COLLÈGE DE FRANCE
1530

CIFAR
CANADIAN INSTITUTE for ADVANCED RESEARCH

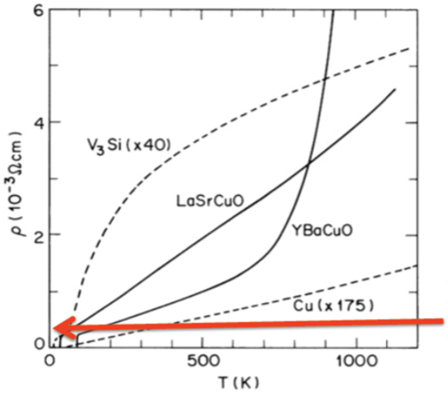
Lecture 2: Doped Mott insulators Strongly correlated superconductivity and its normal phase

André-Marie Tremblay

UNIVERSITÉ DE SHERBROOKE

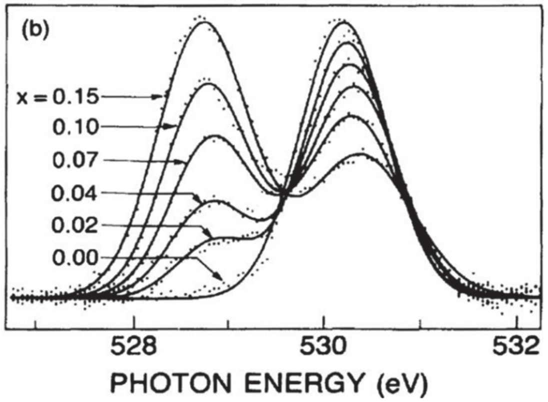
Collège de France, 16 mars 2015
17h00 à 18h30

Last time

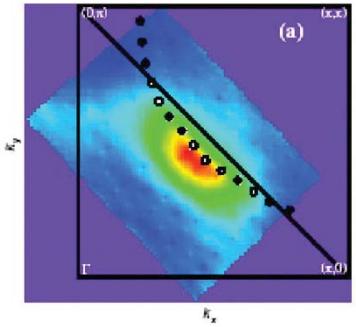


Gurvitch & Fiory
PRL 59, 1337
(1987)

MIR limit
Mean-free path
~ Fermi wavelength



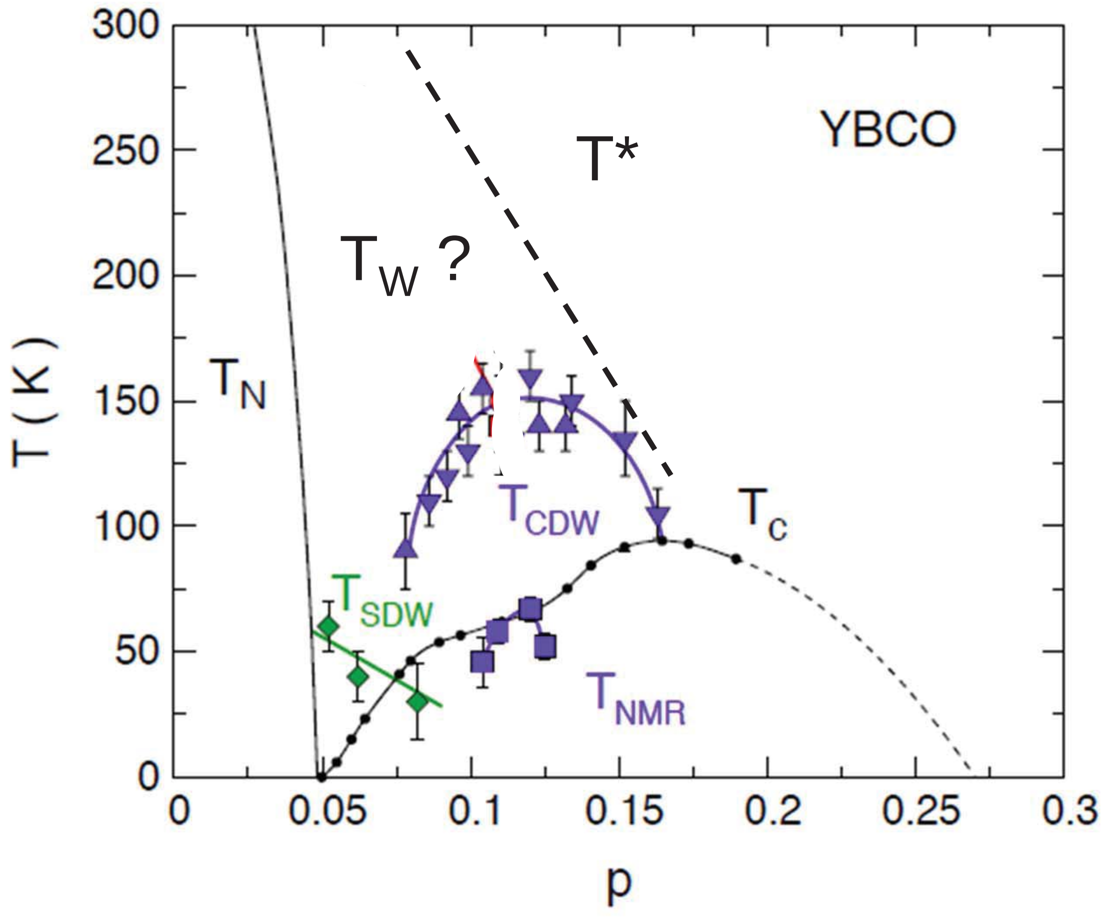
Hole-doped, 10%



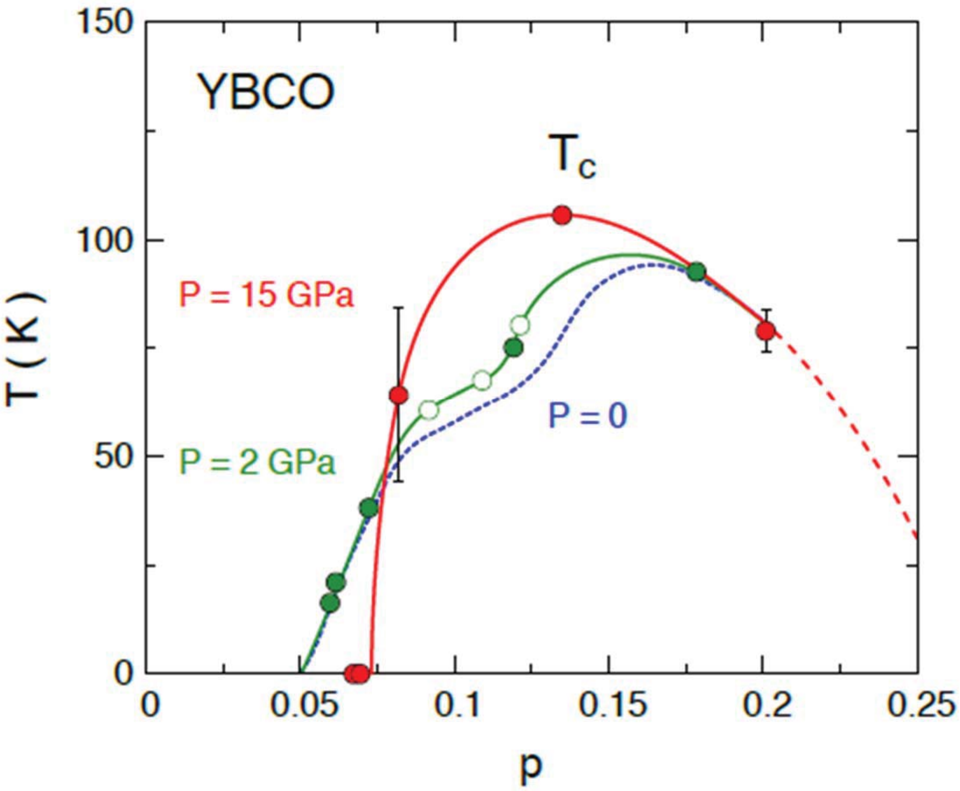
F. Ronning et al. Jan. 2002, $Ca_{2-x}Na_xCuO_2Cl_2$

$$H = \sum_{ij\sigma}(t_{ij} - \delta_{ij}\mu)c^{\dagger}_{i\sigma}c_{j\sigma} + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

Phase diagram for hole-doped cuprates

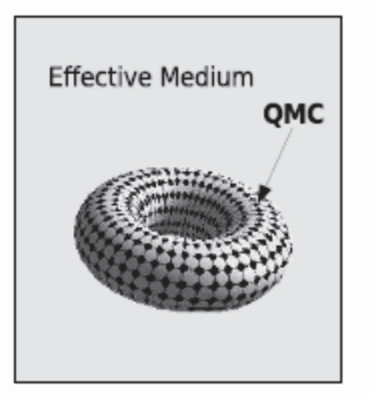


Getting rid of the CDW



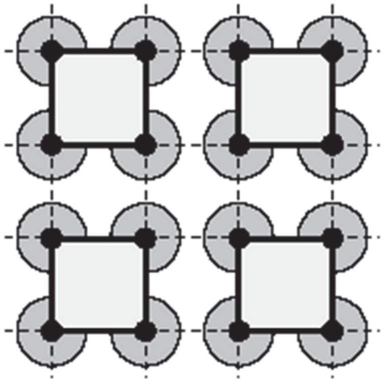
Cyr-Choinière et al, arxiv1503.02033

2d Hubbard: Quantum cluster method

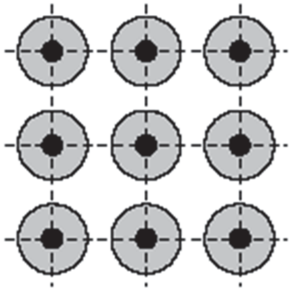


DCA

C-DMFT



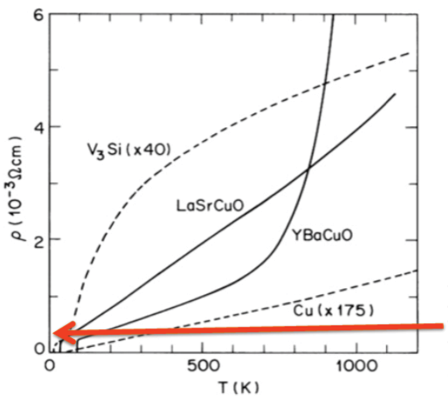
DMFT



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)

Last time



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MIR limit
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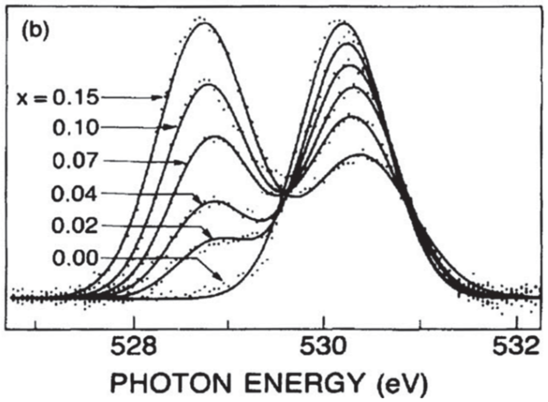
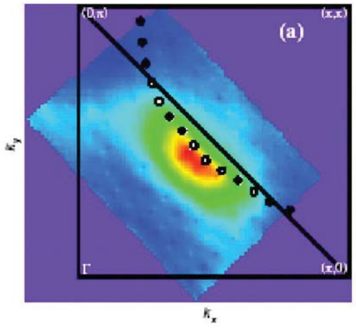
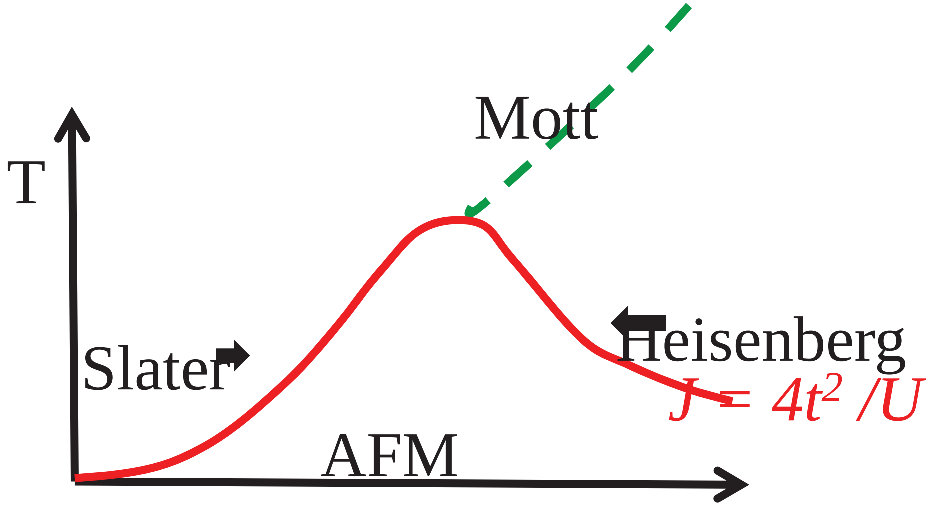


Hole-doped, 10%



F. Ronning et al. Jan. 2002, $Ca_{2-x}Na_xCuO_2Cl_2$

$$H=\sum_{ij\sigma}(t_{ij}-\delta_{ij}\mu)c^{\dagger}_{i\sigma}c_{j\sigma}+U\sum_{i}n_{i\uparrow}n_{i\downarrow}$$



T

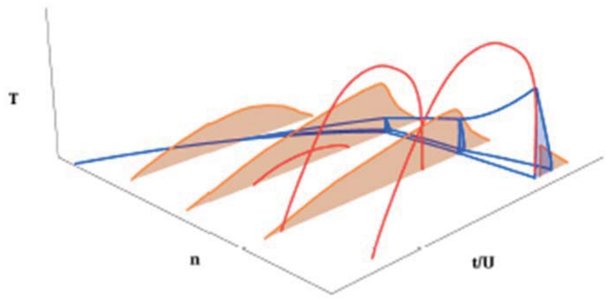
Mott

Slater

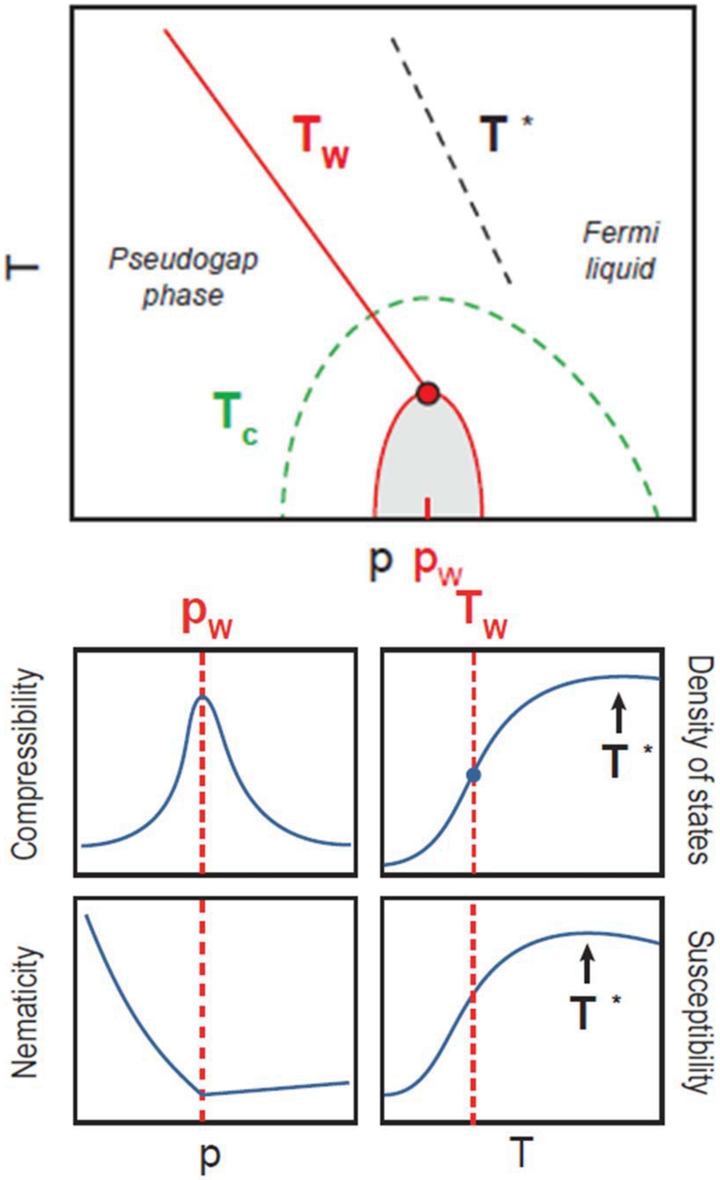
Heisenberg

$J = 4t^2/U$

AFM



CDMFT: Emergent first-order transition



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

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Today

- « Normal » state of cuprates
  - Signatures of Mott physics away from $n=1$
- Superconductivity
  - What is special about strongly correlated SC
  - Origin

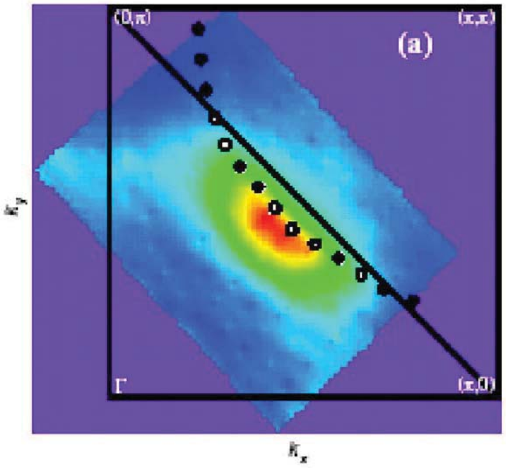
ARPES pseudogap

Strong correlation pseudogap (U > 8t)

- Different from Mott gap that is local (all k) not tied to ω=0.
- Pseudogap close to ω=0 and only in regions nearly connected by (π,π). (e and h),
- Pseudogap is independent of cluster shape (and size) in CPT.
- Not caused by AFM LRO
  - No LRO, few lattice spacings.
  - Not very sensitive to *t'*
  - Scales like *t*.

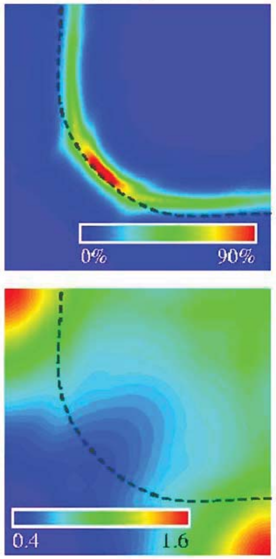
Sénéchal, AMT, PRL **92**, 126401 (2004).

Hole-doped, 10%

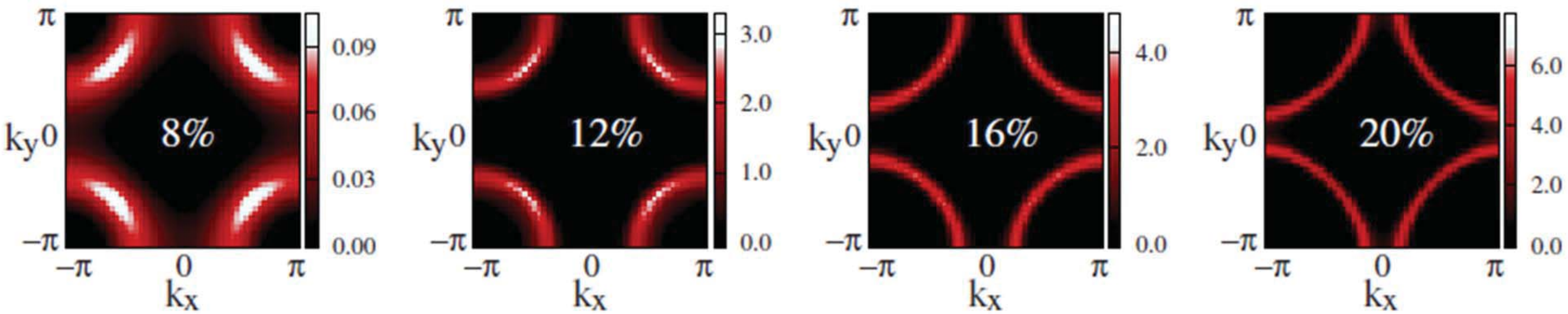


F. Ronning et al. Jan. 2002, $Ca_{2-x}Na_xCuO_2Cl_2$

U= 8



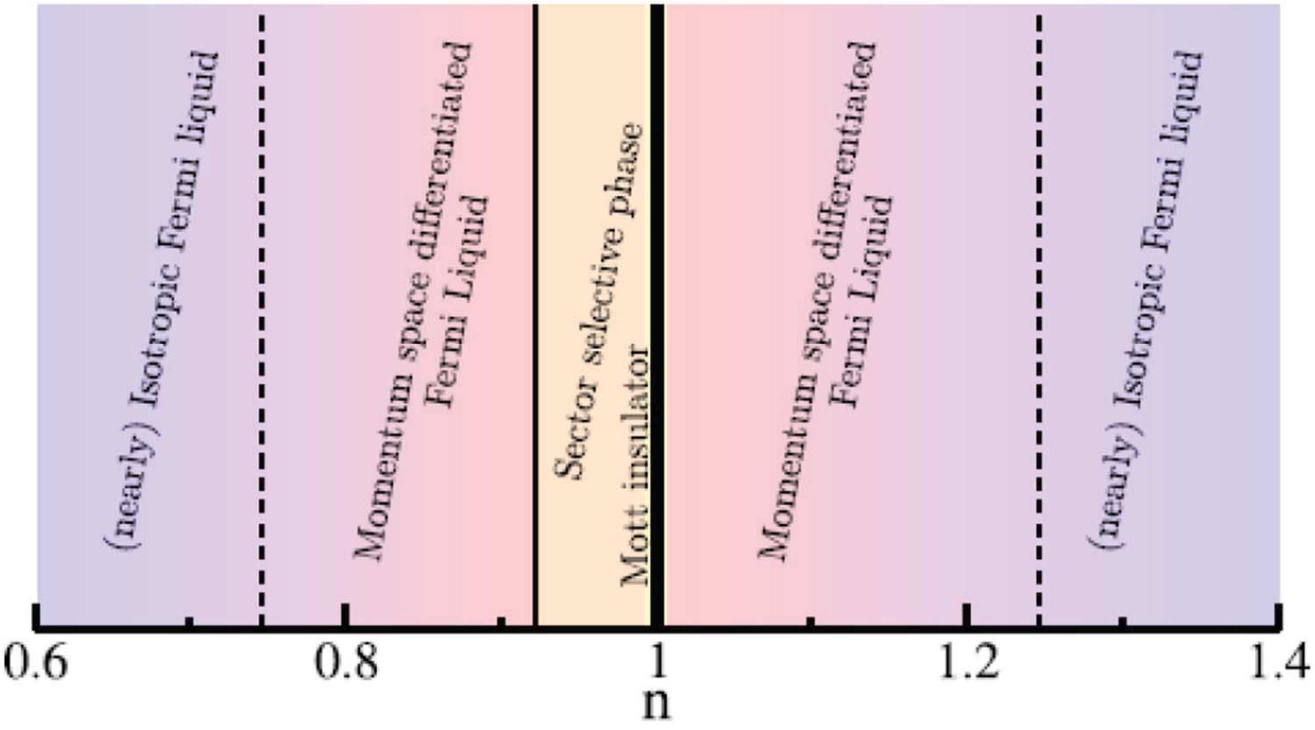
Can be seen with 2 site DCA



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

Momentum dependence of Σ



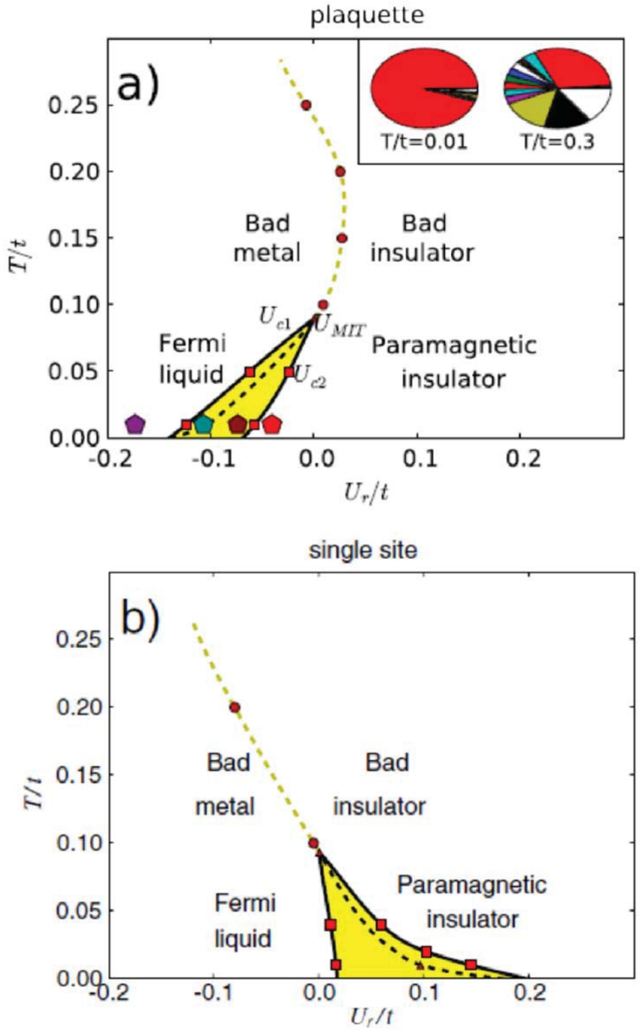
Gull, Werner, Millis, (2009)

Mott transition at $n = 1$

Interaction-induced Mott transition, *n = 1*

4 sites (CDMFT-CTQMC)

$U_{MIT} = 6.05$



Georges, A., and W. Krauth,
PRB **48**, 7167 (1993)

Single site

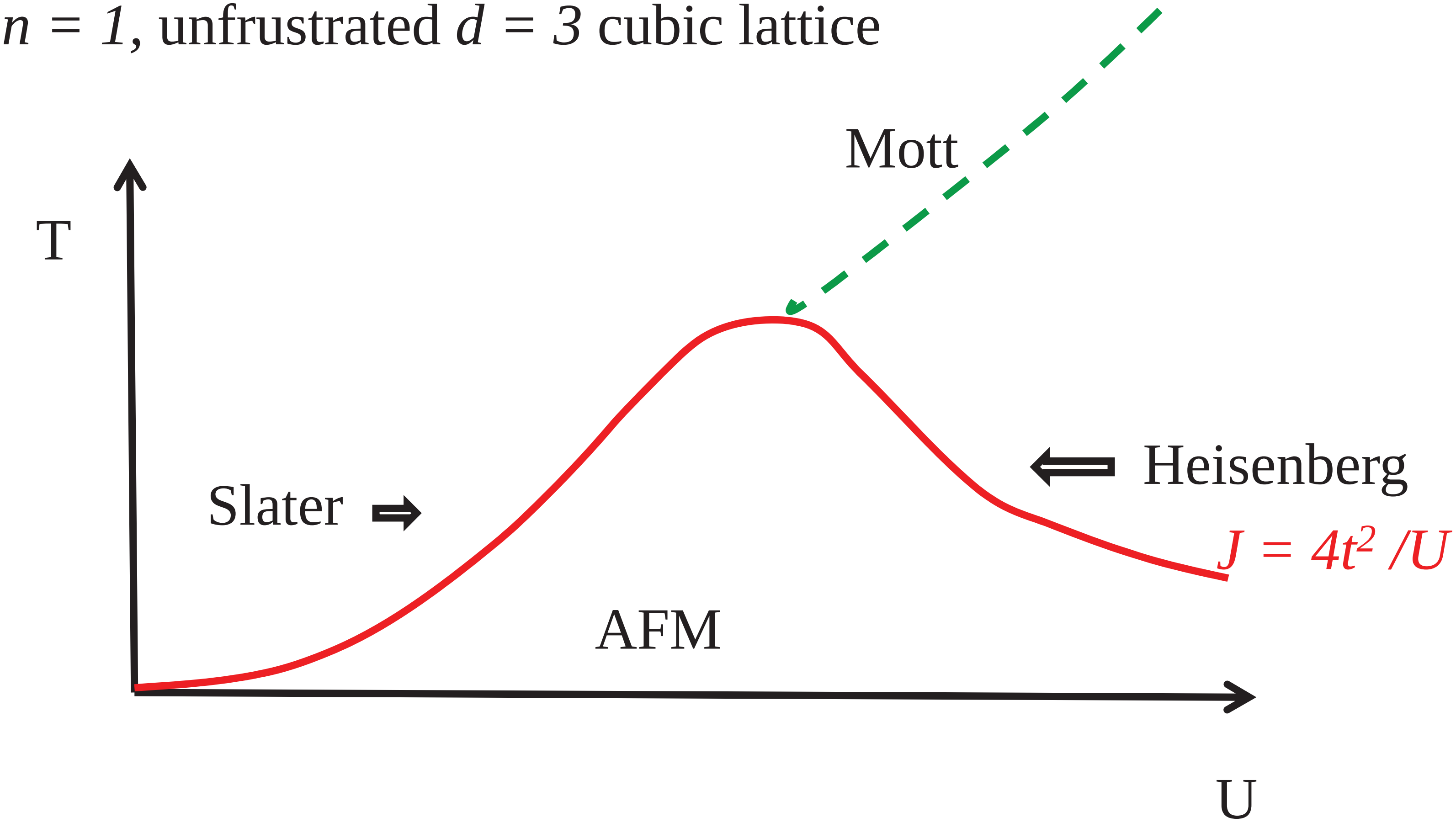
$U_{MIT} \sim 12$

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

H. Park, K. Haule, and G. Kotliar PRL **101**, 186403 (2008)
Balzer, Kyung, Sénécal, Tremblay, Potthof EPL, **85** (2009) 17002

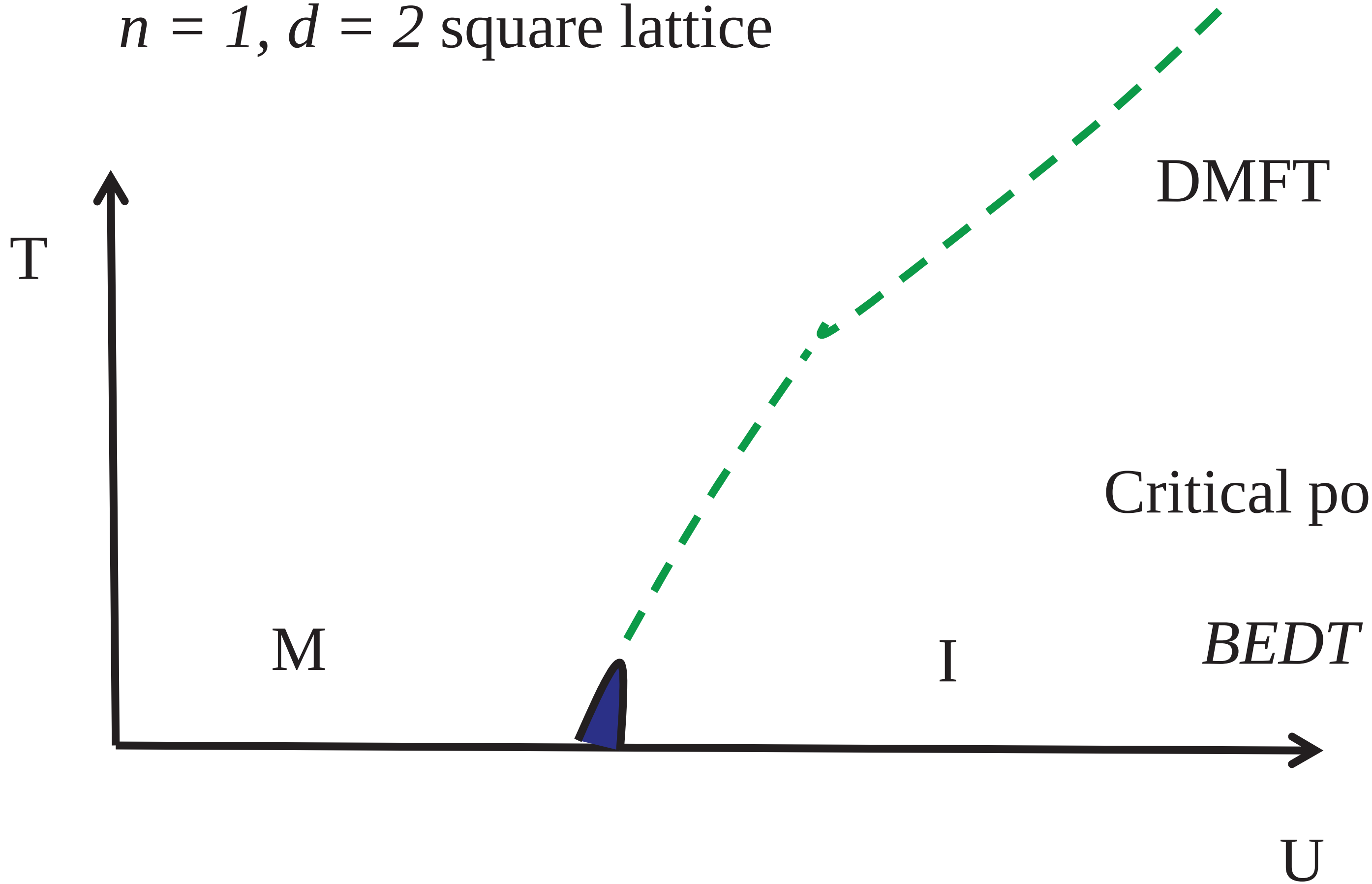
Local moment and Mott transition

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



Local moment and Mott transition

n = *1*, *d* = *2* square lattice



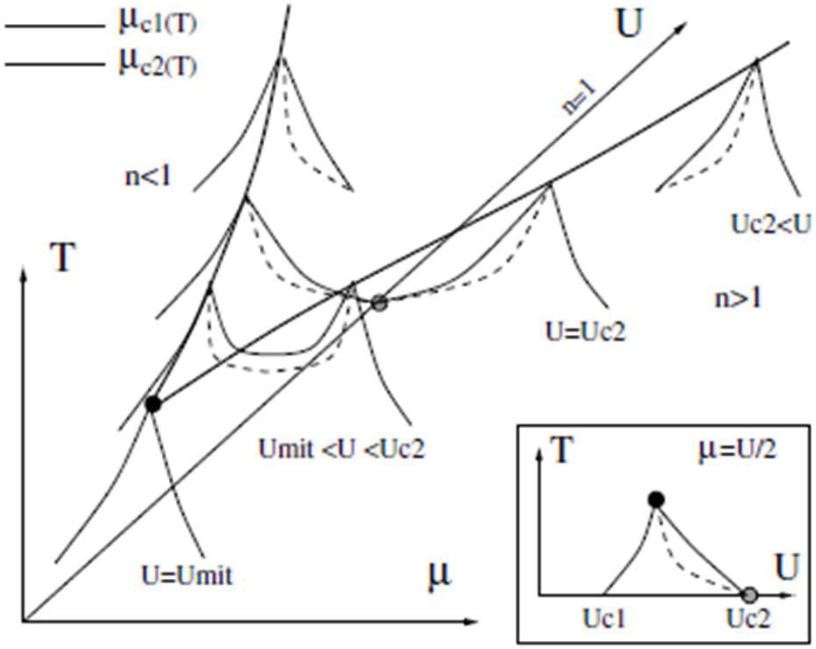
Critical point visible in

BEDT organics

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

Doped Mott insulator

Compressibility divergence at Mott and coexistence (single-site DMFT)



G. Kotliar, S. Murthy, and M. J. Rozenberg, Phys. Rev. Lett. **89**, 046401 (2002).

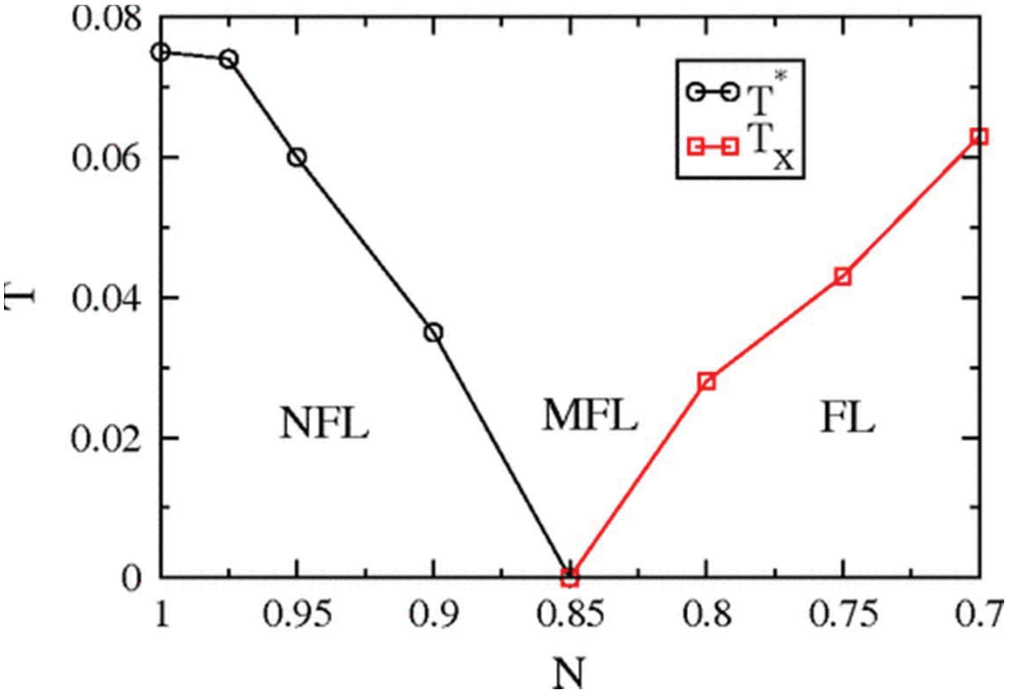
S. Murthy, Rutgers thesis 2004

K. Frikach, M. Poirier, et al.
PRB **61**, R6491 (2000).
S. R. Hassan, A. Georges,
and H. R. Krishnamurthy
PRL **94**, 036402 (2005)

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).
- Momentum selective transition
  - P. Werner et al., PRB 80, 045120 (2009).
  - M. Ferrero et al., EPL 85, 57 009 (2009).
- Competition between Kondo and J
  - 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).

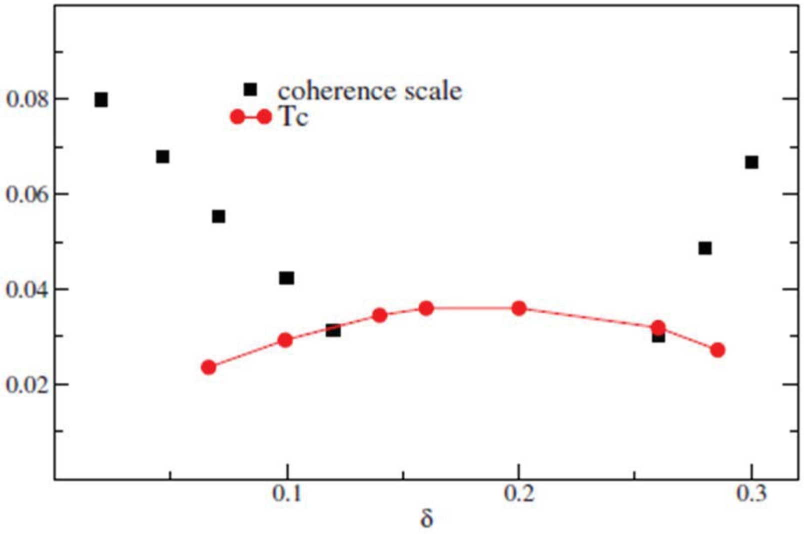
Previous cluster results at finite doping



U = 6, 4x4, t'=0

DCA

N. S. Vidhyadhiraja, A. Macridin, C. Sen, M. Jarrell, and M. Ma, Phys. Rev. Lett. **102**, 206407 (2009).



J = 0.3 (U ~ 13)

EDCA-NCA 2x2

K. Haule and G. Kotliar, Phys. Rev. B **76**, 092503 (2007)

Previous results

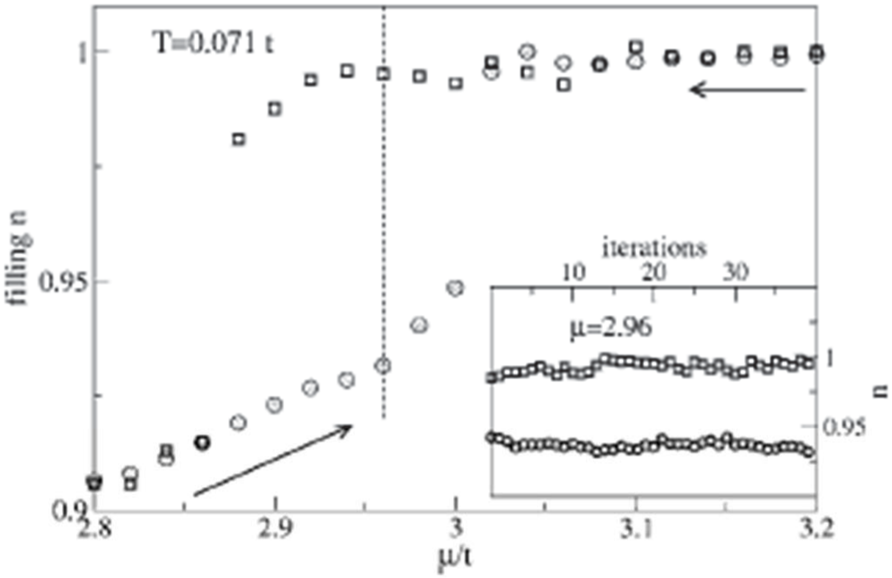
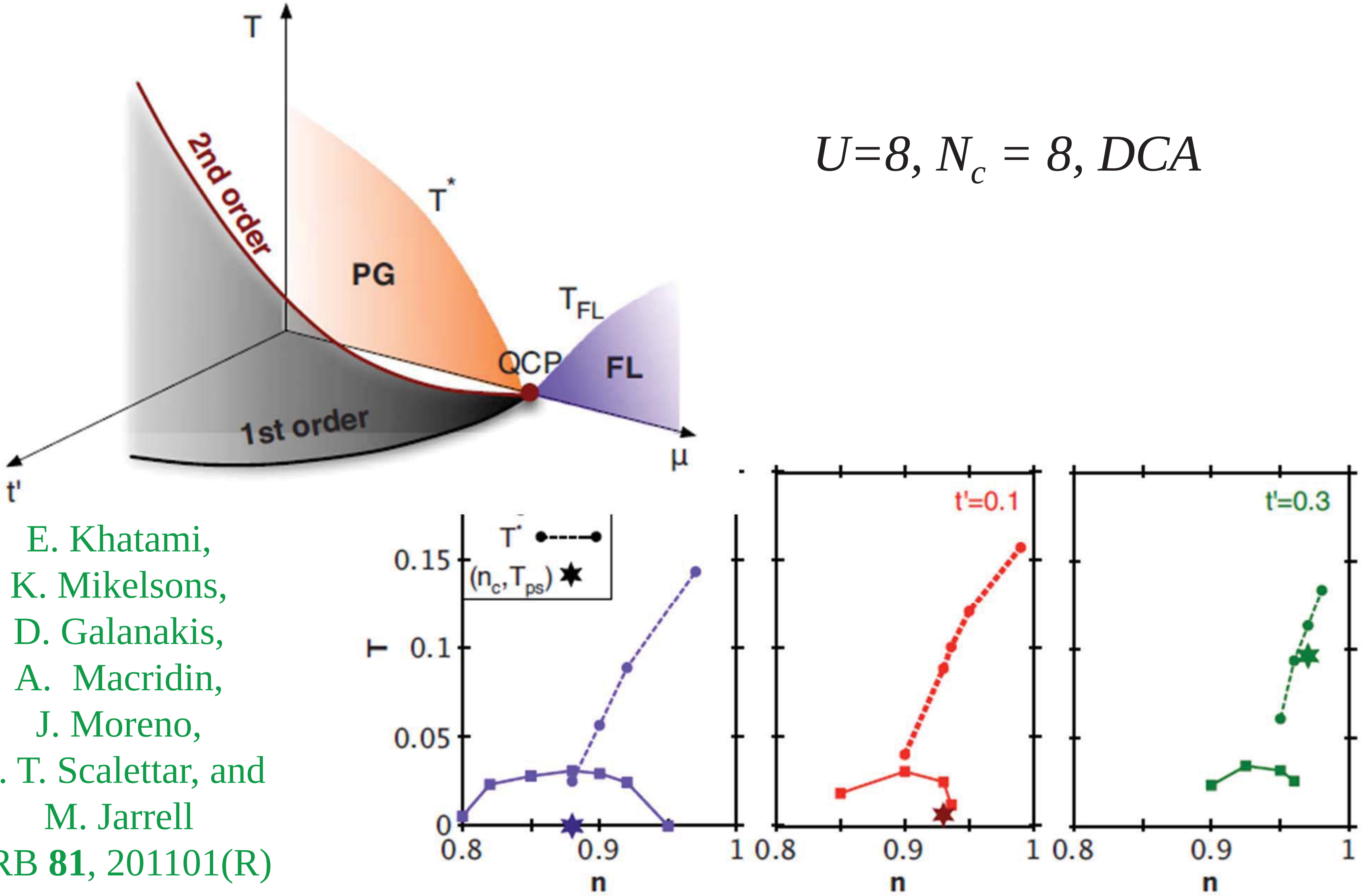


FIG. 2. N_c=8 results. Filling n versus chemical potential below T_c, at T=0.071t. Two solutions describing a hysteresis are found: one incompressible with $n \approx 1$ (squares) and a doped one (circles). Inset: stability of the two solutions versus DCA iterations when μ =2.96t (middle of the hysteresis, corresponding to the dotted line in the main figure).

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

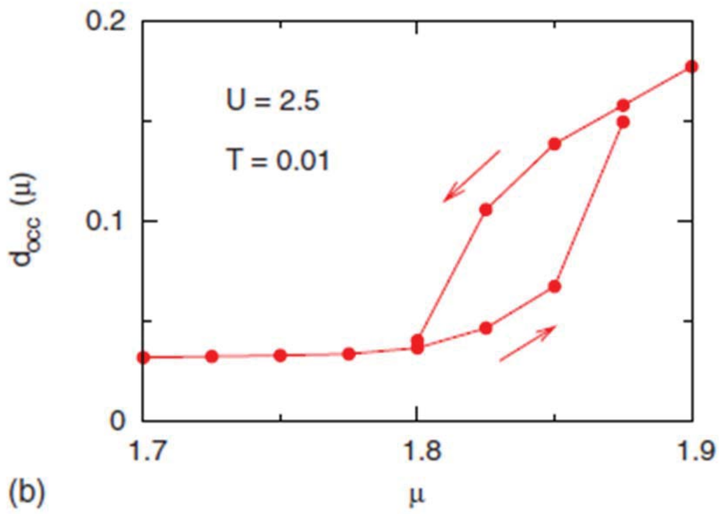
Phase separation on electron-doped side

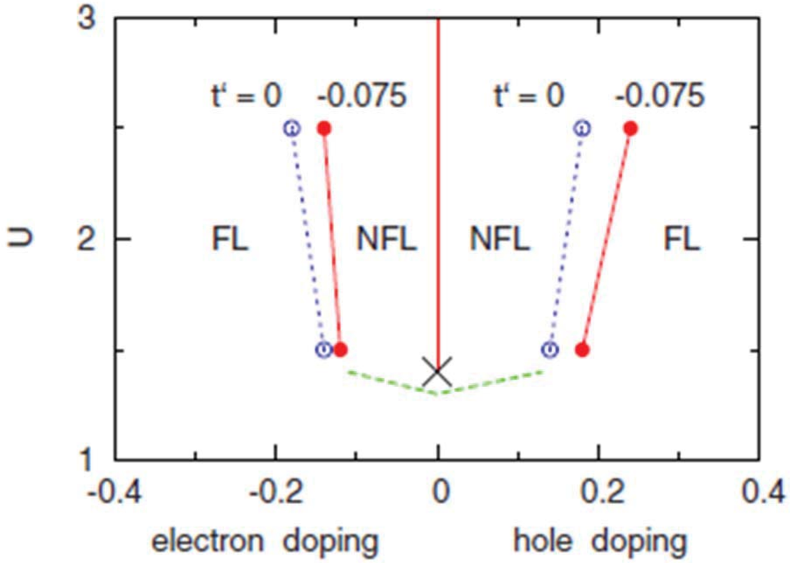


U=8, N_c = 8, *DCA*

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

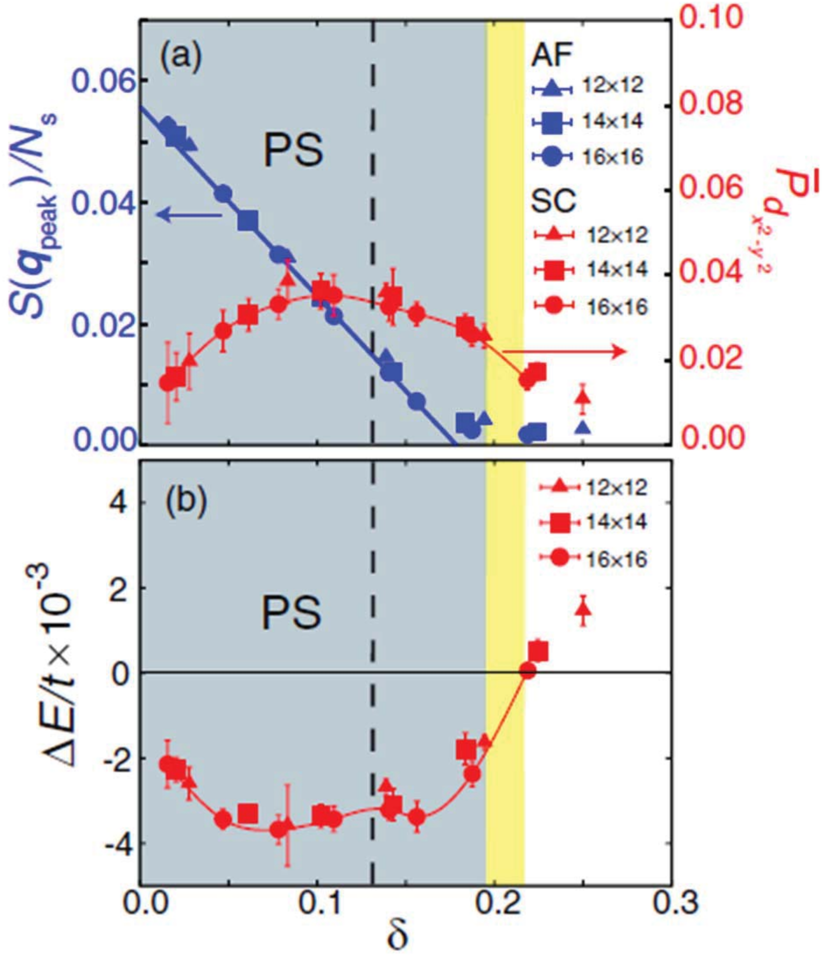
Crossovers and transition



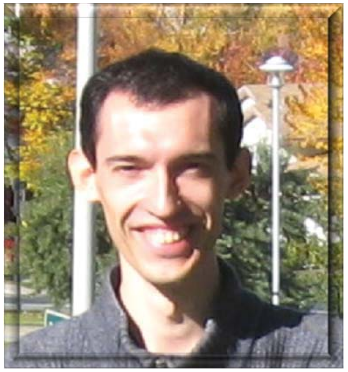


A. Liebsch, N.H. Tong, PRB **80**, 165126 (2009)

Variational Monte Carlo



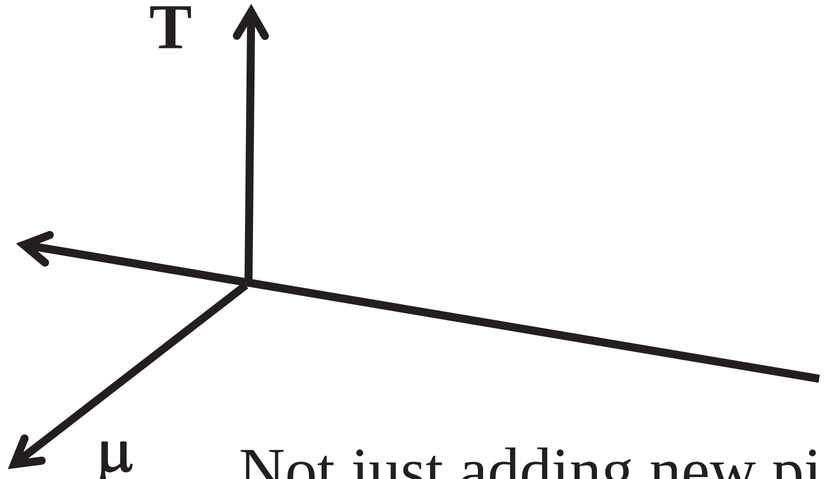
T. Misawa M. Imada PRB **90**, 115137 (2014)



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

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

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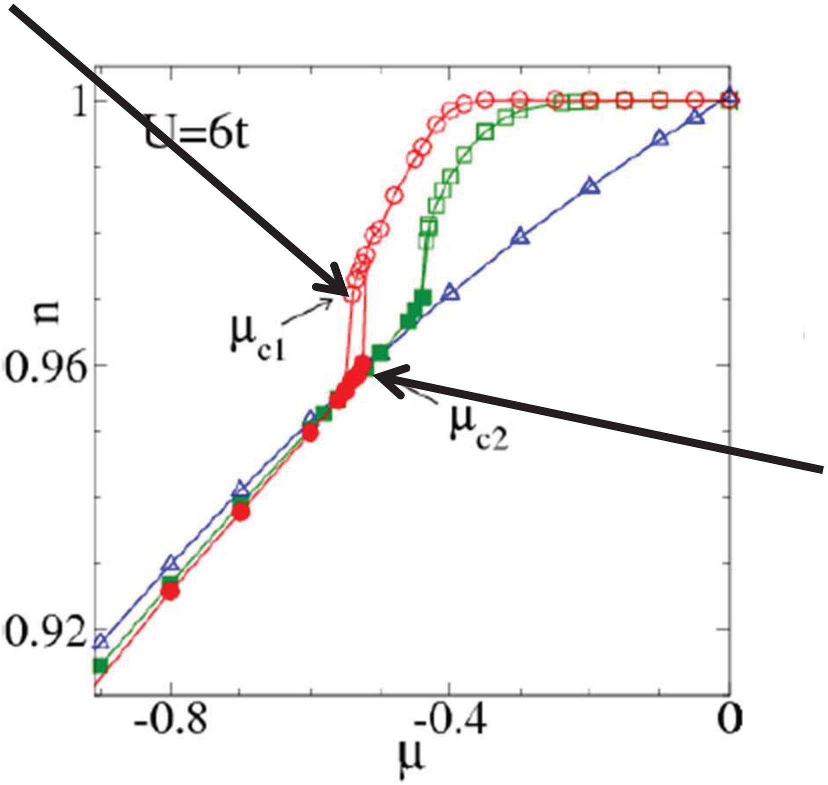
First order transition at finite doping

Spinodals $t' = 0$

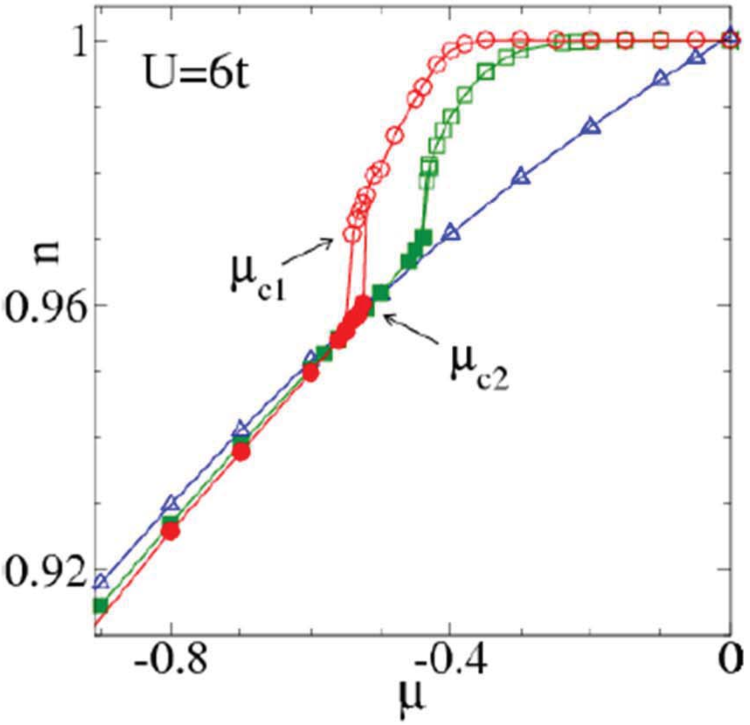


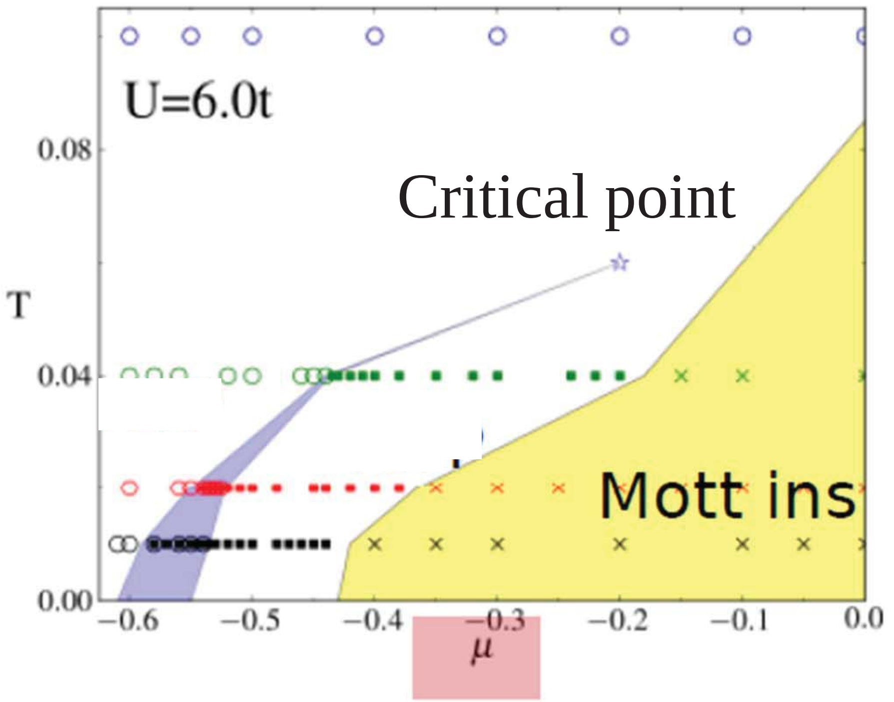
$n(\mu)$ for several temperatures:
$T/t = 1/10, 1/25, 1/50$

Sordi et al. PRL 2010, PRB 2011

First order transition at finite doping

t' = 0





Critical point

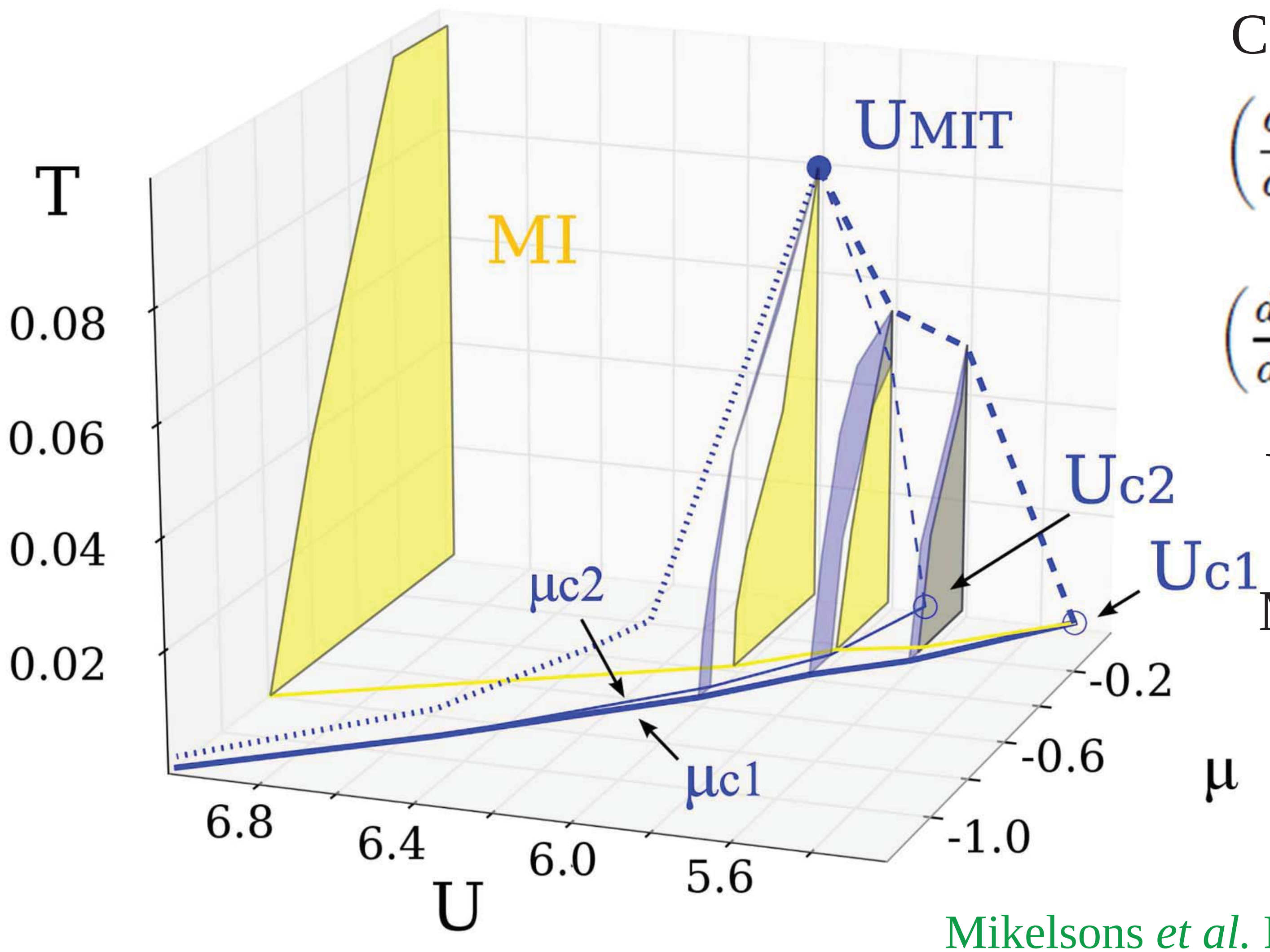
Mott ins

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

Hysteretic behavior: fingerprint first order transition!

Sordi et al. PRL 2010, PRB 2011

Overall phase diagram



Clausius-Clapeyron

$$\left(\frac{dT_c}{d\mu_c}\right)_U = \frac{(n_1 - n_2)}{(S_2 - S_1)}$$

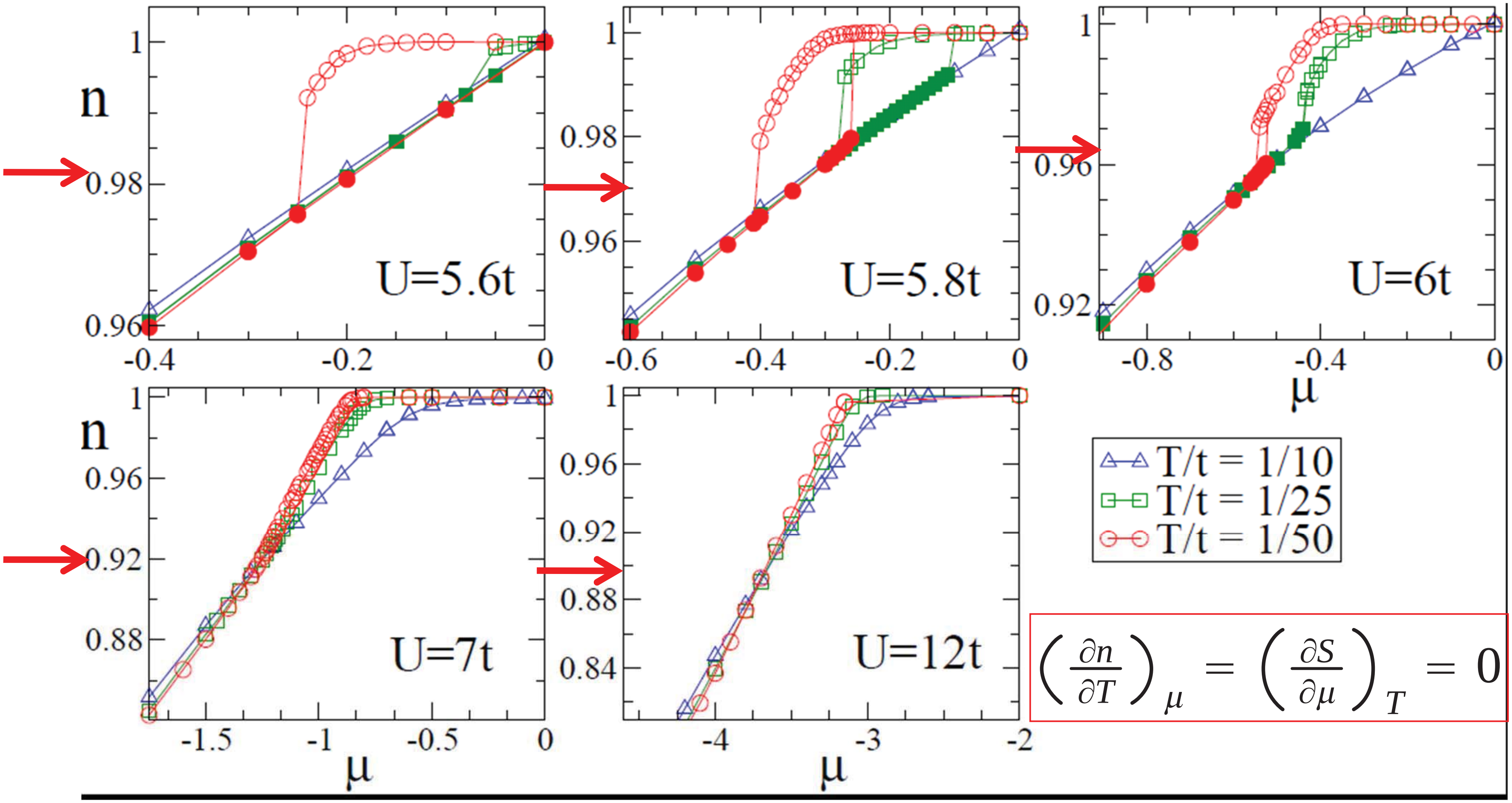
$$\left(\frac{dU_c}{d\mu_c}\right)_T = \frac{(n_1 - n_2)}{(D_1 - D_2)}$$

Underdoped phase
lower *D* and *S*
More compressible

$$\left(\frac{\partial S}{\partial n}\right)_T = 0$$

Mikelsons *et al.* PRB **80**, (2009)

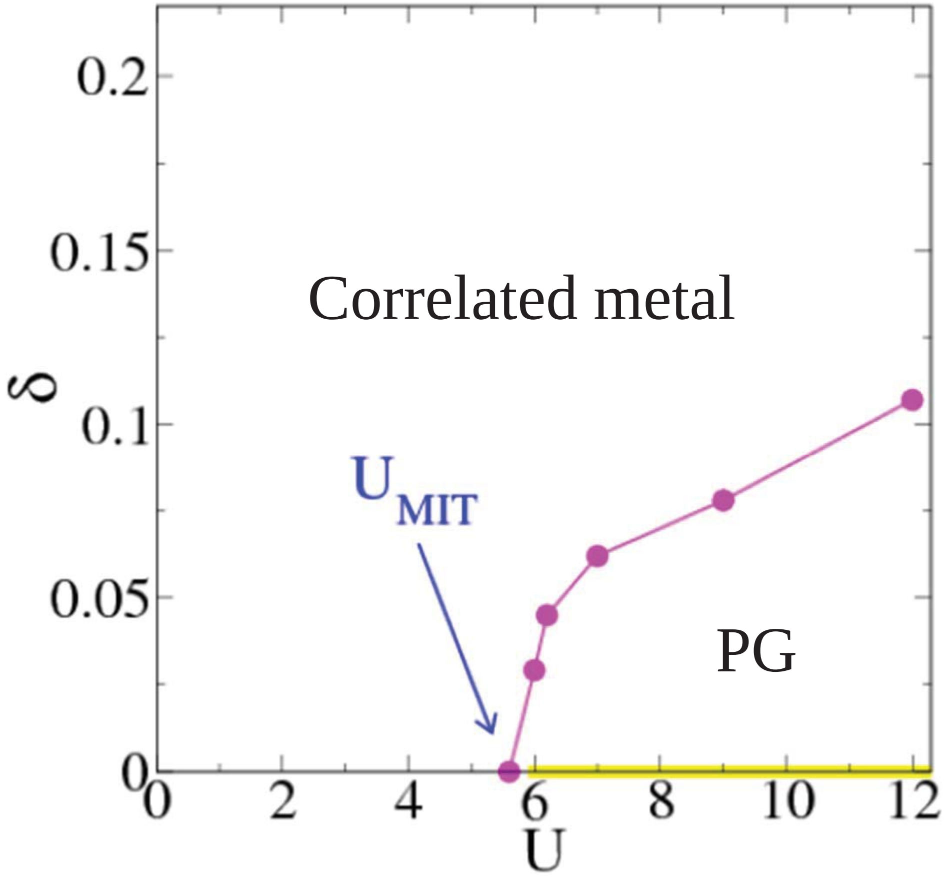
Critical doping as a function of *U* increases

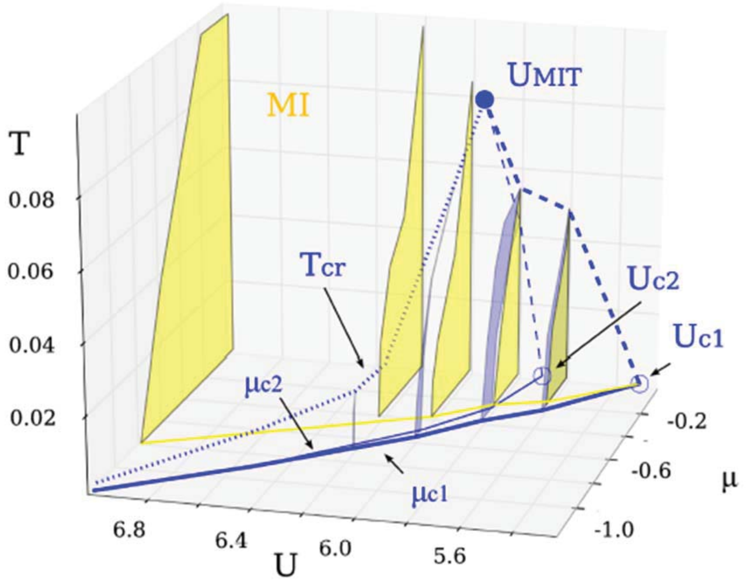


$$\left(\frac{\partial n}{\partial T}\right)_{\mu} = \left(\frac{\partial S}{\partial \mu}\right)_{T} = 0$$

A finite-doping first order transition, linked to Mott transition up to optimal doping

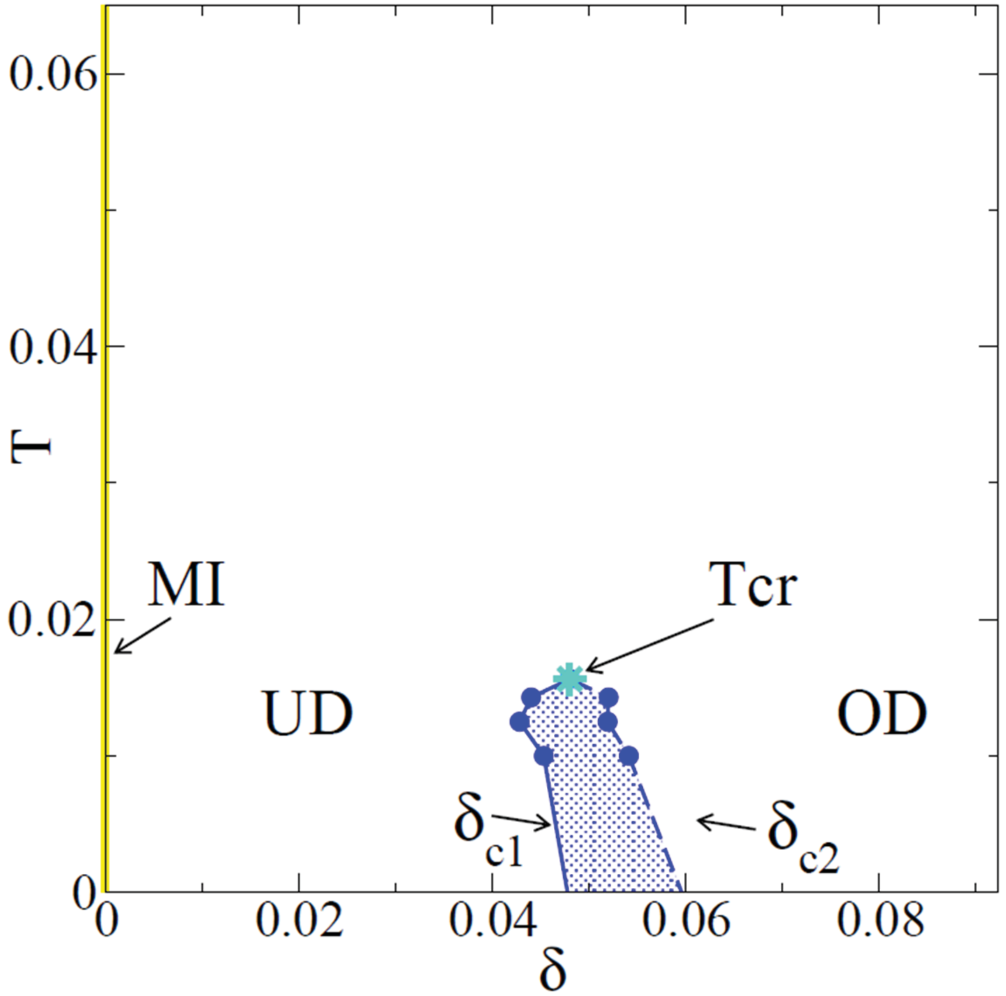
Doping dependence of critical point as a function of *U*





Sordi et al. PRL 2010, PRB 2011

Characterisation of the phases (*U*=6.2*t*)

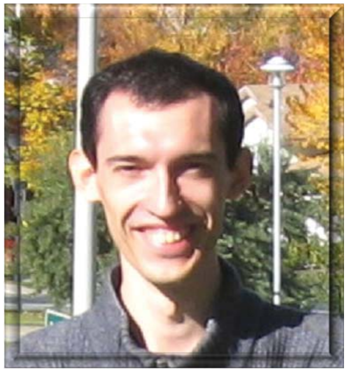


$U > U_{\mathrm{MIT}}$:

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" δ_c = doping at which the 1st order transition occurs

How does the UD phase differ from the OD phase?



Giovanni Sordi

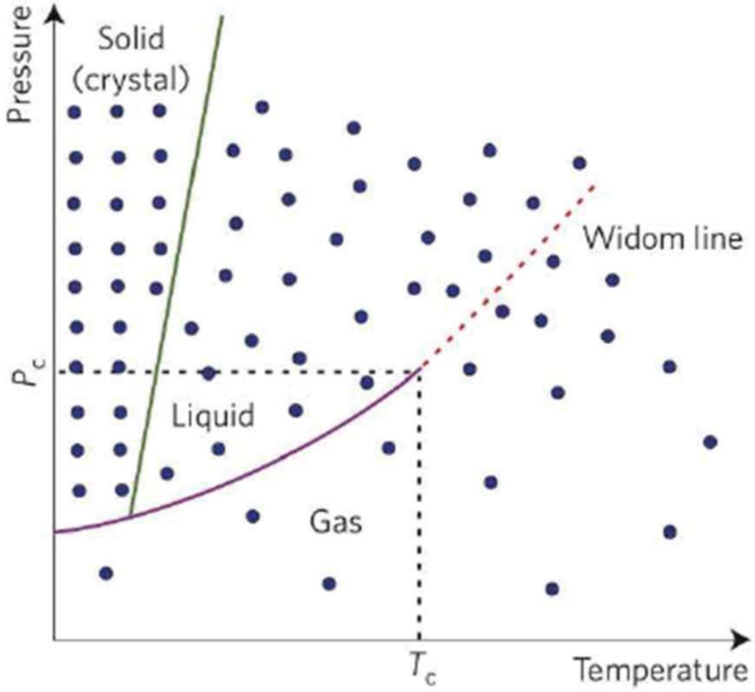
Patrick Sémon

Kristjan Haule

The Widom line *($t'=0$)*

G. Sordi, *et al*. Scientific Reports 2, 547 (2012)

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 $T \rightarrow T_p$
- 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

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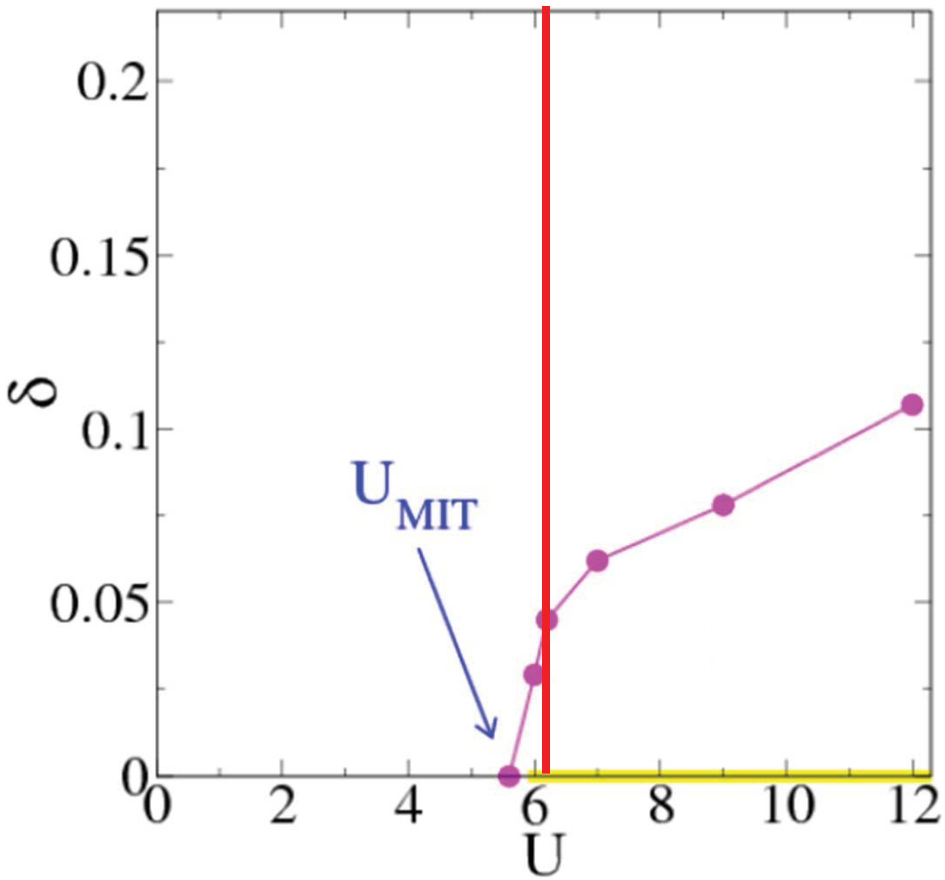
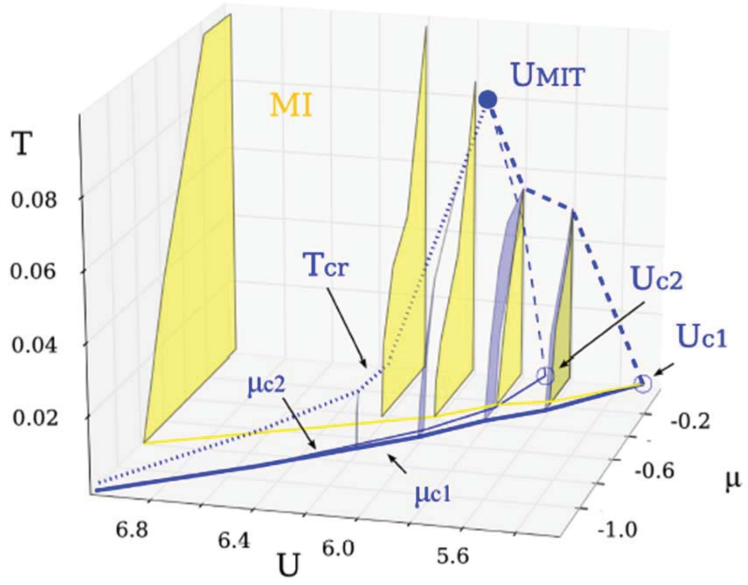
Link to Mott transition up to optimal doping

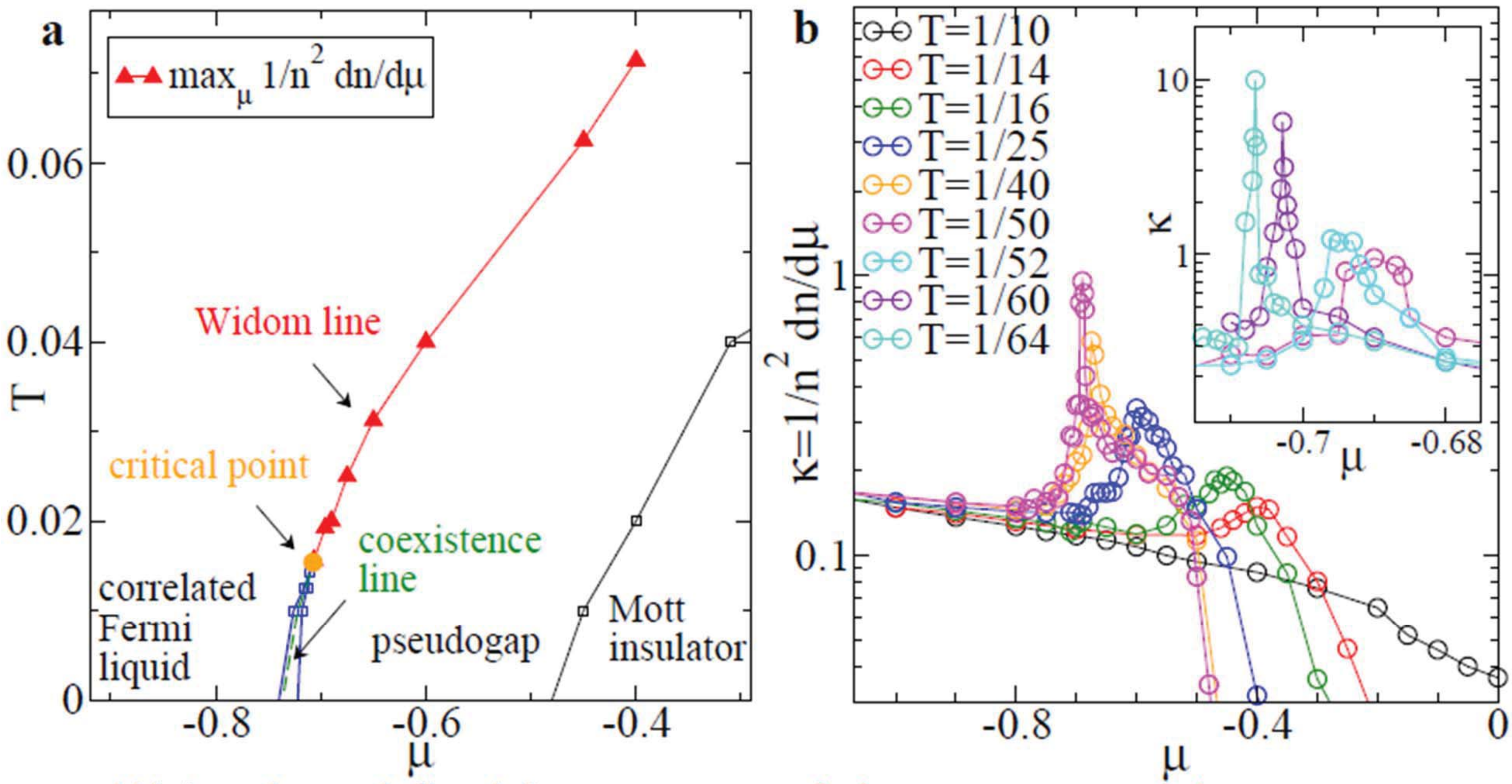
Doping dependence of critical point as a function of *U*





Smaller *D* and *S*

Pseudogap *T** along the Widom line

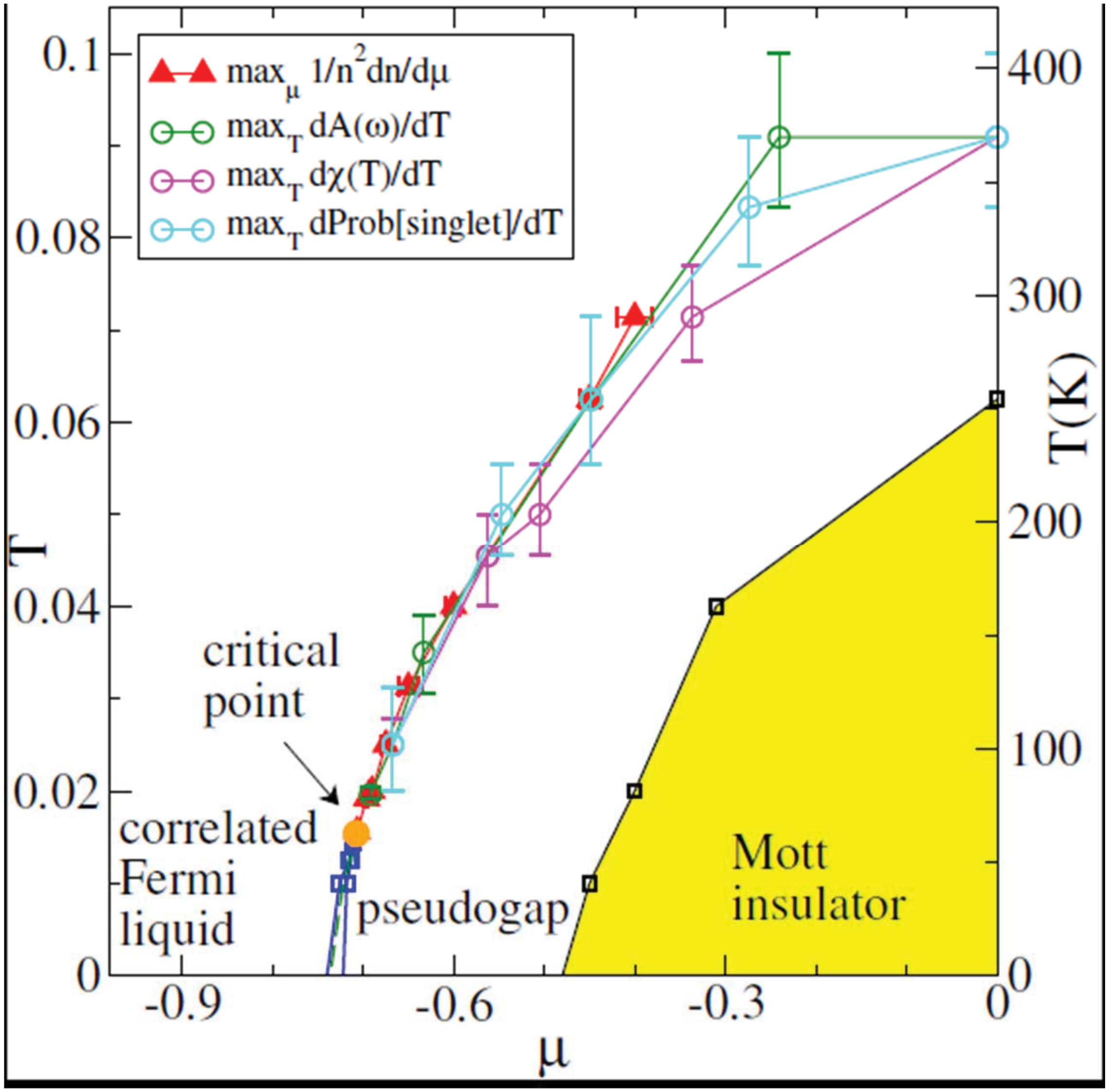


Widom line: defined from maxima of charge compressibility

$\kappa = 1/n^2(dn/d\mu)_T$

divergence of κ at the (classical) critical point!

Rapid change also in dynamical quantities



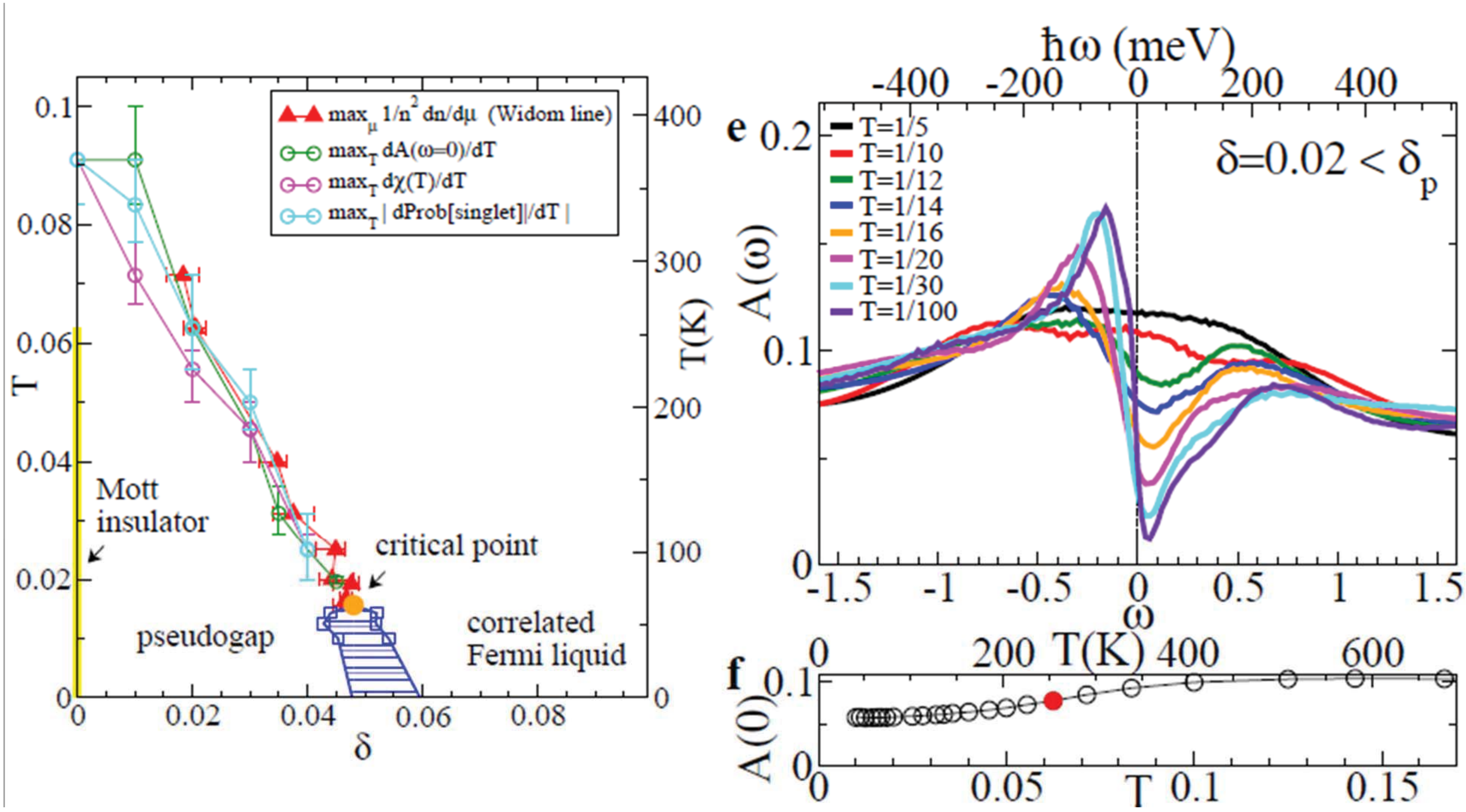
Compare a few results for cuprates

Caveats:

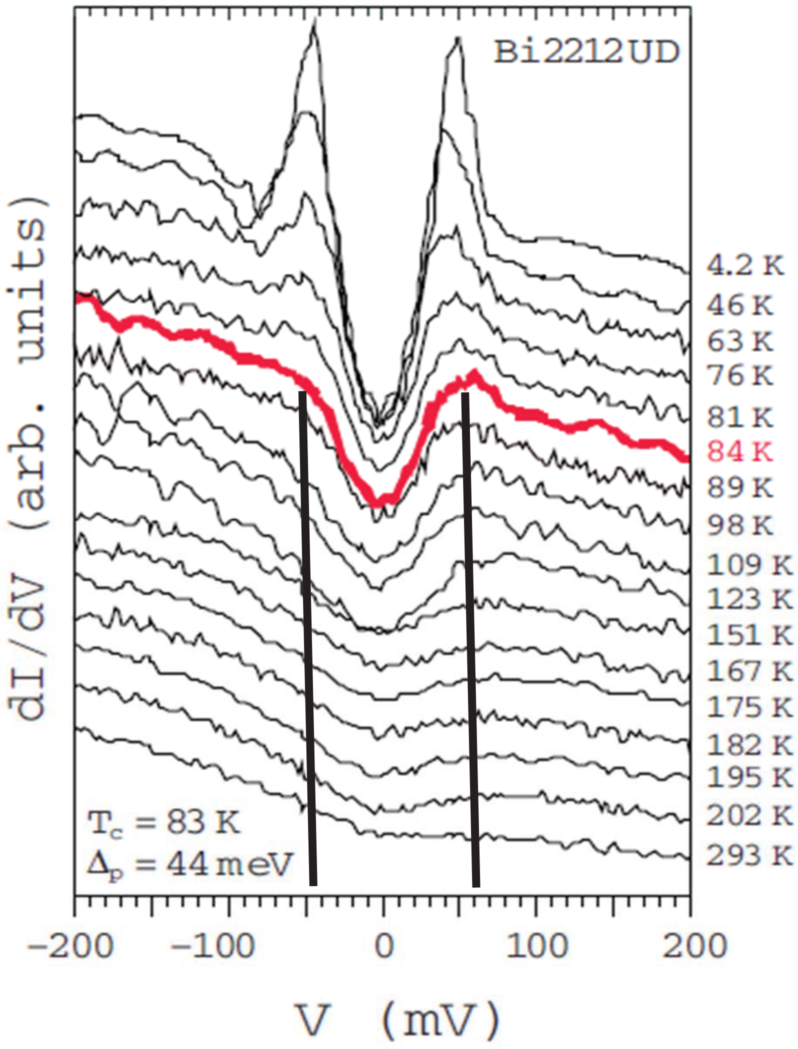
U not large enough

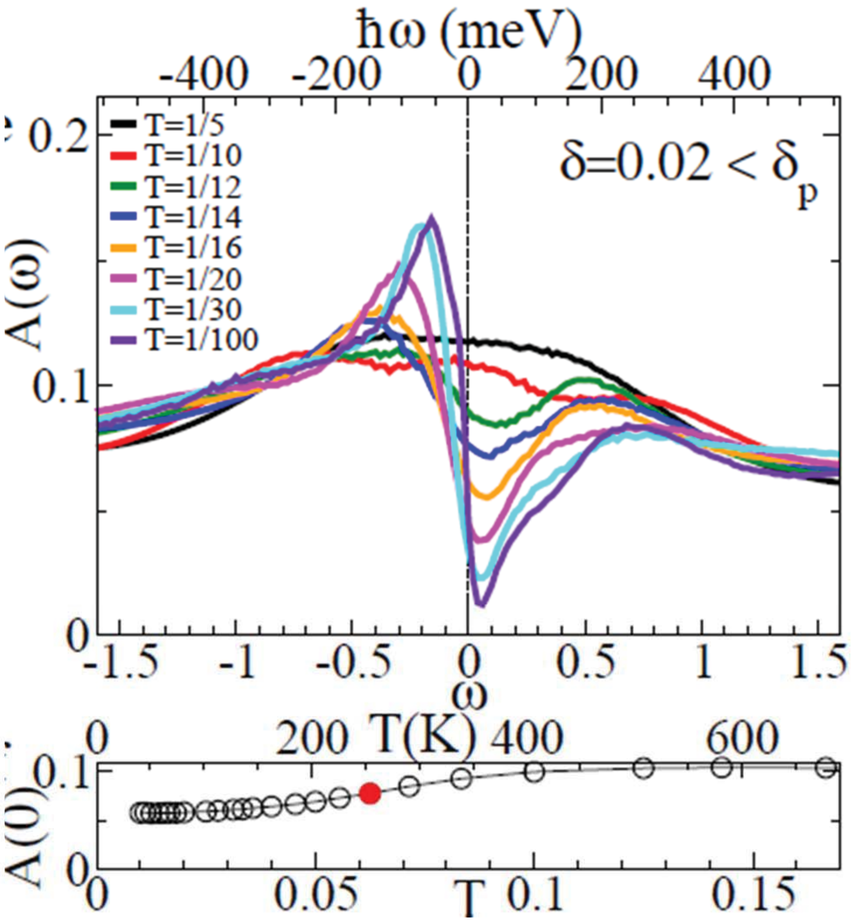
$t'=0$

Density of states



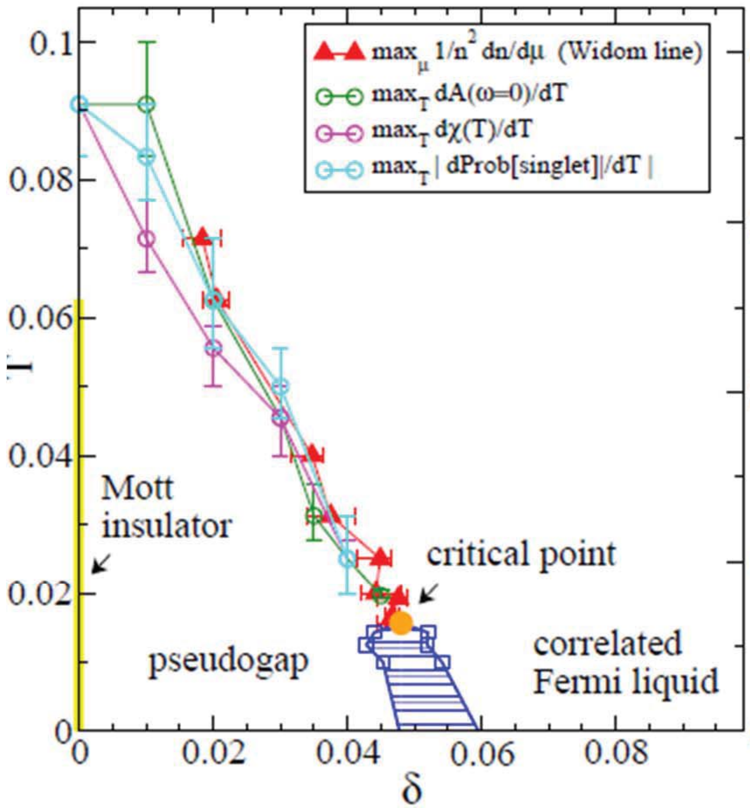
Density of states

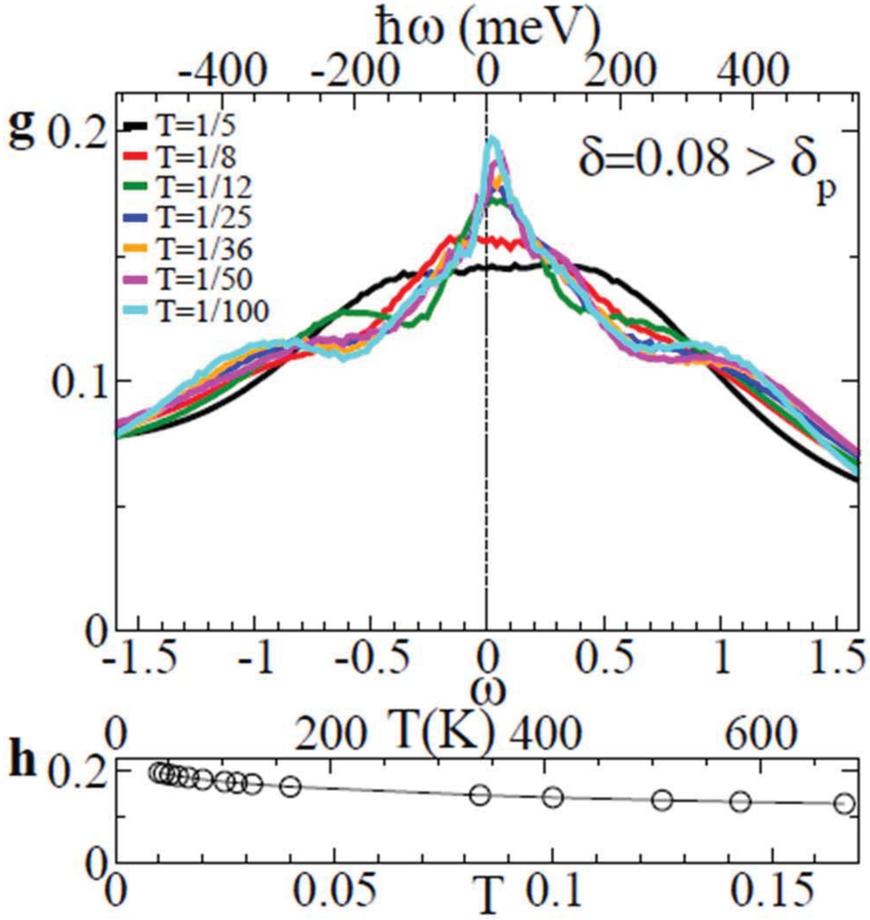




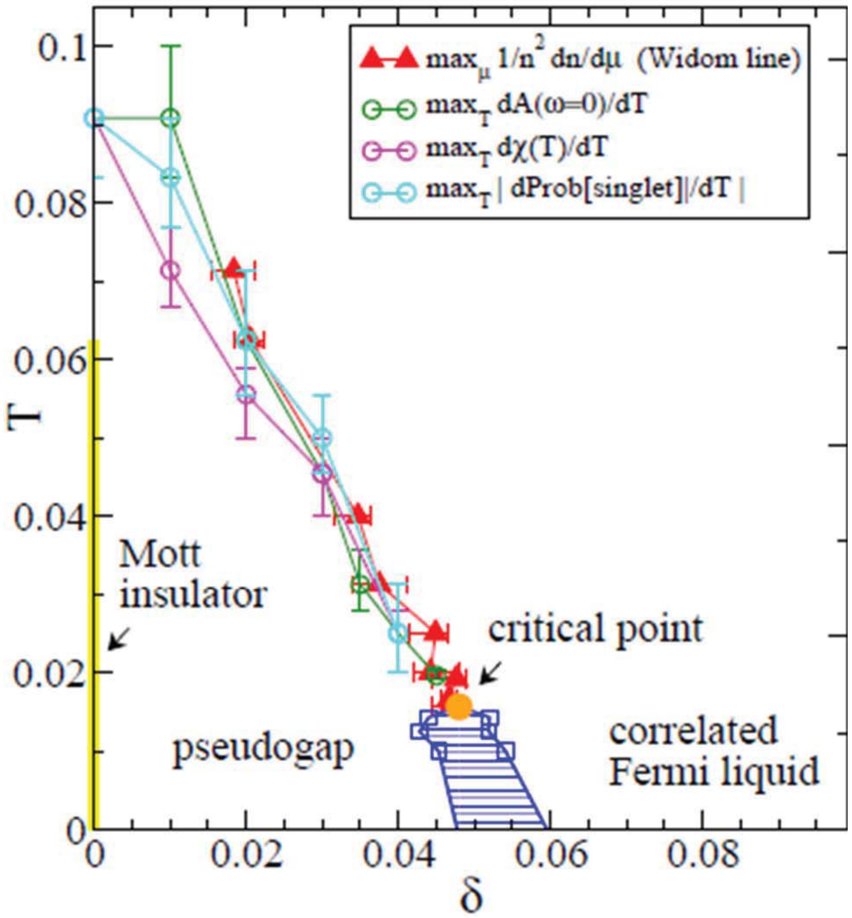
h. Renner, B. Revaz, J.-Y. Genoud,
K. Kadowaki, and Ø. Fischer
PRL 80, 149 (1998)

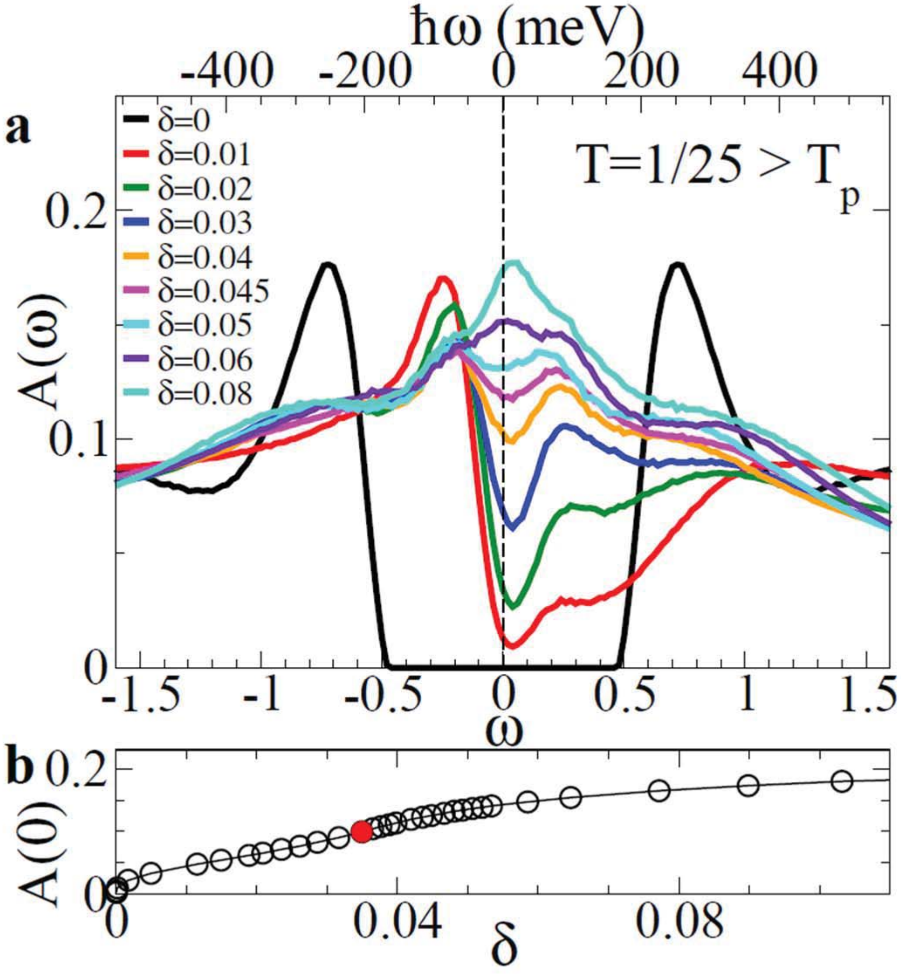
Density of states



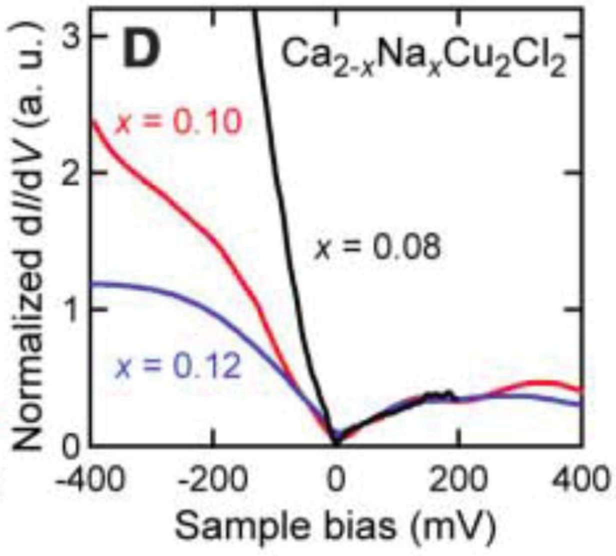


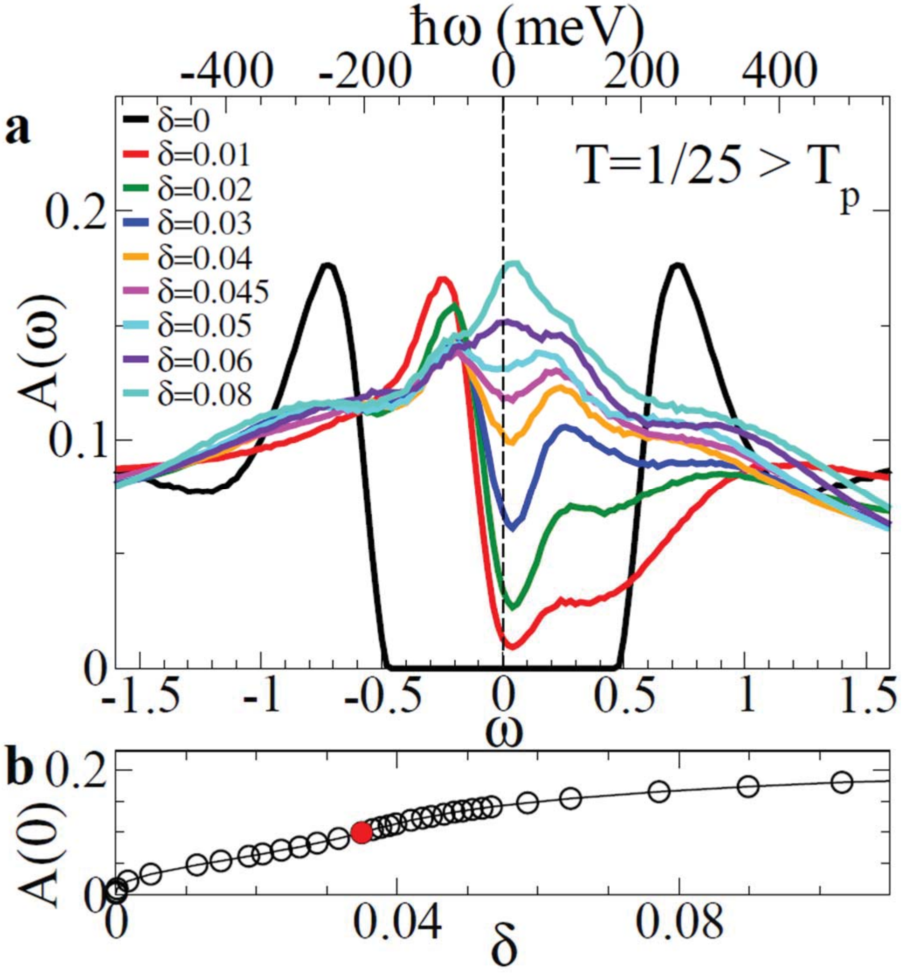
Density of states





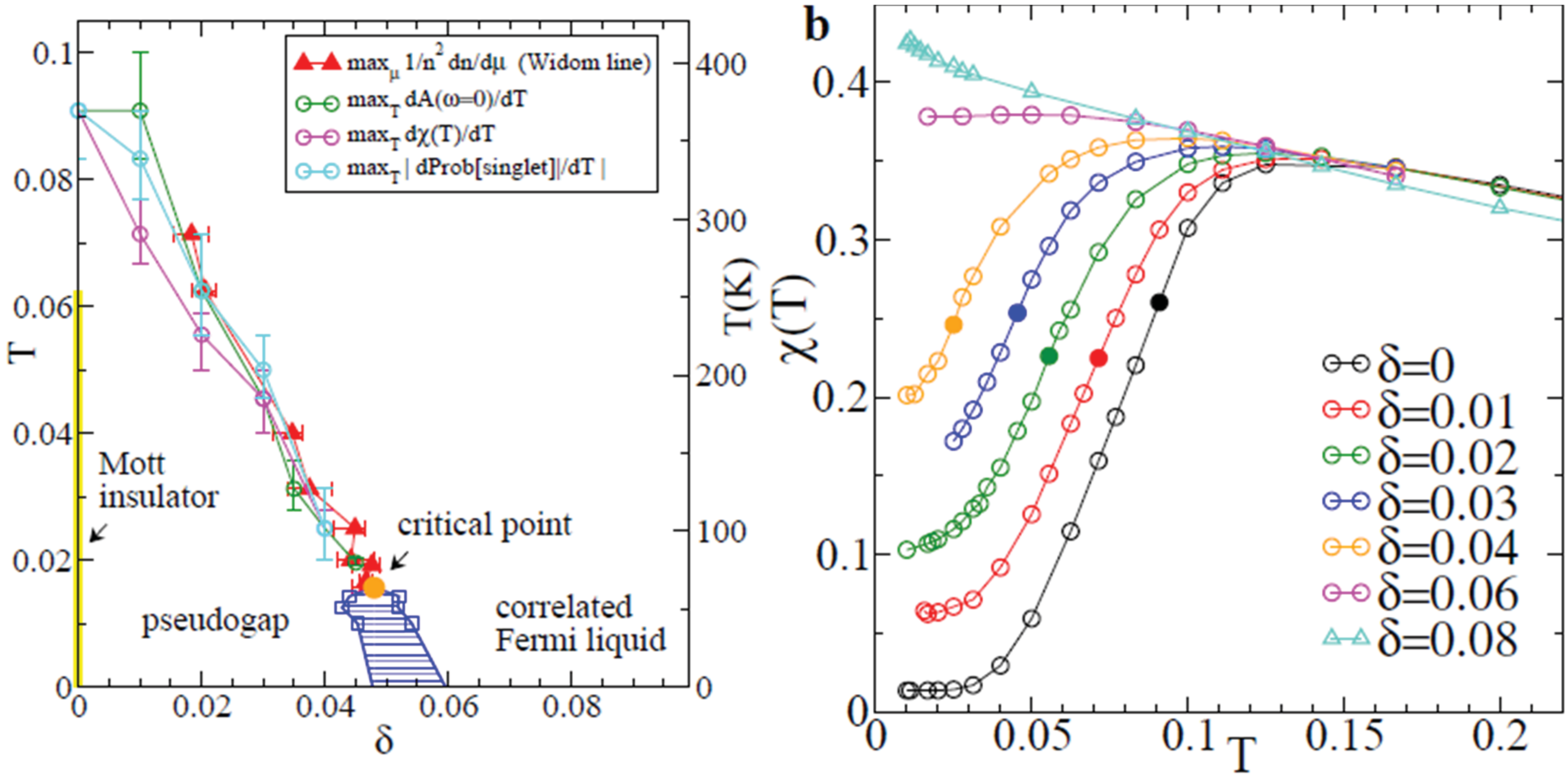
Density of states



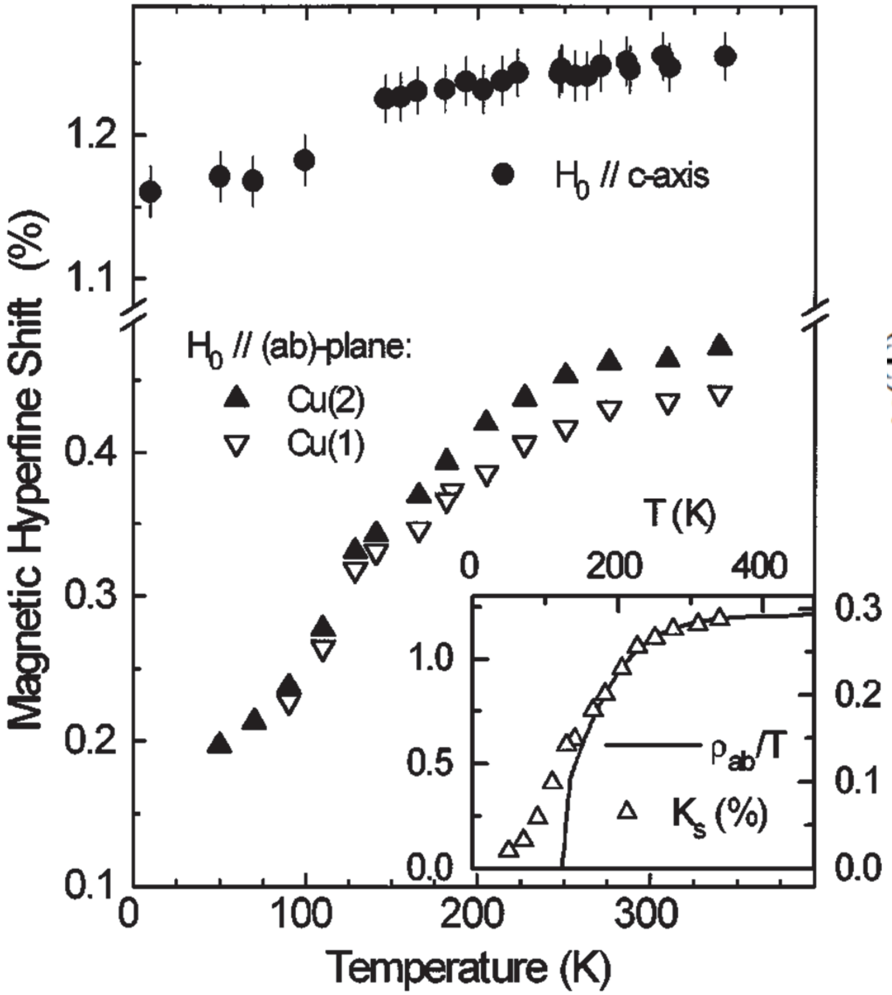


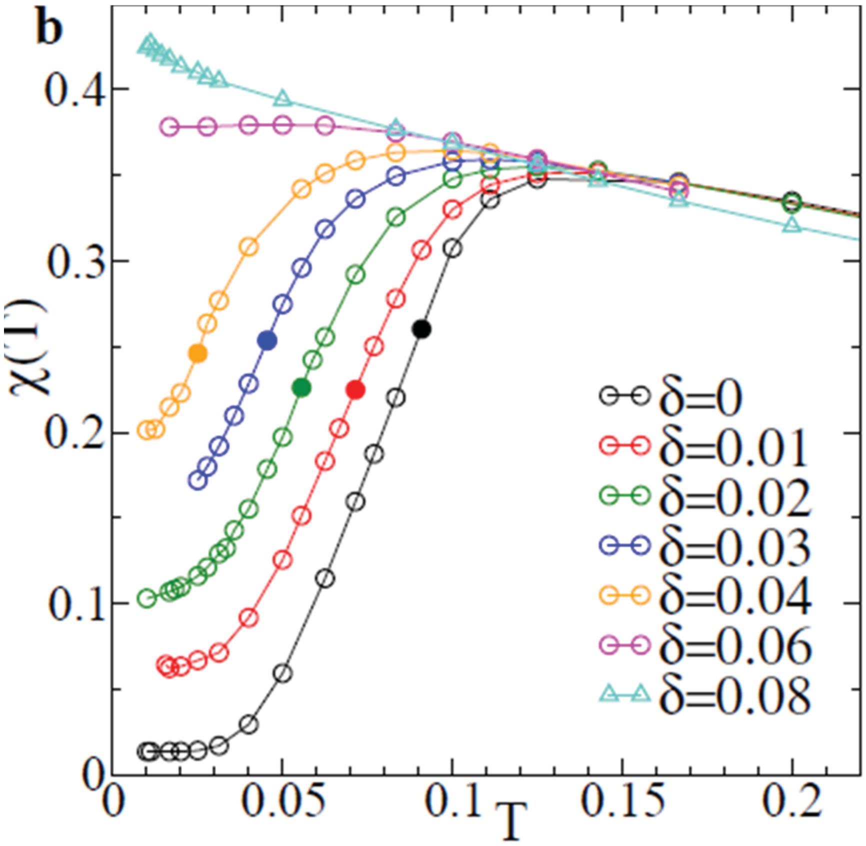
Khosaka et al. *Science* **315**, 1380 (2007);

Spin susceptibility



Spin susceptibility





Underdoped Hg1223

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

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What is the minimal model?

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

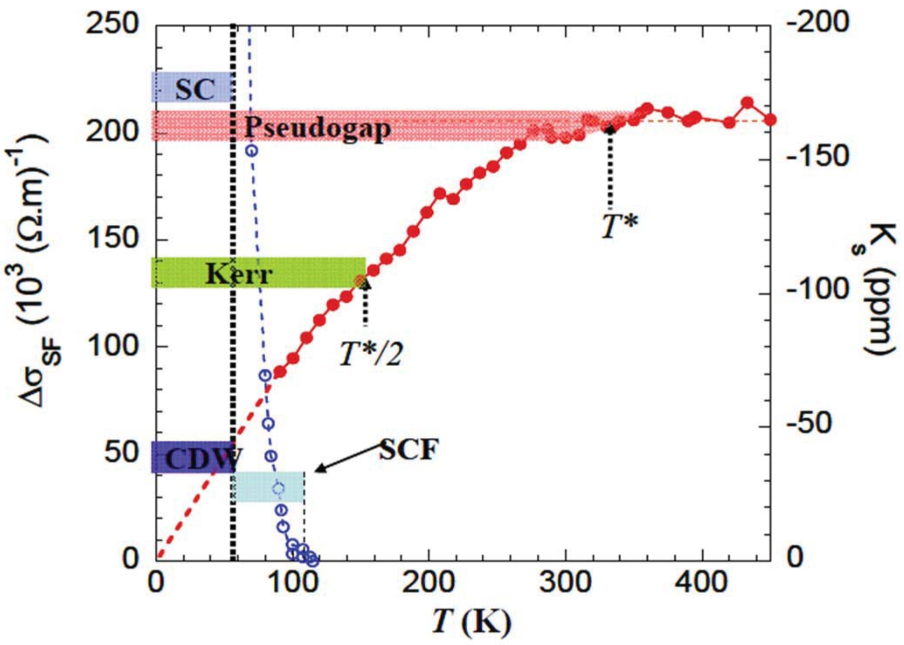
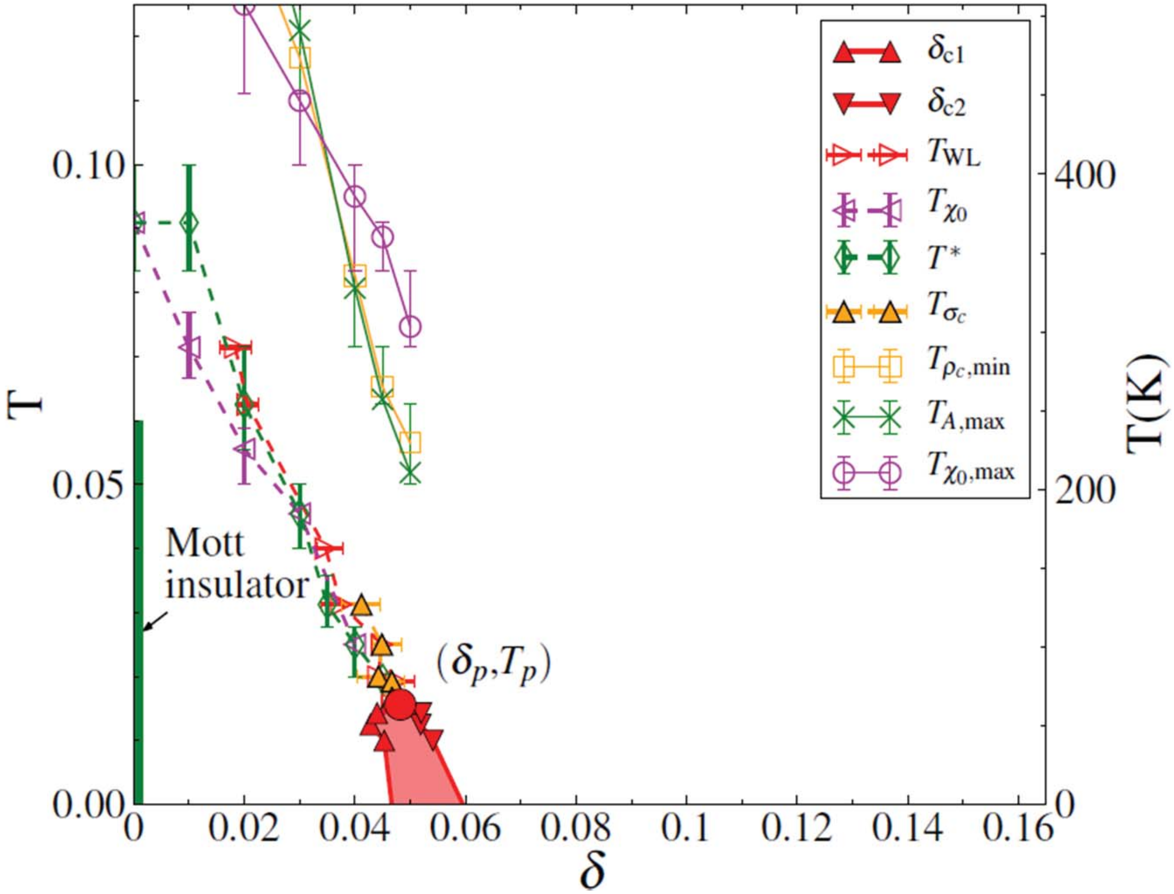


Fig 1 Spin contribution K_s to the ^{89}Y NMR Knight shift [11] for YBCO$_{6.6}$ permit to define the PG onset T^*. Here K_s is reduced by a factor two at $T \sim T^*/2$. The sharp drop of the SC fluctuation conductivity (SCF) is illustrated (left scale) [23]. We report as well the range over which a 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).

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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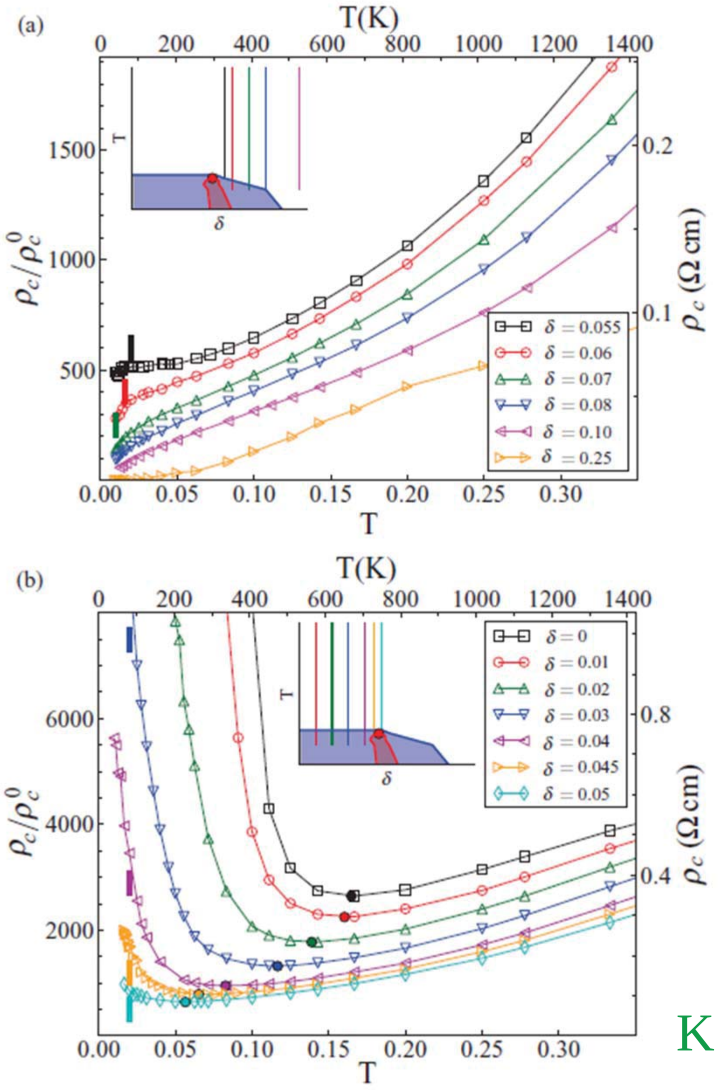
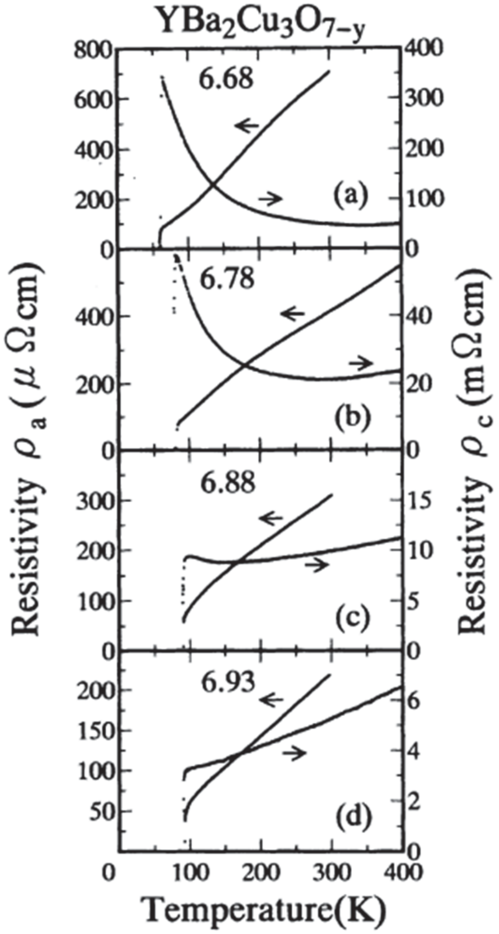
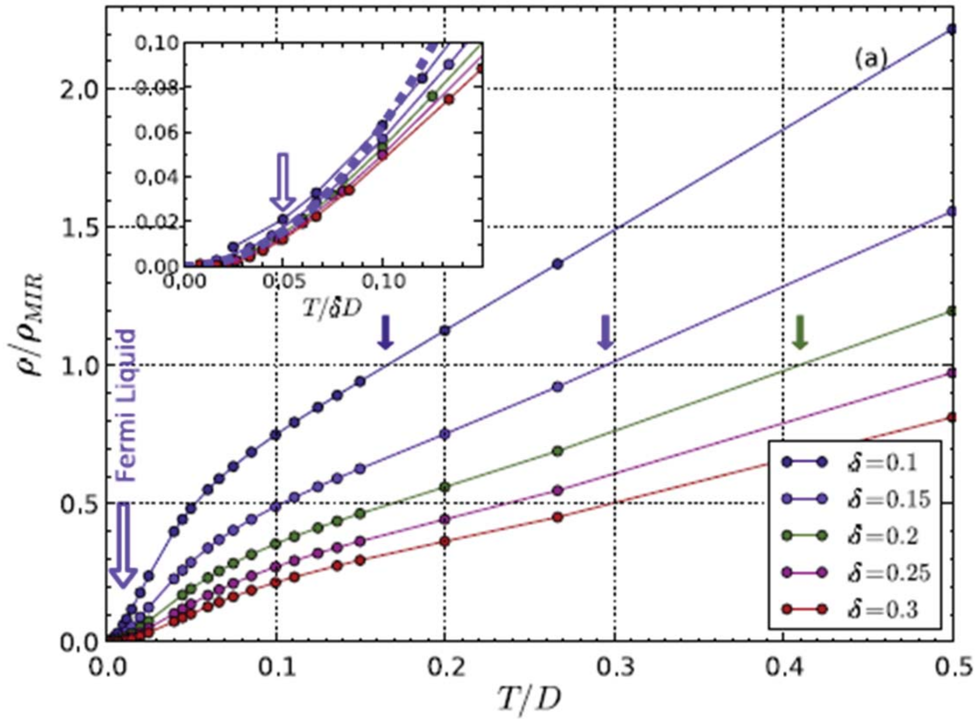
C-axis resistivity





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

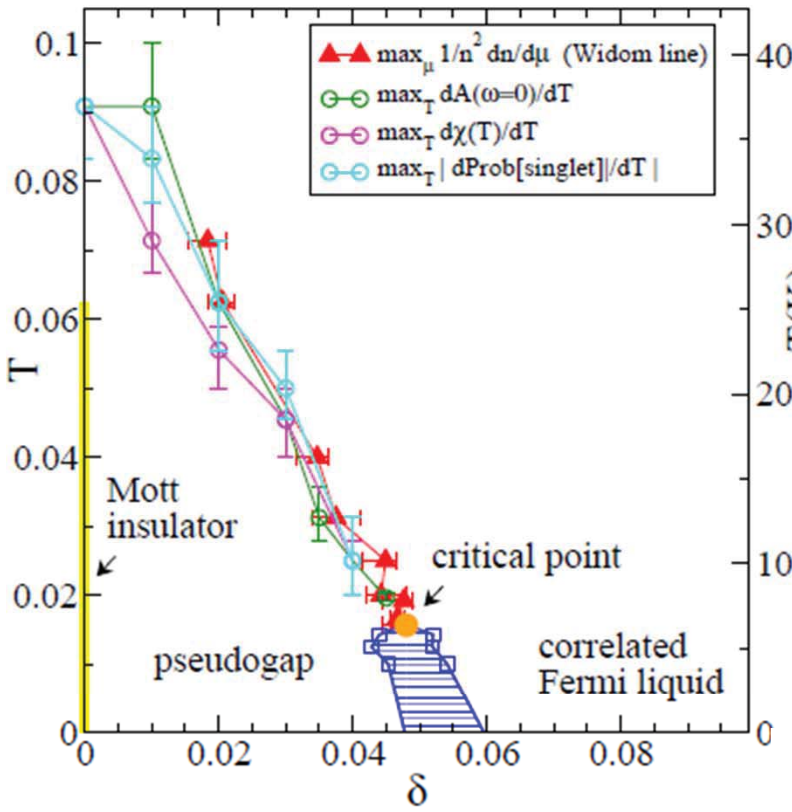
Mott-Ioffe-Regel limit

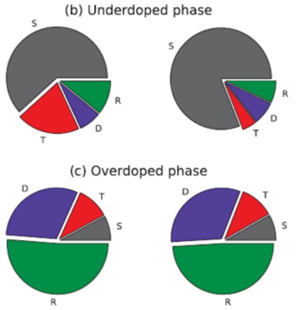


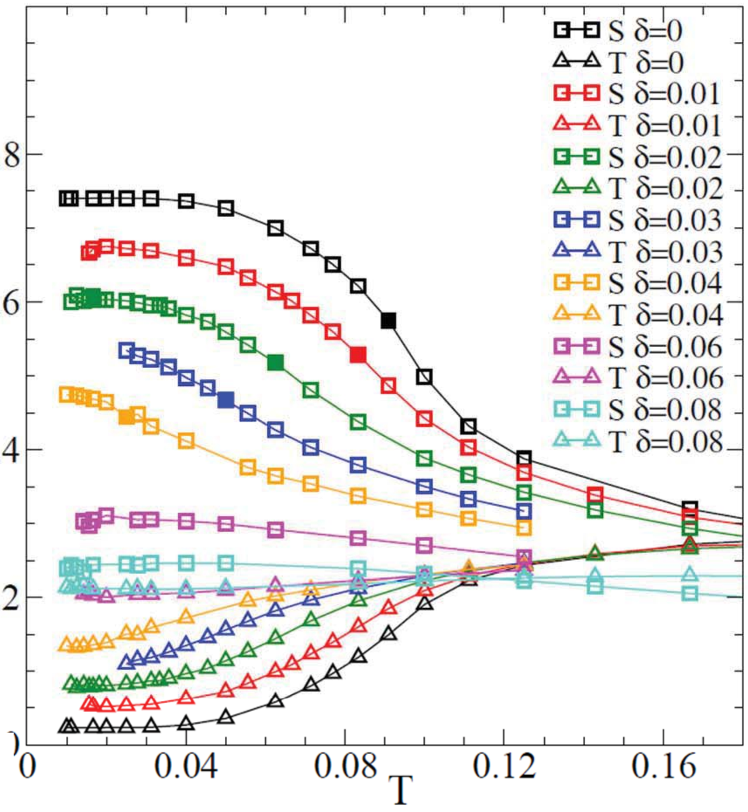
X. Deng, J.j Mravlje, R. Zitko, M. Ferrero, G. Kotliar, and A. Georges
PRL 110, 086401 (2013)

Physics

Plaquette eigenstates

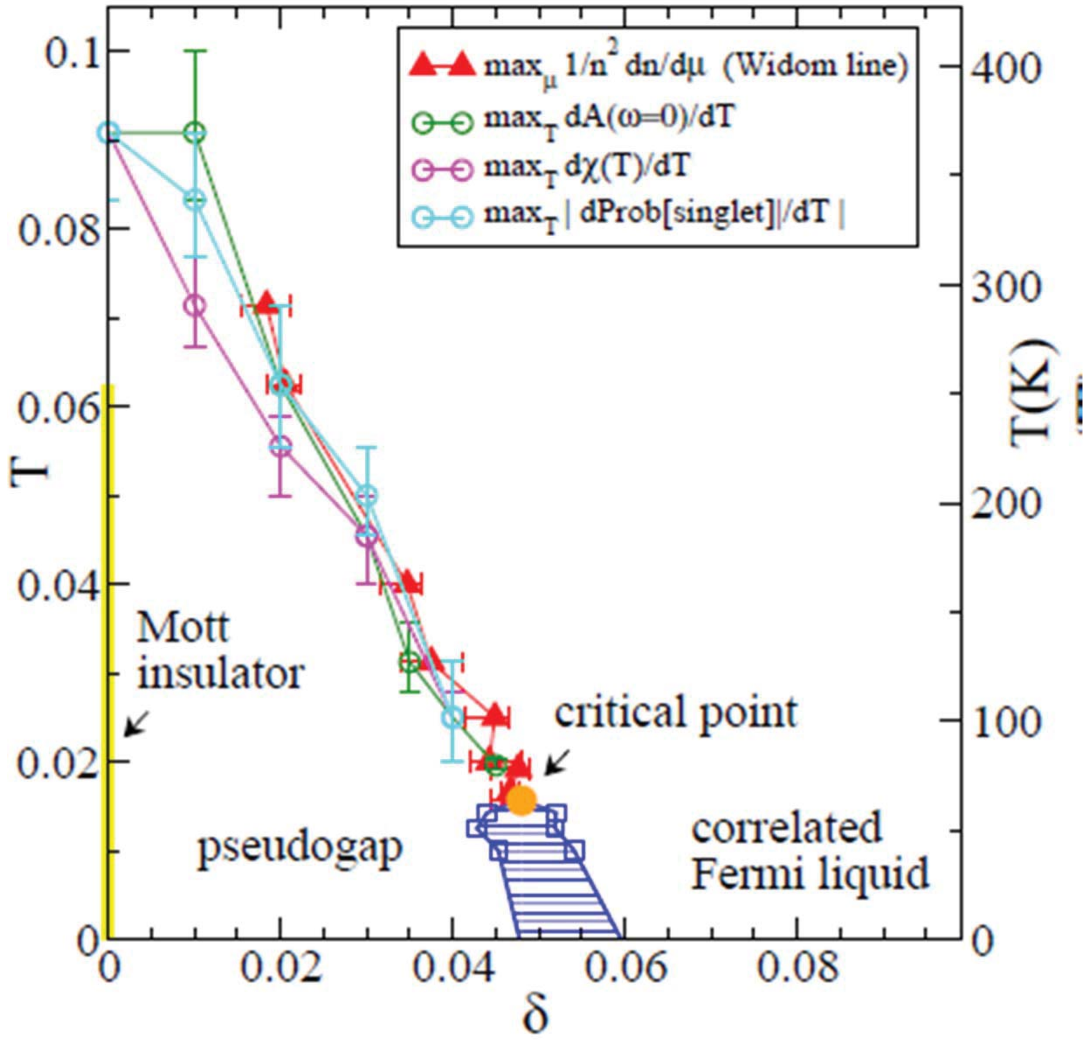




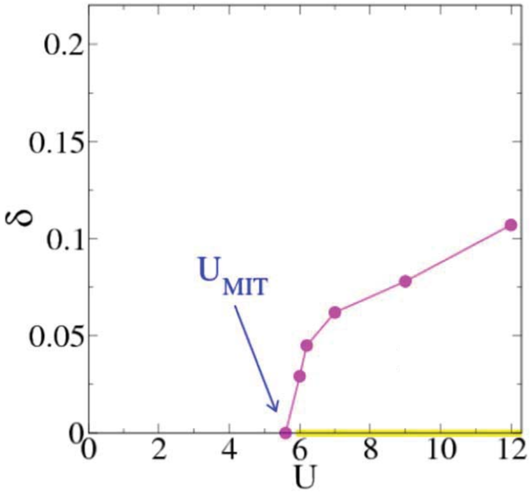


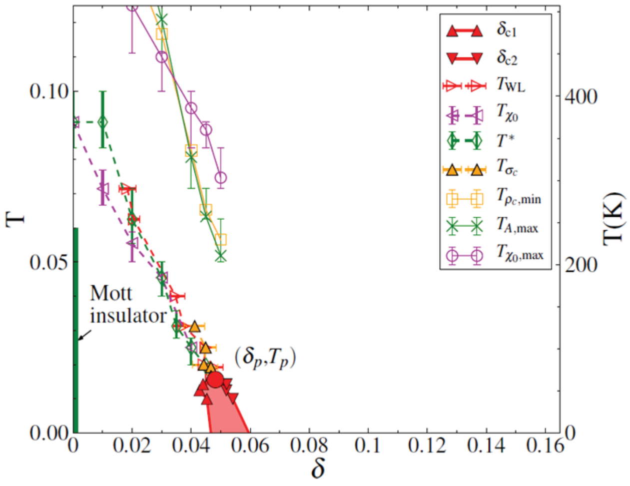
T = 1/10, 1/50

Pseudogap along the Widom line T_W



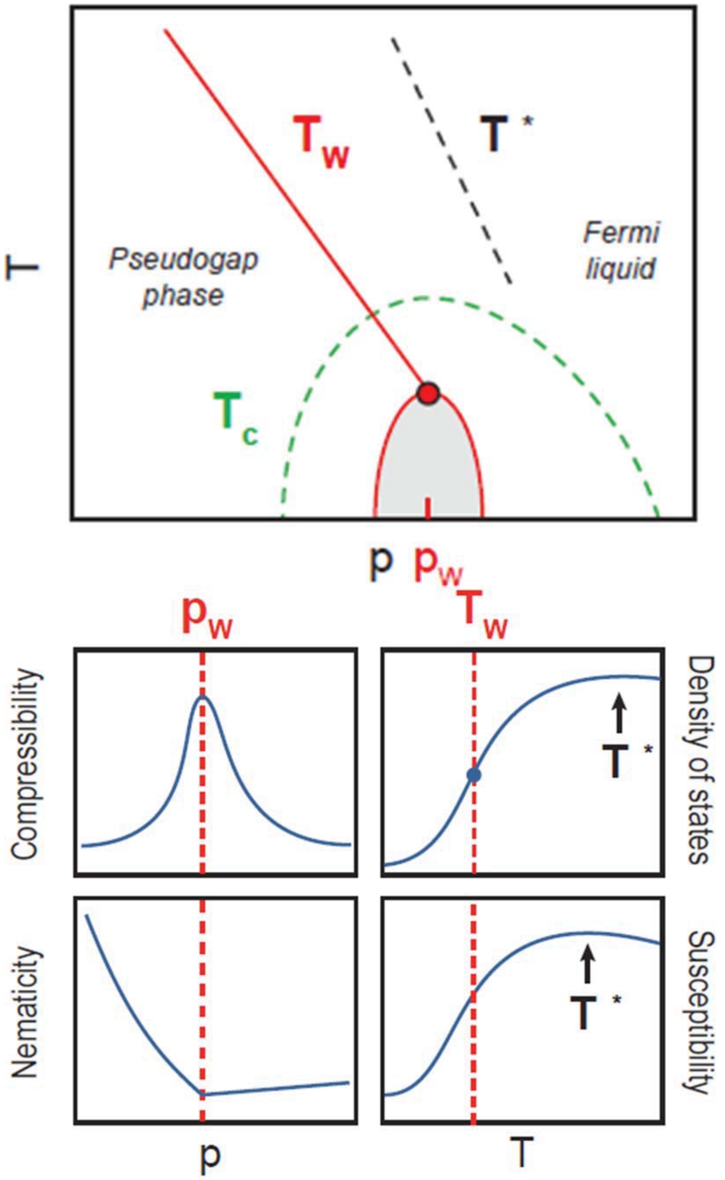
Summary: normal state





- 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?)

Organizing principle



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

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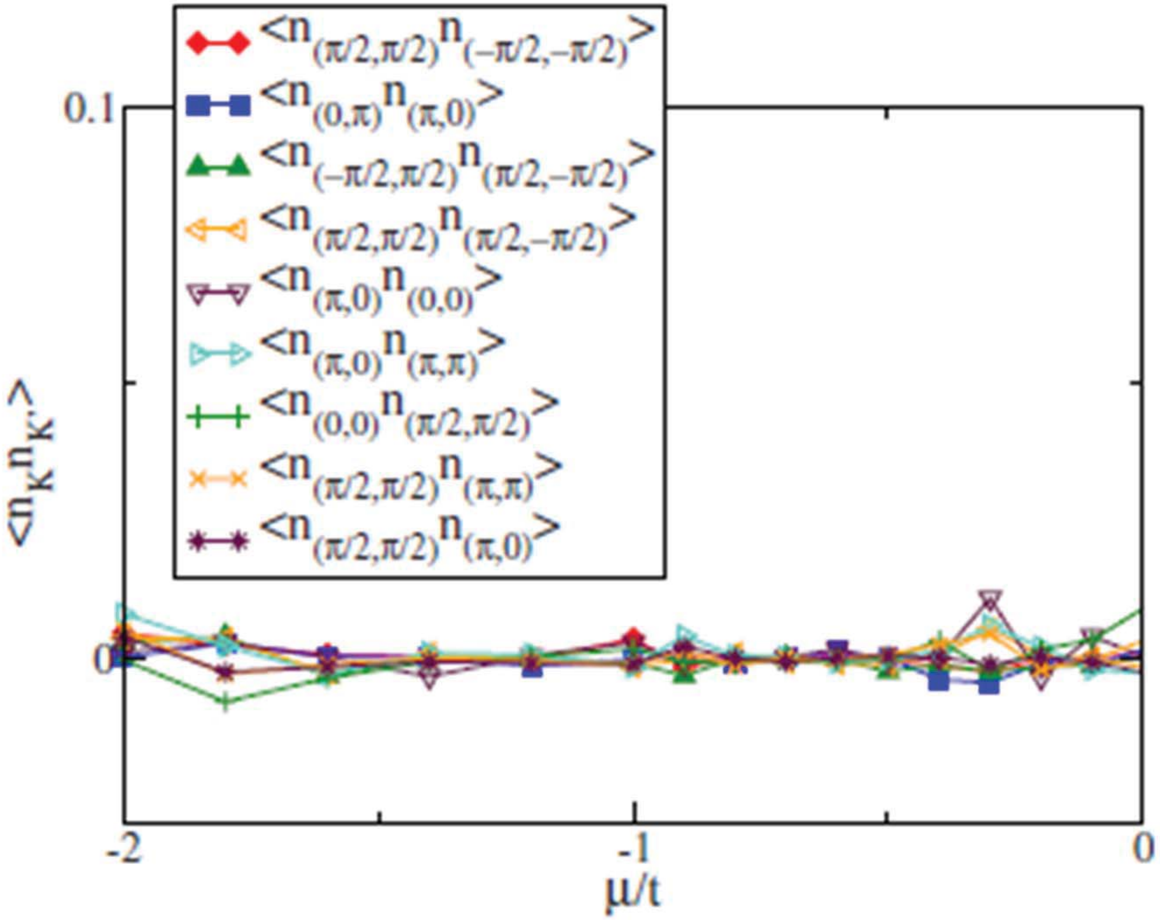
Anisotropy (nematicity)

Normal state and large anisotropy
in an *orthorhombic* crystal

No spontaneous tendency to nematicity in tetragonal crystal



E.Gull, O. Parcollet, P. Werner, and A.J. Millis
PRB **80**, 245102 (2009)

Underdoped metal very sensitive to anisotropy

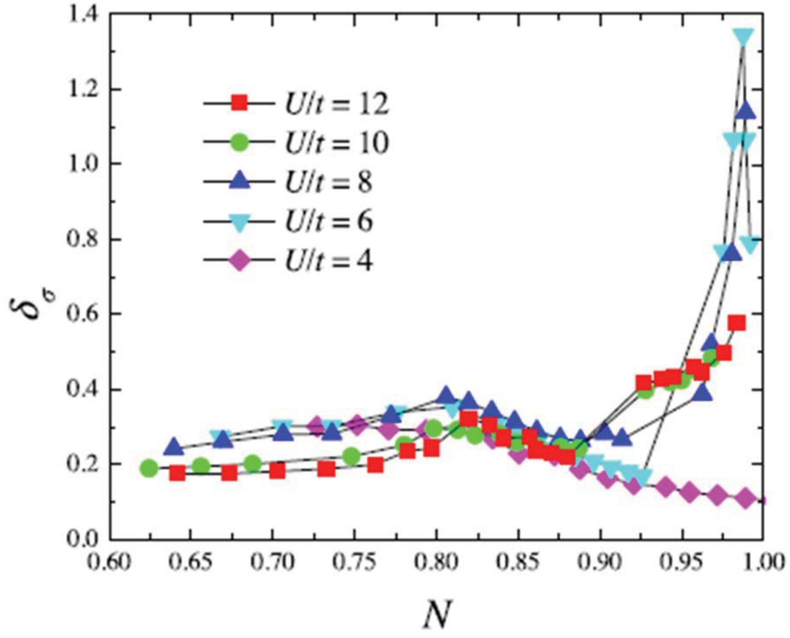
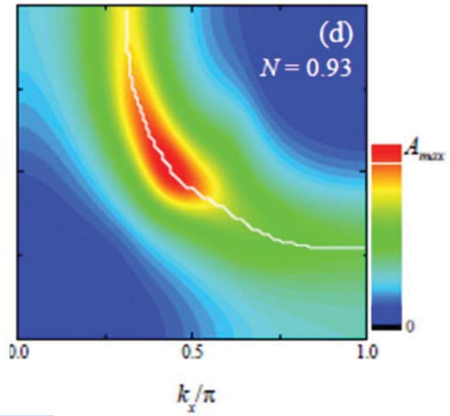
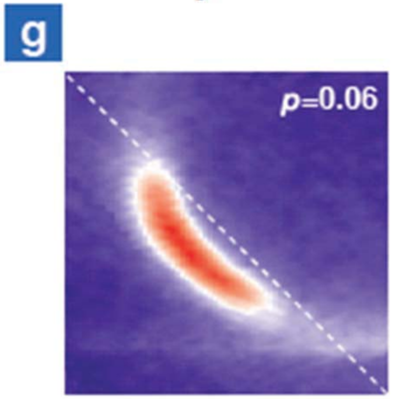


FIG. 3: (Color online) Anisotropy in the CDMFT conductivity $\delta_\sigma = 2\,[\sigma_x(0) - \sigma_y(0)]\,/\,[\sigma_x(0) + \sigma_y(0)]$ as a function of filling N for various values of U and $\eta = 0.1$, $\delta_0 = 0.04$.

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





Satoshi Okamoto

David Sénéchal

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

At finite temperature anisotropy in *Z*

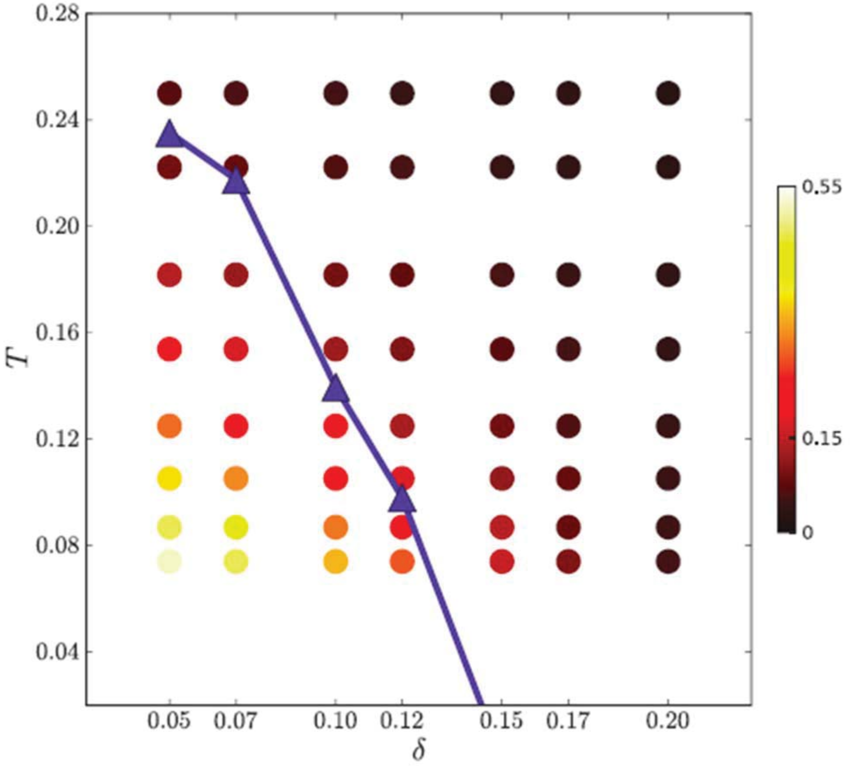
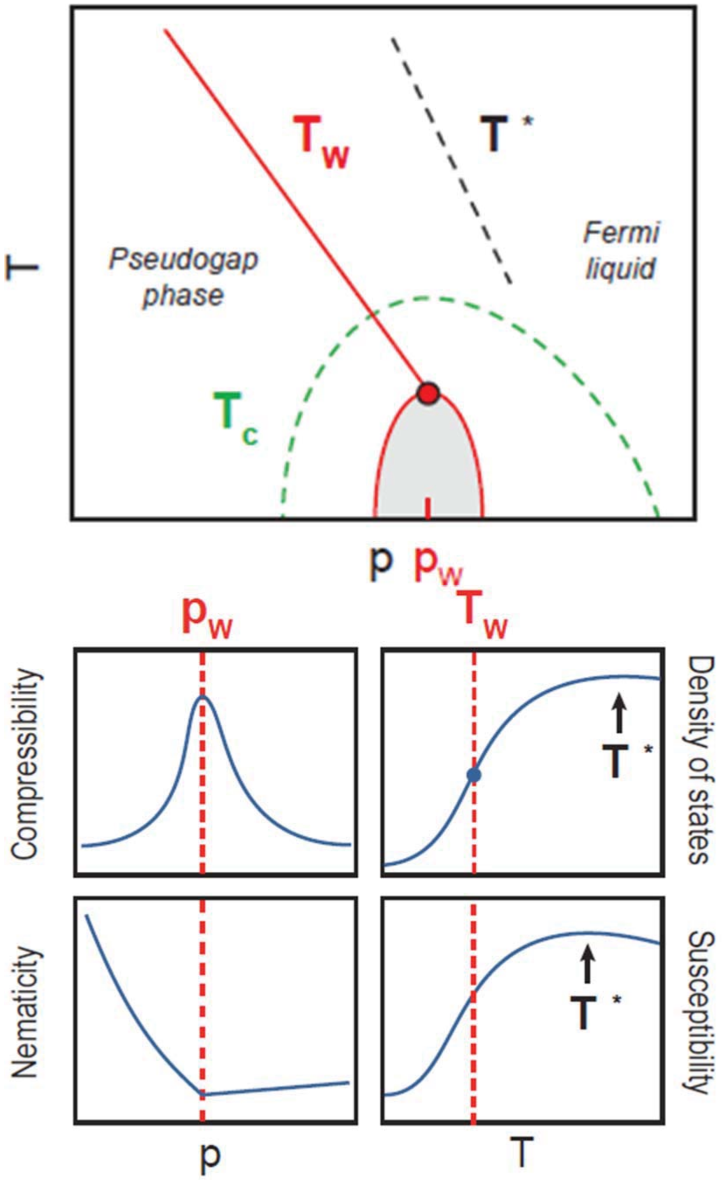


FIG. 3. (Color online) Color map of the anisotropic ratio of the quasiparticle weight σ_Z over the temperature-doping plane, for $U = 6t$. The solid blue curve indicates the pseudogap temperature $T^*(\delta)$ which is obtained as the temperature at which the uniform magnetic susceptibility $\chi_m[q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

U = 6t, DCA, 4x4

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

An emergent phenomenon in CDMFT



- \- Is the pseudogap (PG) a crossover or a phase transition ?
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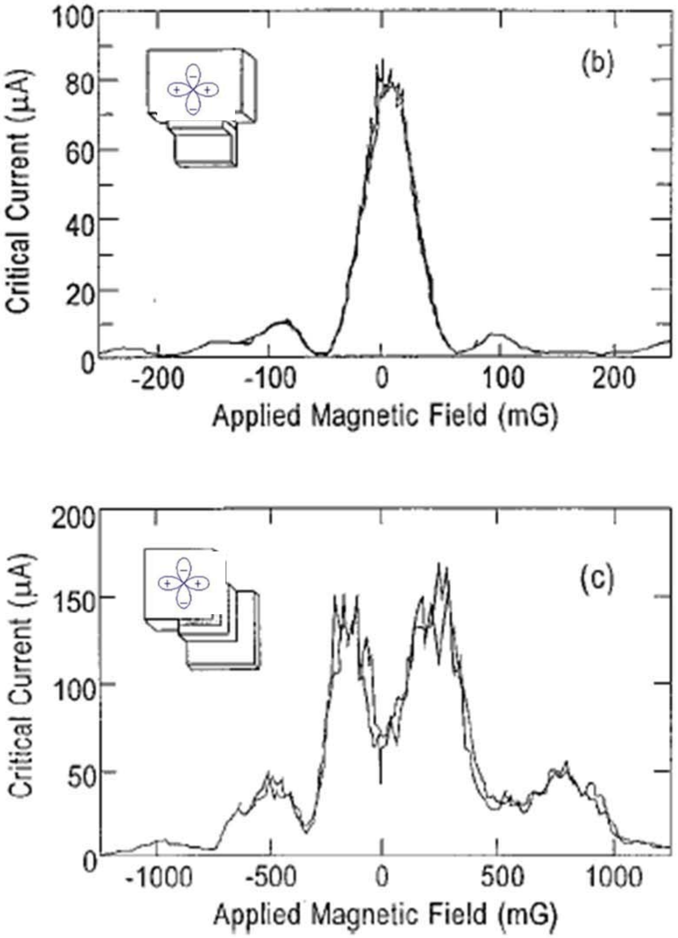
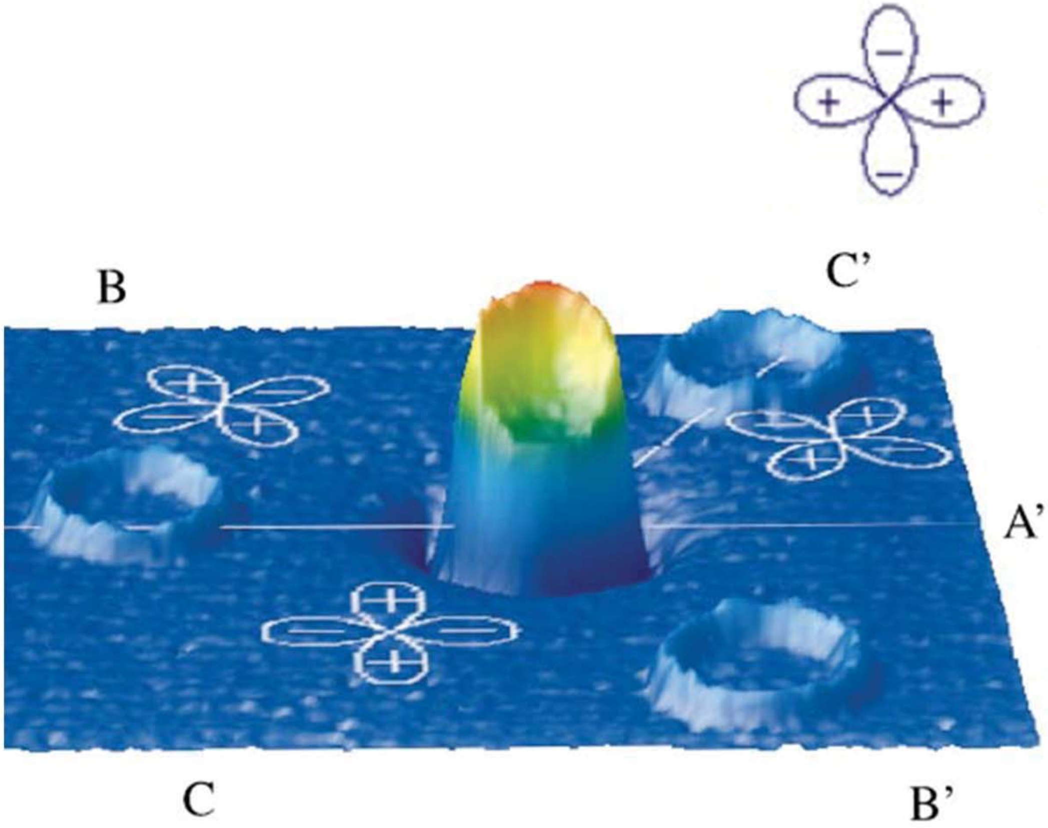
- \- Origin of nematicity ?
- \- Why superconducting ?
- \- Why a dome of SC ?
- \- Does a one-band model capture the key physics ?
- AFM QCP important?
- Lessons from other SC?

d-wave superconductivity

High Tc are d-wave (interference)



Wollman et al. PRL 1993

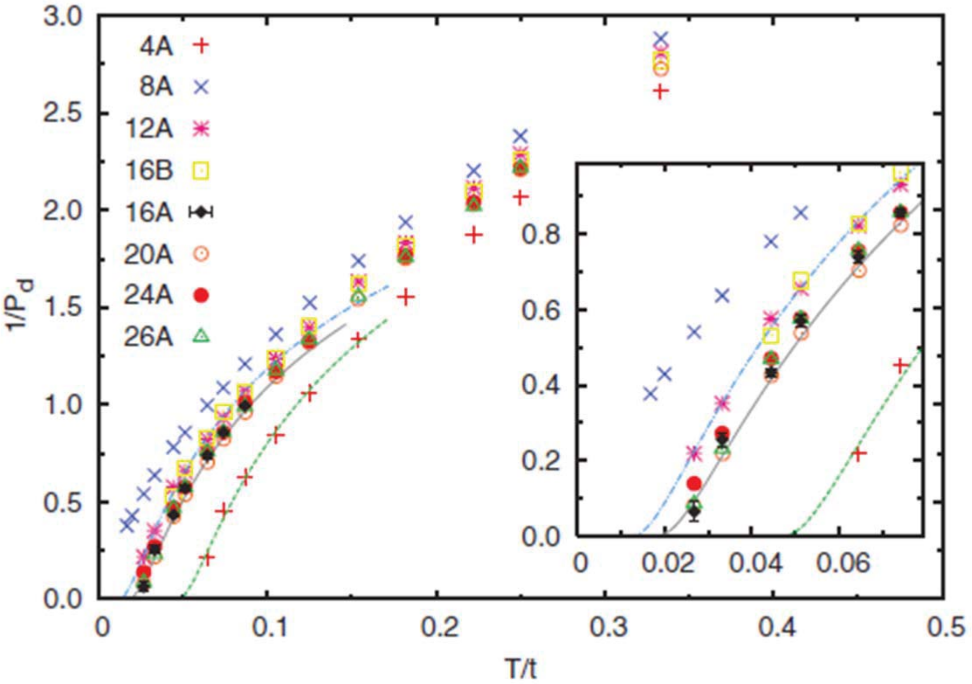


Tsuei Kirtley, Rev. Mod. Phys. 2000

d-wave superconductivity

- Weak coupling
  - C. J. Halboth and W. Metzner, Phys. Rev. Lett. 85, 5162 (2000).
  - B. Kyung, J.-S. Landry, and A. M. S. Tremblay, Phys. Rev. B 68, 174502 (2003).
  - C. Bourbonnais and A. Sedeki, Physical Review B 80, 085105 (2009).
  - D. J. Scalapino, Physica C: Superconductivity 470, Supplement 1, S1 (2010), ISSN 0921-4534, proceedings of the 9th International Conference on Materials and Mech anisms of Superconductivity.
- Renormalized Mean-Field Theory
  - P. W. Anderson, P. A. Lee, M. Randeria, T. M. Rice, N. Trivedi, and F. C. Zhang, Journal of Physics: Condensed Matter 16, R755 (2004).
  - K.-Y. Yang, T. M. Rice, and F.-C. Zhang, Phys. Rev. B 73, 174501 (2006).
- Slave particles
  - P. A. Lee, N. Nagaosa, and X.-G. Wen, Rev. Mod. Phys. 78, 17 (2006).
  - M. Imada, Y. Yamaji, S. Sakai, and Y. Motome, Annalen der Physik 523, 629 (2011)
- Variational approaches
  - T. Giamarchi and C. Lhuillier, Phys. Rev. B 43, 12943 (1991).
  - A. Paramekanti, M. Randeria, and N. Trivedi, Phys. Rev. B 70, 054504 (2004).

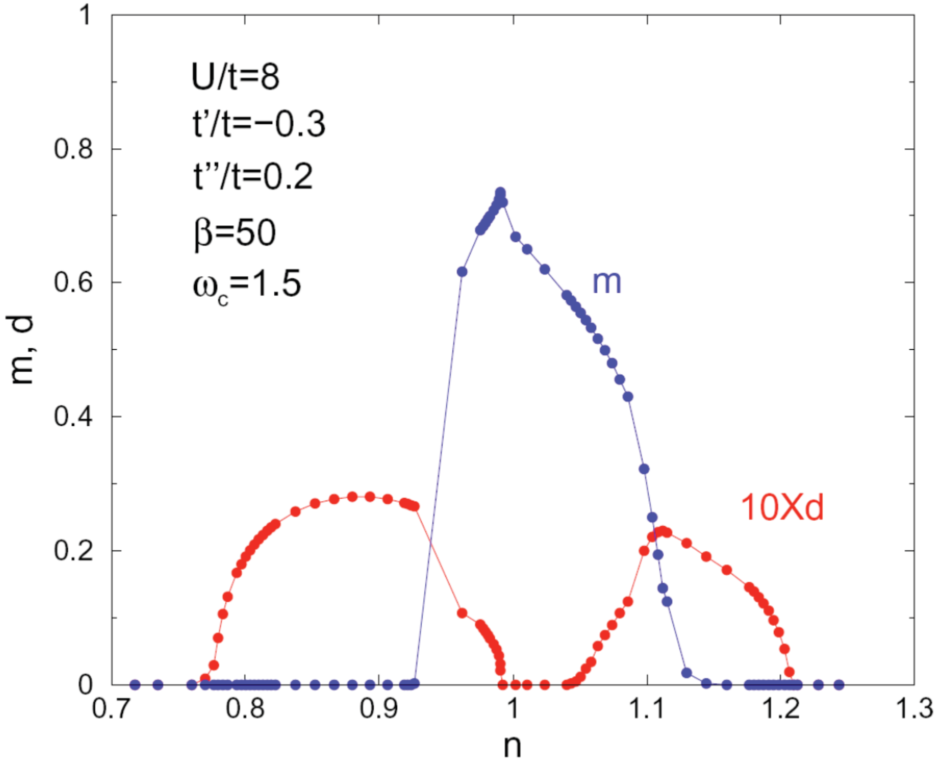
Divergence of d-wave: finite size study



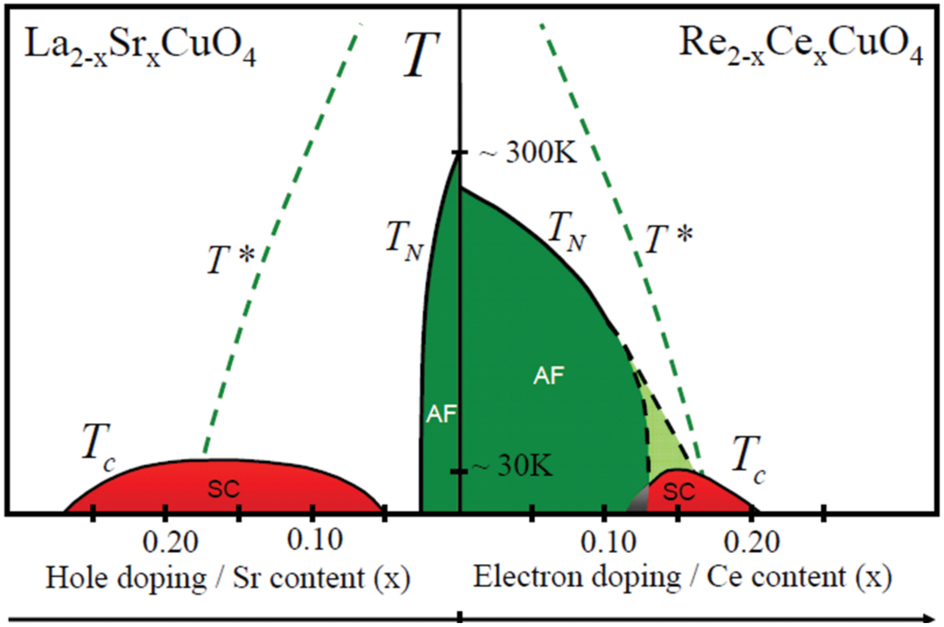
DCA, *U=4*

T. A. Maier, M. Jarrell, T. C. Schulthess,
P. R. C. Kent, and J. B. White PRL **95,** 237001 (2005)

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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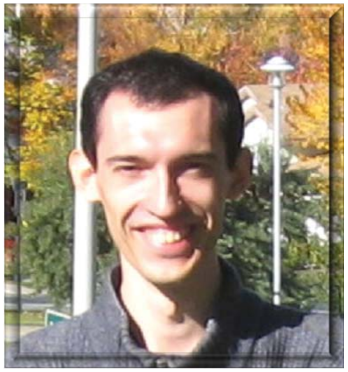

Giovanni Sordi

Patrick Sémon

Kristjan Haule

Finite *T* phase diagram
Superconductivity
t'=0

Sordi et al. PRL **108**, 216401 (2012)

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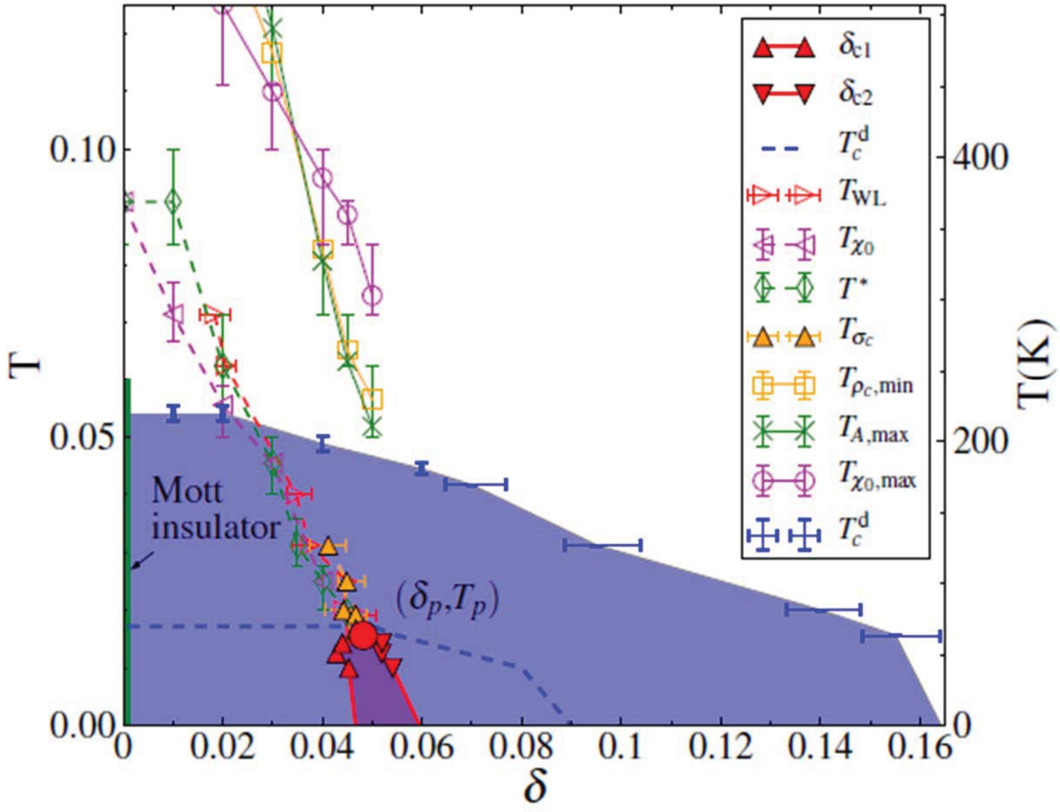
Phase diagram for $U = 6.2\, t$

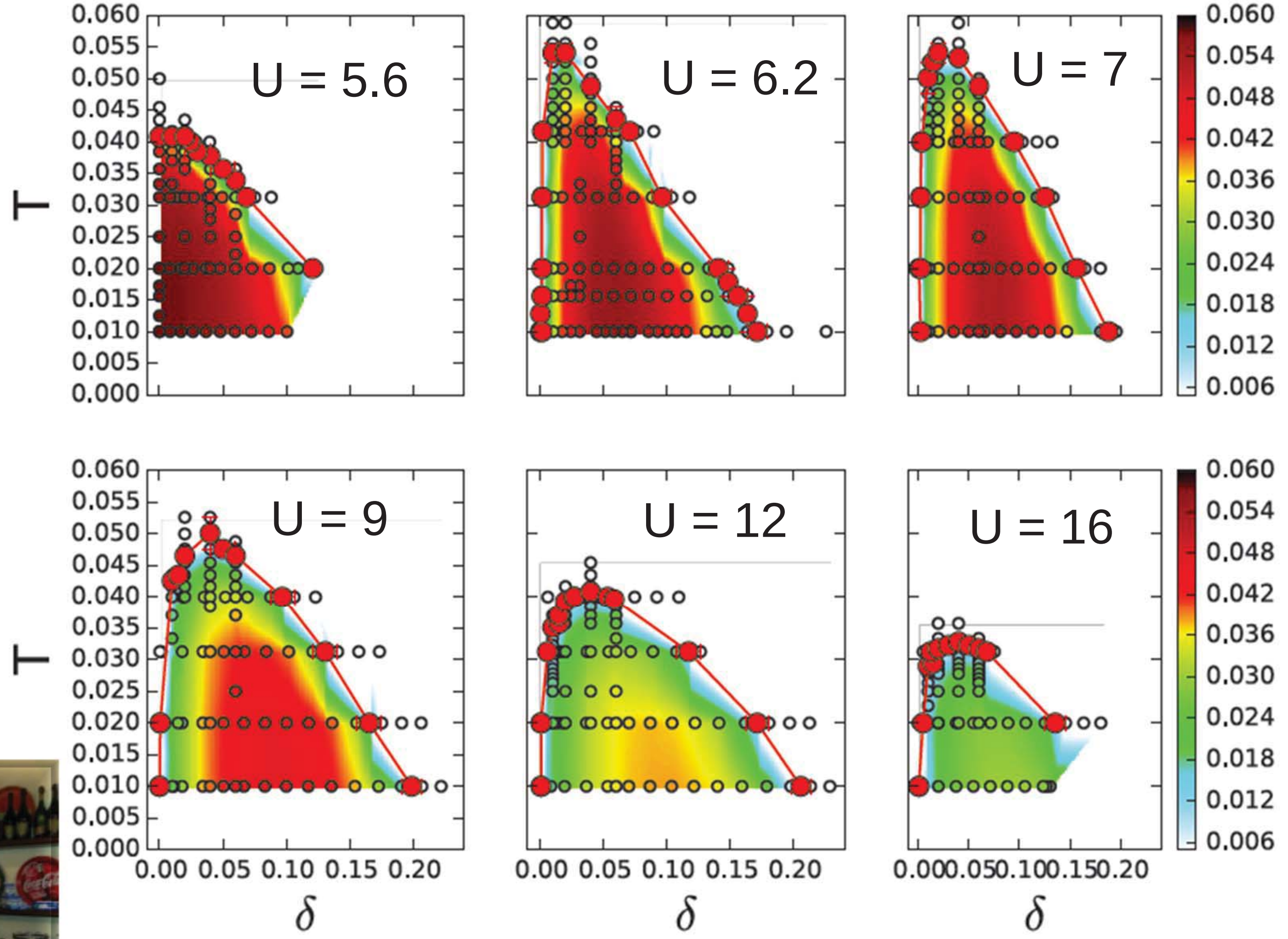
Giovanni Sordi

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)

Order parameter (color) and T_c



Lorenzo Fratino

L. Fratino, G. Sordi (unpublished)

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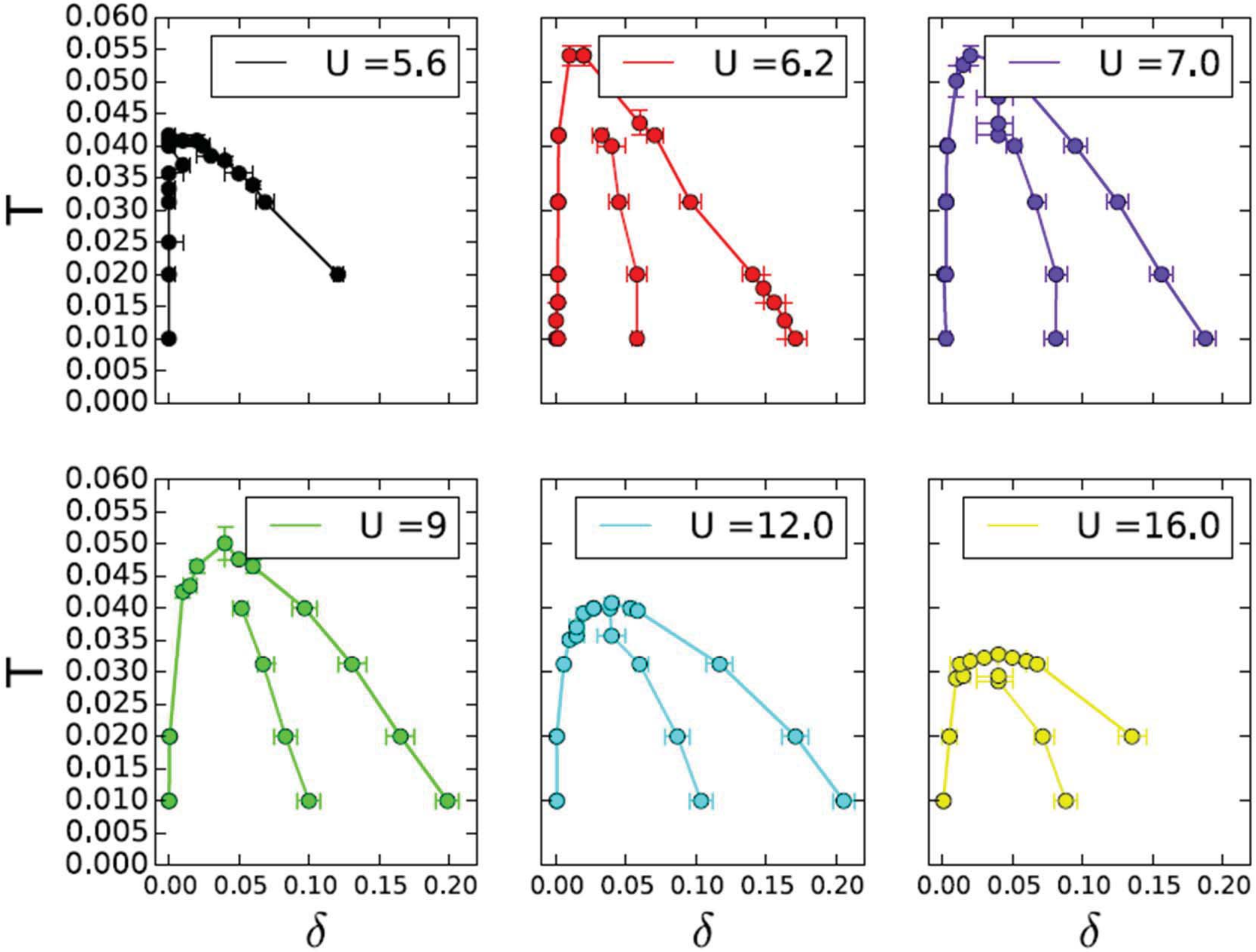
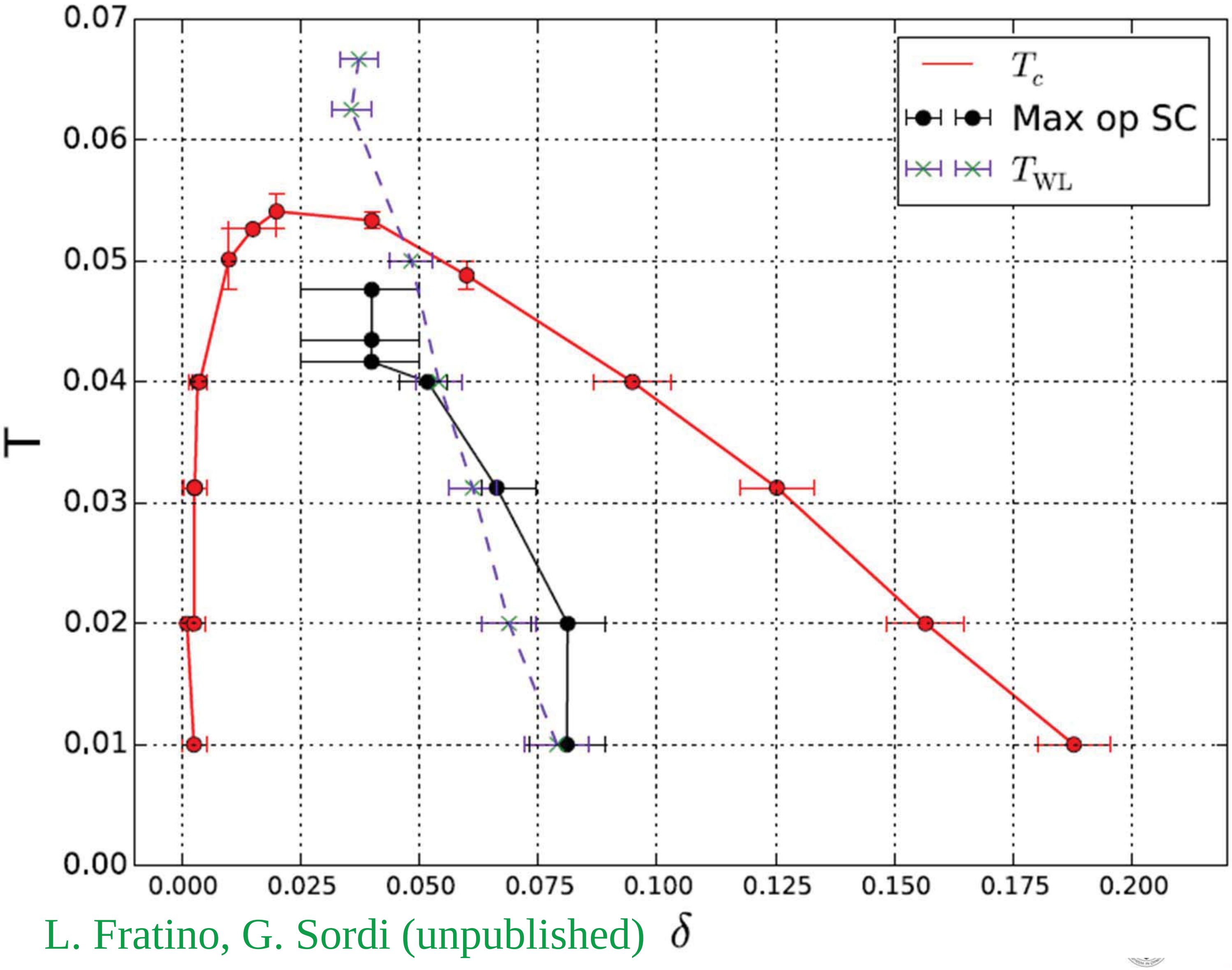
T_c vs $T_{\text{max order parameter}}$



L. Fratino, G. Sordi (unpublished)

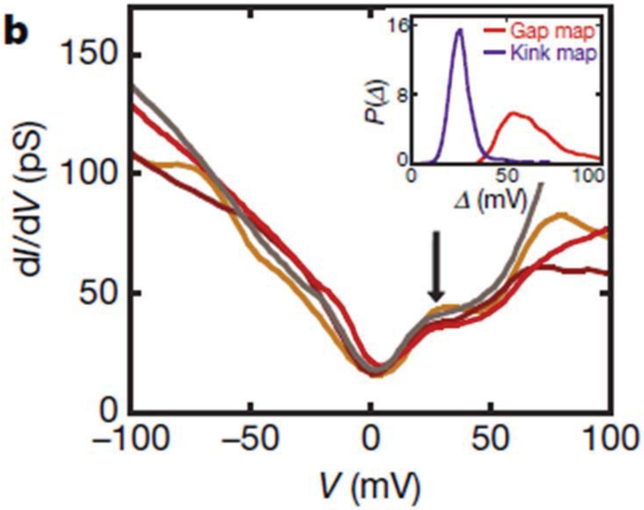
U=7, $\mathrm{T_W}$ vs $\mathrm{T_c}$ vs $\mathrm{T_{max\ order\ parameter}}$



L. Fratino, G. Sordi (unpublished)

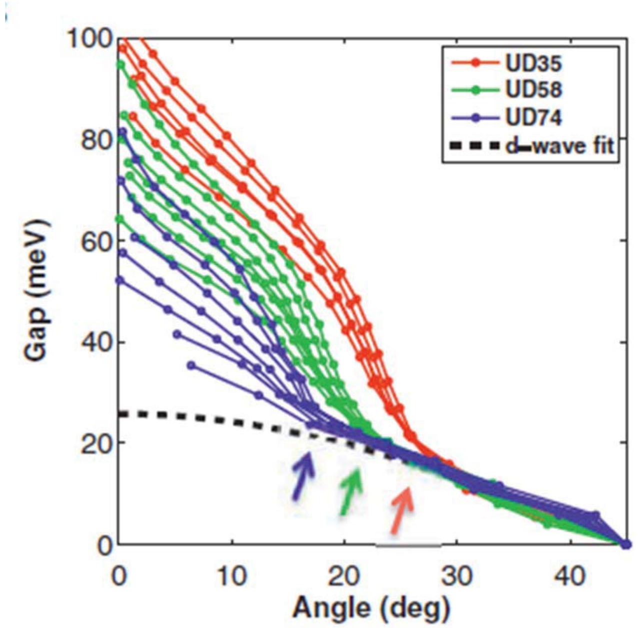
Meaning of T_c^d

- Local pair formation



K. K. Gomes, A. N. Pasupathy, A. Pushp,
S. Ono, Y. Ando, and A. Yazdani,
Nature **447**, 569 (2007)

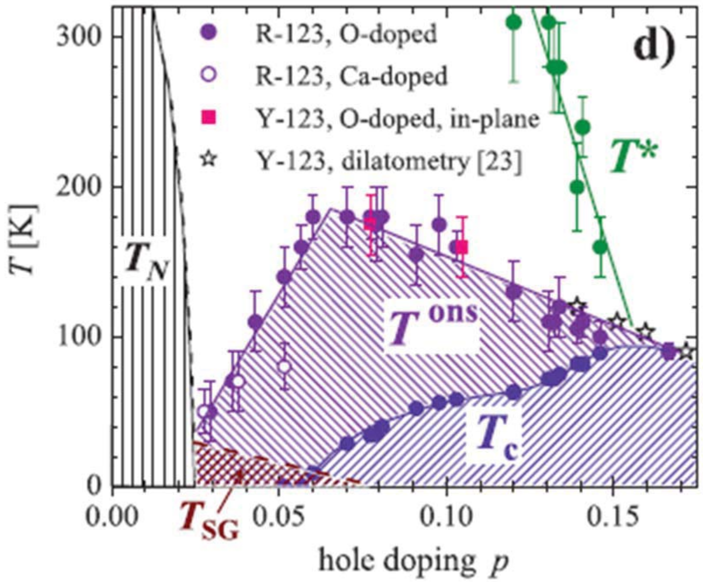
Meaning of T_c^d : Local pair formation



A. Pushp, Parker, … A. Yazdani,
Science **364**, 1689 (2009)

However, our measurements demonstrate that the nodal gap does not change with reduced doping. The pairing strength does not get weaker or stronger as the Mott insulator is approached; rather, it saturates.

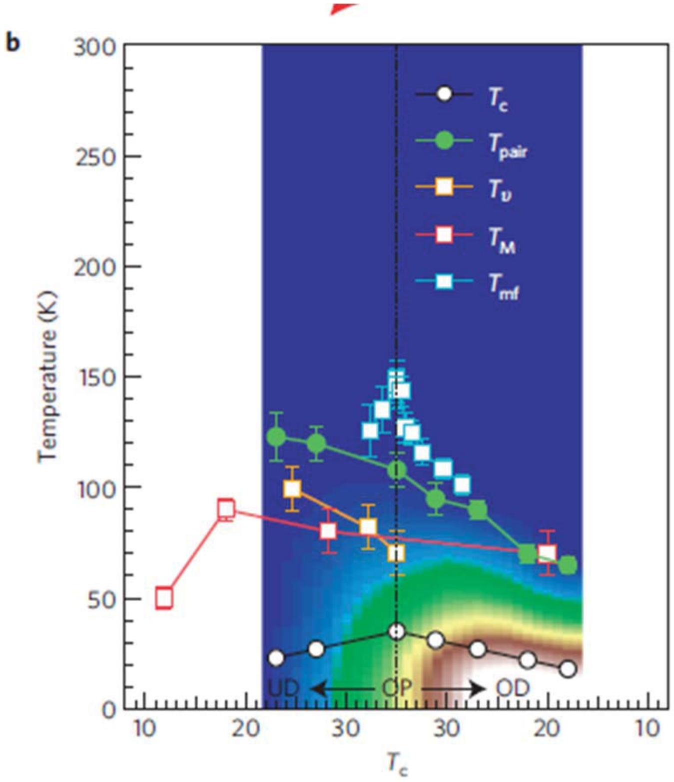
Fluctuating region



Infrared response

Dubroka et al. PRL 106, 047006 (2011)

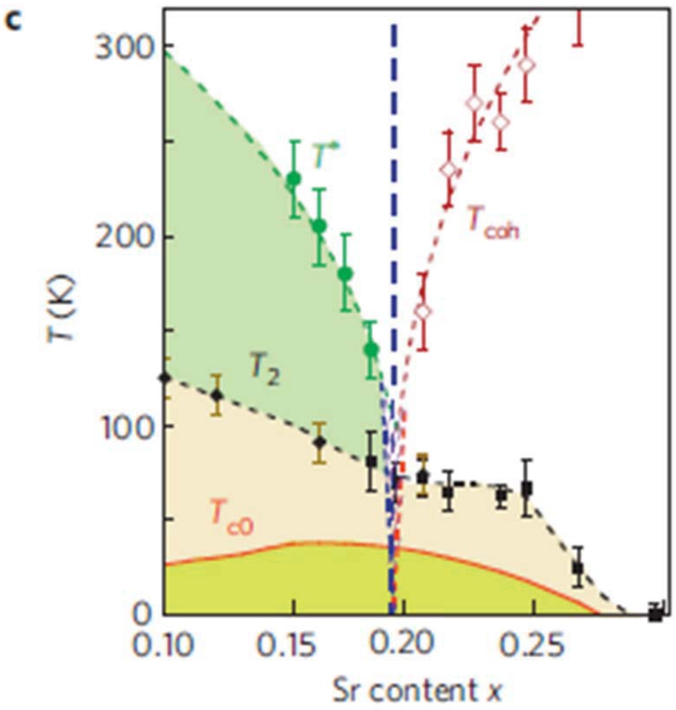
Tpair



ARPES
Bi2212

Kondo, Takeshi, et al. Kaminski Nature Physics **2011**, *7*, 21-25

T_2



Magnetoresistance, LSCO
Fluctuating vortices

Patrick M. Rourke, et al. Hussey Nature Physics 7, 455–458 (2011)

Giant proximity effect

$T_c = 32\ K$
$T_c < 5K$

Morenzoni et al.,
Nature Comms. **2** (2011)

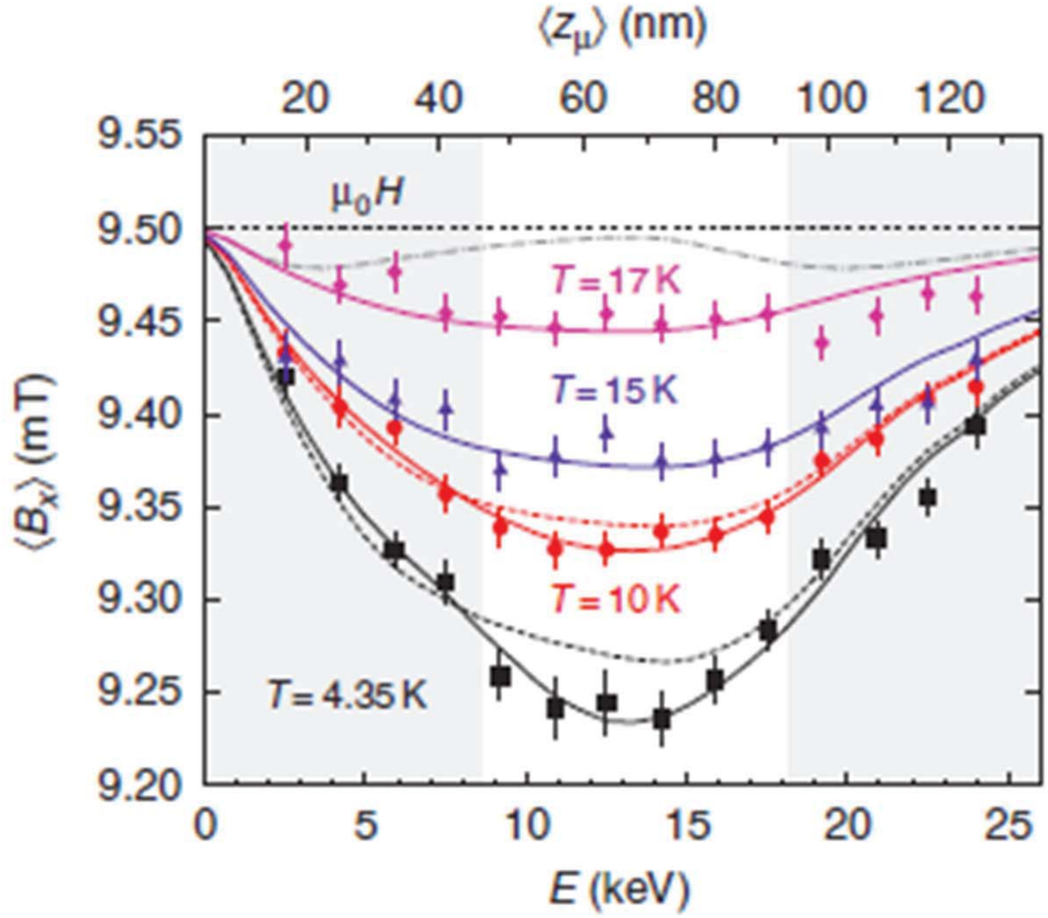


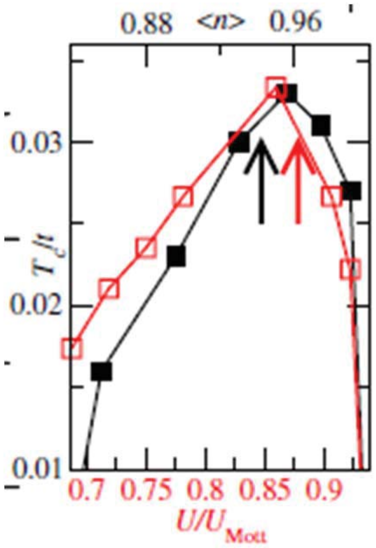
Figure 6 | Depth profile of the local field at different temperatures. The

Actual T_c in underdoped

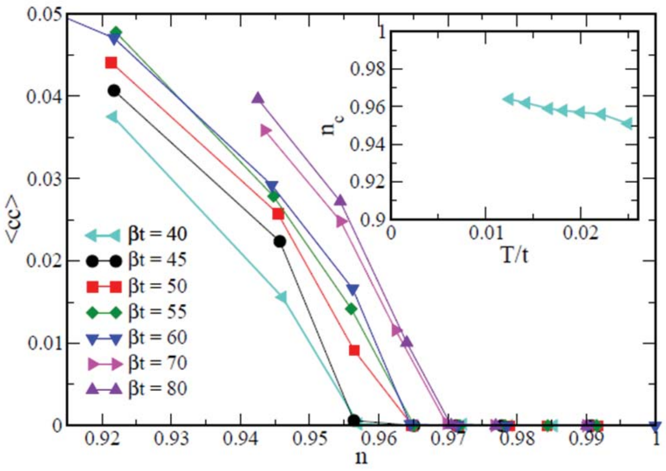
- Quantum and classical phase fluctuations
  - V. J. Emery and S. A. Kivelson, Phys. Rev. Lett. **74**, 3253 (1995).
  - V. J. Emery and S. A. Kivelson, Nature **374**, 474 (1995).
  - D. Podolsky, S. Raghu, and A. Vishwanath, Phys. Rev. Lett. **99**, 117004 (2007).
  - Z. Tesanovic, Nat Phys **4**, 408 (2008).
- Magnitude fluctuations
  - I. Ussishkin, S. L. Sondhi, and D. A. Huse, Phys. Rev. Lett. **89**, 287001 (2002).
- Competing order
  - E. Fradkin, S. A. Kivelson, M. J. Lawler, J. P. Eisenstein, and A. P. Mackenzie, Annual Review of Condensed Matter Physics **1**, 153 (2010).
- Disorder
  - F. Rullier-Albenque, H. Alloul, F. Balakirev, and C. Proust, EPL (Europhysics Letters) **81**, 37008 (2008).
  - H. Alloul, J. Bobro, M. Gabay, and P. J. Hirschfeld, Rev. Mod. Phys. **81**, 45 (2009).

Larger clusters

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



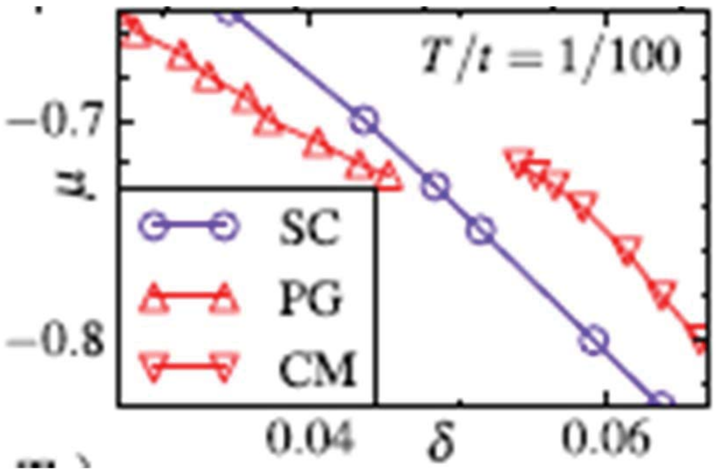
8 site DCA, *U=6t*



8 site DCA, *U=6.5t*

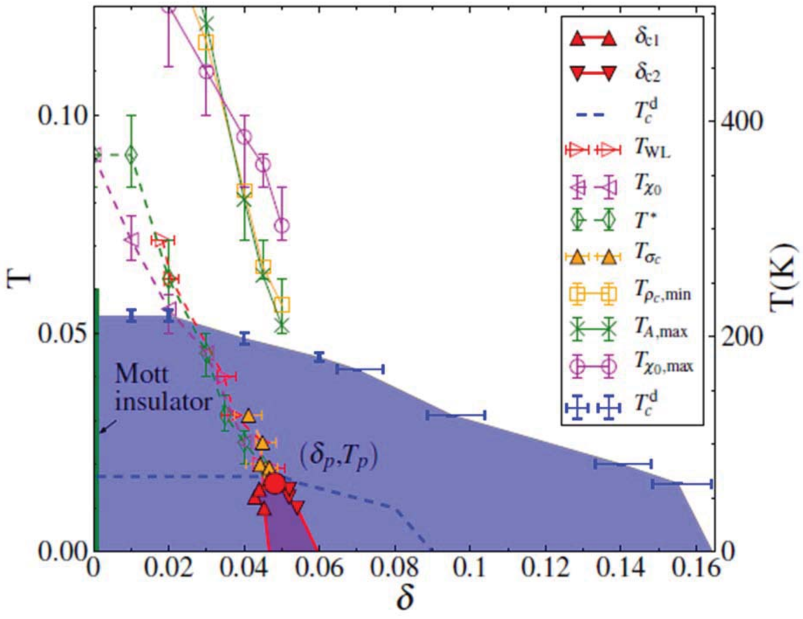
Gull Parcollet Millis,
PRL **110**, 216405 (2013)

Fate of the first order transition in SC state



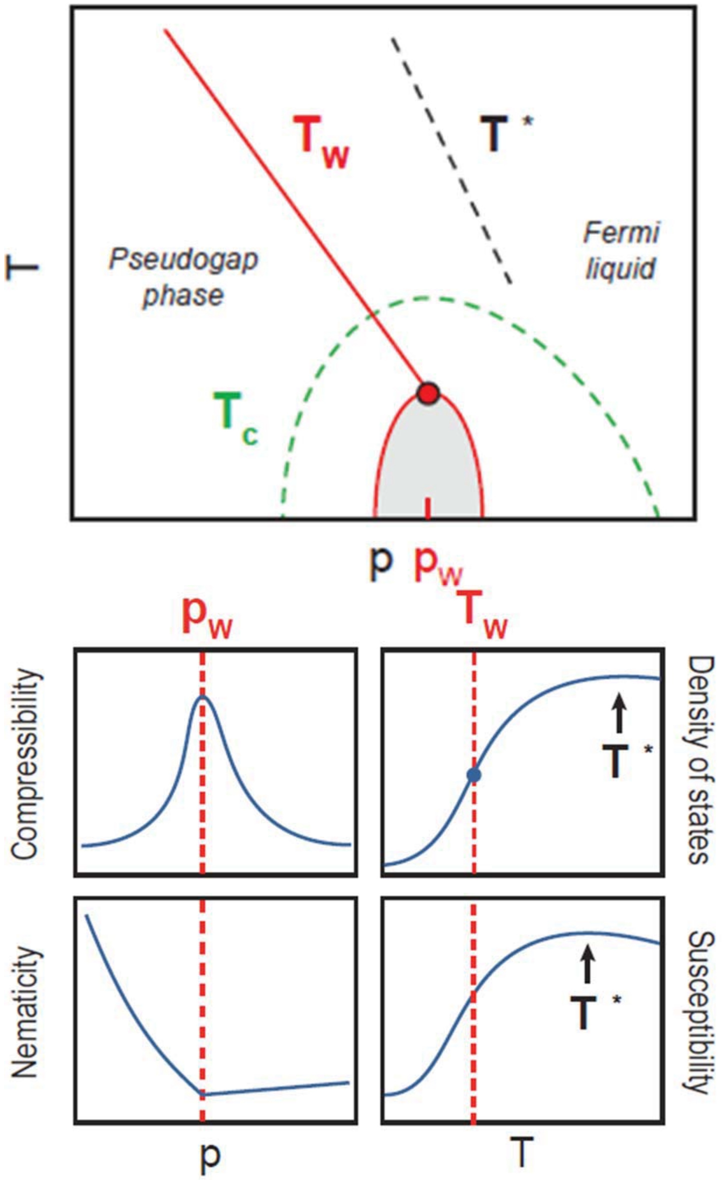
G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)

Summary



- Below the dome, not QCP (but Mott)
- Maximum near Widom line
- T^* different from T_c^d
- First-order transition destroyed (but traces in the dynamics)
- Actual T_c in underdoped
  - Competing order
  - Long wavelength fluctuations (see O.P.)

Organizing principle



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Bio break