Dynamical Mean Field Theory and beyond

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Outline

- Lecture 1 : Introduction to DMFT
- Lecture 2 : Multiorbital DMFT and clusters
  - Towards more realism : multi-orbital DMFT
  - Cluster methods
    - Motivation
    - Formalism : CDMFT, DCA and co.
    - Highlights : a few results with clusters for Hubbard model.
- Lecture 3 : Impurity solvers
- Lecture 4 : Introduction to TRIQS & Hands-on

DMFT equations (1 band paramagnetic)

Lattice model

Ising

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

Hubbard

$$H = -\sum_{\langle ij \rangle} t_{ij} c^\dagger_{i\sigma} c_{i\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow}$$

Effective model

$$H_{\rm eff} = -J h_{\rm eff} \sigma$$

$$m = \langle \sigma \rangle$$

$$S_{\rm eff} = -\int_0^\beta c^\dagger_\sigma(\tau) \mathcal{G}^{-1}_\sigma(\tau - \tau') c_\sigma(\tau') + \int_0^\beta d\tau \; U n_\uparrow(\tau) n_\downarrow(\tau)$$

$$G_{\sigma \rm imp}(\tau) \equiv -\left\langle T c_\sigma(\tau) c^\dagger_\sigma(0) \right\rangle_{S_{\rm eff}}$$

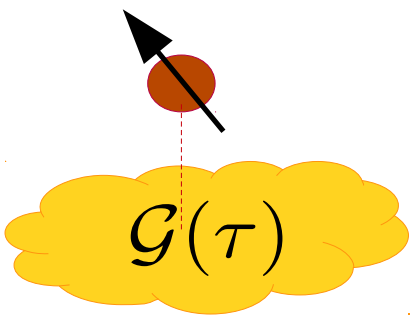
Self consistency condition

$$h_{\rm eff} = zJm$$

$$\Sigma_{\sigma \rm imp}[\mathcal{G}](i\omega_n) \equiv \mathcal{G}^{-1}_\sigma(i\omega_n) - G^{-1}_{\sigma \rm imp}[\mathcal{G}](i\omega_n)$$

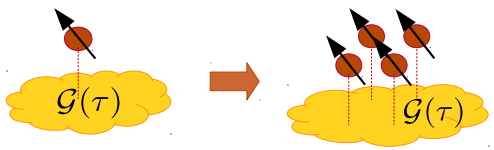
$$G_{\sigma \rm imp}[\mathcal{G}](i\omega_n) = \sum_k \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{\sigma \rm imp}[\mathcal{G}](i\omega_n)}$$

Implicit equation for the bath



DMFT, a family of approximations

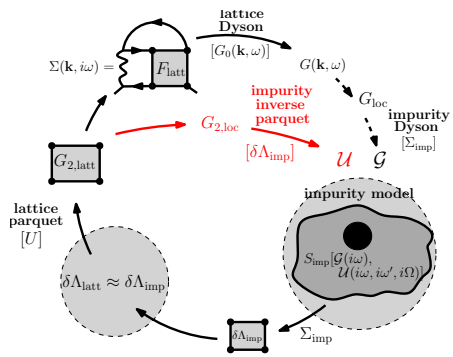
- Cluster DMFT



Control, short range correlation

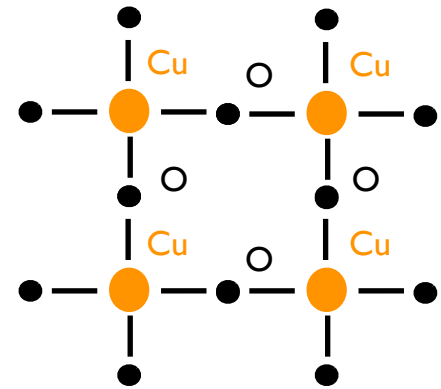
- Beyond cluster DMFT

Self-consistency on vertex
Dual fermions/bosons, Trilex, DΓA



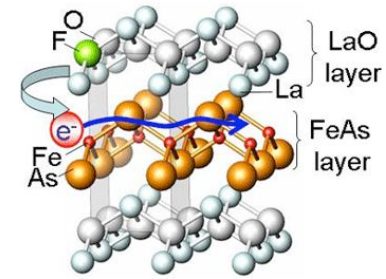
- Multiband/realistic systems

$$\Sigma(\omega) = \begin{pmatrix} \Sigma^{\rm imp}(\omega) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$



- Self-consistency in large unit cell (Cu + 2 O)
  $\Sigma_{ab}(\omega)$ a 3x3 matrix
- Impurity model on Cu, 1 band : $\Sigma^{\rm imp}(\omega)$ 1x1 matrix

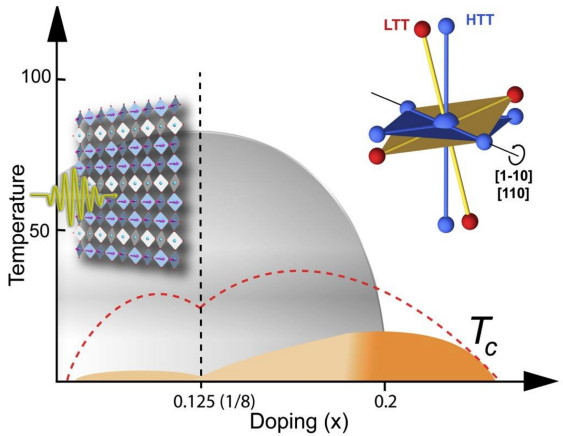
- DFT + DMFT



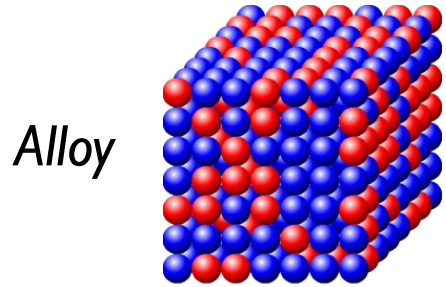
- Interface with electronic structure codes (project on Wannier functions, etc).

DMFT, a family of approximations

- Non equilibrium

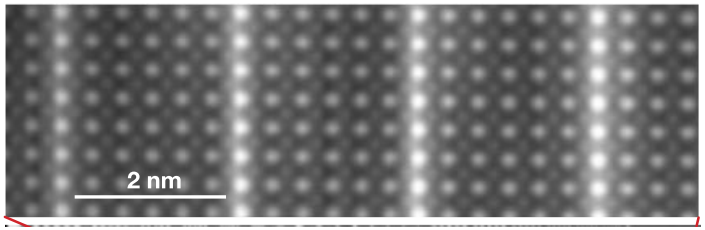


- Disordered systems



- Two impurity models

- Correlated interfaces.



$SrTiO_3/LaTiO_3$

Ohtomo et al, Nature 2002

- One impurity per layer

Towards more realism

Multi-orbital DMFT

- Multiorbital model

$$H = -\sum_{\langle ij \rangle} (t_{ij})_{ab} c^{\dagger}_{i\sigma a} c_{i\sigma b} + H_{\rm int} \qquad (\hat{\epsilon}_k)_{ab}$$

- G, Σ, bath become matrices in the orbital space

$$S_{\rm eff} = -\int_0^\beta \sum_{ab} c^{\dagger}_{\sigma a}(\tau) \mathcal{G}^{-1}_{\sigma,ab}(\tau - \tau') c_{\sigma b}(\tau') + \int_0^\beta d\tau\, H_{\rm int}(\tau)$$

$$G^{\rm imp}_{\sigma ab}(\tau) \equiv -\left\langle T c_{\sigma a}(\tau) c^{\dagger}_{\sigma b}(0) \right\rangle_{S_{\rm eff}}$$

Orbital index

$$\Sigma_{\sigma \rm imp}[\mathcal{G}](i\omega_n) \equiv \mathcal{G}^{-1}_{\sigma}(i\omega_n) - G^{-1}_{\sigma \rm imp}[\mathcal{G}](i\omega_n)$$

Matrix equation

$$G^{\rm imp}_{\sigma}[\mathcal{G}](i\omega_n) = \sum_k \Big((i\omega_n + \mu)\mathbf{1} - \hat{\epsilon}_k - \Sigma^{\rm imp}_{\sigma}[\mathcal{G}](i\omega_n) \Big)^{-1}$$

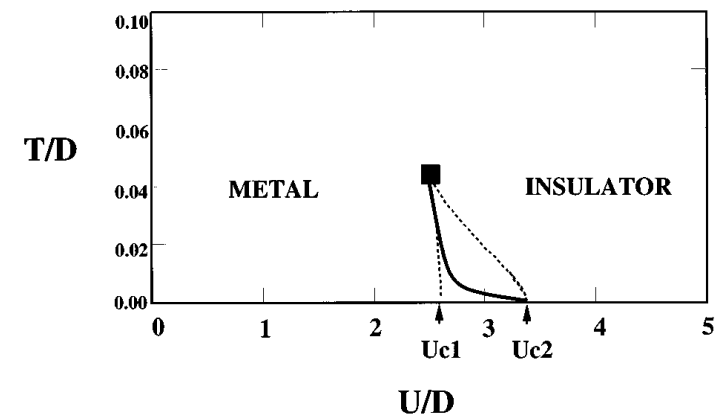
Difference with 1 orbital case

- Fully symmetric model with N orbitals, density-density interaction.

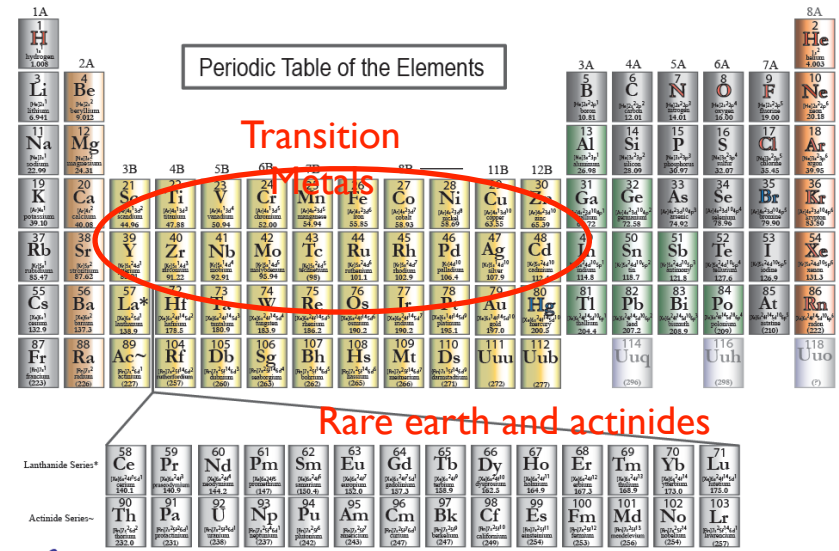
$$H = -\sum_{i,j}\sum_{\sigma=1}^{N} t_{ij} d^{\dagger}_{i\sigma} d_{j\sigma} + \frac{U}{2}\sum_{i}\left[\sum_{\sigma=1}^{N}\left(d^{\dagger}_{i\sigma} d_{i\sigma} - n\right)\right]^2$$

- Similar to N=1. *S. Florens et al. 2002*

$$U_{c1} \sim \sqrt{N} \qquad U_{c2} \sim N$$



- But materials are lot richer.
- H_{int} is not just density-density.
- New physical phenomena, with e.g. Hund's coupling, crystal field splitting.



- e.g. Hund's metal : another route to correlation …

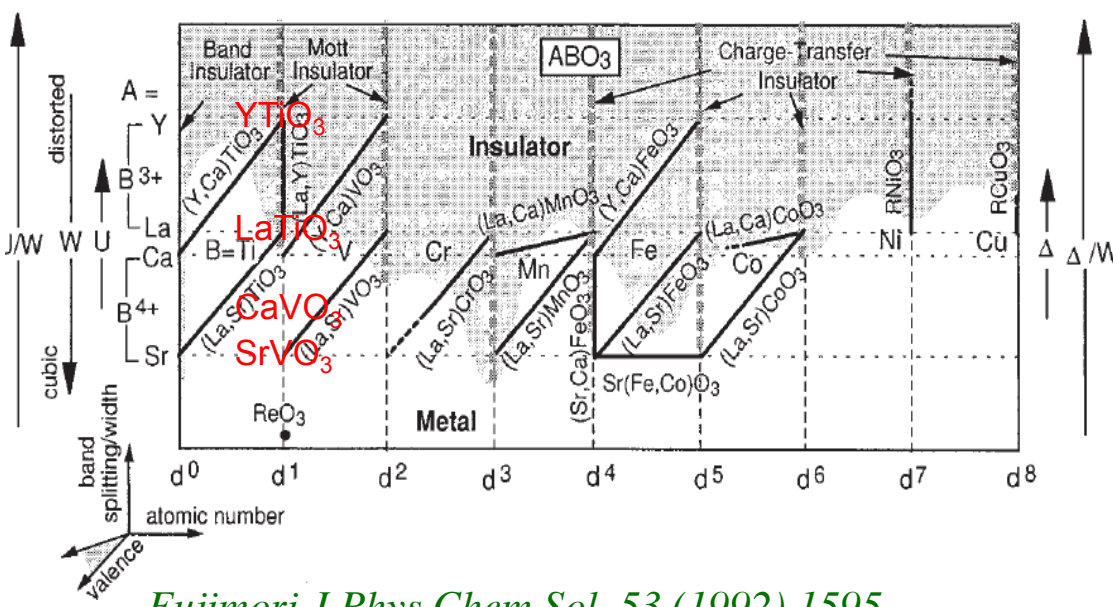
Hund's metal

Cf review A. Georges. L. De Medici, J. Mravlje, arXiv:1207.3033

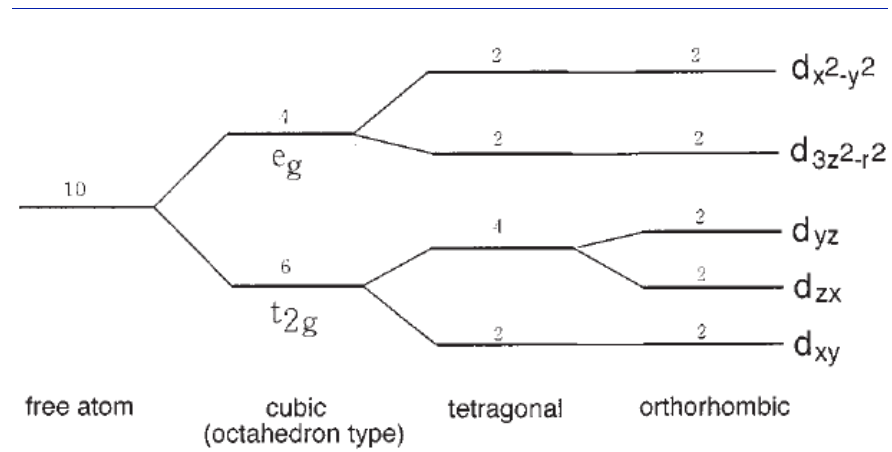
- Kanamori Hamiltonian.

$$H_{\mathrm{K}} = U \sum_{m} \hat{n}_{m\uparrow}\hat{n}_{m\downarrow} + U' \sum_{m\neq m'} \hat{n}_{m\uparrow}\hat{n}_{m'\downarrow} + (U'-J) \sum_{m<m',\sigma} \hat{n}_{m\sigma}\hat{n}_{m'\sigma} +$$
$$-J \sum_{m\neq m'} d^{+}_{m\uparrow} d_{m\downarrow}\, d^{+}_{m'\downarrow} d_{m'\uparrow} + J \sum_{m\neq m'} d^{+}_{m\uparrow} d^{+}_{m\downarrow}\, d_{m'\downarrow} d_{m'\uparrow}$$

- Relevant for a class of materials, e.g. 3d, 4d transition metal oxides



Fujimori J.Phys Chem Sol. 53 (1992) 1595



Hund's metal

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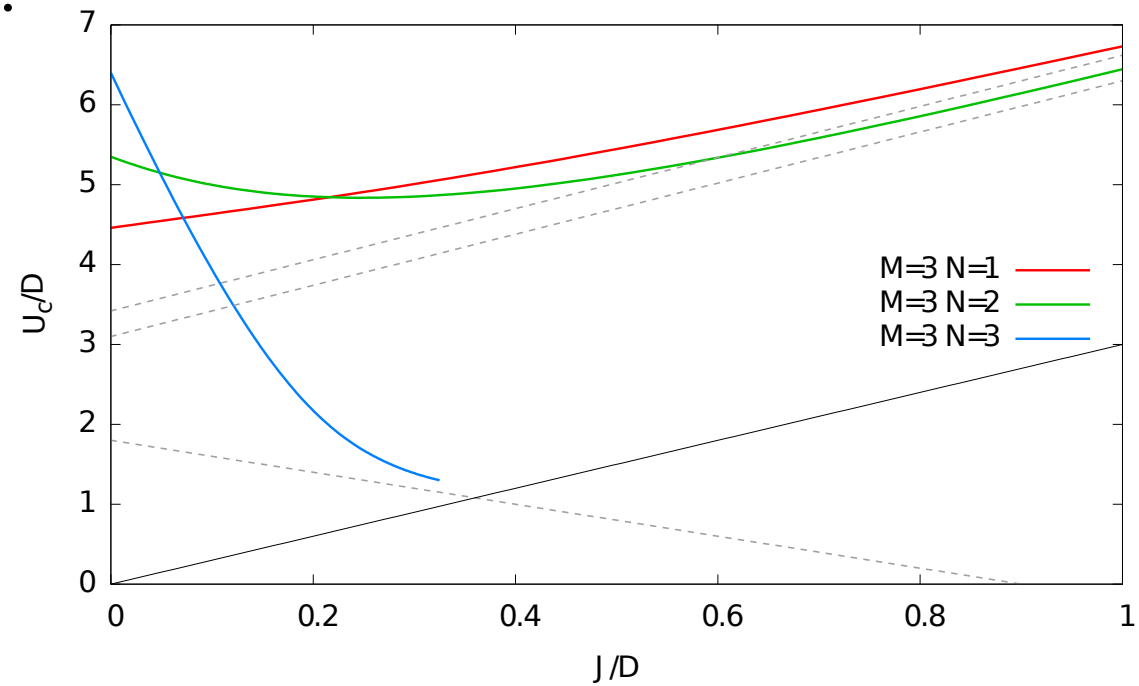
- Kanamori Hamiltonian.

$$H_{\rm K} = U\sum_m \hat{n}_{m\uparrow}\hat{n}_{m\downarrow} + U'\sum_{m\neq m'} \hat{n}_{m\uparrow}\hat{n}_{m'\downarrow} + (U'-J)\sum_{m<m',\sigma} \hat{n}_{m\sigma}\hat{n}_{m'\sigma} +$$
$$-J\sum_{m\neq m'} d^+_{m\uparrow}d_{m\downarrow}\,d^+_{m'\downarrow}d_{m'\uparrow} + J\sum_{m\neq m'} d^+_{m\uparrow}d^+_{m\downarrow}\,d_{m'\downarrow}d_{m'\uparrow}$$

- Effect of Hund's coupling J on the Mott transition and correlation. 3 orbitals, N= 1,2,3 electrons.

  - J enhances U_c away from half-filling (N=1,2)
  - J strongly reduces U_c at half-filling (N=3)



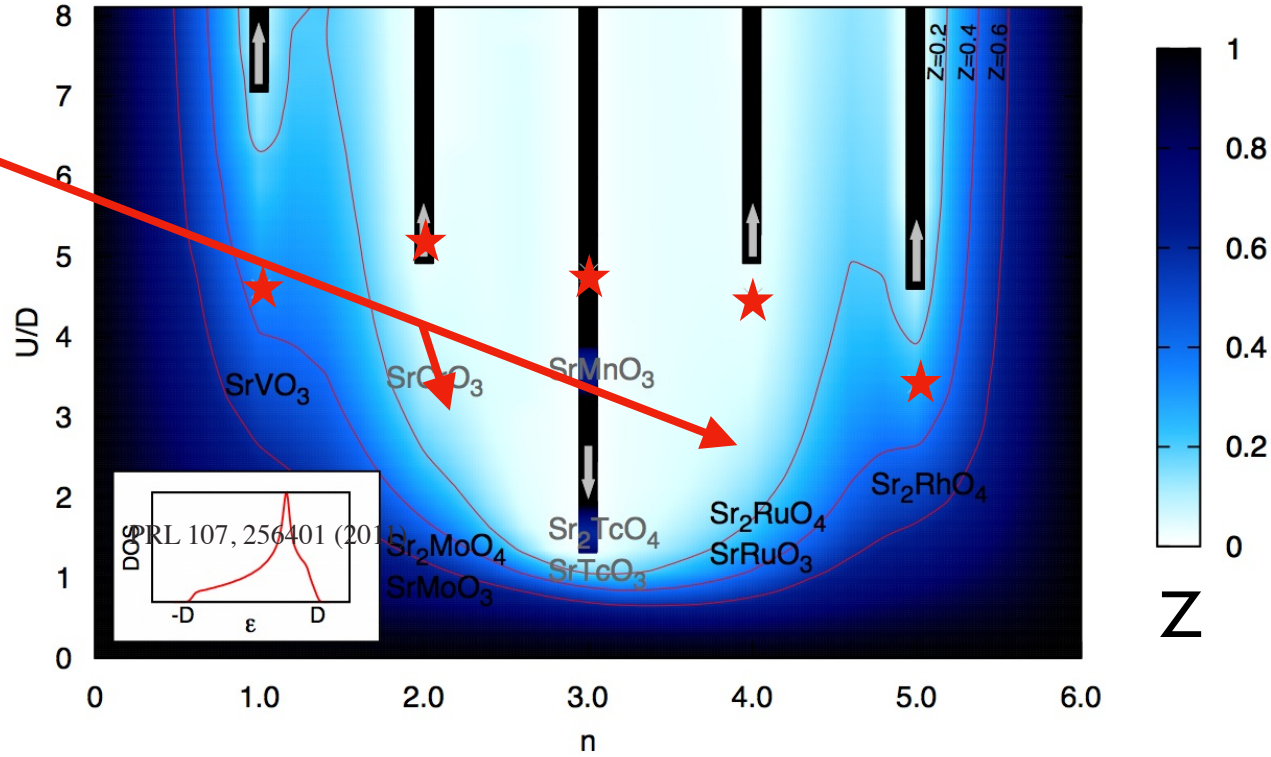
Hands-on : Kanamori 2 bands.

Hund's metal

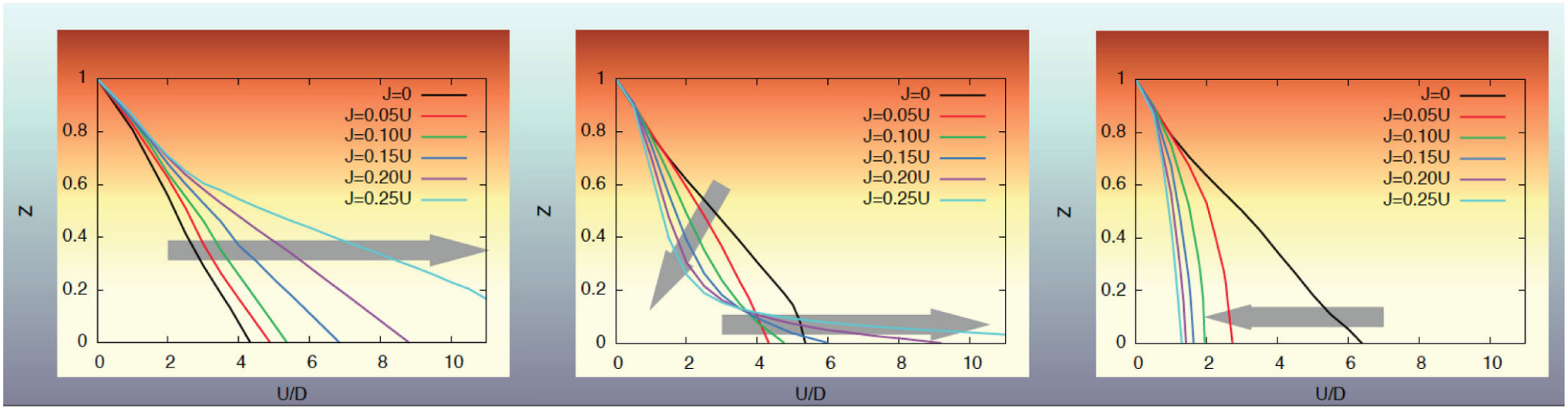
- Strongly correlated metal far from Mott U_c
- Rotationally invariant case $U' = U - 2J$

  J = 0.15U
- Z vs U

T= phase diagram (paramagnetic phase only)



L. De Medici et al. PRL 107, 256401 (2011)



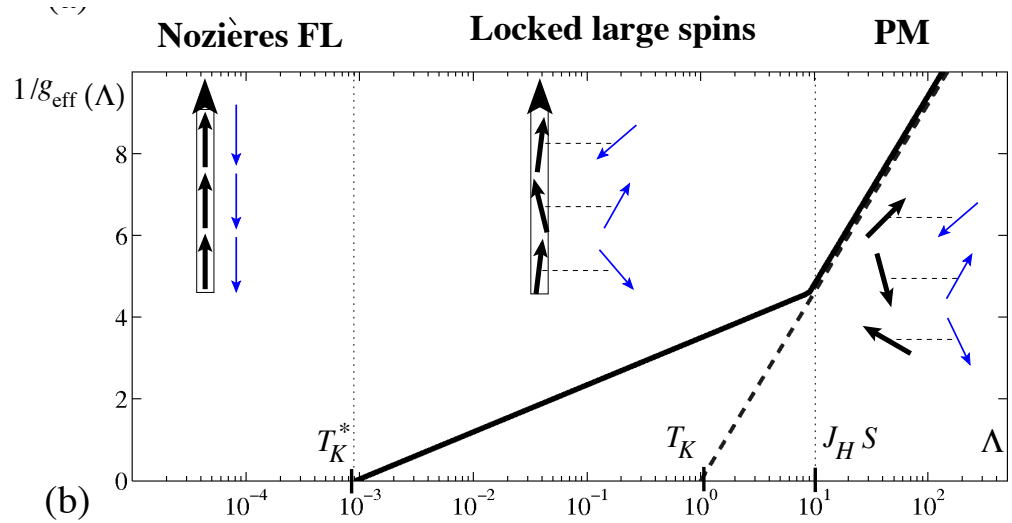
(a) $N = 1$ (b) $N = 2$ (c) $N = 3$

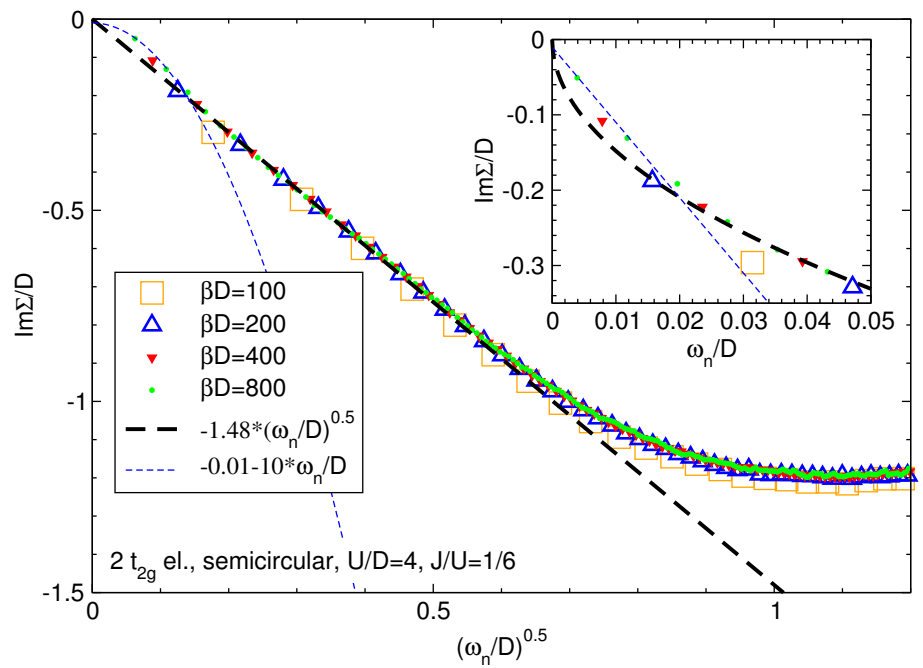
A strongly correlated "Hund metal"

- n=2,4
- J enhances U_c, but reduces coherence temperature
- DMFT : analysis in term of a Kondo impurity.
- Low temperature : Fermi liquid
- Intermediate temperature: non-Fermi liquid, e.g. in self-energy

$$Im\Sigma(\omega) \sim \Gamma + (\omega/D)^{\alpha}$$

Simplified "composite spin" picture

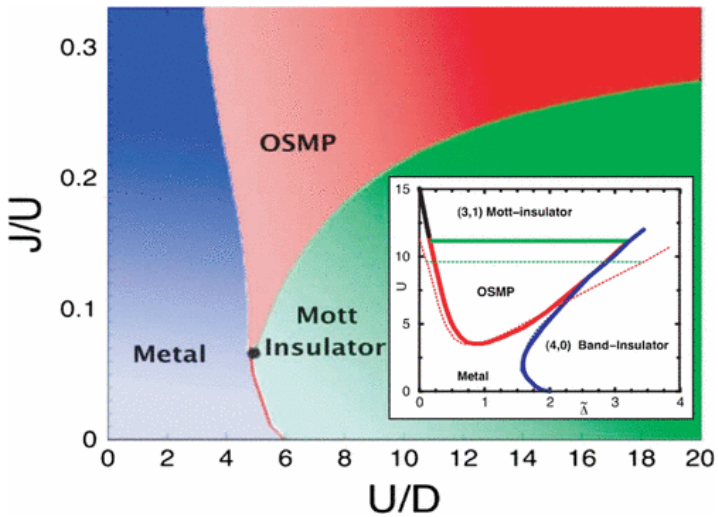


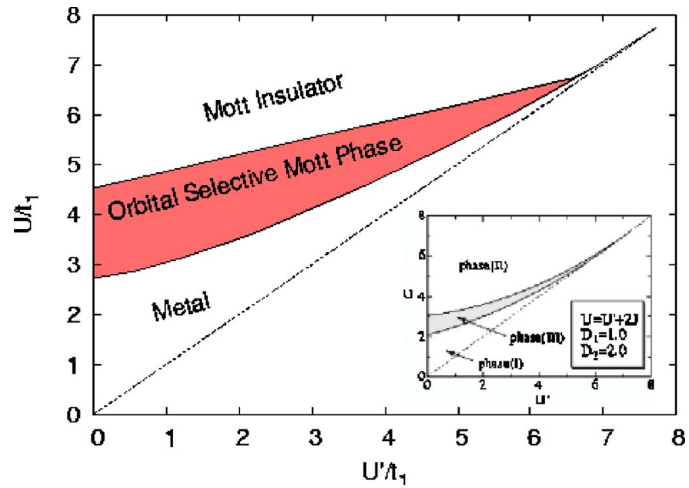


P. Werner et al. Phys. Rev. Lett. 101:166405 (2008)

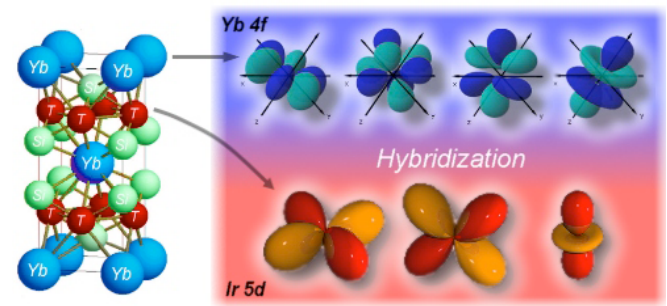
Orbitally selective Mott transition

- Models with different bandwidths and/or crystal field splitting





- Orbitally Selective Mott Phase
  - One orbital localized, other delocalized.
  - The localized orbital can break Fermi Liquid for the delocalized one
    see also e.g. S. Biermann et al., PRL 95 206401 (2005)
    Effective Anderson lattice model.



Towards ab-initio computation : beyond model

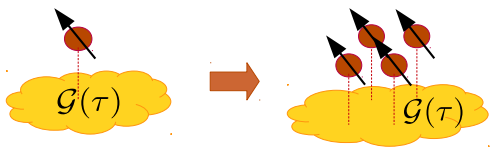
- Mix DFT/LDA + DMFT or GW + DMFT
- Do not start from a model.
- One electron part computed by DFT
- Interaction : U, J_{Hund}
  How to compute U ? e.g. c-RPA.

- An entire subject. Not the topic of this lecture/hands-on.
  Cf Ref 2, Kotliar et al. RMP 2007

Cluster DMFT

DMFT, a family of approximations

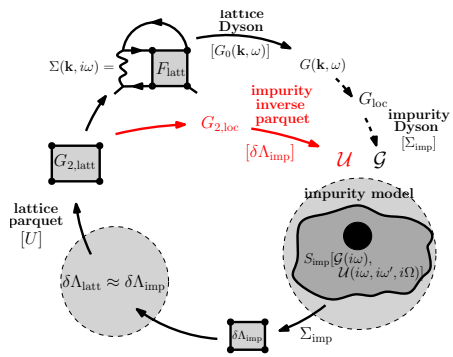
- Cluster DMFT



Control, short range correlation

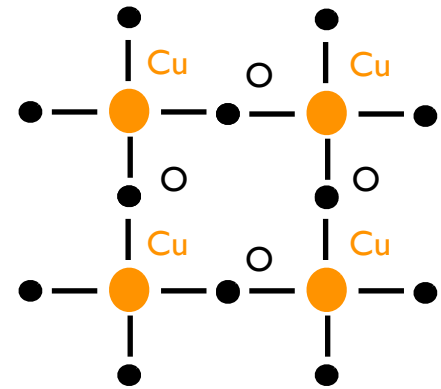
- Beyond cluster DMFT

Self-consistency on vertex
Dual fermions/bosons, Trilex, DΓA



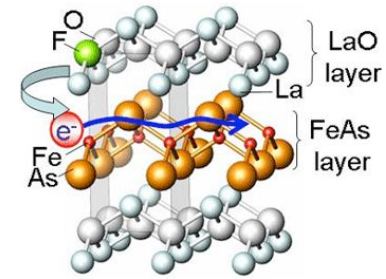
- Multiband/realistic systems

$$\Sigma(\omega) = \begin{pmatrix} \Sigma^{\rm imp}(\omega) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$



- Self-consistency in large unit cell (Cu + 2 O)
  $\Sigma_{ab}(\omega)$ a 3x3 matrix
- Impurity model on Cu, 1 band : $\Sigma^{\rm imp}(\omega)$ 1x1 matrix

- DFT + DMFT

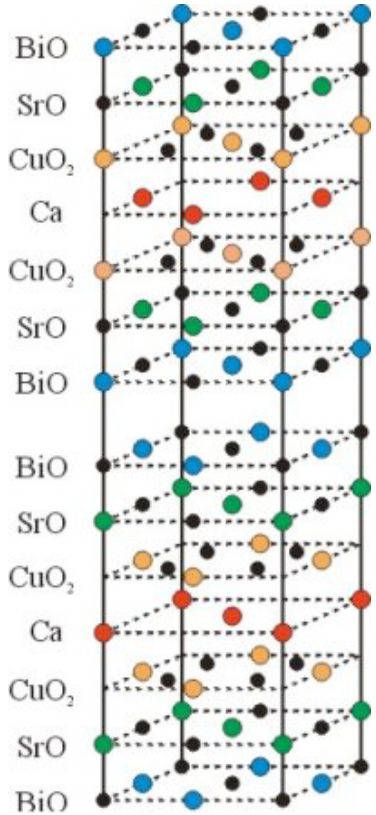


- Interface with electronic structure codes (project on Wannier functions, etc).

Why clusters ?

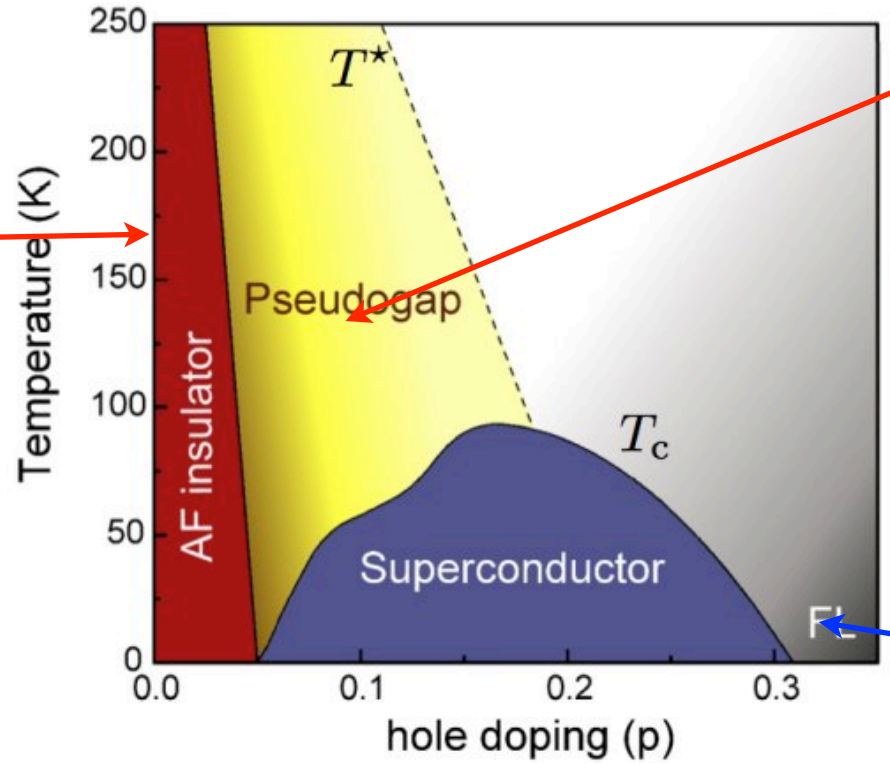
- To overcome some limitations of DMFT
- To get control, possibly a converged solution of e.g. Hubbard model.

Motivation : High Tc superconductors



Mott insulator

High-Tc superconductors.



Unconventional normal metal

Fermi liquid

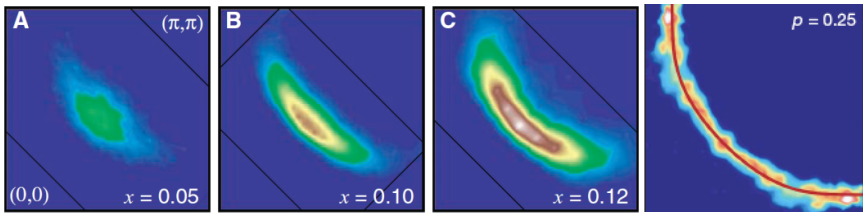
- High Tc superconductors are doped Mott insulators
- We want to use DMFT as a starting point

High Tc superconductors : issues with DMFT

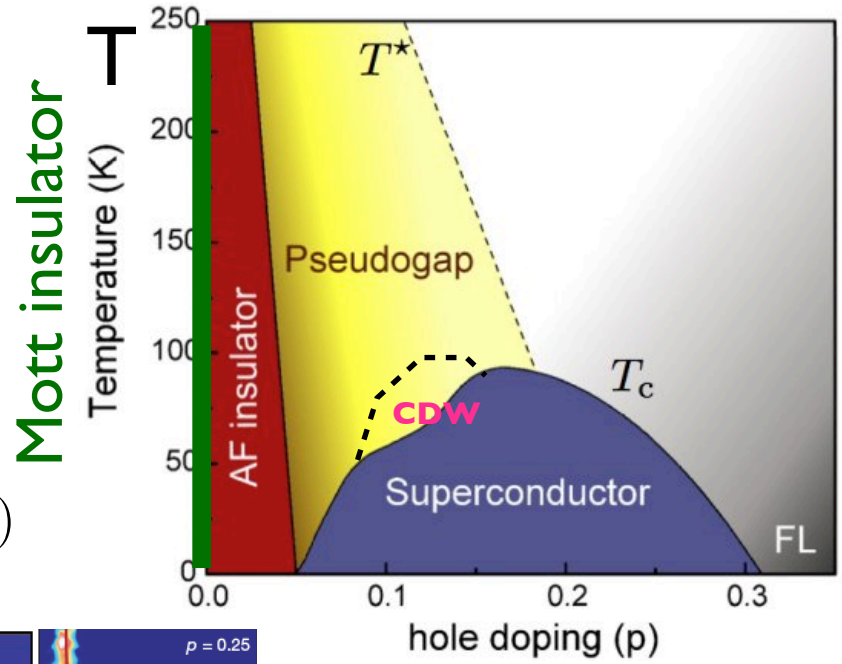
Normal Phase
Local self-energy
is not enough !

DMFT

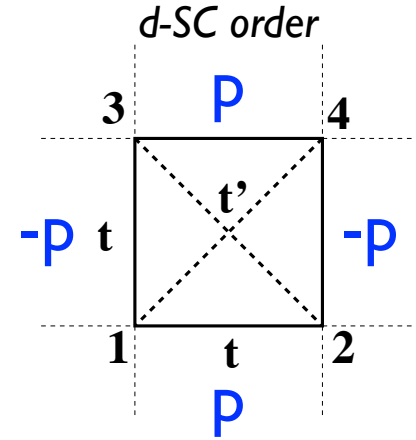
$$\Sigma_{\sigma \mathrm{latt}}(k, i\omega_n) = \Sigma_{\sigma \mathrm{imp}}(i\omega_n)$$



Node Antinode dichotomy in cuprates (ARPES)



SC
d-wave order
1 site is not enough !



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

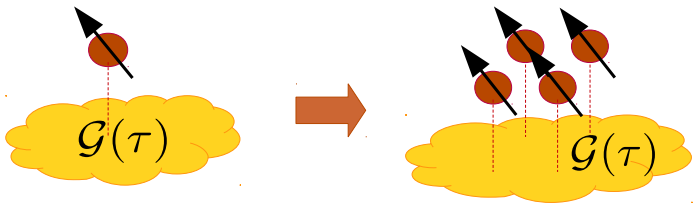
- Σ, Z, m* does depend on k !
- Super-exchange J ? Spin singlets ?
  Cut divergence of m* close to Mott
- Short range spatial correlations ?
- Long range bosonic fluctuations ?
  (e.g. spin fluctuations)

Idea

- Single-site DMFT. Σ is independent of k
- Take a cluster of sites instead of 1 site
- Several cluster methods.
  Different ways to parametrise the k dependence of Σ(k,ω)
- All methods interpolate between DMFT (1 site) and the full lattice problem (infinite number of sites).
  At large cluster size, we have the exact solution
- Two main methods :

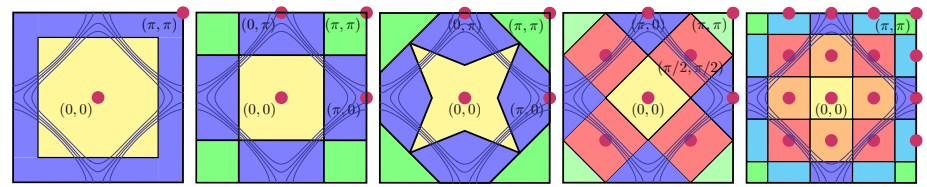
Real space clusters (C-DMFT)

Lichtenstein, Katsnelson 2000
Kotliar et al. 2001



Reciprocal space (DCA)
clusters Brillouin zone patching

Hettler et al. '98, ...

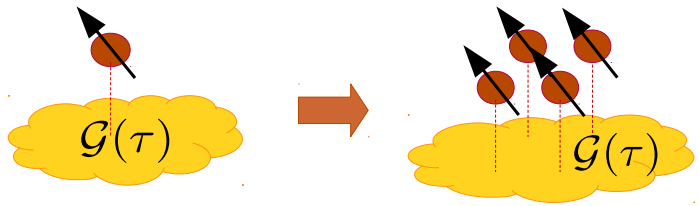


Cellular DMFT (C-DMFT)

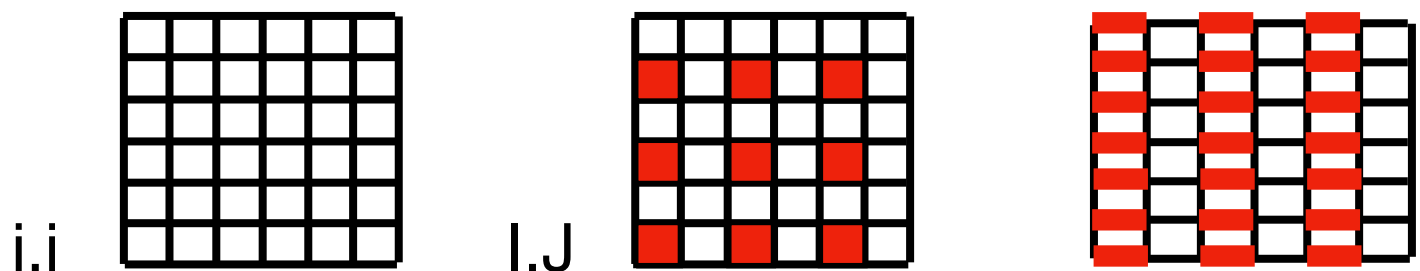
Cellular DMFT (CDMFT)

Lichtenstein, Katsnelson 2000; Kotliar et al. 2001

- Several Anderson impurities coupled to an effective bath



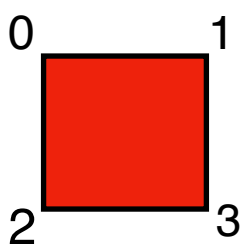
- We tile the lattice with clusters



Superlattice

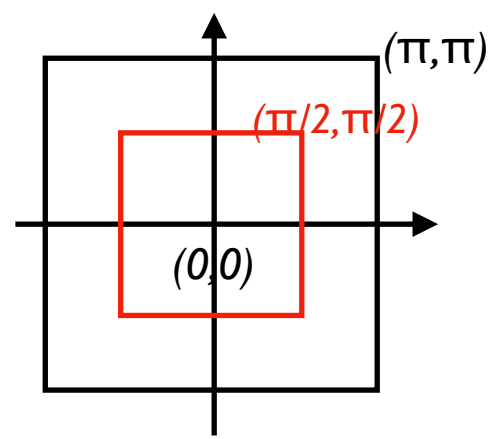
- Superlattice notations

$$i, j \rightarrow (I, J), a = 0, \ldots, 3$$



- Reduced Brillouin zone

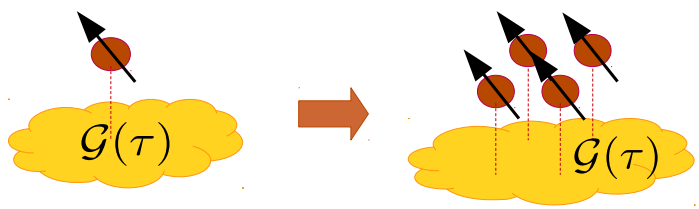
$$\left(\hat{\epsilon}_K\right)_{ab}$$

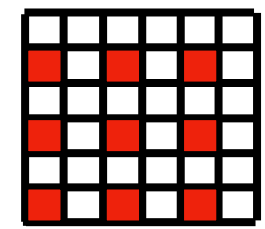


Cellular DMFT (CDMFT)

Lichtenstein, Katsnelson 2000; Kotliar et al. 2001

- Like a multi-orbital DMFT on the superlattice





Cluster index

$$S_{\rm eff} = -\int_0^\beta \sum_{ab} c^\dagger_{\sigma a}(\tau)\mathcal{G}^{-1}_{\sigma,ab}(\tau-\tau')c_{\sigma b}(\tau') + \sum_a \int_0^\beta d\tau\; U n_{\uparrow a}(\tau) n_{\downarrow a}(\tau)$$

$$G^{\rm imp}_{\sigma ab}(\tau) \equiv -\left\langle T c_{\sigma a}(\tau) c^\dagger_{\sigma b}(0)\right\rangle_{S_{\rm eff}}$$

Matrix equation

$$\Sigma_{\sigma \rm imp}[\mathcal{G}](i\omega_n) \equiv \mathcal{G}^{-1}_\sigma(i\omega_n) - G^{-1}_{\sigma\rm imp}[\mathcal{G}](i\omega_n)$$

$$G^{\rm imp}_\sigma[\mathcal{G}](i\omega_n) = \sum_{K\in \text{ RBZ}} \left((i\omega_n+\mu)\mathbf{1} - \hat{\epsilon}_K - \Sigma^{\rm imp}_\sigma[\mathcal{G}](i\omega_n)\right)^{-1}$$

Reduced Brillouin Zone

CDMFT. Translation invariance

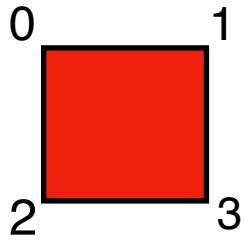
- CDMFT breaks translation invariance !
- (Re)Periodization : Restore translation invariance.
- After the DMFT computation (iterative loop) is converged.

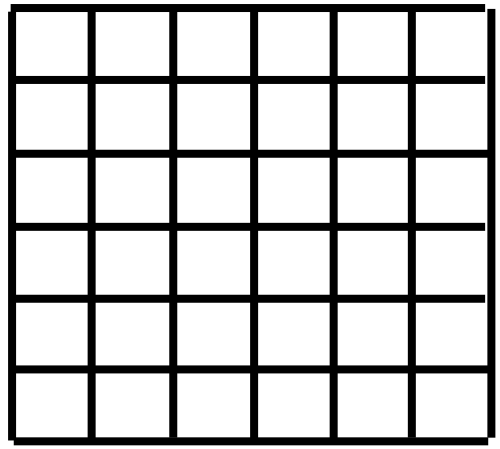
$$\Sigma^{\rm latt}_{i,i} = \Sigma^{\rm imp}_{00}$$

$$\Sigma^{\rm latt}_{i,i} = \frac{1}{2}\Sigma^{\rm imp}_{01}$$

$$\Sigma^{\rm latt}_{i+1,i} = \frac{1}{2}\Sigma^{\rm imp}_{02}$$

$$\Sigma^{\rm latt}_{i+1,i+1} = \frac{1}{4}\Sigma^{\rm imp}_{03}$$



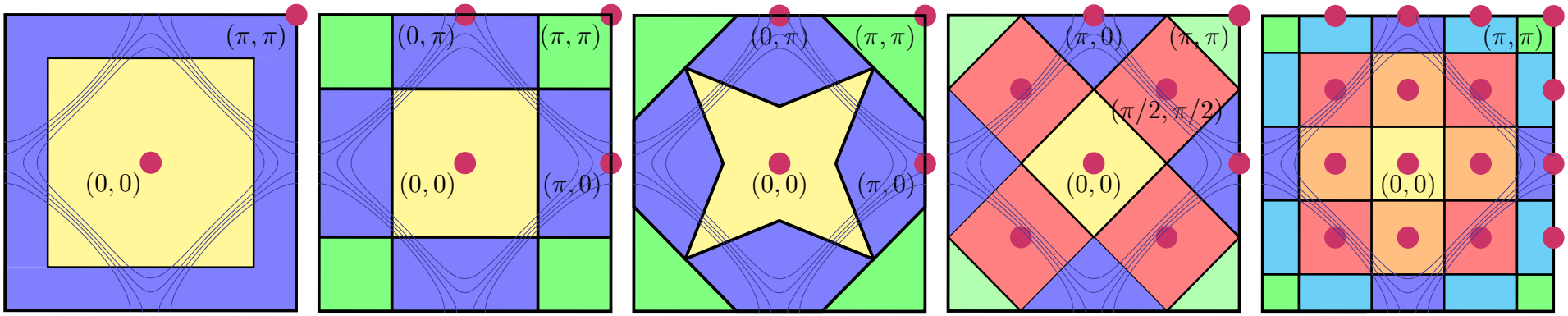


- Factors here to enforce causality property of $\Sigma^{\rm latt}$ (Im $\Sigma^{\rm latt}(\omega) < 0$)
- Ambiguous : Reperiodize self-energy ? G ? Cumulant M ?

DCA

DCA

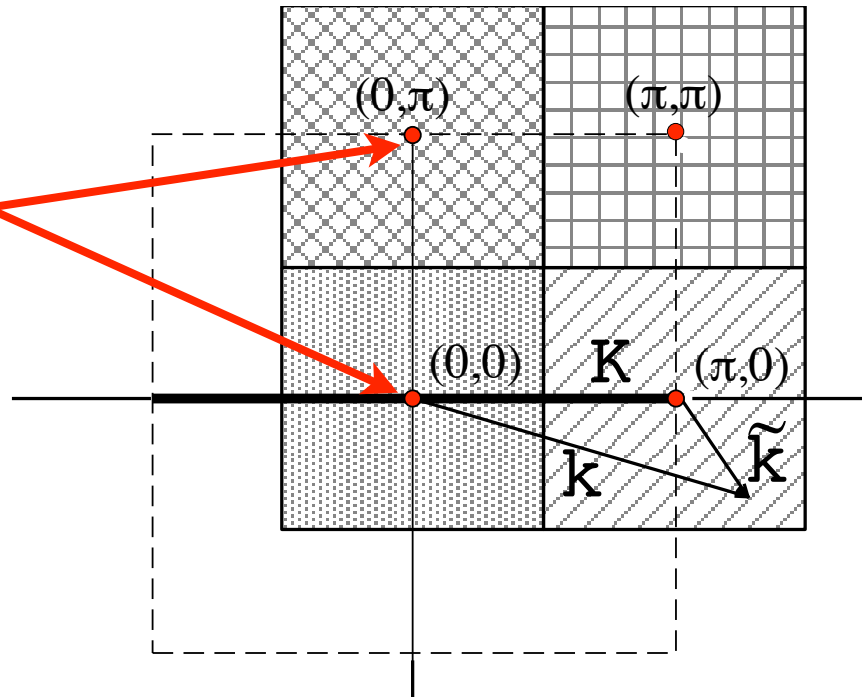
- Idea : take Σ piecewise constant in the Brillouin zone
- Let us cut the BZ in N_c patches (e.g. N_c = 2, 4, 8, 16)



- Red points : centre of the patches : K_c.
- Change coordinate :

$$k \to (K_c, \tilde{k}) \qquad k = K_c(k) + \tilde{k}$$

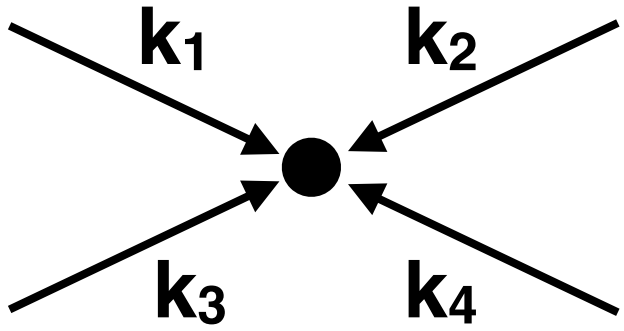
Patch center *In the patch*



DCA : definition

- In the Luttinger-Ward functional **Φ**, coarse grain the momentum conservation.
- Change the vertex :

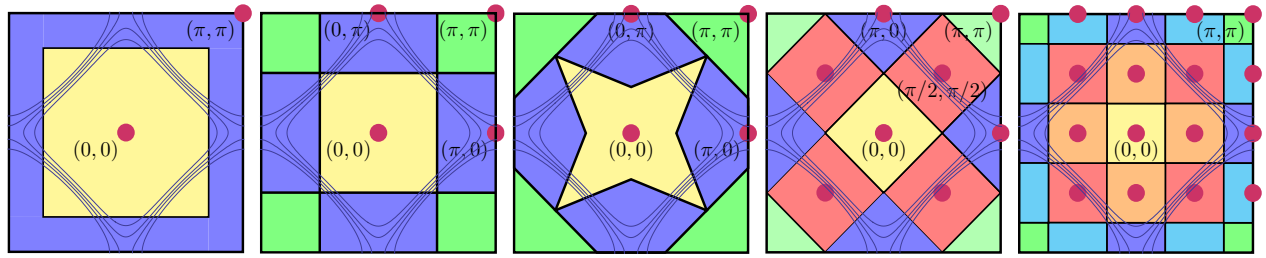
$$\propto \delta(k_1 + k_2 + k_3 + k_4)$$



$$\propto \delta(K_c(k_1) + K_c(k_2) + K_c(k_3) + K_c(k_4))$$

- Yields an approximated $\Phi \approx \Phi_{N_c}$
- $N_c = 1$: DMFT. No k conservation, all propagators are local.
- $N_c = \infty$: Exact
- Ok, but can we solve this with an impurity model ?

DCA : auxiliary impurity model

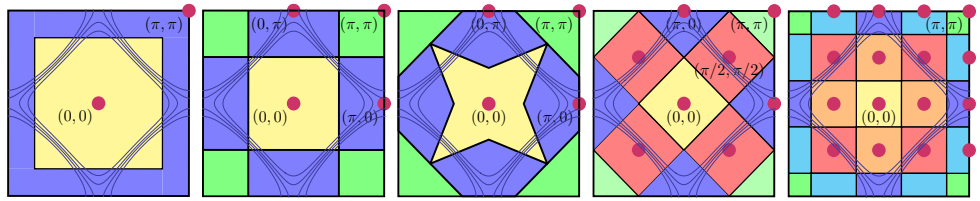


- K_c are exactly the reciprocal lattice of a cyclic finite cluster (e.g. 2x2)
- Take one diagram on the lattice for Φ_{Nc}.
- For each line in the diagram, split the integral on k: $\int dk = \sum_{K_c} \int d\tilde{k}$
- The integral can be done (not constrained at vertex !)
- For each line, we have in fact a full coarse grained propagator

$$G^{\mathrm{imp}}(K_c, i\omega_n) = \int d\tilde{k}\; G^{\mathrm{latt}}(K_c + \tilde{k}, i\omega_n)$$

- Φ_{Nc} is the LW functional of a cyclic finite cluster, evaluated at $G^{imp}(K_c)$

DCA : auxiliary impurity model



- The self-energy on the lattice is given by :

$$\Sigma^{\text{latt}}(k) = \frac{\partial \Phi}{\partial G^{\text{latt}}(k)}$$

$$= \sum_{K_c} \frac{\partial \Phi}{\partial G^{\text{imp}}(K_c)} \underbrace{\frac{\partial G^{\text{imp}}(K_c)}{\partial G^{\text{latt}}(k)}}_{\delta(K_c = K_c(k))}$$

$$= \Sigma^{\text{imp}}(K_c(k))$$

- The self-energy on the lattice is constant by piece on the BZ.
- It has discontinuities in k space. (DCA+ : smooth discontinuities, *Staar et al. Phys. Rev. B 2013, arxiv:1402.4329, arxiv:1601.03838*).
- As in DMFT, we use the impurity model as a machine to compute Φ_{Nc}, the approximation to Φ.

DCA : complete equations

- Impurity model is a cyclic finite cluster
- Like multi-orbital DMFT, but the matrix inversion is diagonal in K_c

$$S_{\text{eff}} = -\int_0^\beta \sum_{ab} c^\dagger_{\sigma a}(\tau)\mathcal{G}^{-1}_{\sigma,ab}(\tau-\tau')c_{\sigma b}(\tau') + \sum_a \int_0^\beta d\tau\ U n_{\uparrow a}(\tau) n_{\downarrow a}(\tau)$$

$$G^{\text{imp}}_{\sigma ab}(\tau) \equiv -\left\langle T c_{\sigma a}(\tau) c^\dagger_{\sigma b}(0)\right\rangle_{S_{\text{eff}}}$$

$$\Sigma_{\sigma\text{imp}}[\mathcal{G}](K_c, i\omega_n) \equiv \mathcal{G}^{-1}_\sigma(K_c, i\omega_n) - G^{-1}_{\sigma\text{imp}}[\mathcal{G}](K_c, i\omega_n)$$

$$G^{\text{imp}}_\sigma[\mathcal{G}](K_c, i\omega_n) = \int d\epsilon D_C(\epsilon) \frac{1}{i\omega_n + \mu - \epsilon - \Sigma^{\text{imp}}_\sigma[\mathcal{G}](K_c, i\omega_n)}$$

Density of state of patch C

$$D_c(\epsilon) \equiv \sum_{\tilde{k}} \delta(\epsilon - \epsilon_{K_c+\tilde{k}})$$

Others cluster methods

- E.g. Nested Clusters *(A. Georges et al. RMP 1996)*
  Self-energy Embedding Theory (SEET) *(D. Zgid, E. Gull 2017)*
- Idea : exhaust the bold 2PI series with local models

$$\Phi_{\text{Hubbard}}[G_{ij}] = \underbrace{\sum_i \phi_1(G_{ii})}_{\textbf{Local = DMFT}} + \underbrace{\sum_{\langle i,j\rangle} \phi_2(G_{i,j}) + \sum_{\langle i,j,k\rangle} \phi_3(G_{i,j}, G_{i,k}, G_{j,k}) + \dots}_{\textbf{Non local = clusters}}$$

- e.g.

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

- Real space, translation invariance. Bethe-Kikuchi at classical limit
- Excellent at weak, moderate coupling.
- Strong coupling : instability of the DMFT iterative cycle, to a non physical solution due to multivaluedness of **Φ**

Application to the Hubbard model

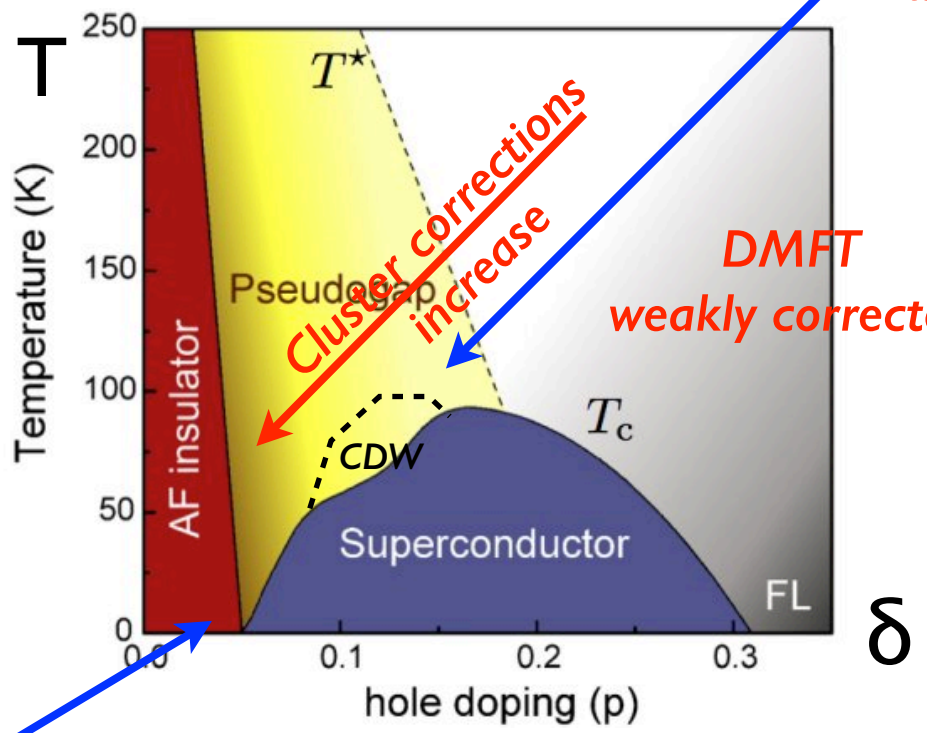
DMFT is high temperature method

"Top to Bottom"

Start from high T/doping

R.G.

Diagrammatic methods

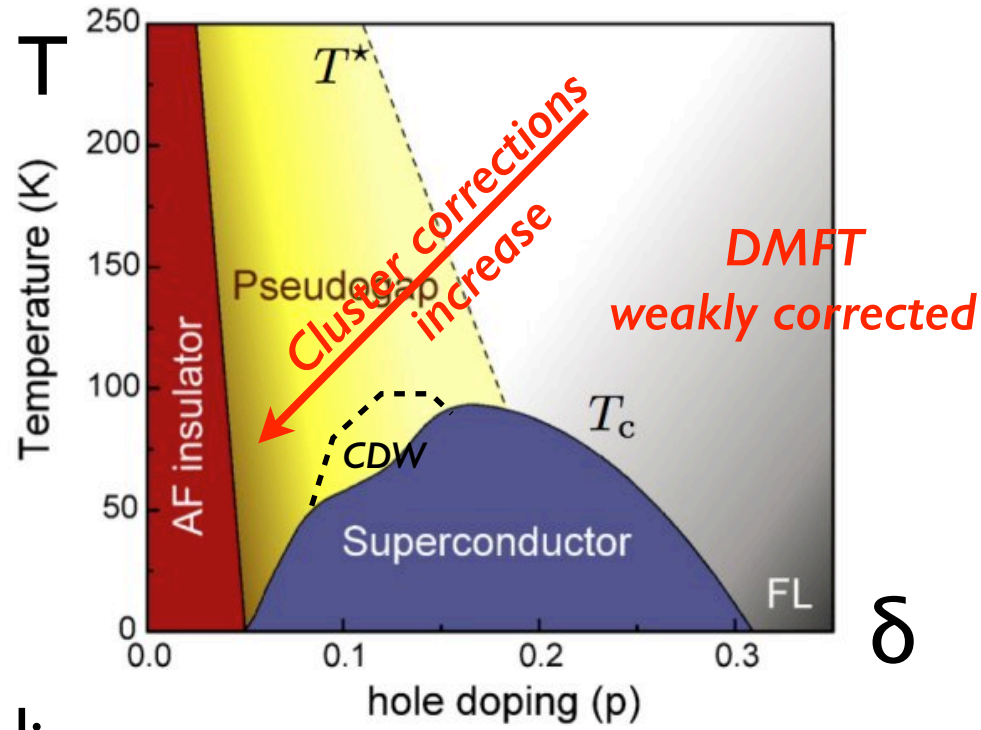


"Bottom to Top"

Study the many-body ground state

DMRG, PEPS, MERA

Large vs minimal clusters



- At high T or δ, intermediate U:
  - Exact solution : can large clusters converge before the sign problem kills the "impurity solver" ?
- At lower T, δ
  - Small clusters capture some important effects (pseudogap, d-SC). Minimal cluster ? Physical picture ?

Cluster DMFT & Hubbard model

- A lot of results on cluster DMFT + Hubbard, with various clusters

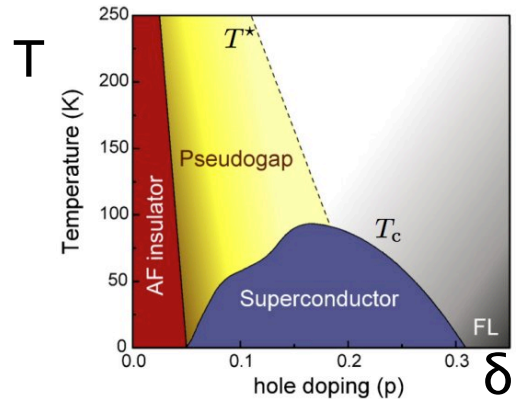
A lot of authors & works since 2000, e.g.
Capone, Civelli, Ferrero, Georges, Gull, Haule,
Imada, Jarrell, Kotliar, Lichtenstein, Katsnelson,
Maier, Millis, Sordi ,Tremblay, Werner, OP, ...

- Let us distinguish:

1. Robust features across various cluster methods
2. Interesting features seen in some cluster methods only
3. Converged (exact) results, at large cluster size.

Cluster DMFT & Hubbard model

- Emergence of some consensus on robust features of the Hubbard model



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Pseudo-gap

- Emerging from Mott insulator
- Nodes/antinodes. Fermi Arcs

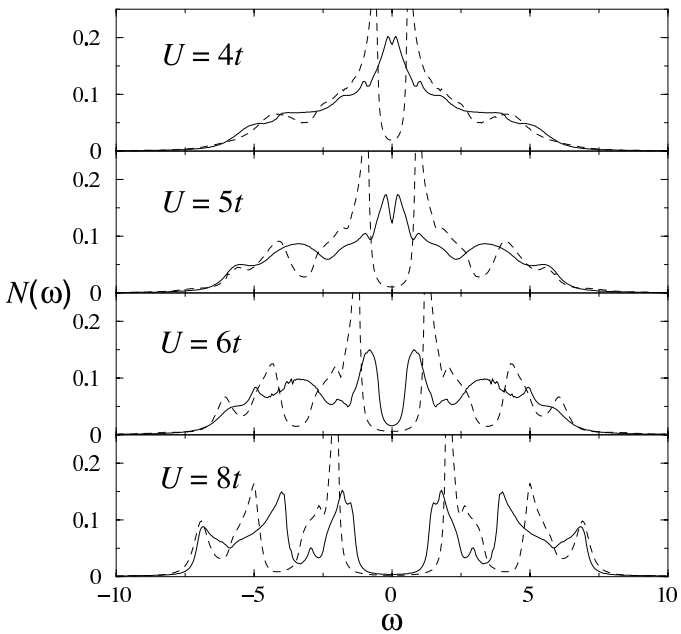
d-wave SC

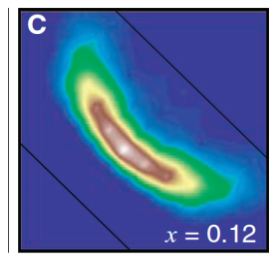
- In various clusters sizes (4, 8, 16, ...).
- Behavior of Tc, gap vs δ

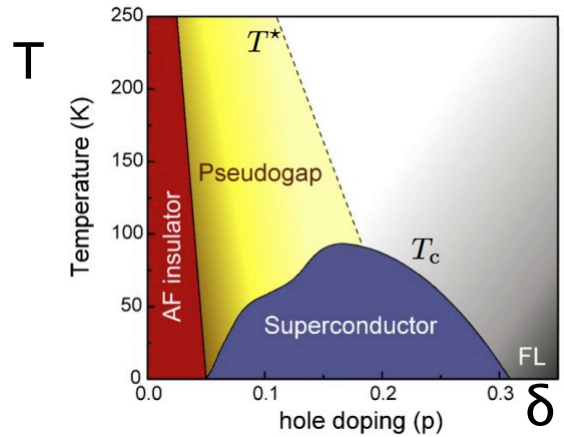
Pseudogap

- CDMFT 2x2 (ED)

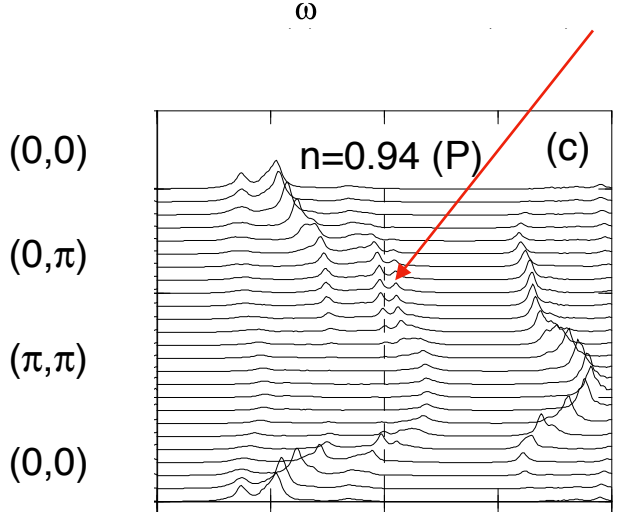
B. Kyung et al. Phys. Rev. B 73, 165114 (2006)



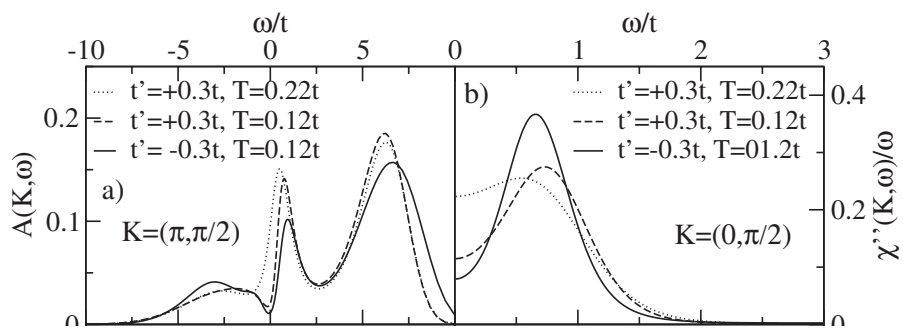


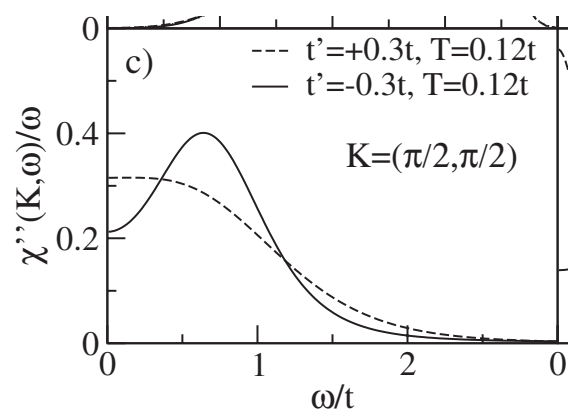


A. Macridin, et al. Phys. Rev. Lett. 97, 036401 (2006)



- DCA, 16 sites, U=8t,

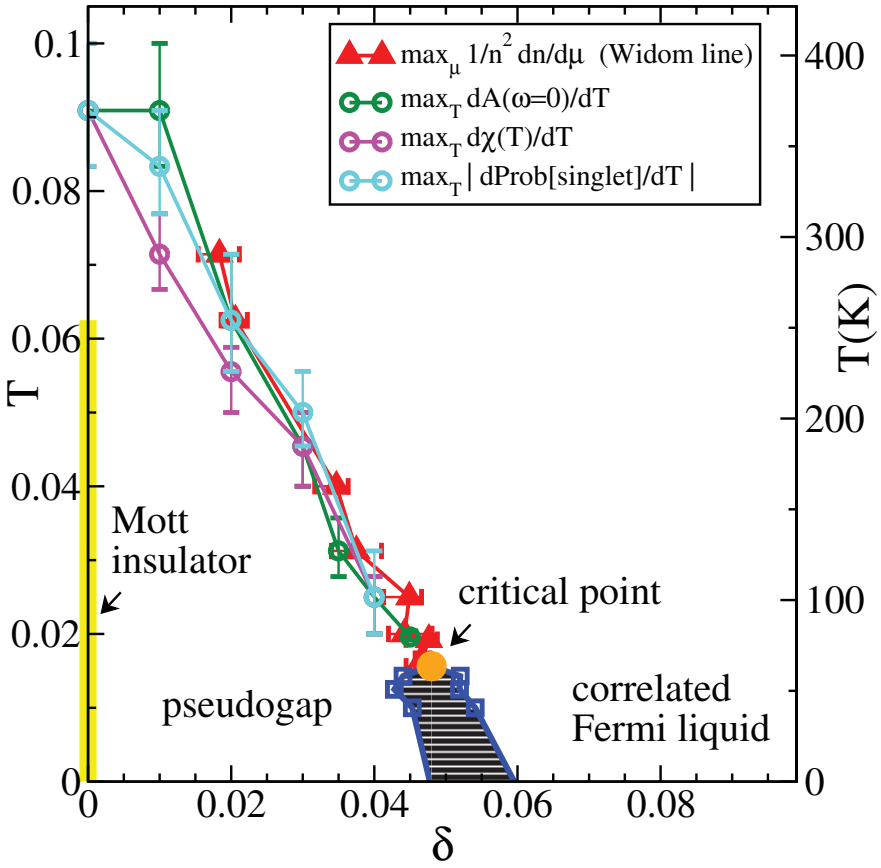


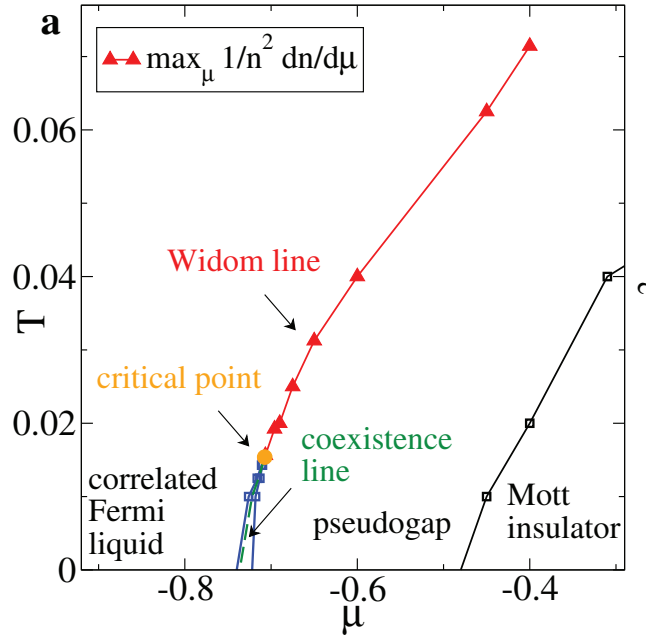


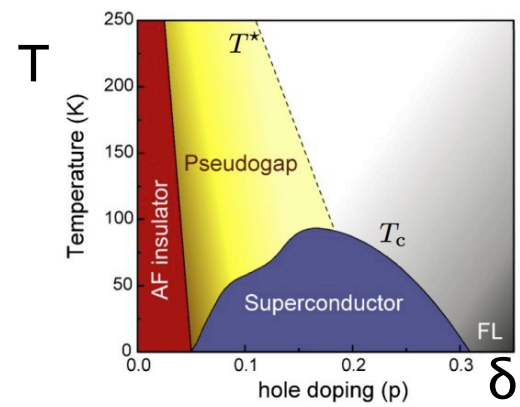
CDMFT 2x2 :Widom line scenario

G. Sordi, P. Sémon, K. Haule & A.-M. S. Tremblay
*Scientific Reports **2**, 547 (2012)*

- CDMFT 2x2 solution, normal phase.







- But cluster is small. Reproduce this with DCA method ?

A minimal example

A quantum dimer in a bath (DCA 2 patches)

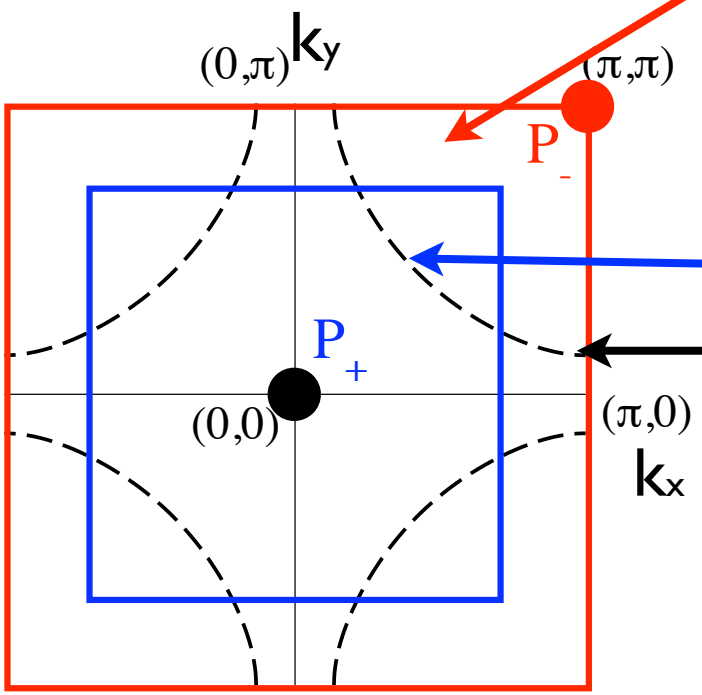
M. Ferrero, P. S. Cornaglia, L. De Leo, O. P. , G. Kotliar, A. Georges, EPL, PRB 2009-2010

Hand-ons

Minimal cluster DMFT for Fermi Arcs

M. Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, A. Georges, EPL and PRB 2009

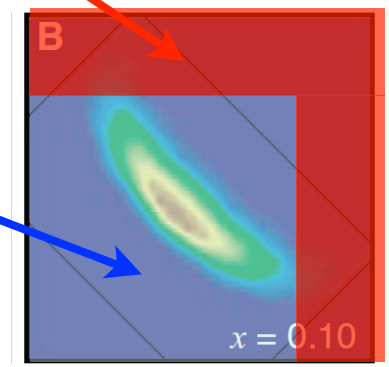
- Two patches patches P+, P- (of equal volume)



Outer patch P- : Antinodes

Inner patch P+ : Nodes

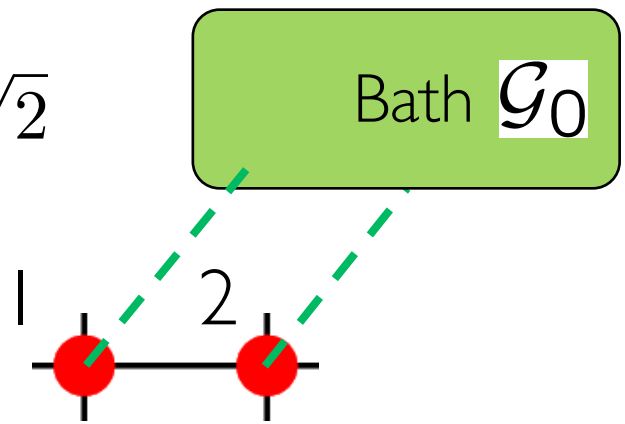
Free Fermi surface



$$\mu = 1, 2$$

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

2-patch DCA



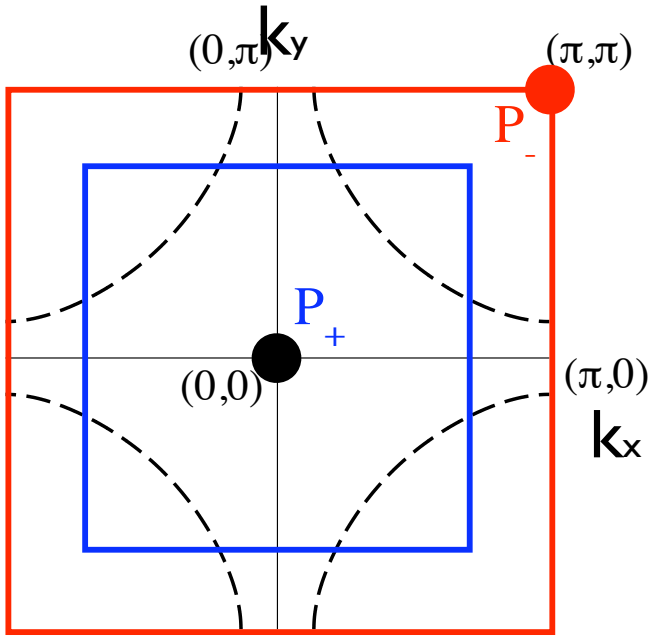
Two-site Anderson impurity model

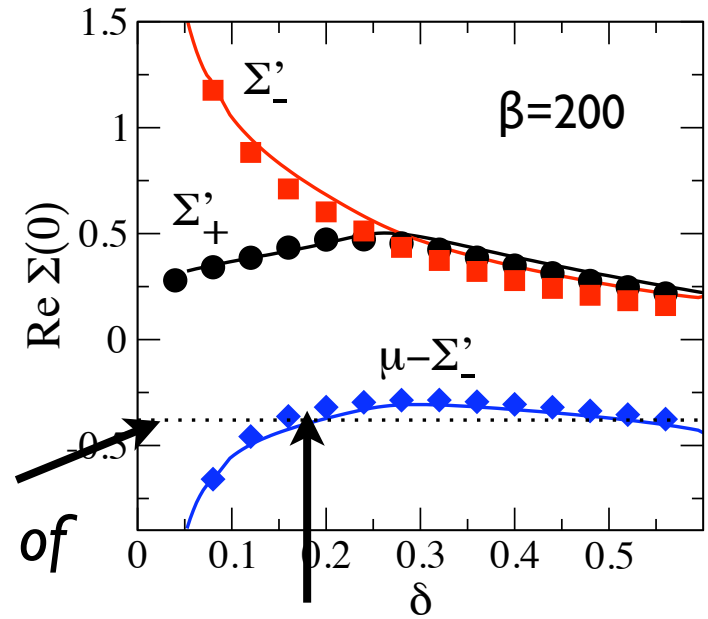
Even (bonding) orbital 1+2 ↔ nodal patch

Odd (antibonding) orbital 1-2 ↔ antinodal patch

Selective Mott 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
- Effective band transition at low energy





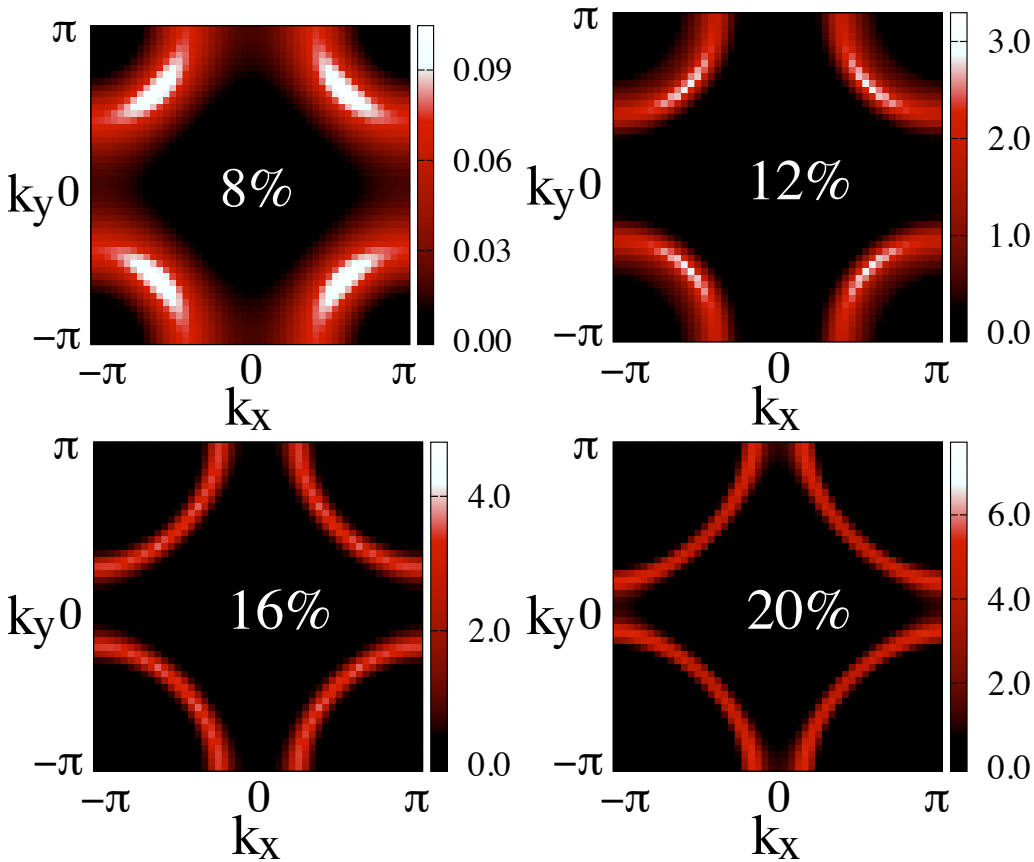
band edge of P- patch

Outer/odd Orbital gets (pseudo-)gapped

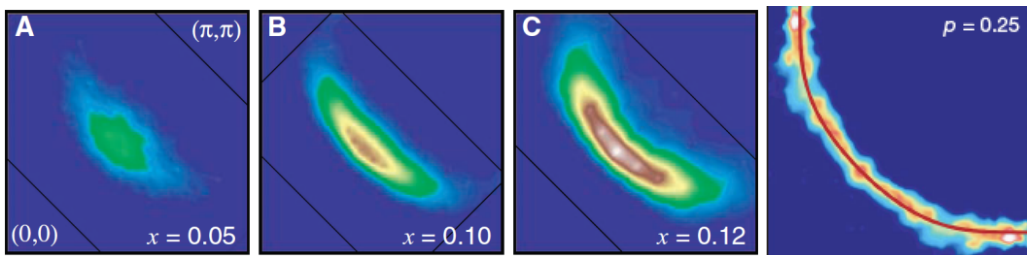
Do it yourself: Hands-on

ARPES intensity maps at Fermi level

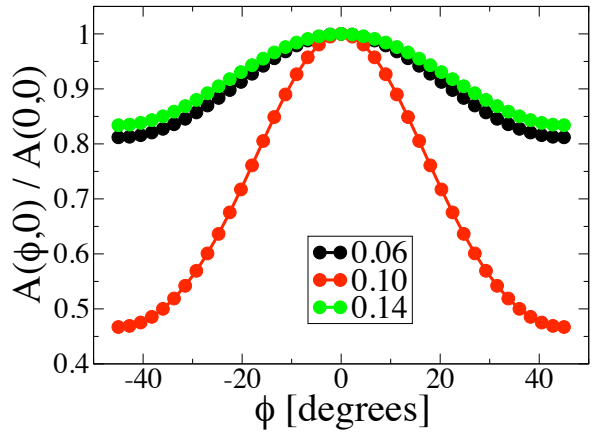
- With "cumulant" interpolation...
- Maximum contrast around 10 %



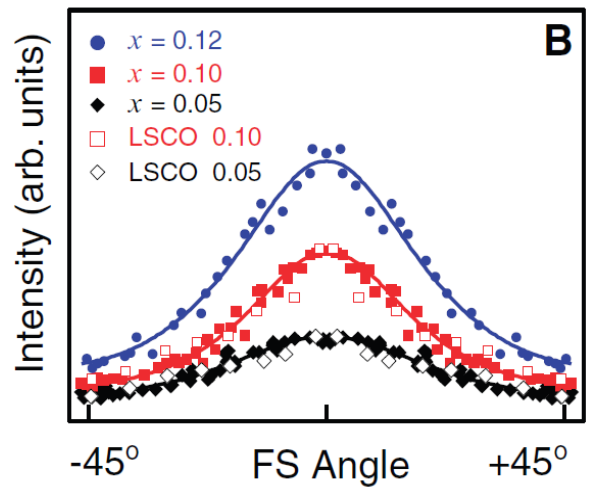
$$A(k, \omega = 0)$$



Theory



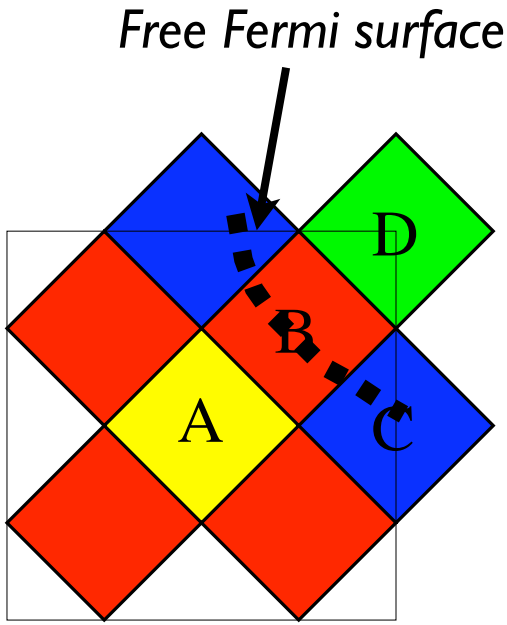
Experiments



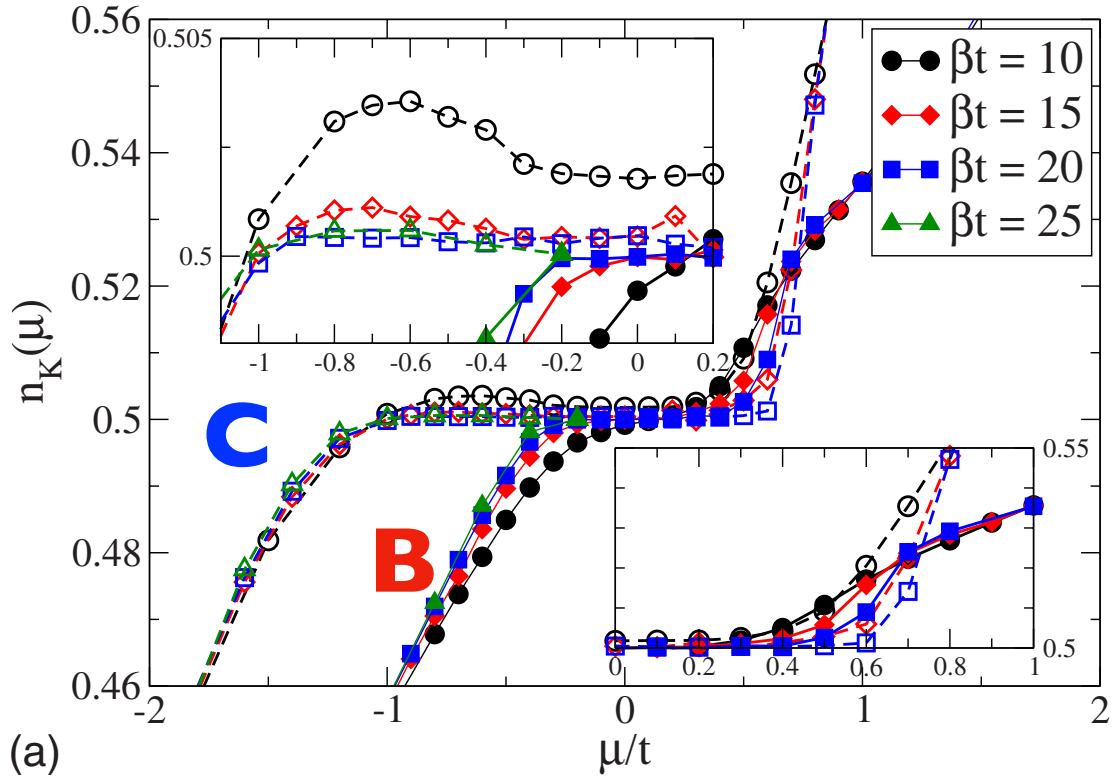
Shen et al. Science 307, 901 (2005)

With 8 sites DCA clusters

E. Gull, P.Werner and A.J. Millis, OP, PRB 2009



Patches for 8 sites clusters

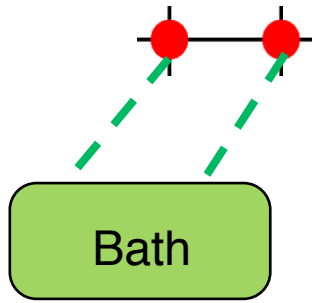


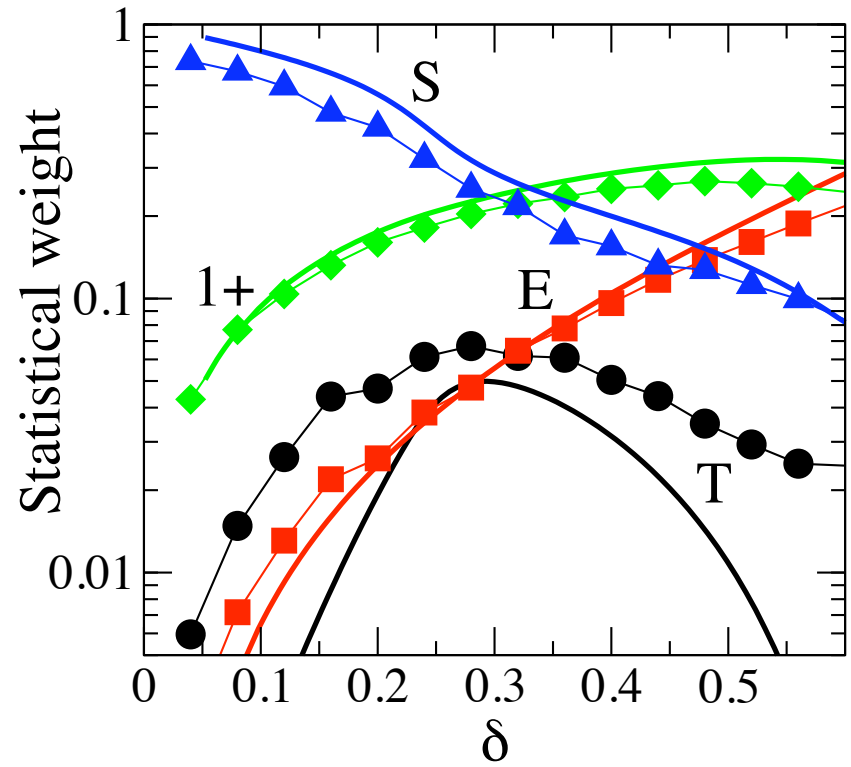
- $n_K(\mu)$: occupation of each patch
- 2 steps transition : at intermediate doping,C insulating, B is metallic.

Having a very small cluster
allows further analysis

Singlet state dominates at low doping

- Relative weight of various cluster states, measured:
  - in the Monte Carlo (time spent in the state in the path integral)
  - in a (rotationally invariant) slave boson solution
    (Lechermann, Georges, Kotliar, OP, 2007)
- Two states of the dimer dominate at low doping :
  - Two spins in a singlet (S)
  - 1 spin 1/2 + 1 hole (1+)

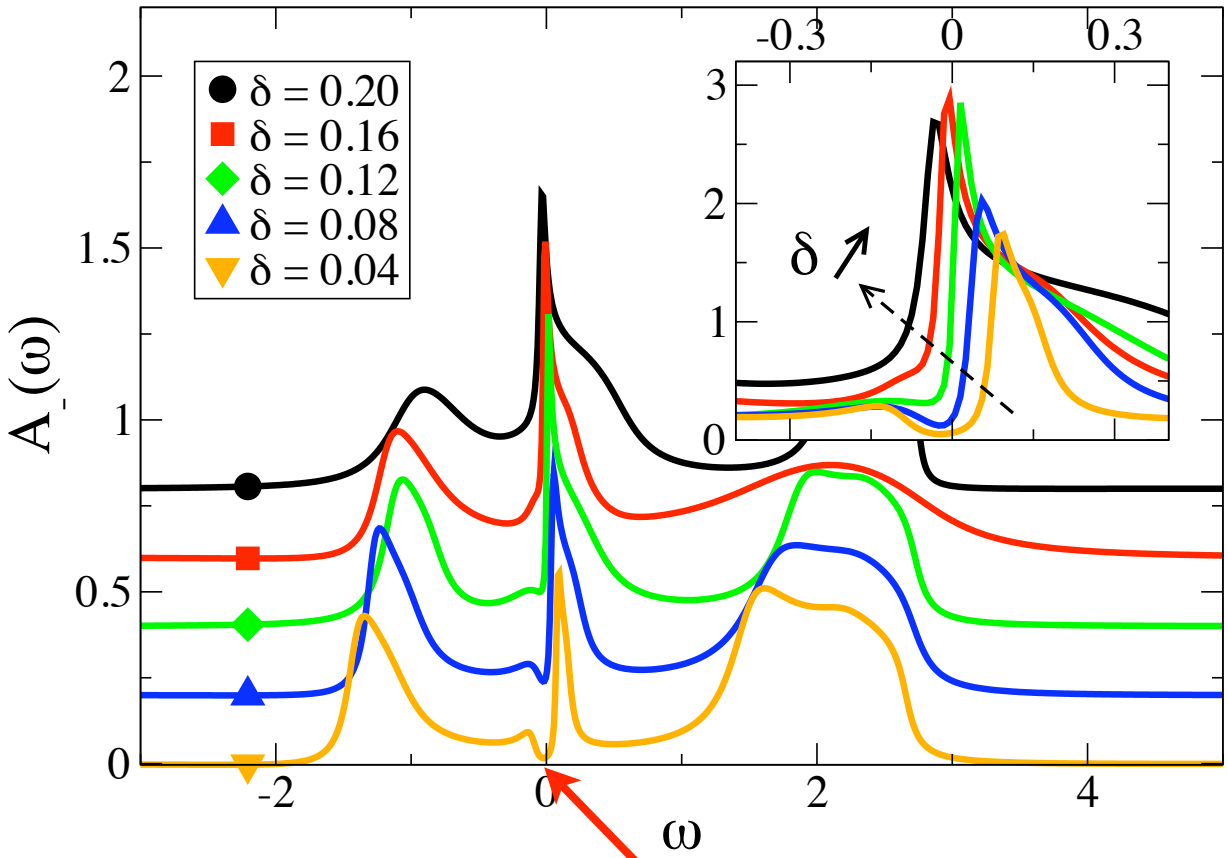


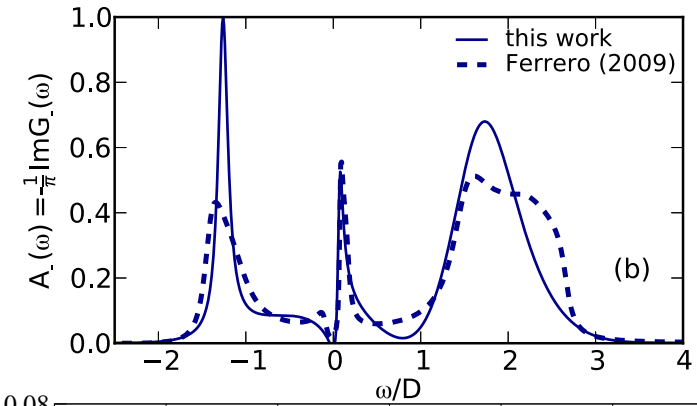


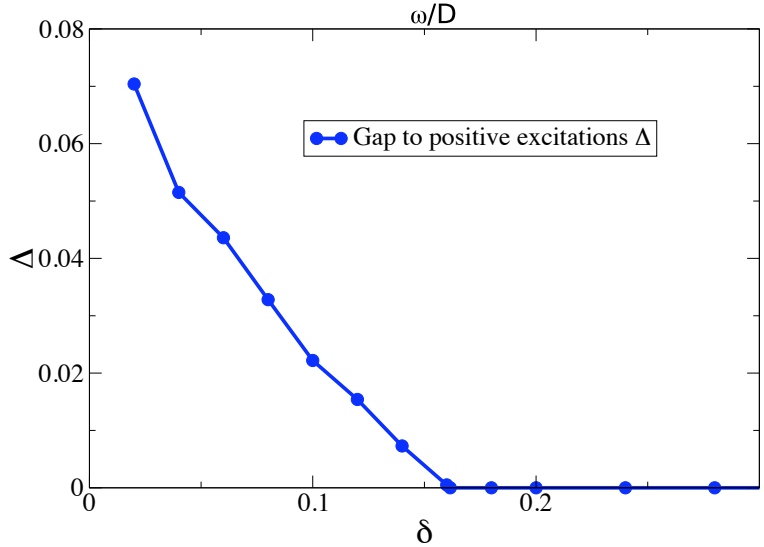
Antinode : not a sharp gap, a pseudogap !

- Effective band transition at low energy, but....

DMRG solver
A. Wolf et al. 2014



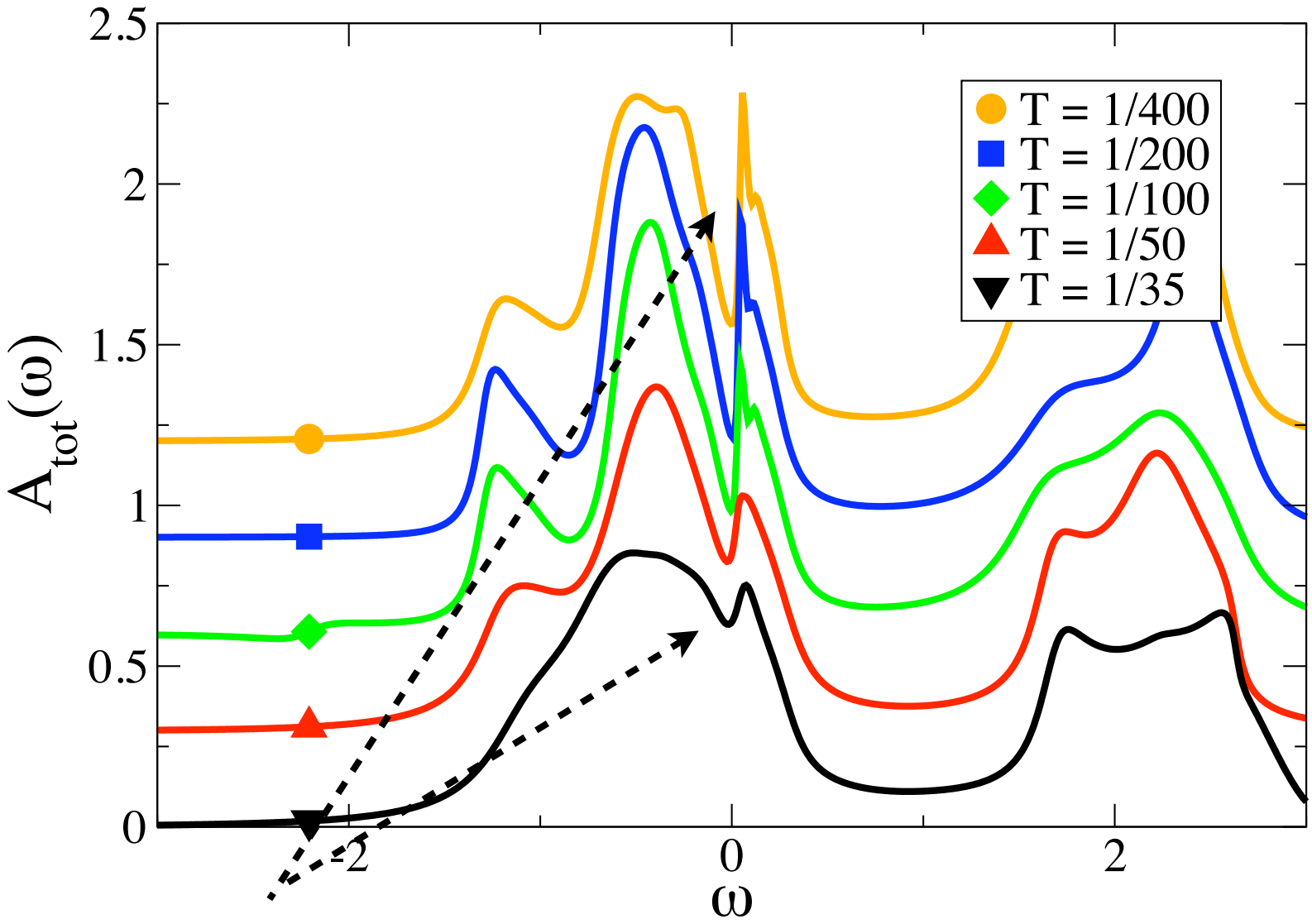




Energy scale of pseudogap on positive energy side

- At the antinode, a pseudogap appears below the transition. Correlations have a strong effect (e.g. prominent Hubbard bands)

Pseudo-gap opens upon cooling



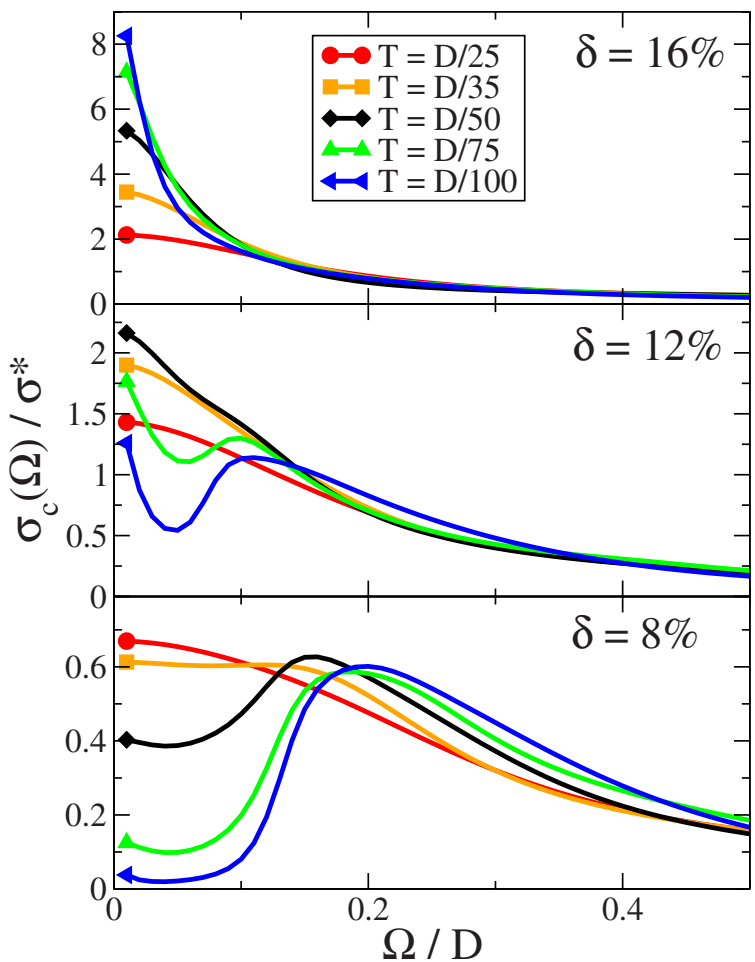
- Total spectral function Atot(ω) for various temperature at δ =0.08. A shift of 0.3 has been added between each curves for clarity.

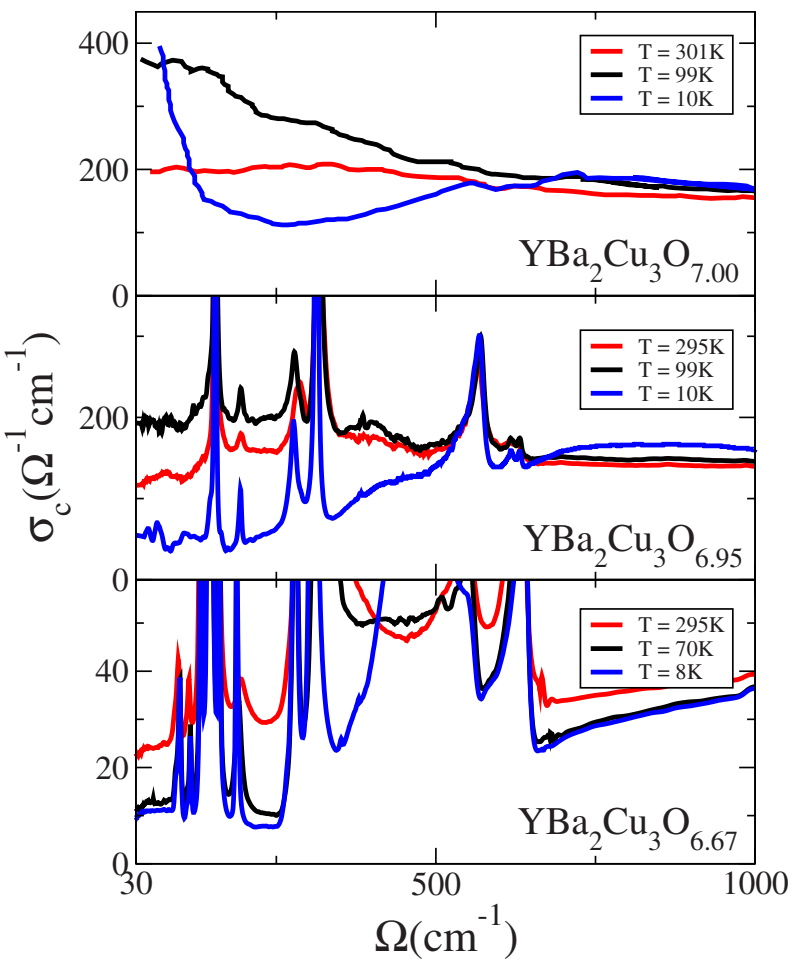
Optics : $\sigma_c(\omega)$

Ferrero, O. P., Georges, Kotliar, Basov, Phys. Rev. B 82 054502 (2010)

- Pseudo-gap in optics. Qualitative agreement with experiments

$$\sigma_c(\Omega) = \frac{2e^2 c}{\hbar ab}\int d\omega \frac{f(\omega) - f(\omega+\Omega)}{\Omega}\frac{1}{N}\sum_{\mathbf{k}} t_\perp^2(\mathbf{k}) A(\mathbf{k},\omega) A(\mathbf{k},\Omega+\omega)$$

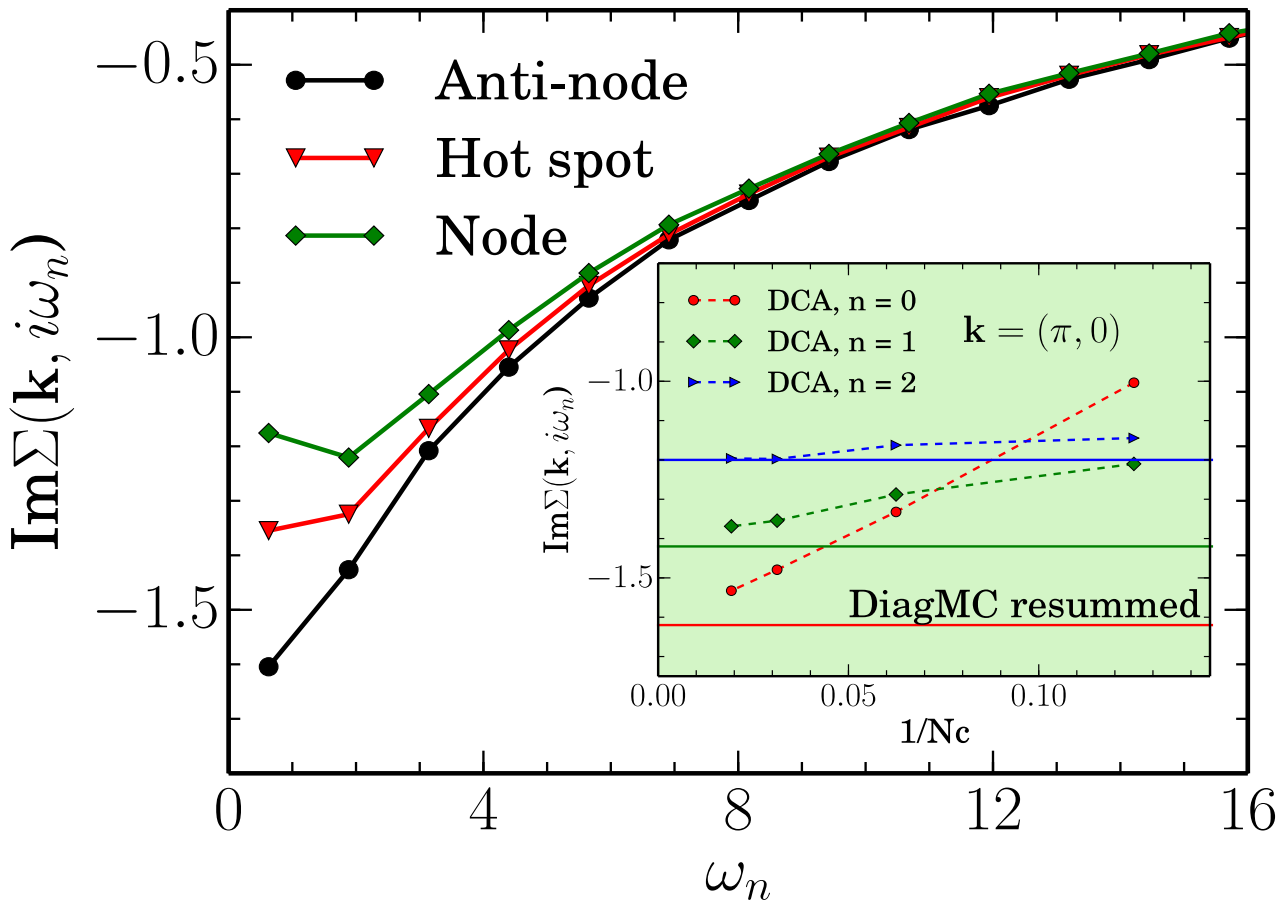




Can we converge the cluster method
in a non-trivial region ?

Pseudogap : exact solution at high temperature

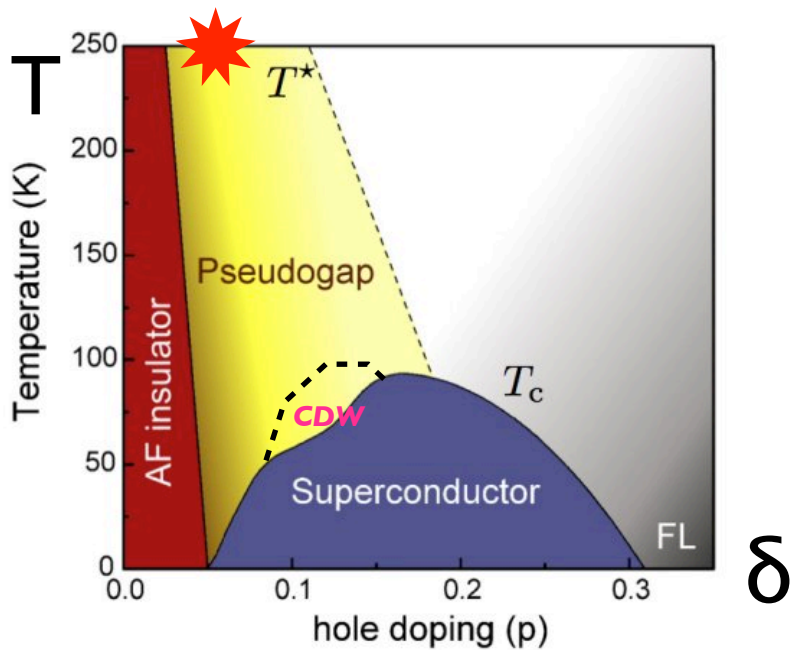
- Exact solution of Hubbard model at a non trivial point with the pseudo-gap !
- Large cluster DCA (converged) or Diagrammatic QMC.

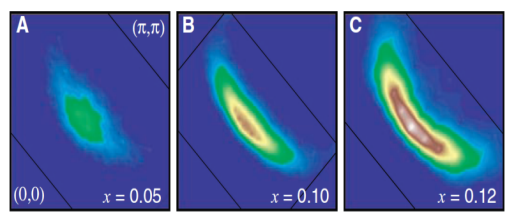


W.Wu, M. Ferrero, A. Georges, E. Kozik. Arxiv:1608.08402

U=5.6t *t'= -0.3t*

δ = *4%* T = *0.2t*





Superconducting phase

d-SC in DMFT

- Need a cluster : 2x2, 8, 16, …, due to symmetry questions.
- Use Nambu spinors

$$\psi_i = \begin{pmatrix} c_{i\uparrow} \\ c^{\dagger}_{i\downarrow} \end{pmatrix}$$

- F : anomalous Green function

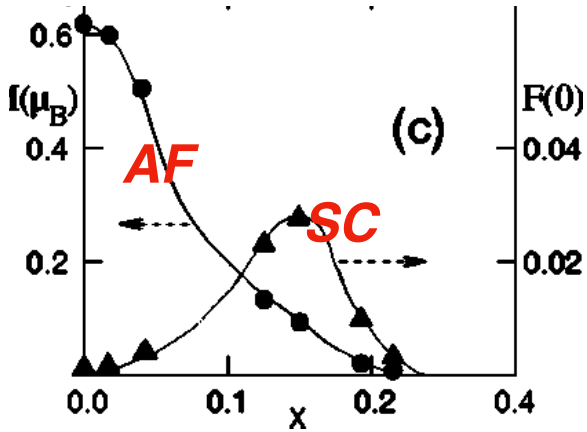
$$\hat{G}(\mathbf{k},\tau) \equiv -\langle T\Psi_{\mathbf{k}}(\tau)\Psi^{+}_{\mathbf{k}}(0)\rangle = \begin{pmatrix} G(\mathbf{k},\tau) & F(\mathbf{k},\tau) \\ F(\mathbf{k},\tau)^{*} & -G(-\mathbf{k},-\tau) \end{pmatrix}.$$

$$F(\mathbf{k},\tau) \equiv -\langle T c_{\mathbf{k}\uparrow}(\tau) c_{-\mathbf{k}\downarrow}(0)\rangle.$$

Anomalous Green function

d-SC and AF

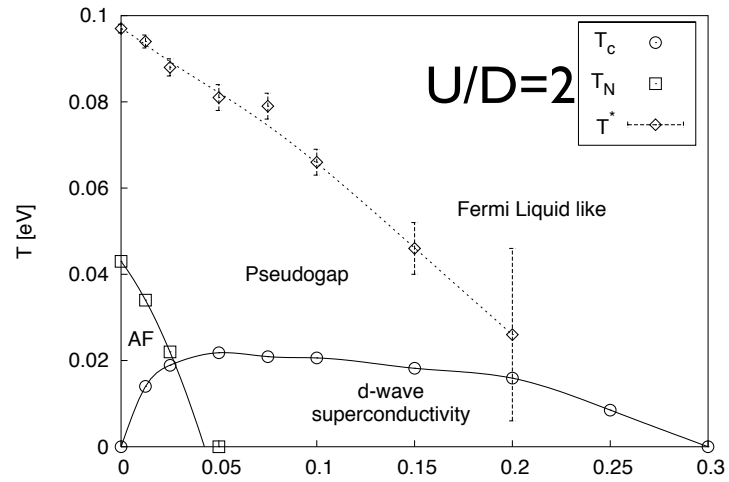
- 4 sites CDMFT



CDMFT

A. Lichtenstein et al. PRB 62, R9283 (2000)

- 4 sites DCA

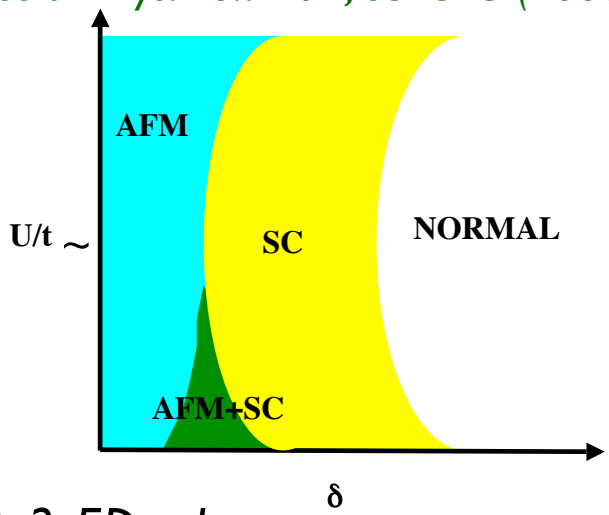


DCA

M. Jarrell et al, PRL 85,1524 (2001)

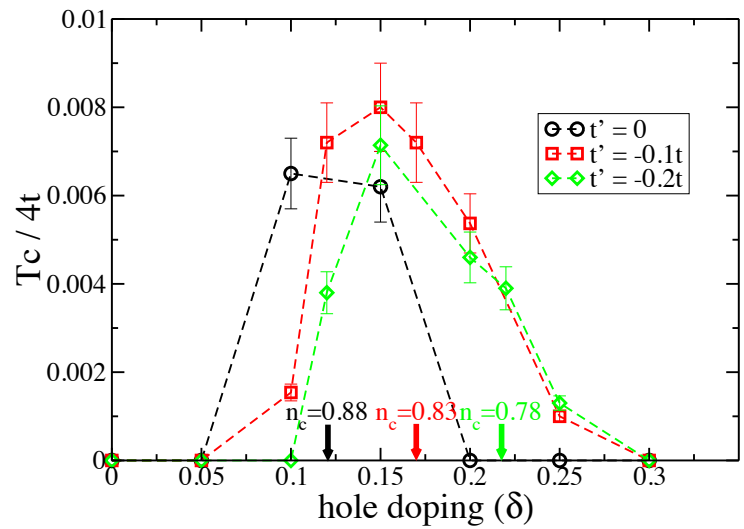
- Coexistence AF, SC

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



CDMFT, 2x2, ED solver

- DCA U=6t, N_c=12, 16.

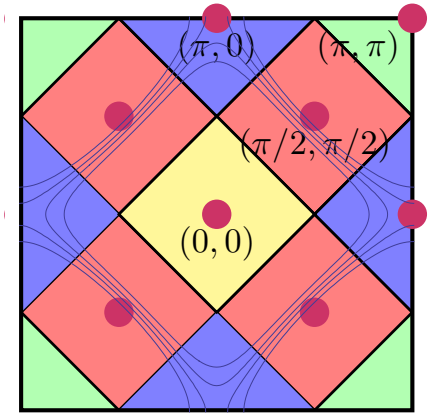


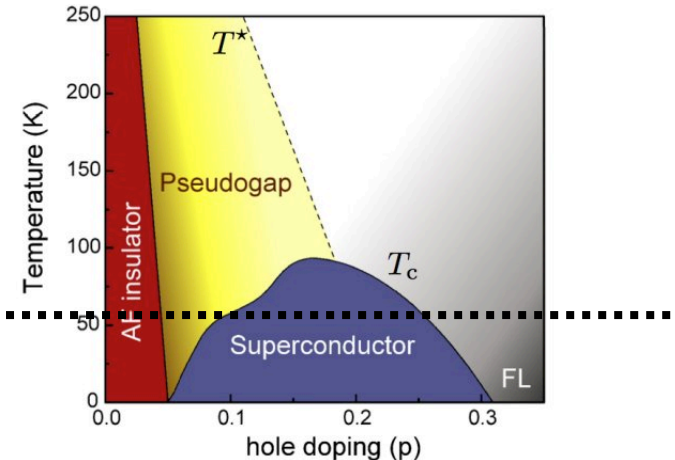
KS Chen et al., Phys. Rev. B 88, 245110 (2013)

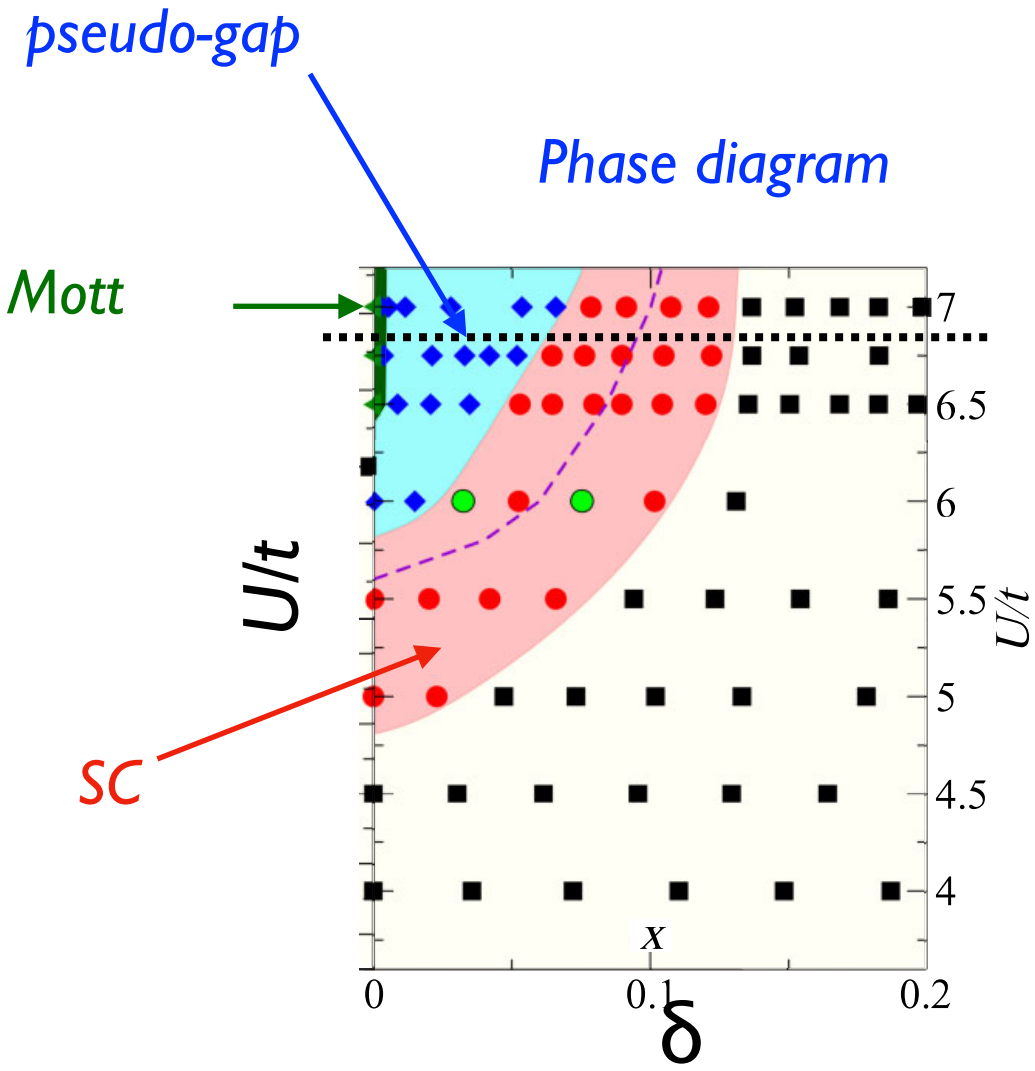
Superconducting phase vs pseudo-gap

E. Gull, O.P., A. Millis PRL 110, 216405 (2013)

- 8 patches DCA
- SC. No AF.



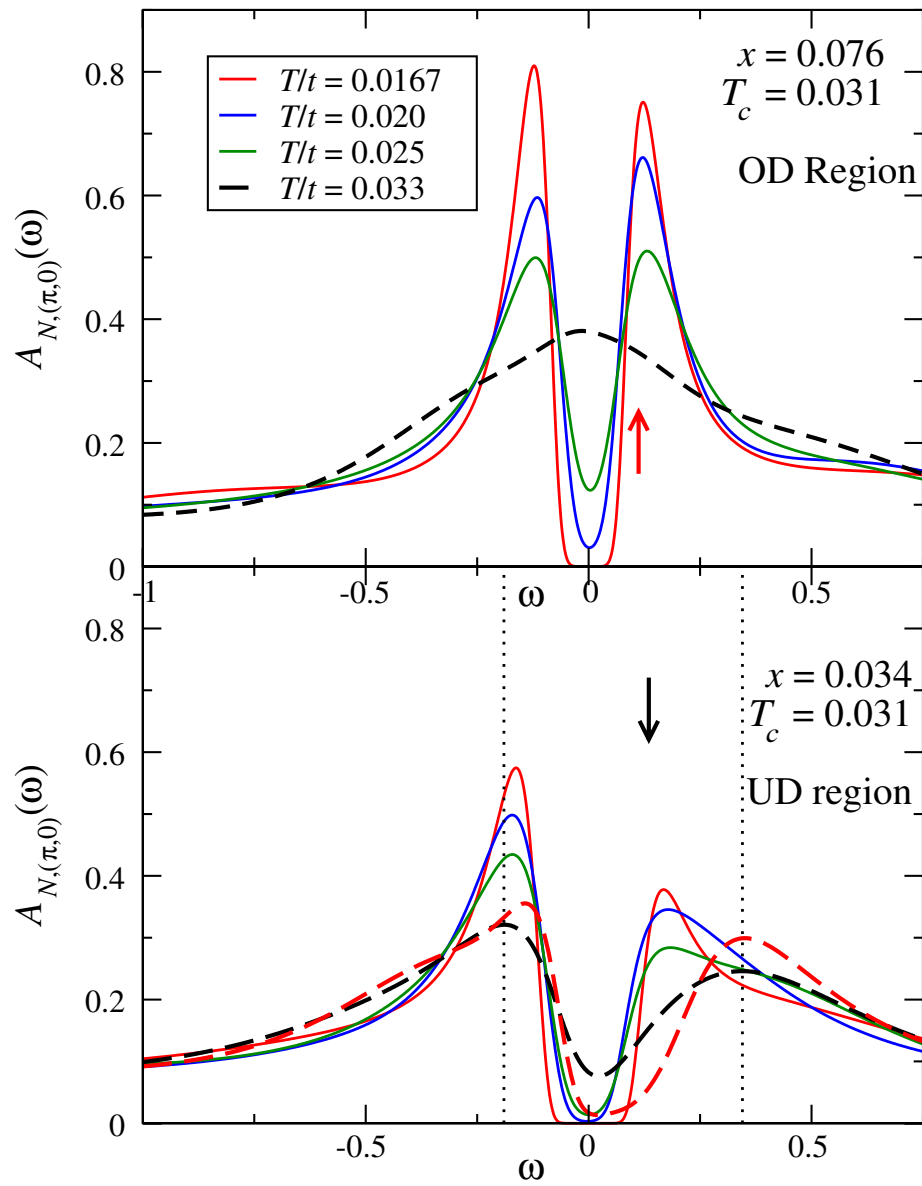


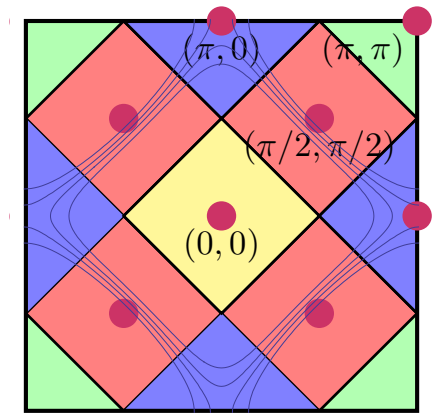


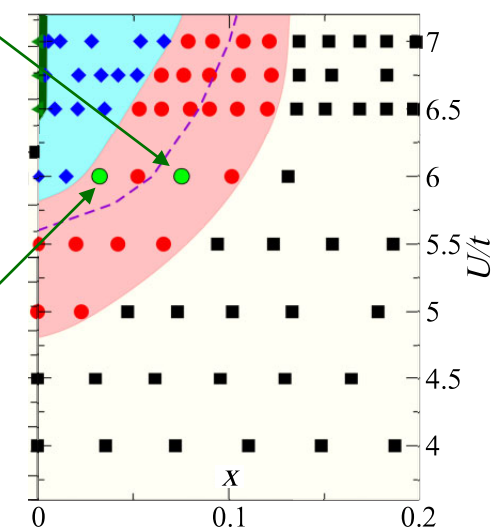
Superconducting phase vs pseudo-gap

E. Gull, O.P., A. Millis PRL 110, 216405 (2013)

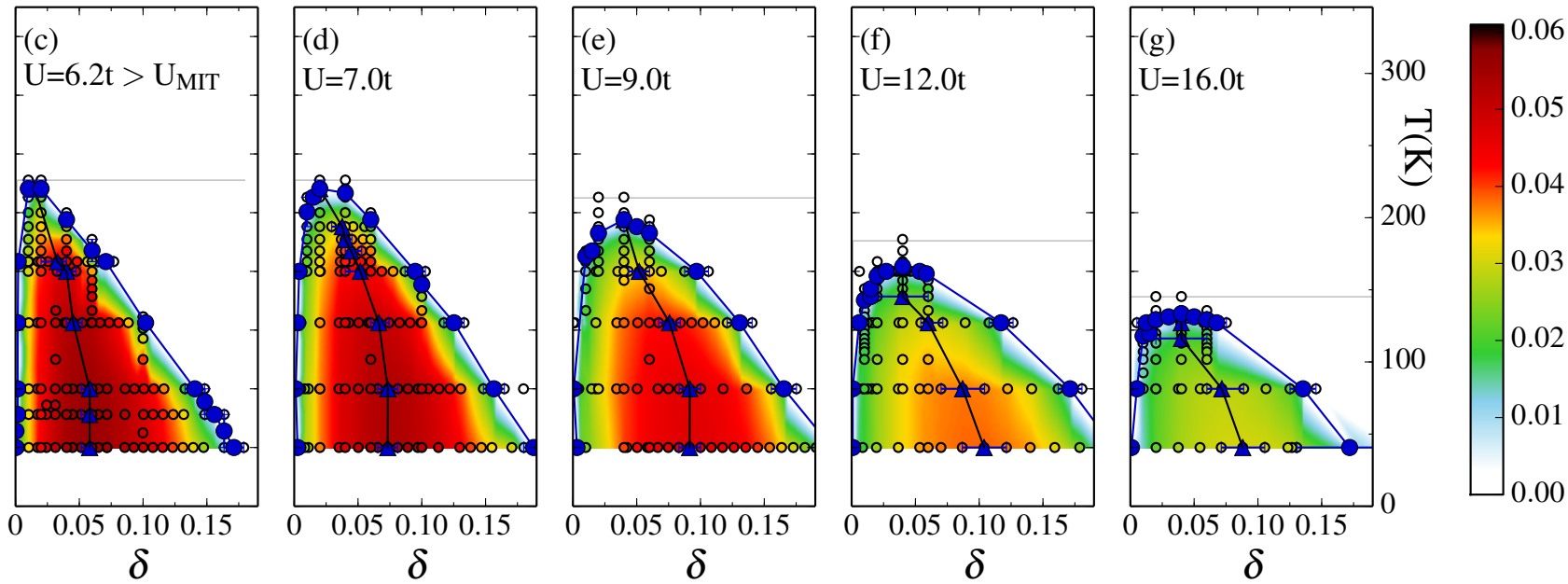
- Pseudo-gap and SC compete with each other







CDMFT 2x2 cluster



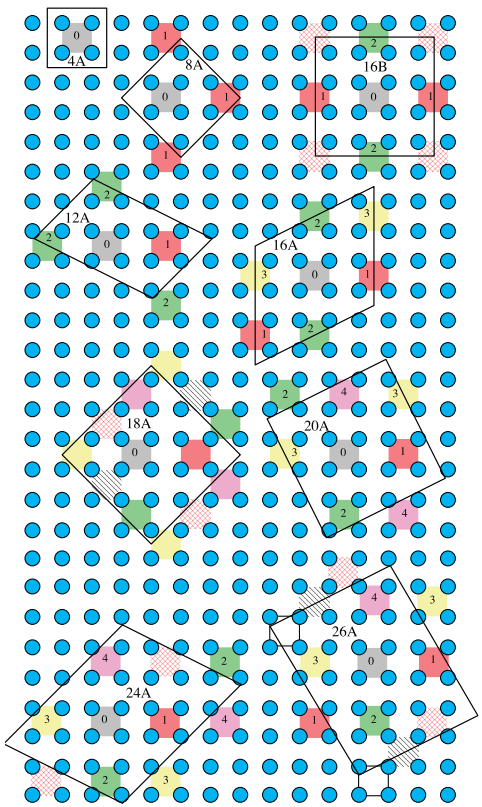
Fratino et al. Scientific Reports 6, 22715 (2016)

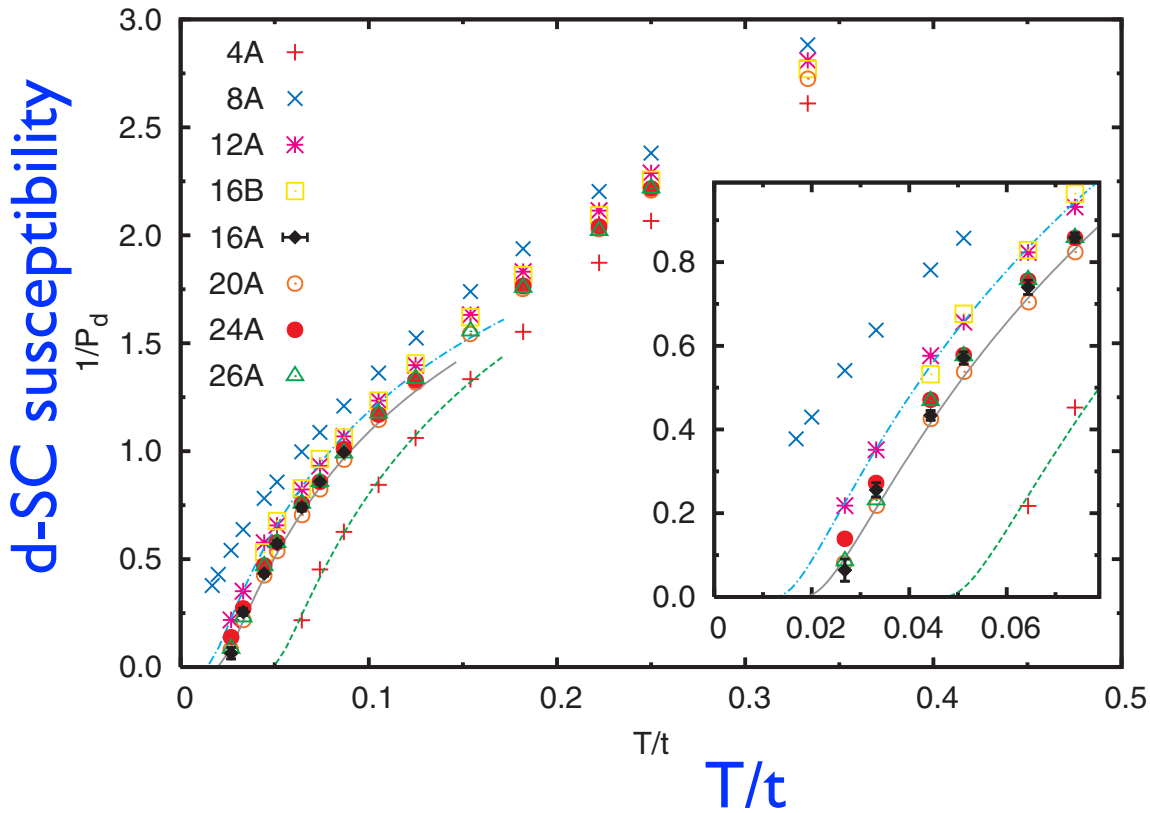
- Plaquette CDMFT
- Asymmetric phase diagram vs doping.
- Related to the phase transition and Widom line observed in normal phase in 2x2 CDMFT ?

Cluster convergence in SC phase

T. Maier et al., PRL 95, 237001 (2005)

- Very large DCA cluster
- U/4t = 1. Low U, below the Mott transition. *Tc ≈ 0.02t*

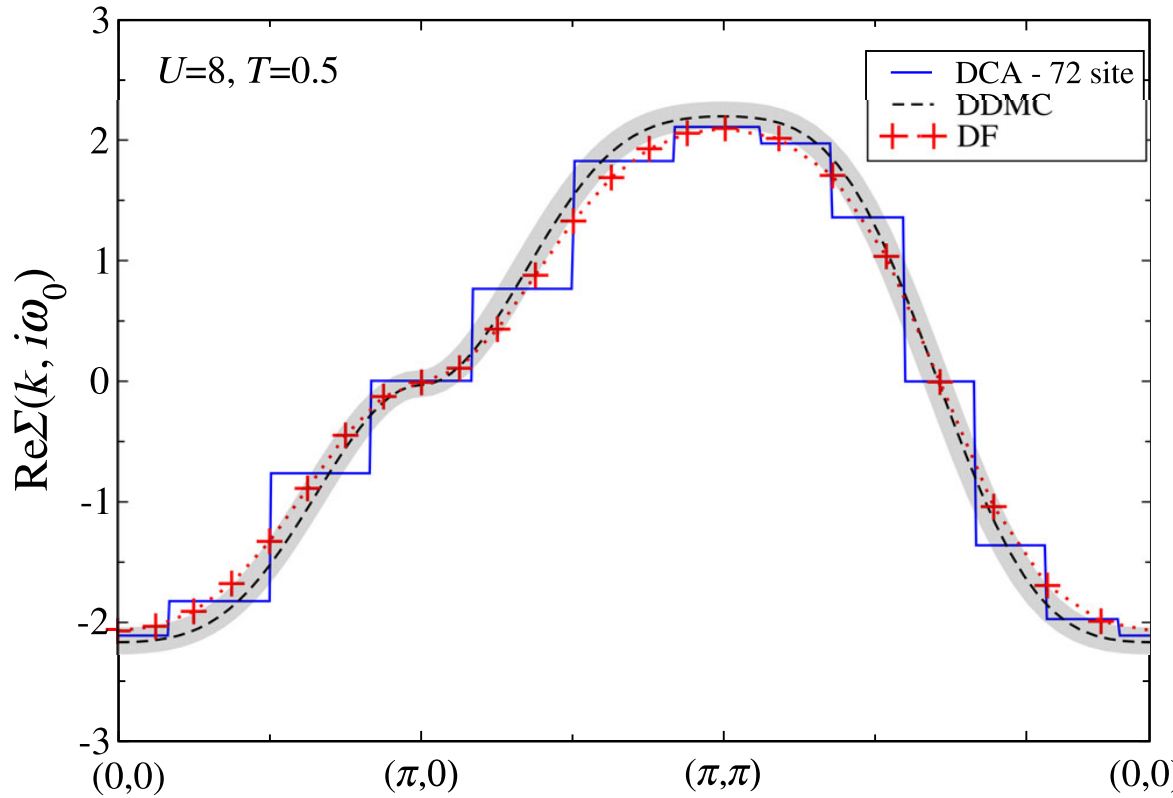




Benchmarks

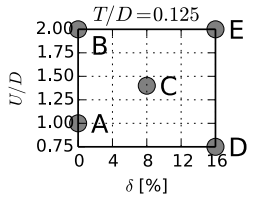
Converging cluster DMFT

- Simons Collaboration Comparison paper
  J. LeBlanc et al. Phys. Rev. X 5, 041041 (2015)
- Where can we converge the cluster DMFT vs size ?
  i.e. obtain the exact solution of e.g. the Hubbard model ?
- Systematic benchmarks of new methods on these points



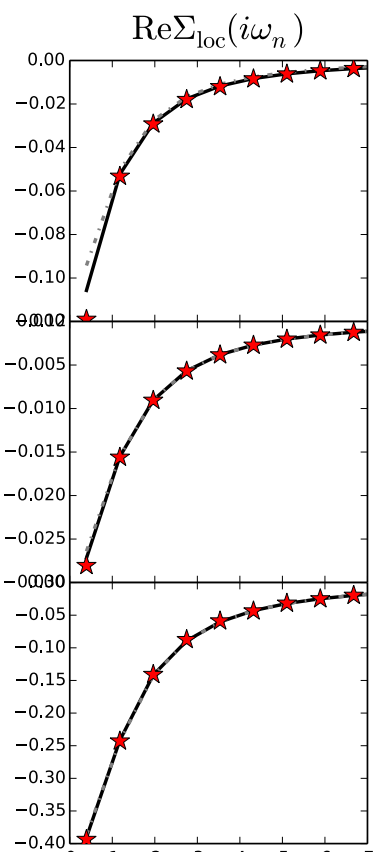
Benchmarking 2x2 CDMFT vs large clusters

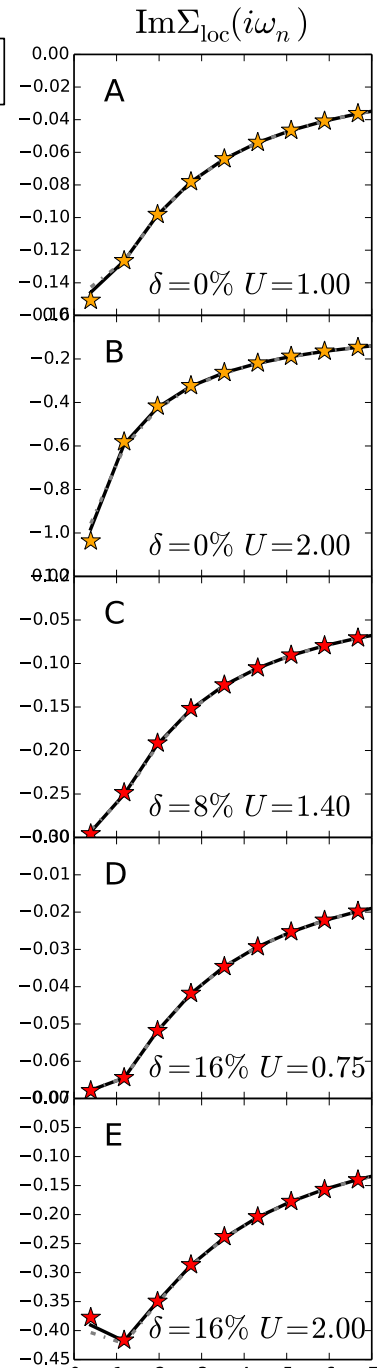
$$\tilde{\Sigma}_k(i\omega_n) \equiv \Sigma(k, i\omega_n) - \Sigma_{\mathrm{loc}}(i\omega_n)$$

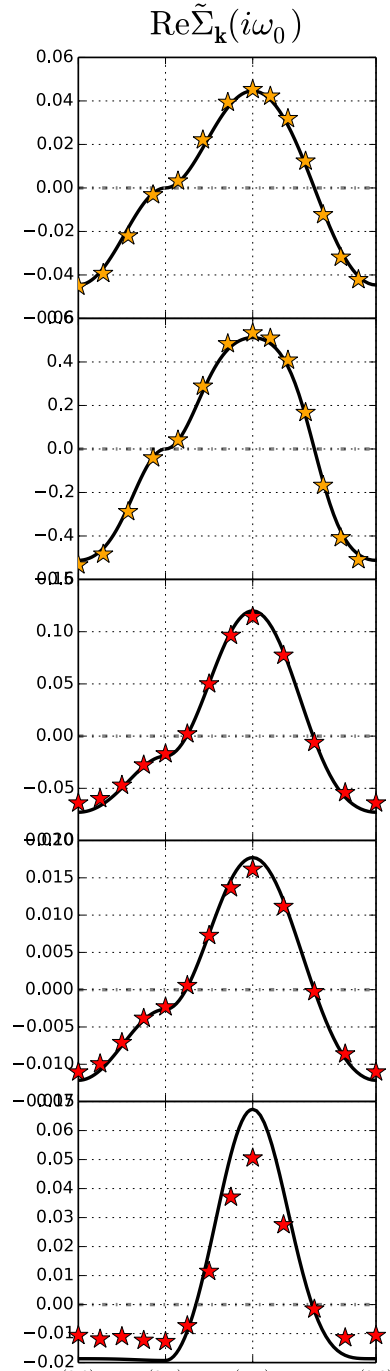


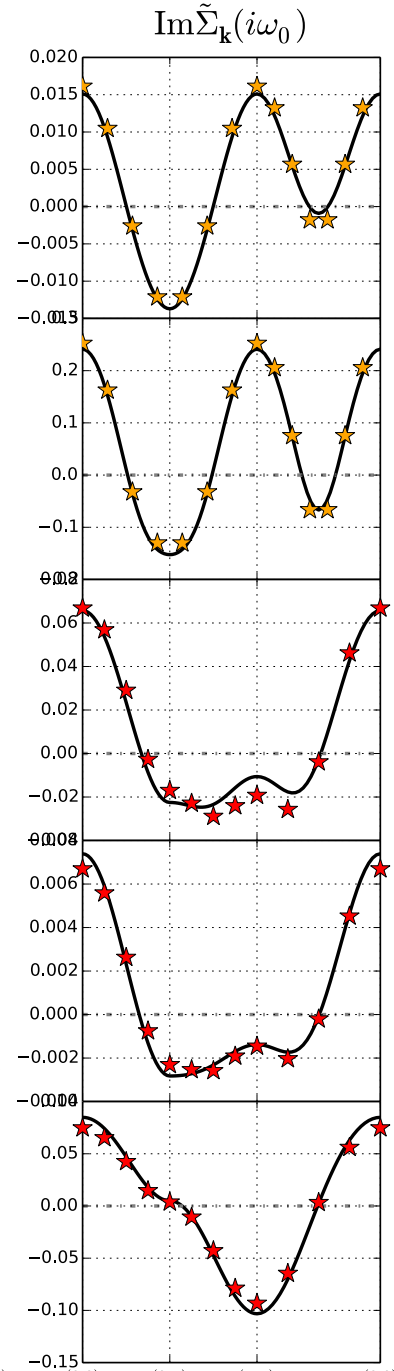
- T/D = 0.125
- CDMFT with reperiodization

From J.Vucicevic 2017









Outline

- Lecture 1 : Introduction to DMFT
- Lecture 2 : Multiorbital DMFT and clusters
  - Towards more realism : multi-orbital DMFT
  - Cluster methods
    - Motivation
    - Formalism : CDMFT, DCA and co.
    - Highlights : a few results with clusters for Hubbard model.
- Lecture 3 : Impurity solvers
- Lecture 4 : Introduction to TRIQS & Hands-on

Thank you for your attention