Mott Physics in Superconductors

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S. Okamoto, B. Kyung, M. Civelli

MIT, 3 October, 2011
How to make a metal

Courtesy, S. Julian
Not always

NiO, Boer and Verway

Peierls, 1937

Mott, 1949
« Conventional » Mott transition

Understood from Hubbard model and dynamical mean field theory

Figure: McWhan, PRB 1970; Limelette, Science 2003
Hubbard model

\[ H = - \sum_{<ij>\sigma} t_{i,j} \left( c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Effective model, Heisenberg: \[ J = 4t^2 \frac{1}{U} \]
Bare Mott critical point in organics

Phase diagram ($X=\text{Cu}[\text{N(CN)}_2]\text{Cl}$)

F. Kagawa, K. Miyagawa, + K. Kanoda
Perspective
Normal state of high-temperature superconductors

Armitage, Fournier, Greene, RMP (2009)

- Competing order
  - Current loops: Varma, PRB 81, 064515 (2010)
  - Stripes or nematic: Kivelson et al. RMP 75 1201(2003); J.C.Davis
  - d-density wave: Chakravarty, Nayak, Phys. Rev. B 63, 094503 (2001); Affleck et al. flux phase
  - SDW: Sachdev PRB 80, 155129 (2009) ...

- Or Mott Physics?

What is under the dome?
Mott Physics away from $n = 1$
Two views (caricature)

Phillips, RMP (2010)

Why $T_c$ decreases?
What is the origin of $T^*$?
What is the strange metal?

Broken symmetry or not.
What lies beneath the dome.
Mott Physics away from $n = 1$
An alternate view (a bit of both)

G. Sordi, K. Haule, A.-M.S.T
PRL, 104, 226402 (2010)
and

Matthias Punk + Subir Sachdev (unpublished)
T. C. Ribeiro and X.-G. Wen,
Outline

• Method
• Normal state
  – First order transition
  – Widom line and pseudogap
• Superconducting state
  – Glue
Method
Mott transition and Dynamical Mean-Field Theory. The beginnings in $d = \text{infinity}$

- Compute scattering rate (self-energy) of impurity problem.
- Use that self-energy ($\omega$ dependent) for lattice.
- Project lattice on single-site and adjust bath so that single-site DOS obtained both ways be equal.

W. Metzner and D. Vollhardt, PRL (1989)
A. Georges and G. Kotliar, PRB (1992)
M. Jarrell PRB (1992)

DMFT, ($d = 3$)
2d Hubbard: Quantum cluster method

Hettler …Jarrell…Krishnamurty PRB 58 (1998)
Kotliar et al. PRL 87 (2001)
Maier, Jarrell et al., Rev. Mod. Phys. 77, 1027 (2005)
Another way to look at this (Potthoff)

\[ \Omega_t[G] = \Phi[G] - Tr[(G_{0t}^{-1} - G^{-1})G] + Tr \ln(-G) \]

\[ \frac{\delta \Phi[G]}{\delta G} = \Sigma \]

\[ \Omega_t[\Sigma] = \Phi[G] - Tr[\Sigma G] - Tr \ln(-G_{0t}^{-1} + \Sigma) \]

Still stationary (chain rule)

\[ \Omega_t[\Sigma] = F[\Sigma] - Tr \ln(-G_{0t}^{-1} + \Sigma) \]

SFT : Self-energy Functional Theory

With \( F[\Sigma] \) Legendre transform of Luttinger-Ward funct.

\[
\Omega_t[\Sigma] = F[\Sigma] + \text{Tr} \ln(-\left(G_0^{-1} - \Sigma\right)^{-1})
\]

is stationary with respect to \( \Sigma \) and equal to grand potential there.

\[
\Omega_t[\Sigma] = \Omega_{t'}[\Sigma] - \text{Tr} \ln(-\left(G_0'^{-1} - \Sigma\right)^{-1}) + \text{Tr} \ln(-\left(G_0^{-1} - \Sigma\right)^{-1}).
\]

Vary with respect to parameters of the cluster (including Weiss fields)

Variation of the self-energy, through parameters in \( H_0(t') \)

Understanding finite temperature phase from a mean-field theory down to $T = 0$

- **Fermi liquid**
  - Start from Fermi sea
  - Self-energy analytical
  - One to one correspondence of elementary excitations
  - Landau parameters

- **Mott insulator**
  - Hubbard model
  - Atomic limit
  - Self-energy singular
  - DMFT
  - How many sites in the cluster determines how low in temperature your description of the normal state is valid.
Mean-field is not a trivial problem! Many impurity solvers.

Here: continuous time QMC

P. Werner, PRL 2006
P. Werner, PRB 2007
K. Haule, PRB 2007
Solving cluster in a bath problem

- Continuous-time Quantum Monte Carlo calculations to sum all diagrams generated from expansion in powers of hybridization.


Mott insulator at finite $T$

M. Vekic and S.R. White, PRB 47, 1160 (1993)
### Interaction-induced Mott transition, $n = 1$

<table>
<thead>
<tr>
<th>Method</th>
<th>$U_{c1}$</th>
<th>$U_c$</th>
<th>$U_{c2}$</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>VCA+ED $2 \times 2 + 8b$</td>
<td>5.25</td>
<td>5.5</td>
<td>6.37</td>
<td>Balzer et al. EPL (2009)</td>
</tr>
<tr>
<td>CDMFT+CTQMC+H $2 \times 2$</td>
<td>5.3</td>
<td></td>
<td>5.7</td>
<td>Park et al. PRL (2008)</td>
</tr>
<tr>
<td>DCA+CTQMC+H $8$</td>
<td>5.7</td>
<td></td>
<td>6.4</td>
<td>Gull et al. cond-mat (2009)</td>
</tr>
<tr>
<td>DCA+CTQMC+H $4$</td>
<td>!</td>
<td>$\sim$4.2</td>
<td>!</td>
<td>Gull et al. EPL (2008)</td>
</tr>
<tr>
<td>Dual fermions</td>
<td>!</td>
<td>$\sim$6.5</td>
<td>!</td>
<td>Hafermann et al. (2008)</td>
</tr>
<tr>
<td>CDMFT+ED $2 \times 2 + 8b$ 15 parameters</td>
<td>?</td>
<td>$\sim$5.6</td>
<td>?</td>
<td>Liebsch, Merino… (2008)</td>
</tr>
<tr>
<td>CDMFT+ED $2,3,4$</td>
<td></td>
<td>$\sim$4</td>
<td></td>
<td>Zhang et al. PRB (2007)</td>
</tr>
<tr>
<td>QMC $6 \times 6$</td>
<td></td>
<td>6</td>
<td></td>
<td>Vekic et al. (1993)</td>
</tr>
</tbody>
</table>
Cuprates as doped Mott insulators
Spectral weight transfer

Meinders et al. PRB 48, 3916 (1993)
Experiment: X-Ray absorption

Number of low energy states above $\omega = 0$ scales as $2x +$
Not as $1+x$ as in Fermi liquid

Chen et al. PRL 66, 104 (1991)

Peets et al. PRL 103, (2009),

Meinders et al. PRB 48, 3916 (1993)
Doping-induced Mott transition ($t' = 0$)

Not just adding new piece:
Lesson from DMFT, first order transition + critical point governs phase diagram
Doping driven Mott transition, $t' = 0$

<table>
<thead>
<tr>
<th>Method</th>
<th>$t'$</th>
<th>Orbital selective</th>
<th>U</th>
<th>Critical point</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>D+C+H 8</td>
<td></td>
<td></td>
<td>7</td>
<td></td>
<td>Werner et al. cond-mat (2009)</td>
</tr>
<tr>
<td>D+C+H 4</td>
<td></td>
<td></td>
<td>7</td>
<td></td>
<td>Gull et al. EPL (2008)</td>
</tr>
<tr>
<td></td>
<td>-0.3</td>
<td></td>
<td>10,6</td>
<td></td>
<td>Liebsch, Merino… (2008)</td>
</tr>
<tr>
<td>D+C+H 8</td>
<td></td>
<td></td>
<td>7</td>
<td></td>
<td>Ferrero et al. PRB (2009)</td>
</tr>
</tbody>
</table>

K. Haule, G. Kotliar, PRB (2008)  
Vildhyadhiraja, PRL (2009)
Doping driven Mott transition

Gull, Werner, Millis, (2009)
First order transition at finite doping

\[ n(\mu) \text{ for several temperatures: } T/t = \frac{1}{10}, \frac{1}{25}, \frac{1}{50} \]
The critical point
Normal state phase diagram

G. Sordi, K. Haule, A.-M.S.T
PRL, 104, 226402 (2010)
Link to Mott transition up to optimal doping

Doping dependence of critical point as a function of $U$
Characterisation of the phases ($U = 6.2t$)

$U > U_{\text{MIT}}$:

1. Mott insulator (MI)
2. Underdoped phase (UD):
   $\delta < \delta_c$
3. Overdoped phase (OD):
   $\delta > \delta_c$
4. Coexistence/forbidden region

Here "optimal doping" $\delta_c =$ doping at which the 1st order transition occurs

How does the UD phase differ from the OD phase?
Pseudogap and the Widom line
The Widom line

Xu et al. PNAS, 102, 46 (2005)
Simeoni et al., Nature Physics 6, 503 (2010)
The Widom line

- a
  - max$_\mu$ 1/n$^2$ dn/d$\mu$
  - Widom line
  - critical point
  - correlated Fermi liquid
  - coexistence line
  - pseudogap
  - Mott insulator

- b
  - $\kappa$ = 1/n$^2$ dn/d$\mu$
  - $T$ = 1/10, 1/14, 1/16, 1/25, 1/40, 1/50, 1/52, 1/60, 1/64
Rapid change also in dynamical quantities
Phase diagram
Phase diagram
Phase diagram
T dependence of the DOS

\[ \delta = 0.02 < \delta_p \]
Phase diagram
Tunneling DOS

Khosaka et al. *Science* **315**, 1380 (2007);
Phase diagram
Spin susceptibility

Underdoped Hg1223
Julien et al. PRL 76, 4238 (1996)
Phase diagram
Plaquette eigenstates
Phase diagram
Local moment and Mott transition

\[ n = 1, \text{ unfrustrated square lattice} \]
Local moment and Mott transition

\[ n = 1, \text{ unfrustrated square lattice} \]
Local singlet and pseudogap transition
Local singlet and pseudogap transition
Another property of the UD phase
Underdoped metal very sensitive to anisotropy

FIG. 3: (Color online) Anisotropy in the CDMFT conductivity $\delta_\sigma = 2 [\sigma_x(0) - \sigma_y(0)] / [\sigma_x(0) + \sigma_y(0)]$ as a function of filling $N$ for various values of $U$ and $\eta = 0.1$, $\delta_0 = 0.04$.

Okamoto, Sénéchal, Civelli, AMST
Phys. Rev. B 82, 180511R 2010

D. Fournier et al. Nature Physics (Marcello Civelli)
Superconductivity

Phase diagram

Exact diagonalization as impurity solver \((T=0)\).
Dome vs Mott (CDMFT)

Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST
CDMFT global phase diagram

Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST

Armitage, Fournier, Greene, RMP (2009)
Consistent with following experiment

H. Mukuda, Y. Yamaguchi, S. Shimizu, … A. Iyo JPSJ 77, 124706 (2008)
Magnetic phase diagram of YBCO

Theoretical phase diagram BEDT

\[ X = \text{Cu}_2(\text{CN})_3 \ (t' \sim t) \]


The glue
Im $\Sigma_{an}$ and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)
The glue


Wakimoto … Birgeneau
PRL (2004)
The glue and neutrons

FIG. 3 (color online). Q-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-$H$ integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i = 140$ meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO 1/8 (open circles) from [2]. The solid lines following data of LSCO $x = 0.25$ and 0.30 are guides to the eyes.

Main collaborators

Giovanni Sordi

Bumsoo Kyung

David Sénéchal

Marcello Civelli

Kristjan Haule

Satoshi Okamoto
$d = 2$ precursors, e-doped

Motoyama et al.

$\zeta^* = 2.6(2)\zeta_{\text{th}}$

Vilk, A.-M.S.T (1997)

Kyung, Hankevych, A.-M.S.T., PRL, sept. 2004

Semi-quantitative fits of both ARPES and neutron
TPSC: general ideas

• General philosophy
  – Drop diagrams
  – Impose constraints and sum rules
    • Conservation laws
    • Pauli principle (\(\langle n_\sigma^2 \rangle = \langle n_\sigma \rangle\))
    • Local moment and local density sum-rules

• Get for free:
  • Mermin-Wagner theorem
  • Kanamori-Brückner screening
  • Consistency between one- and two-particle \(\Sigma G = U\langle n_\sigma n_{-\sigma} \rangle\)

Vilk, AMT J. Phys. I France, 7, 1309 (1997);
*Theoretical methods for strongly correlated electrons* also (Mahan, 3rd)
Resistivity (TPSC)

Dominic Bergeron
Thermoelectric power

Louis-François Arsenault

Sriram Shastry

Patrick Sémon
Heterostructures

Patrick Fournier
Maxime Dion
Simon Verret
Maxime Charlebois
Syed Hassan
David Sénéchal
Retardation effects

\(\Sigma_{i\mu}(k_i^f, \omega)\)

\(\chi''(\omega)\)

\(\delta = 0.04\)

\(\delta = 0.16\)

\(\delta = 0.26\)

\(\delta = 0.29\)  \(\delta = 0.37\)
André-Marie Tremblay

Sponsors:
Mammouth, série
Conclusions

• Tools for Hubbard model, high Tc.
• The influence of Mott Physics extends way beyond half-filling
  – Pseudogap as a phase
  – Effects of critical point at high temperature (Widom line)
  – Superconductivity
    • Dome
    • Retardation effects in pairing come from spin fluctuations.
Merci
Thank you