Cellular Dynamical Mean Field Theory: applications to cuprates and organics

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Outline

- Introduction to Dynamical Mean Field Theory (DMFT).
- Essential elements of a cluster scheme: C-DMFT.
- Hamiltonian and effective action in the cluster variables.
- Self-consistent condition and the C-DMFT algorithm.
- $2 * 2$ sites cluster.
- AFM and Mott transition in cuprates: phase diagram.
- Anisotropies in the self-energy and spectral function.
- DOS and Mott transition in κ-organics.
- Conclusions.

Dynamical Mean Field Theory (DMFT)

DMFT is an extension of the *mean field theory for* classical system (e.g. Ising model) to *quantum system* (e.g. Hubbard model).

DMFT takes into account *local temporal quantum fluctuations* while freezing spatial fluctuations.

DMFT description of the Hubbard model results in a *single-site effective dynamics* (embedded *in a self-consistent bath*) described in terms of an imag. time action S_{eff} at that site

The effective action is parameterized by $G_0(\tau - \tau')$, the

Weiss effective field,

corresponding to the effective magnetic field in the Ising model:

$$\begin{aligned} S_{eff} = & - \int_0^\beta d\tau d\tau' \sum_\sigma c^+_{0\sigma}(\tau) G_0^{-1}(\tau - \tau') c_{0\sigma}(\tau') \\ & + U \int_0^\beta d\tau \, n_{0\uparrow}(\tau) n_{0\downarrow}(\tau) \end{aligned} \quad (1)$$

$G_0(\tau - \tau')$ effective amplitude for a fermion to be created on the isolated site at time τ (coming from the external bath) and being destroyed at time τ' (going back to the bath).

DMFT becomes **exact** in the limit of infinite dimensions (or infinite coordination number).

In practise it works well for 3D systems with large unit cells (as in V_2O_3, $NiSe_xS_{2-x}$ ...)

Some references for DMFT:

• W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989).

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

• R. Chitra and G. Kotliar, Phys. Rev. Lett. **83**, 2386 (1999).

• G. Kotliar, S. Murthy, and M. J. Rozenberg, Phys. Rev. Lett. **89**, 046401 (2002).

Essential elements of a cluster scheme

1) Cluster degrees of freedom $\rightarrow$ impurity degrees of freedom in a bath described by a *Weiss field matrix function* $\widehat{G}_0$.

Solution of the cluster embedded in a medium $\rightarrow$

- cluster Green's function matrix and
- self energy matrix.

2) Expression of the Weiss field in terms of the self energy of the cluster $\rightarrow$

self-consistency condition of the cluster scheme.

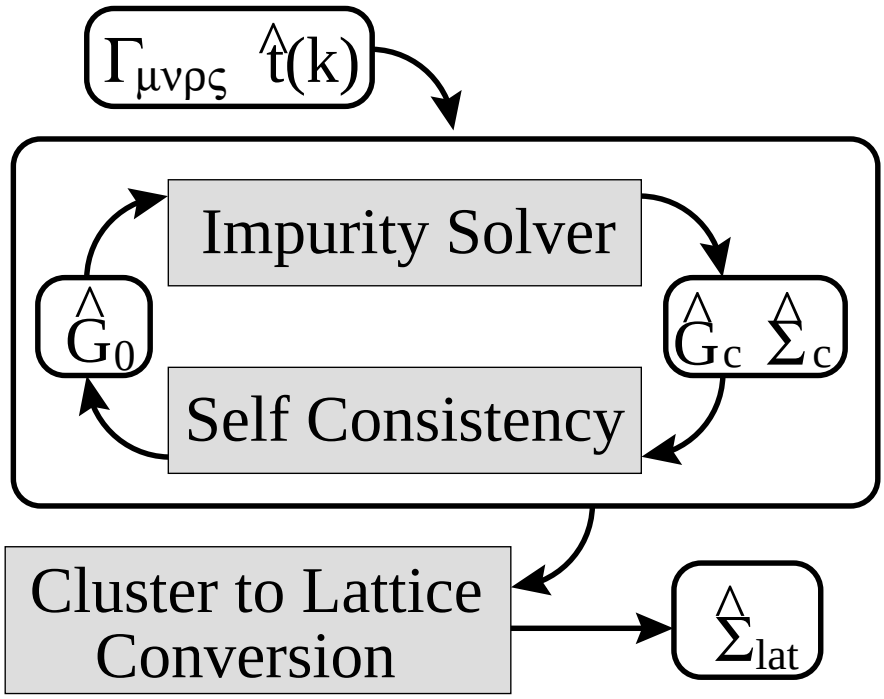
3) Connection between the cluster self energy and the self energy of the lattice.

References on C-DMFT scheme

• G. Kotliar, S. Y. Savrasov, G. Pálsson, and G. Biroli, Phys. Rev. Lett. **87**, 186401 (2001).

• G. Biroli and G. Kotliar, Phys. Rev. B **65**, 155112 (2002).

Schematic C-DMFT algorithm



Selection of cluster variables

(real space formulation of the cluster scheme)

Original lattice $\rightarrow$ *superlattice* of clusters of size $\Pi_{j=1}^{d} \mathrm{L}_j$

R_n new translation vectors .

$|R_n\alpha\rangle$ wave functions (partially) localized around R_n with $\alpha = 1, \ldots, N$ internal *cluster* index.

$S_{R_n\alpha,i\sigma}$ transformation matrix,

$|R_n\alpha\rangle = \Sigma_{i\sigma}|i\sigma\rangle S^{-1}_{i\sigma,R_n\alpha}$.

Creation and annihilation operators of the new basis
$c_{R_n\alpha} = \Sigma_{i\sigma} S_{R_n\alpha,i\sigma} f_{i\sigma}$

and the operators that contain the "local" information that we want to focus our attention on are

$c_\alpha \equiv c_{(R_n=0)\alpha}$ operators of the cluster at the origin.

$O^{mn}_{\mu\nu} = O_{\mu\nu}(R_m - R_n) \equiv \langle R_m\mu|R_n\nu\rangle$ overlap matrix

Hamiltonian in the superlattice

Hamiltonian in terms of the new operators $c_{R_m\mu}$.

$$\begin{aligned} H &= -\sum_{R_m\mu R_n\nu} t_{\mu\nu}(R_m - R_n) c^+_{R_m\mu} c_{R_n\nu} \\ &+ \sum_{R_1\mu R_2\nu R_3\rho R_4\varsigma} U_{\mu\nu\rho\varsigma}(\{R_i\}) c^+_{R_1\mu} c^+_{R_2\nu} c_{R_4\varsigma} c_{R_3\rho}. \end{aligned} \quad (2)$$

$$H = H_c + H_{cb} + H_b$$

H_c involves only the cluster operators,

H_b contains $c_{R_n\mu}$ with $R_n \neq 0$ and plays the role of a "bath",

H_{cb} contains both $c_{R_n\mu}$ with $R_n \neq 0$
and the cluster operators

Partition function

Partition function represented as a functional integral over Grassman variables,

$$Z = \int \prod_{R_n \alpha} Dc^+_{R_n \alpha} Dc_{R_n \alpha} e^{-S} \tag{3}$$

where the action is given by

$$\begin{aligned} S &= \int_o^\beta d\tau \left(\sum_{R_m \mu R_n \nu} c^+_{R_m \mu} O^{mn}_{\mu\nu} \partial_\tau c_{R_n \nu} - H[c^+_{R_m \mu}, c_{R_n \nu}] \right) \\ &\equiv S_c + S_{cb} + S_b. \end{aligned} \tag{4}$$

The effective action for the cluster variables c_μ is obtained by integrating out all the variables $c_{R_n \mu}$ with $R_n \neq 0$

$$\frac{1}{Z_{eff}} e^{-S_{eff}[c^+_\mu c_\mu]} \equiv \frac{1}{Z} \int \prod_{R_m \neq 0, \mu} Dc^+_{R_m \mu} Dc_{R_m \mu} e^{-S}. \tag{5}$$

S_{cb} contains only boundary terms $\rightarrow$ the effects will decrease as the size of the cluster increases.

The effective action is parameterized by

$$G_{0,\mu\nu}(\tau-\tau') \ \textbf{Weiss function of the cluster}$$

$$\begin{aligned} S_{eff} &= -\int_0^\beta d\tau d\tau' \sum_{\mu\nu} c_\mu^+(\tau) G_{0,\mu\nu}^{-1}(\tau-\tau') c_\nu(\tau') \\ &+ \int_0^\beta d\tau_1 d\tau_2 d\tau_3 d\tau_4 \, \Gamma_{\mu\nu\rho\varsigma} c_\mu^+(\tau_1) c_\nu^+(\tau_2) c_\varsigma(\tau_4) c_\rho(\tau_3) \end{aligned} \quad (6)$$

where $\Gamma_{\mu\nu\rho\varsigma} = U_{\mu\nu\rho\varsigma}(\{0\})$.

Using S_{eff} one can calculate the Green's functions of the cluster

$$G_{c,\mu\nu}(\tau-\tau')[\widehat{G}_0] \equiv -\langle T_\tau c_\mu(\tau) c_\nu^+(\tau')\rangle[\widehat{G}_0] \quad (7)$$

and the cluster self energies

$$\widehat{\Sigma}_c \equiv \widehat{G}_0^{-1} - \widehat{G}_c^{-1}. \quad (8)$$

The thermal average $< ... >$ over all configurations is performed by QMC method using the Hirsch-Fye algorithm.

• J. E. Hirsch and R. M. Fye, Phys. Rev. Lett. **56**, 2521 (1986).

Self-consistency condition

Self consistent equations $\rightarrow$ matrix equations expressing the Weiss field in terms of the cluster self energy matrix $\widehat{\Sigma}_c$.

$$\widehat{G}_0^{-1} = \left(\sum_k \frac{1}{(i\omega + \mu)\widehat{O}(k) - \hat{t}(k) - \widehat{\Sigma}_c} \right)^{-1} + \widehat{\Sigma}_c \qquad (9)$$

$\widehat{O}(k)$ is the Fourier transform of the overlap matrix,

$\hat{t}(\mathbf{k})$ is the Fourier transform of the kinetic term of H,

$\mathbf{k}$ is a wave-vector in the reduced Brillouin zone.

Connection to the self energy of the lattice

$$\Sigma_{lat,\sigma\sigma'}(k, \omega_n) = \frac{1}{N_{atoms}} \sum_{\mu\nu} \tilde{S}^{\dagger}_{\sigma,\mu}(k) \Sigma_{c,\mu\nu}(\omega_n) \tilde{S}_{\nu,\sigma'}(k) \qquad (10)$$

$\tilde{S}$ is the Fourier transform of the matrix S with respect to the original lattice indices i.

k is a given wave-vector in the original lattice

C-DMFT with a free cluster (local basis)

(i) The lattice is divided into supercells,

(ii) each supercell is a complex "site" to which one can apply ordinary DMFT.

R_n is the supercell position,

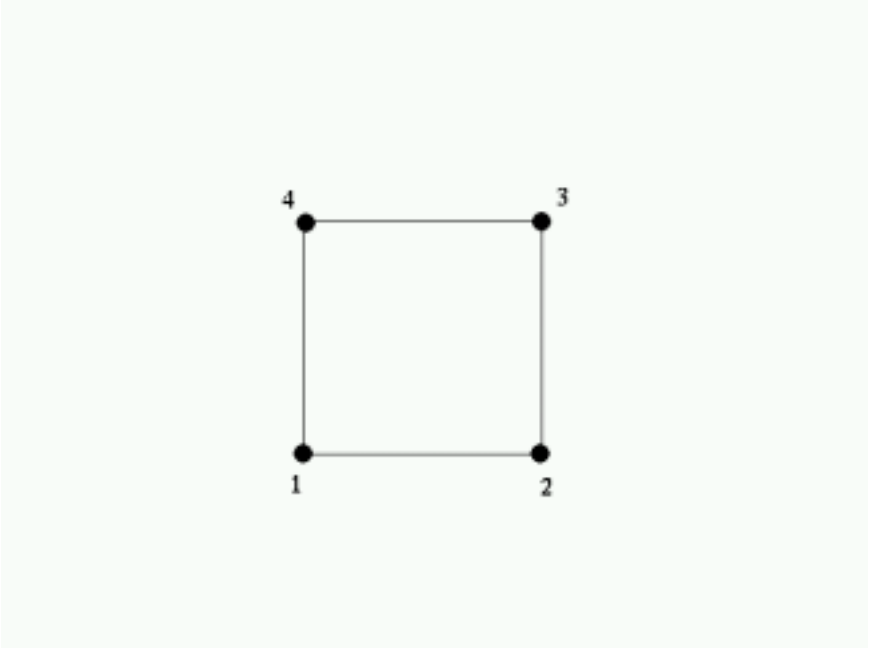
α labels the position l of the different sites within the supercell, and the spin σ, $\alpha = (\sigma, l)$,

$S_{R_n\alpha,i\sigma} = \delta_{\sigma,\sigma'}\delta_{R_n+l,r_i}$

is diagonal in spin and position.

The overlap matrix results, in this case, the identity.

Local basis: $2 * 2$ atoms



The $2 * 2$ local basis is suitable to study both AFM and d-wave SC order parameter on an equal footing.

• A. I. Lichtenstein and M. I. Katsnelson, Phys. Rev. B **62**, R9283 (2000).

Lattice selfenergy:

$$\Sigma_{lat}(k,\omega_n) = \frac{1}{N_{atoms}}(4\Sigma_{11}(\omega_n) + 4(\cos k_x + \cos k_y)\Sigma_{12}(\omega_n) + 4\cos k_x \cos k_y \Sigma_{13}(\omega_n)) \quad (11)$$

Eq. (11) is equivalent to an expantion of the selfenergy in the harmonic of the square lattice up to the second harmonic (*i.e.* second neighbor).

(We assume that all the symmetries of the original lattice are preserved. We don't plug these symmetries in the self-consistency loop, we use them to check the convergency of the C-DMFT algorithm.)

Mott transition and AFM in cuprates

Tight-binding dispersion for $La_{2-x}Sr_xCuO_4$
(fit to ARPES at large doping)

$$\xi(k) = -2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y - \mu \tag{12}$$

Phase diagram for $t' = 0$: Neel temperature T_N as function of U at half filling.

$2 * 2$ cluster is able to take into account AFM correlations without the sublattice construction used in standard DMFT.

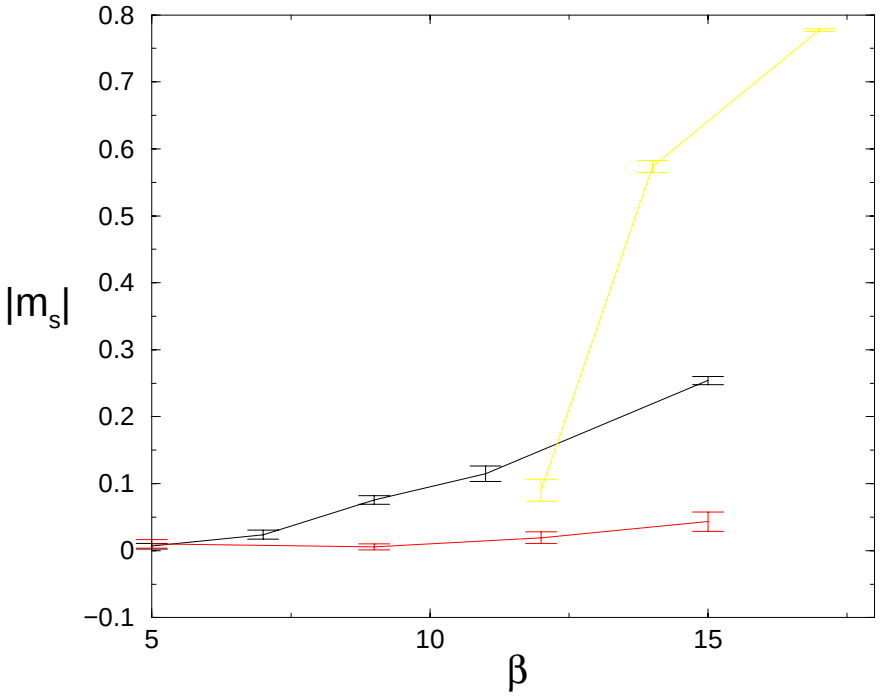
$T_N(U)$ is evaluted finding the temperature where the staggered magnetization $n_\uparrow - n_\downarrow$ starts to be non zero.

$t = 0.25$eV and $t' = 0.15t$, $L = 64$ time slices, $2 * 2$-sites cluster, $\mu = -0.13$eV (0.02eV above the van Hove singularity).

Momentum dependent selfenergy.

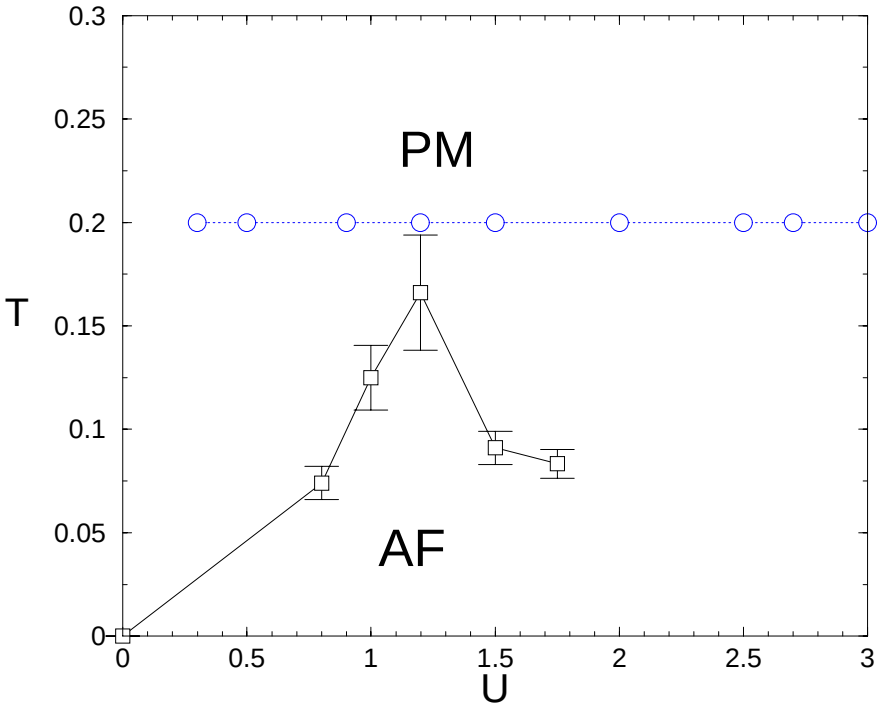
Staggered Magnetization (2x2)

U=0.8 (Red), U=1.2 (Black), U=1.75 (Yellow)



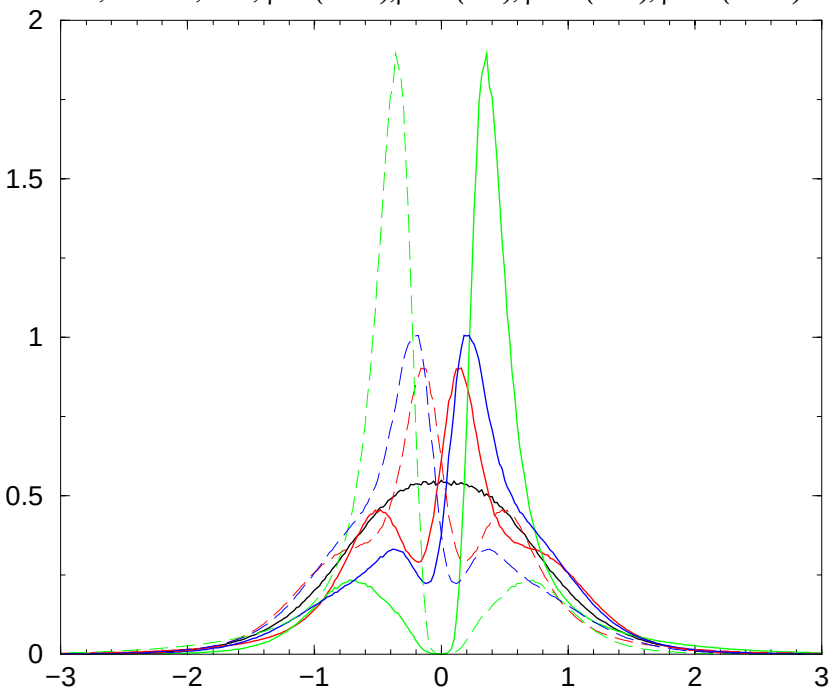
Phase Diagram (2x2)

t=−0.25, t'=0



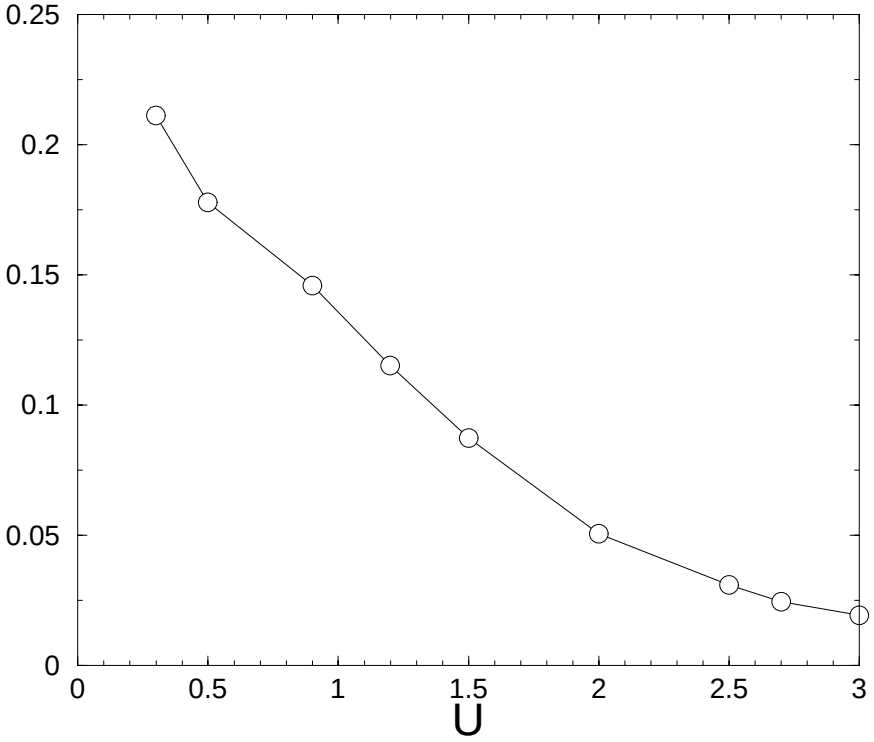
Spectral Density (2x2)

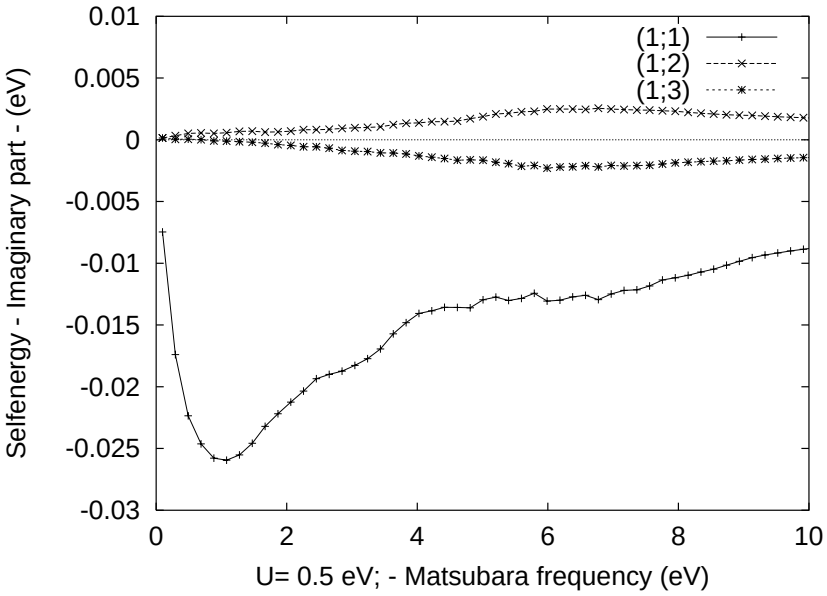
U=1, t=−0.25, t'=0; β=*5 (Black),*β=*12 (Red),* β=*15 (Blue),* β=*20 (Green)*

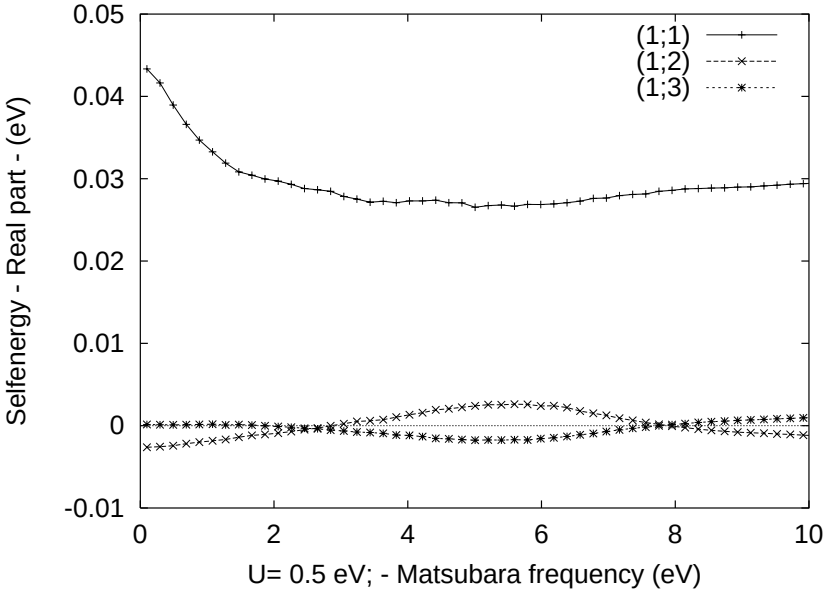


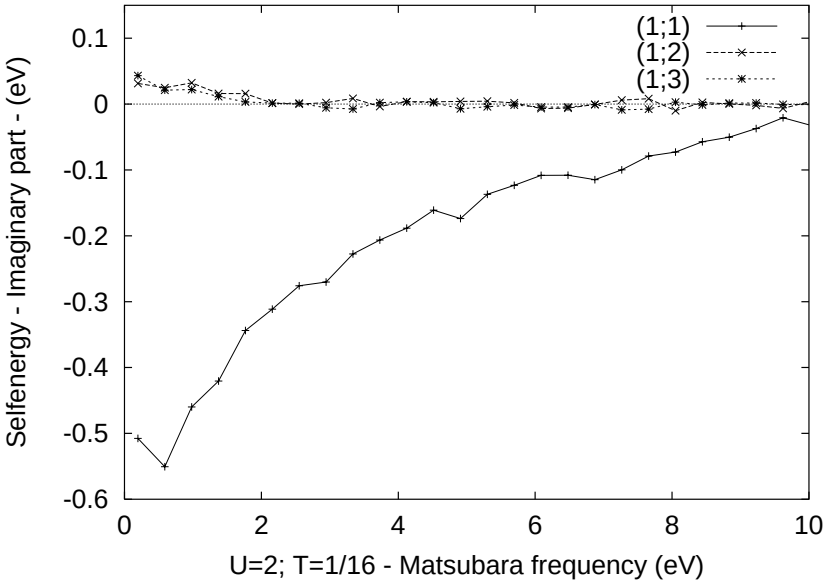
Double Occupancy (2x2)

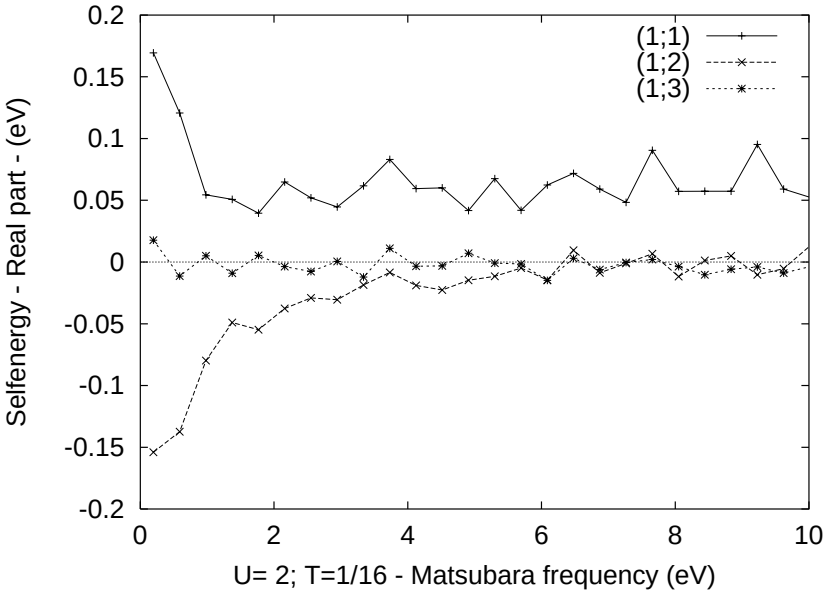
beta=5, t=−0.25, t'=0

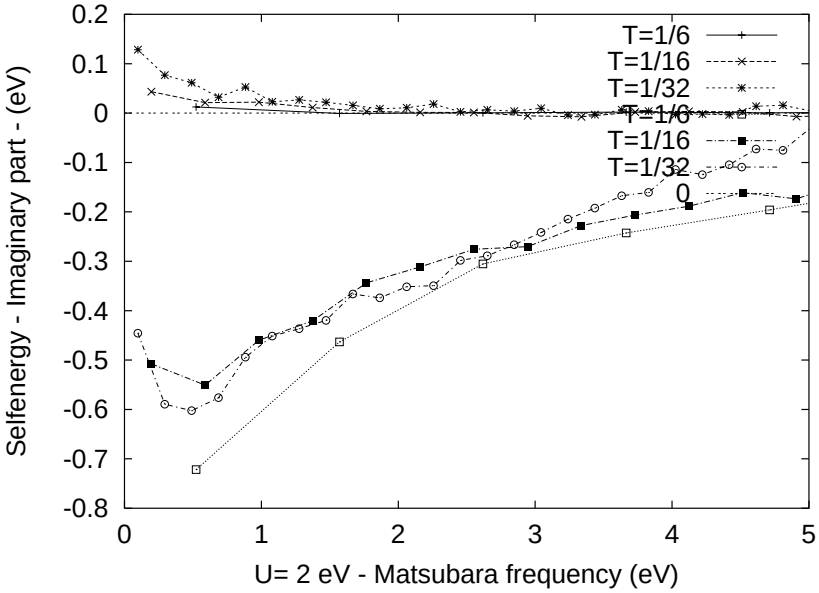


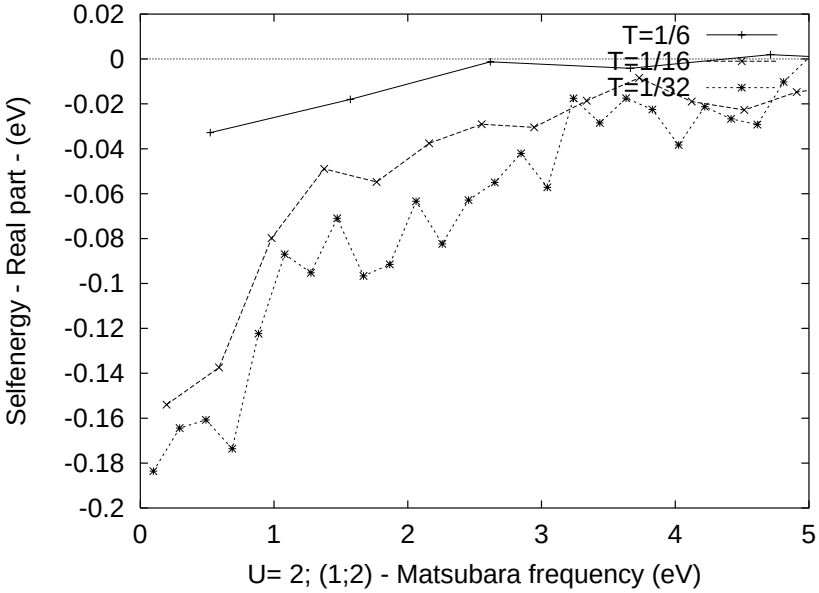

0.01
0.005
0
-0.005
-0.01
-0.015
-0.02
-0.025
-0.03
0
2
4
6
8
10
(1;1)
(1;2)
(1;3)
Selfenergy - Imaginary part - (eV)
U= 0.5 eV; - Matsubara frequency (eV)

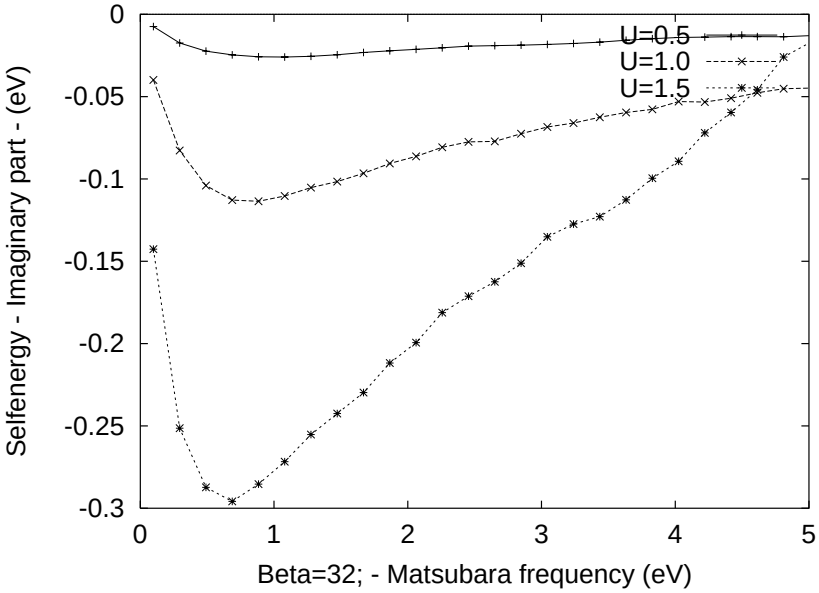

0.05
0.04
0.03
0.02
0.01
0
-0.01
0
2
4
6
8
10
(1;1)
(1;2)
(1;3)
Selfenergy - Real part - (eV)
U= 0.5 eV; - Matsubara frequency (eV)

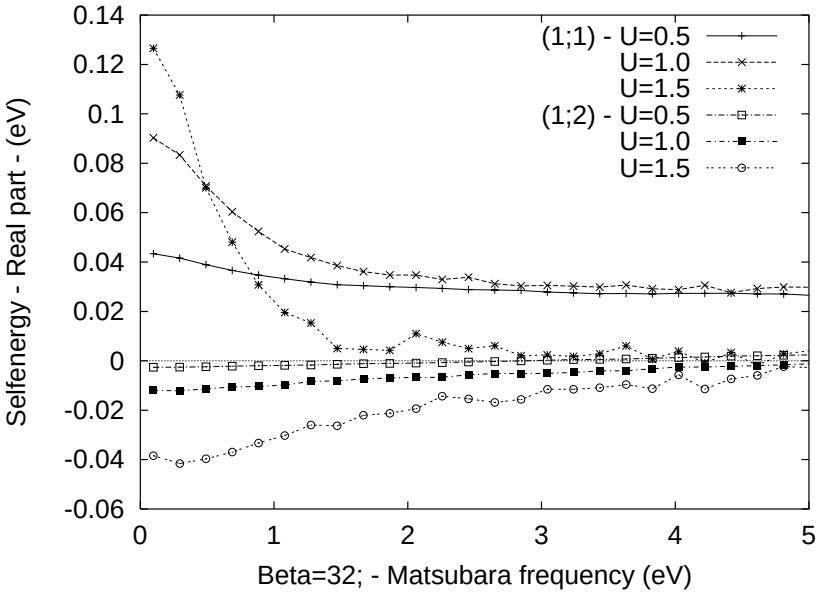

(1;1)
(1;2)
(1;3)
Selfenergy - Imaginary part - (eV)
U=2; T=1/16 - Matsubara frequency (eV)
0.1
0
-0.1
-0.2
-0.3
-0.4
-0.5
-0.6
0
2
4
6
8
10

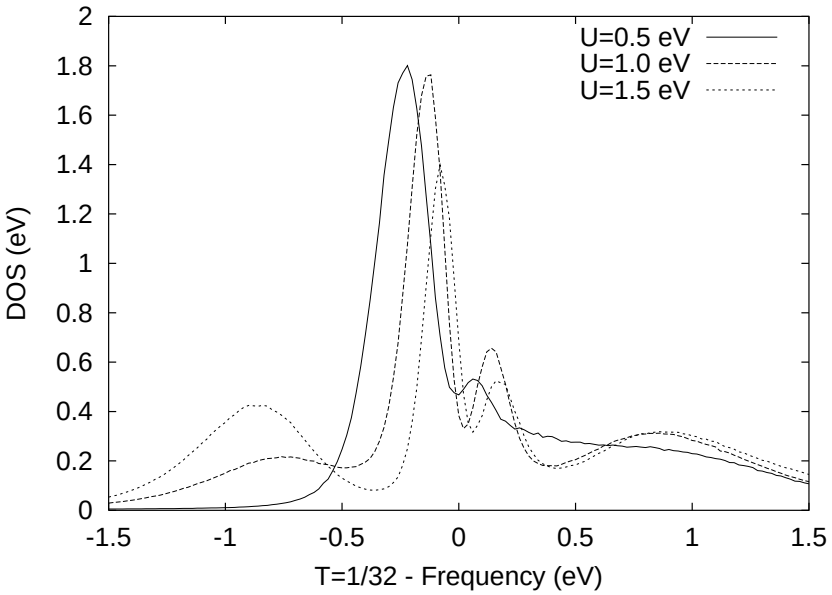

(1;1)
(1;2)
(1;3)
Selfenergy - Real part - (eV)
U= 2; T=1/16 - Matsubara frequency (eV)
0.2
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
-0.2
0
2
4
6
8
10


Selfenergy - Imaginary part - (eV)
U= 2 eV - Matsubara frequency (eV)
T=1/6
T=1/16
T=1/32
T=1/6
T=1/16
T=1/32
0


Selfenergy - Real part - (eV)
U= 2; (1;2) - Matsubara frequency (eV)
T=1/6
T=1/16
T=1/32


Selfenergy - Imaginary part - (eV)
Beta=32; - Matsubara frequency (eV)
U=0.5
U=1.0
U=1.5
0
-0.05
-0.1
-0.15
-0.2
-0.25
-0.3
0
1
2
3
4
5


Selfenergy - Real part - (eV)
Beta=32; - Matsubara frequency (eV)
(1;1) - U=0.5
U=1.0
U=1.5
(1;2) - U=0.5
U=1.0
U=1.5
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
-0.02
-0.04
-0.06
0
1
2
3
4
5



Spectral function $A(k, \omega)$ and density of states $\rho(\omega)$ evaluated with the maximum entropy algorithm for analytic continuation of data with statistical error.

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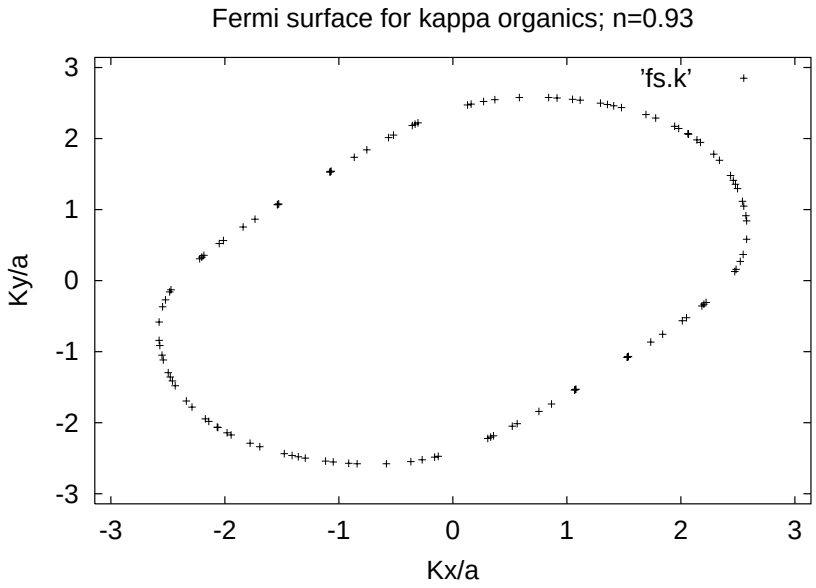
High temperature limit ($T \sim U$):

DMFT is valid $\rightarrow$ we have verified that the off-diagonal elements of the cluster selfenergy are zero and the resulting lattice selfenergy is wave-vector independent.

Low temperature limit ($T < t^2/U$):

off-diagonal selfenergies are finite and the lattice selfenergy is wave-vector dependent: C-DMFT is able to capture short-range correlations (such as AFM correlations) and the wave-vector dependence of the band structure and Fermi surface, going beyond DMFT.

Mott transition in 2D k-organics



Tight-binding dispersion for 2D-κ-organics

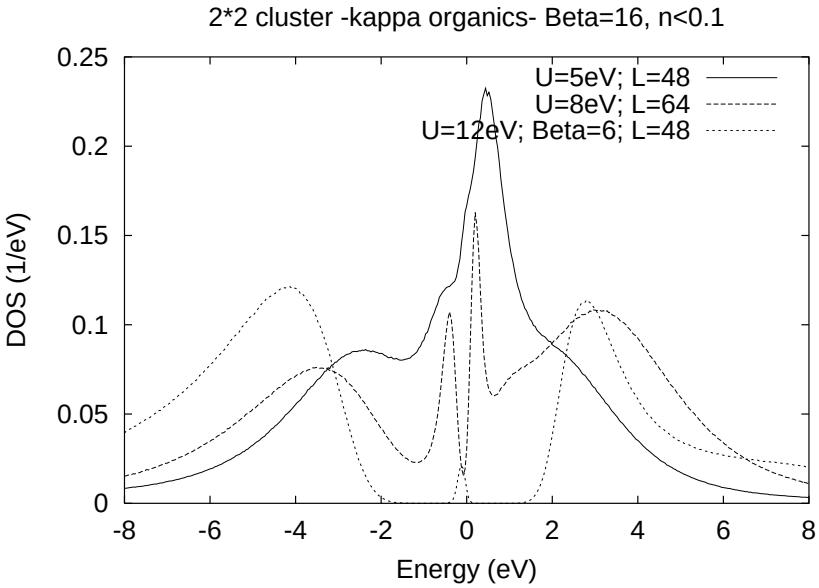
- K. Kuroki and H. Aoki, Phys. Rev. B **60**, 3060 (1999).

$$\xi(k) = -2t(\cos k_x + \cos k_y) + \qquad (13)$$
$$2t'_1 \cos(k_x + k_y) + 2t'_2 \cos(k_x - k_y) - \mu$$

The next-nearest-neighbor hopping is strongly anisotropic.

Typical values here considered:

$t = 1\text{eV}$, $t'_1 = 0.7t$, $t'_2 = -0.11t$
$2 * 2$ cluster to include AFM correlations


2*2 cluster -kappa organics- Beta=16, n<0.1
U=5eV; L=48
U=8eV; L=64
U=12eV; Beta=6; L=48
DOS (1/eV)
Energy (eV)
0.25
0.2
0.15
0.1
0.05
0
-8
-6
-4
-2
0
2
4
6
8

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Conclusions

- $2 * 2$ sites cluster.
- AFM and Mott transition in cuprates: phase diagram.
- Wave-vector dependence in the self-energy.
- DOS and Mott transition in κ-organics.

DMFT has produced a wealth of information in problems where the physics is local. **Cluster methods** promise to be equally fruitful in more complex problems where **correlations between more sites and orbitals** need to be taken into account. All the techniques which have been used for the solution of the single site DMFT are applicable to this cluster extension.

A1. Connection to impurity models

As in single site DMFT, it is very convenient to view the cluster action as arising from a Hamiltonian,

$$\begin{aligned} H_{imp} &= \sum_{\rho\varsigma} \widehat{E}_{\rho\varsigma} c^+_\rho c_\varsigma + \sum_{\mu\nu\rho\varsigma} \Gamma_{\mu\nu\rho\varsigma} c^+_\mu c^+_\nu c_\rho c_\varsigma \\ &+ \sum_{k\lambda} \epsilon_{k\lambda} a^+_{k\lambda} a_{k\lambda} + \sum_{k\lambda,\mu} \left(V_{k\lambda,\mu} a^+_{k\lambda} c_\mu + h.c. \right). \end{aligned} \quad (14)$$

$\epsilon_{k\lambda}$ is the dispersion of the auxiliary band,
$V_{k\lambda,\mu}$ are the hybridization matrix elements describing the effect of the medium on the impurity.
When the band degrees of freedom are integrated out, the effect of the medium is parameterized by a

hybridization function

$$\Delta_{\mu\nu}(i\omega_n)[\epsilon_{k\lambda}, V_{k\lambda}] = \sum_{k\lambda} \frac{V^*_{k\lambda,\mu} V_{k\lambda,\nu}}{i\omega_n - \epsilon_{k\lambda}}. \quad (15)$$

The hybridization function is related to the Weiss field function by expanding Eq. 9 in high frequencies:

$$\widehat{G}_0^{-1}(i\omega_n) = i\omega_n \bar{O} - \widehat{E} - \widehat{\Delta}(i\omega_n) \quad (16)$$

$\bar{O} = \left[\Sigma_k \widehat{O}_k^{-1}\right]^{-1}$ is the overlap matrix indicating that the impurity model has been written in a non-orthogonal local basis.

A2. Other examples of C-DMFT approach

a) Multiorbital DMFT in a non-orthogonal basis: Another important special case of our general construction is the implementation of single-site DMFT in a non-orthogonal basis. In this case the supercell is a single site, but the wave functions defining the cluster operators are chosen so that they are very localized in real space.
In fact, an implementation of this method, has resulted in new advances in the theory of Plutonium. Here the flexibility in the choice of basis is crucial for the success of the DMFT program.

b) Partial localized bases: This method would allow its formulation in terms of wave functions which are partially localized in real and momentum space such as wavelet functions. This flexibility is most appealing for treating problems such as the Mott transition where both the particle-like and the wave-like aspect of the electron need to be taken into account requiring a simultaneous consideration of real and momentum space.

A3. C-DMFT *vs* DCA

Cluster defined in real space and

the self energy matrices could be taken to be cyclic in the cluster indices so that the matrix equations could be diagonalized in a cluster momentum basis,

Eq. (9) for C-DMFT would reduce to the DCA equation.

However, in the DMFT construction, the clusters have free and not periodic boundary conditions, and we treat a more complicated problem requiring additional matrix inversions. A comparison can be found in
G. Biroli and G. Kotliar, Phys. Rev. B **65**, 155112 (2002).

References on DCA

• C. Huscroft *et al.*, cond-mat/9910226;

• H. Hettler, M. Mukherjee, M. Jarrell and H. R. Krishnamurthy, cond-mat/9903273;

• T. Maier, M. Jarrell, T. Pruschke, J. Keller, Eur. Phys. J. B **13**, 613 (2000);

• M. H. Hettler *et al.*, Phys, Rev. B **58**, R7475 (1998).