Introduction to Cluster DMFT methods

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Outline

1. Why? Motivations for cluster extensions of DMFT.
3. A selection of a few results.
General references for Cluster DMFT

- **DMFT (in particular section IX).**

- **Cluster DMFT (methods, results).**

- **Electronic structure calculations with DMFT (Cf cluster section IIB)**
Reminder: Mott transition

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

\[ H = - \sum_{\langle ij \rangle, \sigma=\uparrow, \downarrow} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U n_{i\uparrow} n_{i\downarrow}, \quad n_{i\sigma} \equiv c_{i\sigma}^{\dagger} c_{i\sigma} \]

- An intermediate coupling problem

How is the metal destroyed close to a Mott transition?

\( \delta = 1 - \langle n^{\uparrow} + n^{\downarrow} \rangle \)
Reminder : DMFT (I)

- Baym-Kadanoff functional of the Green function $G_{ij}$

$$\Gamma_{BK}[G_{ij}] = \text{Tr} \ln G_{ij} - \text{Tr}(g_{0ij}^{-1}G_{ij}) + \Phi_{BKLW}[G_{ij}]$$

$$G_{ij}(t) \equiv -\langle T c_i(t)c_j^\dagger(0) \rangle \quad \Sigma_{ij} = \frac{\delta\Phi_{BKLW}}{\delta G_{ij}}$$

$g_{0ij}^{-1}$: Free Green function


$$\Phi_{BKLW}[G_{ij}] \approx \phi_{AIM}(G_{ii})$$

- Exact in large dimension (Metzner-Vollhardt, 1989)
Reminder : DMFT (II)

- Self consistent Anderson impurity formulation *(Kotliar-Georges 1992)*
  
  =
  
  a method to solve the local approximation on $\Phi$

**Weiss**

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

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

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

$$m = \tanh(\beta h_{\text{eff}})$$

$$h_{\text{eff}} = z J m$$

**DMFT**

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

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

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

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

$$G_0^{-1}(i\omega_n) = \left( \sum_k \frac{1}{i\omega_n + \mu - t(k) - \Sigma(i\omega_n)} \right)^{-1} + \Sigma(i\omega_n)$$
Reminder: DMFT (III)

• Lattice quantities versus impurity quantities.

\[ G_{\text{latt}}(k, \omega) = \frac{1}{\omega + \mu - \epsilon_k - \Sigma_{\text{latt}}(k, \omega)} \]

\[ \Sigma_{\text{latt}}(k, \omega) = \Sigma(\omega) \equiv G_0^{-1} - G_c^{-1} \]

• In DMFT, \( \Sigma_{\text{latt}} \) is independent of \( k \).

• Consequences:
  • Effective mass and \( Z \) are linked \( Z = \frac{m}{m^*} \)
  • Finite temperature lifetime, \( Z \) are constant along the FS.
When is single-site DMFT not sufficient?
Mott transition in DMFT

- Cf. D. Vollhardt’s lecture. Compares nicely to some experiments.

Schematic DMFT phase diagram (with frustration)

Valid beyond DMFT? e.g. Paramagnetic insulator

PRL 91, 016401 (2003)
High temperature superconductors

- A family of copper oxides: \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \), \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta} \), with 2d Cu-O planes
High Tc cuprates are doped Mott Insulators

• A generic phase diagram, with 5 regions:

AF Mott insulator

No FL strange metal

AF order

AF

PG

SC

FL

Tc

under doped

over doped

A Mean Field picture of cuprates based on DMFT?
Superconducting phase

- d-wave gap (with nodes)

\[ \Delta(k) \propto \Delta_0 (\cos(k_x) - \cos(k_y)) + \Delta'_0 (\cos(2k_x) - \cos(2k_y)) + \ldots \]

![Graph showing the d-wave gap](image)

**Antinodal direction**

**Nodal direction**

**ARPES**

Ding et al, 1996
One site is not enough!

- d-wave superconductivity: need 4 sites cluster
- 1 site: a trivial representation of the lattice group
- Same would be true for a (spin) Peierls phase. Cf. Lecture by S. Biermann on VO$_2$

Clusters fix this problem (e.g. allowing d-SC order)
Pseudo-gap region

- Fermi “arcs” (ARPES)
  - Fermi liquid below and above coherence scale
  - Variations of along the Fermi surface of $Z, m^*, T_{coh}$

\[ Z, m^*, T_{coh} \]

\[ T \]

\[ M \]

\[ ky \]

\[ 0 \]

\[ kx \]

\[ \pi \]

\[ \text{Bi2212 : Kanigel et al. 2,447 (2006)} \]

\[ \text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2 \]

\[ A(k, \omega = 0^+) \]

\[ T = 110K \quad T_c = 70K \]

\[ k_z (\pi, \pi) \]

\[ k_z (0,0) \quad x = 0.05 \]

\[ x = 0.10 \]

\[ \text{Shen et al. Science 307, 901 (2005)} \]
Why a Dynamical Mean Field?

- Fermi liquid with low coherence scale: \( \epsilon_F^* = ZD \)
- Coherent and incoherent part
- Transfer of spectral weight from low to high \( \omega \)
- Beyond a low energy quasi-particle description (slave bosons)
- Price: solve a quantum impurity model.

Hubbard model, DMFT, (IPT), \( T=0, \delta=0 \)

\[
\rho(\omega) \equiv -\frac{1}{\pi} \text{Im} G(\omega)
\]

\( U/D = 1 \)
\( U/D = 2 \)
\( U/D = 2.5 \)
\( U/D = 3 \)
\( U/D = 4 \)

Metal
Mott insulator
Hubbard band (incoherent)
QP peak (coherent)
• \( T > T_{coh} \) : the Kondo peak “melts” \( \rightarrow \) bad metal.

• DMFT can describe a metal with a low coherence temperature, and above this coherence temperature.
Local self-energy is not enough!

- In DMFT: no $k$-dependence of the self-energy.
- Finite temperature lifetime, $Z$ are constant along the FS.
- Effective mass $m^*$ has to diverge when $Z \rightarrow 0$ \[ Z = \frac{m}{m^*} \]

Clusters reintroduce some $k$-dependence in $\Sigma$

*Shen et al. Science 307, 901 (2005)*
Summary of motivations for cluster DMFT

- Describe orders that single-site DMFT can not handle (e.g. d-SC)
- Some k-dependence of the self-energy : variations of Z, effective mass, lifetime along the Fermi surface.
- Non trivial paramagnetic insulators (frustrated magnets ?)
- Keep short range correlations (e.g. AF fluctuations).
- Effect of J in the paramagnet not in DMFT
e.g. cut divergence of the effective mass
(See slave-bosons or large N, e.g. G. Kotliar, Les Houches 1991).
- Systematic corrections beyond mean field for Mott transition.
Clusters : an interpolation between mean field and d=2,3
Outline

1. Motivations for cluster extensions of DMFT.
2. Introduction to cluster methods.
3. A few results...
Cluster extensions of DMFT

- **Principle**: a finite number of sites in a self consistent bath.
  - *local quantum fluctuations* → *short range quantum fluctuations*

- Interpolate between DMFT and finite dimensions
- Finite size systems BUT with “boundary conditions” G0.
- **Many choices**:
  - Type of clusters (e.g. shape, size)
  - Self-consistency condition: \( G_0(i\omega_n) = \mathcal{F}_{\text{lattice}}[G_c](i\omega_n) \)
  - How to approximate lattice quantities from cluster quantities?

**Cluster DMFT is not unique**
How to build cluster extensions of DMFT?

• **Strategy**: Higher approximation on $\Phi$ than DMFT

\[ \Phi \approx \phi_{AIM}(G_{ii}) \]

• $\Phi$-derivability $\Rightarrow$ conservative approximation (Baym-Kadanoff)
  
  In particular, Luttinger Theorem. (Cf. M. Katsnelson’s lecture).

• **Two of the main difficulties**:
  
  • Find impurity models to solve the approximation on $\Phi$.
  
  • Do not break causality!
First attempt: Nested Scheme


- Approximate Luttinger Ward functional by:

\[ \Phi = \sum_i \tilde{\phi}_1(G_{ii}) + \sum_{<ij>} \tilde{\phi}_2(G_{ii}, G_{jj}, G_{ij}) + \cdots \]

- Apply it to a 1 site and a 2 site problem:

\[
\begin{align*}
\phi_{1\text{site}}(G_{ii}) &= \tilde{\phi}_1(G_{ii}) \\
\phi_{2\text{sites}}(G_{ii}, G_{jj}, G_{ij}) &= \tilde{\phi}_2(G_{ii}, G_{jj}, G_{ij}) + \tilde{\phi}_1(G_{ii}) + \tilde{\phi}_1(G_{jj})
\end{align*}
\]

- Introducing z, the connectivity of the lattice:

\[ \Phi_{\text{Nested}} \approx (1 - z) \sum_i \phi_{1\text{site}}(G_{ii}) + \sum_{<ij>} \phi_{2\text{sites}}(G_{ii}, G_{jj}, G_{ij}) \]

- Leads to Bethe-Kikuchi method in the classical limit

BUT...
Causality problem!

- **Causality** $= \text{Im } \Sigma < 0$ (definite negative matrix)
- **Strong Causality property**: guarantee that $\text{Im } \Sigma < 0$ for any bath $G_0$
  Hence there will not be any causality violation at any step in the DMFT iterative loop.
- Quantum impurity problem is causal by construction: the problem lies in the self-consistency.
- It is not obvious to have a causal scheme: **Nested schemes lead to causality violations** (Ingersent; Kotliar, Georges)
- **Origin of the causality problem**:
  See also A. Fuhrmann, S. Okamoto, H. Monien, and A. J. Millis PRB 75, 205118 (2007)
- So let’s try something else!
C-DMFT
(G. Kotliar et al. PRL 87 186401 2001)

• DMFT on a superlattice. Similar to a multiorbital model.

Superlattice

Cluster site labeling

1 ≤ μ, ν ≤ 4

• R, R′: position of the cluster.
  μ, ν= cluster site labels.

\[ \Phi_{C\text{-DMFT}}(G) = \sum_{R} \Phi_{4\text{sites}}(G_{μ,R;ν,R} | G_{ρ,R;λR′} = 0) \]
C-DMFT equations

- 4 Anderson impurities coupled to an effective bath

\[ S_{\text{eff}} = - \int \int_{0}^{\beta} d\tau d\tau' c_{\mu}^\dagger(\tau)G_{0,\mu\nu}^{-1}(\tau, \tau')c_{\nu}(\tau') + \int_{0}^{\beta} d\tau U(n_{i\uparrow}n_{i\downarrow})(\tau) \]

\[ G_{c\mu\nu}(\tau) = -\langle T c_{\mu}(\tau)c_{\nu}^\dagger(0) \rangle_{S_{\text{eff}}} \]

\[ \Sigma_{c} = G_{0}^{-1} \quad - G_{c}^{-1} \]

\[ G_{0}^{-1}(i\omega_n) = \left[ \sum_{K \in \text{R.B.Z.}}' \left( i\omega_n + \mu - \hat{t}(K) - \Sigma_{c}(i\omega_n) \right)^{-1} \right]^{-1} + \Sigma_{c}(i\omega_n) \]
DCA

• Cluster method in k-space: $\Sigma$ piecewise constant on B.Z.

• Example for 2x2 cluster on square lattice.

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

Cluster momenta $k_c$

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

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

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

• Same multiple impurity problem than in C-DMFT.

\[ S_{\text{eff}} = - \int \int_{0}^{\beta} d\tau d\tau' c_{\mu}^{\dagger}(\tau) G_{0,\mu\nu}^{-1}(\tau, \tau') c_{\nu}(\tau') + \int_{0}^{\beta} d\tau U n_{\mu \downarrow} n_{\mu \uparrow}(\tau) \]

\[ G_{c\mu\nu}(\tau) = - \langle T c_{\mu}(\tau)c_{\nu}^{\dagger}(0) \rangle_{S_{\text{eff}}} \]

\[ \Sigma_c = G_0^{-1} - G_c^{-1} \]

• \( G, \Sigma \) cyclic on the cluster

• Cluster translation invariance.

• Translation invariance not broken (k-space)

\[ G_0^{-1}(k_c, i\omega_n) = \left( \sum_{\tilde{k}} \frac{1}{i\omega_n + \mu - t(\tilde{k}) - \Sigma(k_c, i\omega_n)} \right)^{-1} + \Sigma_c(k_c, i\omega_n) \]

\[ T. \text{Maier et al, Rev. Mod. Phys. 77, 1027 (2005)} \]
DCA in real space


• Similar self-consistency as in CDMFT.
  Change the hopping function.

\[
S_{\text{eff}} = - \int \int_0^\beta d\tau d\tau' c_\mu^\dagger(\tau) G_{0,\mu\nu}^{-1}(\tau, \tau') c_\nu(\tau') + \int_0^\beta d\tau U n_{\mu \downarrow} n_{\mu \uparrow}(\tau)
\]

\[
G_{c\mu\nu}(\tau) = - \langle T c_\mu(\tau) c_\nu^\dagger(0) \rangle_{S_{\text{eff}}}
\]

\[
\Sigma_c = G_0^{-1} - G_c^{-1}
\]

\[
G_0^{-1}(i\omega_n) = \left[ \sum_{K \in R.B.Z.} \left( i\omega_n + \mu - \hat{t}_{\text{DCA}}(K) - \Sigma_c(i\omega_n) \right)^{-1} \right]^{-1} + \Sigma_c(i\omega_n)
\]

\[
t_{\alpha\beta}^{\text{DCA}}(K) = \sum_{k_c} e^{i k_c (\alpha - \beta)} t(K + k_c)
\]

• It is “easy” to switch method.
Evaluation of lattice quantities.

- DCA: need to interpolate between the value at $K_c$.
- CDMFT: more severe, since it breaks translation invariance. Need to restore it by re-periodization.

- Which quantity should we periodize (or interpolate)?
  - Most irreducible ($\Sigma$ rather than $G$!), most local.
  - NB: breaks $\Phi$-derivability.
C-DMFT : $\Sigma$-Periodization

- The original proposal (G. Kotliar et al. PRL 87 186401 2001)
- Example : 2x2 cluster on a square lattice

$$\Sigma^{Lattice}(k) = \frac{1}{4} \sum_{i=1}^{4} \Sigma^{Cluster}_{ii} + \frac{1}{2} \left[ (\Sigma^{Cluster}_{12} + \Sigma^{Cluster}_{34}) \cos(k_x) + (\Sigma^{Cluster}_{24} + \Sigma^{Cluster}_{13}) \cos(k_y) + \Sigma^{Cluster}_{14} \cos(k_x + k_y) + \Sigma^{Cluster}_{23} \cos(k_x - k_y) \right]$$

Cluster quantities $\Leftrightarrow$ harmonics on the lattice

Size of cluster = resolution in $k$ space
C-DMFT : $\Sigma$-Periodization (2)

- $\Sigma$- periodization generates spurious mid-gap states in Mott insulator
  \textit{(B. Kyung, A.M. Tremblay et al)}

- In fact $\Sigma$ can be singular in an insulator.
  e.g. Atomic Green function (1 Hubbard site, ph symmetric)

\[
G(i \omega_n)_{\text{at}} = \frac{1/2}{i \omega_n + U/2} + \frac{1/2}{i \omega_n - U/2}.
\]

\[
\Sigma(i \omega_n) \sim \frac{U^2}{i \omega_n}
\]

- $\Sigma$ is irreducible and simple in a perturbative expansion in the interaction.

- What is the analogous of $\Sigma$ in an expansion in $t$?
C-DMFT : M-Periodization

- Definition of the irreducible cumulant:
  *Sum of all diagrams 1-particle irreducible in an expansion around the atomic limit (i.e. in \( t \), not in \( U \)).*

- For a presentation of this diagrammatics: *(W. Metzner, PRB 43, 8549 1991)*

- Relation with the self-energy:
  \[
  M^{-1}(k, \omega) = \omega + \mu - \Sigma(k, \omega)
  \]

- The Green function is:
  \[
  G(k, \omega) = \left( t(k) - M^{-1}(k, \omega) \right)^{-1}
  \]
C-DMFT : M-Periodization (2)

(T. Stanescu, G. Kotliar PRB 74, 125110, 2006)

- In DMFT, $\Sigma$ and $M$ are local.
- Hubbard, 1/2 filled, 2x2 CDMFT, U/D = 2, ED solver, cluster quantities

$M$ is more localized than $\Sigma$. 

![Diagram showing comparison of $M$ and $\Sigma$](image-url)
C-DMFT : M-Periodization (3)

(T. Stanescu, G. Kotliar PRB 74, 125110, 2006)

⇒ Periodize the irreducible cumulant

• Same formula as for the self-energy:

\[
M^{\text{Lattice}}(k) = \frac{1}{4} \sum_{i=1}^{4} M_{ii}^{\text{Cluster}} + \frac{1}{2} \left[ (M_{12}^{\text{Cluster}} + M_{34}^{\text{Cluster}}) \cos(k_x) + (M_{24}^{\text{Cluster}} + M_{13}^{\text{Cluster}}) \cos(k_y) + M_{14}^{\text{Cluster}} \cos(k_x + k_y) + M_{23}^{\text{Cluster}} \cos(k_x - k_y) \right]
\]

• A non-linear relation ⇒ \( \Sigma_{\text{lattice}}(k, 0) \) can have singularity!

Some CDMFT results rely on using this periodization
Many cluster methods!

- Nested Schemes, DCA (Reciprocal space), CDMFT : Real space
- Self-energy functional \( (M. Potthoff \text{ et al. See e.g. condmat 0511729}) \)
- Extended cluster DMFT (Extended DMFT + cluster) \( (\text{see e.g. K. Haule}) \)
- Cluster perturbation theory : CPT, VCPT (not self-consistent) \( \text{A.M. Tremblay, D. Sénéchal.} \)
- PCDMFT : use \( \Sigma(k,\omega) \) in the self-consistency \( \text{(G. Biroli et al. PRB, 69,205108 (2004); see also A. Lichtenstein and M. Katsnelson, PRB 62, R9283 (2000))} \)
- For a review, see : \( T. Maier \text{ et al, Rev. Mod. Phys. 77,1027 (2005)} \)
Can we test cluster methods?
Test the cluster method in one dimension

- One dimensional physics (*Cf Book by T. Giamarchi, Oxford University Press*).
- Low energy (large distance): Luttinger liquid physics, spin-charge separation.
- Some correlated models (e.g. Hubbard model) can be solved analytically (by Bethe Ansatz) for the thermodynamics.
- The dynamical correlations can be computed with DMRG.
- Let us solve the 1d Hubbard model with 1 and 2 site CDMFT and compare to the exact result.
- Computation of short range physics, thermodynamics.
- DMFT can NOT capture Luttinger liquid large distance physics.
Test the cluster method in one dimension (2)

- Occupation vs chemical potential (2 sites cluster)
  

BA = Bethe Ansatz
Test the cluster method in one dimension (3)

- Dynamical quantities.

Comparison to DMRG (in Matsubara, with Hallberg's algorithm)

How to solve (cluster) DMFT equations?
Impurity solvers

\[ S_{\text{eff}} = -\int_{\beta}^{0} d\tau d\tau' c^{\dagger}_{\mu}(\tau) G_{0,\mu\nu}^{-1}(\tau, \tau') c_{\nu}(\tau') + \int_{0}^{\beta} d\tau U(n_{i\uparrow} n_{i\downarrow})(\tau) \]

\[ G_{c\mu\nu}(\tau) = -\langle T c_{\mu}(\tau) c^{\dagger}_{\nu}(0) \rangle_{S_{\text{eff}}} \]

- Many different solvers (Cf D. Vollhardt & M. Troyer’s lectures).
  - Quantum Monte-Carlo (Hirsch-Fye, CTQMC).
    \[ P.\text{Werner et al. PRL 97, 076405 (2006)} \]
  - Exact diagonalisation (ED).
  - Renormalization group methods: NRG, DMRG.
  - Approximate methods (IPT, NCA,...)
- By far the hardest part in DMFT (will be hidden here).
- No “best” solver (T=0 or finite, real \( \omega \) or Matsubara, etc...)
Why is DMFT harder than usual impurity problems?

- Bath can have a structure at low energy ...
- ... while most analytical solvers (e.g. Bethe Ansatz, CFT) use a flat band!

Valid in universal regime \( T, \omega, T_K \ll D \)

Not sufficient to solve DMFT
Outline

1. Motivations for cluster extensions of DMFT.
2. Introduction to cluster methods.
3. A few results:
   - Cluster correction to DMFT picture of Mott transition
   - Phase diagram of Hubbard model
   - Two energy scales in the SC phase.
Is the DMFT picture of Mott transition corrected by clusters?
**U-driven Mott transition**

- Signature of Mott transition in double occupancy in 1 site DMFT. (A. Georges, W. Krauth, PRL 69, 1240 (1992))

\[ d \equiv \langle n_i^\uparrow n_i^\downarrow \rangle \]

(Kotliar et al. condmat/0003016)
• Similar result in cluster. (See also B. Kyung, AM. Tremblay, 2005)

• Frustration is essential! (hard for QMC-Hirsch-Fye)

U-driven Mott transition

DMFT

C-DMFT (2x2)

(Kotliar et al. condmat/0003016)

O. P. et al. PRL 2003

But....
Cluster corrections close to Mott transition

- Fixed $T/D = 45 > T_c$, various $U$.
- Anisotropic Hubbard model

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

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

$\text{Teff} = D/128, U=16t$

t,t' isotropic

Hubbard model
2x2 CDMFT

$\text{DMFT metal}$

$\text{Anisotropic metal}$

$n=1 : \text{Mott}$

Hole doped

Electron doped

Highly frustrated

$M. \text{Civelli, M. Capone, S. S. Kancharla, O.P and G. Kotliar} \quad \text{Phys. Rev. Lett. 95, 106402 (2005)}$
Generic features

• DMFT metal at small $U$, large doping : no cluster corrections.

• Approaching to Mott transition, cluster effects becomes more and more important.

• Observed also in other cluster methods :
  DCA (see e.g. T. Maier et al, Rev. Mod. Phys. 77, 1027 (2005)),
  CPT, VCPT (See A.M. Tremblay et al).

• .. and e.g. in Functionnal RG (W. Metzner et al.)
Phase diagram of the Hubbard model
Does the Hubbard model have d-SC?

- d-SC in 2x2 cluster


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

- 2x2 CDMFT (M. Civelli, K. Haule). \( T_c \approx \frac{t}{100} \ll T_c^{\text{DCA} \ 2x2} \)

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

All cluster methods consistently predicts d-SC, AF, with different \( T_c \)
AF, d-SC : coexistence or competition?


- Hubbard model (various $U$, ED solver).
- Qualitative difference between large and small $U$.
  - Small $U$ : coexistence between AF + d-SC
  - Higher $U$, first order transition.
Nature of the SC phase
**“Standard” simplest RVB picture**


\[
\Delta(k) \propto \Delta_0\left(\cos(k_x) - \cos(k_y)\right) \quad \text{with} \quad \Delta_0(\delta) \uparrow \quad \text{for} \quad \delta \to 0
\]

\[
\Delta_0(\delta) \propto T_c(\delta) \quad \text{unlike BCS}
\]
High-Tc SC phase

• Two energy scales in SC phase

• Raman experiments. *M. LeTacon et al., Nature Physics, 2, 537, 2006*

• See also ARPES experiments. *Tanaka., Science 314, 1910, (2006)*

• Gap at antinode (maximum) increases for $\delta \to 0$.

• Gap around node (slope) decreases for $\delta \to 0$, like $T_c$.

What does Cluster DMFT gives ?
2 gaps in high-Tc superconductors


- Solution of Hubbard model, 2x2 CDMFT, ED solver, SC phase
- Cluster quantities:

  \[ \text{Re} \Sigma_{12}^{\text{ano}}/t \]

  \[ \text{Im} G_{11}/\pi \]

- Anomalous self-energy non-monotonic in \( \delta \) and decreases at low \( \delta \)
- Gap of local \( G \) increases close to the Mott insulator.

\[ \Rightarrow 2 \text{ energy scales} \]
2 gaps in high-$T_c$ superconductors


- Analyze ARPES spectrum at (anti)node with/without anomalous $\Sigma$

![Graph A: Nodal spectrum](image)

![Graph B: Antinodal spectrum](image)

![Graph C: Anomalies at node and antinode](image)

![Graph D: Anti-nodal behavior](image)
Nodal region


\[ A(k, \omega) \simeq Z_{nod} \delta \left( \omega - \sqrt{v_{nod}^2 k_\perp^2 + v_\Delta^2 k_\parallel^2} \right) \]

QP velocity \( \perp \) to FS

\[ v_{nod} = Z_{nod} |\nabla_k \xi^0_k| \]

Anomalous velocity \( \parallel \) to FS

\[ v_\Delta = Z_{nod} |\nabla_k \Sigma^{ano}(k)| \]

Slope of the gap at the node

\[ \delta \]

\[ v_{nod}/(a_0 t) \quad v_\Delta/(a_0 t) \]
Antinodal region: decomposition of the gap

- Nor: anomalous $\Sigma = 0$.
- Tot: full gap
- Sc: contribution of anomalous $\Sigma$

$$\Delta_{sc} = \sqrt{\Delta_{tot}^2 - \Delta_{nor}^2}$$
$$\Delta_{sc}(k) \sim Z_{anod} |\Sigma_{ano}(k, 0)|$$

$$G_{k\sigma}^{-1}(\omega) = \begin{pmatrix}
\omega - \varepsilon_k - \Sigma_{\sigma}^{nor}(k, \omega) & -\Sigma_{\sigma}^{ano}(k, \omega) \\
-\Sigma_{\sigma}^{ano}(k, \omega) & \omega + \varepsilon_k + \Sigma_{\sigma}^{nor}(k, -\omega)
\end{pmatrix}$$

Cluster DMFT and ab-initio methods.

- Cluster DMFT can be mixed with e.g. LDA, like DMFT. e.g.

- Dynamical Singlets and correlation-assisted Peierls transition in VO$_2$
  (S. Biermann, A. I. Poteryaev, A. I. Lichtenstein, A. Georges, PRL 94, 026404 (2005))
  Cf Lecture by S. Biermann.

- Metal-Insulator transition in Ti$_2$O$_3$
  (A. I. Poteryaev, A. I. Lichtenstein, G. Kotliar, PRL 93, 086401 (2004))
Conclusion

• **Good:**
  • More orders than DMFT (d-SC)
  • Node/Antinode dichotomy: some (limited) k-resolution
  • DMFT based: coherent, incoherent features.

• **Limitations:**
  • Still hard to solve (large size, large U).
  • k-resolution still limited. Various different cluster methods.
  • No “large distance” physics (e.g. Luttinger in 1d).

• **Open questions:**
  • 2 impurities have richer physics (RKKY vs Kondo). QCP?
  • Low energy effective theories. Simple picture of the “mechanism”.