Remnant of the first order Mott transition at finite doping as an organizing principle for strongly correlated superconductors

André-Marie Tremblay

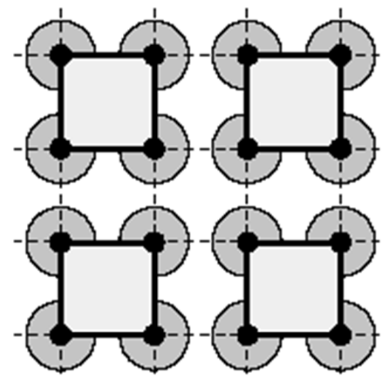
UNIVERSITÉ DE SHERBROOKE

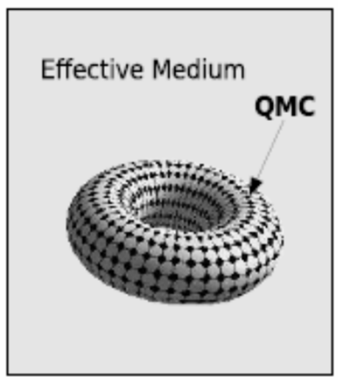
Collège de France, 26 mars 2015
17h45 à 18h15

Method

2d Hubbard: Quantum cluster method

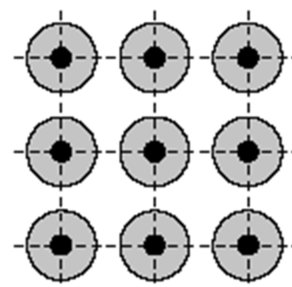
C-DMFT





DCA

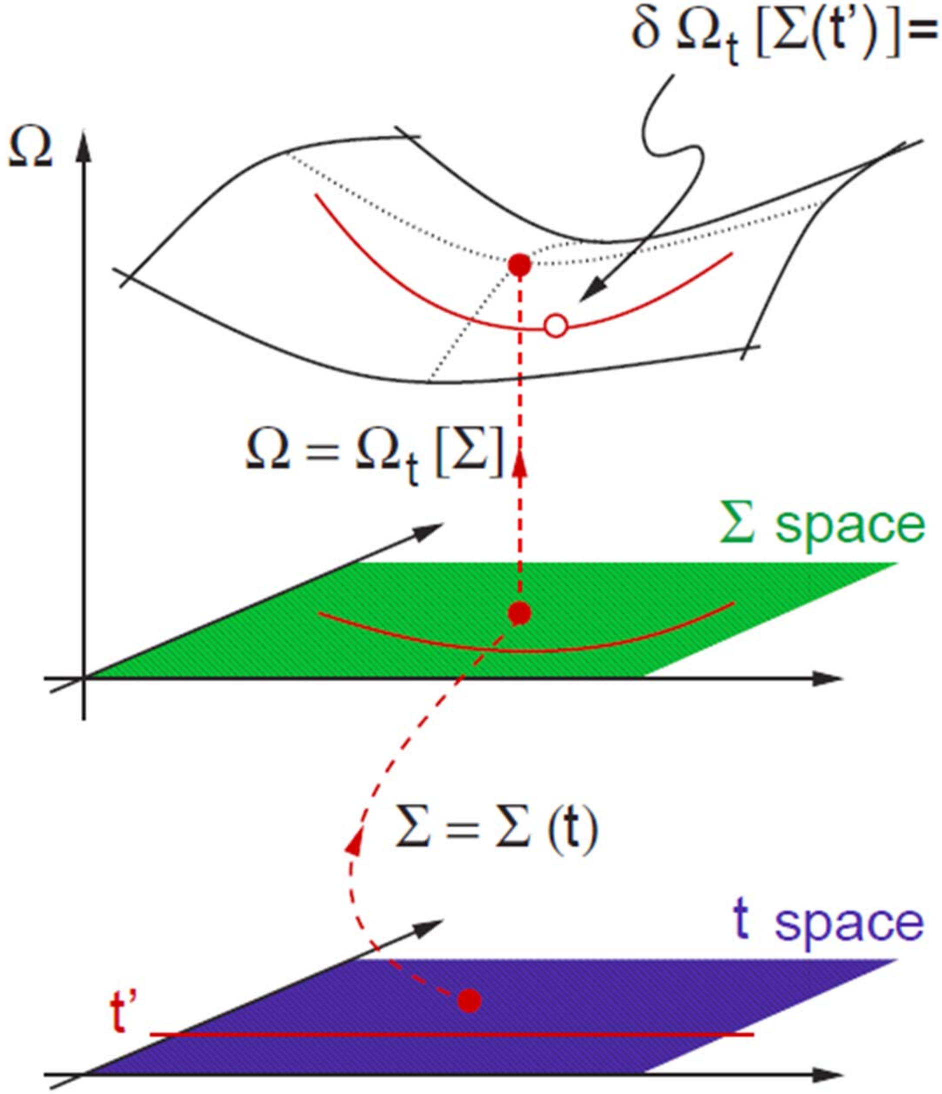
DMFT



Hettler …Jarrell…Krishnamurty PRB **58** (1998)
Kotliar et al. PRL **87** (2001)
M. Potthoff *et al.* PRL **91,** 206402 (2003).

REVIEWS
Maier, Jarrell et al., RMP. (2005)
Kotliar *et al.* RMP (2006)
AMST *et al.* LTP (2006)

DMFT as a stationnary point

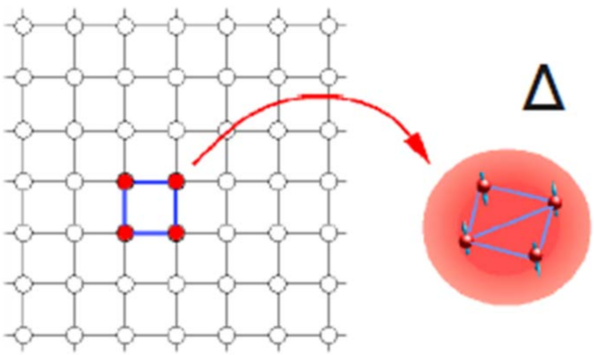


M. Potthoff, Eur. Phys. J. B 32, 429 (2003).

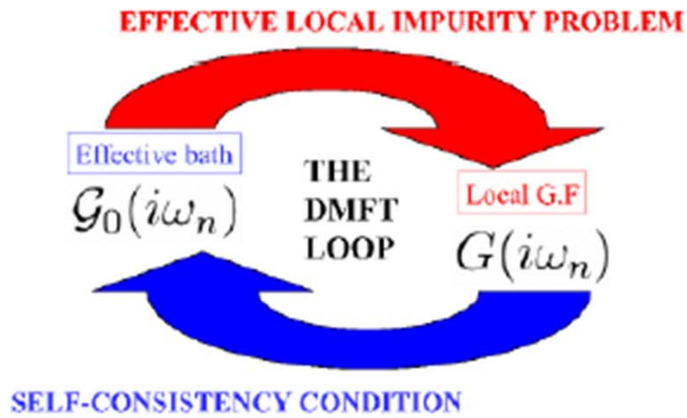
+ and -

- Long range order:
  - Allow symmetry breaking in the bath (mean-field)
- Included:
  - Short-range dynamical and spatial correlations
- Missing:
  - Long wavelength p-h and p-p fluctuations

C-DMFT



$$Z = \int \mathcal{D}[\psi^\dagger, \psi]\, \mathrm{e}^{-S_c - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\mathbf{K}} \psi^\dagger_{\mathbf{K}}(\tau)\Delta_{\mathbf{K}}(\tau,\tau')\psi_{\mathbf{K}}(\tau')}$$



Mean-field is not a trivial problem! Many impurity solvers.

Here: continuous time QMC

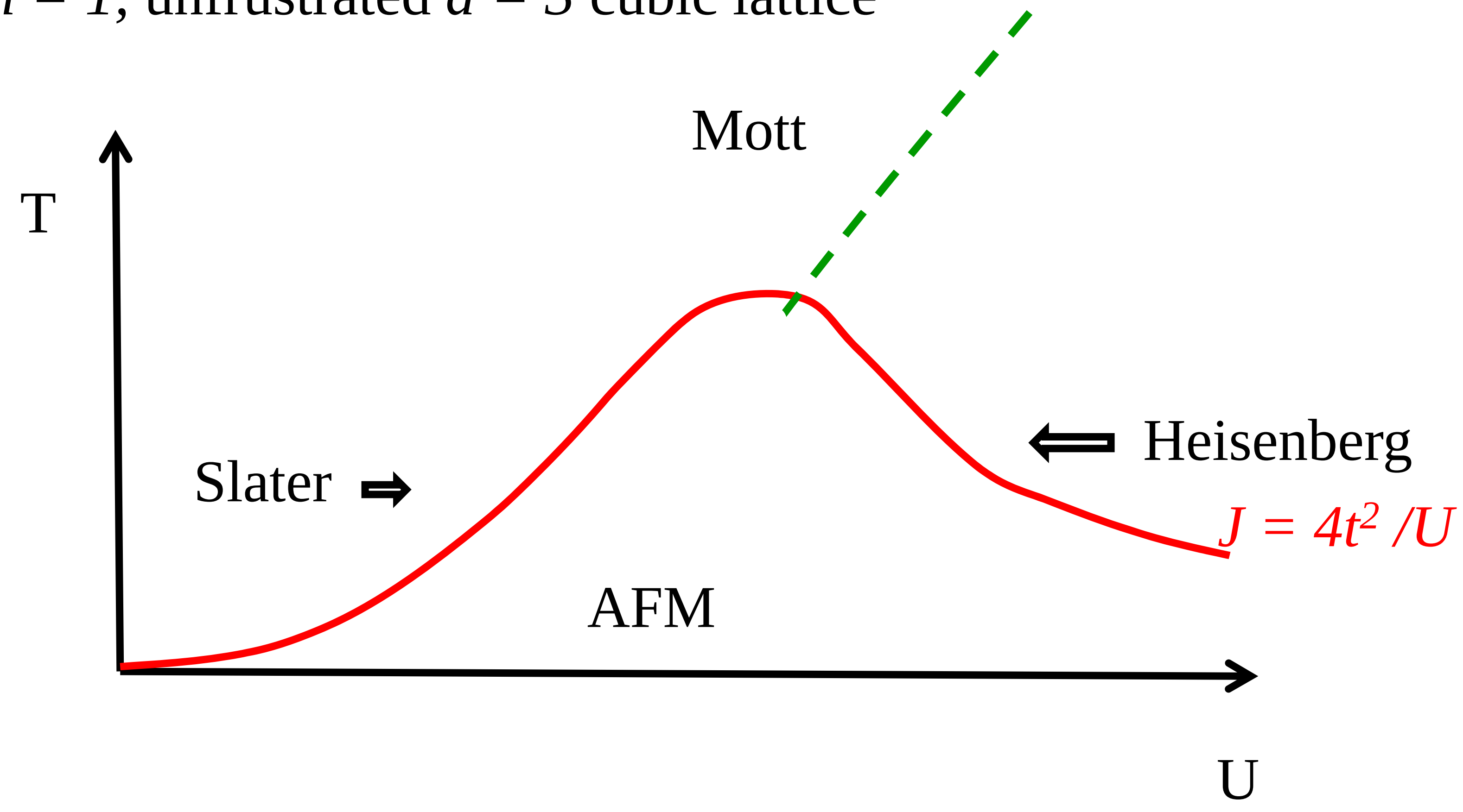
P. Werner, PRL 2006
P. Werner, PRB 2007
K. Haule, PRB 2007

$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n) - \left[\sum_{\tilde{k}} \frac{1}{i\omega_n + \mu - t_c(\tilde{k}) - \Sigma_c(i\omega_n)}\right]^{-1}$$

Mott physics (half-filling)

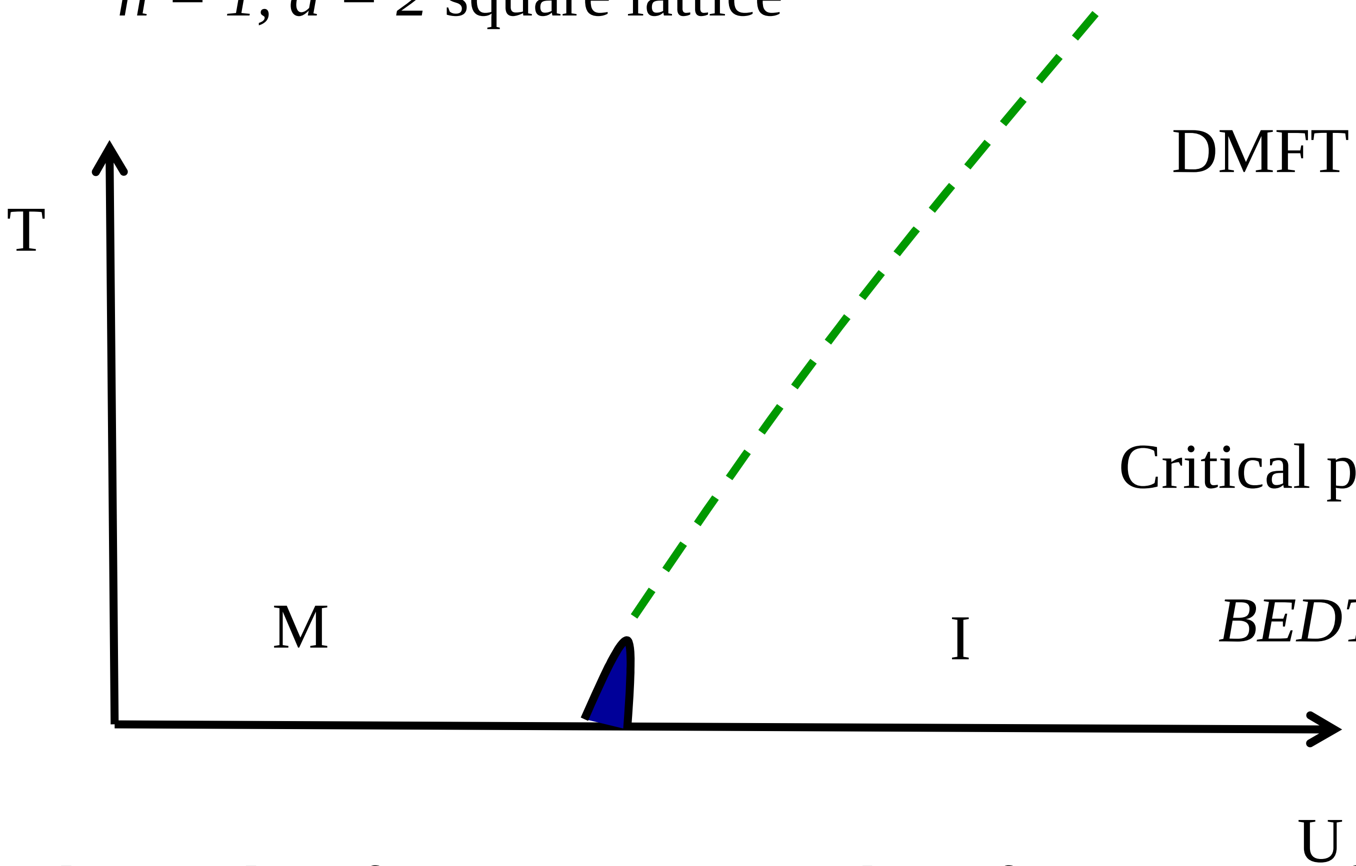
Local moment and Mott transition

$n = 1$, unfrustrated $d = 3$ cubic lattice



Local moment and Mott transition

n = 1, d = 2 square lattice



Critical point visible in

BEDT organics

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

Doped Mott insulator : normal state

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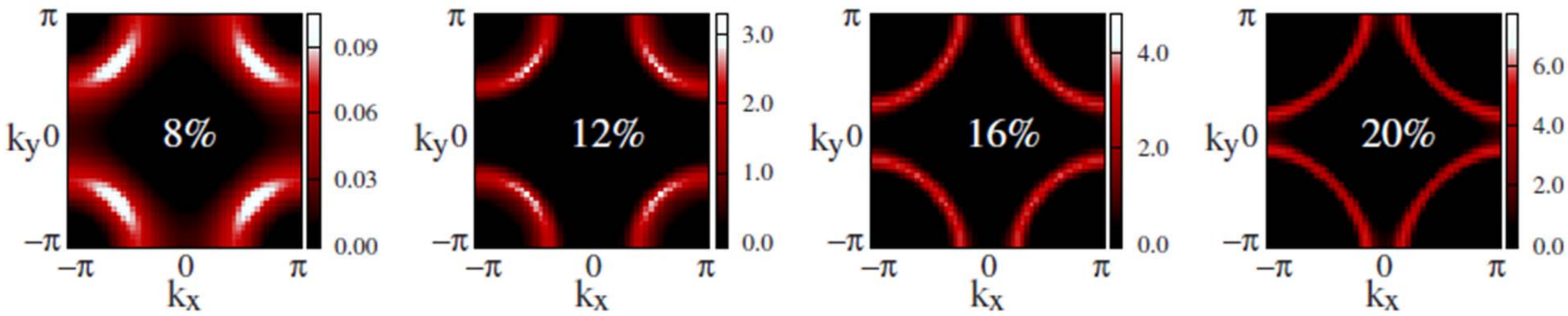
Anomalous metallic state near half-filling (examples)

- Pseudogap
  - B. Kyung et al., PRB 73, 165114 (2006).
  - N. S. Vidhyadhiraja et al., PRL 102, 206407 (2009).
  - A. Liebsch and N.-H. Tong, PrB 80, 165126 (2009).
  - D. Sénéchal, AMST, PRL **92** (2004)
- Momentum selective transition
  - P. Werner et al., PRB 80, 045120 (2009).
  - M. Ferrero et al., EPL 85, 57 009 (2009).
- Competition between Kondo and superexchange
  - K. Haule and G. Kotliar, Phys. Rev. B 76, 104509 (2007).
  - M. Ferrero et al., Europhys. Lett. 85, 57 009 (2009).
  - K. Haule and G. Kotliar, Phys. Rev. B 76, 092503 (2007).

Pseudogap



Michel Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, A. Georges
PRB **80**, 064501 (2009)

Seen by all groups and DCA, CDMFT

Gull, Werner, Millis, PRB (2009)

Sénéchal, AMT, PRL **92**, 126401 (2004).

C. Huscroft, M. Jarrell, Th. Maier, et al. PRL **86**, 139 (2001)

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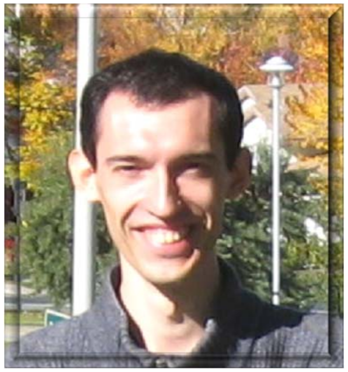
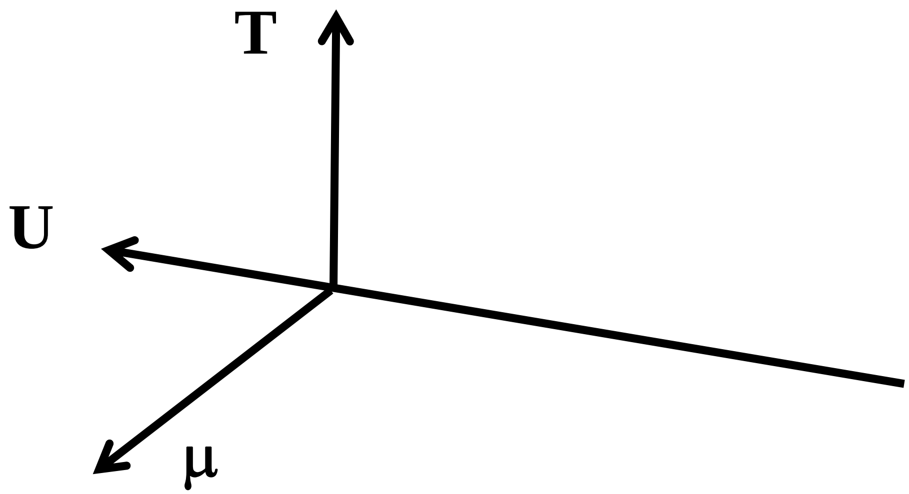


Giovanni Sordi

G. Sordi, K. Haule, A.-M.S.T
PRL, **104**, 226402 (2010)
and
Phys. Rev. B. **84**, 075161 (2011)

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



Kristjan Haule

Lesson from DMFT, first order transition + critical point governs phase diagram

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A first order transition?

At positive *t'*

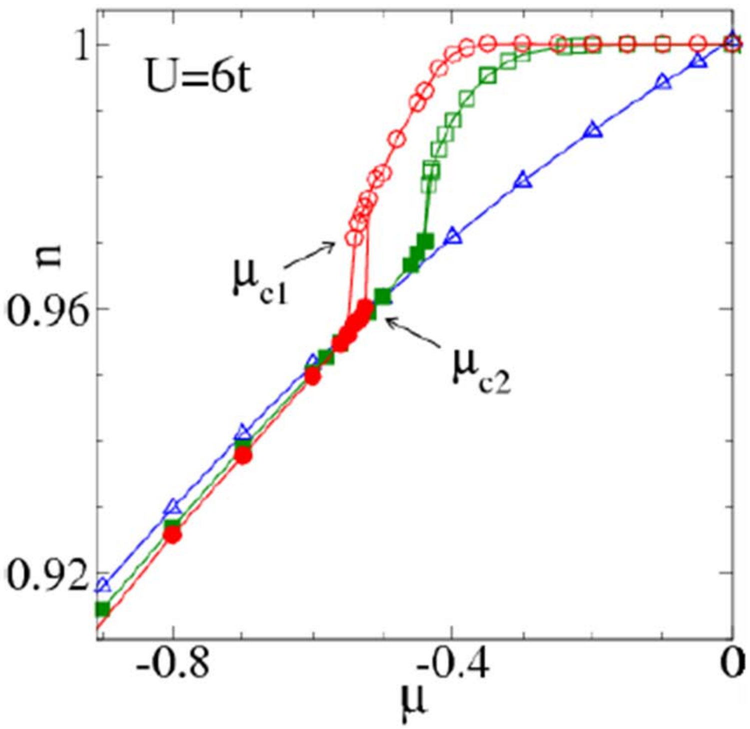
A. Macridin, M. Jarrell, and T. Maier,
Phys. Rev. B **74**, 085104 (2006)

E. Khatami, K. Mikelsons, D. Galanakis, A. Macridin, J. Moreno,
R. T. Scalettar, and M. Jarrell
PRB **81**, 201101(R) 2010

A. Liebsch, N.H. Tong, PRB **80**, 165126 (2009)

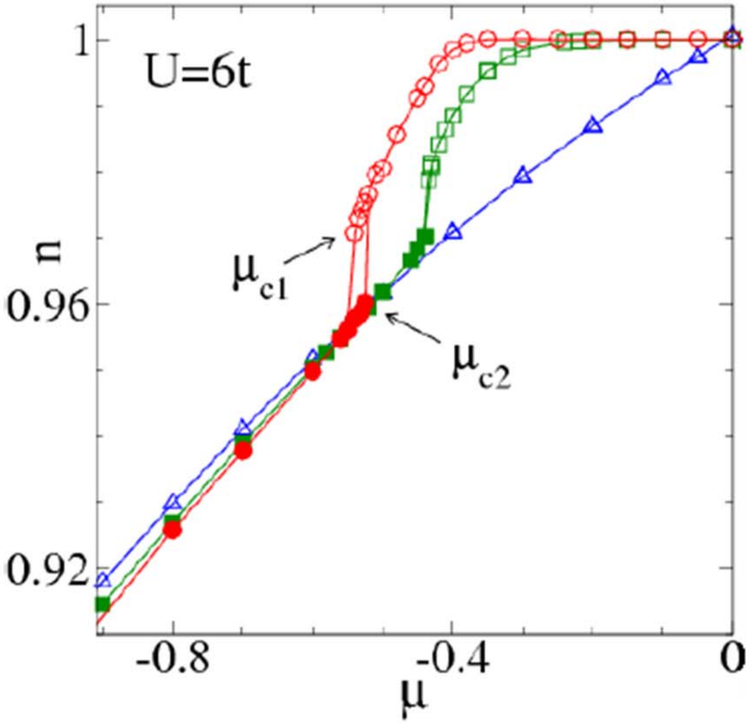
Here *t'=0*

First order transition at finite doping

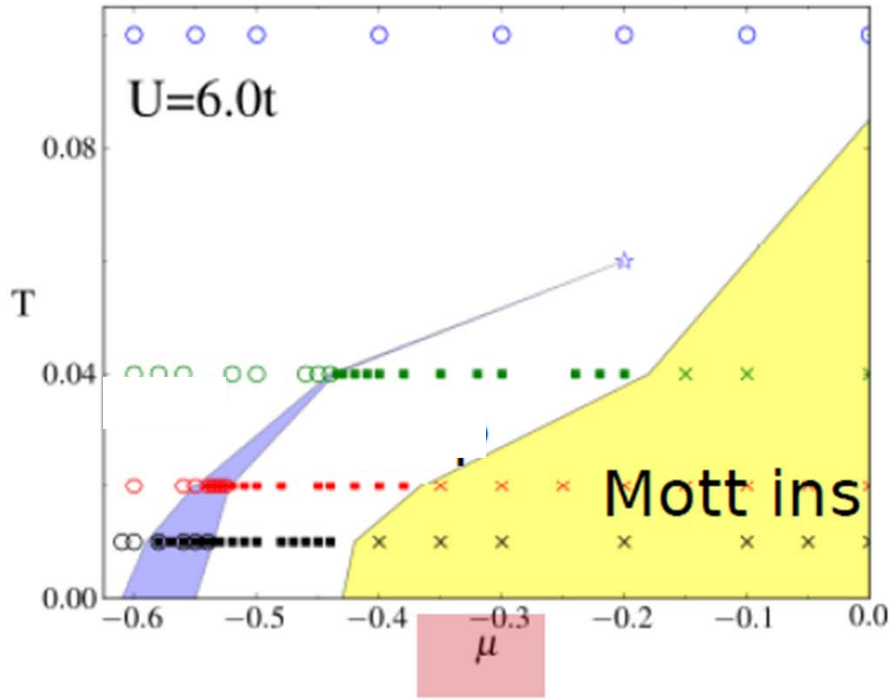


$n(\mu)$ for several temperatures:
$T/t =$1/10, 1/25, 1/50

First order transition at finite doping

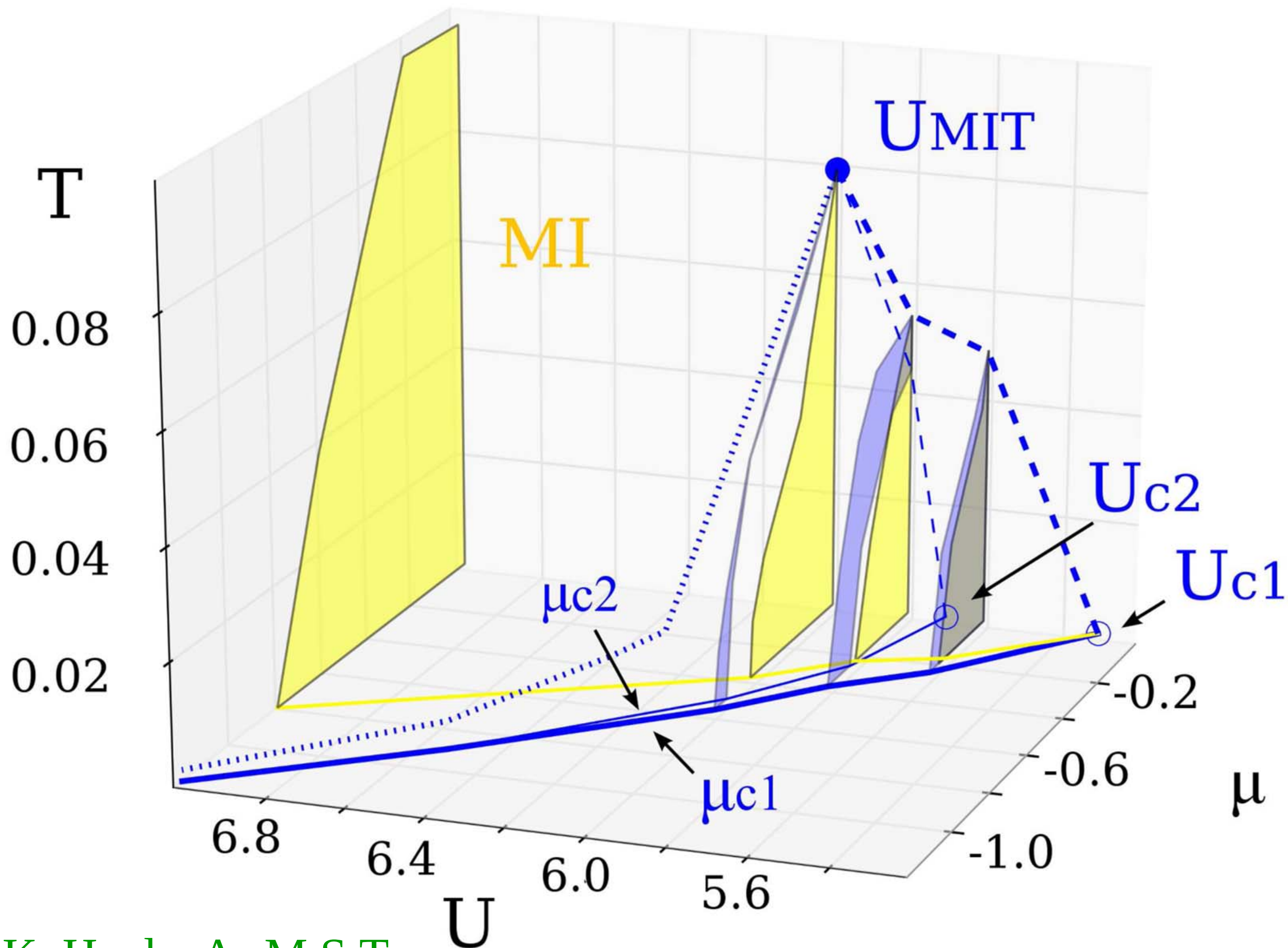


$n(\mu)$ for several temperatures: $T/t = 1/10,\ 1/25,\ 1/50$



Hysteretic behavior: fingerprint first order transition!

Normal state phase diagram



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

$\mu = 0$, H. Park, K. Haule, and G. Kotliar, Phys. Rev. Lett. 101, 186403 (2008).

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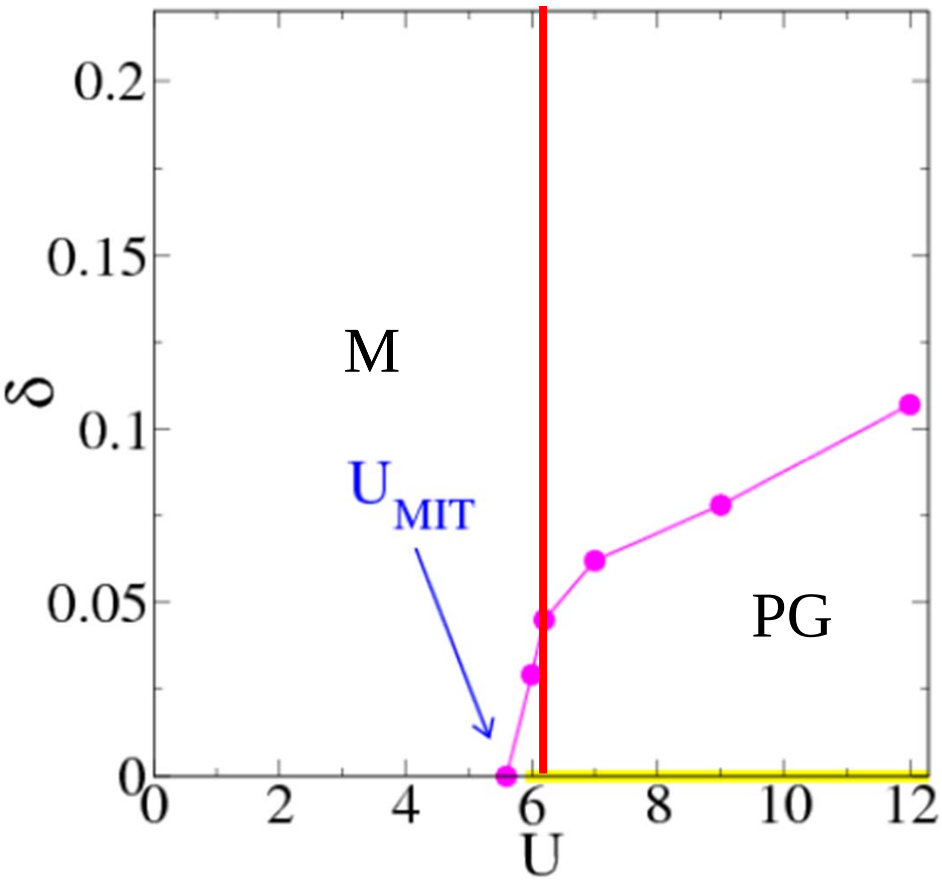
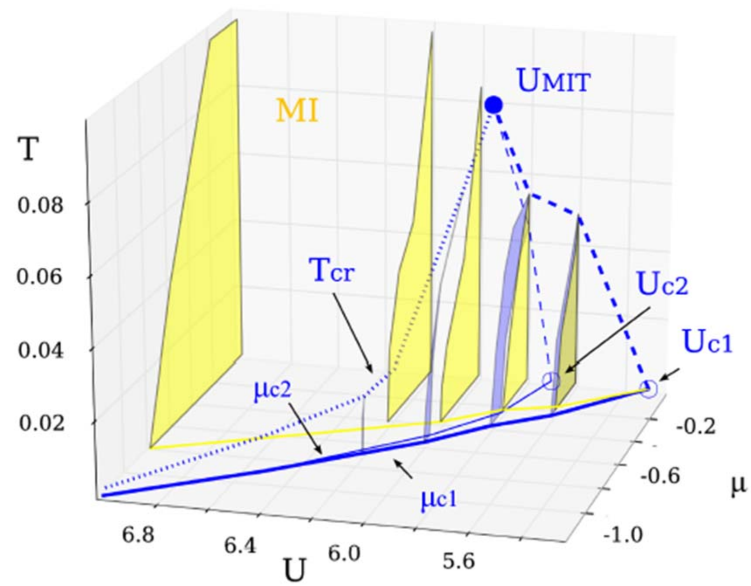
Link to Mott transition up to optimal doping

Doping dependence of critical point as a function of *U*



Smaller *D* and *S*



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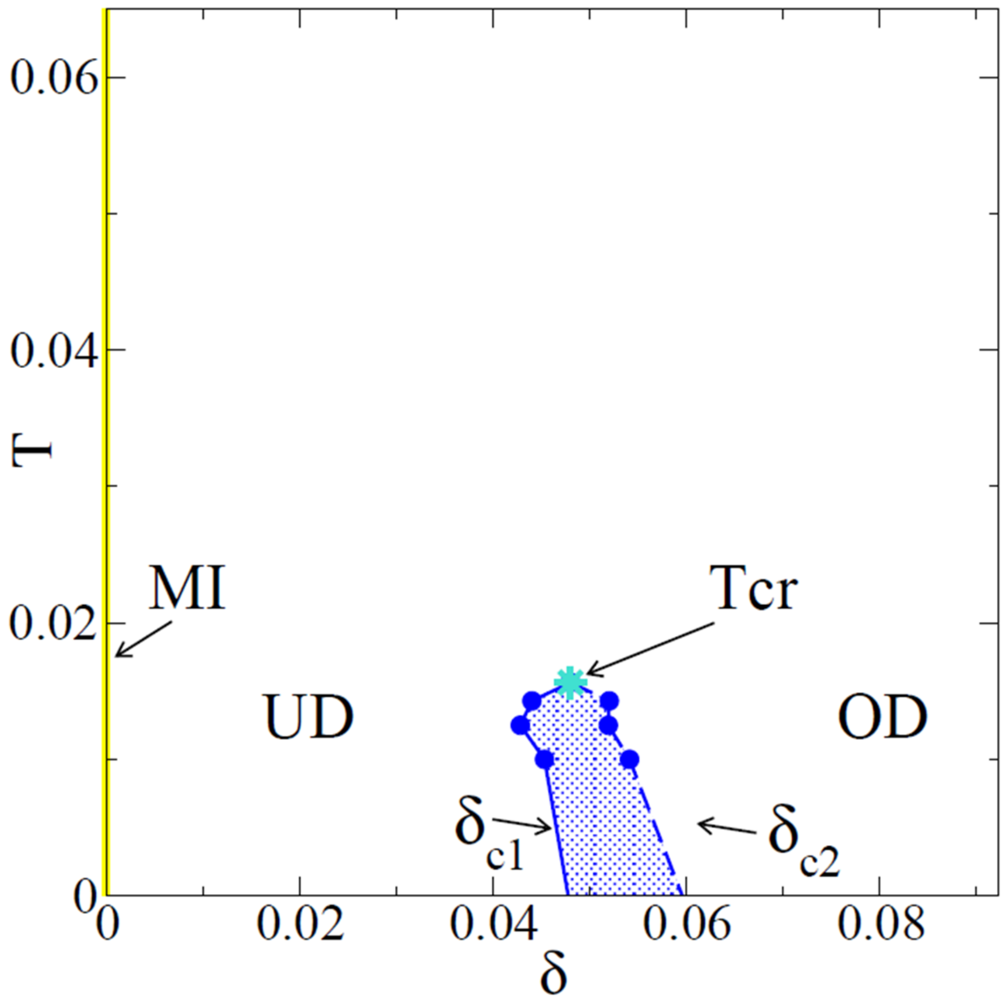
Characterisation of the phases (U=6.2t)



Giovanni Sordi

Patrick Sémon

Kristjan Haul

Widom line *(t' = 0)*

Pseudogap in the normal state and the Widom line

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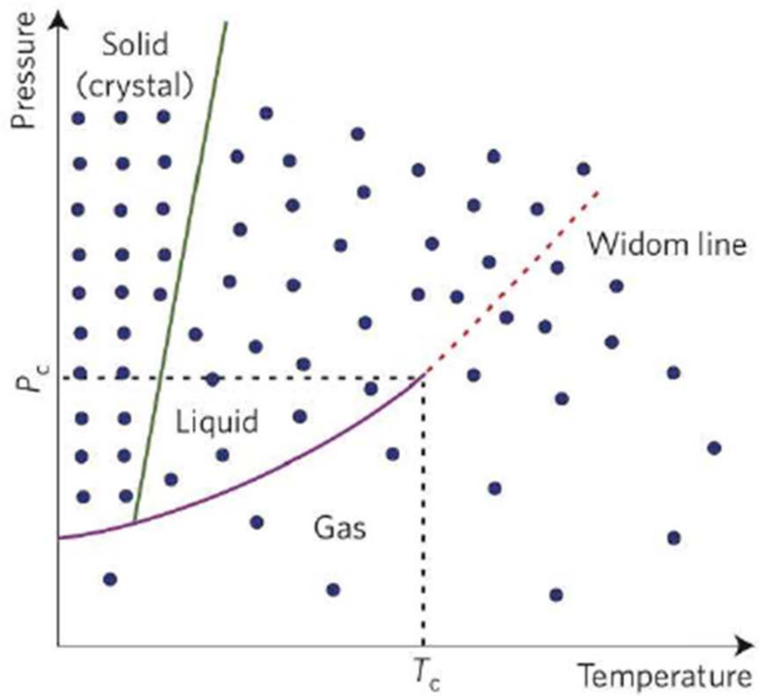
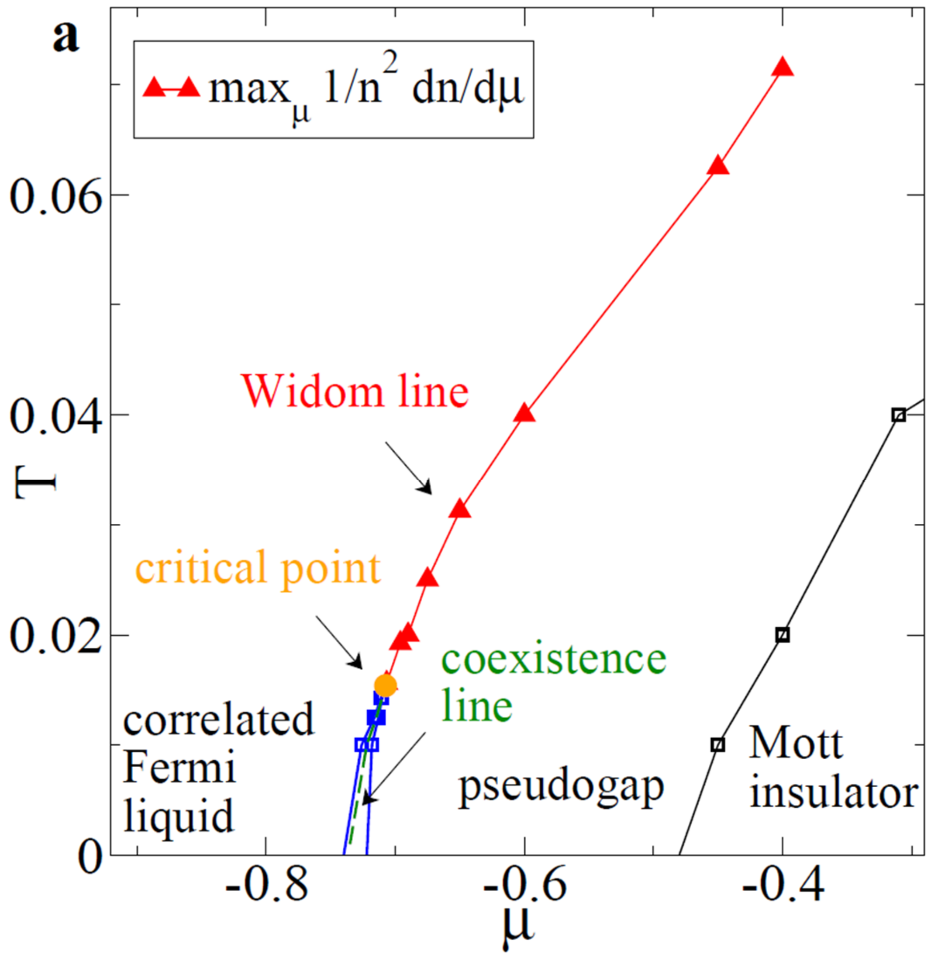
What is the Widom line?

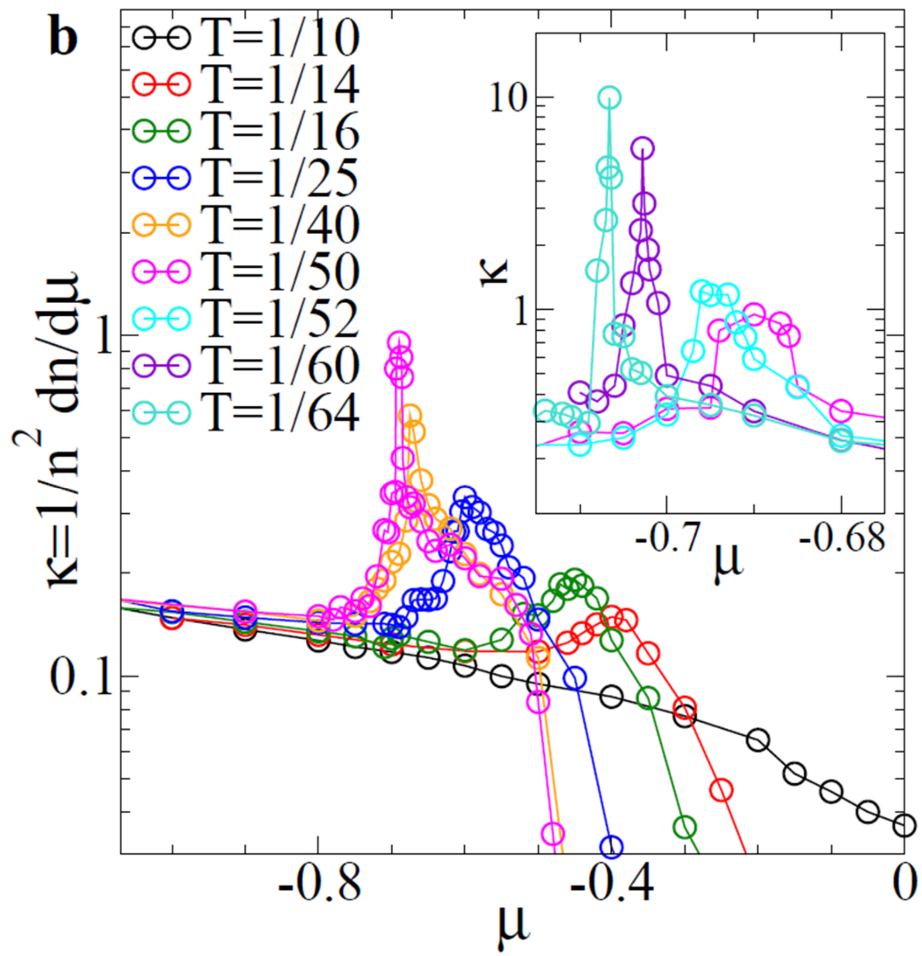


McMillan and Stanley, Nat Phys 2010

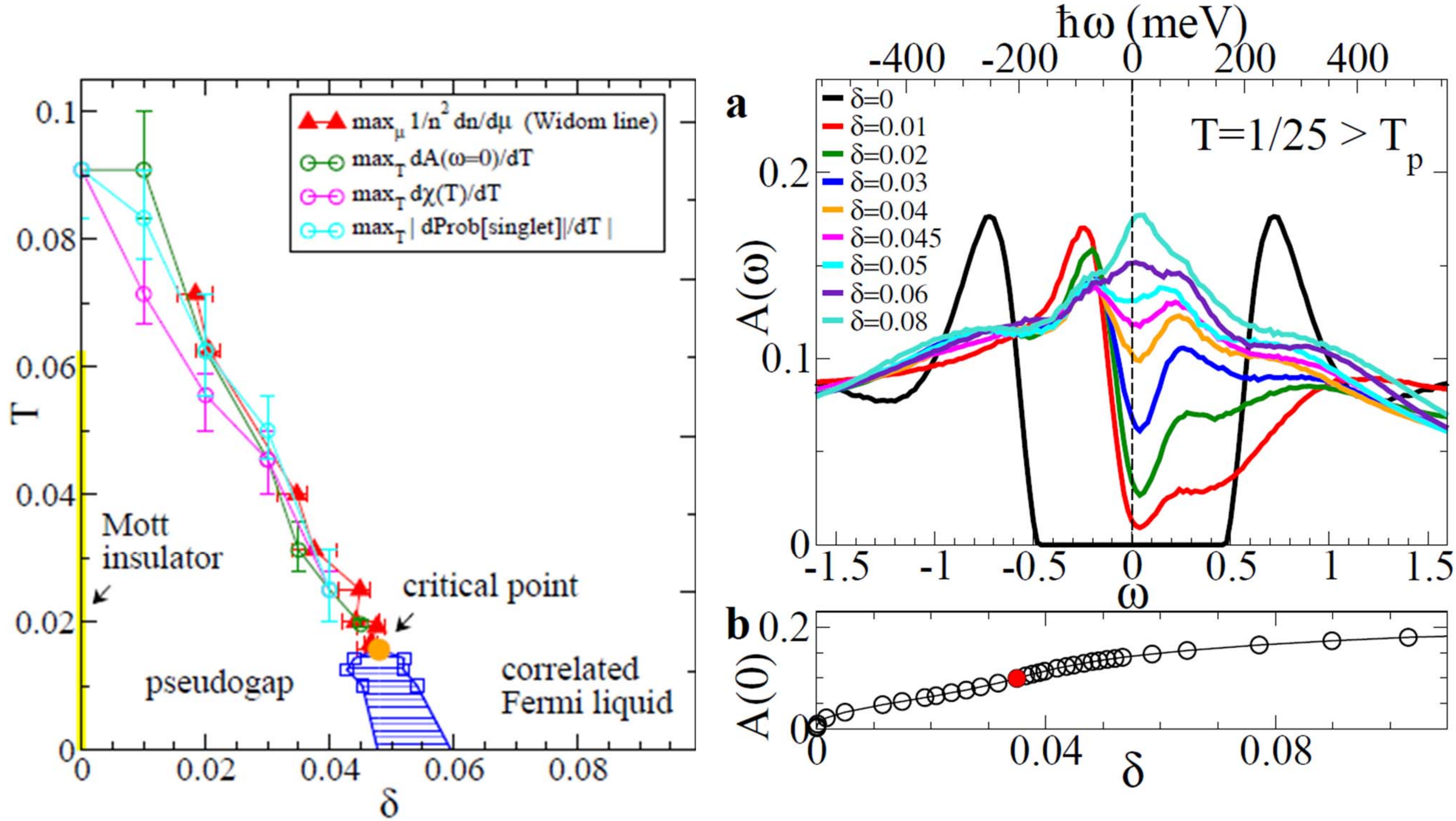
- it is the continuation of the coexistence line in the supercritical region
- line where the maxima of different response functions touch each other asymptotically as $T \to T_p$
- liquid-gas transition in water: max in isobaric heat capacity C_p, isothermal compressibility, isobaric heat expansion, etc
- DYNAMIC crossover arises from crossing the Widom line!
  water: Xu et al, PNAS 2005, Simeoni et al Nat Phys 2010

The Widom line

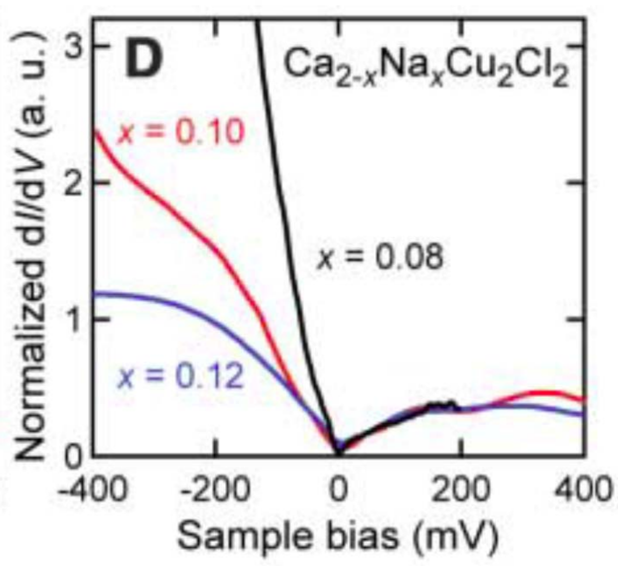


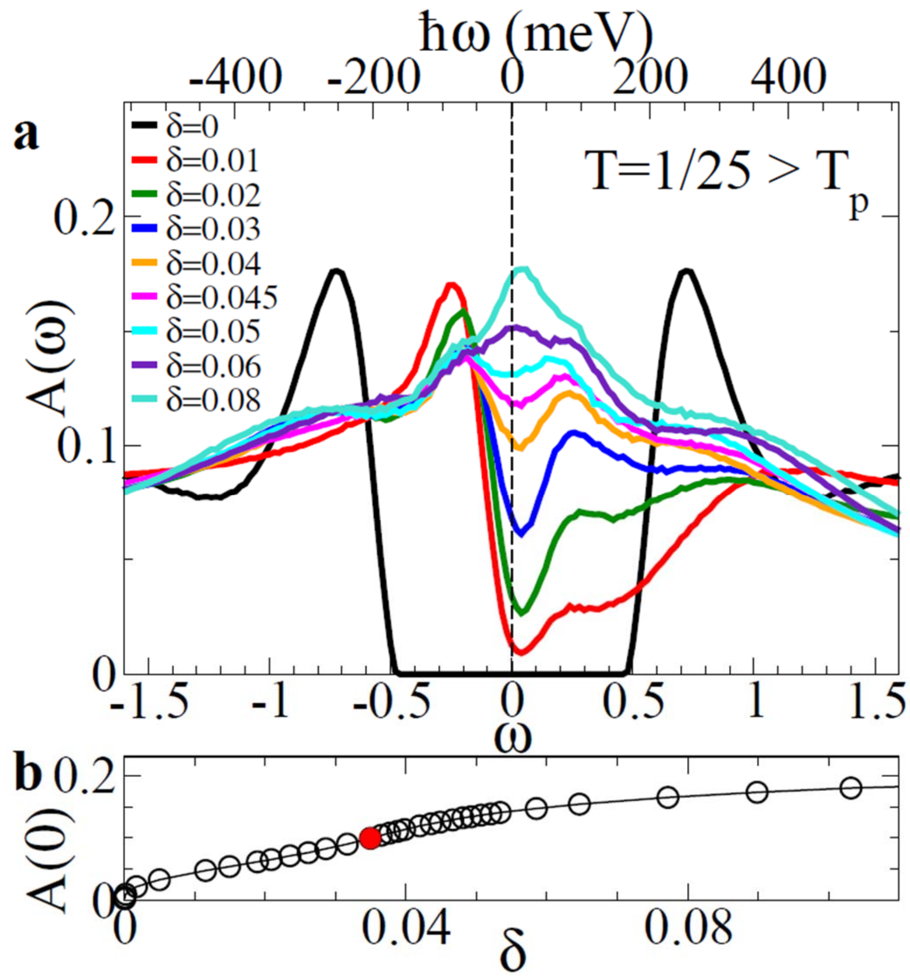


Density of states



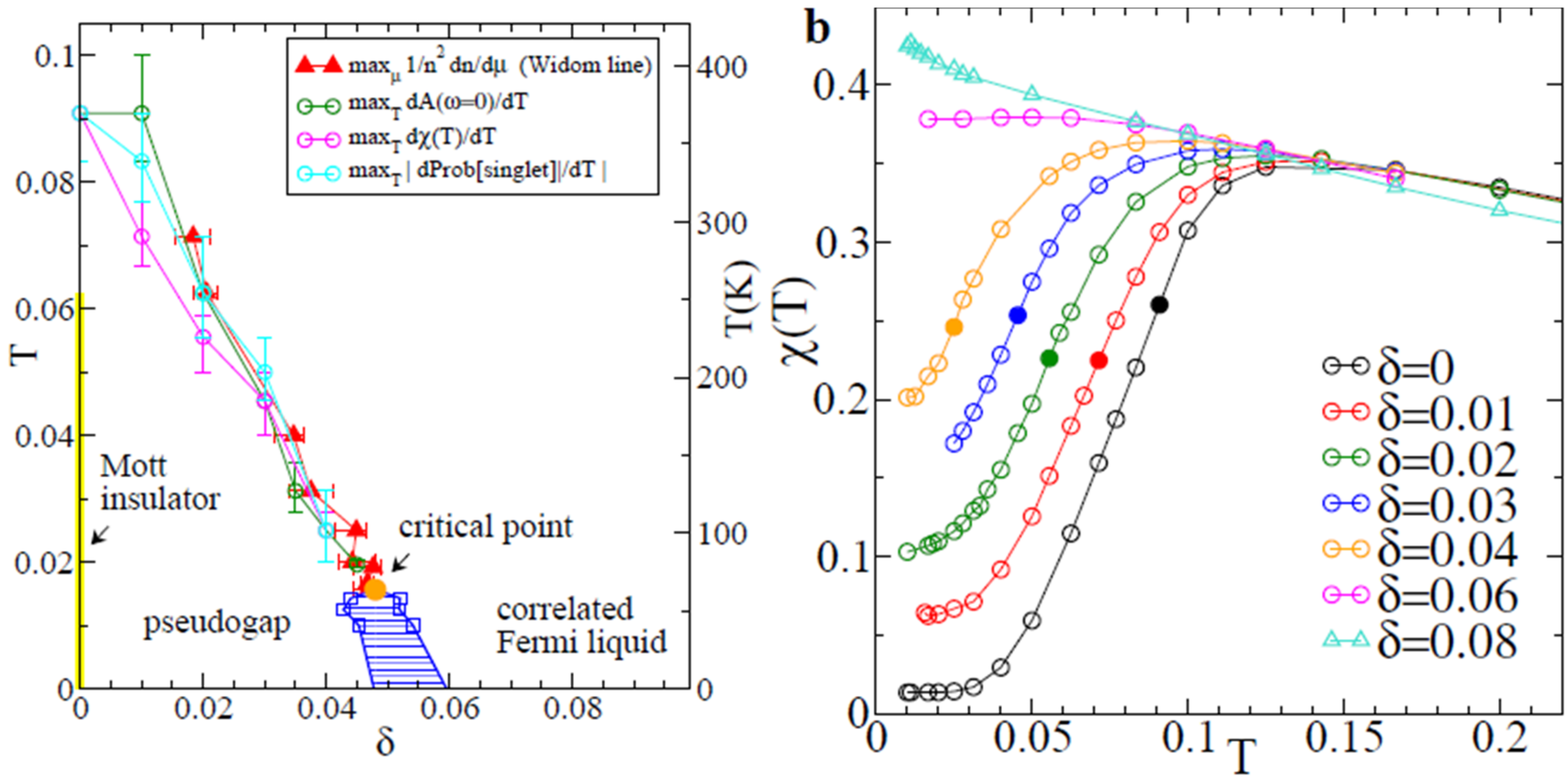
Density of states





Khosaka et al. *Science* **315**, 1380 (2007);

Spin susceptibility



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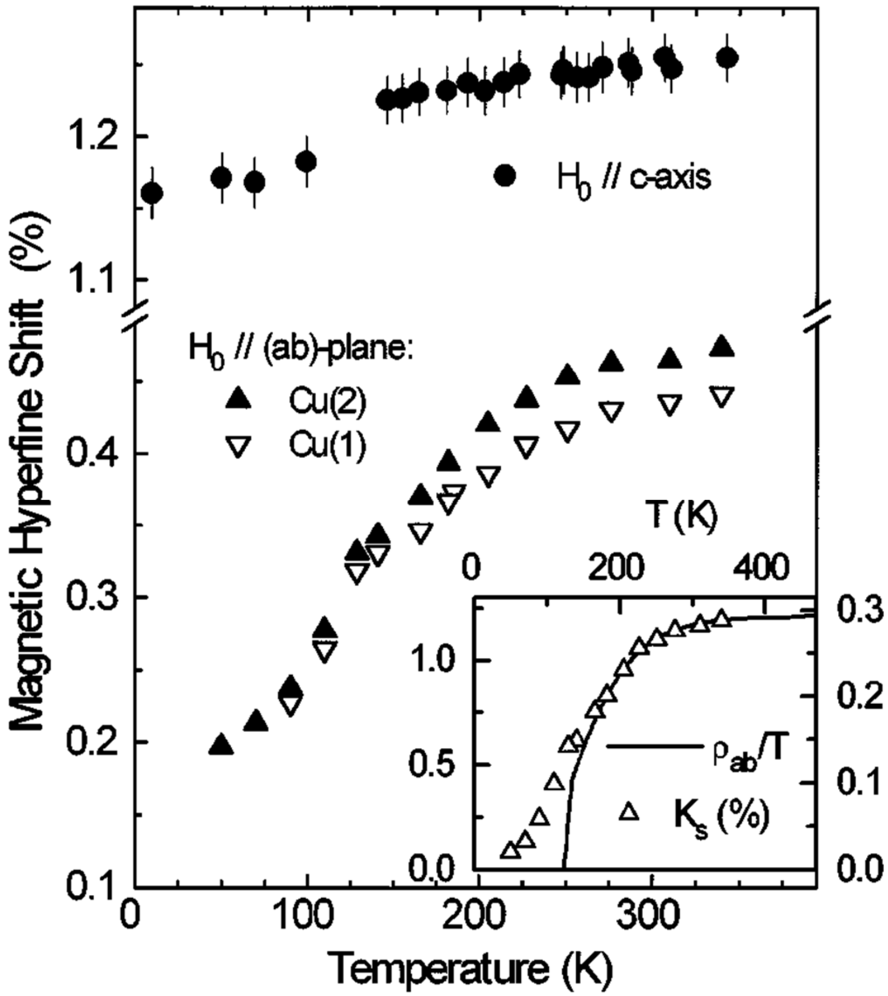
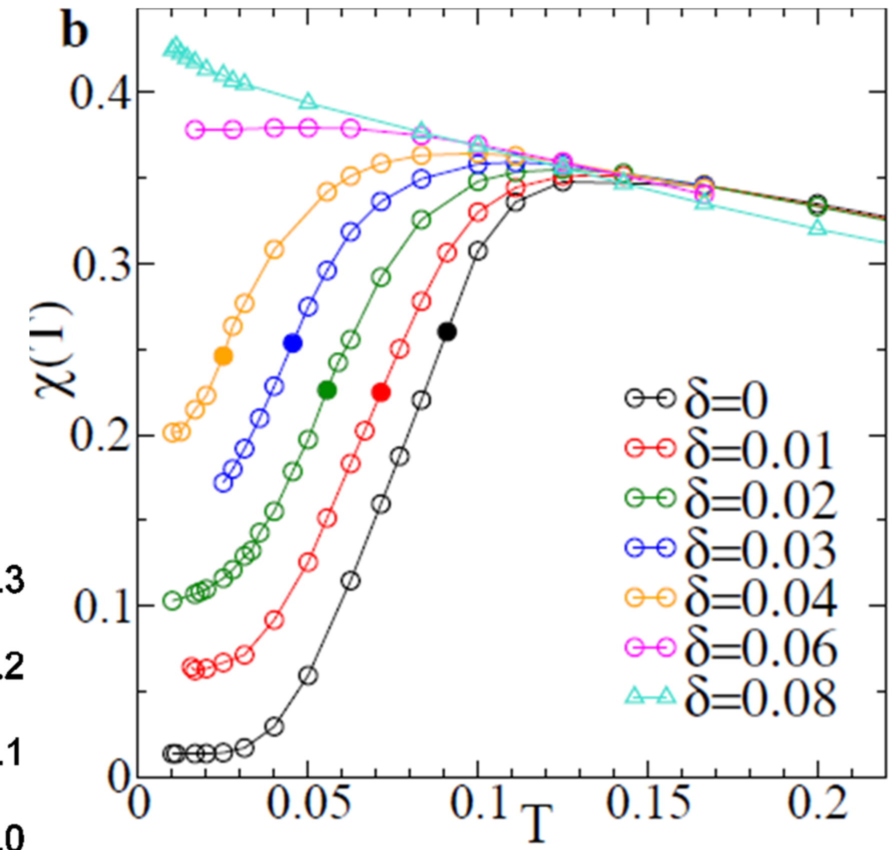
Spin susceptibility





Underdoped Hg1223

Julien et al. PRL **76,** 4238 (1996)

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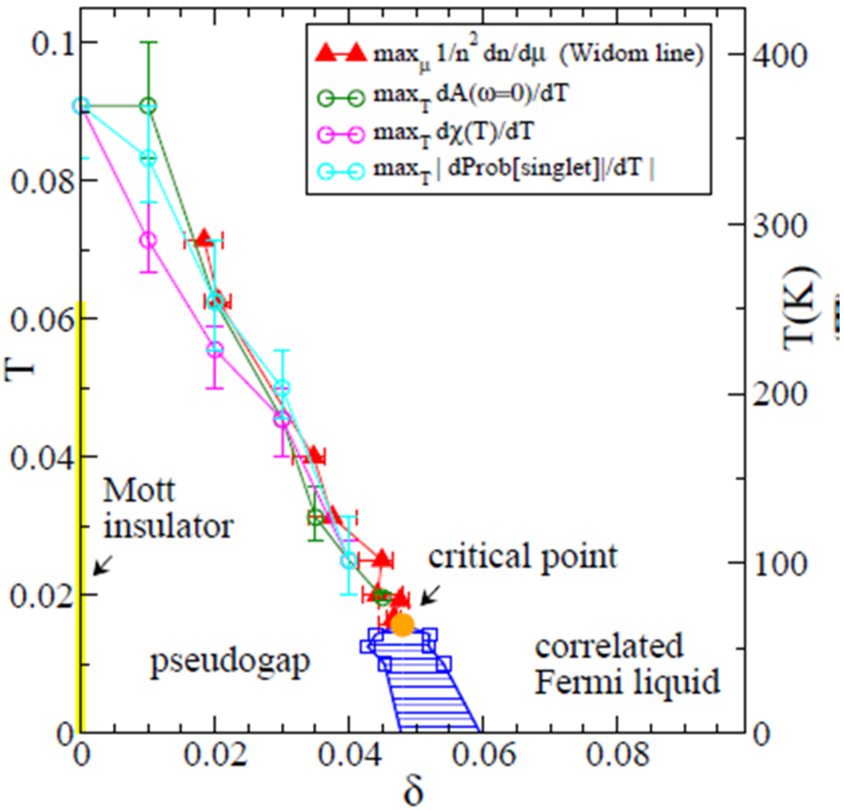
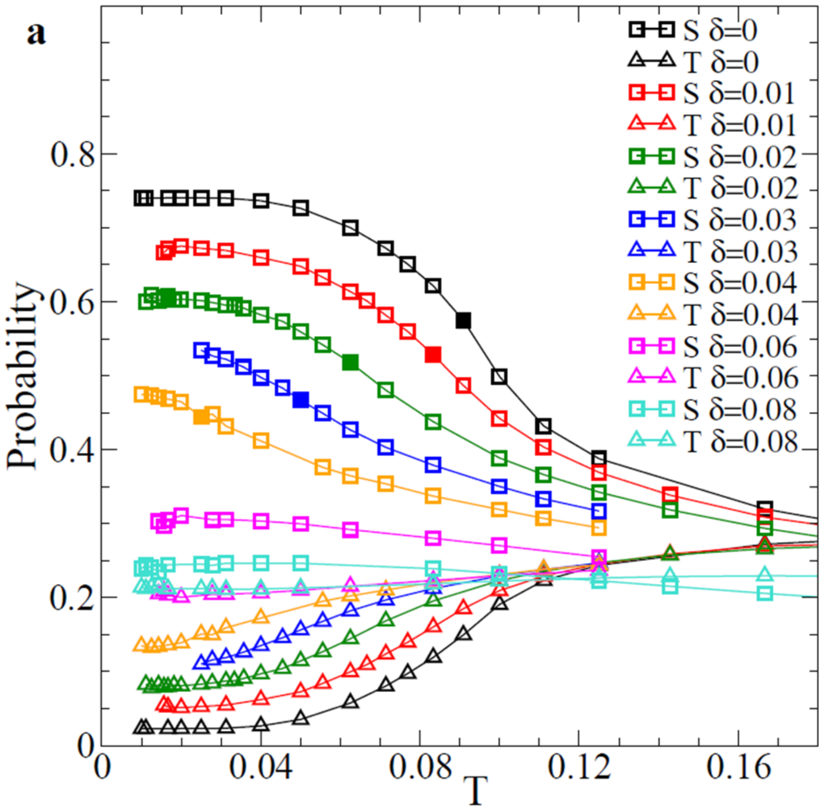
Physics

Plaquette eigenstates





See also:

Michel Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, A. Georges
PRB **80**, 064501 (2009)

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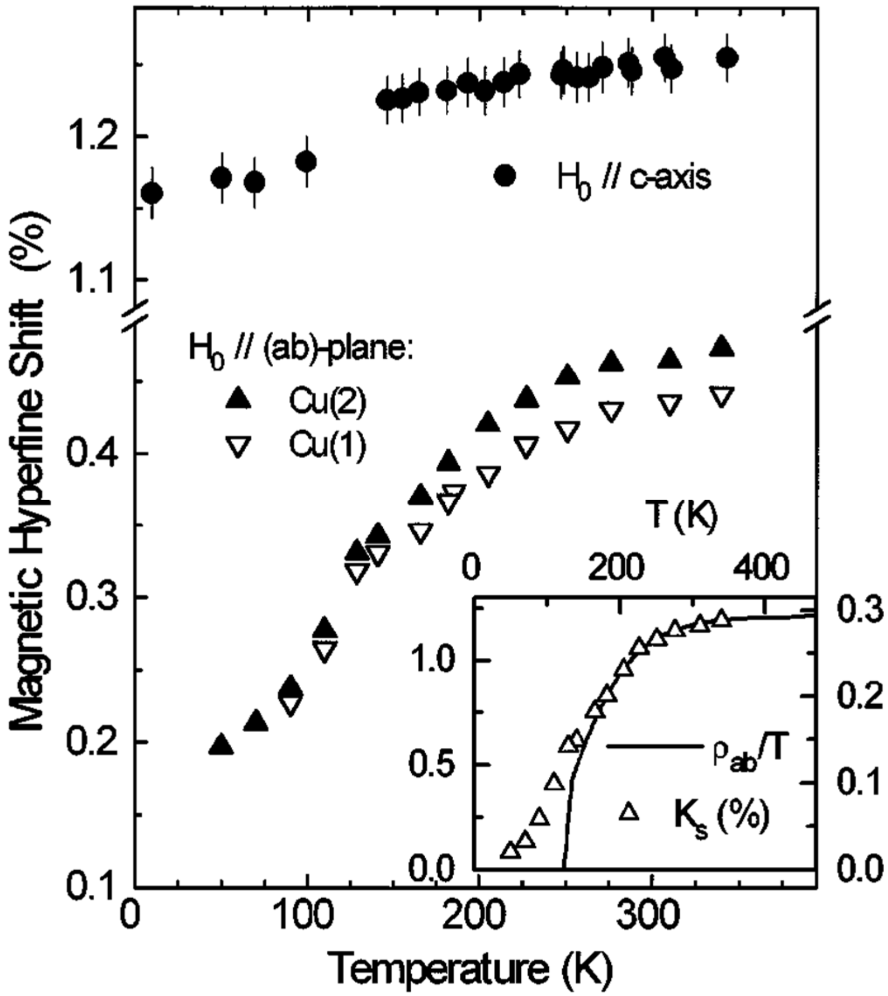
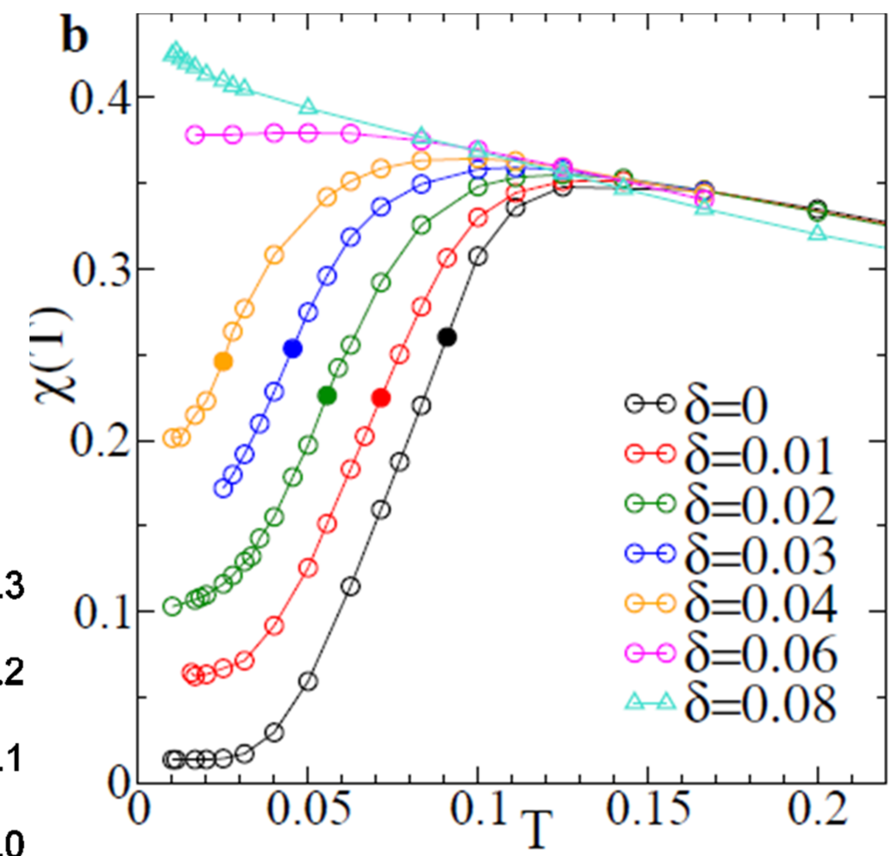
Spin susceptibility





Underdoped Hg1223

Julien et al. PRL **76,** 4238 (1996)

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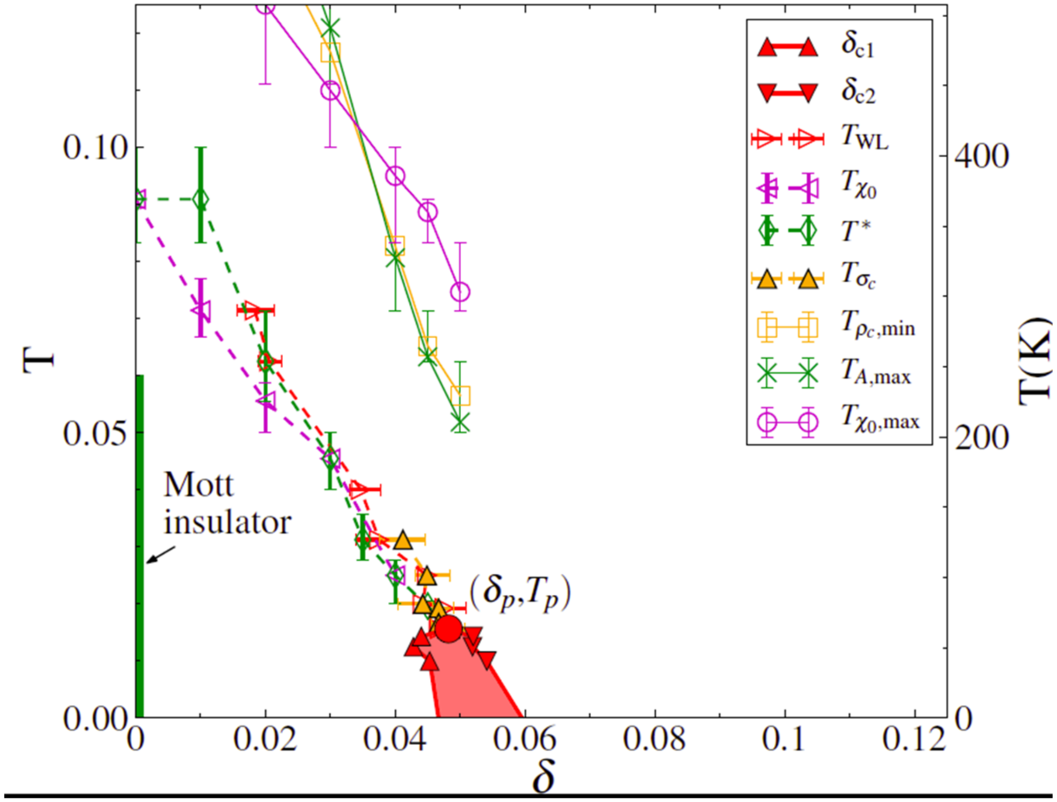
Two crossover lines

Giovanni Sordi

Patrick Sémon



G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)

P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B **89**, 165113/1-6 (2014)

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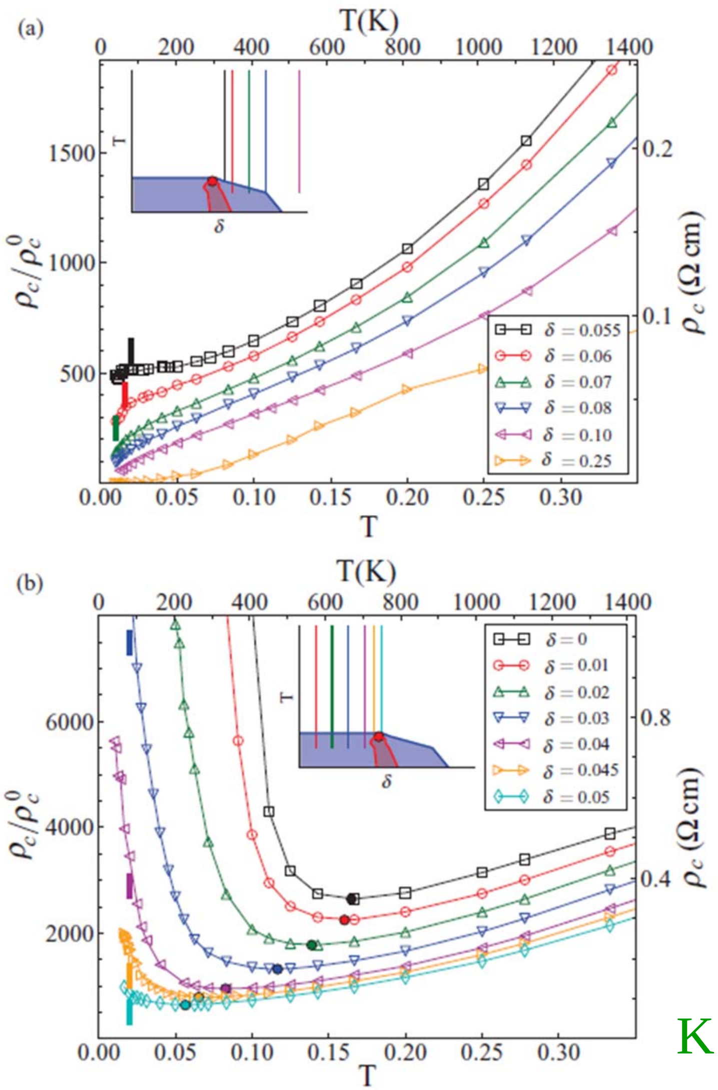
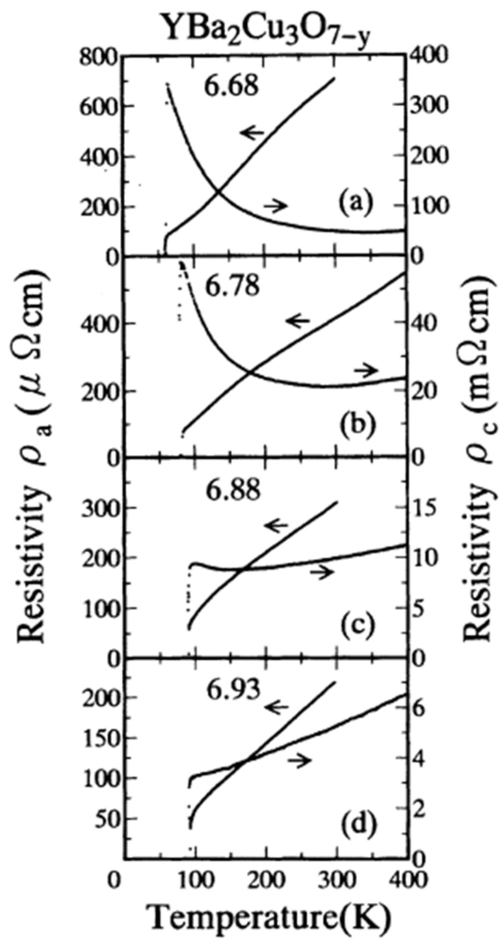
c-axis resistivity





K. Takenaka, K. Mizuhashi, H. Takagi, and S. Uchida, Phys. Rev.B 50, 6534 (1994).

What is the minimal model?

H. Alloul arXiv:1302.3473
C.R. Académie des Sciences, (2014)

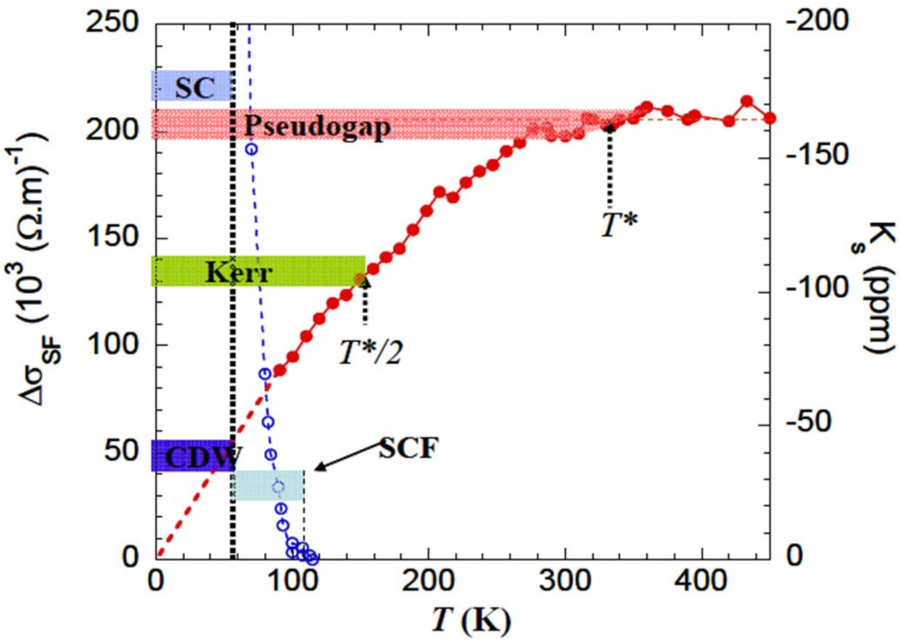


Fig 1 Spin contribution K_s to the ^{89}Y NMR Knight shift [11] for $YBCO_{6.6}$ permit to define the PG onset T^*. Here K_s is reduced by a factor two at $T \sim T^*/2$. The sharp drop of the SC fluctuation conductivity (SCF) is illustrated (left scale) [23]. We report as well the range over which a Kerr signal is detected [28], and that for which a CDW is evidenced in high fields from NMR quadrupole effects [33] and ultrasound velocity data [30]. (See text).

Anisotropy (nematicity)

Normal state and large anisotropy
in an *orthorhombic* crystal

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Underdoped metal very sensitive to anisotropy

$$\delta_\sigma = \frac{\sigma_x - \sigma_y}{(\sigma_x + \sigma_y)/2} \qquad t_{x,y} = t(1 \pm \delta_0/2)$$

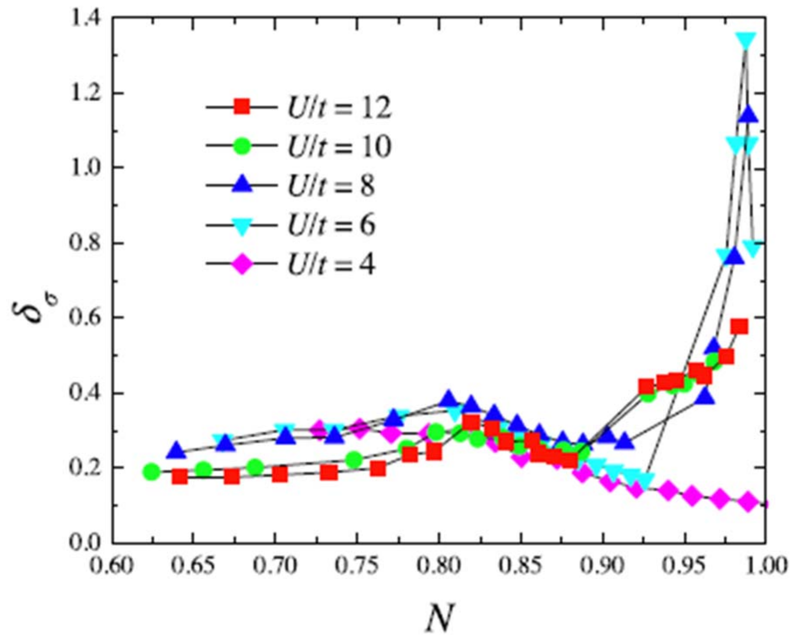
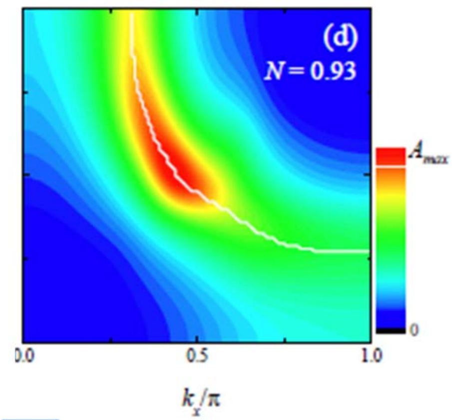
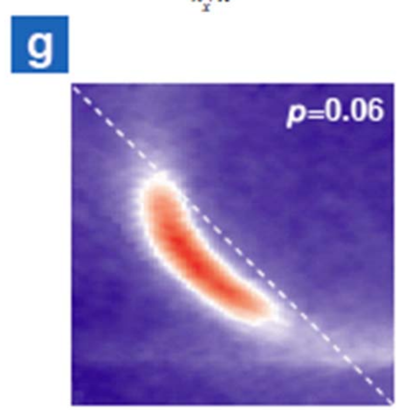


FIG. 3: (Color online) Anisotropy in the CDMFT conductivity $\delta_\sigma = 2\,[\sigma_x(0) - \sigma_y(0)]\,/\,[\sigma_x(0) + \sigma_y(0)]$ as a function of filling N for various values of U and $\eta = 0.1$, $\delta_0 = 0.04$.





Satoshi Okamoto

David Sénéchal

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

D. Fournier *et al.* Nature Physics (Marcello Civelli

At finite temperature anisotropy in Z

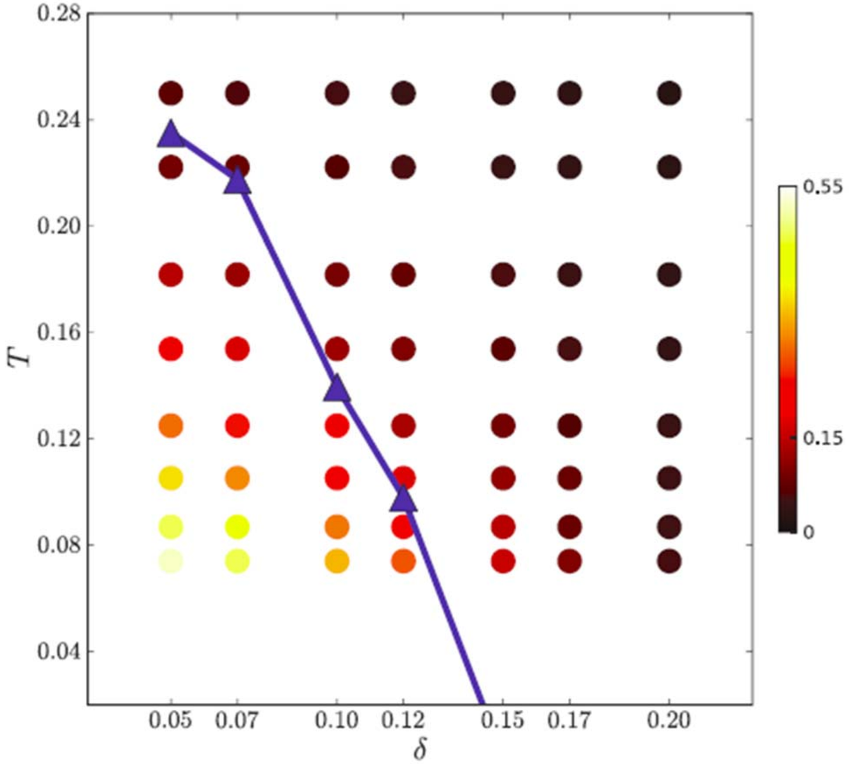


FIG. 3. (Color online) Color map of the anisotropic ratio of the quasiparticle weight σ_Z over the temperature-doping plane, for $U = 6t$. The solid blue curve indicates the pseudogap temperature $T^*(\delta)$ which is obtained as the temperature at which the uniform magnetic susceptibility $\chi_m[q = (0,0), T]$ has a maximum.

U = 6t, DCA, 4x4

Su, Maier, PRB **84**, 220506(R) (2011)

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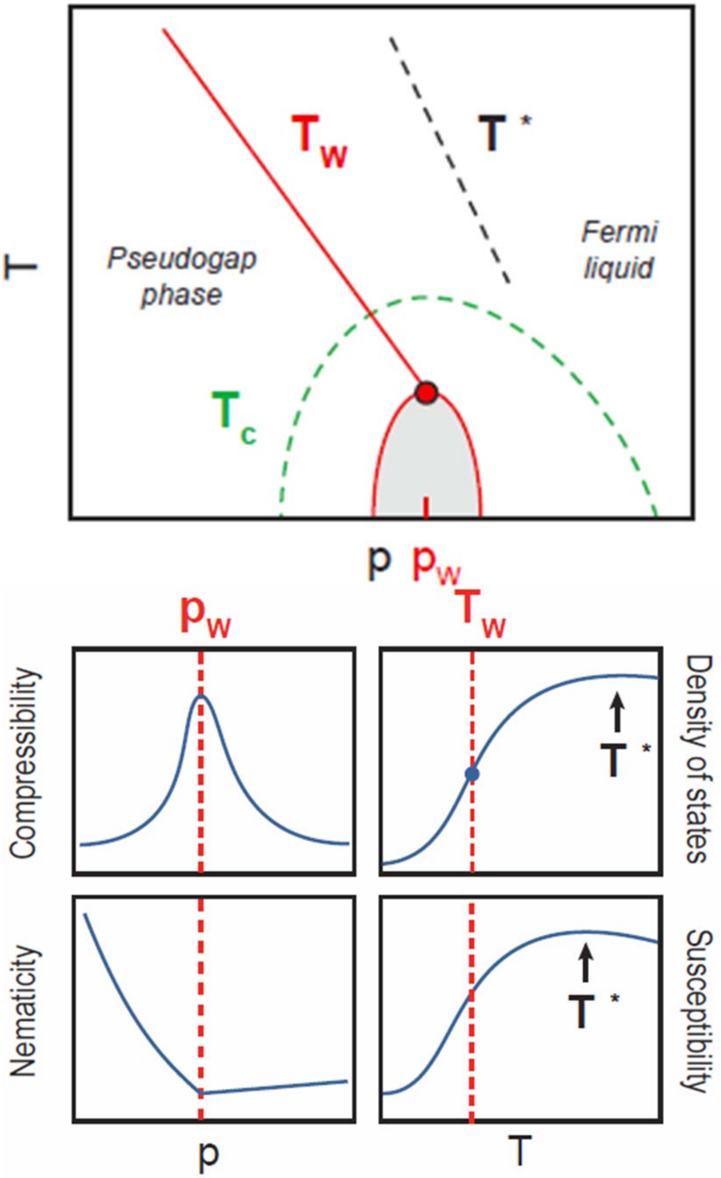
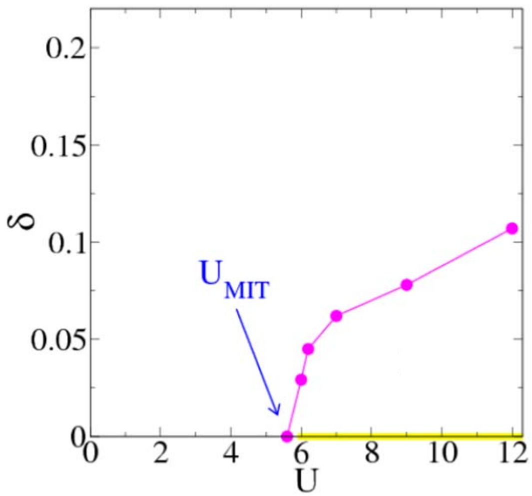
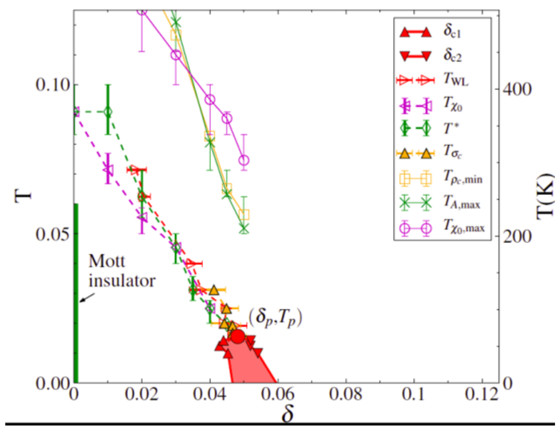
CDMFT: Emergent first-order transition



Summary: normal state





- Signatures of Mott physics extend way beyond half-filling
- Pseudogap is a phase
- Pseudogap *T** controlled by a Widom line and its precursor
- High compressibility (stripes?)
- Widom line
  - Thermodynamics (Susceptibility)
  - Transport (c-axis resistivity)
  - DOS

Superconductivity

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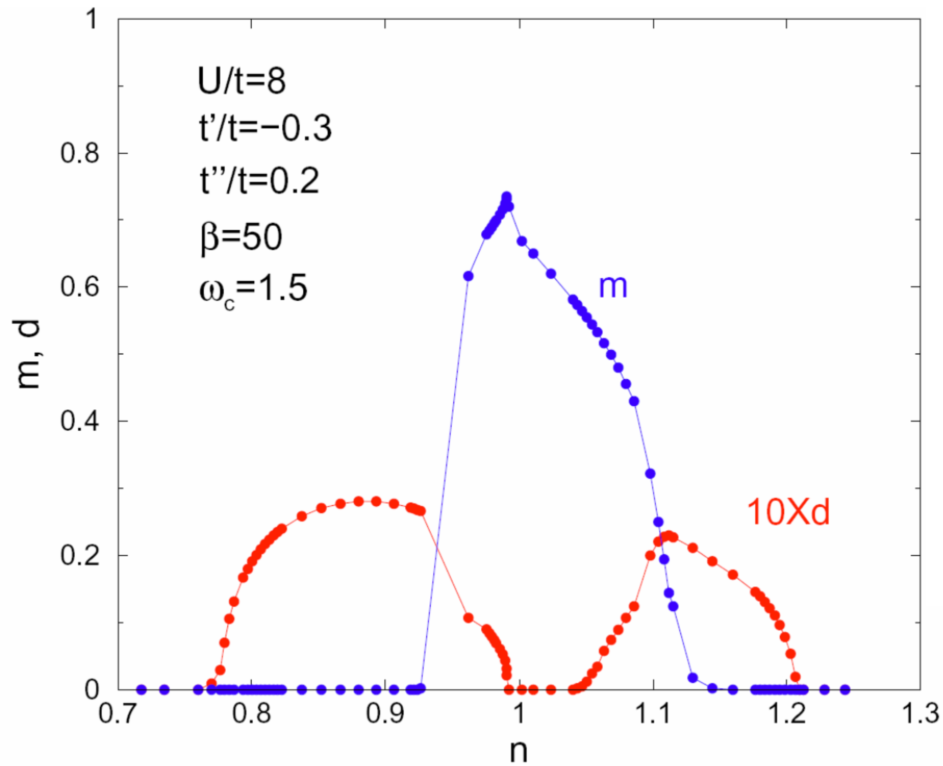
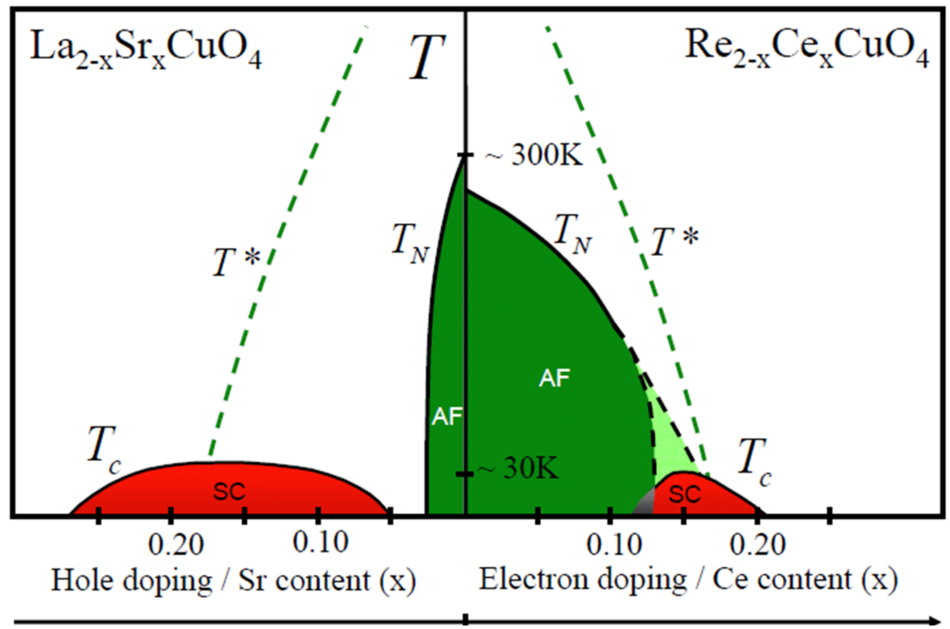
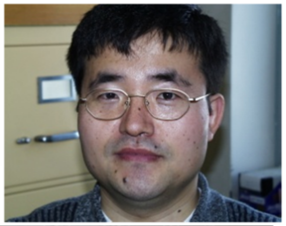
CDMFT global phase diagram



Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008)
AND Capone, Kotliar PRL (2006)



Armitage, Fournier, Greene, RMP (2009)



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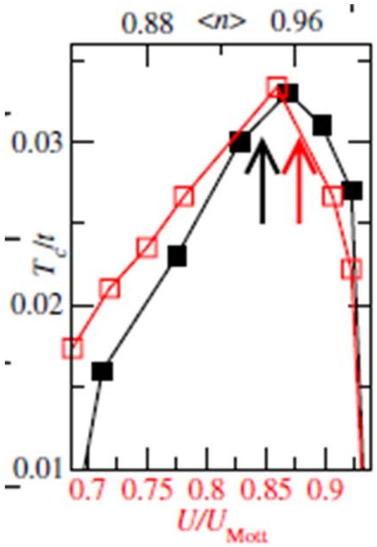
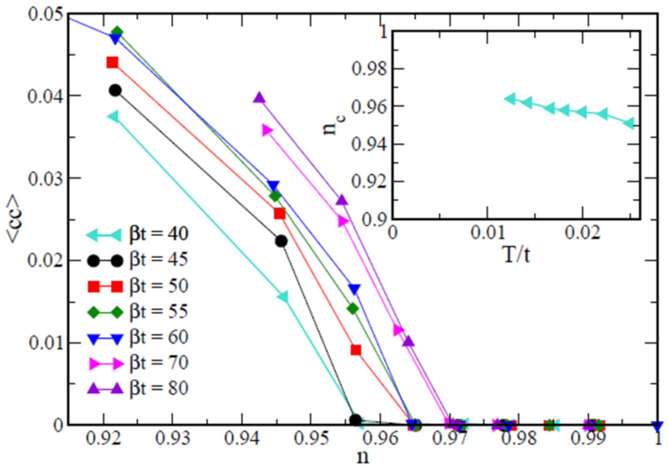
8 site clusters

8 site DCA, *U=6t*



Gull Parcollet Millis
PRL **110**, 216405 (20…

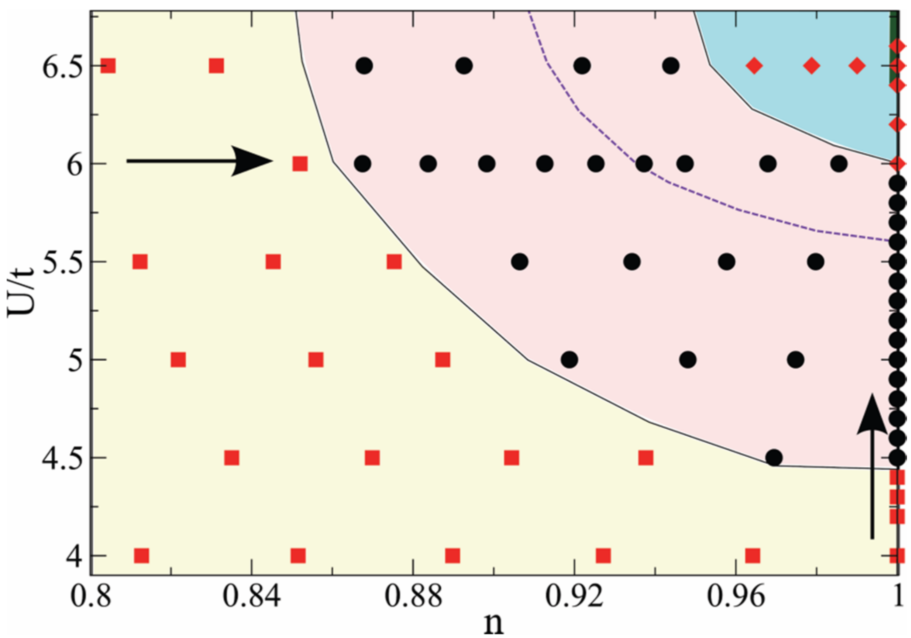
8 site DCA, *U=6.5t*

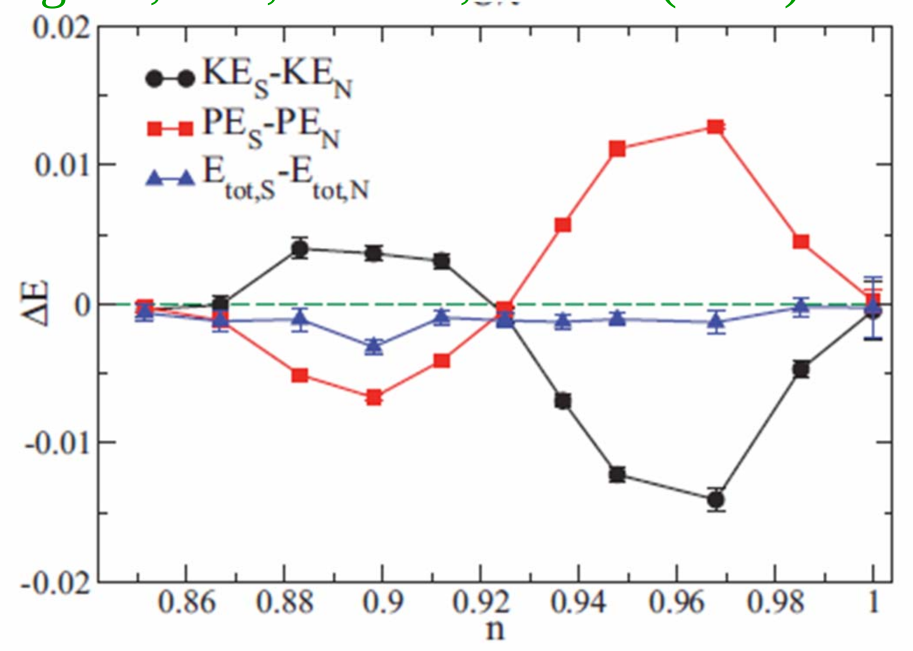


- In 2x2 T_c vanishes extremely close to half-filling. In larger cluster, earlier.
- Local pairs in underdoped (2x2)

Condensation energy

Experiments: Guy Deutscher, Phys. Rev. B 72, 092504(2005)
N. Bontemps et al. Annals of Physics 321 (2006) 1547–1558
F. Carbone, A. B. Kuzmenko, H. J. A. Molegraaf, et al, PRB **74**, 064510 (2006)





U = 6t, T = 1/60, 8 sites – DCA

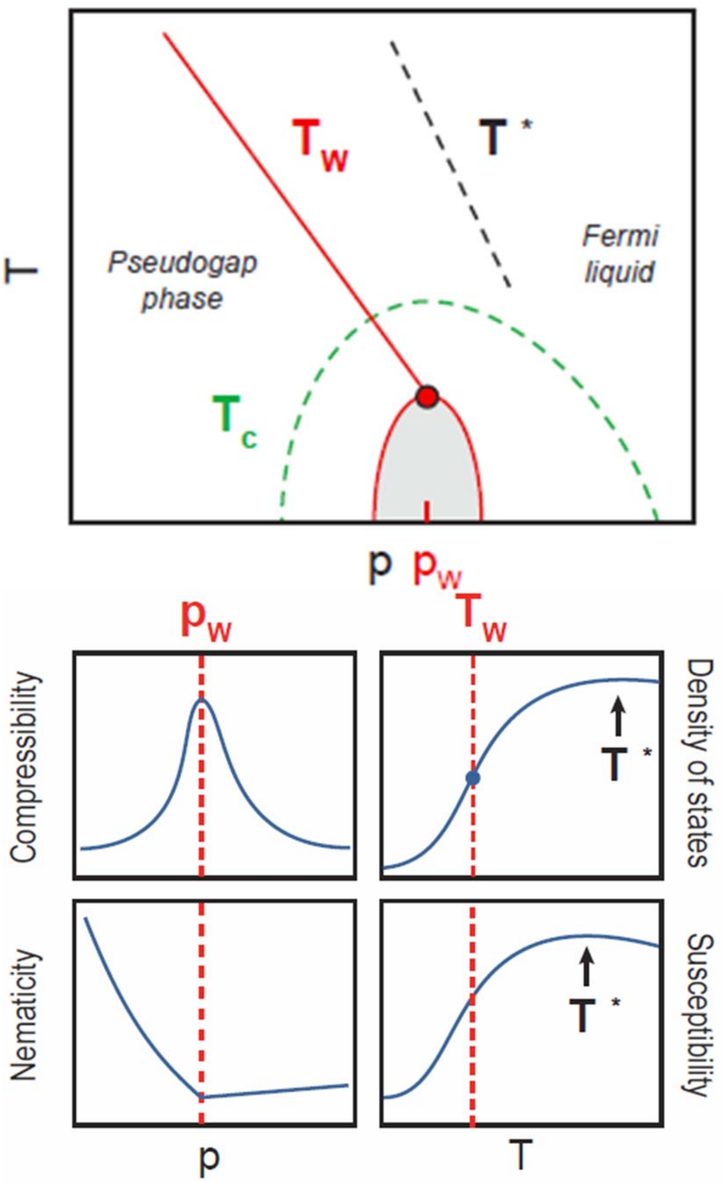
E. Gull, A. Millis, PRB **86**, 241106(R) (2012)

See also

Th. A. Maier, M. Jarrell, et al. PRL **92,** 027005 (2004)
K. Haule, G. Kotliar EPL, 77 (2007) 27007

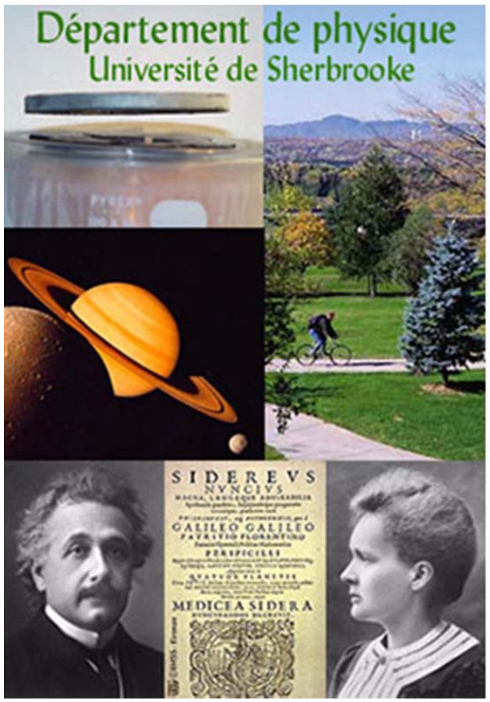
Summary

CDMFT: Emergent first-order transition



- Is the pseudogap (PG) a crossover or a phase transition ?
- Origin of nematicity ?
- Why a dome of SC ?
- Why superconducting ?
- Does a one-band model capture the key physics ?
- Lessons from other SC?
  - Organics
  - Heavy fermions
- AFM QCP important?
- Relation between CDW and the PG ?
- Why CDW peaked at 12% doping ?

André-Marie Tremblay



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Merci

Thank you