Quantum dimer

Dynamical Mean Field Theory and beyond

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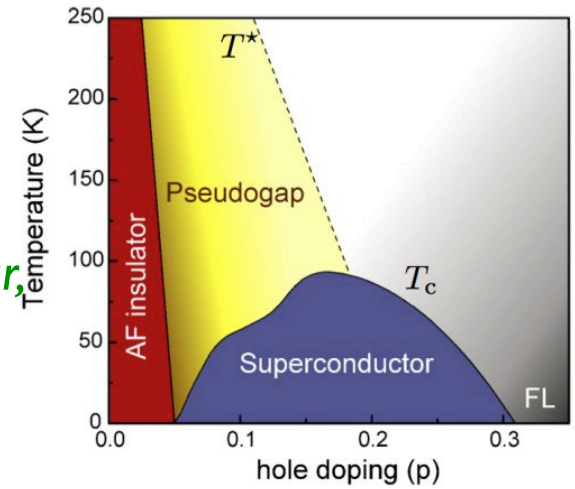
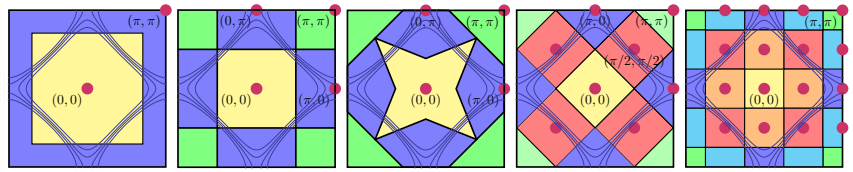
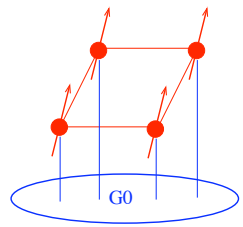
Cluster DMFT & Hubbard model: robust features

Cf talks by Millis, Kotliar, Tremblay

Many authors: Civelli, Ferrero, Georges, Gull, Haule, Jarrell, Kotliar, Lichtenstein, Katsnelson, Maier, Millis, Sordi, Tremblay, OP, ...







Pseudo-gap

d-wave SC

- Emerging from Mott insulator.
- k-space differentiation nodes/ antinodes. Fermi Arcs.
- No long range order
- Role singlets. RVB ?

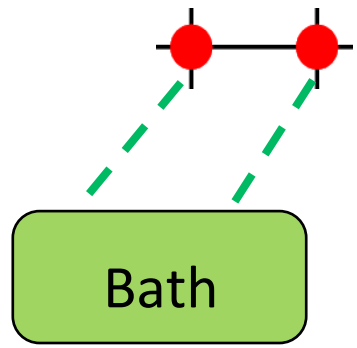
- Robust in various clusters: 2x2, 8, 16, larger cluster at small U.
- Dome vs doping.
- Role of J in the pairing mechanism ?

Many observed features in pseudo-gap and SC phase

Many open questions (low T, CDW, ...)

Outline

- A minimal picture of the pseudo-gap with a dimer in a bath.
  - Liquid of singlets/dimers (RVB)
  - Mean field with a dimer in a bath ?



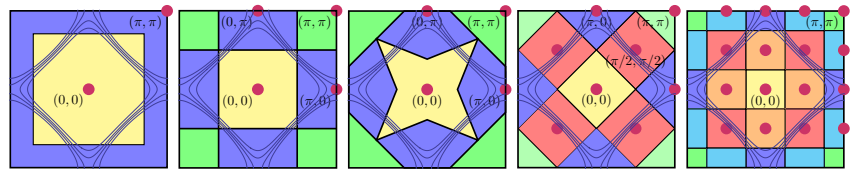
- Spin-fluctuation and Mott physics : a unified framework
  - Motivations:
    - DMFT clusters miss effect of long-range (spin) fluctuations.
    - k resolution for $A(k,\omega)$, $\Sigma(k,\omega)$ is still poor.
    - Convergence is too slow with cluster size in e.g. pseudo-gap region. Sign problem.
    - Better use of a little impurity/dimer in a bath ?

Quantum dimer in a bath ....

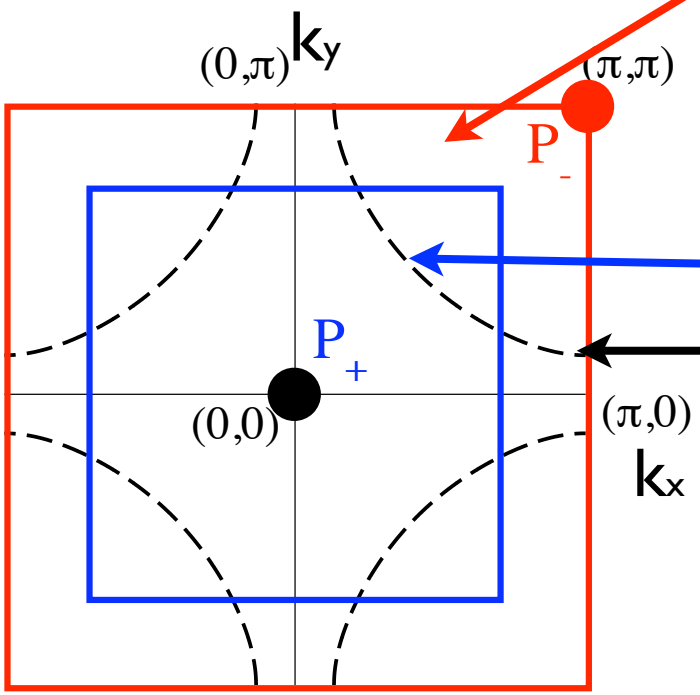
M. Ferrero, P. S. Cornaglia, L. De Leo, O. P. , G. Kotliar, A. Georges, EPL, PRB 2009-2010

Two sites in a self-consistent bath ...

- Cut the Brillouin zone into two patches P+, P- (of equal volume)

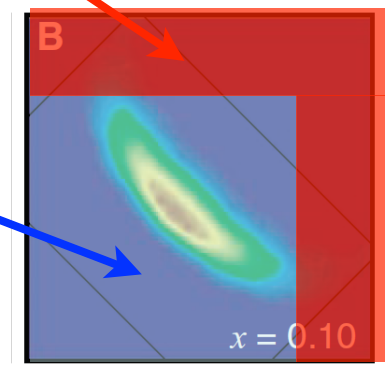


Outer patch P- : Antinodes



Inner patch P+ : Nodes

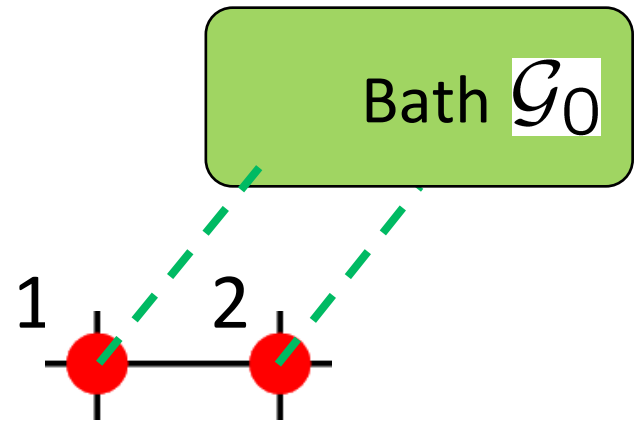
Free Fermi surface



2-patch "DCA" construction

Even (bonding) orbital 1+2 ↔ nodal patch

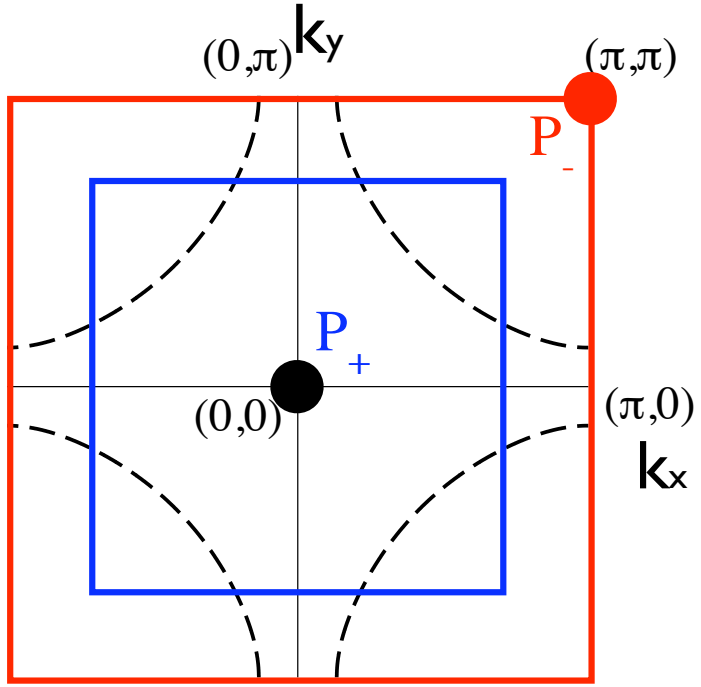
Odd (antibonding) orbital 1-2 ↔ antinodal patch

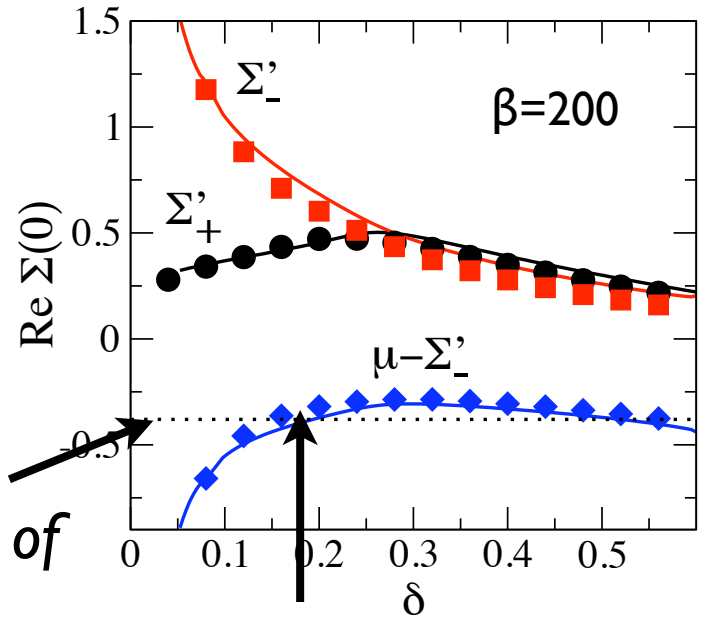


Two-site Anderson impurity model

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





band edge of P- patch

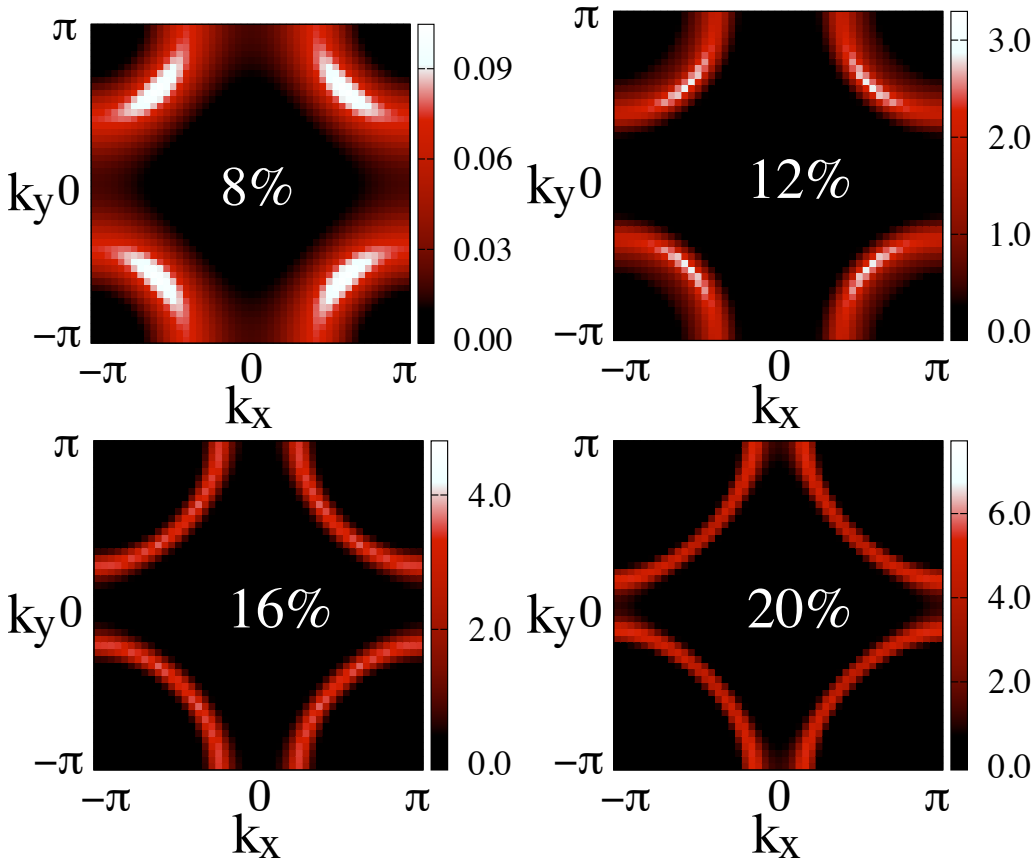
Outer/odd Orbital gets (pseudo-)gapped

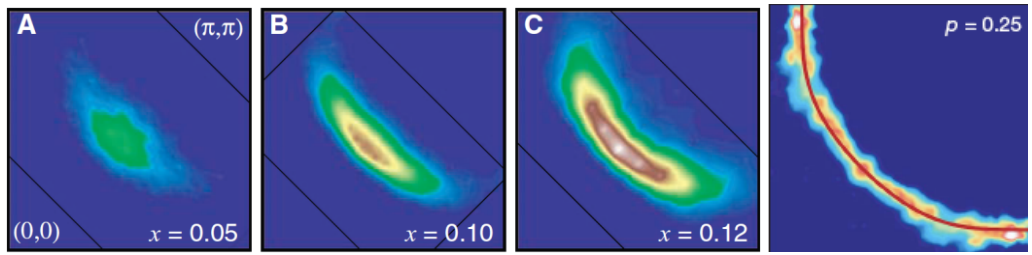
Effective band transition at low energy

ARPES intensity maps at Fermi level

- With "cumulant" interpolation...

$A(k, \omega = 0)$

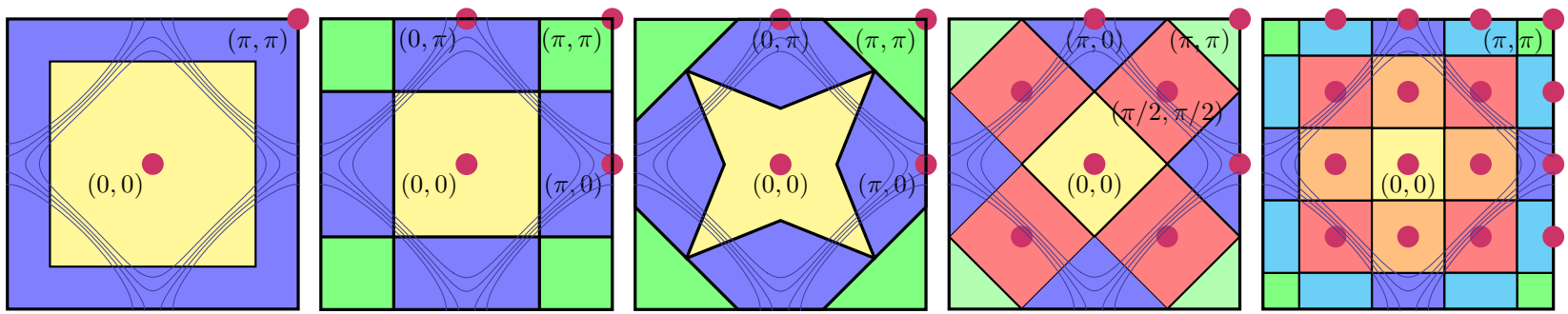




- Rough resolution.
  Two k points only :
  node & antinode,
  the rest is interpolation.

Compatible with larger clusters

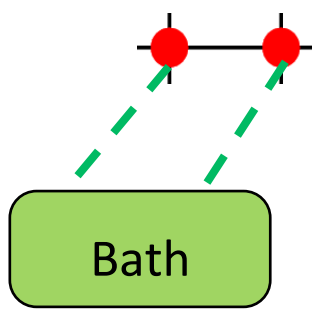
- Selective Mott transition in k-space also with 8, 16 clusters
  Cf Millis' talk.
- Appearance of Arcs due to Mott, short range correlation.
- Probably not a real transition at large cluster size

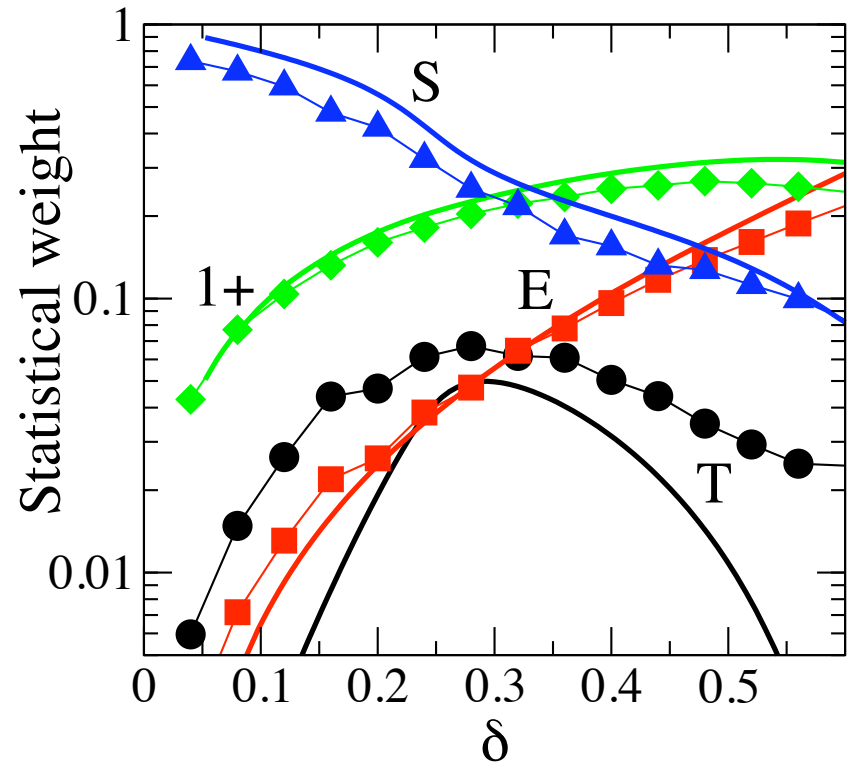


- Gull, OP, Millis Phys. Rev. Lett. 110 216405 (2013)
- Gull, OP, Werner, Millis Phys. Rev. B 80 245102 (2009)
- Werner, Gull, OP, MillisPhys. Rev. B 80 045120 (2009)
- Gull, Ferrero, OP, Georges, Millis Phys. Rev. B 82 155101 (2010)

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+)

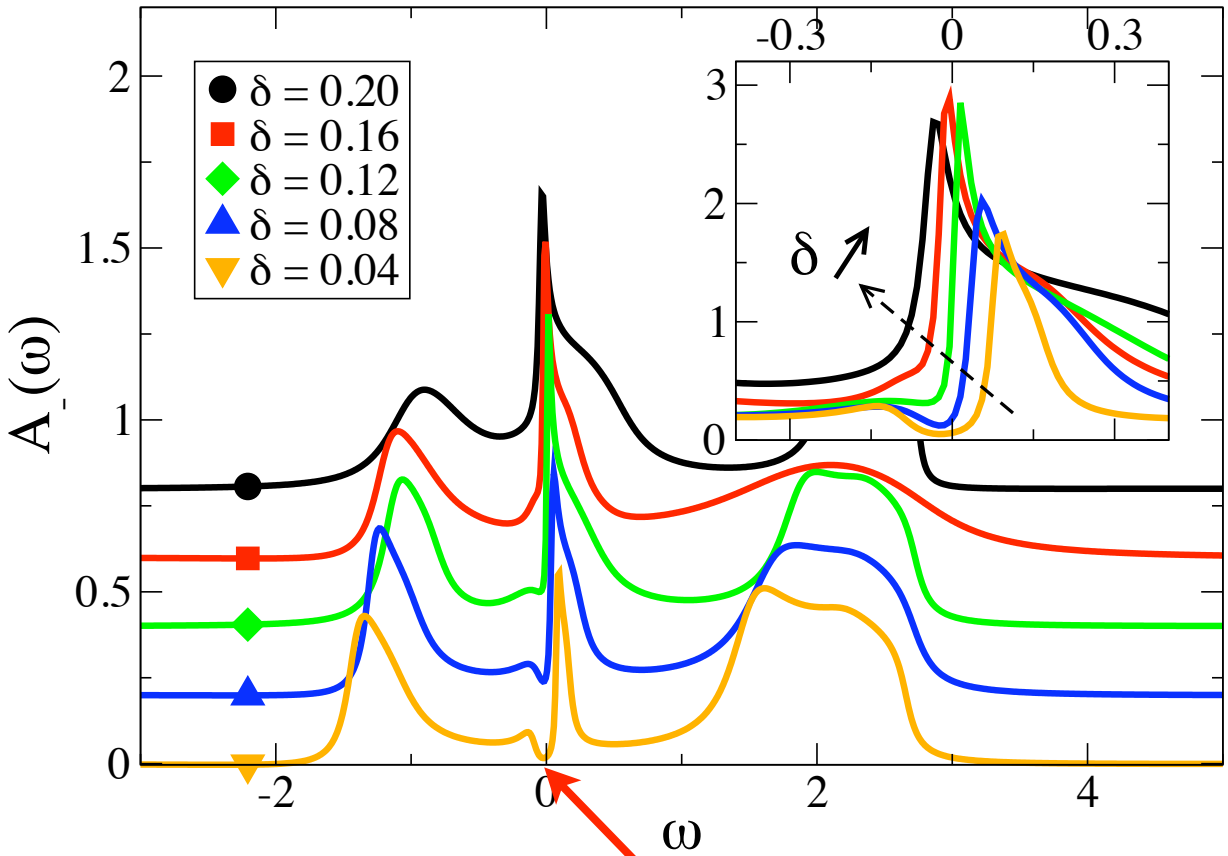


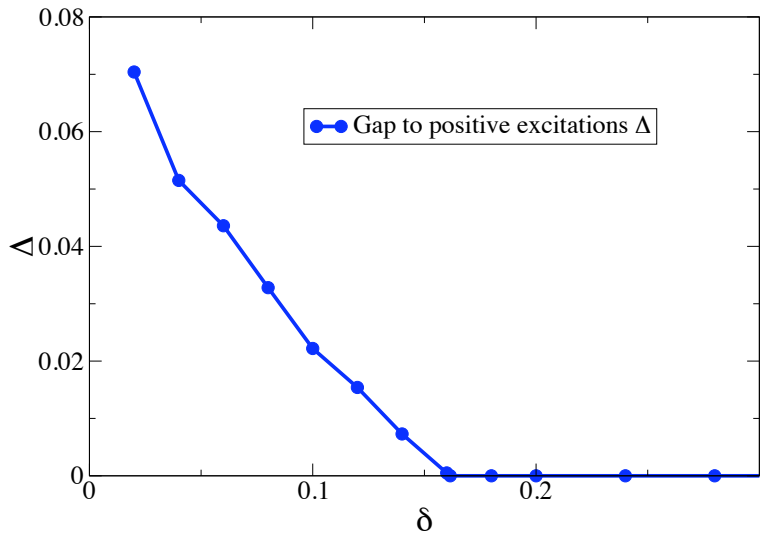


Cf Sachdev's talk.

Antinode : not a sharp gap, a pseudogap !

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

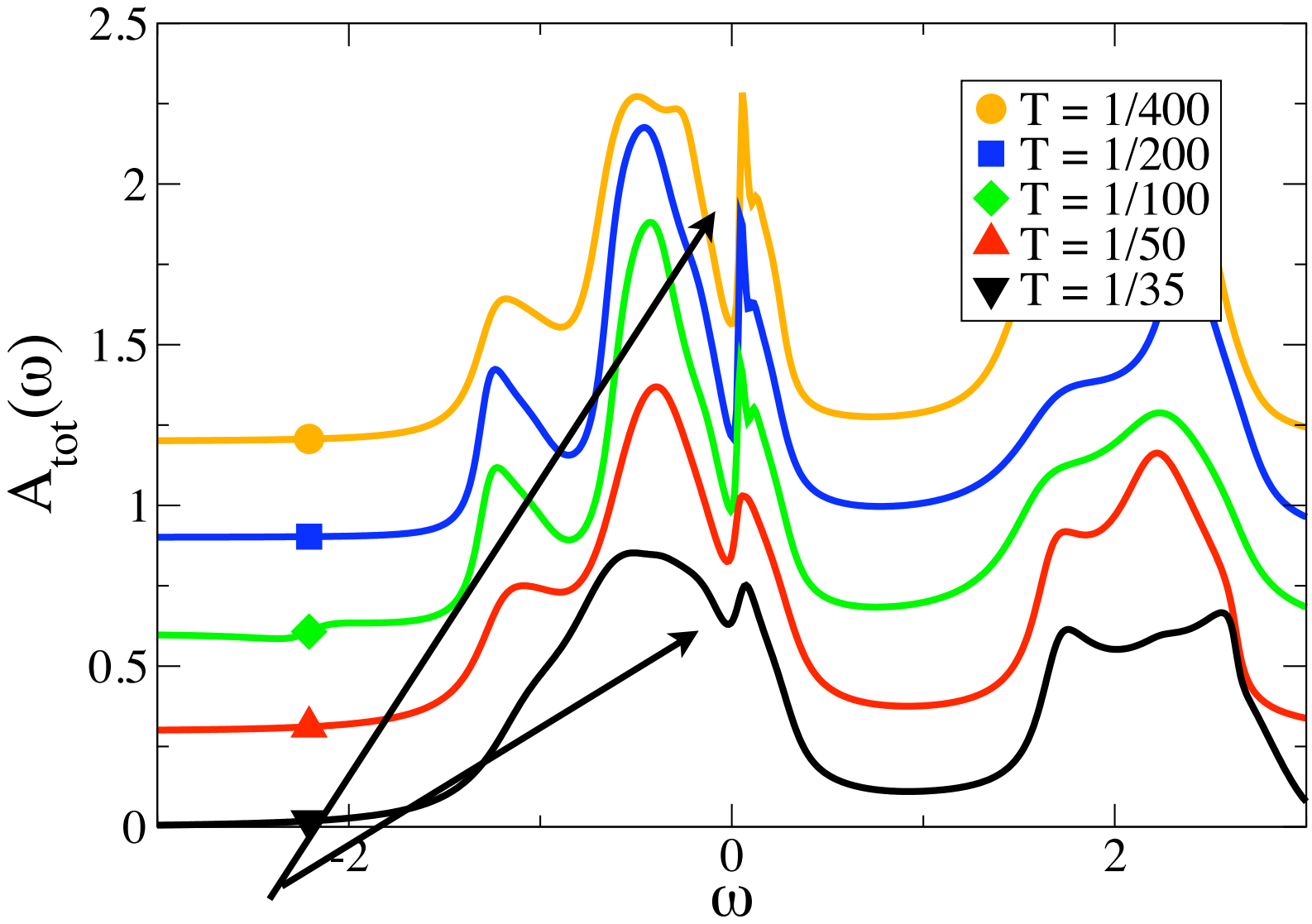




Energy scale of pseudogap on positive energy side

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

Pseudo-gap opens upon cooling



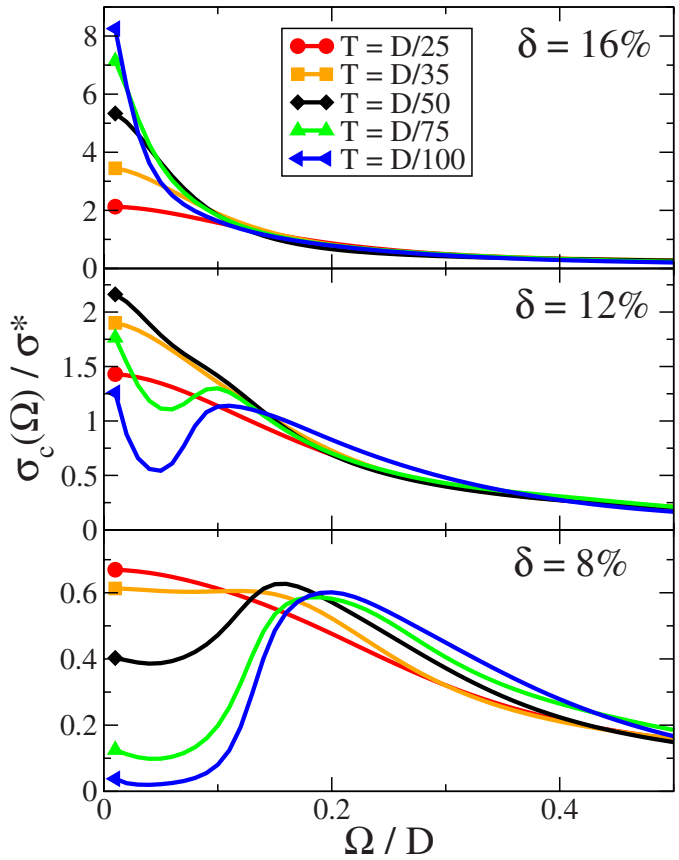
- Total spectral function Atot(ω) for various temperature at δ =0.08. A shift of 0.3 has been added between each curves for clarity.

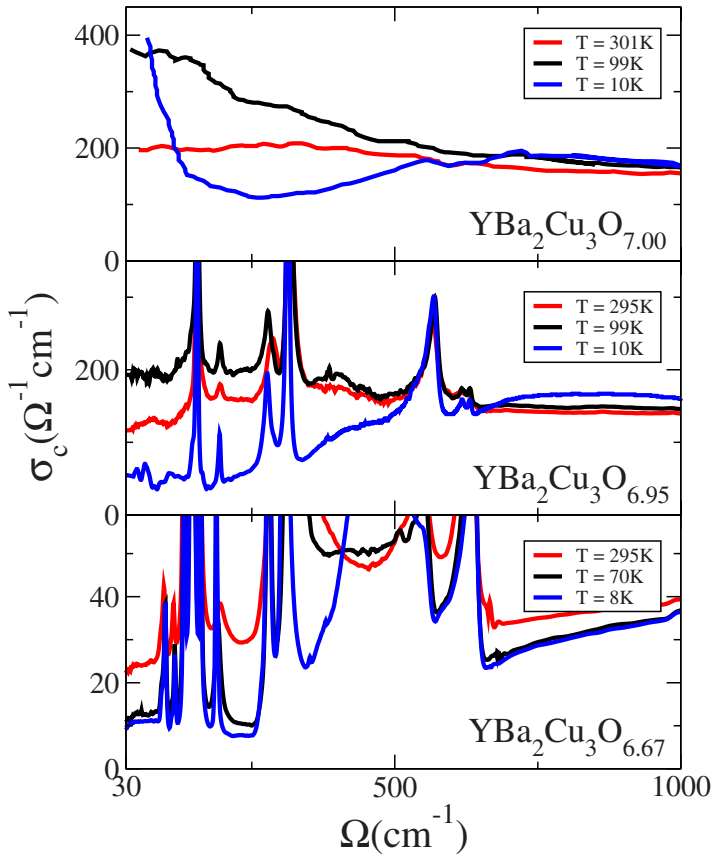
Optics : σc(ω)

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

- Pseudo-gap opening in optics.
  Qualitative agreement with experiments

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





Partial summary

- Two impurities in a self-consistent bath à la DMFT capture basic features of pseudo-gap:
  - Selective Mott transition in k-space.
  - Node-antinode differentiation, Fermi Arcs
  - Pseudogap in spectral function vs ω, optics (σ_c)
  - Dominated by singlet & (spin 1/2; hole) states.
- How to do better ? Improve resolution ?

Spin fluctuations and Mott physics

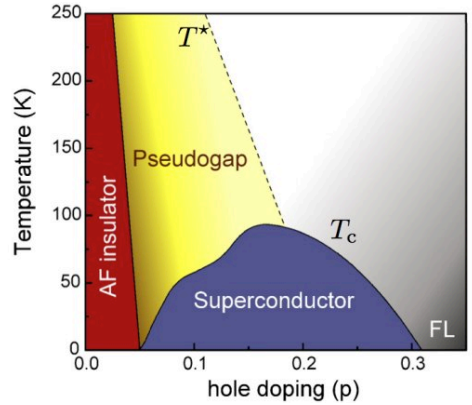
Marry spin-fluctuation and Mott physics ?
Better use of a little impurity/dimer in a bath ?

T. Ayral, O.P.: arxiv/1503.07724

Spin fluctuations vs Mott physics

Cf talks by Chubukov, Pépin,

Many authors e.g.: Pines, Chubukov, Pépin, Onufrieva, Pfeuty, Sachdev, ...



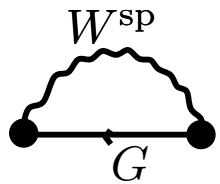
Cf talks by Millis, Kotliar, Tremblay

Many authors: Civelli, Ferrero, Georges, Gull, Haule, Jarrell, Kotliar, Maier, Millis, Sordi, Tremblay, OP, ...

Spin fluctuation

- Effect on the (long-range) AF fluctuations on electrons. QCP.
- Simplest diagrammatic form.

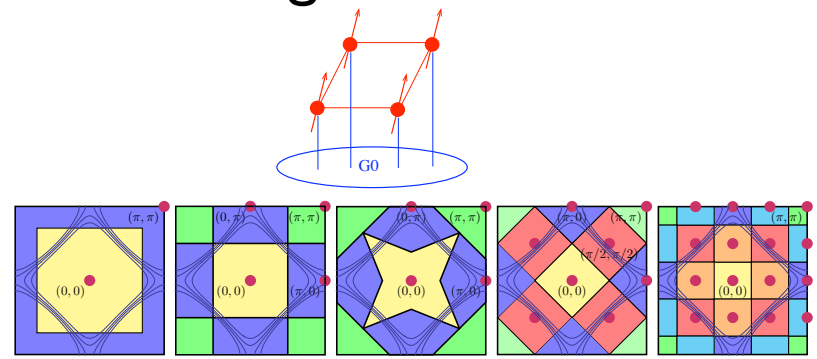
$$\Sigma(k, i\omega) \approx$$



- Hot/cold spots, d-SC, ...
- No Mott physics

Mott physics

- Describe doped Mott insulator.
- Cluster DMFT methods : Mott, short range fluctuations.



- Miss the effect of long range AF fluctuations.

Both in the same formalism ?

Electron-boson interaction vertex

- Decouple the interaction with a boson, in charge/spin channels.

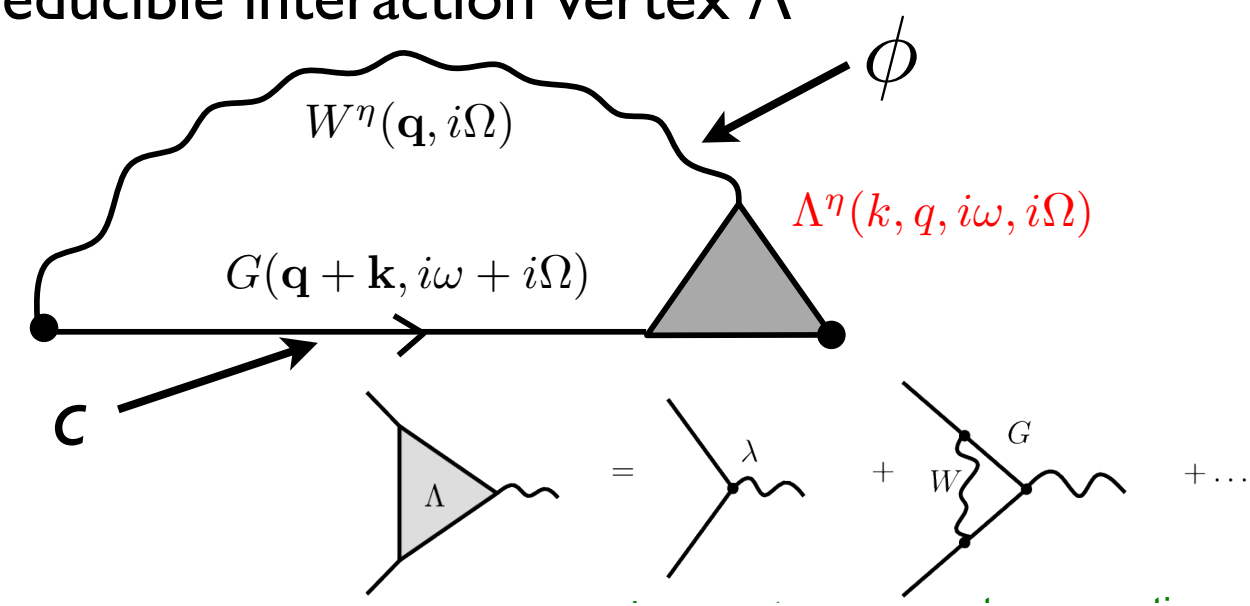
$$S_{\rm latt} = \int_0^\beta d\tau \sum_{ij} c^*_{i\sigma\tau} \left\{ \partial_\tau + t_{ij} \right\} c_{j\sigma\tau} + \sum_{i,I=0,x,y,z} \left[\frac{1}{2} (U^I)^{-1} \phi^I_{i\tau} \phi^I_{i\tau} + \lambda^I \phi^I_{i\tau} n^I_{i\tau} \right]$$

$$\lambda^I = 1$$

- Central object : 1PI irreducible interaction vertex Λ

$$W = \langle \phi\phi \rangle$$

$$\Sigma(\mathbf{k}, i\omega) = \sum_{\eta=ch,sp}$$



- Approximation : local Λ computed via a self-consistent impurity model

$$\Lambda^\eta(\mathbf{q}, \mathbf{k}, i\omega, i\Omega) \approx \Lambda^\eta_{\rm imp}(i\omega, i\Omega)$$

- Approximation for the vertex Λ, not for self-energy Σ like DMFT.
  (Cf also, DΓA, dual fermions/bosons)

Definition

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

- Two simple limits :
  - Atomic limit : t=0, isolated atoms
  - Weak coupling limit : U=0, free electrons.

DMFT

- A local approximation of the Luttinger-Ward functional Φ (2-particle irreducible diagrams) *(Georges-Kotliar '92).*

$$F(G) = Tr \ln G - Tr(G_0^{-1} G) + \Phi(G)$$

$$\Sigma = \frac{\delta \Phi}{\delta G}$$

- DMFT definition:

$$\Phi(G) \approx \sum_i \phi_{atomic}(G_{ii}) \quad \text{+ cluster corrections}$$

- DMFT is exact for U=0 and in the atomic limit (t=0).
- Impurity model in a self-consistent bath: an auxiliary problem, like Kohn-Sham potential in DFT, *Cf Kotliar et al. RMP 2007*
- Which quantity of the quantum many-body problem shall I approximate with the atomic quantity ?
- A functional of the vertex Λ ?

TRILEX (triply-irreducible local expansion).

- A functional of the vertex *De Dominicis-Martin, Math. Phys. 1, '64*,

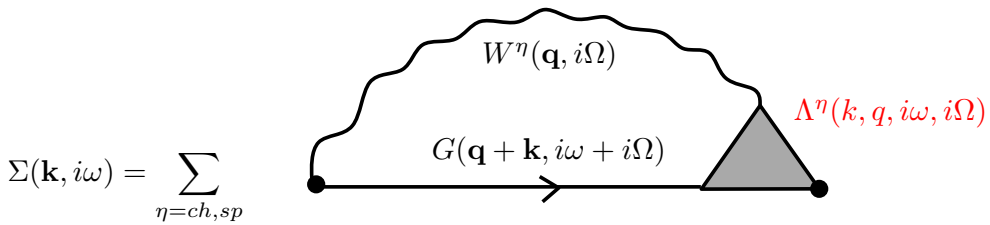
$$F(G,W,\Lambda) = F_0(G,W,\Lambda) + \mathcal{K}(G,W,\Lambda) \qquad \Lambda - 1 = \frac{\delta \mathcal{K}}{\delta \Lambda}$$

Explicit — *Vertex corrections*

3-particle irreducible diagrams

- Trilex definition :

$$\mathcal{K}(G,W,\Lambda) \approx \sum_i \mathcal{K}_{atomic}(G_{ii}, W_{ii}, \Lambda_{iii}) \quad \text{+ cluster corrections}$$



"Weak coupling", U ⟶0

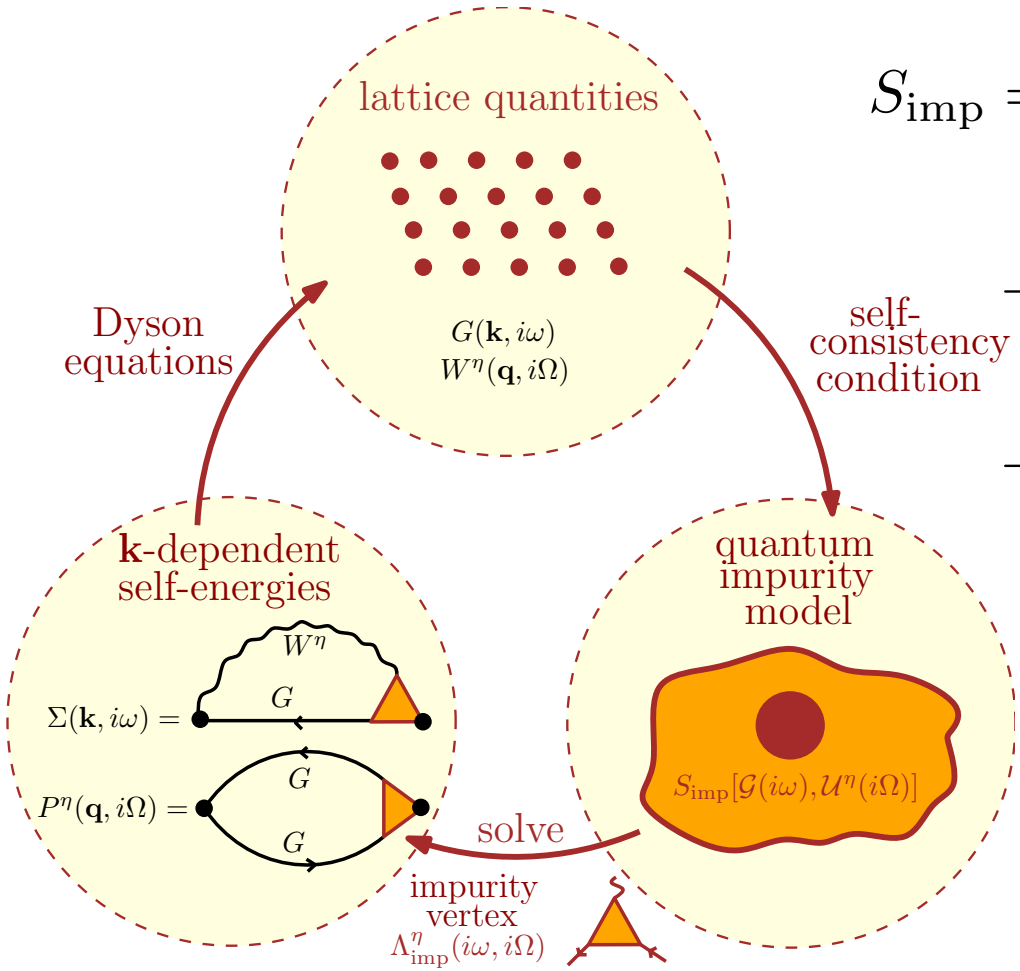
- No vertex correction: Λ = 1
- Spin fluctuation diagram

Atomic limit, t⟶0

- Exact in this limit
- Mott physics (DMFT)

Spin-fluctuation and DMFT are two "asymptotic" regimes of TRILEX.

Self-consistent impurity model



bath

$$S_{\rm imp} = -\iint_0^\beta d\tau d\tau' \sum_\sigma c^*_{\sigma\tau} \mathcal{G}(\tau - \tau') c_{\sigma\tau'}$$
$$+ \frac{1}{2} \iint_0^\beta d\tau d\tau' \mathcal{U}^{ch}(\tau - \tau') n(\tau) n(\tau')$$
$$+ \frac{1}{2} \iint_0^\beta d\tau d\tau' \mathcal{U}^{sp}(\tau - \tau') \vec{S}(\tau) \cdot \vec{S}(\tau')$$

Retarded interaction (including spin-spin)

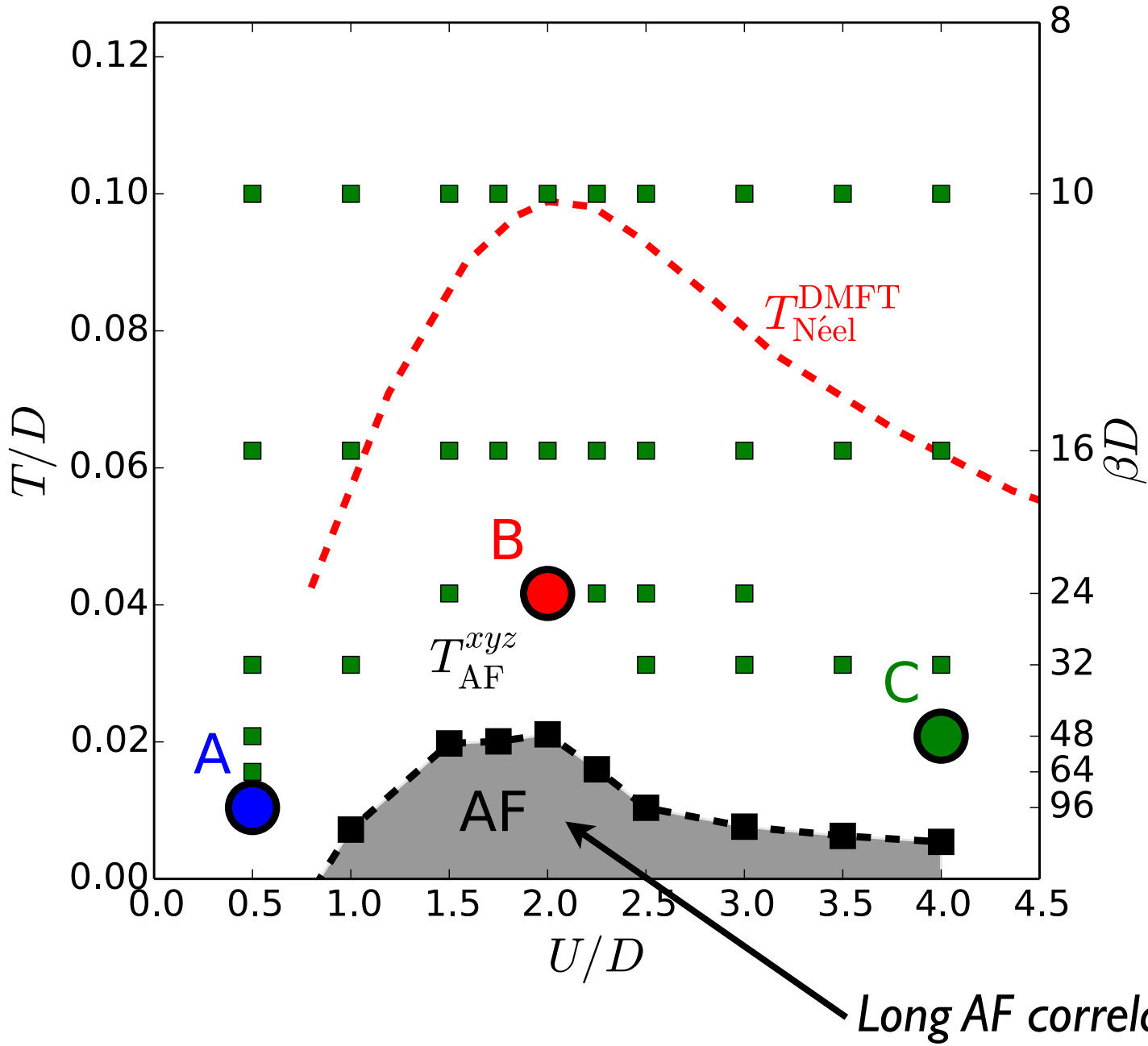
- Compute Λ from three point correlation. Boson integrated here.
- A single site (E)DMFT, much faster to solve than cluster
- Algorithm : CTQMC-HYB with double expansion (J. Otsuki, 2013). No sign problem.

Features: theory summary

- Spin fluctuations and Mott Physics built in, as two asymptotic regimes.
- k-dependent self-energies
- Susceptibilities (charge, spin), fnt (q,ω)
- The central object is the vertex Λ, i.e. effective interaction between electrons and bosonic fluctuation. Mechanisms ?
- Controlled by clusters, up to the exact solution, like cluster DMFT.
- Solvable with today's algorithms ...

Some results ...

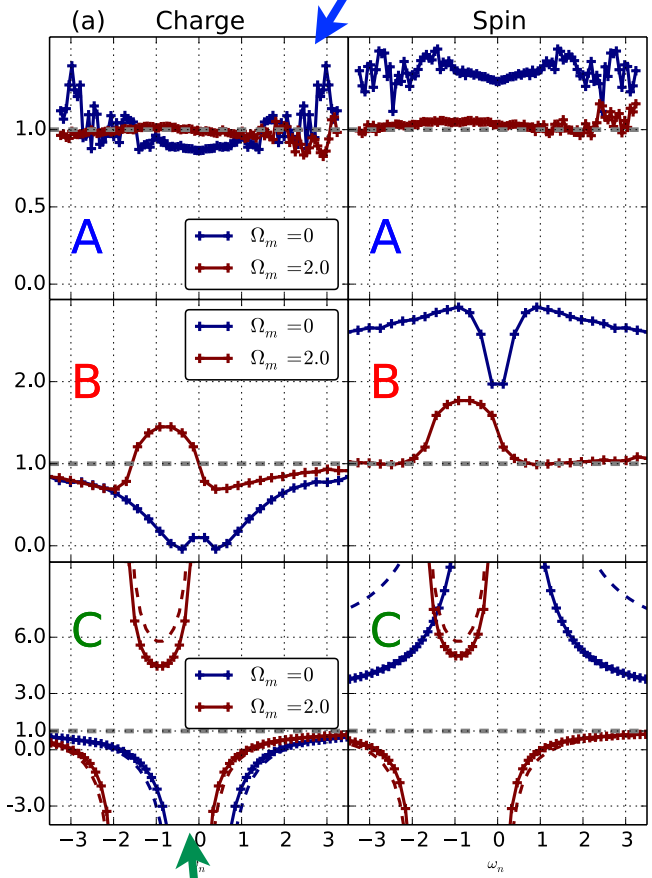
Phase diagram at half-filling



Metal to insulator

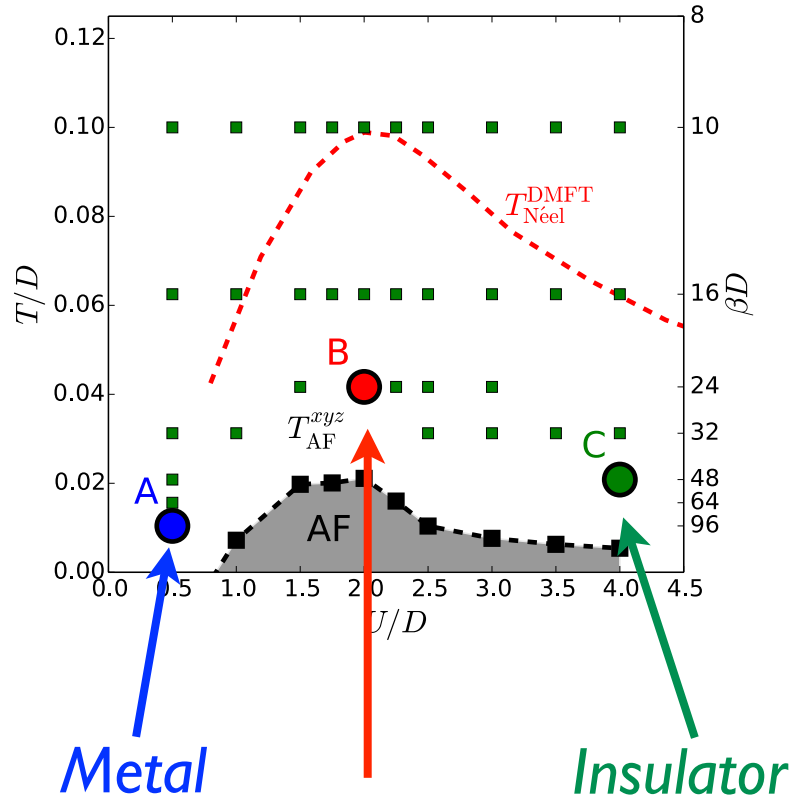
$\Lambda_{imp}(i\omega, i\Omega)$

Λimp=1



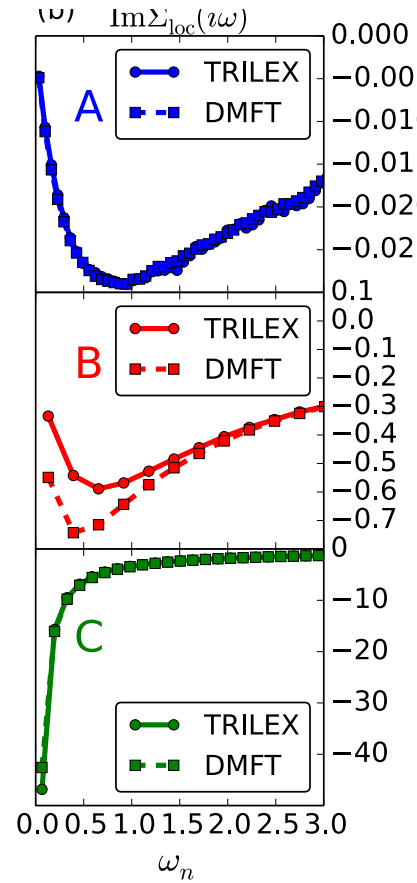
Λimp=Λatomic

ω



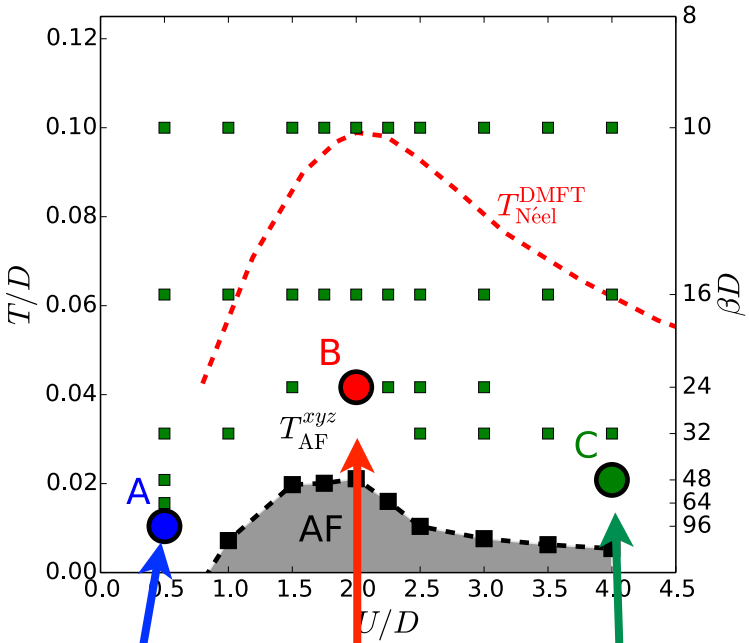
Correlated metal

$\mathrm{Im}\Sigma_{loc}(i\omega)$



Vertex Λ drives the Mott transition

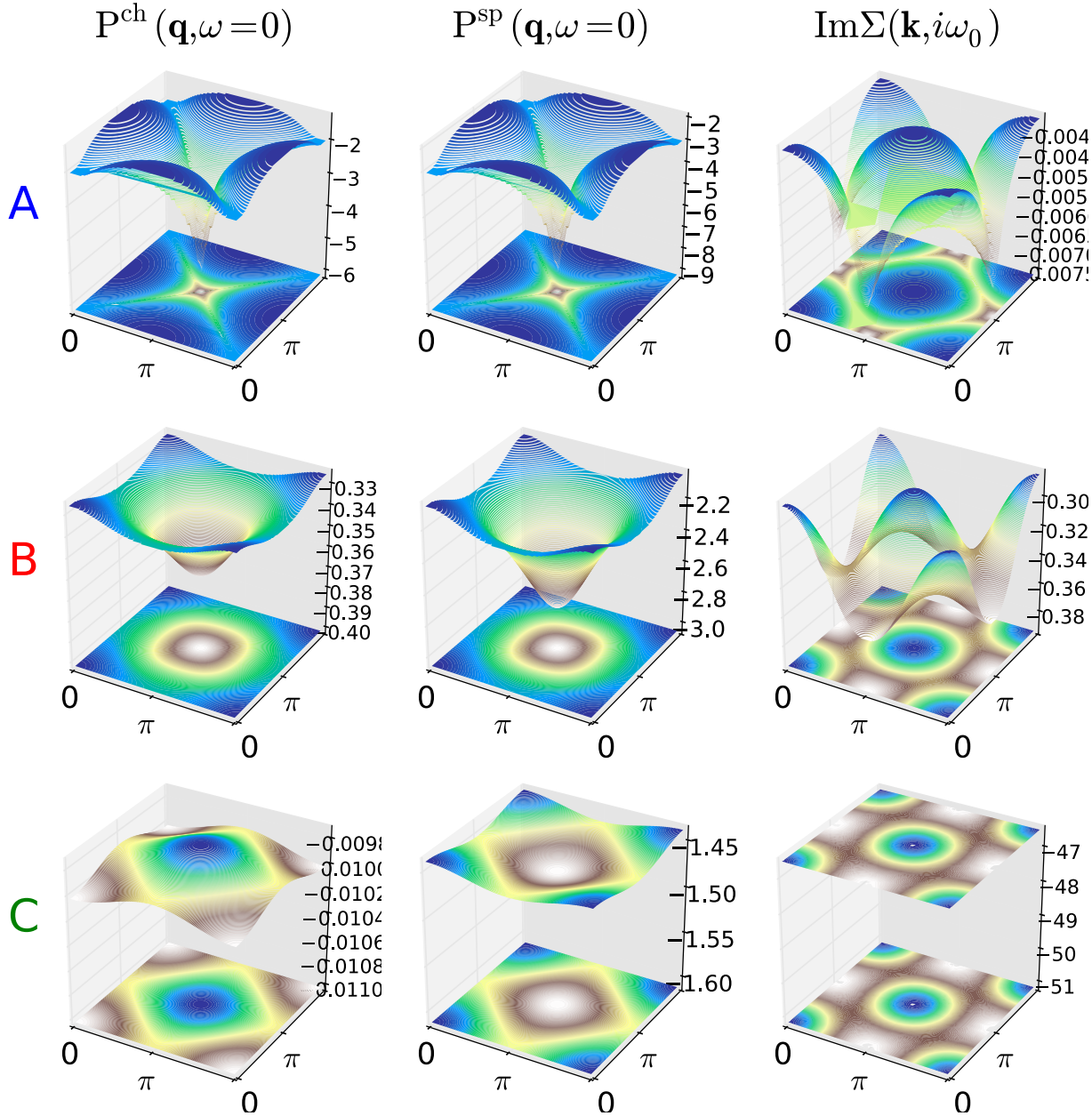
k-dependent self-energy and polarization



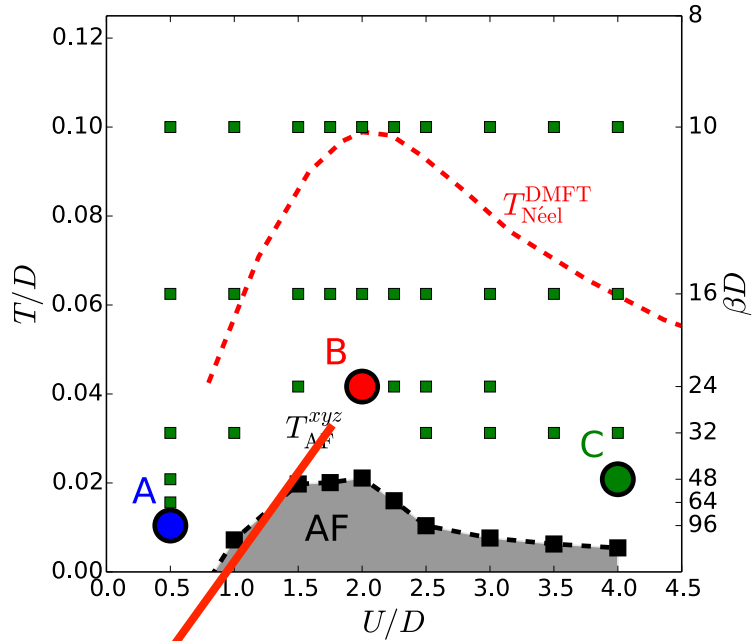
Metal
Σ(k,ω)

Insulator
Σ almost local
≈ DMFT

Correlated metal
Vertex correction
Not DMFT,
k dependent Σ

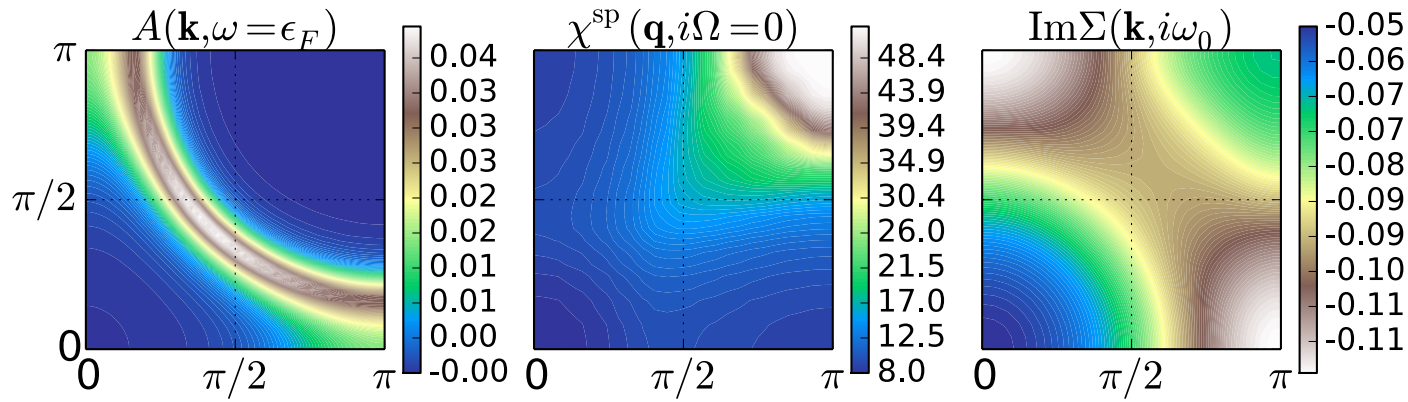


Doping at intermediate U



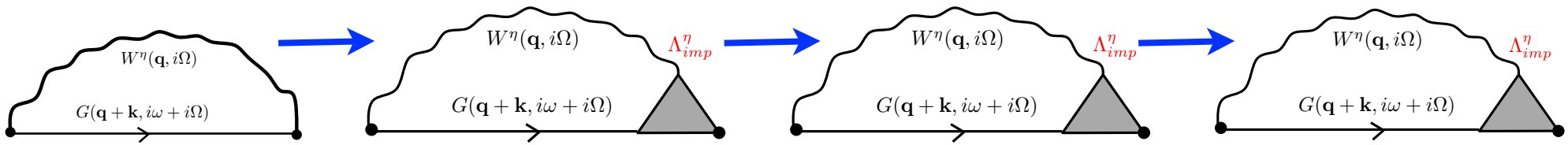
- t'=-0.4t, δ=10%, βD=96

Fermi Arc



Where is the dimer ?

- Systematic cluster corrections for TRILEX.



No vertex — *1 impurity* — *Dimer* — *Cluster*

Spin-fluctuation	Spin-fluctuation Mott Physics	Spin-fluctuation Mott Physics Local singlets	Spin-fluctuation Mott Physics Local singlets Control

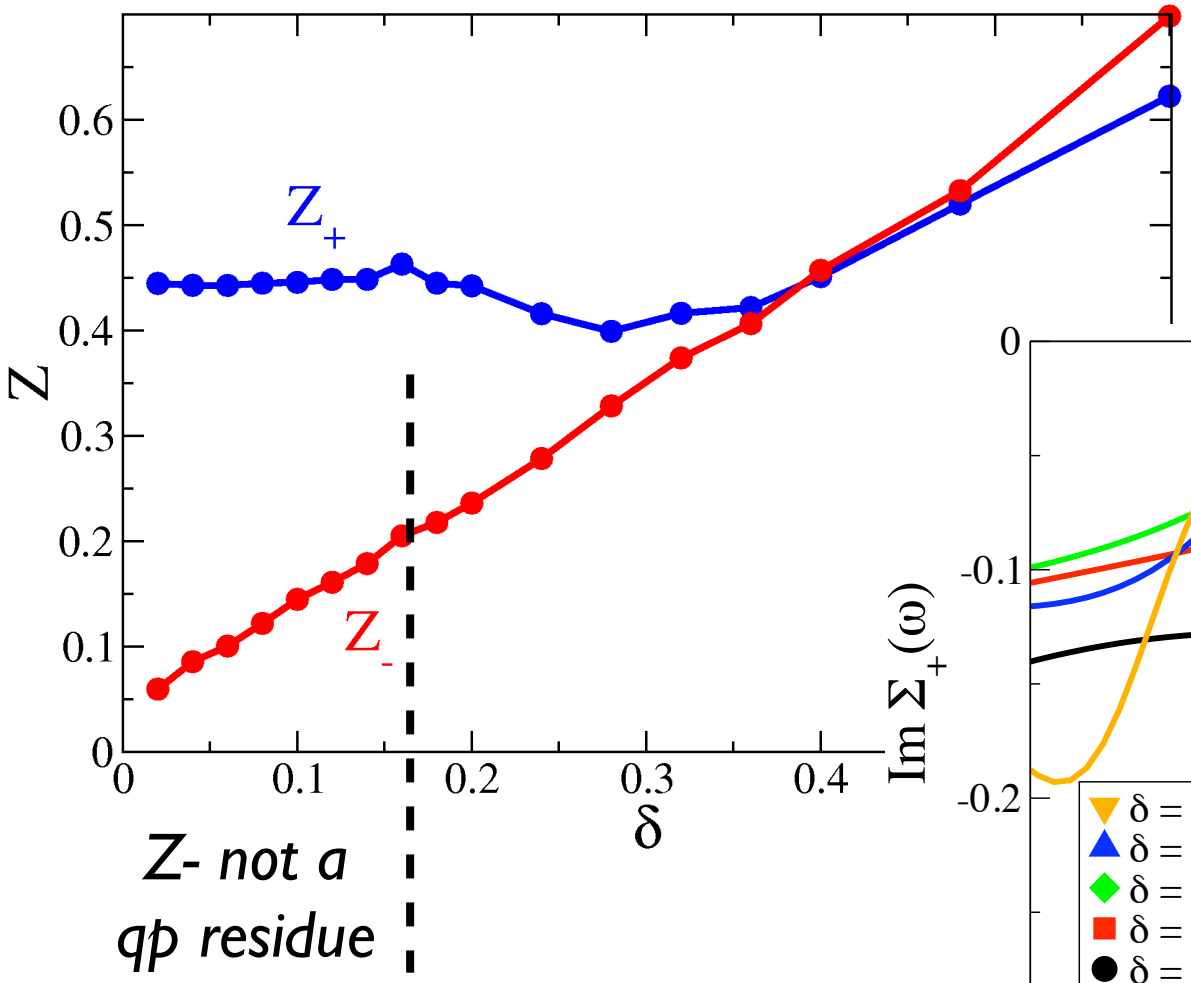
- Decoupling in the physically relevant channel (spin, charge ...) leads to a much faster convergence vs cluster size ?

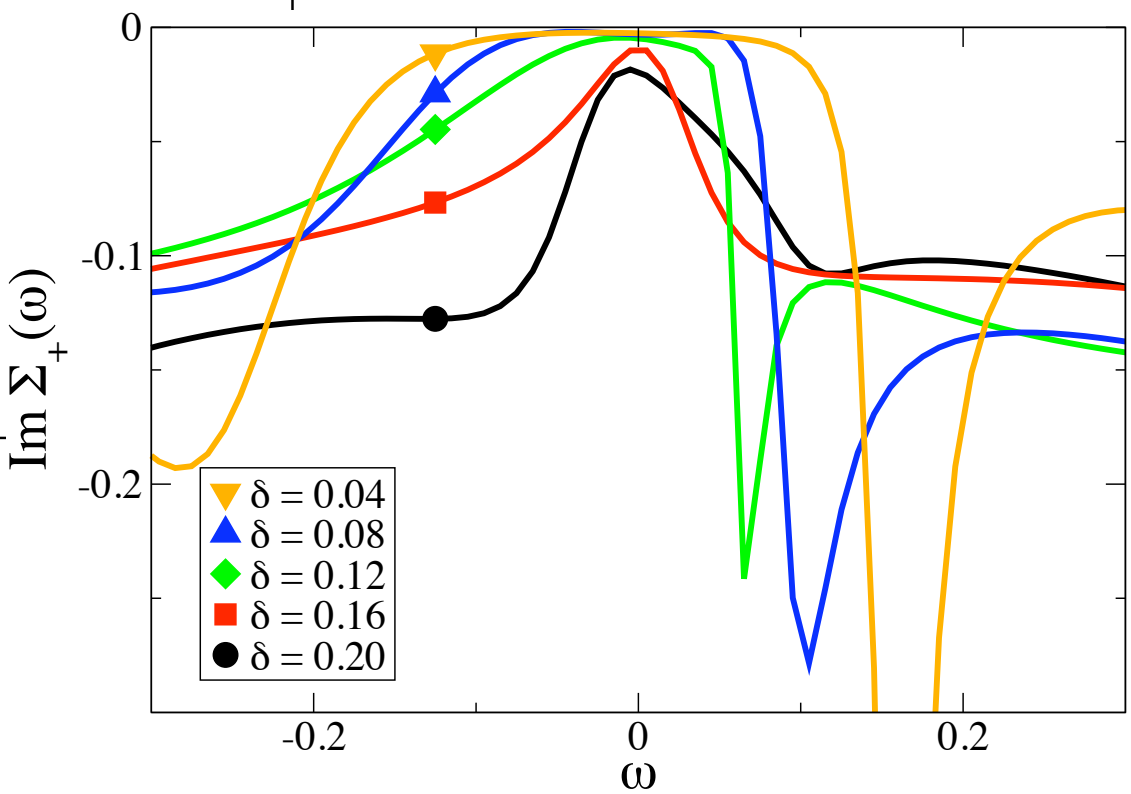
Conclusion

- Two impurities in a bath : a minimal approach to pseudogap
- TRILEX : Spin-fluctuations and Mott physics in the same framework
  - k-dependant self-energies
  - Mott physics
  - Long range spin/charge fluctuations
  - Materials ? Multiorbitals ? Easier to solve than clusters ?
- Work in progress :
  - d-SC in TRILEX
  - Dimer and cluster corrections
  - Systematic benchmark of the method.

Thank you for your attention

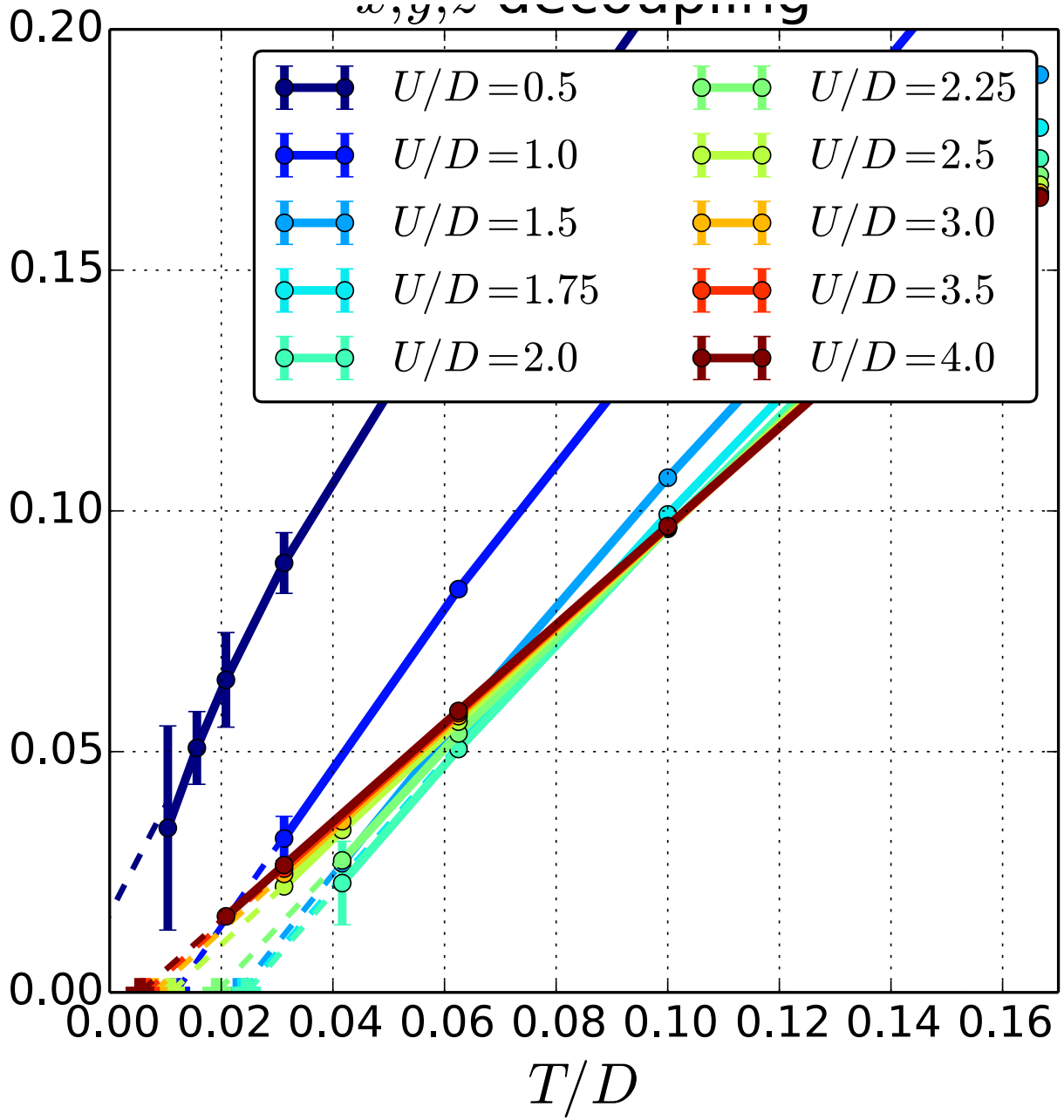
Quasiparticle weights and lifetime: node "protected"





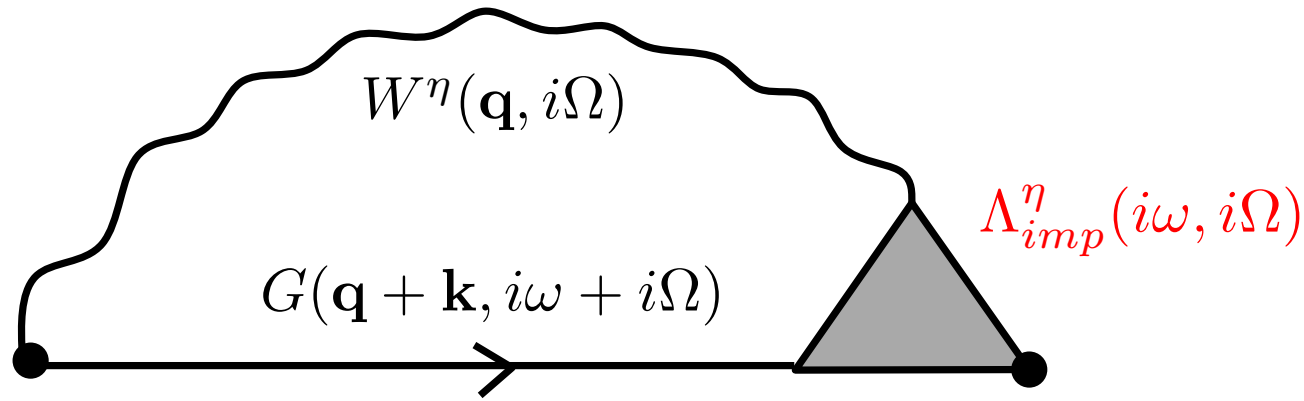
- Below the critical doping, when the odd orbital is insulating, the even (nodal) orbital has a roughly constant quasiparticle residue: it is "protected"

Computation of T_AF



Two "simple" limits

$$\Sigma(\mathbf{k}, i\omega) = \sum_{\eta=ch,sp}$$



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

"Weak coupling", U ⟶0

$$\Lambda_{imp} \approx \lambda$$

- No vertex correction.
- Spin fluctuation diagram

Atomic limit, t⟶0

$$\Lambda_{imp}(i\omega, i\Omega) \approx \Lambda_{atomic}(i\omega, i\Omega)$$

- Exact in this limit
- Mott physics (DMFT)

Spin-fluctuation and DMFT are two "asymptotic" regimes of TRILEX.

Functionals ...

- DMFT is a local approximation of the Luttinger-Ward functional Φ (2-particle irreducible diagrams) *(Georges-Kotliar '92).*

$$\Phi(G) \approx \phi_{atomic}(G_{ii})$$ *DMFT*

$$\Sigma = \frac{\delta \Phi}{\delta G}$$

- Here, we make a similar approximation on the higher-order functional introduced in *De Dominicis-Martin, Math. Phys. 1, '64*, made of 3-particle irreducible diagrams ...

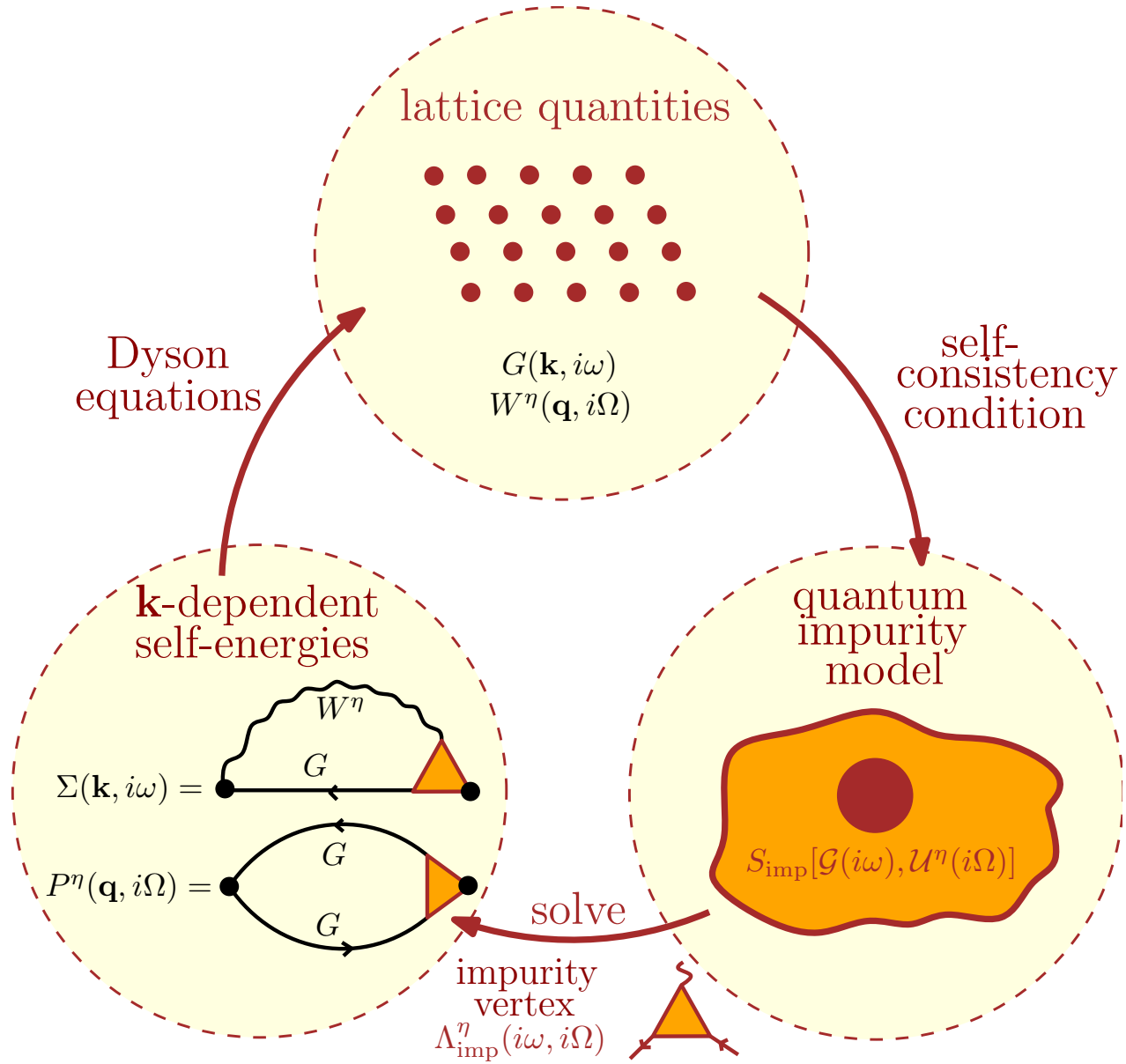
$$\Lambda - 1 = \frac{\delta \mathcal{K}}{\delta \Lambda}$$

$$\mathcal{K}(G, W, \Lambda) \approx \mathcal{K}_{atomic}(G_{ii}, W_{ii}, \Lambda_{iii})$$

TRILEX (triply-irreducible local expansion).

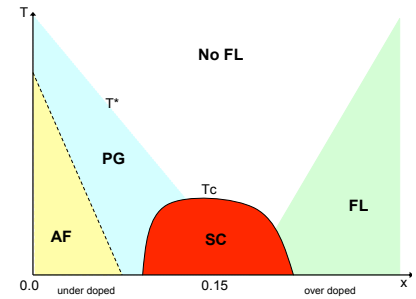
TRILEX : overview

- Solved via a self-consistent, auxiliary quantum impurity model

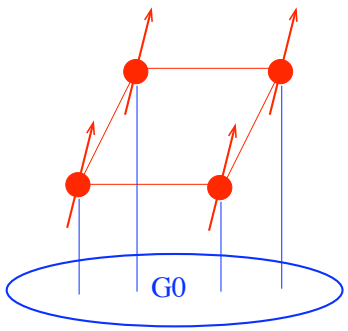


DMFT & clusters ...

- Cluster DMFT : a systematic approach to study Mott physics.
  - Mott physics and short-range fluctuations.
  - One control parameter :
    Nc, size of cluster or number of patches
  - Better algorithms for large clusters *(Gull, Werner, OP, Troyer 2008)*

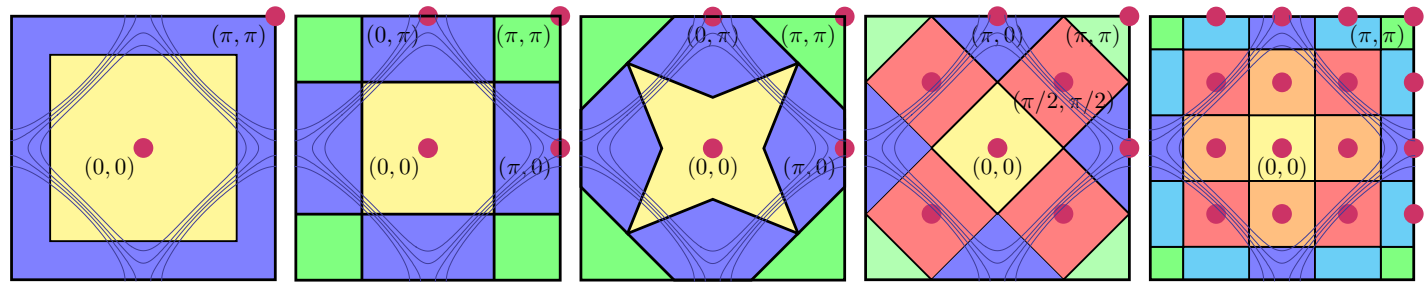


Various cluster shapes



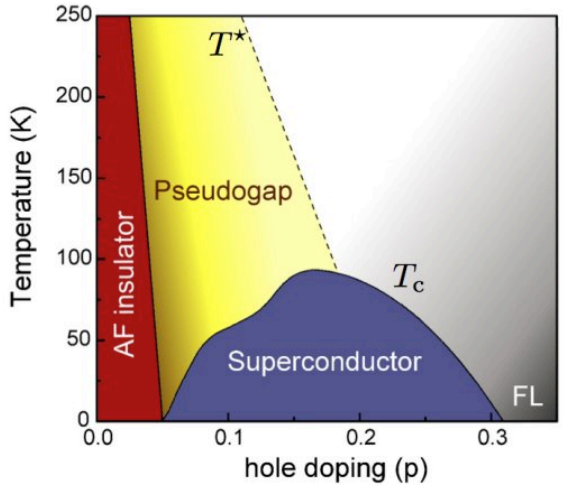
Real space

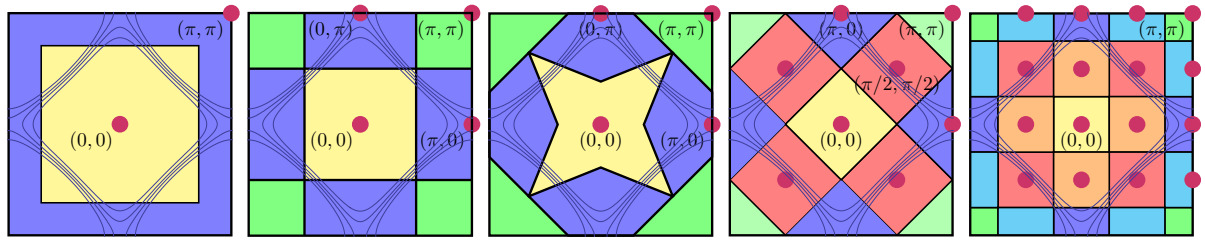
Nc = 2 *Nc = 4* *Nc = 4* *Nc = 8* *Nc = 16*

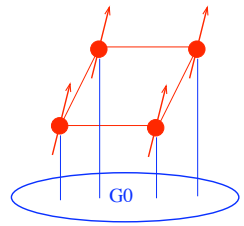


Reciprocal space

Cluster DMFT & Hubbard model







- *Pionneering work 2x2 clusters*
  - *Lichtenstein, Katsnelson PRB 62, R9283 (2000).*
  - *Maier, Jarrell, Pruschke, Keller, PRL 85, 1524 (2000).*
- DCA method *M. H. Hettler, M. Mukherjee, M. Jarrell, and H. R. Krishnamurthy Phys. Rev. B 61, 12739 (2000)*
- *Rutgers Group ; Kotliar, Haule, et al.*
- *8 sites* : Gull, OP, Millis (2009-2013).