Cluster Dynamical Mean Field Analysis of the Mott transition

O. Parcollet

CEA-Saclay

FRANCE

“Dynamical Breakup of the Fermi Surface in a doped Mott Insulator”
M. Civelli, M. Capone, S. S. Kancharla, O.P., G. Kotliar. cond-mat/0411696

“Cluster Dynamical Mean Field Analysis of the Mott Transition”

“Cluster dynamical mean-field theories: Causality and classical limit”
Mott transition

- Metal-Insulator transition due to interactions.
- Relevant for e.g.:
  - $V_2O_3$.
  - High-Tc Cuprates are doped Mott insulators.
  - Explanation of pseudo-gap, d-SC mechanism?
- DMFT: a successful method for Mott transition.
  - Realistic calculations (in combination with band theory): e.g.
    - Pu: S. Savrasov, G. Kotliar, E. Abrahams, Nature 410, 793 (2001)
    - “Correlation-assisted Peierls transition in VO$_2$”
      S. Biermann, A. Poteryaev, A. I. Lichtenstein, A. Georges, cond-mat/0410005
- In this talk: Beyond DMFT with cluster methods
## DMFT: a self-consistent impurity problem

<table>
<thead>
<tr>
<th>Local Quantity</th>
<th>Effective problem</th>
<th>Weiss Field</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ising</td>
<td>$m = \langle S_i \rangle$</td>
<td>Ising spin in field $h_{\text{eff}}$ [ m = \tanh(\beta h_{\text{eff}}) ]</td>
</tr>
<tr>
<td>DMFT</td>
<td>Local Green function $G$</td>
<td>Quantum impurity</td>
</tr>
<tr>
<td></td>
<td>$G(t) \equiv -\langle T c_i(t) c_i^\dagger(0) \rangle$</td>
<td>$G_0 = F[G]$</td>
</tr>
</tbody>
</table>

### Hamiltonians

- **Ising**
  
  \[ H_{\text{Ising}} \equiv -J \sum_{\langle i, j \rangle} S_i S_j \]

- **Hubbard**
  
  \[ H_{\text{Hubbard}} = - \sum_{i,j,\sigma} t_{ij} c_{i \sigma}^\dagger c_{j \sigma} + U n_{i \uparrow} n_{i \downarrow} \]

---

A. Georges, G. Kotliar (1992)
Why a **dynamical** Mean Field?

- **DMFT**: a mean field on the local Green function $G(\omega)$

- DMFT describes:
  - Fermi liquid with low coherence scale $\epsilon_F^* = ZD$.
  - Coherent and incoherent part
  - Transfer of spectral weight from low to high $\omega$

$$\rho(\omega) \equiv -\frac{1}{\pi} \text{Im}G(\omega), \delta = 0$$

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

**DMFT goes beyond a low energy quasi-particle description.**
Mott transition in DMFT: Phase diagram

Frustrated Hubbard model at half filling: \( \delta = 0 \), paramagnet

DMFT, a starting point for some SCES?

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

Cluster DMFT (1)

- Missing in DMFT . . .
  - Various orders: e.g. d-SC, DDW, stripes
  - $k$ dependence of $\Sigma(k, \omega) \implies Z \sim \frac{m}{m^*}$.
  - Variations of $Z, m^*, \tau(T), T_{coh}$ along the Fermi surface.
  - Non magnetic insulators (frustrated magnets?)
  - Non-local interactions. Short range AF correlations.
- . . . but present in cluster methods

\[ \text{short range spatial quantum fluctuations} \]

DMFT

Cluster DMFT
Cluster DMFT (2)

- Interpolate between DMFT and 2d/3d when cluster size $\rightarrow \infty$.
- Finite size systems BUT:
  - in a bath $G_0$ (like “Boundary Conditions”)
  - in thermodynamic limit (phase transitions)
- Static (Hartree-Fock) approximation possible at longer distance.
- Choices:
  - Type, shape of clusters (e.g. (linear) size $L_c$).
  - How to compute lattice quantities from cluster quantities.
- Various cluster methods: $\neq$ parametrisations of $\Sigma(k)$
  - CDMFT (G. Kotliar, S. Savrasov, G. Pálsson, G. Biroli PRL (2001))
  - Nested Cluster Schemes, PCDMFT, Fictive impurity models, ...
In this talk

• Questions:
  • Is the DMFT picture of the Mott transition stable? (Cluster as $1/d$ corrections).
  • Existence of anisotropic FL (due to interactions)?
    $$Z(k), T_{\text{coh}}(k), (m^*/m_{\text{band}})(k)$$
  • Renormalization of the Fermi Surface?
  • Orders: AF, d-SC, ...?

• Study CDMFT, $2 \times 2$ cluster, Hubbard model on square lattice for various $U$, $t'/t$, $\delta$
  using QMC (Hirsch-Fye) and ED (exact diagonalization)

Isotropic model:

Anisotropic model:
CDMFT

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

\[ S_{\text{eff}} = - \int \int_0^\beta d\tau d\tau' c_{\mu}^+(\tau)G_{0,\mu \nu}^{-1}(\tau, \tau')c_{\nu}(\tau') + \int_0^\beta d\tau U_{\alpha \beta \gamma \delta}(0)(c_{\alpha}^+ c_{\beta}^+ c_{\gamma}^+ c_{\delta})(\tau) \]

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

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

\[ G_0^{-1}(i\omega_n) = \left[ \sum_{K \in R.B.Z.} \left( i\omega_n + \mu - \hat{t}(K) - \Sigma_c(i\omega_n) \right)^{-1} \right]^{-1} + \Sigma_c(i\omega_n) \]
CDMFT (2)

- Lattice quantities ≠ cluster quantities
- Lattice self energy is computed at the end
- Restore translation invariance on lattice (2 × 2 clusters):

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

- Cluster self-energies parameterize the \( k \) dependence.
- Prescription not unique: cumulants (T. Stanescu et al. To appear),
  periodize the Green function (B. Kyung et al. condmat/0502565, S12-7).
Mott transition in DMFT : Phase diagram

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


- Without frustration, Néel temperature $T_N$ is large.

Frustration is essential to see this Mott transition
Paramagnetic solutions of CDMFT

- In DMFT:
  Paramagnetic sol. for $t' = 0 \sim$ Paramagnetic solution for $t'/t \sim 1$

- In Cluster DMFT: different type of paramagnets
  - Paramagnet for $t' = 0$
    - Strong AF fluctuations inside the cluster.
    - Paramagnet with short range AF fluctuations at low resolution?
  - Paramagnet for $t'/t \sim 1$
    - Similar to DMFT solution
    - Can only be reached by solving a frustrated model.
    - QMC solution, but sign problem at low temperature.
    - Anisotropic model, $t'/t = 0.9$
A DMFT-like Mott transition ...

- Double occupation $d_{occ} = \sum_i \langle n_i^\uparrow n_i^\downarrow \rangle$. No AF order

---

**DMFT**

![Graph showing double occupation vs. $U$]

**CDMFT**

![Graph showing double occupation vs. $U$]

- Application: "Interactions-induced adiabatic cooling and antiferromagnetism of cold fermions in optical lattices" F. Werner, OP, A. Georges, S. Hassan, to appear


$T/D = 1/20, 1/30, 1/40, 1/44$
...with $k$-dependent self-energy

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

---

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

---

![Graph showing metal, crossover, and insulator regions](image-url)
Self-energies in imaginary time

\[ U = 2, 2.1, 2.2, 2.25, 2.29, 2.31, 2.34, 2.43, 2.5 \quad T/D = 1/44. \]
Hot and Cold regions

- $A(k, \omega = 0)$ in the metallic region: $U/D = 2.0, 2.25$
Quasi-particle residue and effective mass

Close to the Mott transition, \( Z \neq \frac{m}{m^*} \)

![Graph showing the relationship between \((m/m^*)Z\) and \(U\) for different temperatures.](image)
Fermi liquid at $T = 0$?

- Conjecture: for $T \to 0$, $\text{Im} \Sigma_{14} \to 0$
- $Z_{(\pi,\pi)} \neq Z_{(0,\pi)}$
  $k$-dependence in $Z$ due to the proximity of the Mott insulator.
- QMC inefficient for low $T$ and high $U$.
  $\implies$ Exact Diagonalization method.
Exact diagonalization

- Hamiltonian representation of the bath $G_0$ with free electrons.
- Hoppings and energies of the Bath determined self-consistently.
- For $2 \times 2$ clusters: 8 sites in the bath

Not limited by frustration or large $U$.
- “$T = 0$” calculation but at finite EFFECTIVE temperature $T_{\text{eff}}$.
- Size of the bath is small.
Exact diagonalization : Comparison with QMC

\( t' = 0, \delta = 0.1, U = 8t, \beta D = 50, D = 4t = 1, \) paramagnet.
Hot and cold regions

\[ A(k, \omega = 0^+) \]. \[ T_{\text{eff}} = D/128, U = 16t, \] isotropic model. Condmat/0411696

- \[ t' = -0.3t \]
  \[ n = 0.73, 0.89, 0.96 \]

- \[ t' = +0.3t \]
  \[ n = 0.70, 0.90, 0.95 \]

- \[ t' = +0.9t \]
  \[ n = 0.69, 0.92, 0.96 \]
Renormalization of the Fermi Surface

- \( t_{\text{eff}}(k) = t(k) - \text{Re} \Sigma_{\text{lattice}}(k, 0) \)
- Fermi Surface is renormalized by interactions close to the Mott transition.
- Details are model dependent.

Bare \( t, t' \) can not be extracted simply from ARPES data
Fermi liquid or Non Fermi Liquid at $T = 0$?

- Pseudo-gap at $T = 0$?  
  B. Kyung et al., condmat/0502565, S12-7

- $\omega$-resolution problem in ED: $\Delta \omega \approx 0.1t \implies T_{\text{eff}} \sim D/40 \sim T_{\text{Mott}}$.

- Solution at $T = 0$ is still an open question
d-SC in CDMFT

- d-SC order present at $T = 0$ (M. Capone and S. S. Kancharla, private communication)
Conclusion

- Cluster methods add $k$ resolution to DMFT.
- Mott transition in frustrated systems in CDMFT:
  - DMFT-like Mott transition ...
  - ... with Hot-Cold regions due to the proximity of Mott transition.
- Renormalization of the Fermi surface.
- d-SC phase at $T = 0$.

Open questions

- Complete solution of $2 \times 2$ clusters ($T = 0$) ?
- Fermi liquid or Non Fermi liquid ?
- Nature of the Mott insulator ?