What lies beneath the dome

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G. Sordi, D. Sénéchal, K. Haule,
S. Okamoto, B. Kyung, M. Civelli

Aspen, 13 July 2011
Two views (caricature)

Phillips, RMP (2010)

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

Long correlation length 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
arXiv:1102.0463
Method
Bare Mott critical point in organics

\[ G(k, \omega) = \frac{1}{\omega - \varepsilon_k - \Sigma(k, \omega)} \rightarrow \Sigma''(k, \omega) \rightarrow \infty \]

F. Kagawa, K. Miyagawa, + K. Kanoda

Phase diagram (X=Cu[N(CN)₂]Cl)
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.
Solving cluster in a bath problem

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


See also

**CDMFT**
- Park-Haule-Kotliar 4
- Liebsch-Tong 4
- Imada-Motome 4

**DCA**
- Ferrero, Georges, Kotliar 2
- Jarrell 8 and more
- Millis-Gull 8
4 sites is already quite good
Interaction-induced Mott transition, $n = 1$

4 sites (CDMFT-CTQMC)

$U_{MIT} = 6.05$

$U_r = (U - U_{MIT})/U_{MIT}$


$U_{MIT} \sim 12$
Mott insulator at finite $T$

M. Vekic and S.R. White, PRB 47, 1160 (1993)
Spectral weight transfer

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

Chen et al. PRL 66, 104 (1991)

Peets et al. PRL 103, (2009), Phillips, Jarrell arXiv

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

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

G. Sordi, K. Haule, A.-M.S.T
PRL, 104, 226402 (2010)
and
arXiv:1102.0463
First order transition at finite doping

$n(\mu)$ for several temperatures:
$T/t = 1/10, 1/25, 1/50$
We do not see critical point anymore
In the T=0 plane

![Diagram showing the T=0 plane with critical points and the CDMFT region.](image)
Cuts for T dependence

![Graphs showing cuts for T dependence](image)
Cuts for T dependence

(U=6.2t) 

(U=7.0t)

\(T_{cr}\) 

\(\mu_{ci}(T)\) 

\(\mu_{c2}(T)\)
Normal state phase diagram

G. Sordi, K. Haule, A.-M.S.T
PRL, 104, 226402 (2010)
first order transition at finite doping between two metals
it is associated to Mott physics: all signatures of the first order transition can be traced back to Mott critical point
⇒ signature of the Mott transition in the 2D Hubbard model extends way beyond half filling!
Another property of the UD phase
Underdoped metal very sensitive to anisotropy

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

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

• The influence of Mott Physics extends way beyond half-filling

• Conjecture that quantum-critical like behavior is constant $U$ cut of our phase diagram, i.e. very low $T$ critical point.