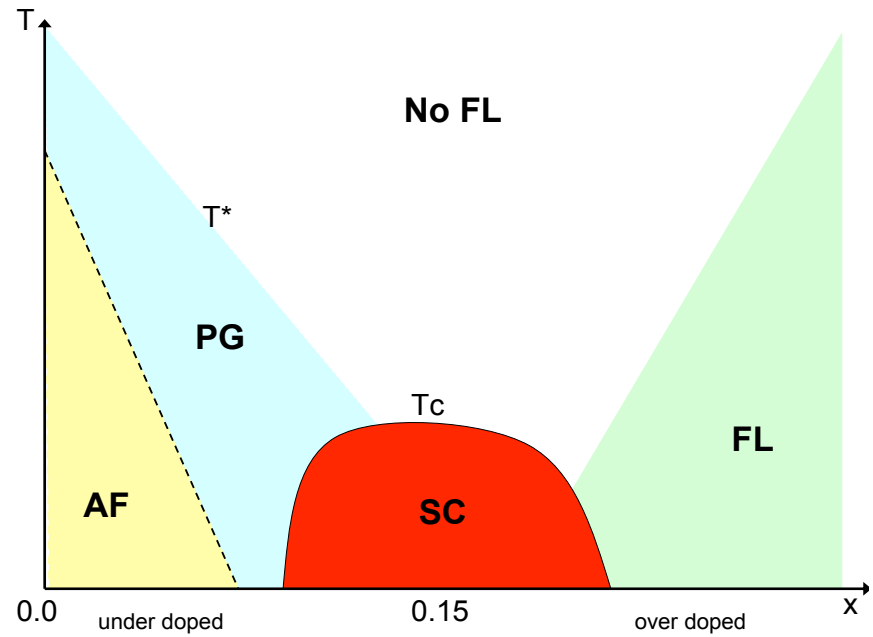
Antinodal direction

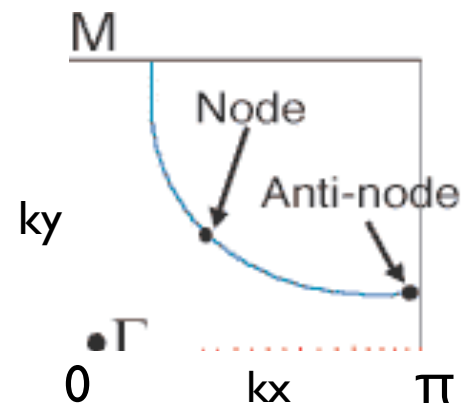
Nodal direction



← ARPES

Ding et al,1996



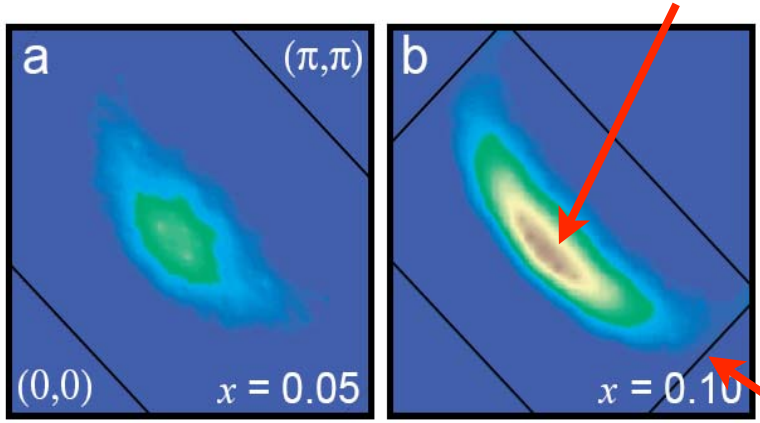


Fermi Arcs

- Spectral intensity map at Fermi level (ARPES) $A(k, \omega = 0)$

Bi2212 : Kanigel et al. Nature 2,447 (2006)

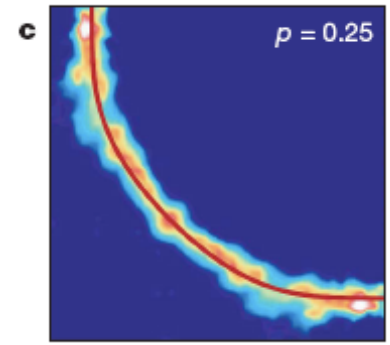
$Ca_{2-x}Na_xCuO_2Cl_2$



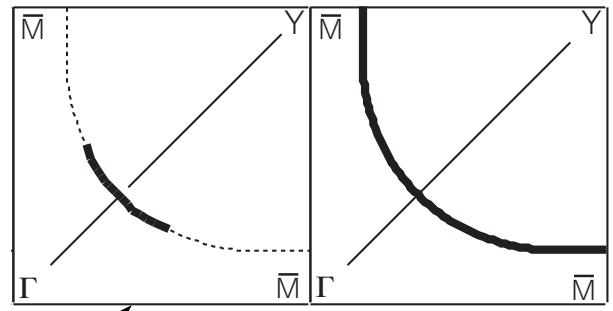
Quasi-Particle

No Quasi-Particle

Shen et al. Science 307, 901 (2005)



"Good" Fermi liquid

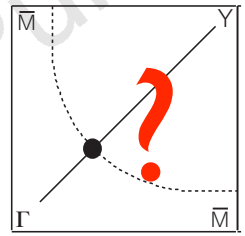


δ↘

Arcs shrinks for δ→0

Nature of the Fermi Arcs ?

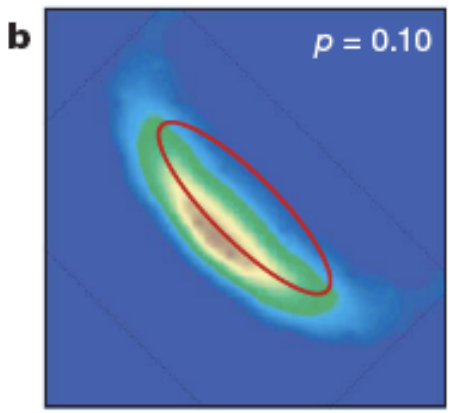
- What is the low temperature normal state ?
- Vanishing arcs at T=0 ? Nodal liquid ?
  Kanigel et al. Nature 2,447 (2006)



- Fermi liquid with strong variations of Z, T_{coh}, m* along the Fermi surface ?

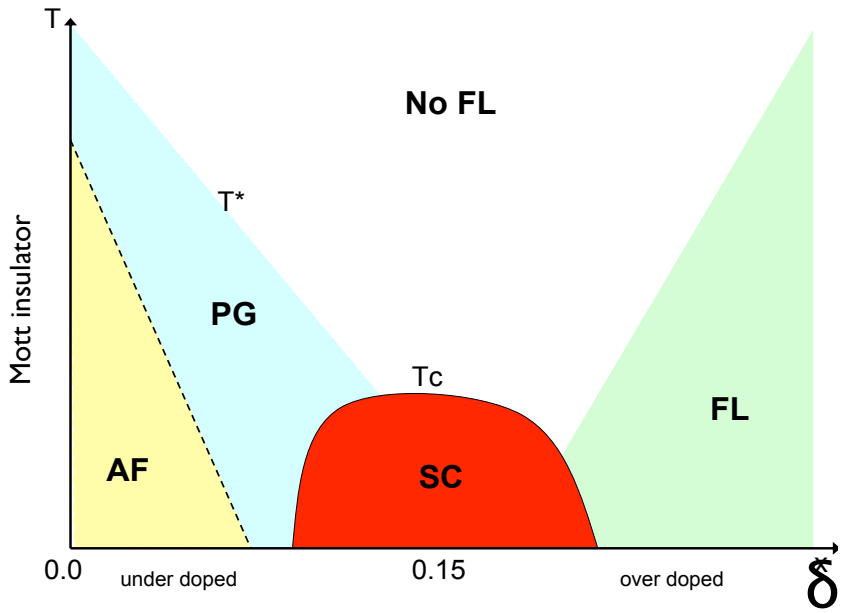
$$T_{\rm coh}^{\rm Antinode} < T < T_{\rm coh}^{\rm Node} \quad ?$$

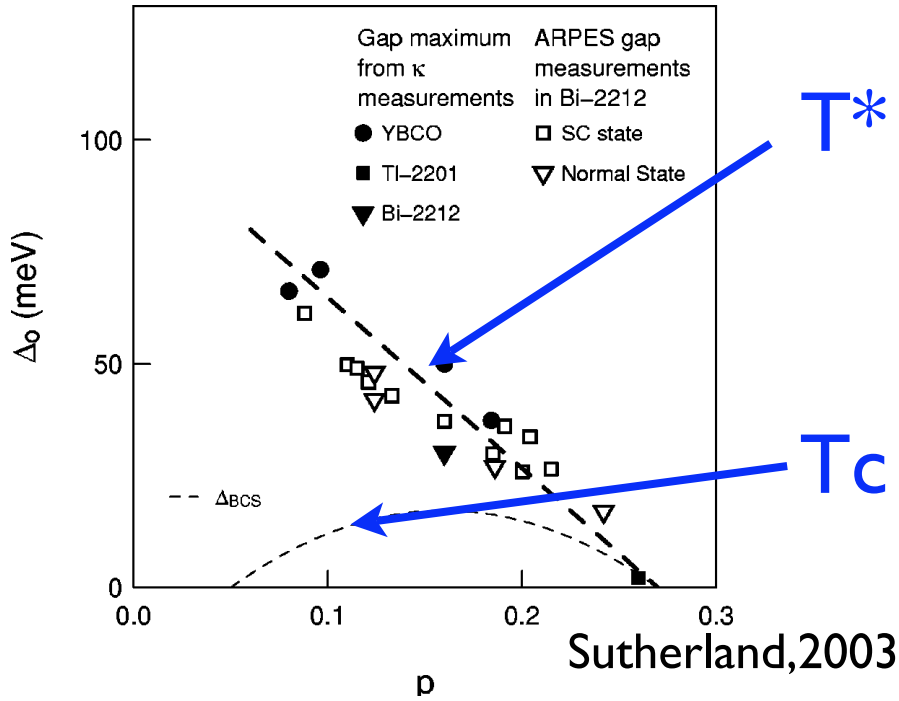
- Quantum oscillations in strong magnetic field (Shubnikov-de Haas) *N. Doiron-Leyraud at al, Nature, 2007*
  - Low temperature, suppress SC with field
  - Pocket Fermi surface in the normal state ?



SC phase

- Evolution of the superconducting gap with doping δ
- Non-BCS behaviour : $\Delta_0(\delta) \not\propto T_c(\delta)$





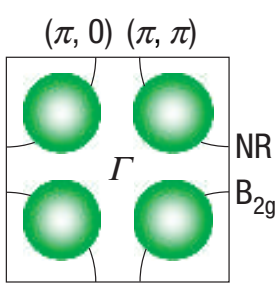
- But recent experiments suggest this is too simple ....

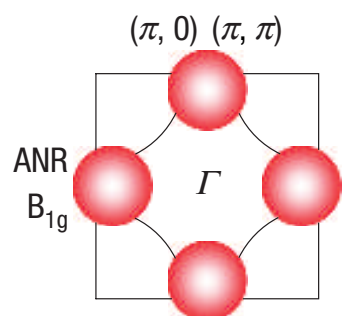
Electronic Raman spectroscopy

$\chi''(\omega)$

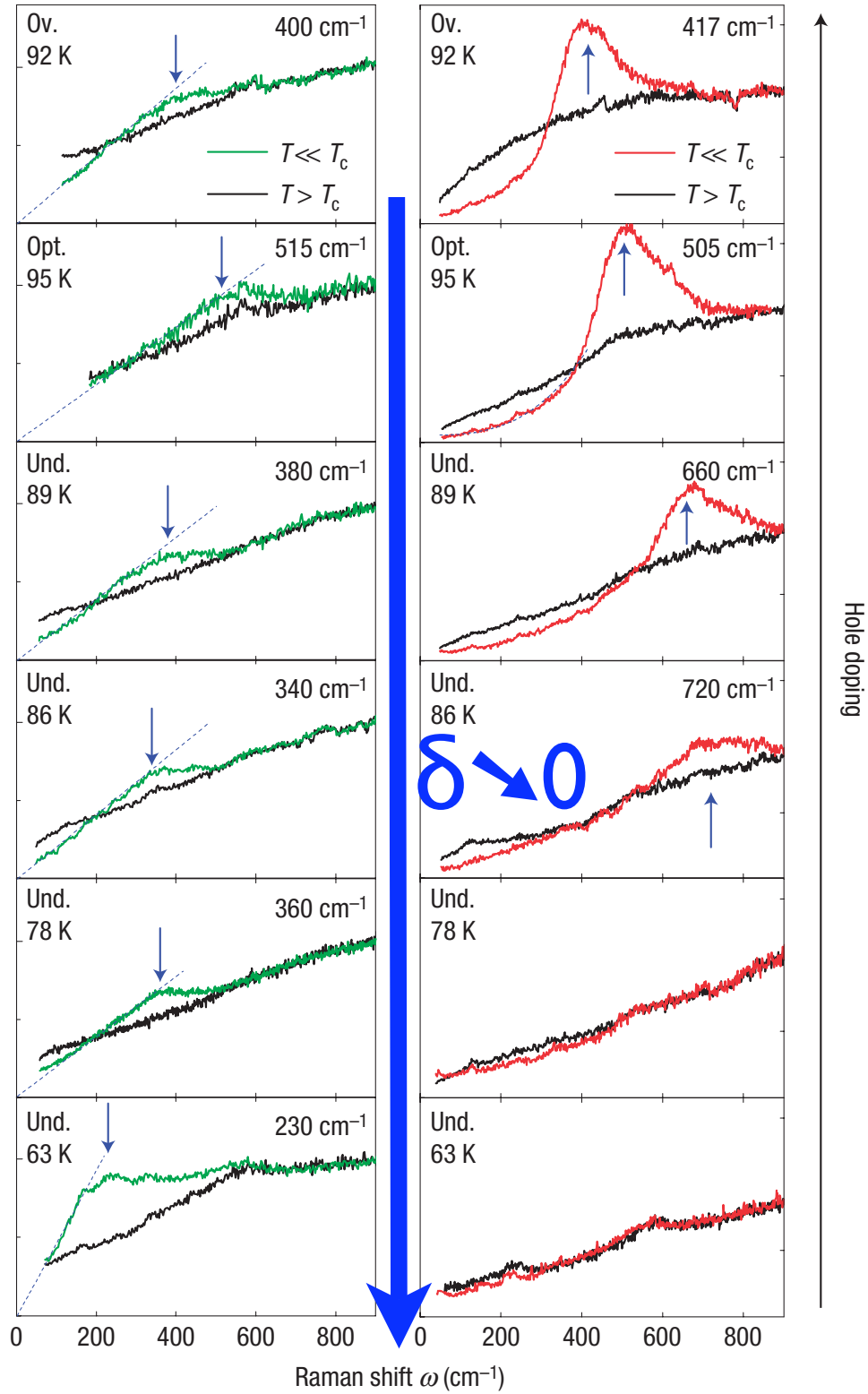
M. LeTacon, A. Sacuto, A. Georges, G. Kotliar, Y Gallais, D. Colson and A. Forget, Nature Physics, 2, 537,2006

- $HgBa_2CuO_{4+\delta}$
- 2 set of measures, probing Nodal Region (NR) and Antinodal Region (ANR)

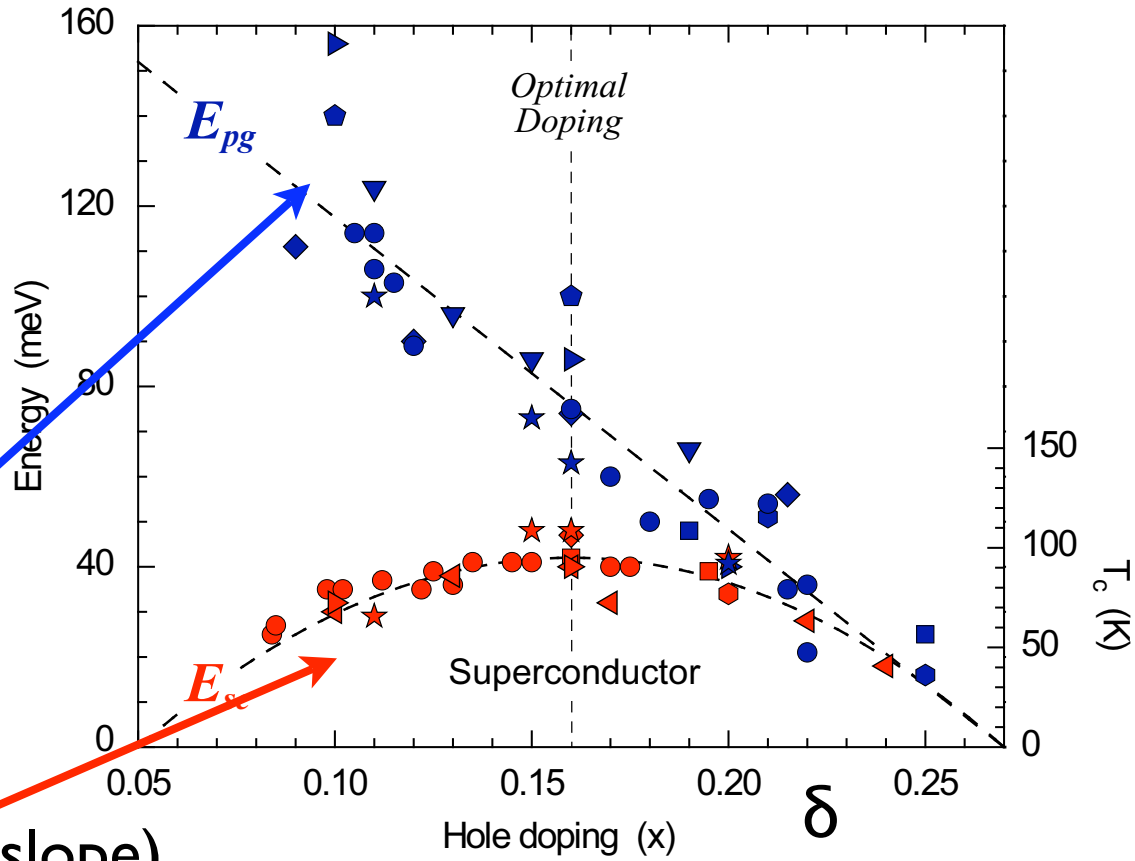




- No BCS fit
- Two energy scales in the SC phase



"Two gaps" in SC phase ?



- Gap at antinode (maximum) increases for δ→0.
- Gap close to node (slope) decreases for δ→0, like Tc.

picture from arXiv:0706.4282

- Raman experiments.
  M. LeTacon et al., Nature Physics, 2, 537,2006
- See also ARPES experiments.
  Tanaka et al,Science 314, 1910, (2006)

$$v_\Delta = \left.\frac{d\Delta(\phi)}{d\phi}\right|_{\text{Node}} \to 0 \text{ for } \delta \to 0$$

- Still debated...

Nodal-Antinodal dichotomy : summary

- *Normal phase* :
  - Fermi Arcs
  - Quasi-particle in the nodes, pseudogap in the antinode
- *Superconducting phase* :
  - Two behaviours of the gap of 1-particle Green function(?)
- Phenomenological idea :
  - Node like an ordinary Fermi liquid/SC
  - Antinode more like an insulator
- Can we understand this from a systematic microscopic calculation e.g. of Hubbard model ?
- What is the mechanism ?

In this talk : DMFT approach

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1. Physical motivations
2. DMFT and clusters
3. Selective Mott transition in k space
4. Two gaps in the SC phase

Dynamical Mean Field Theory

A. Georges, G. Kotliar, W. Krauth and M. Rozenberg, Rev. Mod. Phys. 68, 13, (1996)
G. Kotliar, S.Y. Savrasov, K. Haule, V. S. Oudovenko, OP, C. Marianetti, Rev. Mod. Phys. 78, 865 (2006)

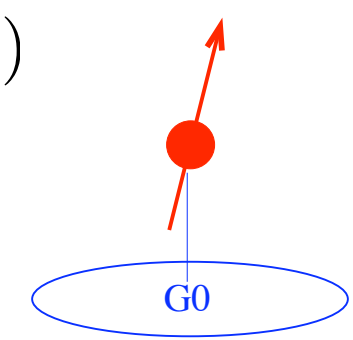
- *Ising model* (Weiss) : A single spin in an effective field.
- *Fermionic Hubbard model* (Kotliar-Georges, 92)
  Anderson impurity with an effective band determined self-consistently

$$H = \underbrace{\epsilon_0 \sum_{\sigma=\uparrow,\downarrow} c^\dagger_\sigma c_\sigma + U n_\uparrow n_\downarrow}_{\text{Local site}} + \underbrace{\sum_{k,\sigma=\uparrow,\downarrow} V_{k\sigma} \xi^\dagger_{k\sigma} c_\sigma + h.c. + \sum_{k,\sigma=,\downarrow} \epsilon_{k\sigma} \xi^\dagger_{k\sigma} \xi_{k\sigma}}_{\text{Coupled to an effective electronic bath}}$$

$$\Updownarrow$$

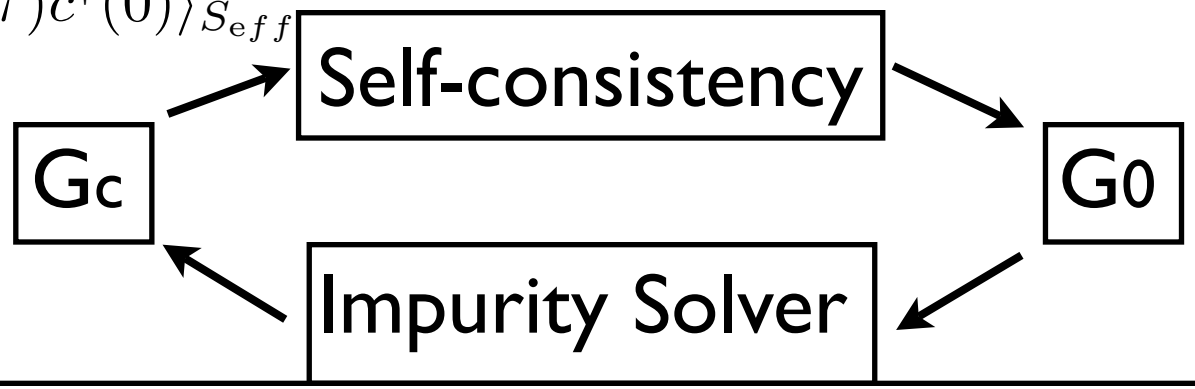
$$S = -\int_0^\beta c^\dagger_\sigma(\tau) G^{-1}_{0\sigma}(\tau - \tau') c_\sigma(\tau') + \int_0^\beta d\tau U n_\uparrow(\tau) n_\downarrow(\tau)$$

Bath → "Weiss field" $G^{-1}_{0\sigma}(i\omega_n) \equiv i\omega_n + \epsilon_0 - \sum_k \frac{|V_{k\sigma}|^2}{i\omega - \epsilon_{k\sigma}}$



DMFT

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



$$S_{\text{eff}} = -\int_0^\beta c_\sigma^\dagger(\tau) G_0^{-1}(\tau - \tau') c_\sigma(\tau') + \int_0^\beta d\tau U n_\uparrow(\tau) n_\downarrow(\tau)$$

- *Continuous Time QMC* : Sum diagrams with Monte-Carlo
  - Expansion in U : *A.N. Rubtsov et al., Phys. Rev. B (2005)*
  - Expansion around atomic limit : [P. Werner's talk]
    P. Werner, A. Comanac, L. de' Medici, M. Troyer, A. J. Millis, PRL (2006)
  - CT-AUX [P. Werner's talk]: *E.Gull et al., EPL (2008)*
  - No sign problem (1 site DMFT).
- *Exact diagonalization M.Caffarel and W. Krauth PRL (1994)*

DMFT equations (simplest case)

Ising	*Hubbard*
$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$	$H = -\sum_{\langle ij \rangle \sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow}$
$m = \langle \sigma \rangle$	$G_c(\tau) = -\langle T c(\tau) c^\dagger(0) \rangle_{S_{eff}}$
$H_{\rm eff} = -J h_{\rm eff} \sigma$	$S_{\rm eff} = -\int_0^\beta c^\dagger_\sigma(\tau) G_0^{-1}(\tau - \tau') c_\sigma(\tau') + \int_0^\beta d\tau U n_\uparrow(\tau) n_\downarrow(\tau)$
$h_{\rm eff} = zJm$	$\Sigma(i\omega_n) \equiv G_0^{-1}(i\omega_n) - G_c^{-1}(i\omega_n)$ $G_0^{-1}(i\omega_n) = \underbrace{\left(\sum_k \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma(i\omega_n)} \right)^{-1}}_{G_{\rm lattice}(k, i\omega_n)} + \Sigma(i\omega_n)$

- The self-energy on the lattice is local : in metals, Z, m*, coherence temperature, finite temperature lifetime are constant along the Fermi surface.

A diagrammatic point of view

$$\Sigma_{ij} = \frac{\delta \Phi}{\delta G_{ji}}$$

De Dominicis, Martin (1964)

$$\Phi_{\text{Hubbard}}[G_{ij}] = \sum 2 \text{ particle-irreducible (2PI) diagrams}$$

$$= \underbrace{\sum_i \phi_1(G_{ii})}_{\textbf{Local}} + \underbrace{\sum_{\langle i,j \rangle} \phi_2(G_{i,j}) + \sum_{\langle i,j,k \rangle} \phi_3(G_{i,j}, G_{i,k}, G_{j,k}) + \dots}_{\textbf{Non local}}$$

- DMFT approximation (exact in d→∞ limit) *Metzner, Vollhardt (1989)*

$$\Phi_{\text{Hubbard}}(G_{ij}) \approx \sum_i \phi_1(G_{ii})$$

- Local 2PI diagrams of Hubbard = 2PI diagrams of Anderson impurity

$$\phi_1(G_{ii}) = \Phi_{\text{Anderson}}(G_{ii})$$ *Kotliar, Georges (1992)*

DMFT sums local 2 PI diagrams, with a sign-free QMC.

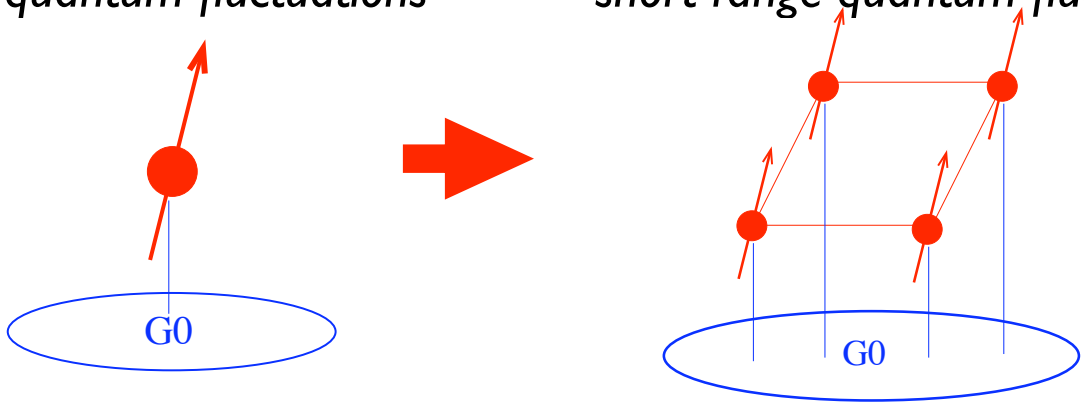
From Mean Field to a controllable method : clusters

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

- *Principle* : systematic interpolation between Φ_{Hubbard} and Φ_{DMFT} with a finite number of sites in a self consistent bath.

- One way to bring control to DMFT [See also A. Lichtenstein's talk]

local quantum fluctuations *short range quantum fluctuations*

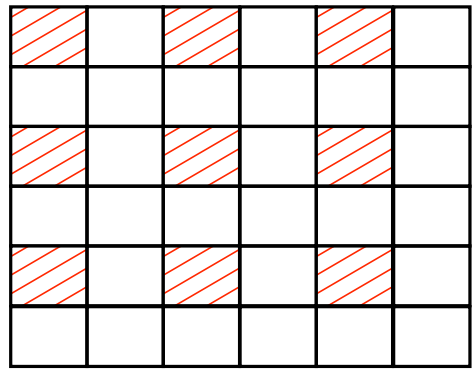


- *Real space cluster (CDMFT)*
  DMFT on a superlattice
  A. Lichtenstein and M. Katsnelson, PRB 62, R9283 (2000)
  G. Kotliar et al. PRL 87 186401 2001,

- *Reciprocal space cluster method (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)

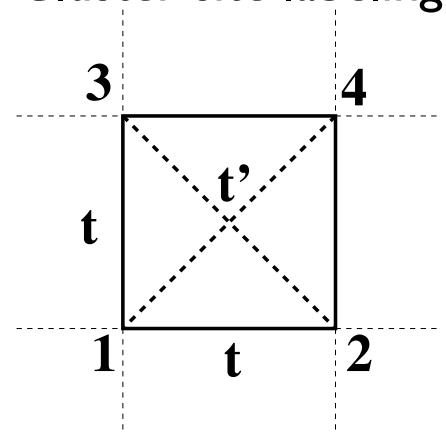
C-DMFT

- DMFT on a superlattice of clusters.



Superlattice

Cluster site labeling



$$1 \leq \mu, \nu \leq 4$$

- R,R' : position of the cluster.
  μ,ν= cluster site labels.

$$\Phi_{CDMFT}(G) = \sum_R \Phi_{4sites}(G_{\mu,R;\nu,R} | G_{\rho,R;\lambda R'} = 0)$$

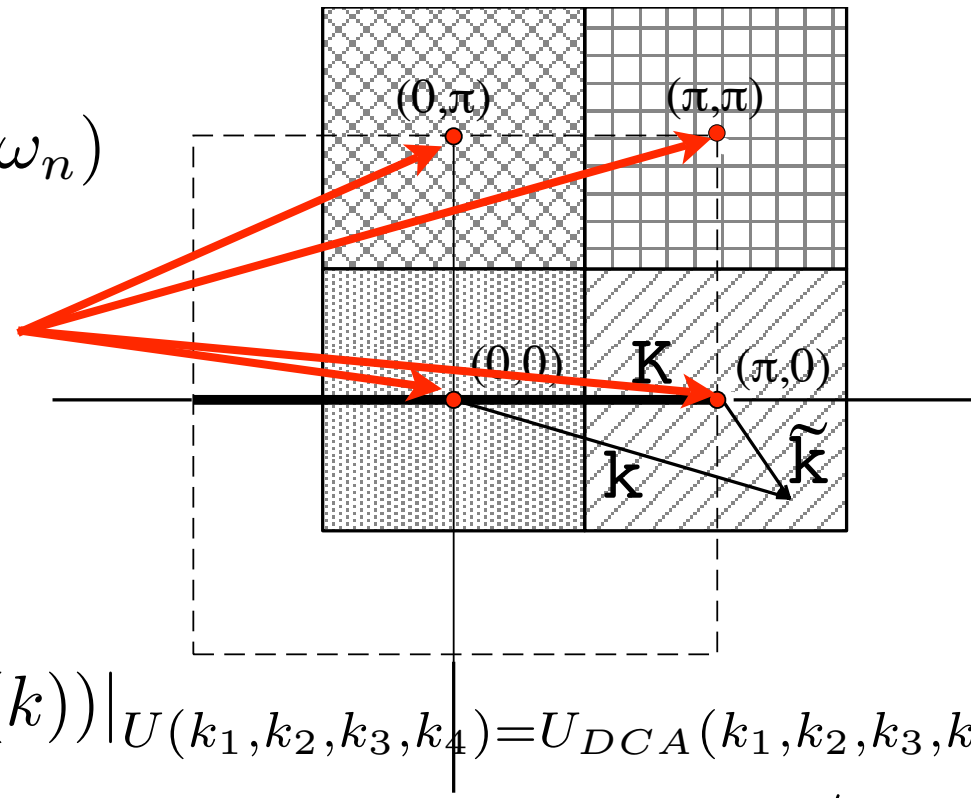
- Same equations as multiorbital DMFT (4 sites as orbitals)

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.

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

Cluster momenta k_c



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

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

Cluster size = momentum resolution

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

Is DMFT a good starting point ?

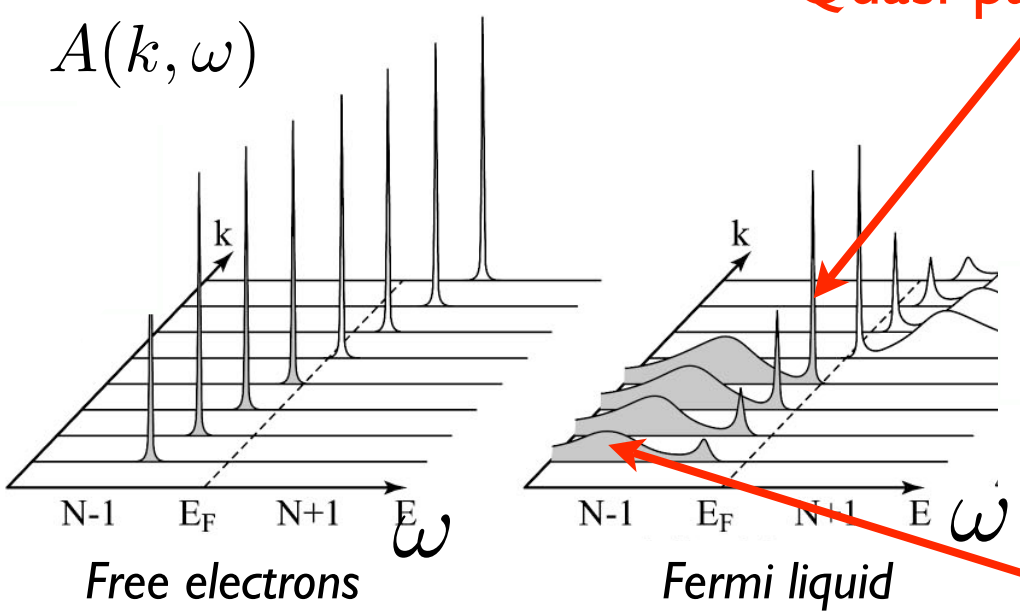
- Compare to experiments...
- Cluster corrections small at small U, high T, large doping
  e.g. good for ultra-cold fermions.
- Why ? ...

DMFT : a good starting point for Mott physics

Lattice

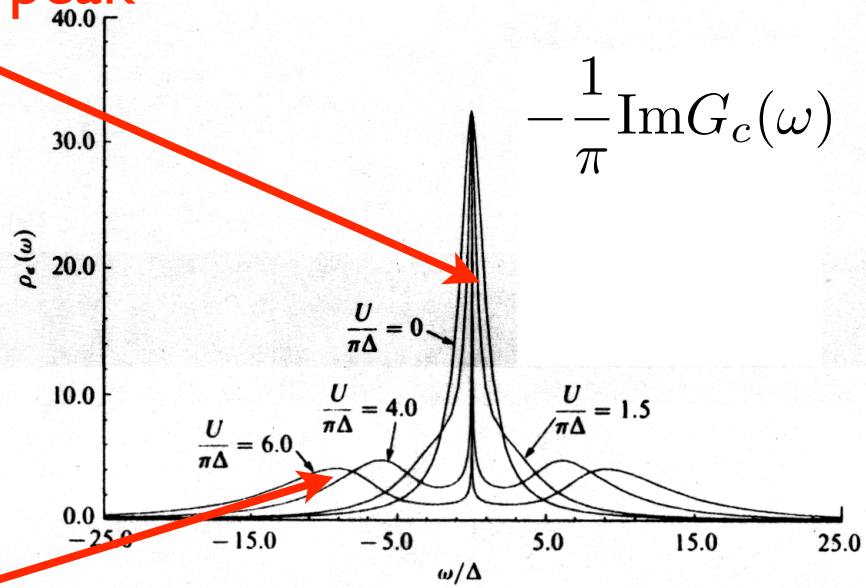
Anderson impurity

Quasi-particle-peak



Free electrons

Fermi liquid



Hubbard bands

Mott physics :
Hubbard band (localized)
vs
Q.P. peak (delocalized)

- Abrikosov-Suhl resonance
- Local Fermi liquid with coherence temperature T_K
  Nozières, 1974

DMFT : from an analogy to a mean field formalism

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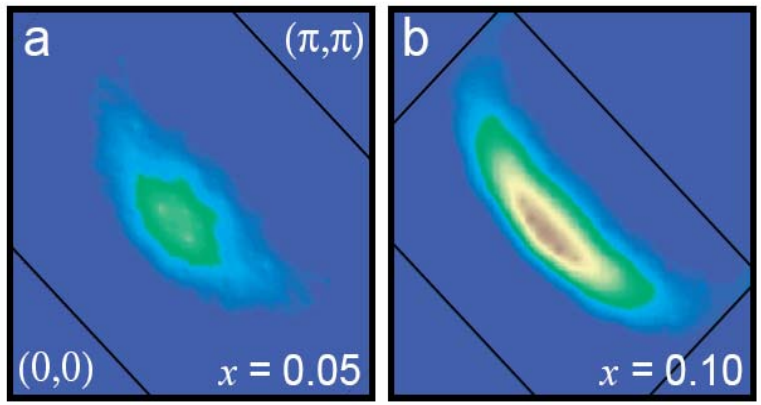
Minimal cluster DMFT approach to normal phase

- Two complementary points of view on cluster DMFT :
  - A systematic numerical method (largest cluster)
    e.g. 16 sites : *A. Macridin et al., PRL 97, 036401 (2006)*
  - A mean field method (smallest cluster)
    M. Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, A. Georges, arxiv:0806.4383

$Ca_{2-x}Na_xCuO_2Cl_2$



Shen et al. Science 307, 901 (2005)

- Goal : Describe the normal phase (Fermi arcs, pseudogap) with a minimal cluster of 2 sites.
  Search for a simple (analytical) picture of the mechanism.

Orbital selective transition in k-space

M. Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, A. Georges, arxiv:0806.4383

- DCA method with two patches of equal volume

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

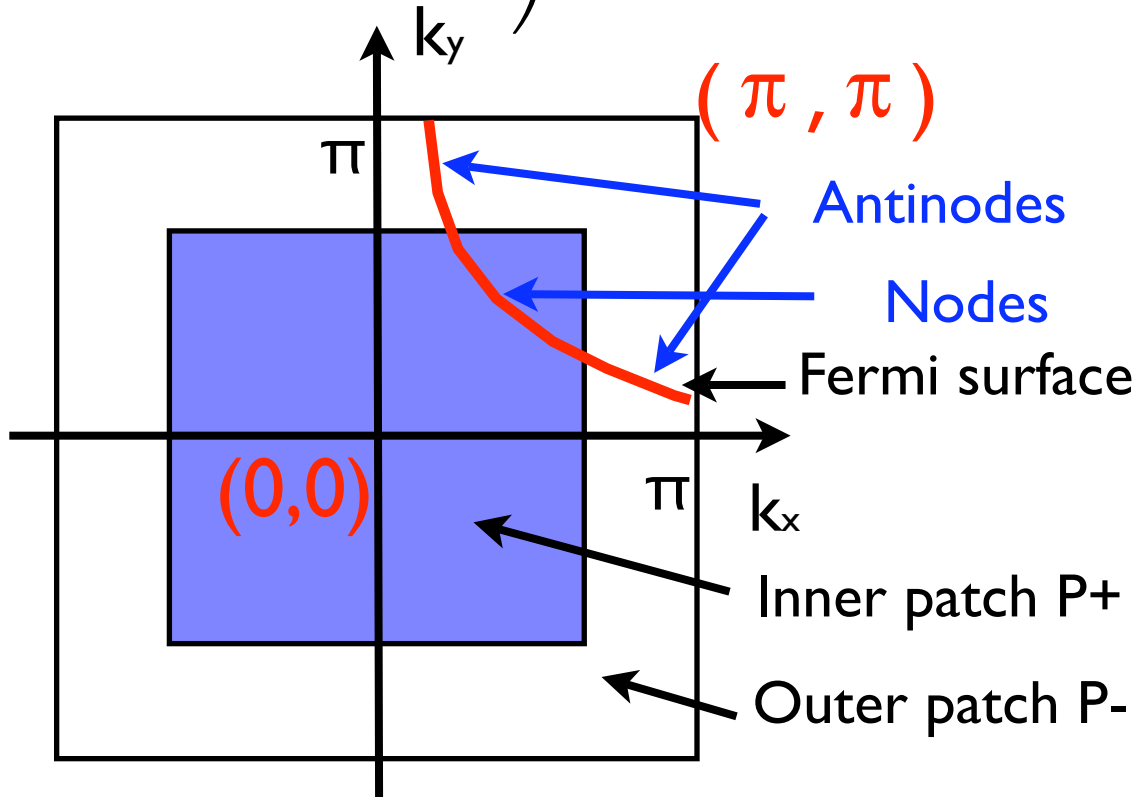
$$G^{-1}_{0\pm}(i\omega_n) = \left(\sum_{k\in P_\pm} \frac{1}{i\omega_n + \mu - \epsilon(k) - \Sigma_\pm(i\omega_n)} \right)^{-1} + \Sigma_\pm(i\omega_n)$$

- Using even/odd basis

$$\mu = 1, 2$$

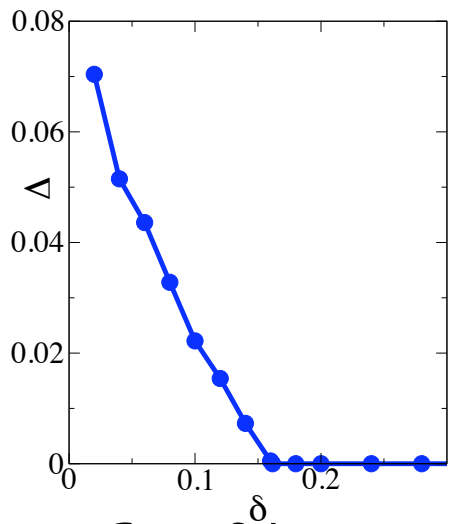
$$c_\pm = (c_1 \pm c_2)/\sqrt{2}$$

- Two cluster momenta : (0,0) and (π , π)
- CTQMC solution using Werner's et al algorithm

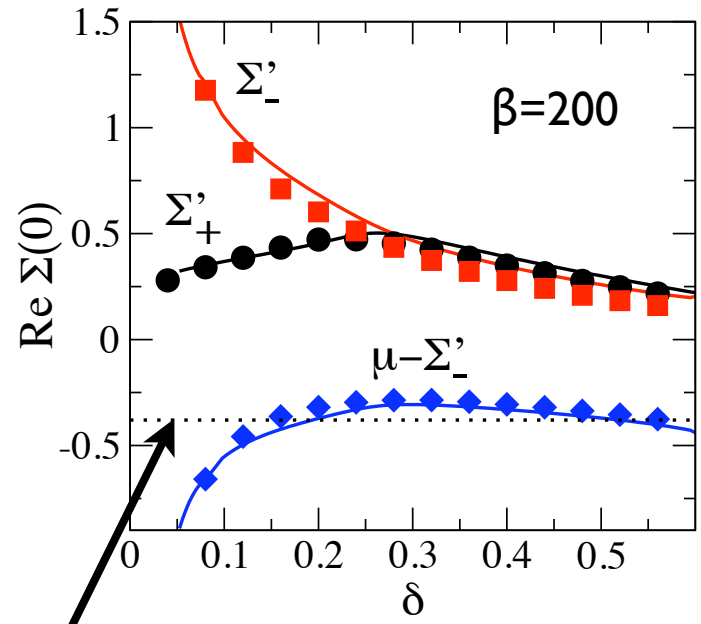


Orbital selective transition in k-space

- At high doping/temperature, DMFT not corrected by cluster terms.
- Around 16%, orbital corresponding to outer patch P- becomes insulating : μ - Σ_(0) reaches the band edge of P- patch
- Quasi-particles only exists in the inner patch



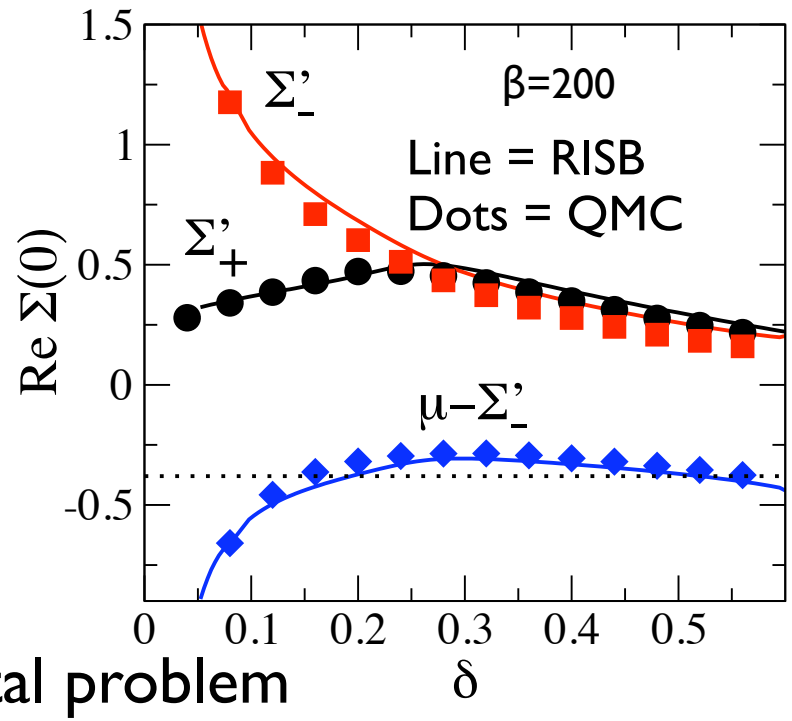
*Gap of the outer Green function G_*



band edge of P- patch

Orbital selective transition in k-space

- Ordinary slave boson mean field : $c_\sigma^\dagger = b f_\sigma^\dagger, \qquad \sum_\sigma f_\sigma^\dagger f_\sigma + b^\dagger b = 1$
  - RVB theory of cuprates
    Anderson, Science (1987), G. Kotliar, J. Liu Phys. Rev. B 38, 5142 (1988)
  - Low energy solution of 1 site DMFT (Brinkman-Rice)
  - No k dependence of Σ !
- Here, low energy is given by Rotationnally Invariant Slave Bosons
  F.Lechermann, A. Georges, G. Kotliar, OP, PRB (2007)

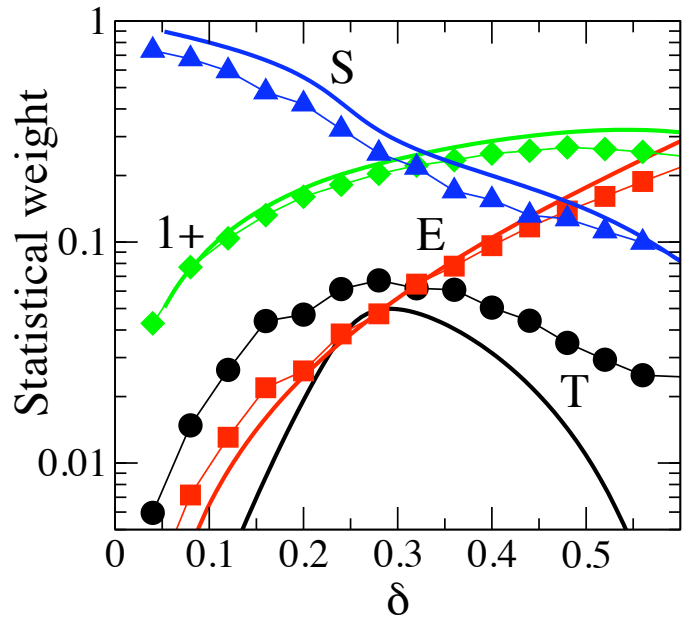


- Cluster : k dependency as a multiorbital problem
  + RISB : slave bosons for multiorbital problem

⇒ Cluster + RISB = a slave boson method with k dependency

Orbital selective transition in k-space

- With CTQMC and Rotationnally Invariant Slave Bosons methods, it is possible to compute the relative weight of various cluster states.
- Singlet state dominates at low doping
- Some similarities with RVB approach
  Anderson, Science (1987), G. Kotliar, J. Liu Phys. Rev. B 38, 5142 (1988)
  but here self-energy depends on k (impossible to get with ordinary slave bosons).



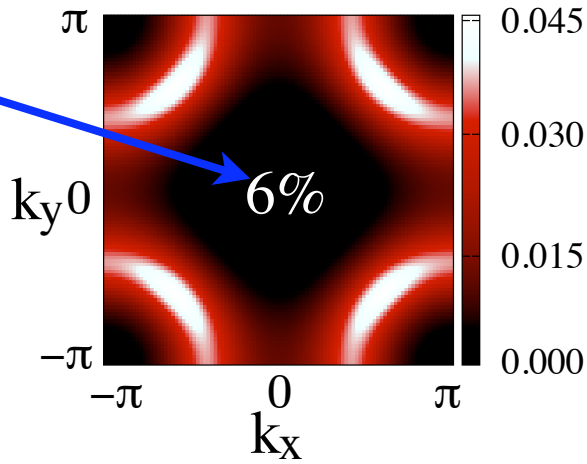
Minimal cluster approach to Fermi Arcs

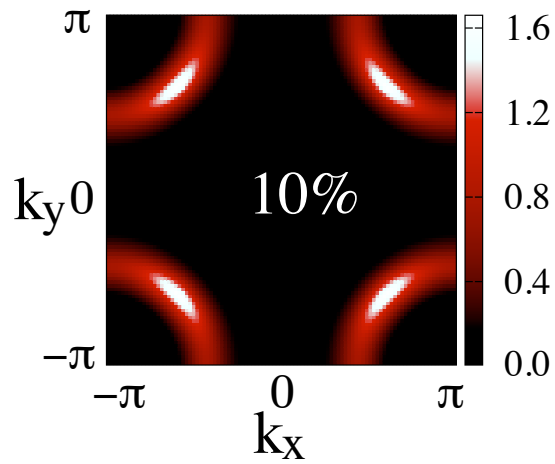
M. Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, A. Georges, arxiv:0806.4383

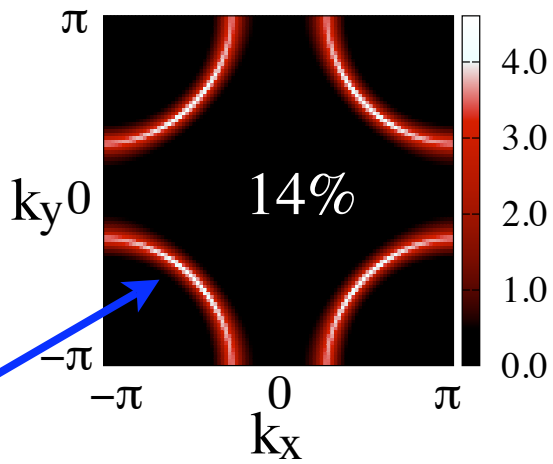
- Spectral function at Fermi level (DCA + interpolation ...)
- Maximum contrast around 10 %

Doping

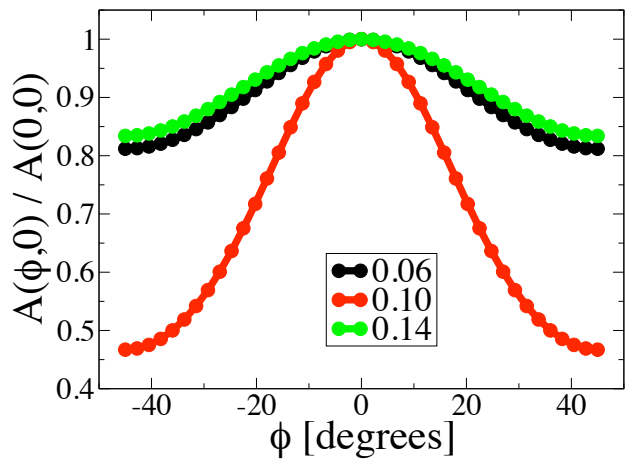
$A(k, \omega = 0)$



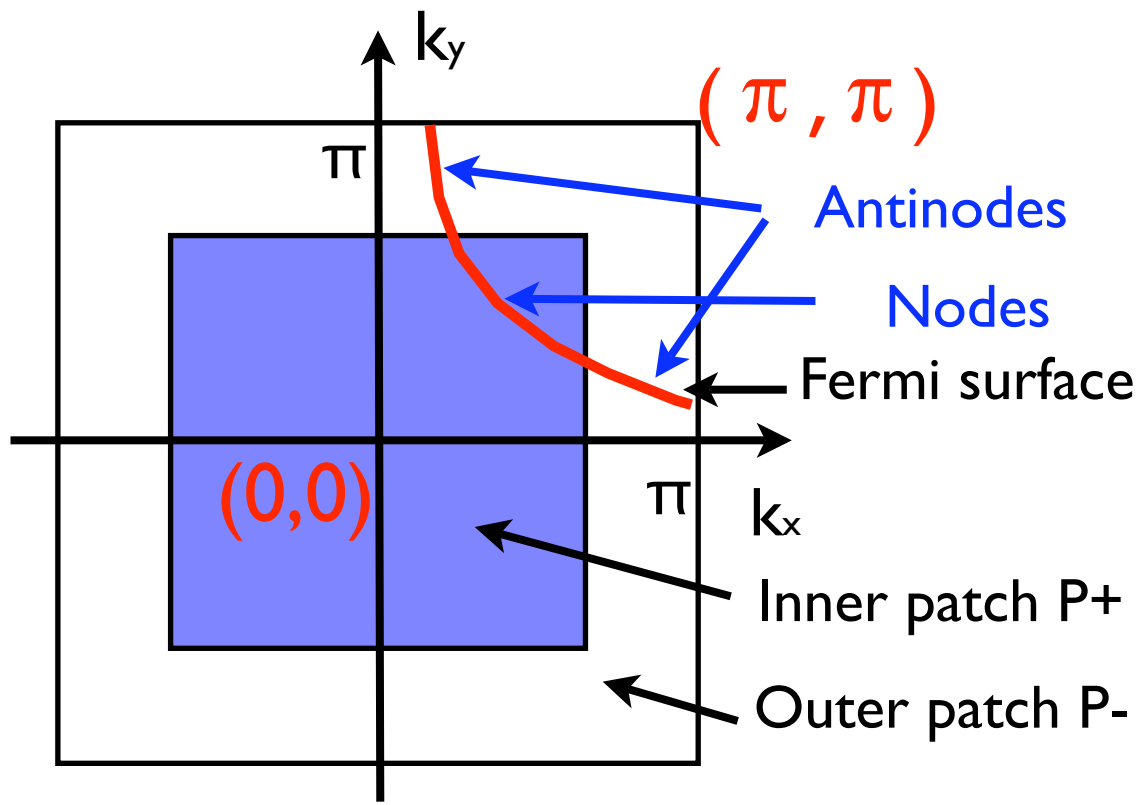




DMFT metal



Comparison with larger clusters ...

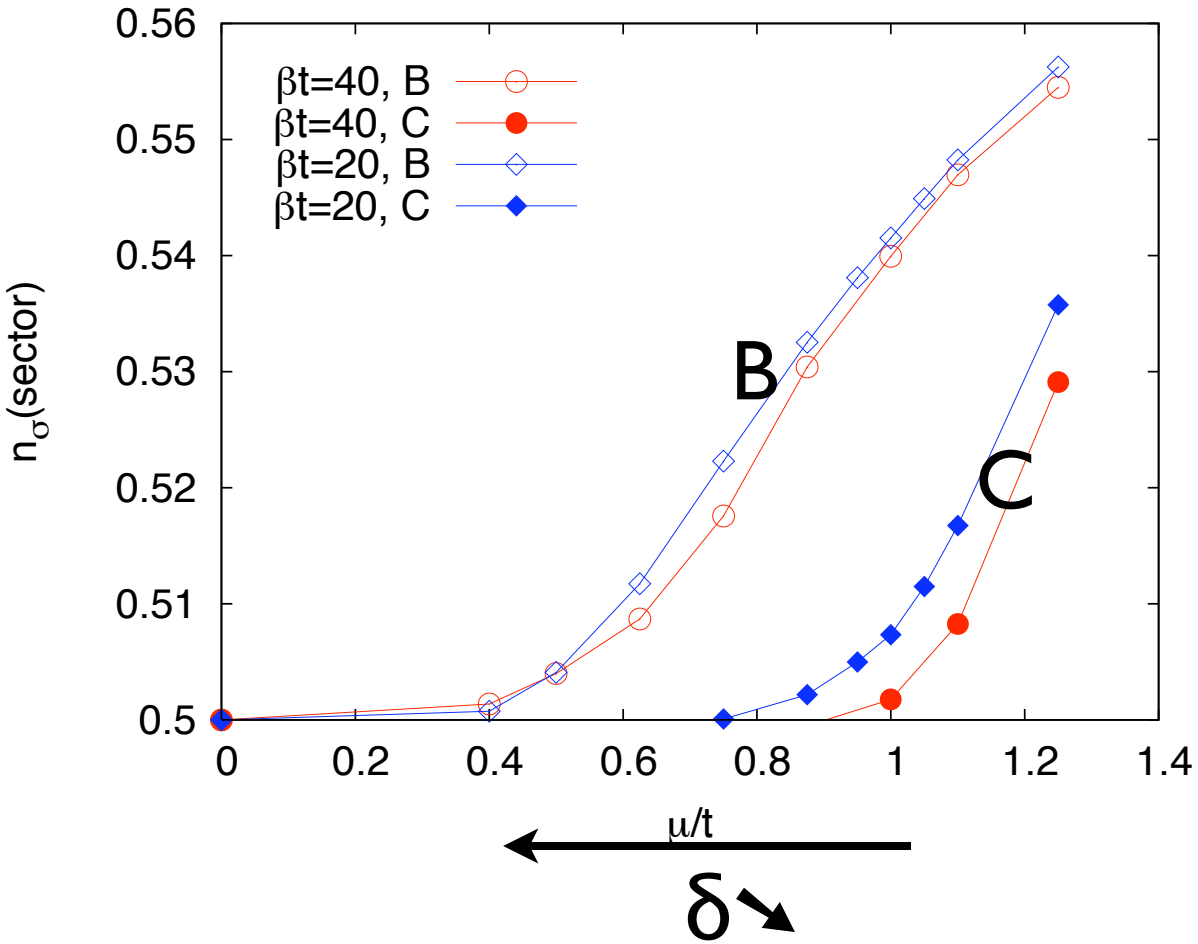


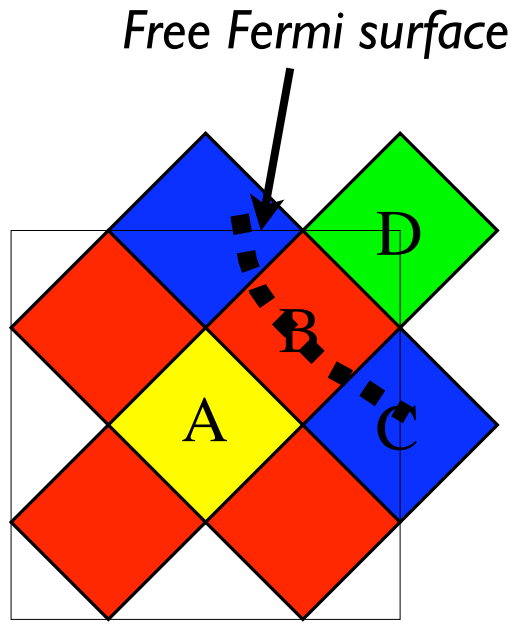
- Only two cluster momenta :
  (0,0) and (π , π) far from Fermi surface !

Compare with 8 sites calculations

E. Gull, P.Werner and A.J. Millis, OP

- Solution of 8 sites DCA with CTAUX algorithm
- Doping driven transition
- 2 steps transition : sector C before sector B



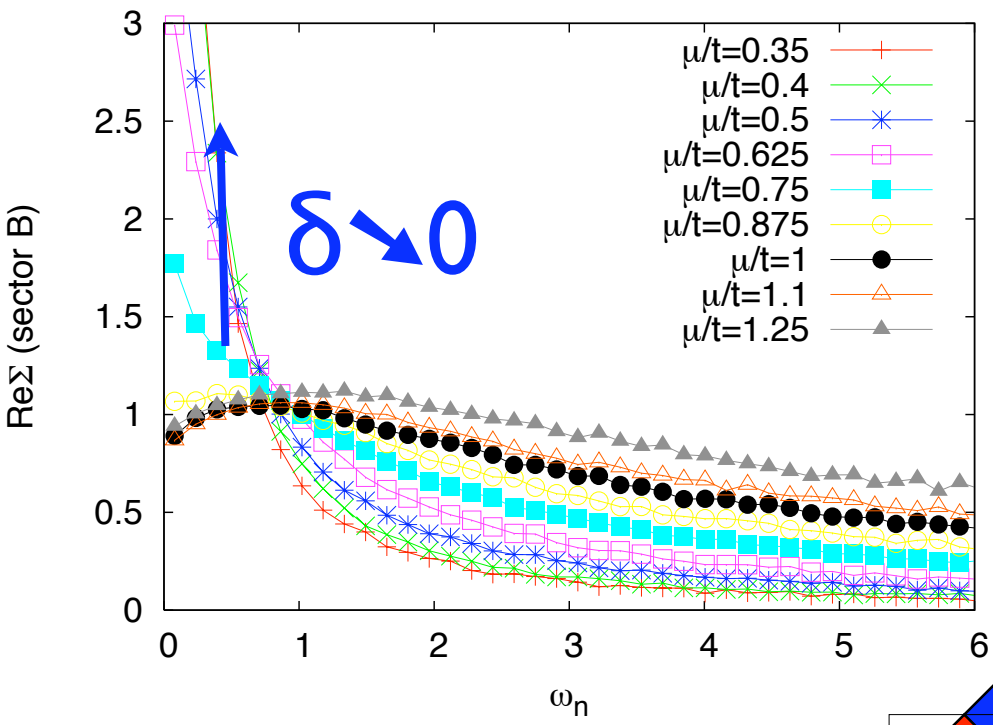


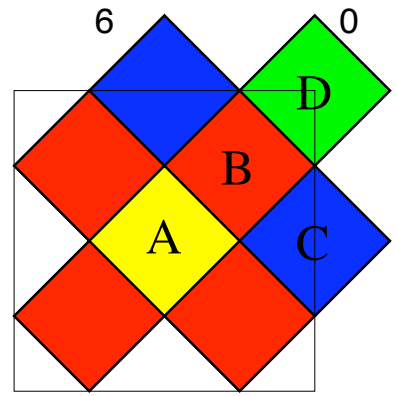
Patches for 8 sites clusters

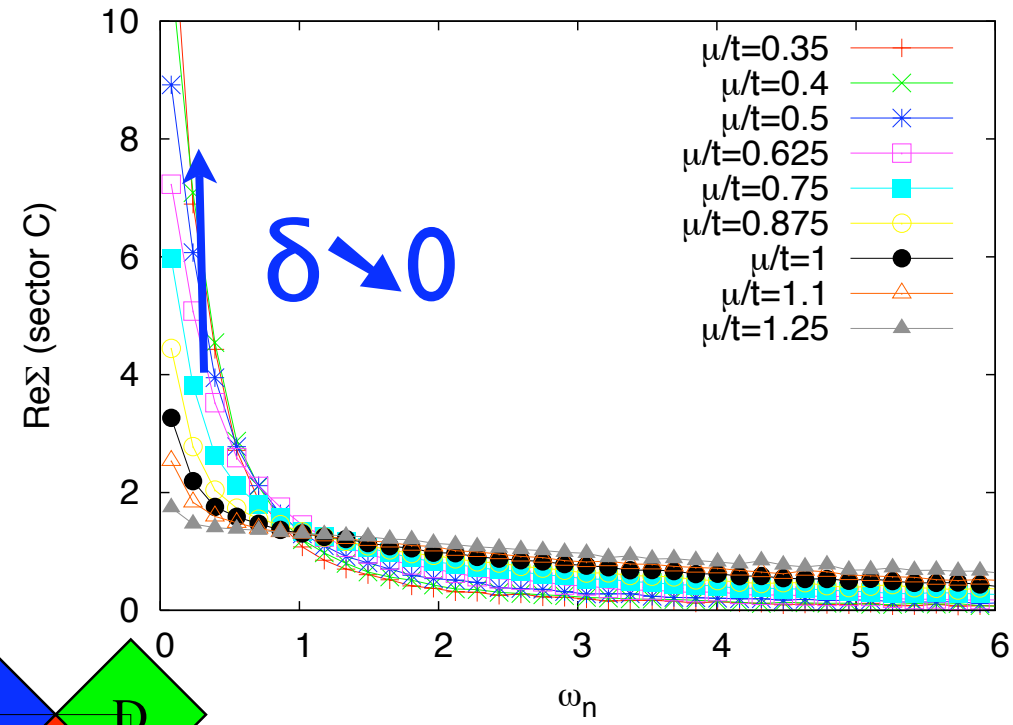
Compare with 8 sites calculations (II)

E. Gull, P. Werner and A.J. Millis, OP

- Similar mechanism : Re Σ(0) getting large, out of bands







Confirmation of the picture found in 2 sites

Test interpolation

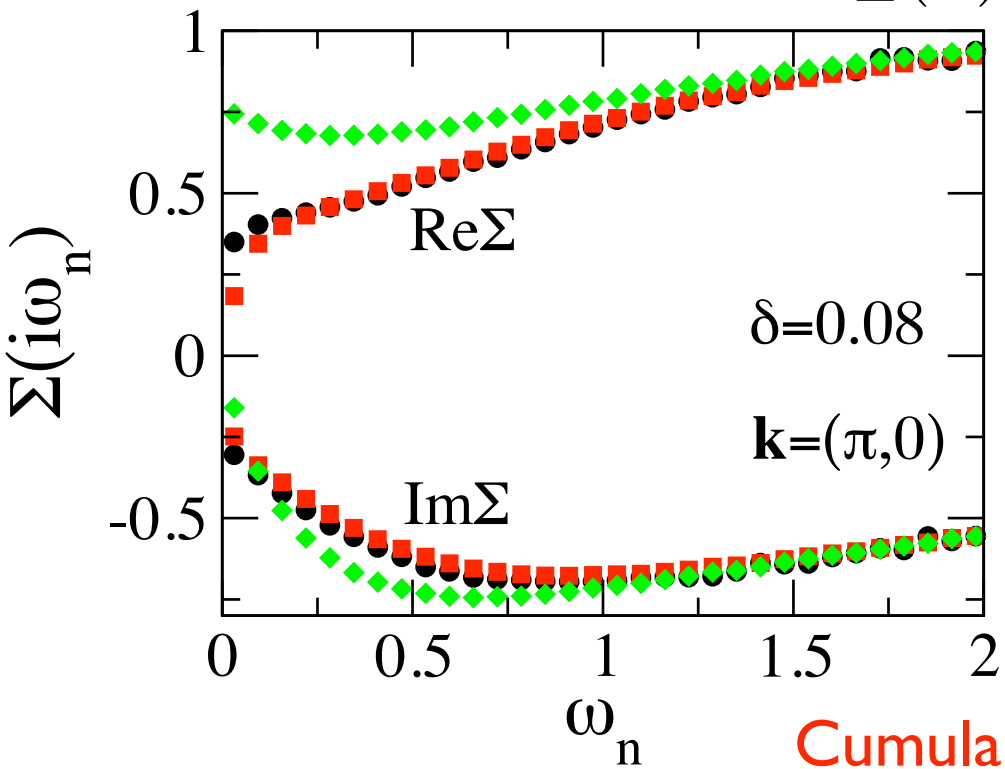
M. Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, A. Georges, arxiv:0806.4383

- Interpolate the self-energy and the cumulant at (π,0) and compare with 4 sites DCA at (π,0) (black curve)

$$\Sigma(\mathbf{k},\omega) = \Sigma_+(\omega)\alpha_+(\mathbf{k}) + \Sigma_-(\omega)\alpha_-(\mathbf{k})$$

$$M(\mathbf{k},\omega) = M_+(\omega)\alpha_+(\mathbf{k}) + M_-(\omega)\alpha_-(\mathbf{k})$$

$$\alpha_\pm(\mathbf{k}) = \frac{1}{2}\{1 \pm \frac{1}{2}[\cos(k_x) + \cos(k_y)]\}$$



Cumulant interpolation is a lot better

Outline

1. Physical motivations
2. DMFT and clusters
3. Selective Mott transition in k space
4. Two gaps in the SC phase

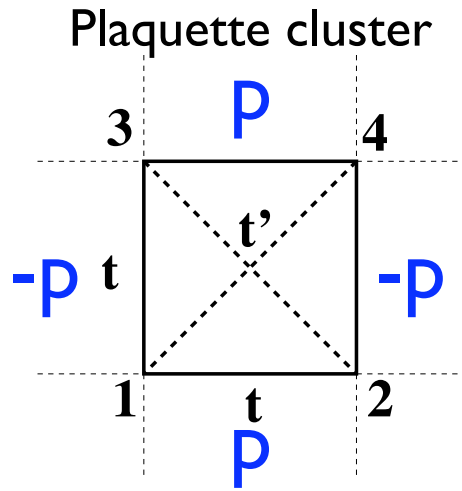
d-SC phase in cluster DMFT

- CDMFT and DCA have a phase diagram with AF and d-SC
  A. Lichtenstein and M. Katsnelson, PRB 62, R9283 (2000);
  M. Jarrell et al, PRL 85,1524 (2001)

- Large Clusters at U/D=1 (DCA), up to 26 sites : *Tc ≈ 0.023t*
  T. Maier et al., PRL 95, 237001 (2005)

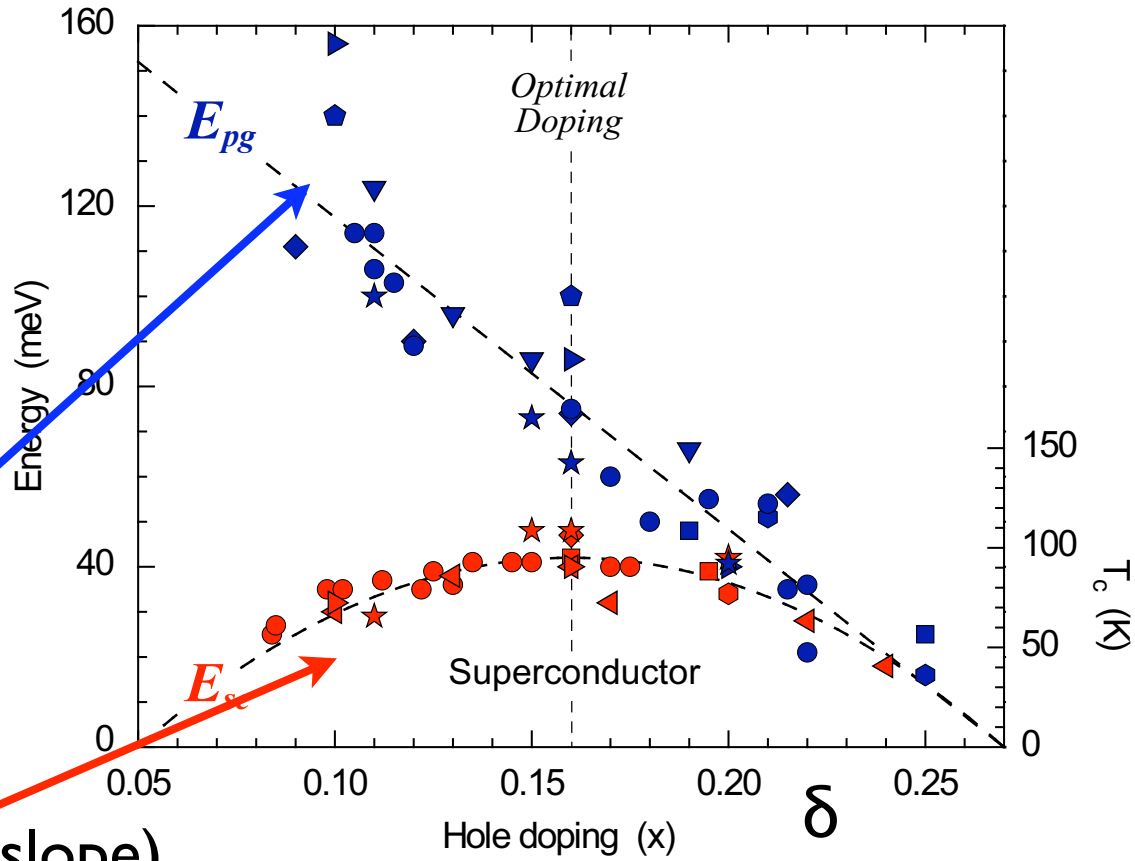
- Smallest cluster : 2x2 plaquette

$p = \langle c^{\dagger}_{1\uparrow} c^{\dagger}_{2\downarrow} \rangle$



- Here : a <u>minimal</u> cluster approach :
  - Two gaps picture ? Doping dependence of the gap ?

"Two gaps" in SC phase : reminder



- Gap at antinode (maximum) increases for δ→0.
- Gap close to node (slope) decreases for δ→0, like Tc.

picture from arXiv:0706.4282

- Raman experiments.
  M. LeTacon et al., Nature Physics, 2, 537,2006
- See also ARPES experiments.
  Tanaka et al,Science 314, 1910, (2006)

$$v_\Delta = \left.\frac{d\Delta(\phi)}{d\phi}\right|_{\text{Node}} \to 0 \text{ for } \delta \to 0$$

- Still debated...

CDMFT result (4 sites)

M. Civelli, M.Capone, A. Georges, K. Haule, O. Parcollet, T Stanescu, G. Kotliar, PRL (2008)

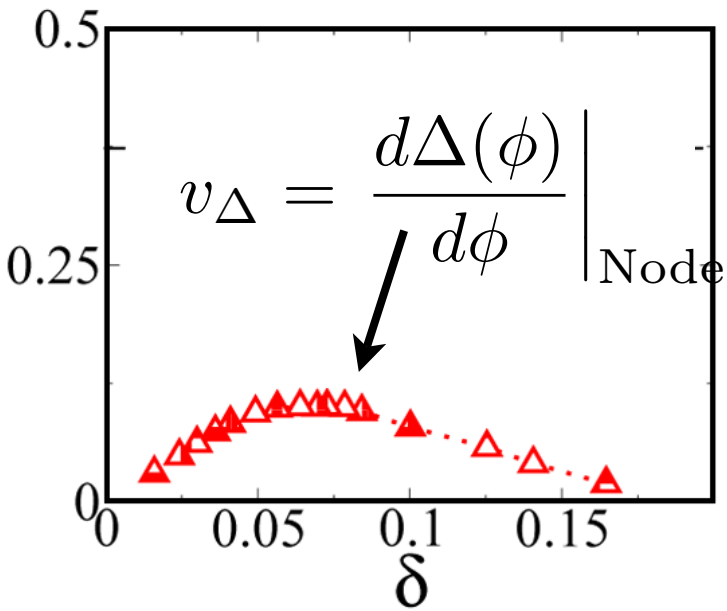
Nodes

t'=-0.3t; U = 12t; ED solver

Antinodes

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

$$v_\Delta = \mathcal{Z}_{nod}|\nabla_k \Sigma^{\rm ano}(k)|$$

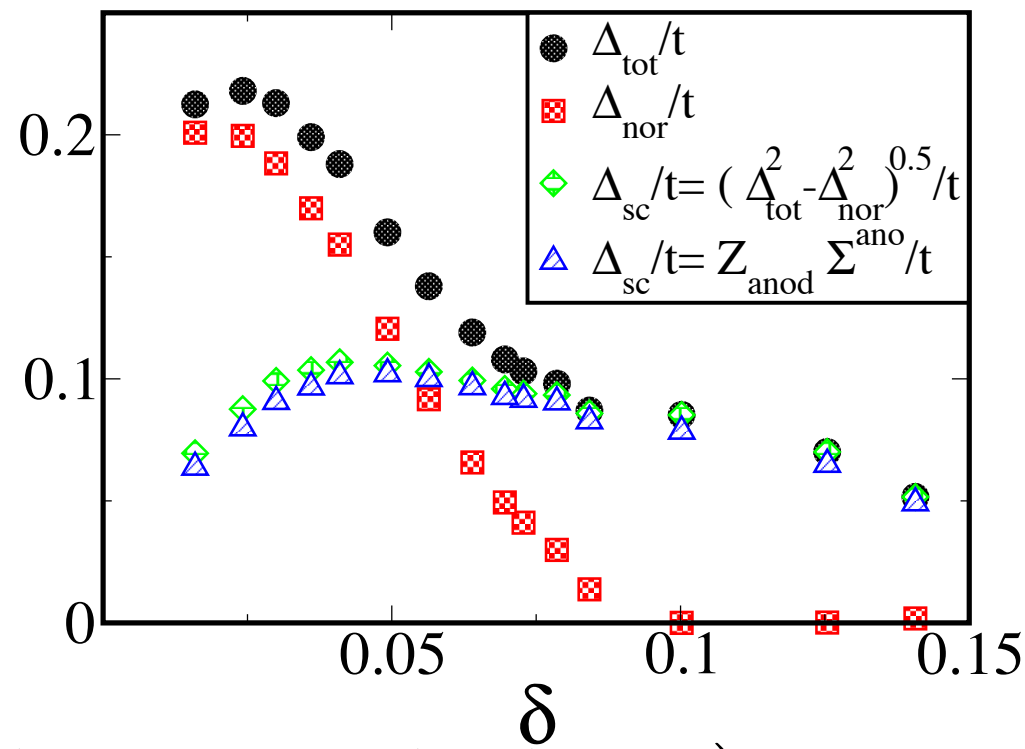


full gap

$\Sigma_{ano}=0$

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

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



$$G^{-1}_{k\sigma}(\omega) = \begin{pmatrix} \omega - \varepsilon_k - \Sigma^{\rm nor}_\sigma(k,\omega) & -\Sigma^{\rm ano}(k,\omega) \\ -\Sigma^{\rm ano}(k,\omega) & \omega + \varepsilon_k + \Sigma^{\rm nor}_\sigma(k,-\omega)^* \end{pmatrix}$$

Conclusion

- Clusters : a systematic expansion around DMFT
- Useful for Mott physics
- A lot of recent progress on methods to solve DMFT equations.
- Strong differences between Nodes and Antinodes :
  - Normal phase : destruction of quasi-particles at antinodes in a transition selective in k-space.
  - SC phase : two components SC gap.