What lies beneath the dome

A.-M. Tremblay

G. Sordi, D. Sénéchal, K. Haule,

S. Okamoto, B. Kyung, M. Civelli

CIFAR
CANADIAN INSTITUTE for ADVANCED RESEARCH

UNIVERSITÉ DE SHERBROOKE

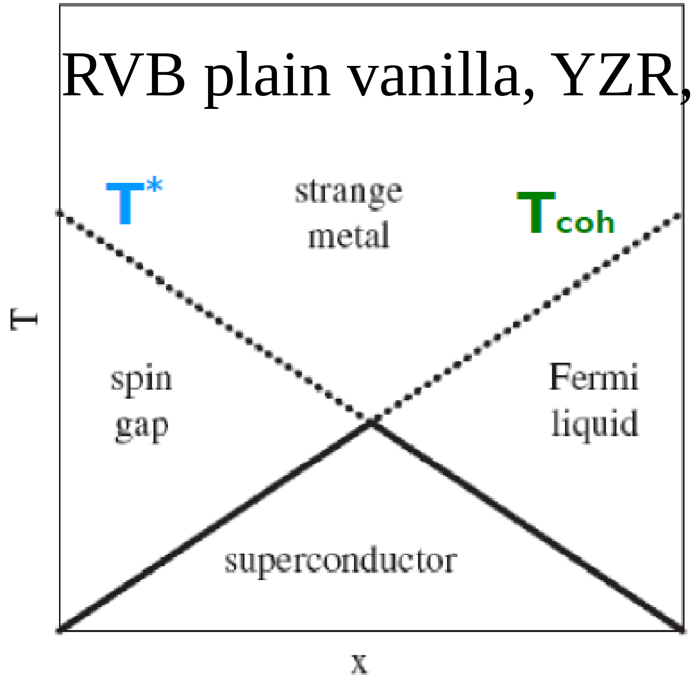
Aspen, 13 July 2011

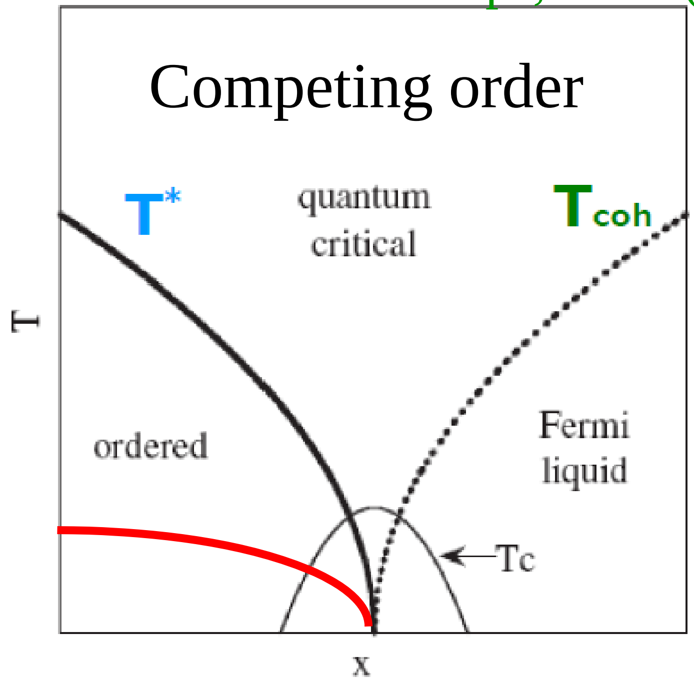
VERITATEM IN CHARITATE

UNIVERSITÉ DE SHERBROOKE

Two views (caricature)

Norman, Adv. Phys. (2005)
Broun, Nat. Phys. (2006)
Phillips, RMP (2010)



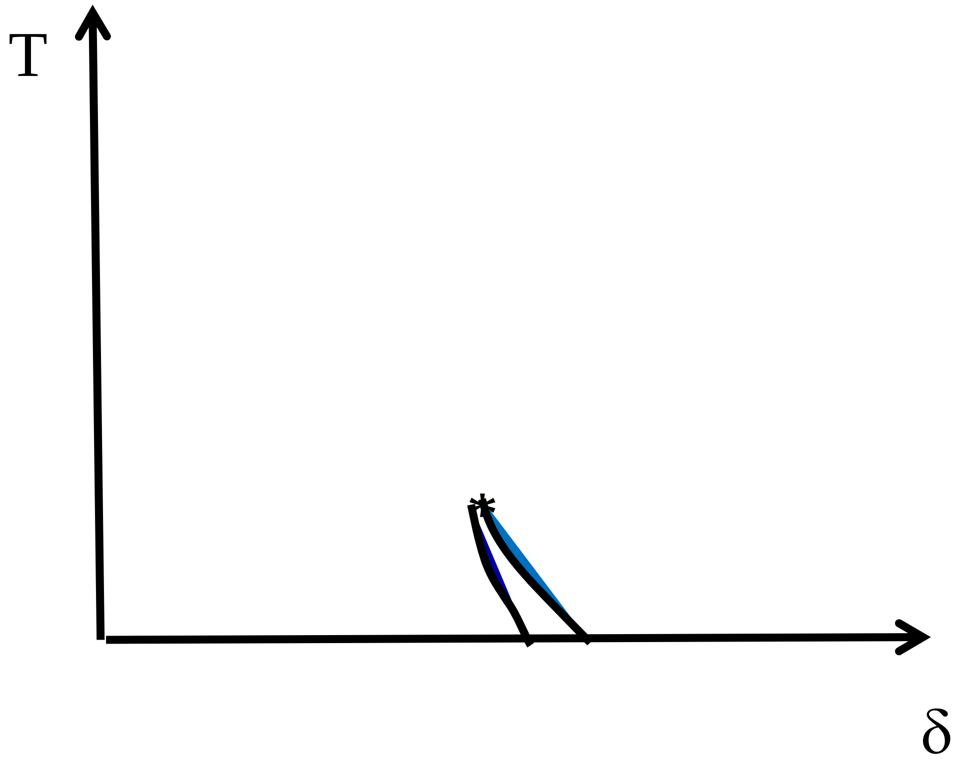


Why T_c decreases?
What is the origin of T^*?
What is the strange metal?

Long correlation length or not.
What lies beneath the dome.
Mott Physics away from $n = 1$

UNIVERSITÉ DE SHERBROOKE

An alternate view (a bit of both)

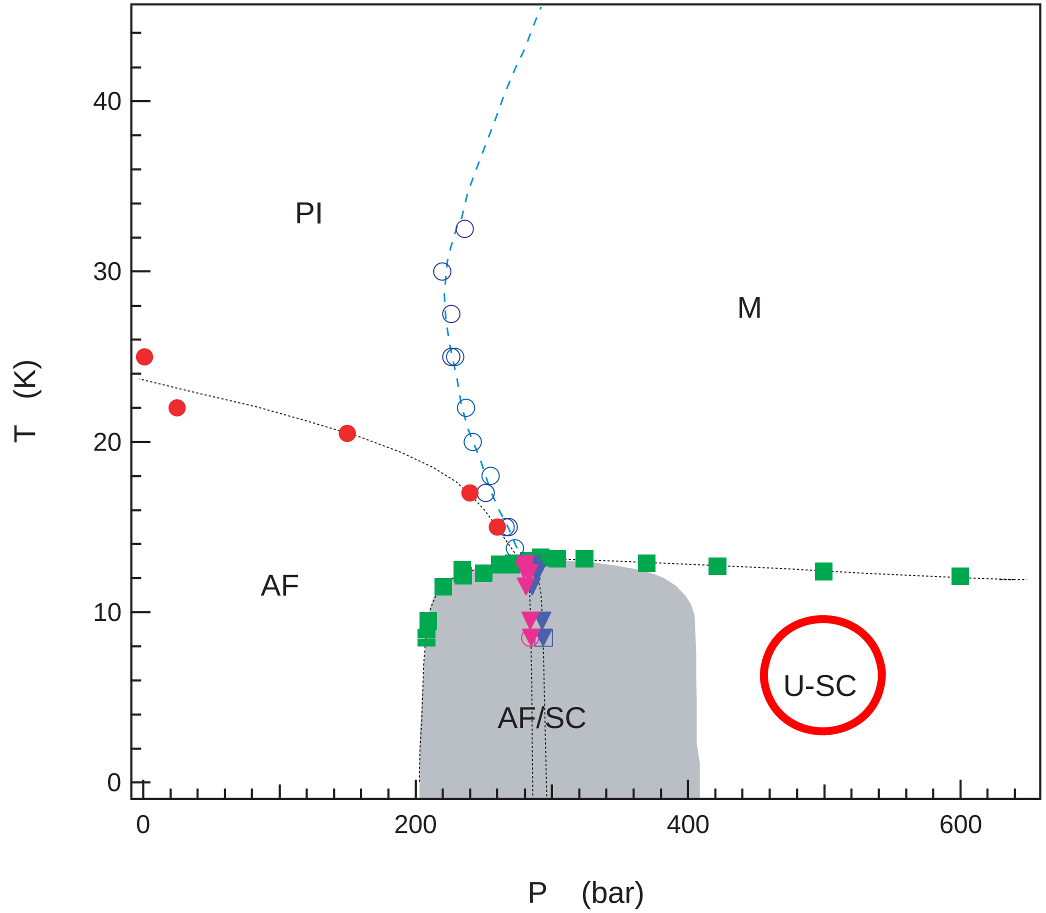


G. Sordi, K. Haule, A.-M.S.T
PRL, **104**, 226402 (2010)
and
arXiv:1102.0463

UNIVERSITÉ DE SHERBROOKE

Method

Bare Mott critical point in organics



$$G(\mathbf{k},\omega) = \frac{1}{\omega - \varepsilon_{\mathbf{k}} - \Sigma(\mathbf{k},\omega)} \rightarrow \Sigma''(\mathbf{k},\omega) \rightarrow \infty$$

F. Kagawa, K. Miyagawa, + K. Kanoda
PRB **69** (2004) +Nature **436** (2005)

Phase diagram (X=Cu[N(CN)$_2$]Cl)

S. Lefebvre et al. PRL **85**, 5420 (2000), P. Limelette, et al. PRL **91** (2003)

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.
  - P. Werner, A. Comanac, L. de' Medici, M. Troyer, and A. J. Millis, Phys. Rev. Lett. **97**, 076405 (2006).
  - K. Haule, Phys. Rev. B **75**, 155113 (2007).

See also

CDMFT

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

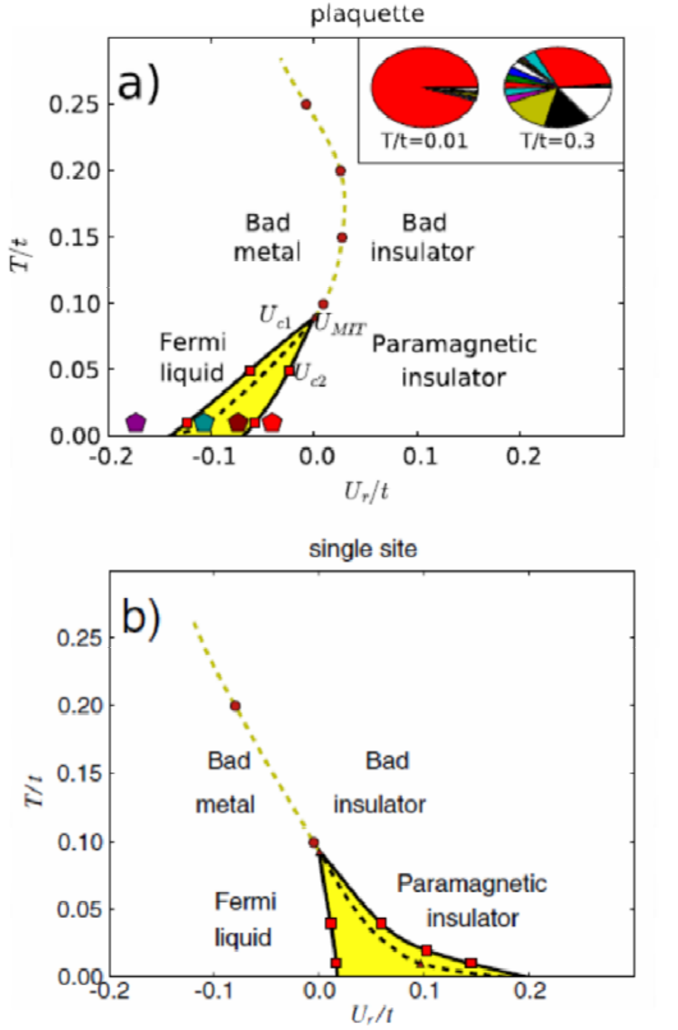
DCA

- 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)



$U_{MIT} = 6.05$

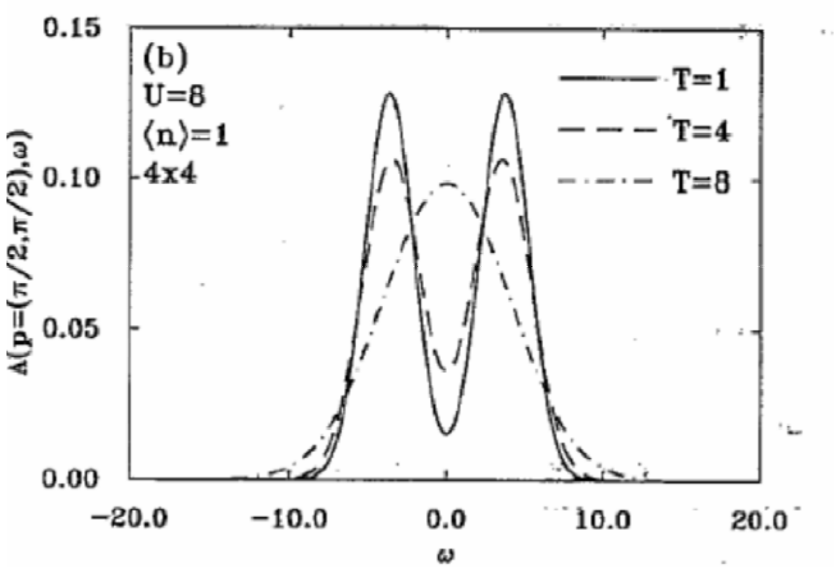
Single site

$U_{MIT} \sim 12$

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

H. Park, K. Haule, and G. Kotliar PRL **101**, 186403 (2008)

Mott insulator at finite *T*



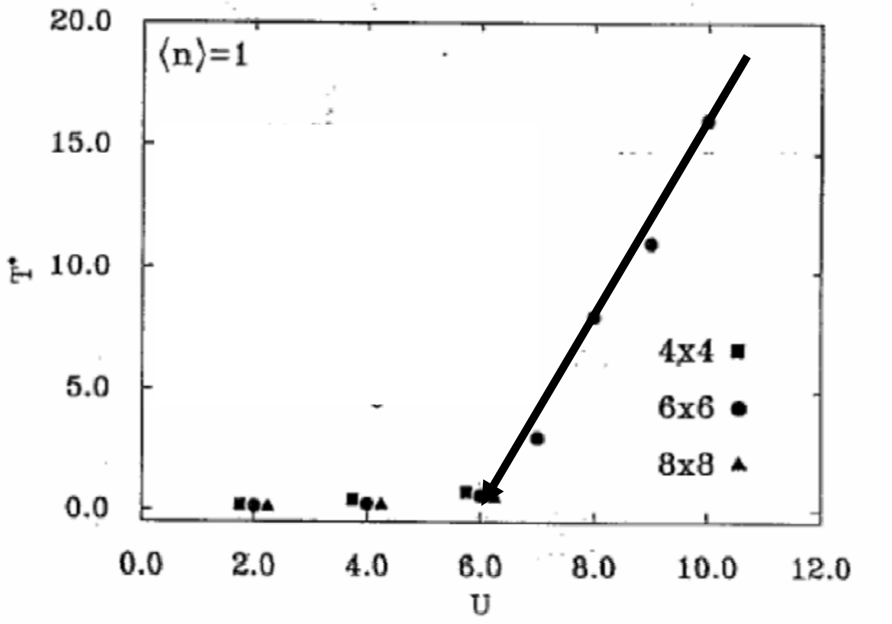
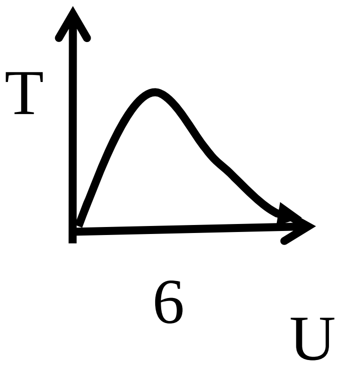


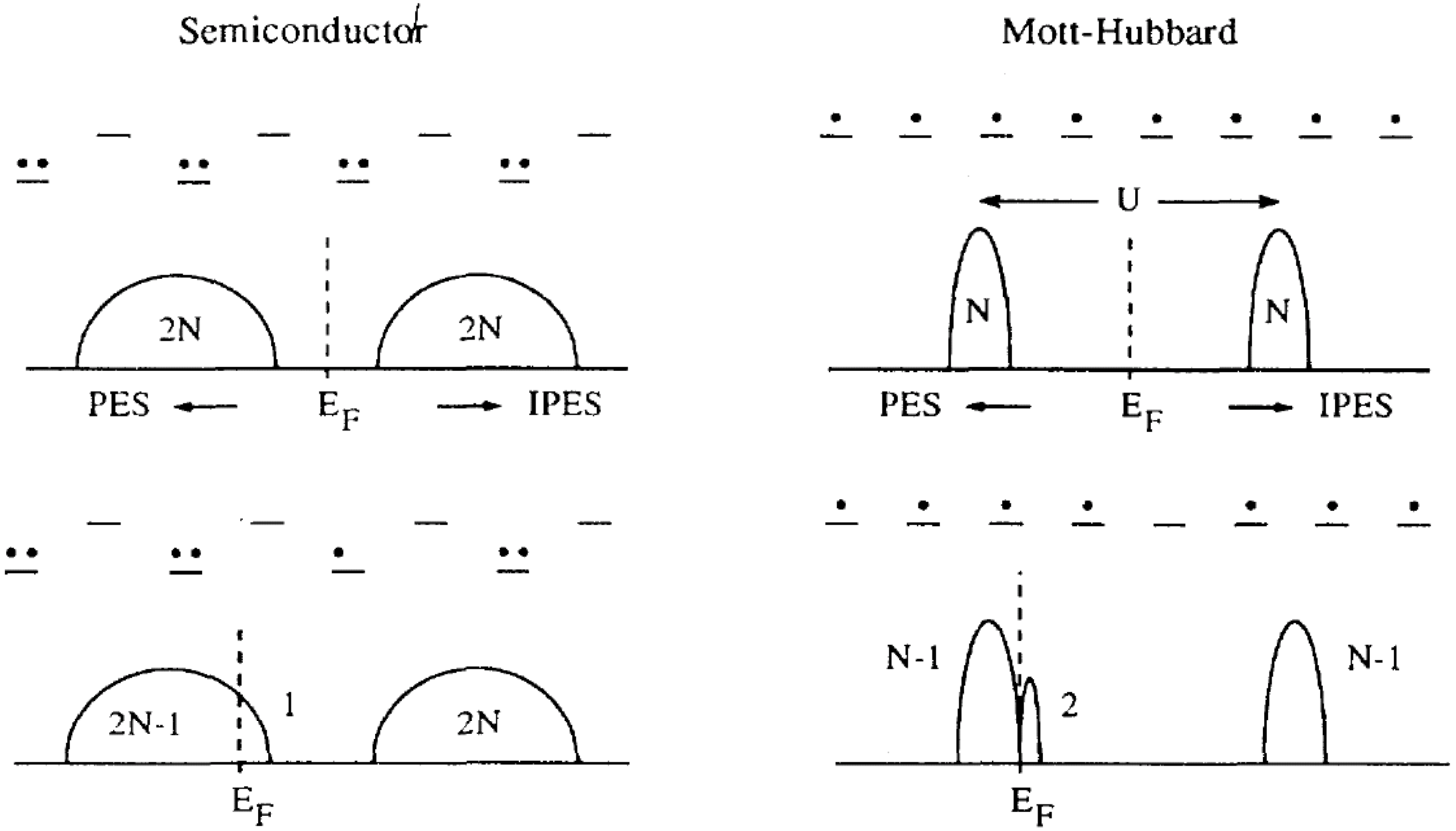
FIG. 5. The temperature T^* at which the gap develops vs U for 4×4, 6×6, and 8×8 lattices.



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

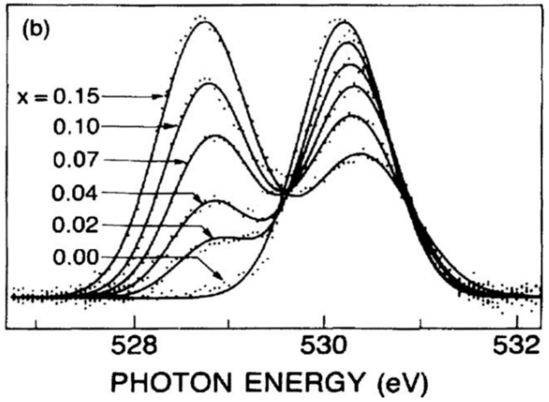
UNIVERSITÉ DE SHERBROOKE

Spectral weight transfer

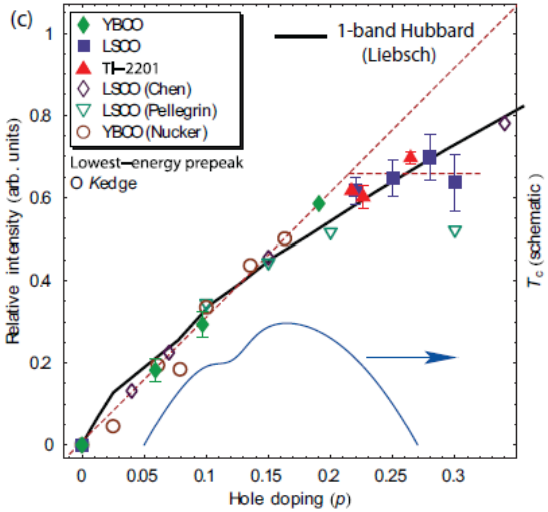


Meinders *et al.* PRB **48**, 3916 (1993)

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 ω = 0 scales as *2x* +

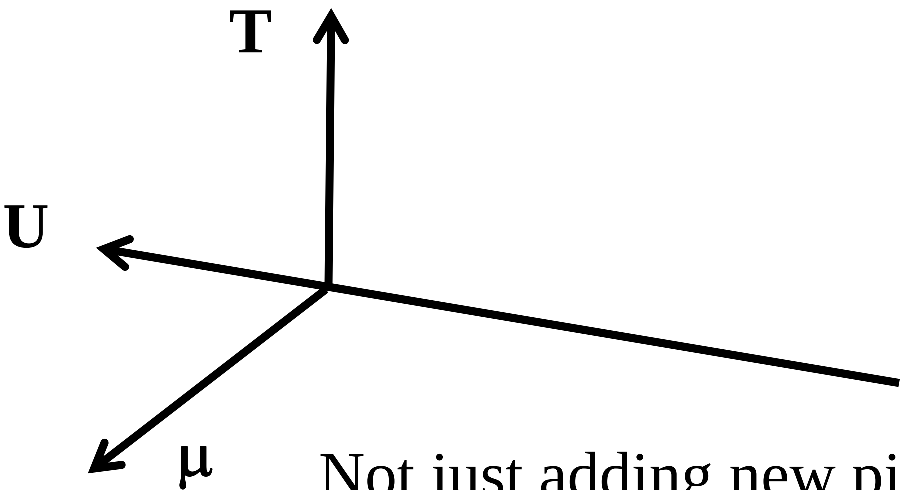
Not as 1+x as in Fermi liquid

Meinders *et al.* PRB **48**, 3916 (1993)

Giovanni Sordi

G. Sordi, K. Haule, A.-M.S.T
PRL, **104**, 226402 (2010)
and
arXiv:1102.0463

Doping-induced Mott transition (*t'=0*)

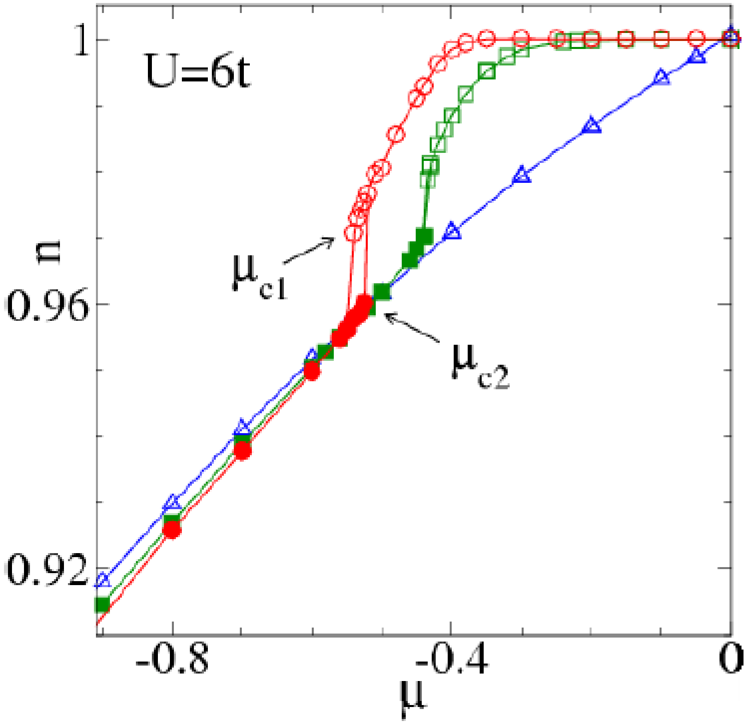


Not just adding new piece:
Lesson from DMFT, first order transition + critical point governs phase diagram

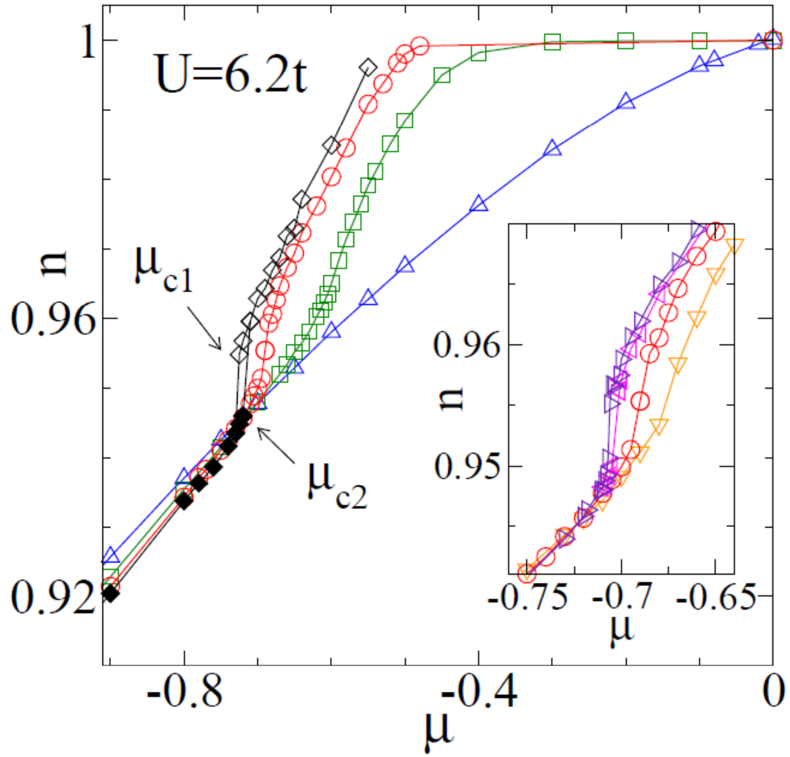
Kristjan Haule

UNIVERSITÉ DE SHERBROOKE

First order transition at finite doping

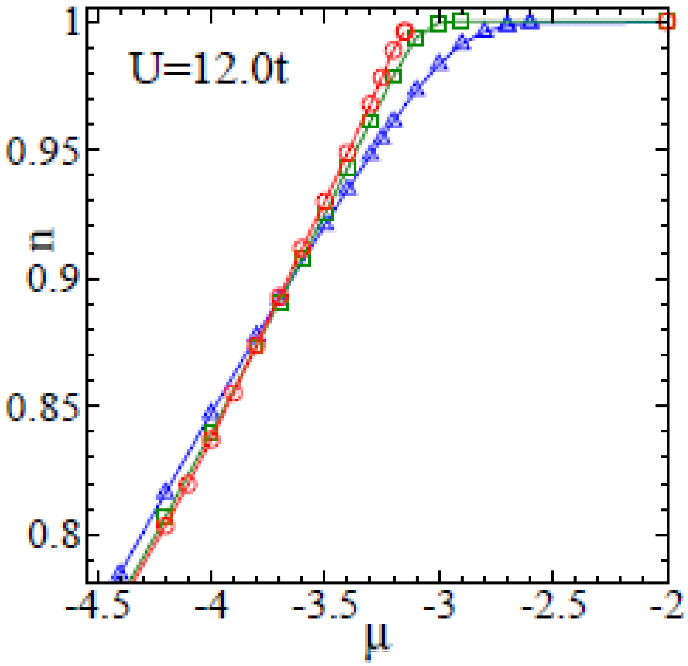


$n(\mu)$ for several temperatures:
$T/t = 1/10,\ 1/25,\ 1/50$



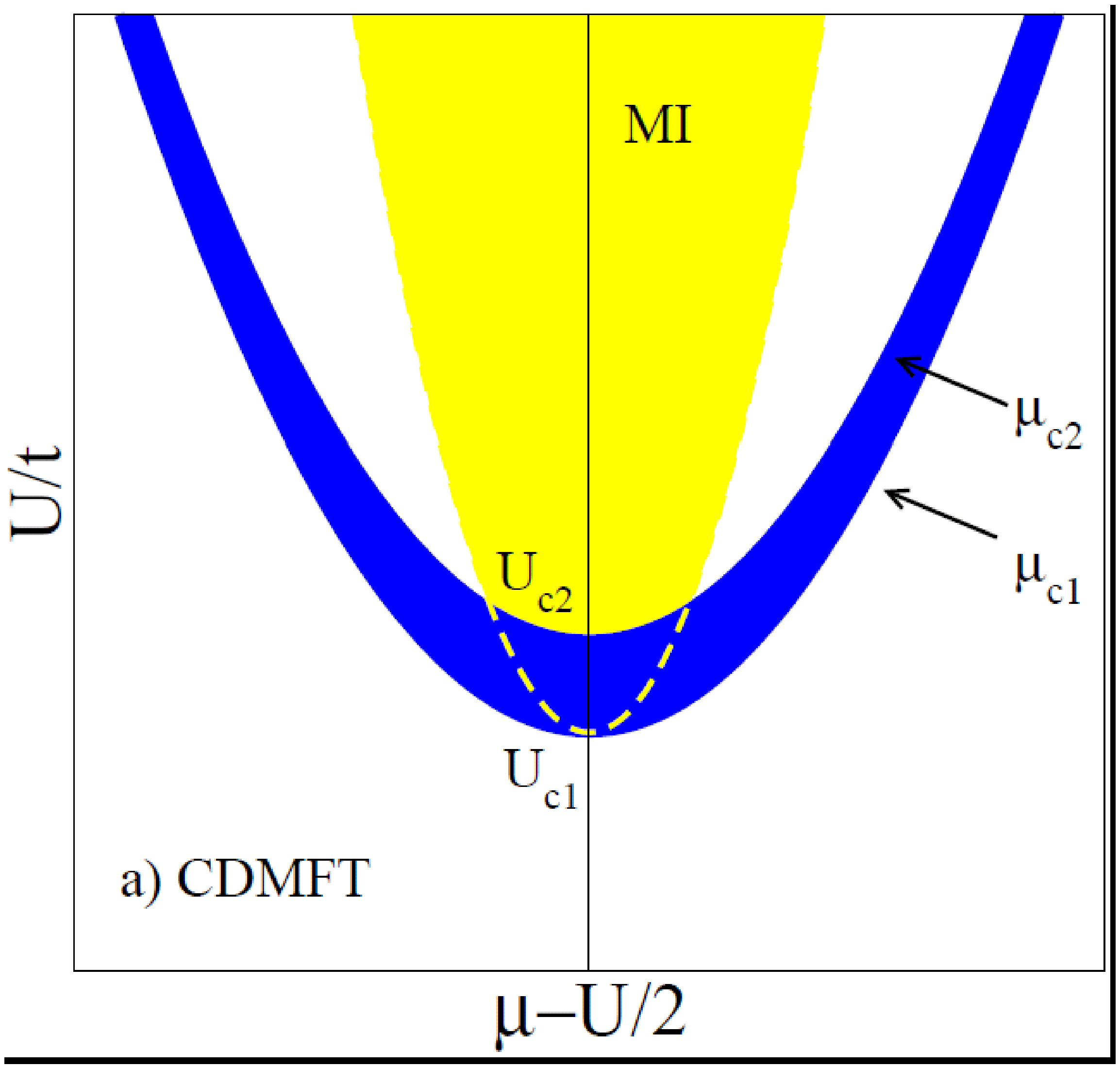
UNIVERSITÉ DE
SHERBROOKE

We do not see critical point anymore

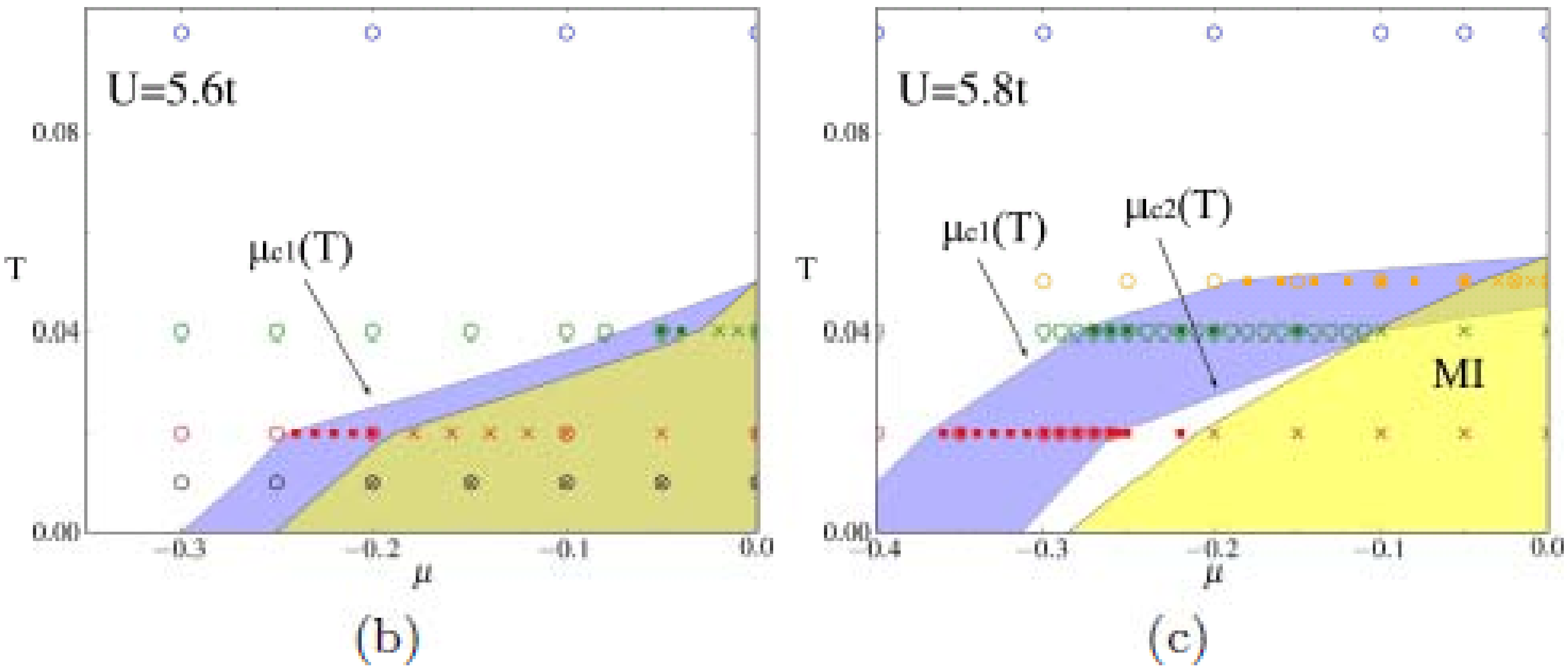


(h)

In the T=0 plane

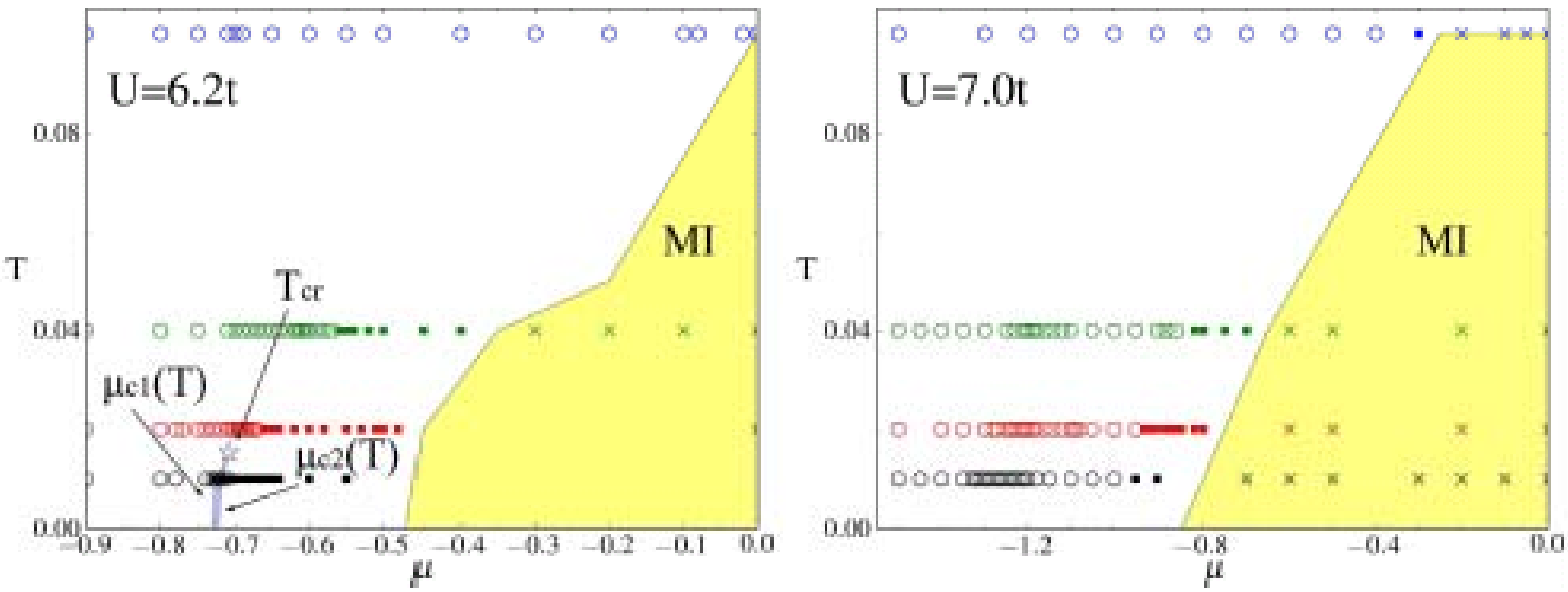


Cuts for T dpendence



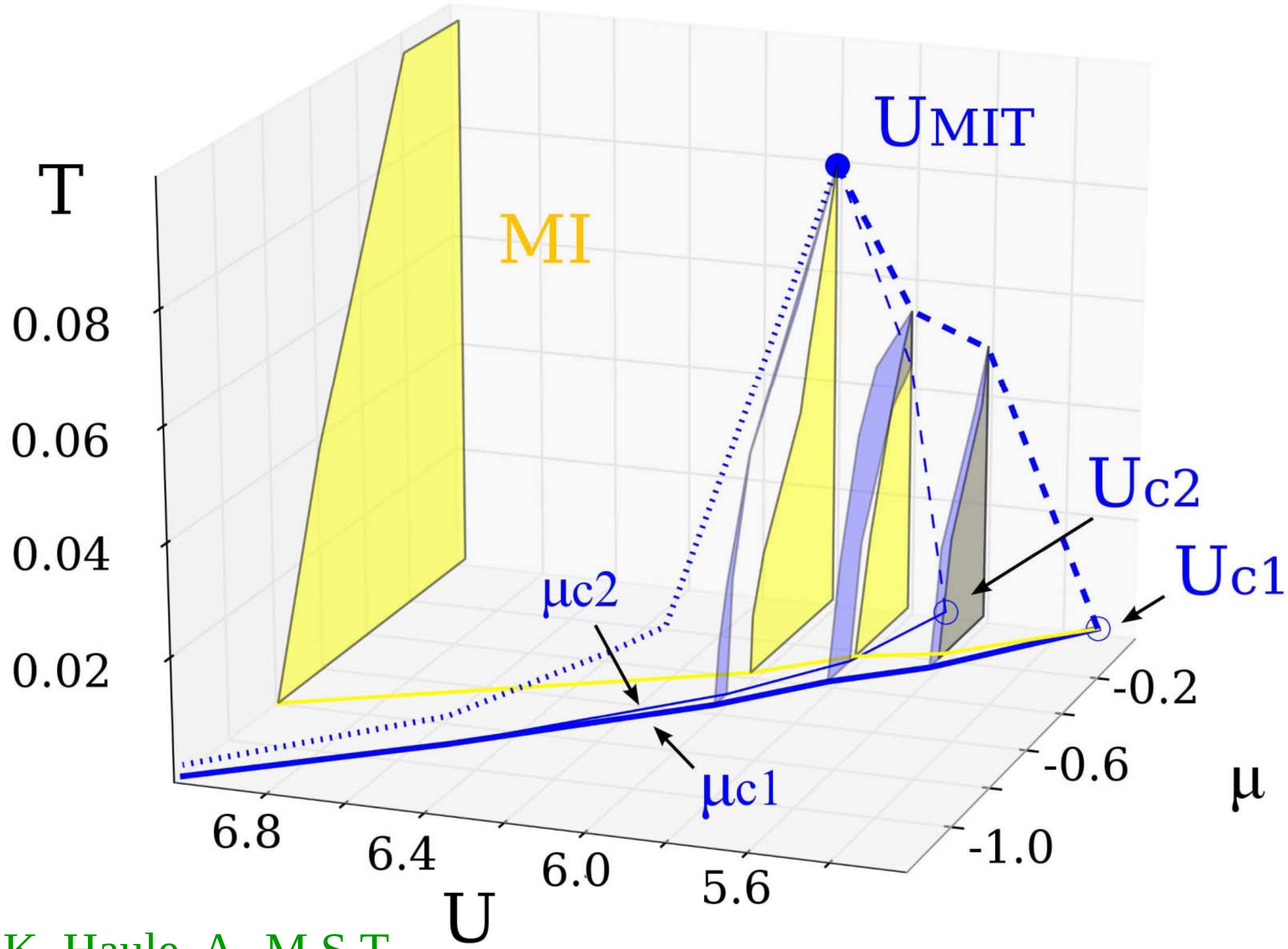
UNIVERSITÉ DE SHERBROOKE

Cuts for T dependence



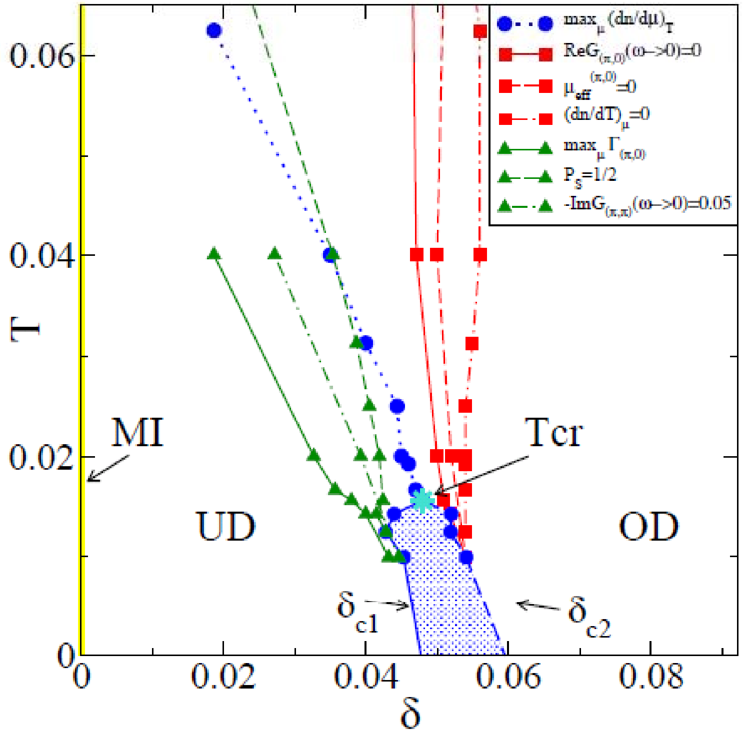
(e) (f)

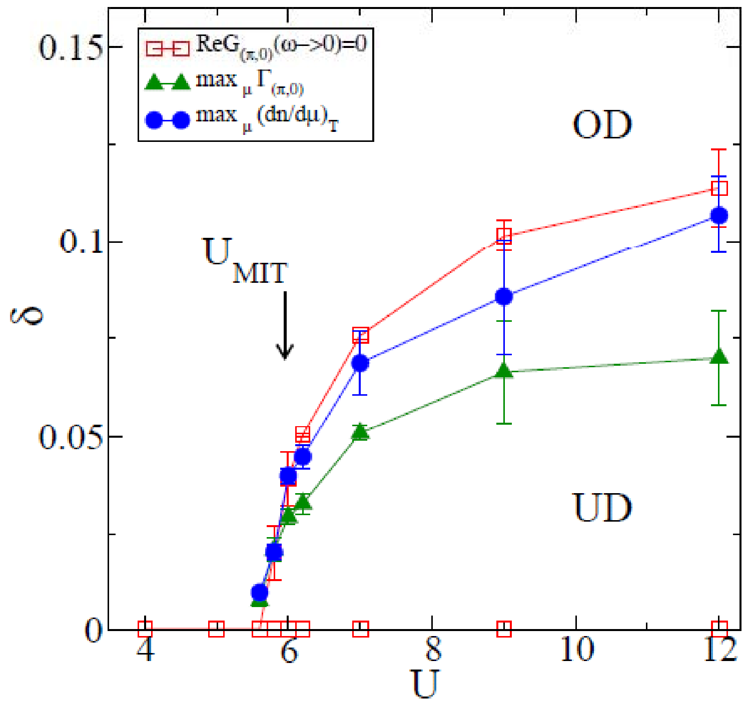
Normal state phase diagram



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

Summary





- 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

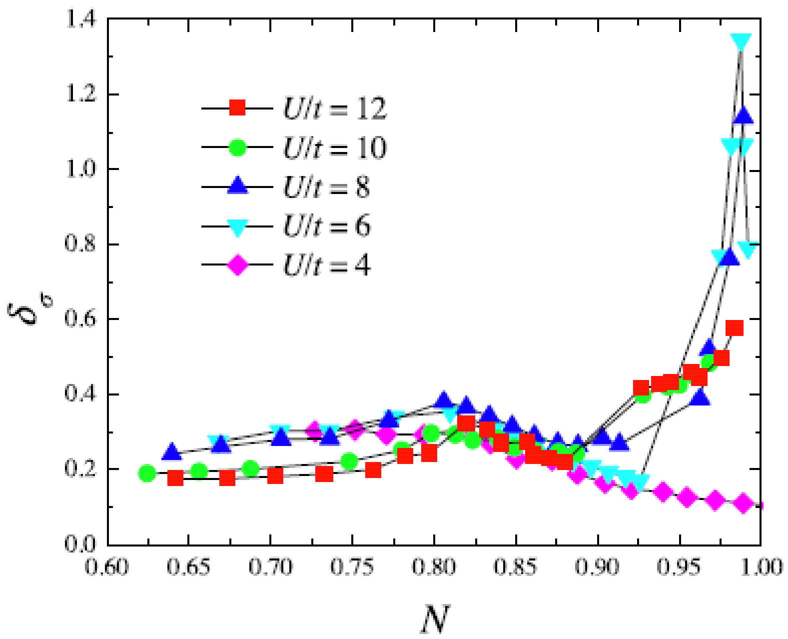
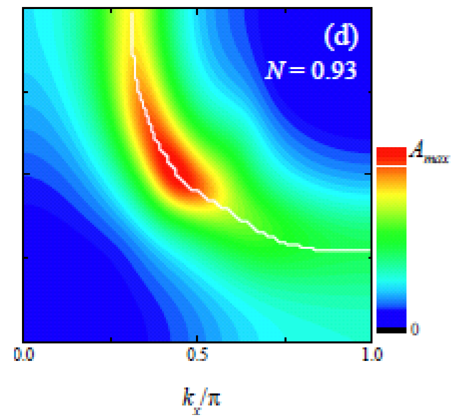
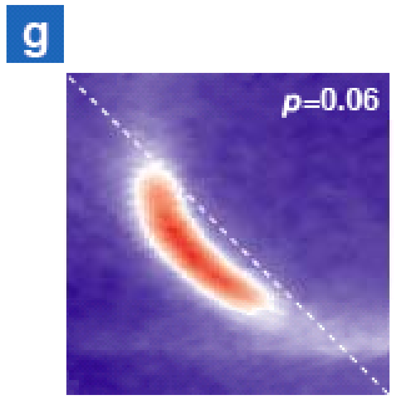


FIG. 3: (Color online) Anisotropy in the CDMFT conductivity $\delta_\sigma = 2\,[\sigma_x(0) - \sigma_y(0)]\,/\,[\sigma_x(0) + \sigma_y(0)]$ as a function of filling N for various values of U and $\eta = 0.1$, $\delta_0 = 0.04$.





Satoshi Okamoto

David Sénéchal

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.