Pseudogap $T^*$ along the Widom line of a first-order transition in doped Mott insulators

A.-M. Tremblay
G. Sordi, K. Haule, P. Sémon

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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 $n = 1$
Hubbard model

1931-1980

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

Effective model, Heisenberg: \( J = 4t^2 / U \)
Method
Mott transition and Dynamical Mean-Field Theory. The beginnings in $d = \infty$

- 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)
Kotlier et al. PRL 87 (2001)

REVIEWS
Maier, Jarrell et al., RMP. (2005)
Kotlier et al. RMP (2006)
AMST et al. LTP (2006)
Not perfect!

• Missing:
  – Long wavelength fluctuations

• Included:
  – Short-range dynamical and spatial correlations

• Long range order:
  – Allow symmetry breaking in the bath (mean-field)
$n = 1$, unfrustrated cubic lattice

$J = 4t^2 / U$
Local moment and Mott transition

\( n = 1 \), unfrustrated square lattice
Outline

• Method
• Finite \( T \) phase diagram
  – Normal state (no LRO, what is below the dome)
    • First order transition
    • Widom line and pseudogap
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>
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<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>
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<tr>
<td>D+C+H 4</td>
<td>-0.3</td>
<td></td>
<td>10,6</td>
<td></td>
<td>Gull et al. EPL (2008)</td>
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<tr>
<td>D+C+H 8</td>
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<td>7</td>
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<td>Liebsch, Merino… (2008)</td>
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<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)
Continuous-time Quantum Monte Carlo calculations to sum all diagrams generated from expansion in powers of hybridization.


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
First order transition at finite doping

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

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

μ = 0, H. Park, K. Haule, and G. Kotliar,
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" $\delta_c = \ldots$

doping at which the 1st order transition occurs

How does the UD phase differ from the OD phase?

Smaller $D$ and $S$
Density of states

Graph a shows the density of states as a function of energy (hω) for different values of δ, with T = 1/25 > Tp. The graph indicates a transition from Mott insulator to correlated Fermi liquid as δ increases.

Graph b presents the behavior of A(0) as a function of δ, showing a crossover from a pseudogap to a critical point.
Density of states

Khosaka et al. *Science* **315**, 1380 (2007);
Density of states
Density of states
Spin susceptibility
Spin susceptibility

Underdoped Hg1223
Julien et al. PRL 76, 4238 (1996)
Plaquette eigenstates
Pseudogap $T^*$ along the Widom line
The Widom line

arXiv:1110.1392
What is the Widom line?

- it is the continuation of the coexistence line in the supercritical region
- line where the maxima of different response functions touch each other asymptotically as $T \to T_p$
- liquid-gas transition in water: max in isobaric heat capacity $C_p$, isothermal compressibility, isobaric heat expansion, etc.
- DYNAMIC crossover arises from crossing the Widom line!
  
Pseudogap \( T^* \) along the Widom line

Widom line: defined from maxima of charge compressibility
\[
\kappa = 1/n^2 (dn/d\mu)_T
\]
divergence of \( \kappa \) at the (classical) critical point!
Rapid change also in dynamical quantities
Phase diagram
Summary

- Mott physics extends way beyond half-filling
- Pseudogap is a phase
- Pseudogap $T^*$ is a Widom line
- High compressibility (stripes?)
André-Marie Tremblay

Sponsors:
Mammouth
Merci
Thank you