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Workshop on
Novel States and Phase Transitions in Highly Correlated Matter

12 - 23 July 2004

Cluster extensions of dynamical mean field theory

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Cluster Extensions of Dynamical Mean Field Theory

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1. DMFT : a starting point for some SCES ?
2. Clusters extensions
3. Mott transition in frustrated systems

Coll: G. Kotliar (Rutgers), M. Civelli (Rutgers), G. Biroli (Saclay)

DMFT : a functional definition

- Approximations on effective action for a local physical quantity
- Ising model $H_{\text{Ising}} \equiv -J \sum_{\langle i,j \rangle} S_i S_j$

  Local Magnetisation: $m_i = \langle S_i \rangle$, $\Gamma[m_i] \approx \Gamma_{\text{Mean Field}}[m_i]$
- Weakly correlated electronic systems

  Local density $n(x)$. Density Functional Theory, LDA.
- Strongly correlated systems :

  $H_{\text{Hubbard}} = -\sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U n_{i\uparrow} n_{i\downarrow}$

$$\Gamma[G_{ij}] = \mathsf{Tr} \ln G_{ij} - \mathsf{Tr}(g^{-1}_{0ij} G_{ij}) + \Phi_{LW}[G_{ij}]$$

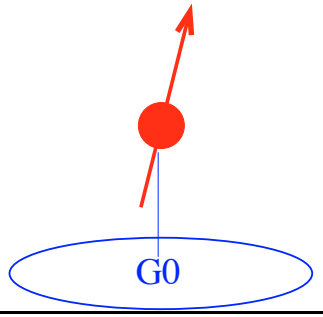
$$G_{ij}(t) \equiv -\left\langle T c_i(t) c^\dagger_j(0) \right\rangle \qquad \Sigma_{ij} = \frac{\delta \Phi_{LW}}{\delta G_{ij}}$$

Local Green Function $G(t) \equiv G_{ii}(t)$

Dynamical Mean Field Theory (DMFT) : $\Phi_{LW}[G_{ij}] \approx \phi[G_{ii}]$

A. Georges, G. Kotliar, W. Krauth, M. Rozenberg RMP (1996)

DMFT : a self-consistent impurity problem

	Local Quantity	Effective problem	Weiss Field
Ising	$m = \langle S_i \rangle$	Ising spin in field h_{eff} $m = \tanh(\beta h_{\text{eff}})$	$h_{\text{eff}} = Jzm$
DMFT	Local Green function G $G(t) \equiv -\left\langle T c_i(t) c_i^\dagger(0) \right\rangle$	**Quantum impurity** 	**Bath** $G_0(t)$ $G_0 = F[G]$

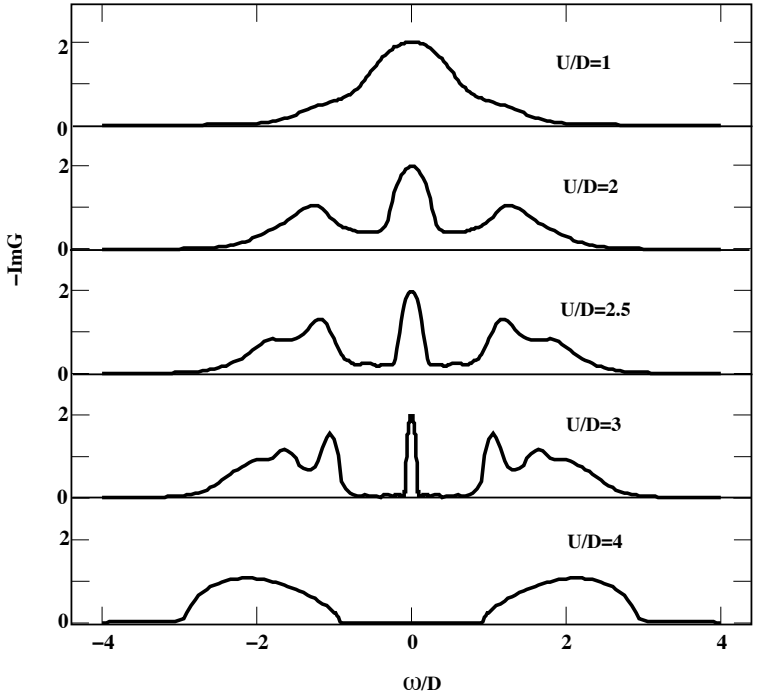
A. Georges, G. Kotliar (1992)

- Explicit realisation as a limit $d \to \infty$ W. Metzner, D. Vollhardt PRL (1989)

Mott transition in DMFT

- Why is the local Green function $G(\omega)$ the "order parameter " ?

$\rho(\omega) \equiv -\frac{1}{\pi}\mathrm{Im}G(\omega)$ vs. U (Hubbard model, DMFT,IPT,$T = 0$)

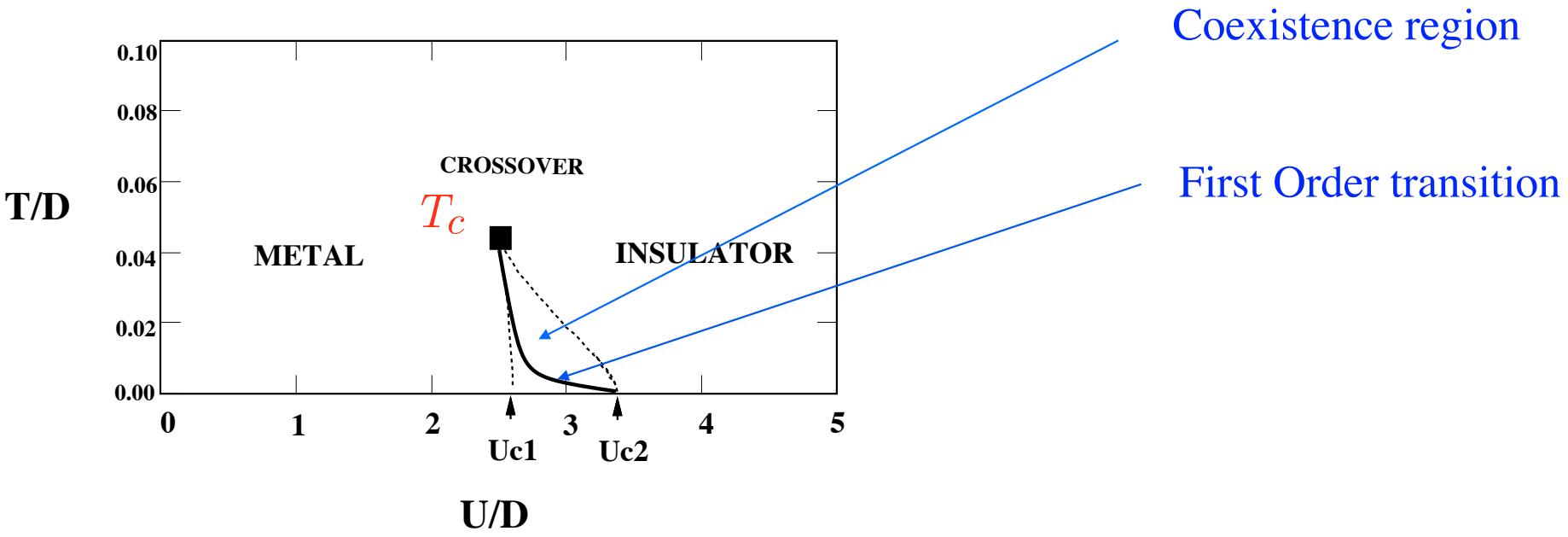


- Transfer of spectral weight.
- Fermi liquid with low coherence scale $\epsilon_F^* = ZD$.
- Coherent and incoherent part
- Describe low and high ω

Mott transition in DMFT : Phase diagram

- Frustrated Hubbard model at half filling : $\delta = 0$, paramagnet

A. Georges, G. Kotliar, W. Krauth, M. Rozenberg RMP (1996)



- $U \sim 1/p$ (p : pressure) in experiments

Frustration is essential to see this Mott transition

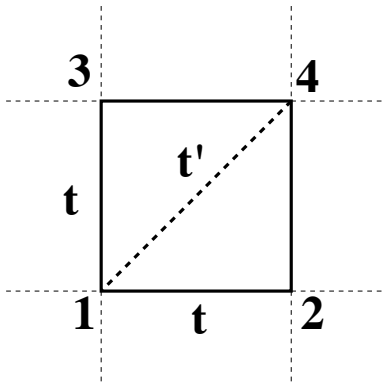
DMFT, a starting point for some SCES ?

- 2D organics : $\kappa-$(BEDT-TTF)$_2$Cu[N (CN)$_2$]Cl).
- Modelisation with a 2d frustrated Hubbard model

  $t'/t \approx 1$

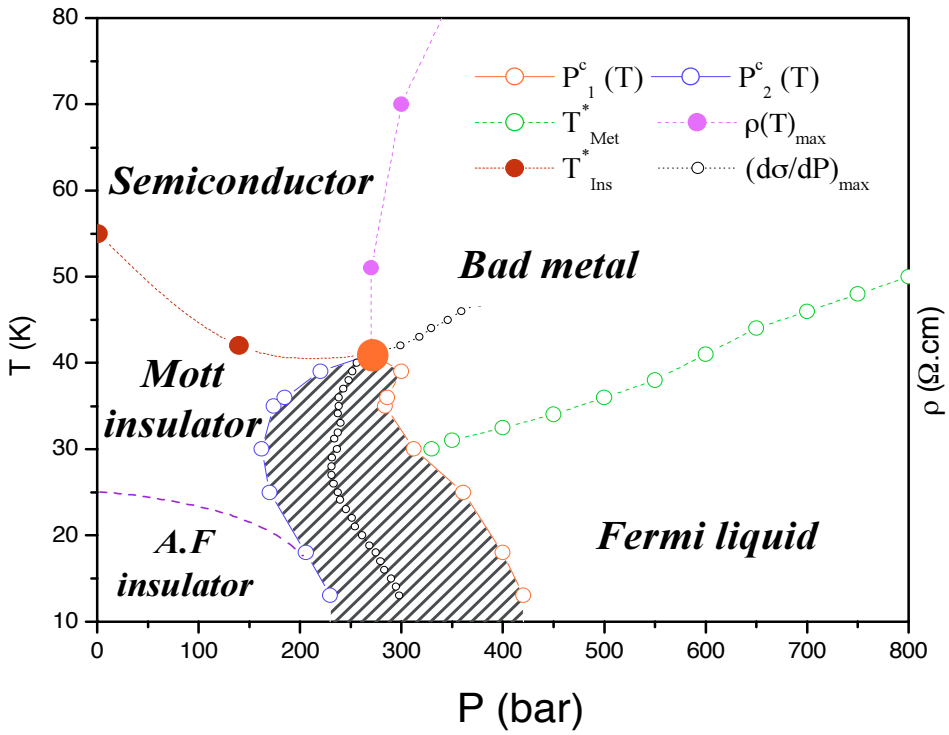
H. Kino, H. Fukuyama J. Phys. Soc. Jpn.65 2158 (1996)

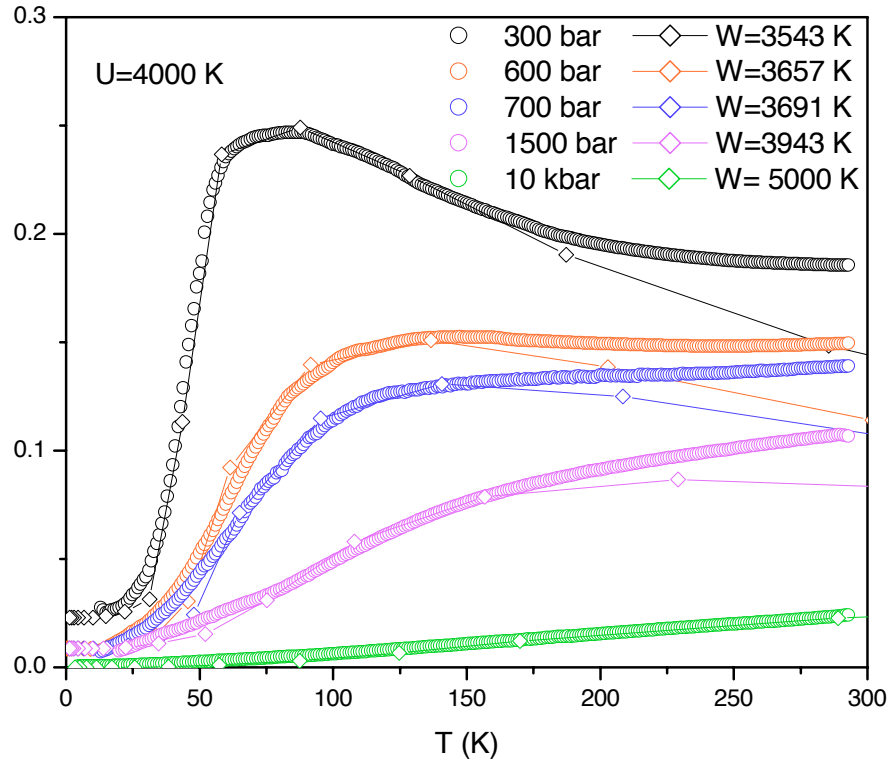
$$H = -\sum_{i,j,\sigma} t_{i,j} c^{\dagger}_{i,\sigma} c_{j,\sigma} + \sum_{i} U \left(n_{i\uparrow} - \frac{1}{2} \right) \left(n_{i\downarrow} - \frac{1}{2} \right)$$



DMFT, a starting point for some SCES ?

- 2D organics : $\kappa-(\text{BEDT-TTF})_2\text{Cu}[\text{N}(\text{CN})_2]\text{Cl}$





P.Limelette, P.Wzietek, S.Florens, A.Georges, T.A.Costi, C.Pasquier, D.Jérome, C.Mézière, P.Batail PRL (2003)

- Stability of the DMFT picture ?
- Shape of the transition line ?
- Critical point : not Ising ($\neq$ 3D V_2O_3) ? K. Kanoda et al.

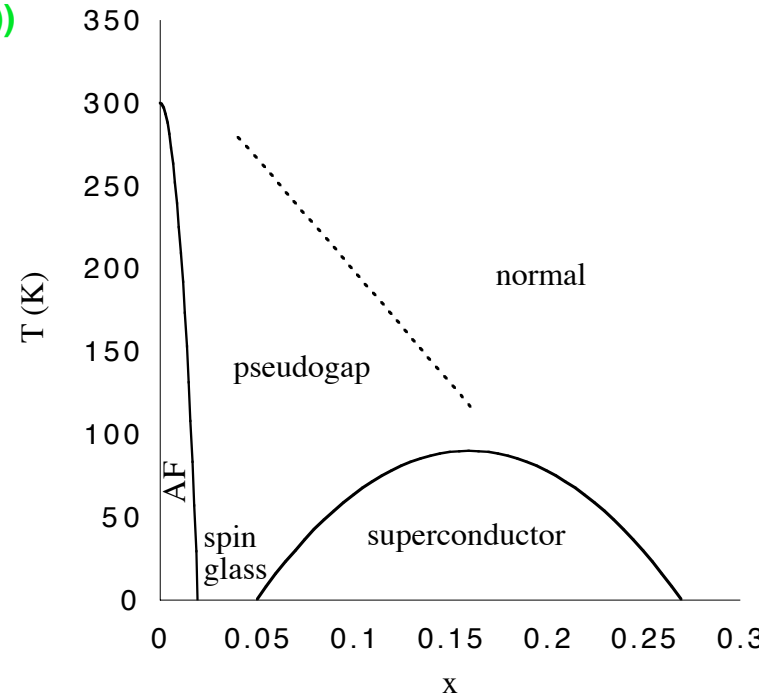
DMFT, a starting point for some SCES ?

- 2D organics : $\kappa-$(BEDT-TTF)$_2$Cu[N (CN)$_2$]Cl).
- V_2O_3
- Pu (Realistic computations)

(S. Savrasov, G. Kotliar, E. Abrahams, Nature 410, 793 (2001))

- High-Tc Cuprates

  - Doped Mott insulators.
  - Short range correlation
  - SCS Cf M. Capone's talk

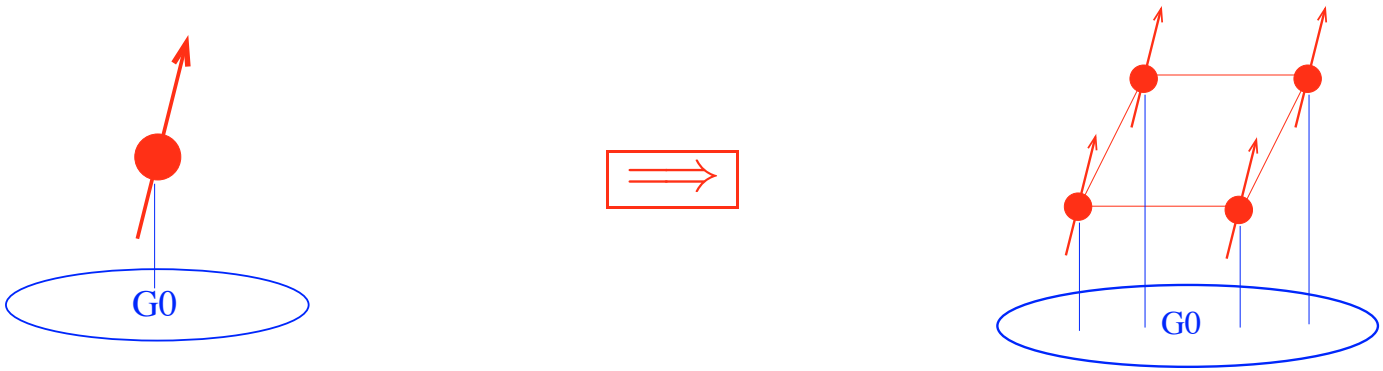


Cluster DMFT (1)

- Missing in DMFT . . .
  - Various orders : e.g. d-SC,DDW, (AF).
  - k dependence of $\Sigma(k,\omega) \Longrightarrow Z \sim \frac{m}{m^*}$
  - Variations of Z, m^*, τ on the Fermi surface.
  - Non trivial insulators (frustrated magnets ?)
  - Non-local interactions (e.g. nearest neighbours).
- . . . but present in cluster methods

spatially short range quantum fluctuations

DMFT **Cluster DMFT**



Cluster DMFT (2)

- Interpolate between DMFT and finite dimensions.
- Finite size systems BUT :
  - in a bath G_0 (like “Boundary Conditions”)
  - in thermodynamic limit
- Static (Hartree-Fock) approximation possible at longer distance.
- Choices :
  - Type, shape of clusters (*e.g.* (linear) size L_c).
  - Self-consistency condition : $G_0 = F[G]$.
  - How to compute lattice quantities from cluster quantities.
  - Various possible parametrisations of $\Sigma(k)$

Cluster DMFT is not unique

Many Cluster Schemes

- CDMFT (Cellular DMFT) (G. Kotliar, S. Savrasov, G. Pálsson, G. Biroli PRL (2001))

  Real space clusters.
- PCDMFT : Periodised CDMFT. (G. Biroli, OP, G. Kotliar, PRB 2004)
- DCA (M.H. Hettler, A.N. Tahvildar-Zadeh, M. Jarrell, T. Pruschke,H.R. Krishnamurthy PRB (1998))

  Reciprocal-space cluster. $\Sigma(k)$ piecewise constant in B.Z.
- NCS : Nested Cluster Scheme. (G. Kotliar, A. Georges, RMP (1996))

$$\Phi_{PS} = (1-z)\sum_i \phi_{1site}(G_{ii}) + \sum_{<ij>} \phi_{pair}(G_{ii}, G_{jj}, G_{ij})$$

- Chain DMFT (S. Biermann, A. Georges,A. Lichtenstein, T. Giamarchi PRL (2001))

  $1d$ chain in a self-consistent bath. Quasi-1d materials.
- CPT (not self-consistent) (S. Pairault, D. Sénéchal, A.M. Tremblay PRL (1998))
- Fictive impurity models (S. Okamoto, A.J. Millis, H. Monien, A. Fuhrmann PRB (2003))

Requirements for a good cluster method

- Convergence to the exact solution for large cluster.
- Ordered phases possible : AF, (d-)SC, CDW, DDW, stripes. . .
- Causality :
  - Im$\Sigma(\omega)$, Im$G(\omega) \leq 0$
  - CDMFT, PCDMFT and DCA are causal.
  - Recent proof using t'Hooft-Veltman-Cutkovsky "cutting rules".

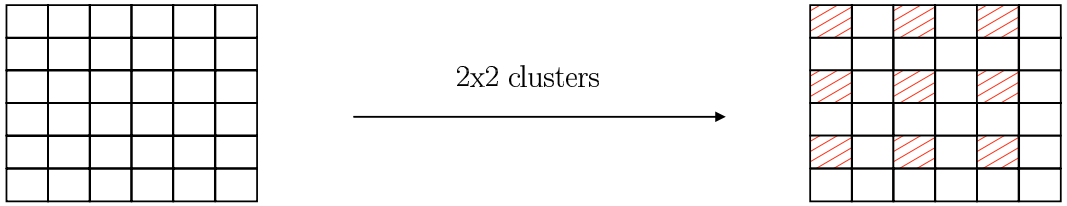
    (G. Biroli, OP,G. Kotliar, PRB 2004)
  - NCS are not causal in general.
  - Causality violation appear in metallic phase, for small size.
- CDMFT (and variants e.g. PCDMFT) and DCA pass the tests.
- Comparisons in 1d, classical limit, large-N ...

DMFT equations

Hubbard model	Ising model
$H = -\sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U n_{i\uparrow} n_{i\downarrow}$	$H = -J \sum_{ij} \sigma_i \sigma_j$
$G(\tau) = -\langle T c(\tau) c^\dagger(0) \rangle_{S_{\text{eff}}}$	$m = \langle \sigma \rangle$
$S_{\text{eff}} = -\int_0^\beta c^\dagger_\sigma(\tau) G_0^{-1}(\tau - \tau') c_\sigma(\tau') + U \int_0^\beta d\tau n_\uparrow n_\downarrow$	$H_{\text{eff}} = -J h_{\text{eff}} \sigma$
$\Sigma = G_0^{-1} - G_c^{-1}$	
	$m = \tanh(\beta h_{\text{eff}})$
$G_0^{-1}(i\omega_n) = \left(\sum_k \frac{1}{i\omega_n + \mu - t(k) - \Sigma(i\omega_n)} \right)^{-1} + \Sigma(i\omega_n)$	$h_{\text{eff}} = z J m$

CDMFT

$$H = -\sum_{R_m \mu R_n \nu} \hat{t}_{\mu\nu}(R_m - R_n) c^+_{R_m \mu} c_{R_n \nu} + \sum_{\substack{R_1 \mu R_2 \nu \\ R_3 \rho R_4 \varsigma}} U_{\mu\nu\rho\varsigma}(\{R_i\}) c^+_{R_1 \mu} c^+_{R_2 \nu} c_{R_4 \varsigma} c_{R_3}$$



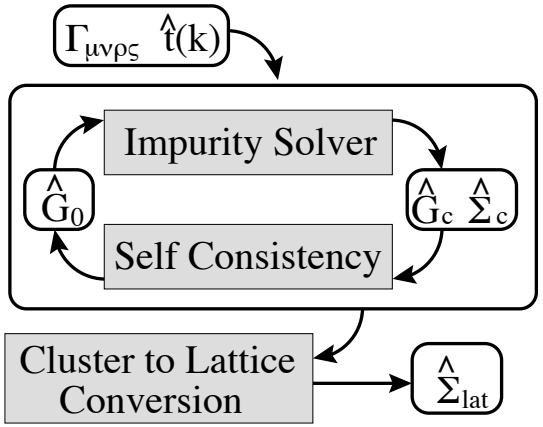
$$S_{\text{eff}} = -\int\int_0^\beta d\tau d\tau' c^\dagger_\mu(\tau) G^{-1}_{0,\mu\nu}(\tau,\tau') c_\nu(\tau') + \int_0^\beta d\tau U_{\alpha\beta\gamma\delta}(0)(c^\dagger_\alpha c_\beta c^\dagger_\gamma c_\delta)(\tau)$$

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

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

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

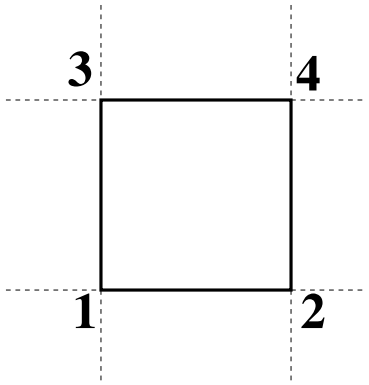
CDMFT (2)



- Lattice quantities $\neq$ cluster quantities
- Lattice self energy is computed at the end
- Restore translation invariance on lattice :

$$\Sigma_{ij}^{lattice} = \sum_{\alpha,\beta:\alpha-\beta=i-j} w_{\alpha,\beta}(\Sigma_c)_{\alpha\beta} \qquad w>0, \sum_{\alpha\beta;\alpha-\beta=x} w_{\alpha,\beta} \to 1 \quad \forall x$$

- Simplest case : 2×2 clusters



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

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

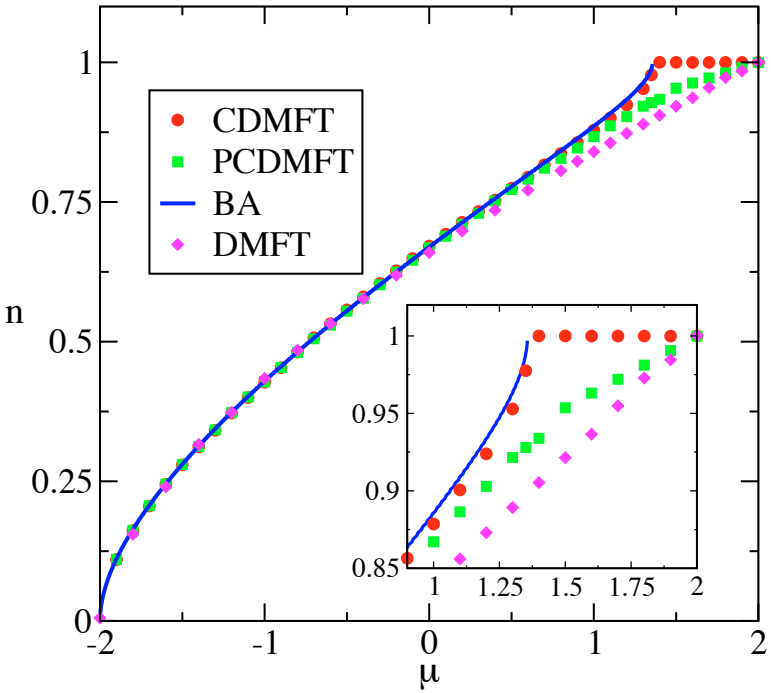
- Phase with broken translation invariance captured by the cluster.

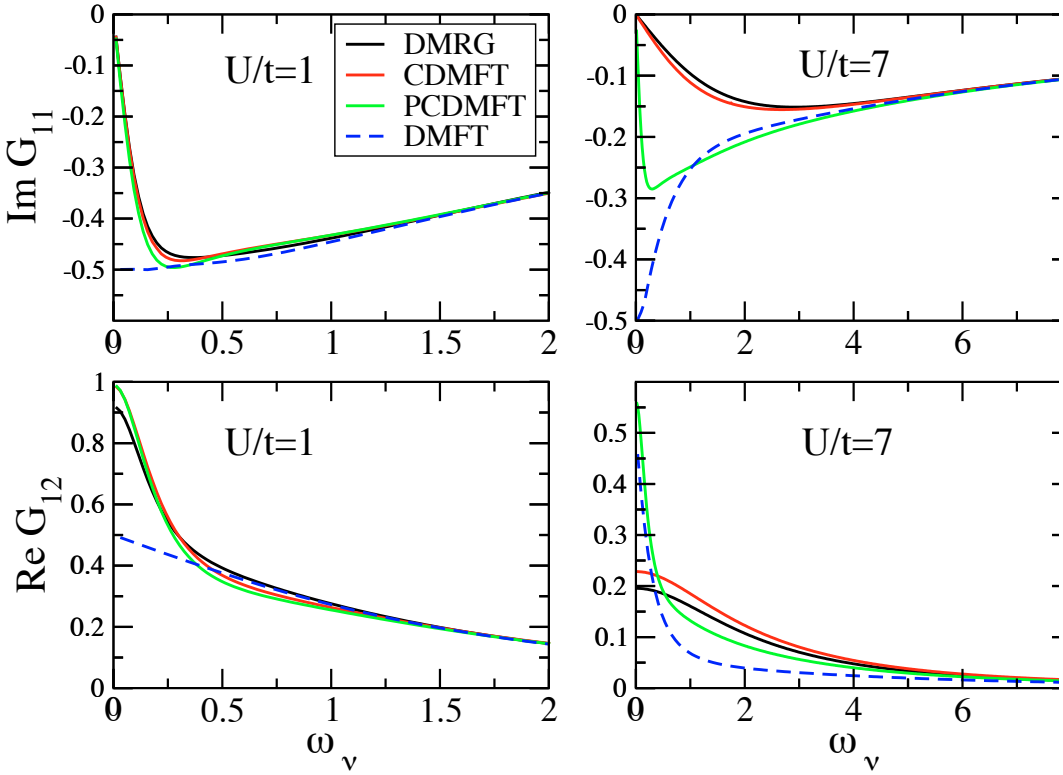
Test in one dimension

- Solve the 1D Hubbard model with 2 sites clusters and E.D. solver

  Compare with Bethe Ansatz solution and DMRG.

M. Capone, M. Civelli, S.S. Kancharla, C.Castellani,G. Kotliar PRB (2004)





$n(\mu)$ for $U/t = 4$, $N_{\text{cluster}} = 2$,$N_{\text{bath}} = 8$

Some results on the 2d Hubbard model

- AF + $d-$wave SC
  - Variant of PCDMFT.

    A. Lichtenstein, M. Katsnelson, PRB (2000)
  - DCA **M. Jarrell, T. Maier et al.**
  - CDMFT : d-SC, $T_c < T_c^{\mathrm{DCA}}$.

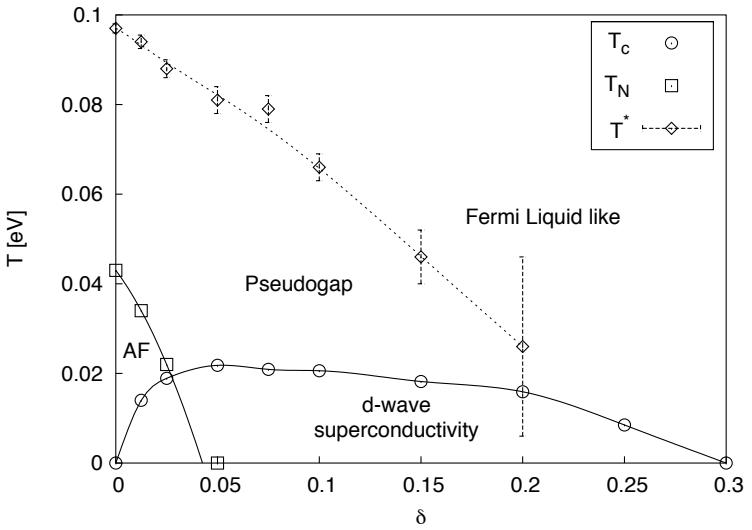
    Recent results with E.D.

    M. Capone
- Pseudogap phase

  $\chi_c(\omega)$, $\chi_s(\omega)$

  Recent work with CPT : **A.M. Tremblay et al.**, CDMFT **S. Kancharla**.
- Mott transition in frustrated Hubbard model **OP, G. Biroli, G. Kotliar, PRL (2004)**

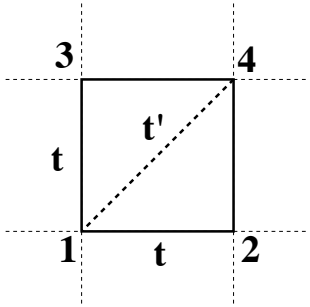
DCA, 2×2 clusters



Cluster solution of a frustrated Hubbard model

O.P, G. Biroli, G. Kotliar, PRL (2004)

- Frustrated Hubbard model for organics $t'/t = 0.9$, $\delta = 0$.
- Solve CDMFT for 2×2 cluster with QMC.

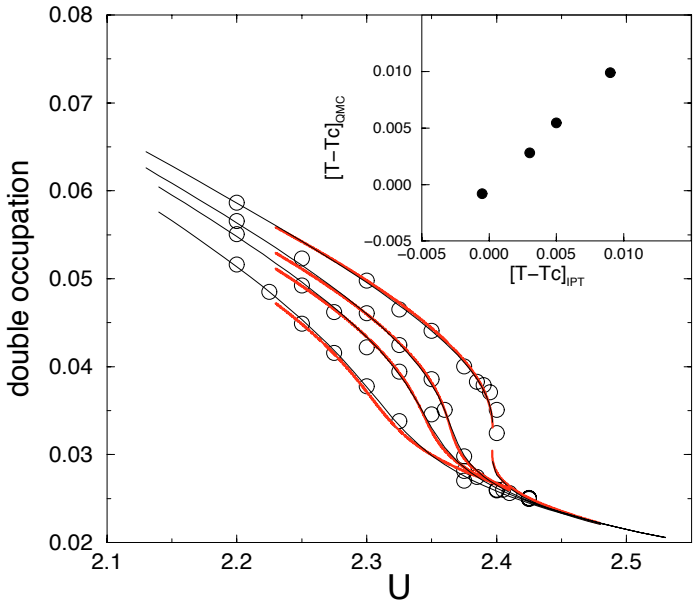


- In DMFT, paramagnetic solutions of an unfrustrated model are solutions of a frustrated model
- But in CDMFT one must solve a frustrated model

A DMFT-like Mott transition ...

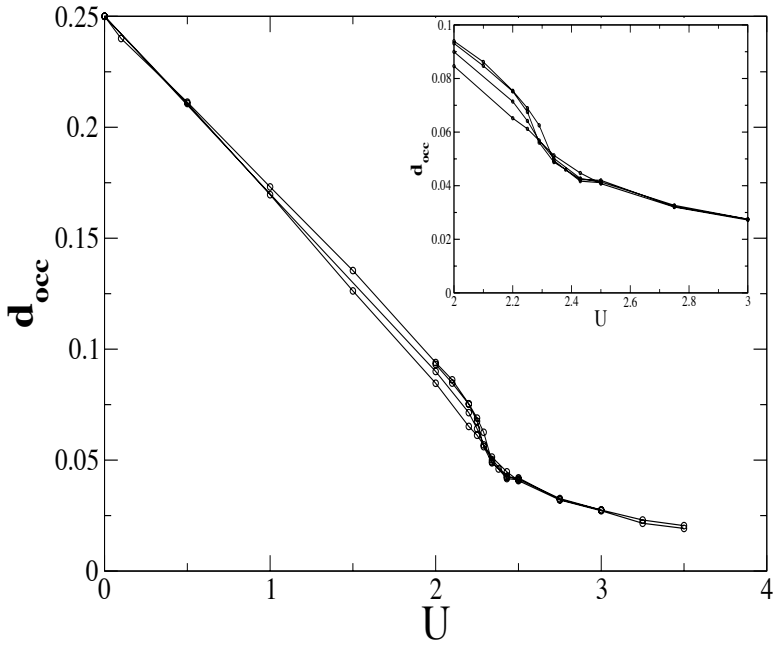
- No AF order (at the temperature of the QMC).
- DMFT-like Mott transition. Double occupation $d_{occ} = \sum_i \langle n_{i\uparrow} n_{i\downarrow} \rangle$

DMFT



G. Kotliar, E. Lange, M. J. Rozenberg et al. PRL (2000)

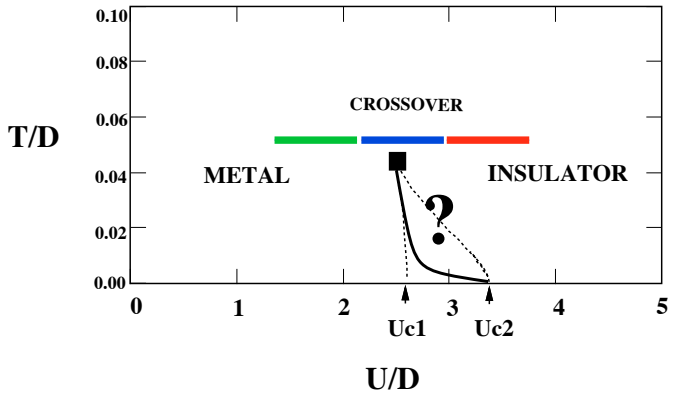
CDMFT



$T/D = 1/20, 1/30, 1/40, 1/44$

. . . with k-dependent self-energy

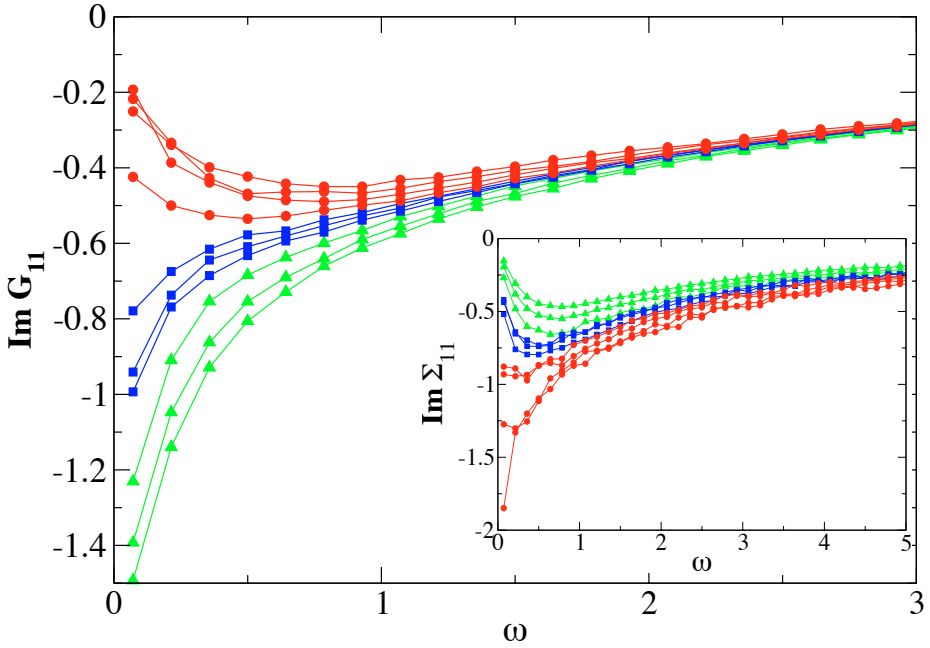
- Fixed $T/D = 45 > T_c$, various U : 3 regions in U.

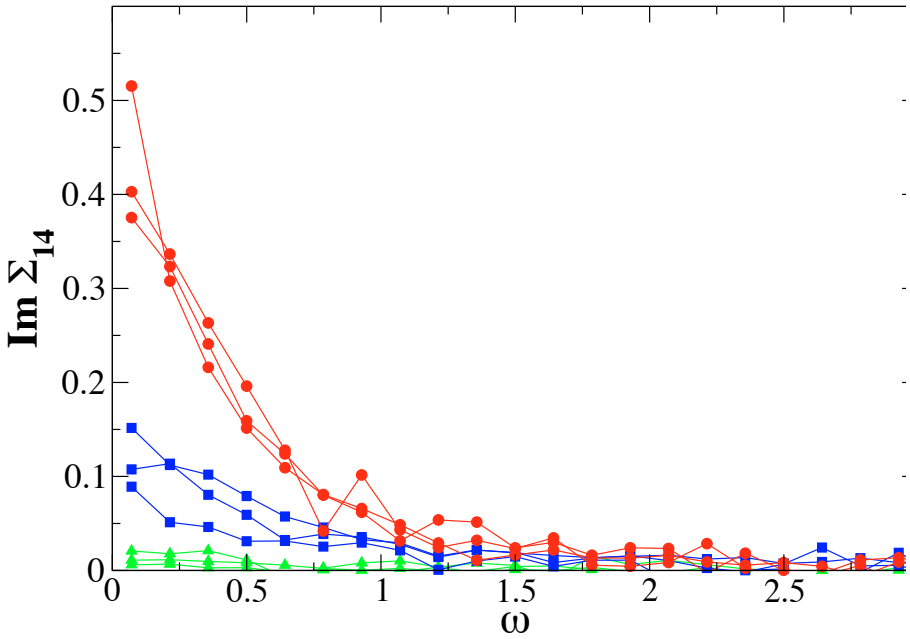


DMFT metal	Metal. Hot-Cold spots	Finite T insulator
$U/D \leq 2.2$	$2.25 \leq U/D \leq 2.3$	$2.35 \leq U/D$
$\Sigma''_{11} \sim c_1 + \left(1 - \frac{1}{Z}\right) i\omega_n$	$\Sigma''_{11} \sim c_2 + \left(1 - \frac{1}{Z}\right) i\omega_n$	$\Sigma''_{11} \sim c_3$
$\Sigma''_{12}, \Sigma''_{14} \approx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

- $\Sigma'(\omega = 0) \neq 0 \Longrightarrow t'_{eff}$ more isotropic

Self-energies in imaginary time

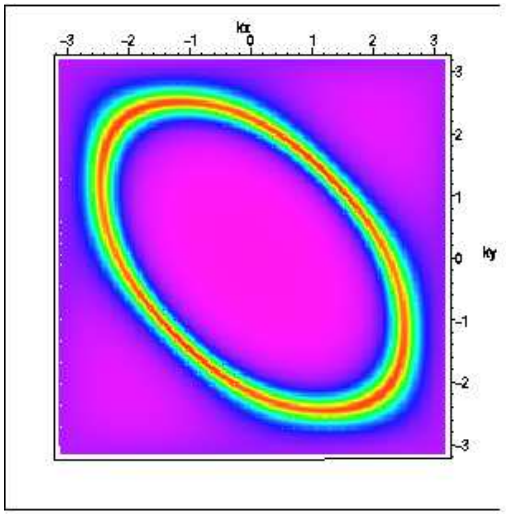


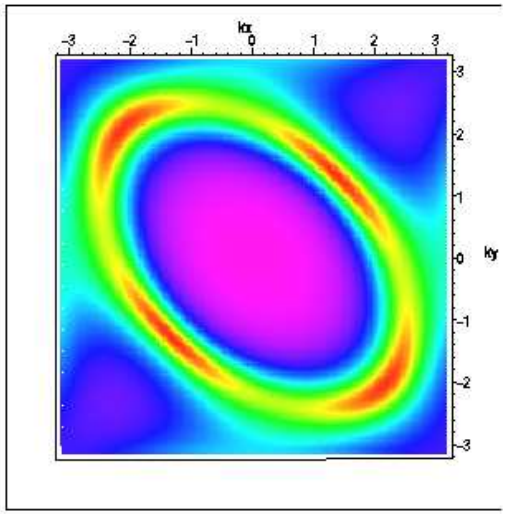


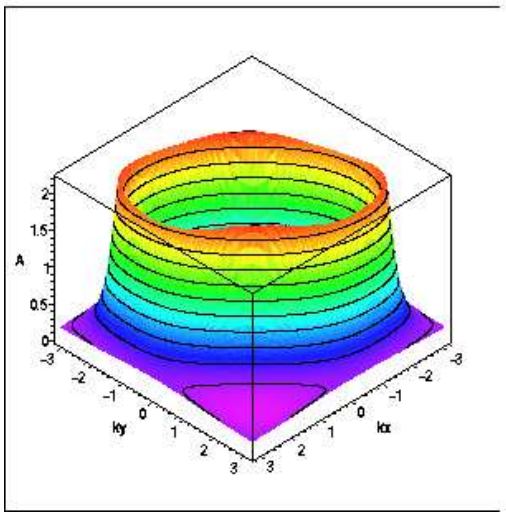
$U = 2, 2.1, 2.2, 2.25, 2.29, 2.31, 2.34, 2.43, 2.5 \qquad T/D = 1/44.$

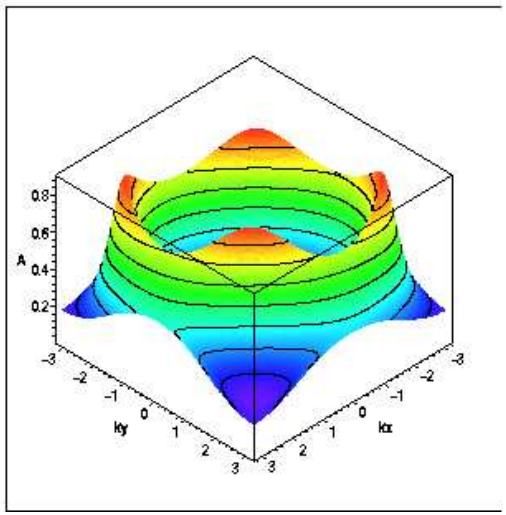
Hot and Cold regions

- $A(k, \omega = 0)$ in the metallic region : $U/D = 2.0, 2.25$









A possible scenario

- For $T \to 0$, Im$\Sigma_{14} \to 0$: $Z_{(\pi,\pi)} \neq Z_{(0,\pi)}$
- Above T_c, continuity from metal to insulator.

  k-dependence is due to the proximity of the Mott insulator.
- Different coherence temperatures for (π, π) and $(0, \pi)$ directions.
- Strong frustration : weak AF fluctuations.

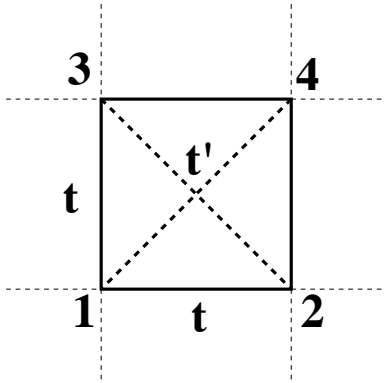
- Need for solutions for lower T and higher U
- Problem : QMC is inefficient (sign problems).

  $\Longrightarrow$ Exact Diagonalisation at $T = 0$.

Preliminary results at $T = 0$ (1)

Coll : M. Civelli, S. Kancharla, M. Capone

- On isotropic model, 2×2 clusters, CDMFT.



- 8 Sites in the bath ($2\times$ cluster size)
- Coexistence Metal-Insulator like in DMFT.
- Non magnetic insulator for $U/D > 3$.

  Does not break translation symmetry.

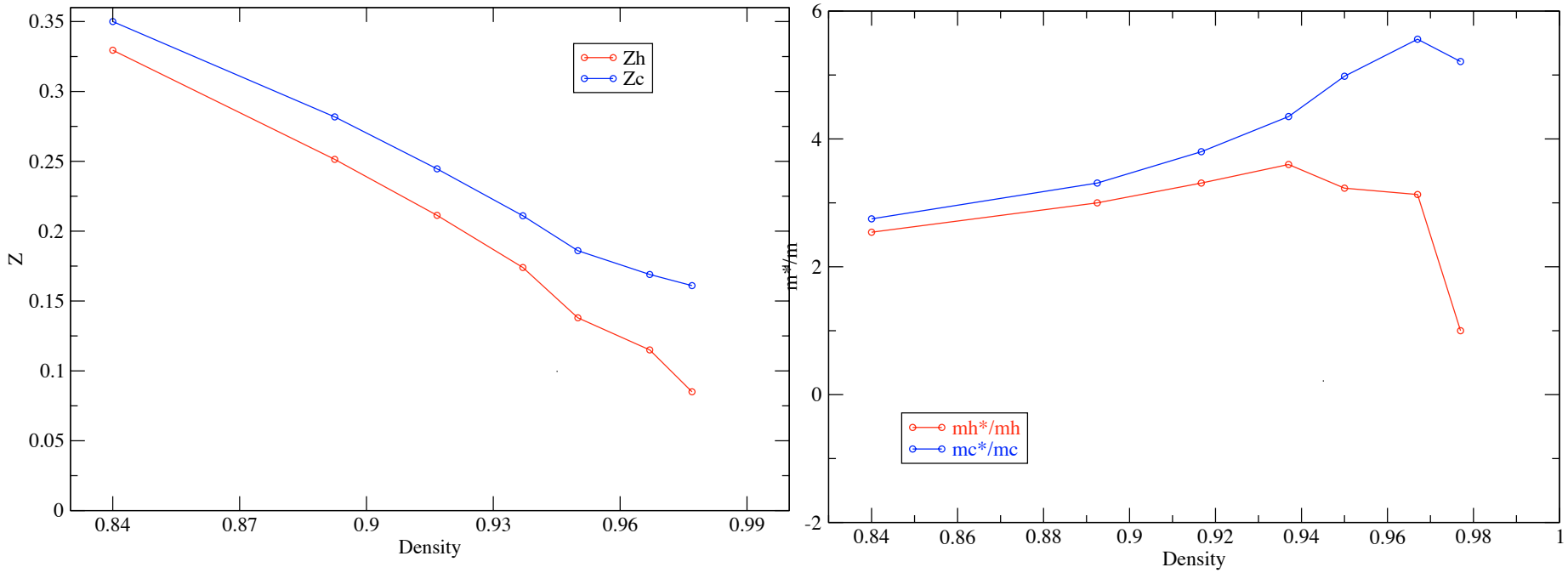
Preliminary results at $T = 0$ (2)

- Close to the Mott transition, for large U : $U/D = 4$:

$$Z_{(0,\pi)} > Z_{(\pi,\pi)}$$

$m^*_{(\pi,\pi)}$ does not diverge.

Z $\qquad\qquad$ m^*/m



Conclusion

- DMFT as a starting point for SCES.
- Many DMFT cluster methods...
- Mott transition in frustrated systems in CDMFT.
  - DMFT-like Mott transition ...
  - ... with cluster corrections close to CP and large U.
  - Hot-Cold regions.

- Open questions
  - Nature of the Mott insulator : VBS ? Spin liquids ?
  - Complete phase diagram
  - Shape of the transition line
  - Transport.