



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

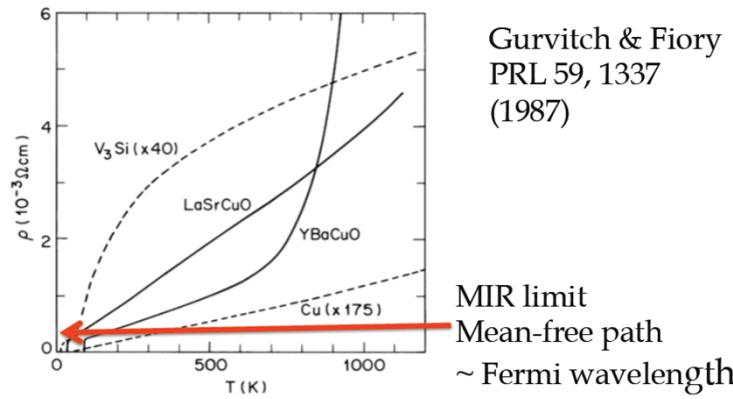
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Collège de France, 16 mars 2015
17h00 à 18h30



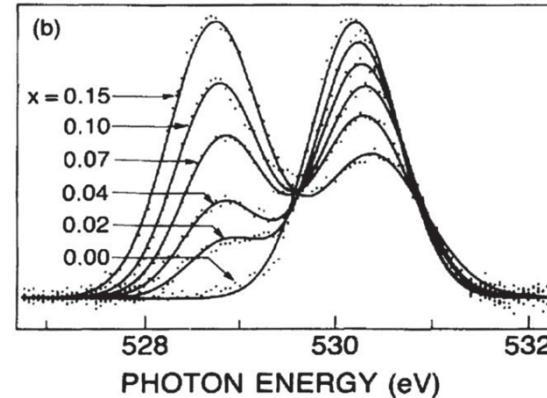
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Last time

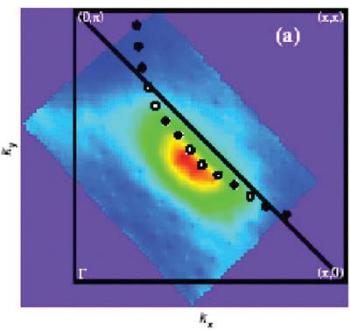


Gurvitch & Fiory
PRL 59, 1337
(1987)

MIR limit
Mean-free path
~ Fermi wavelength



Hole-doped, 10%



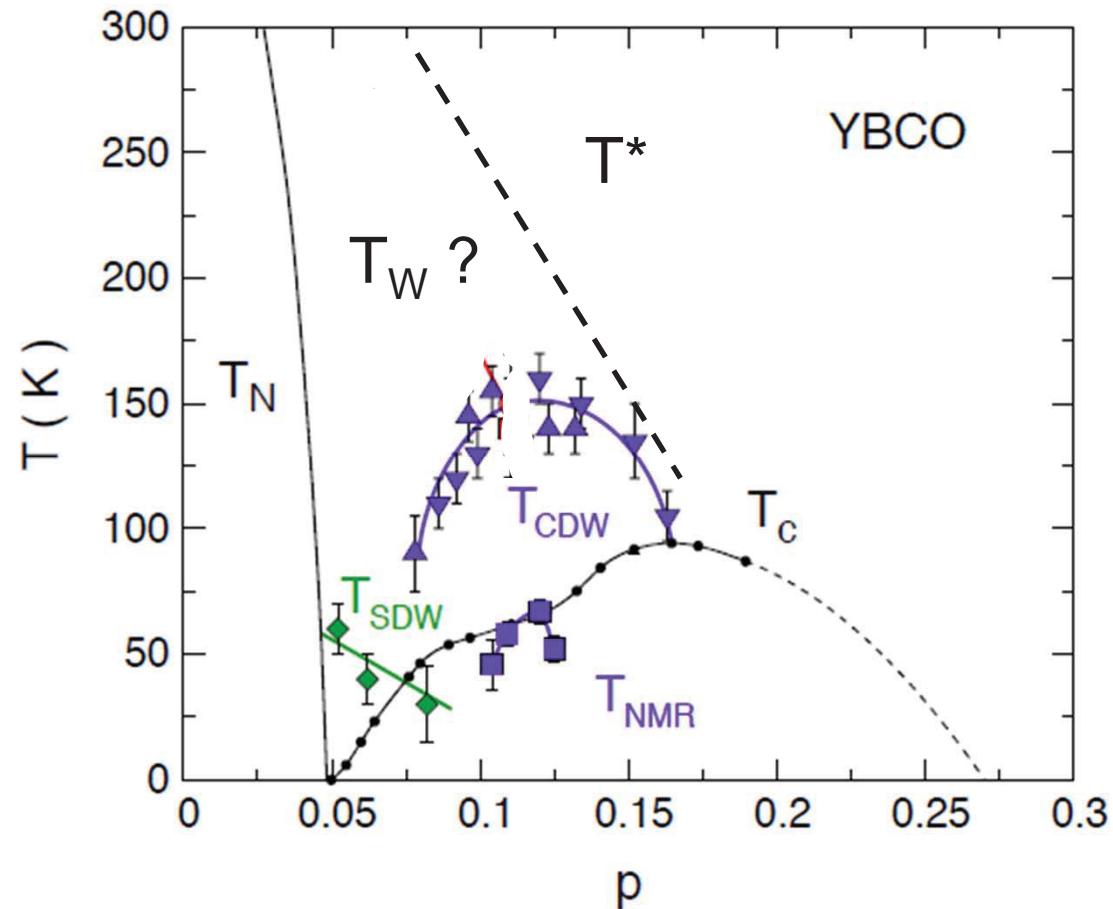
F. Ronning et al. Jan. 2002, $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$

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

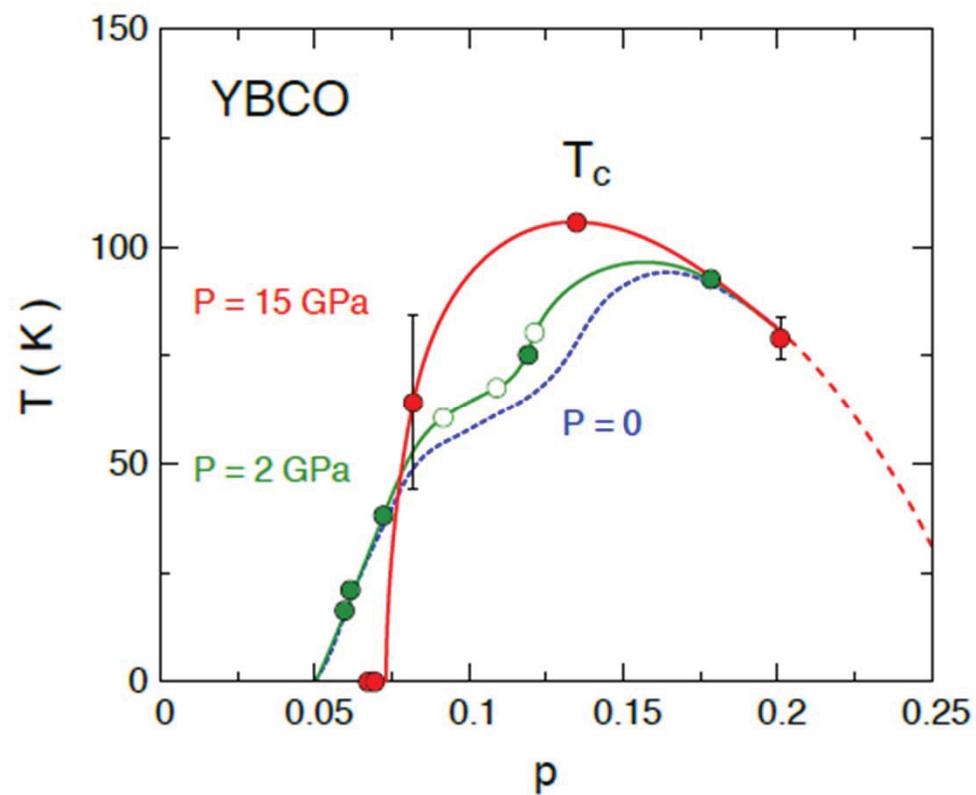


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Phase diagram for hole-doped cuprates

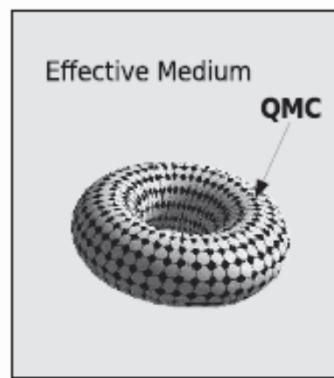


Getting rid of the CDW



Cyr-Choinière et al, arxiv1503.02033

2d Hubbard: Quantum cluster method

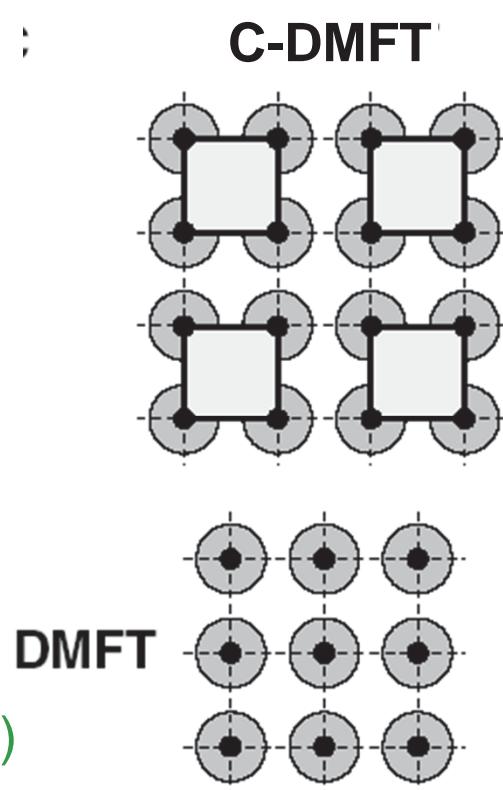


DCA

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)

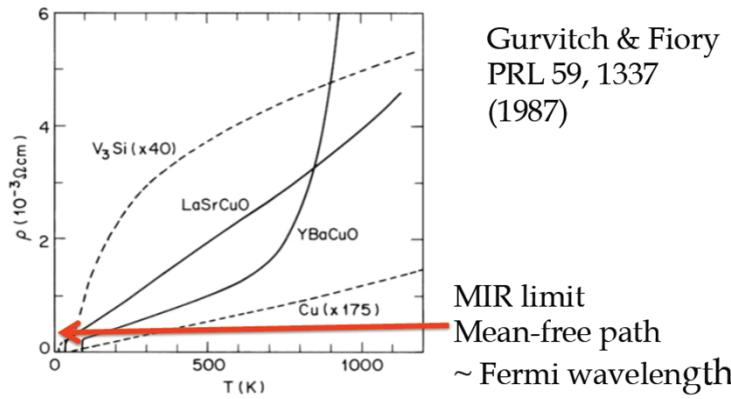
Kotliar et al. RMP (2006)

AMST et al. LTP (2006)



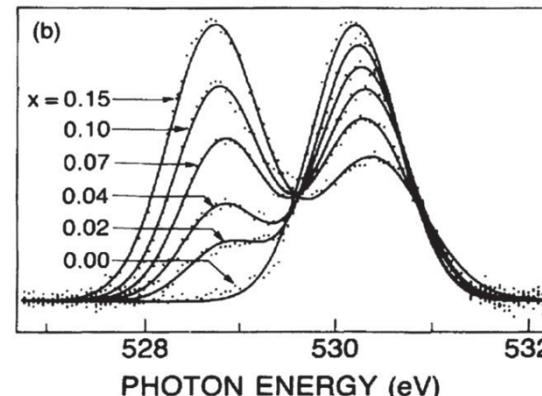
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Last time

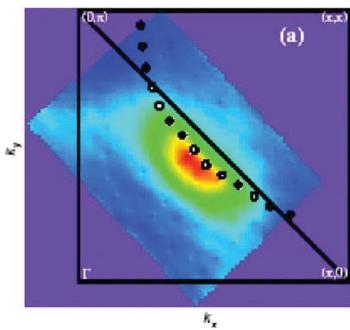


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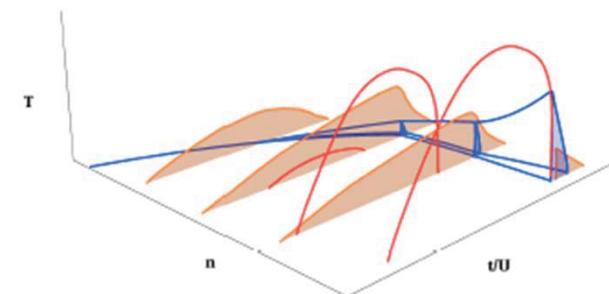
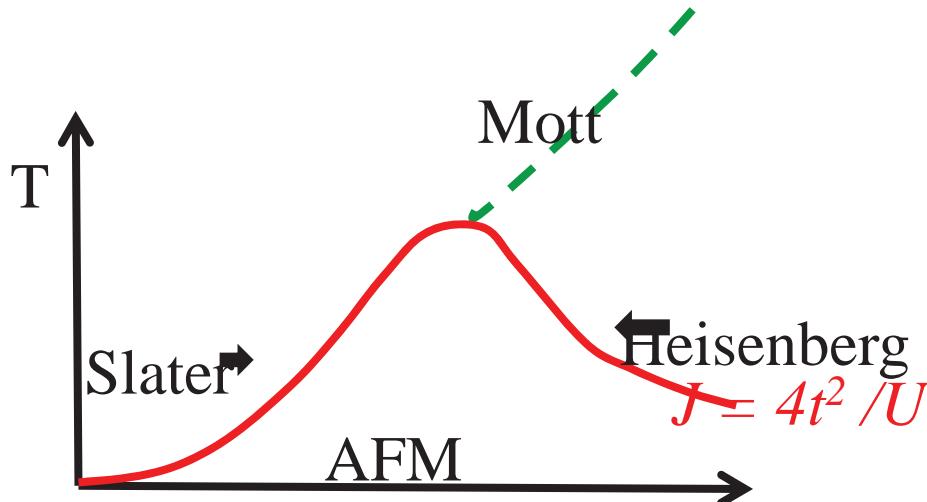


Hole-doped, 10%



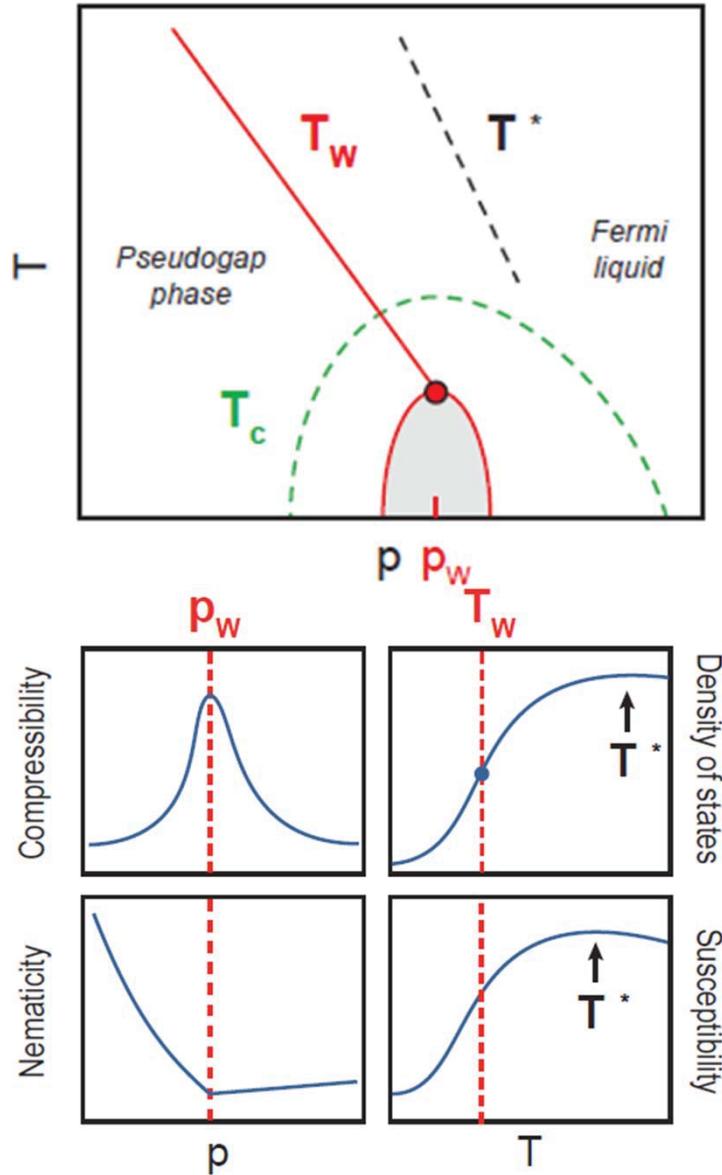
F. Ronning et al. Jan. 2002, $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$

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



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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?



Today

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

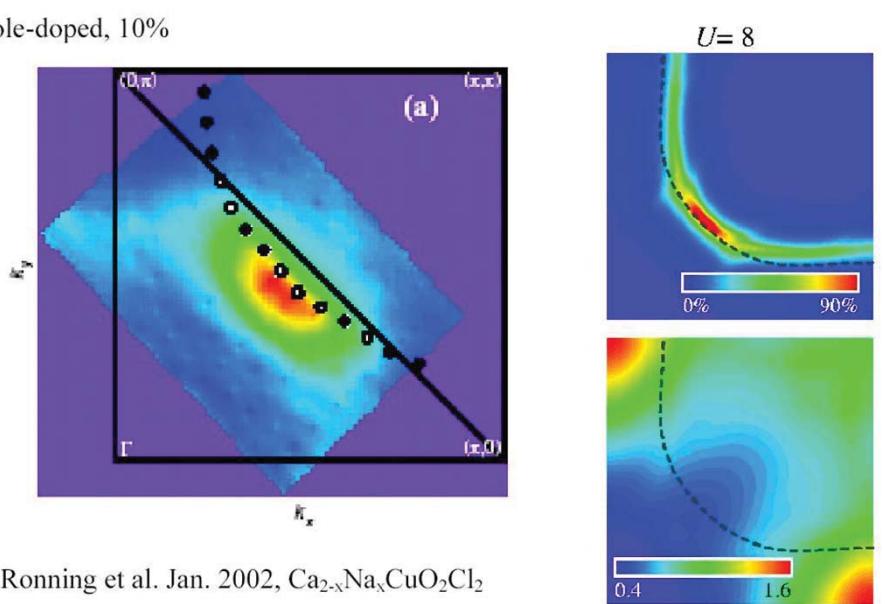


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ARPES pseudogap

Strong correlation pseudogap ($U > 8t$)

- Different from Mott gap that is local (all k) not tied to $\omega=0$.
- Pseudogap close to $\omega=0$ 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 .



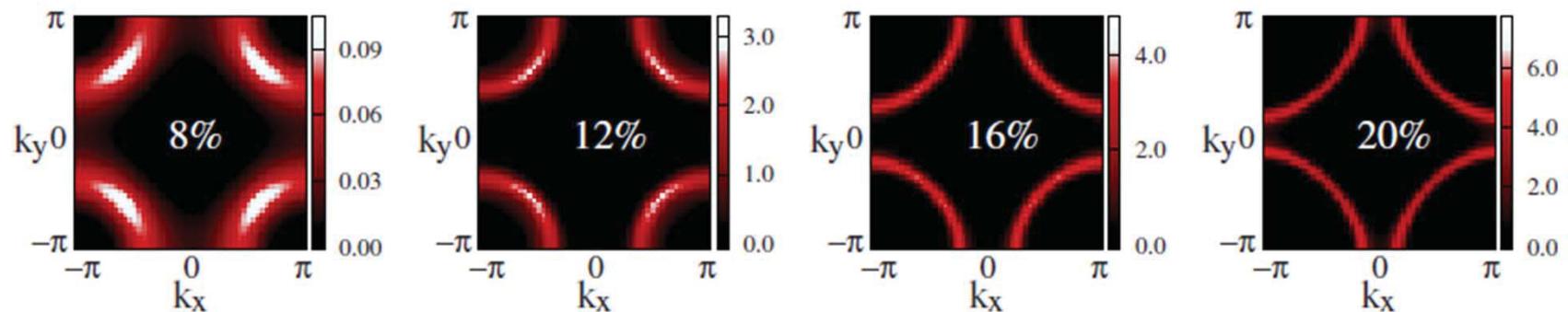
F. Ronning et al. Jan. 2002, $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$

Sénéchal, AMT, PRL 92, 126401 (2004).



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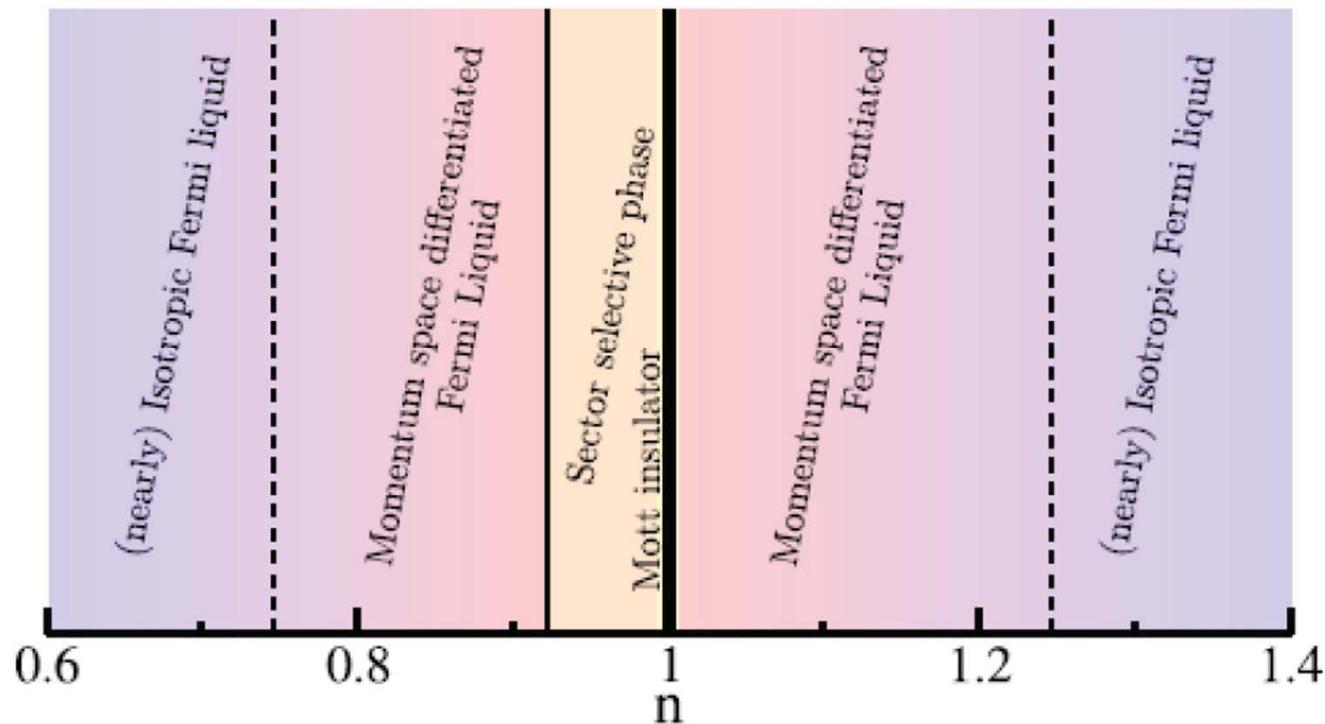
Can be seen with 2 site DCA



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)



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Mott transition at $n = 1$

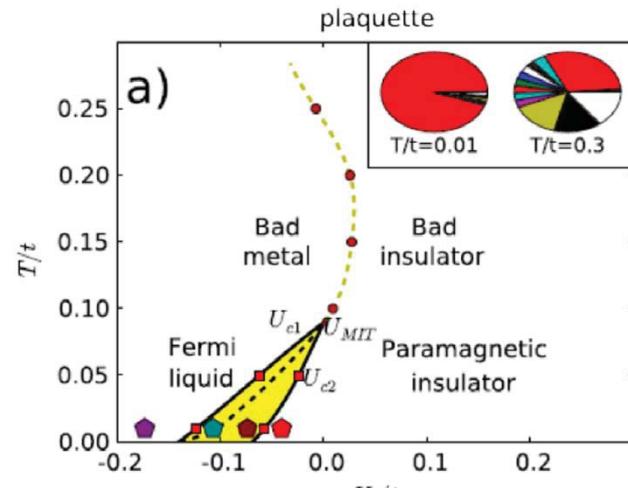
Interaction-induced Mott transition, $n = 1$

4 sites (CDMFT-CTQMC)

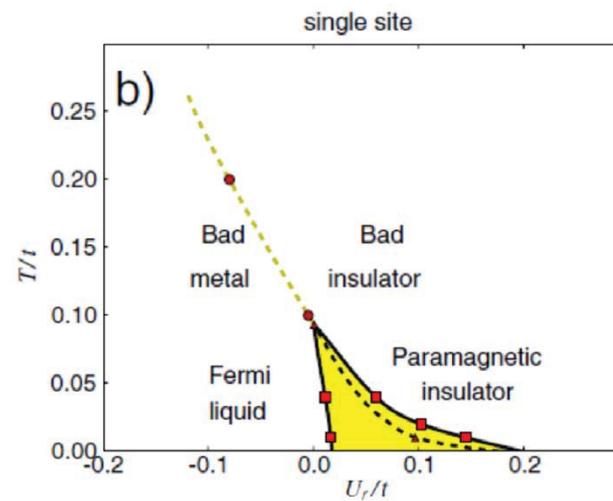
Georges, A., and W. Krauth,
PRB **48**, 7167 (1993)

Single site

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



$$U_{MIT} = 6.05$$

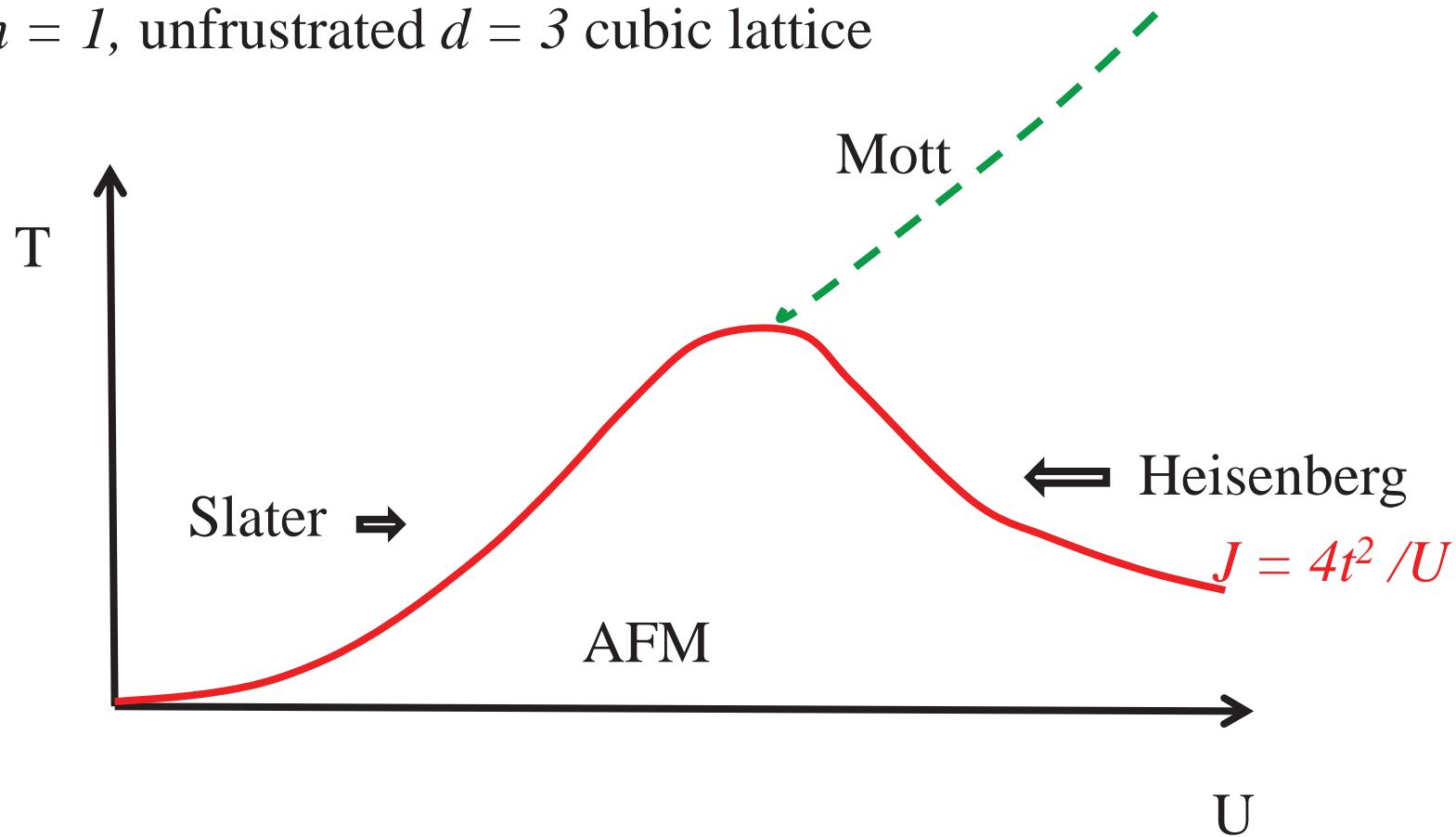


$$U_{MIT} \sim 12$$

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

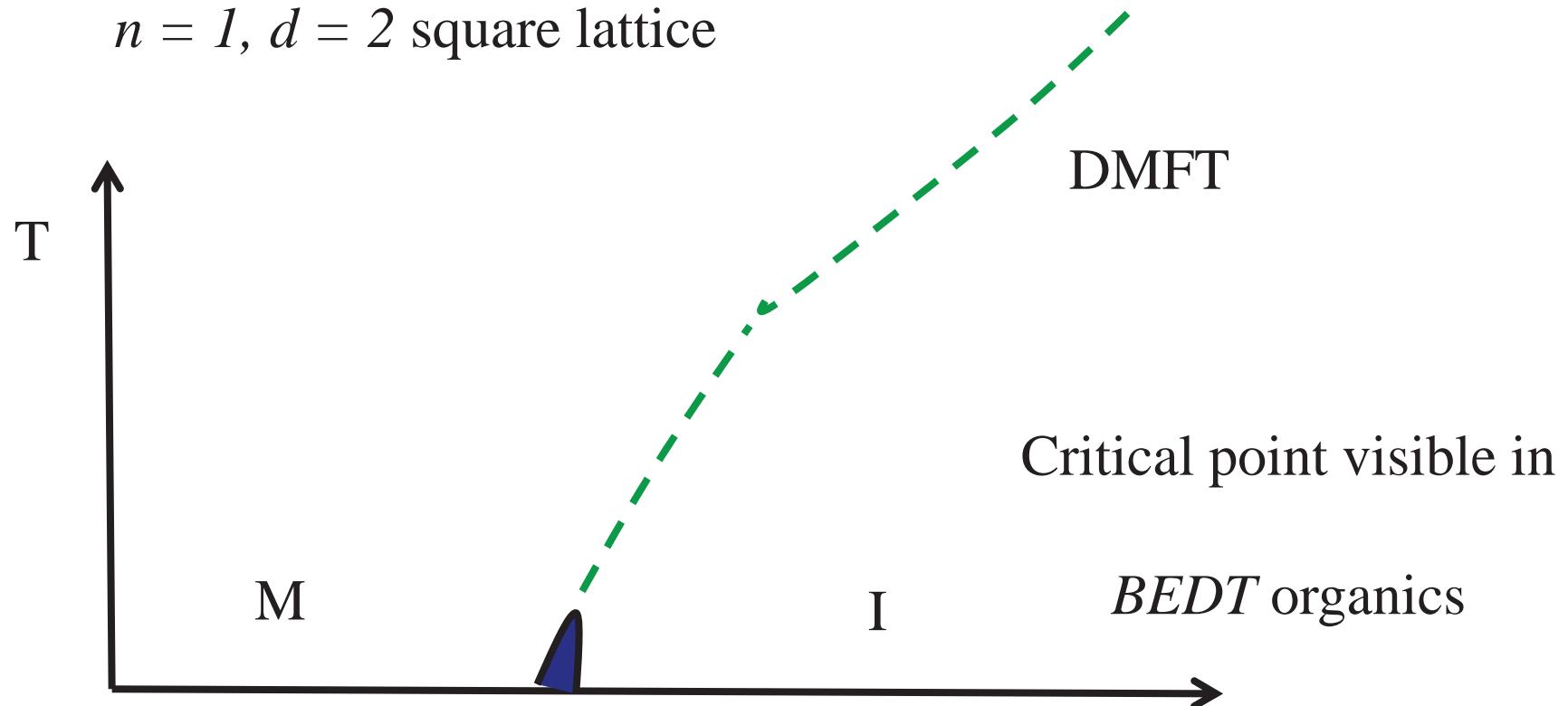
Local moment and Mott transition

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



Local moment and Mott transition

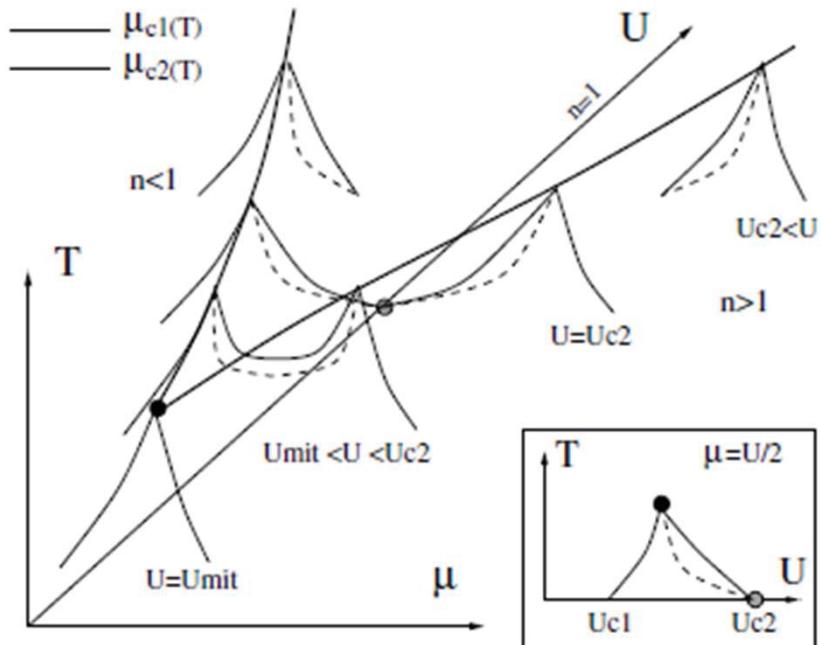
$n = 1, d = 2$ square lattice



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).

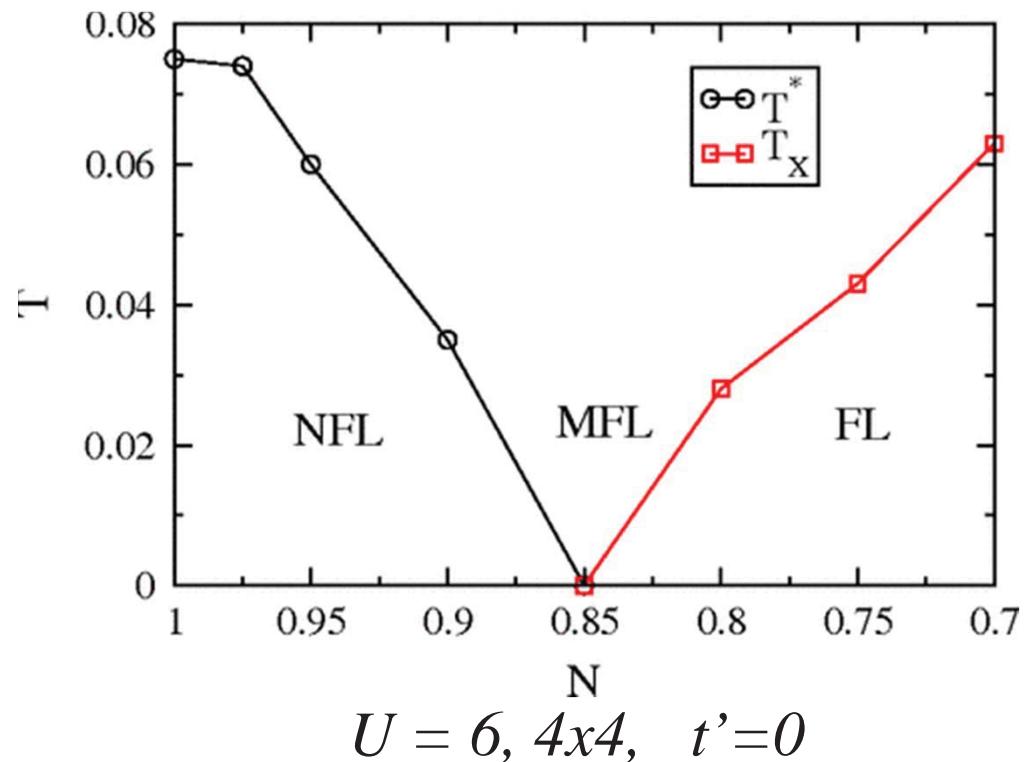
S. Murthy, Rutgers thesis 2004

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

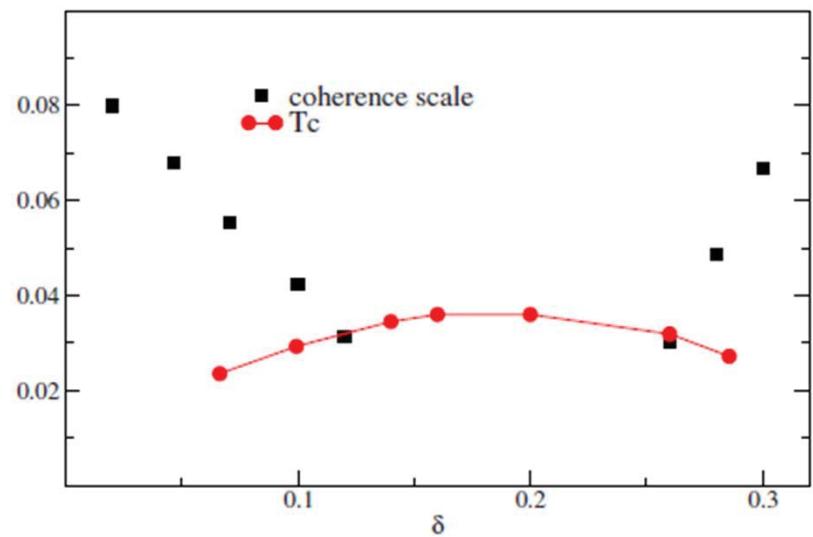
Anomalous metallic state near half-filling (examples)

- 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



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



$J = 0.3 (U \sim 13)$
EDCA-NCA 2x2

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

Previous results

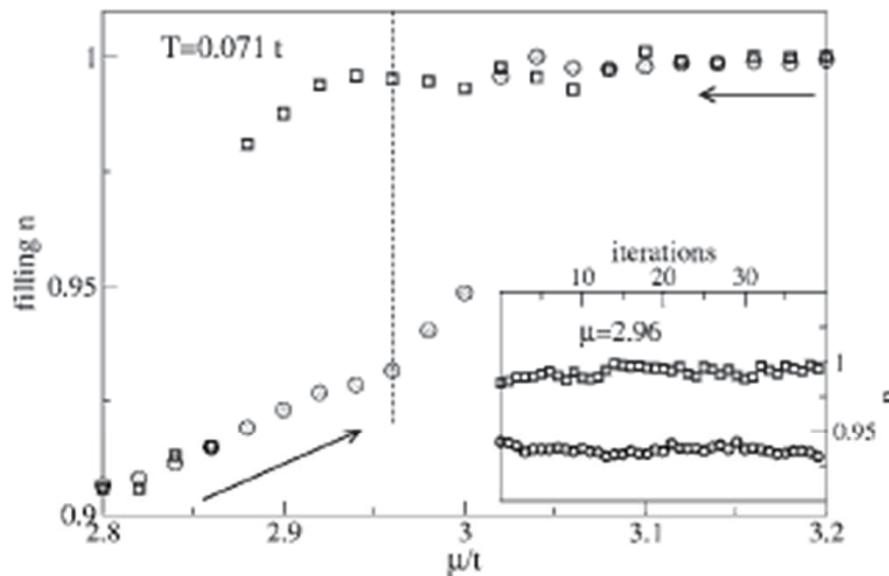
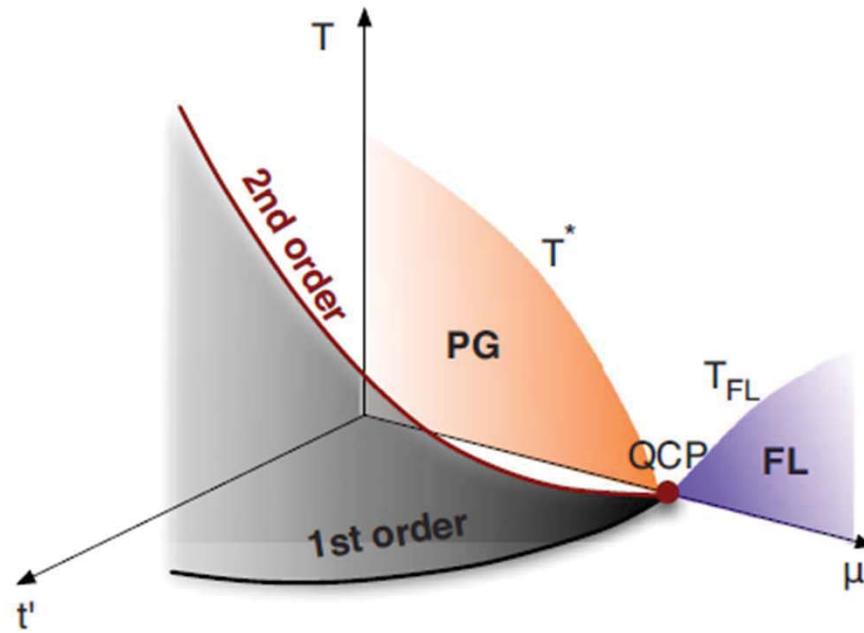


FIG. 2. $N_c=8$ results. Filling n versus chemical potential below T_c , at $T=0.071t$. Two solutions describing a hysteresis are found: one incompressible with $n \approx 1$ (squares) and a doped one (circles). Inset: stability of the two solutions versus DCA iterations when $\mu = 2.96t$ (middle of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

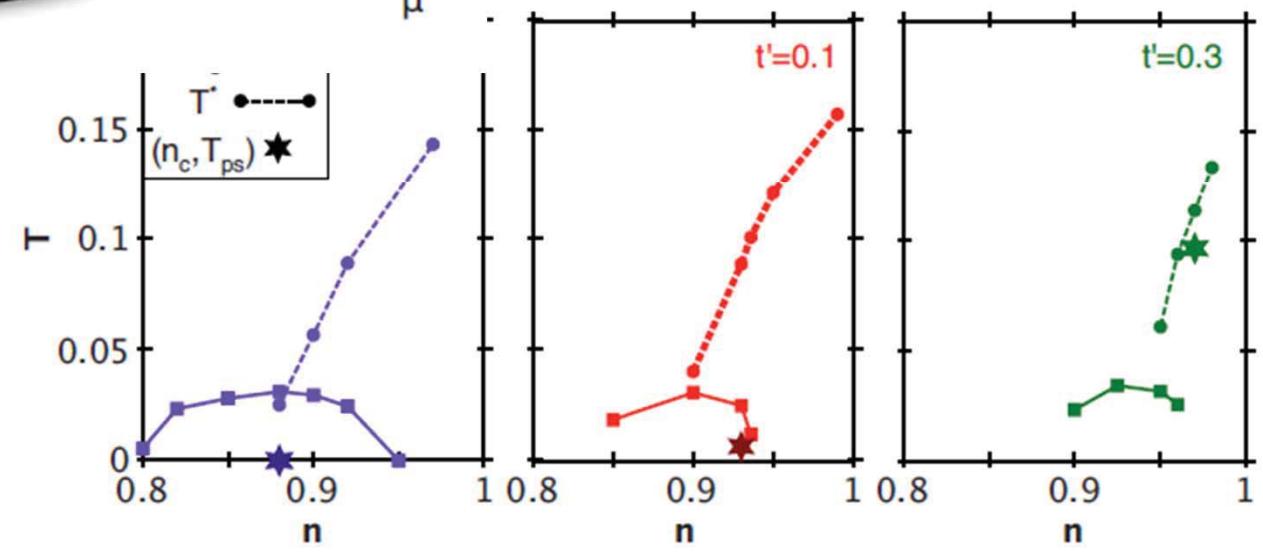
A. Macridin, M. Jarrell, and T. Maier,
Phys. Rev. B **74**, 085104 (2006)

Phase separation on electron-doped side

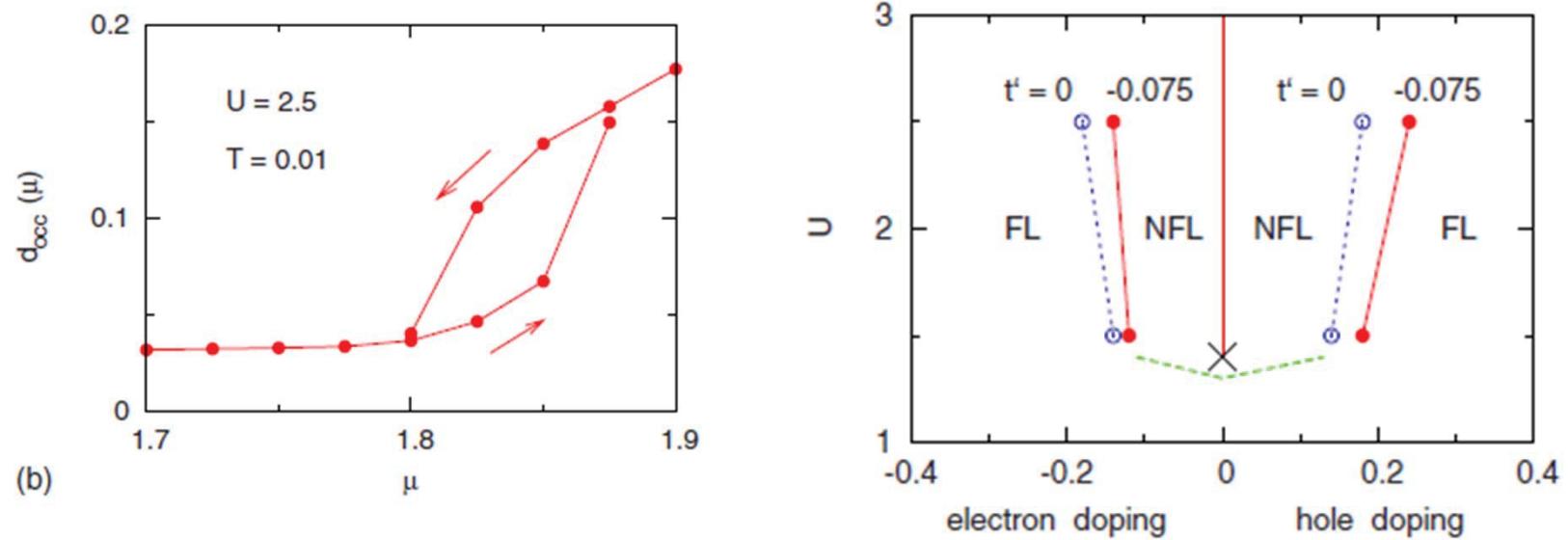


$U=8, N_c = 8, DCA$

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

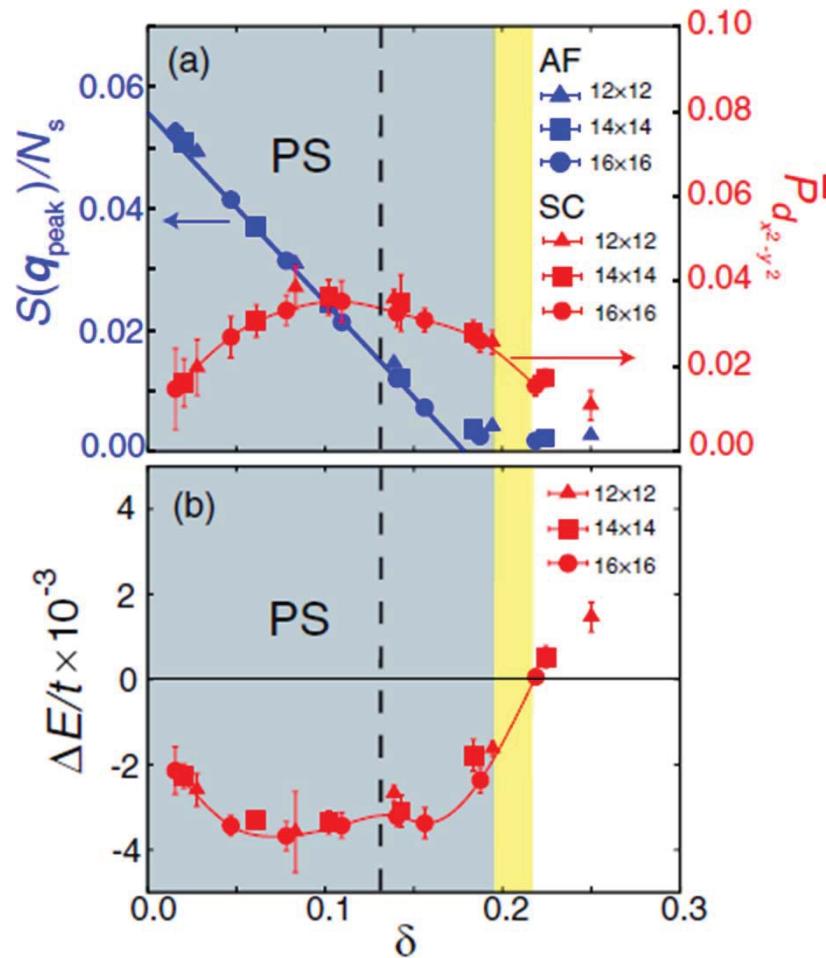


Crossovers and transition



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

Variational Monte Carlo



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

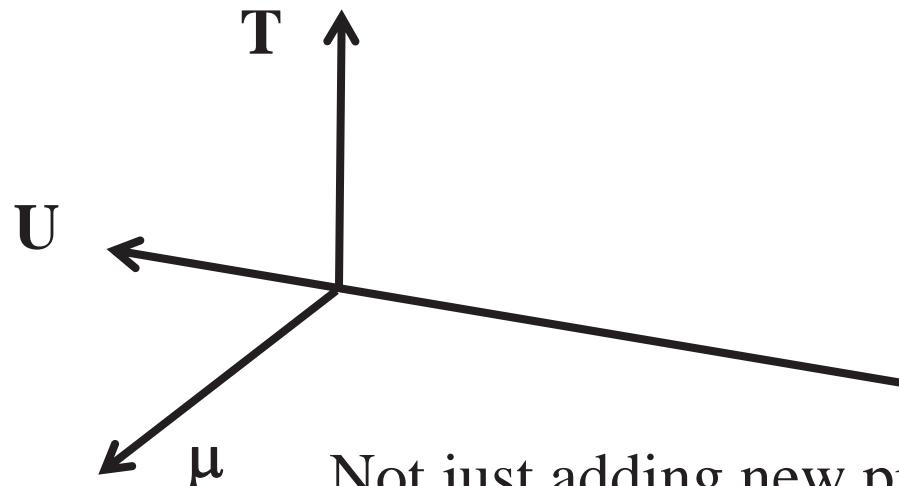


Giovanni Sordi

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

Phys. Rev. B, **84**, 075161 (2011)

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



Not just adding new piece:

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

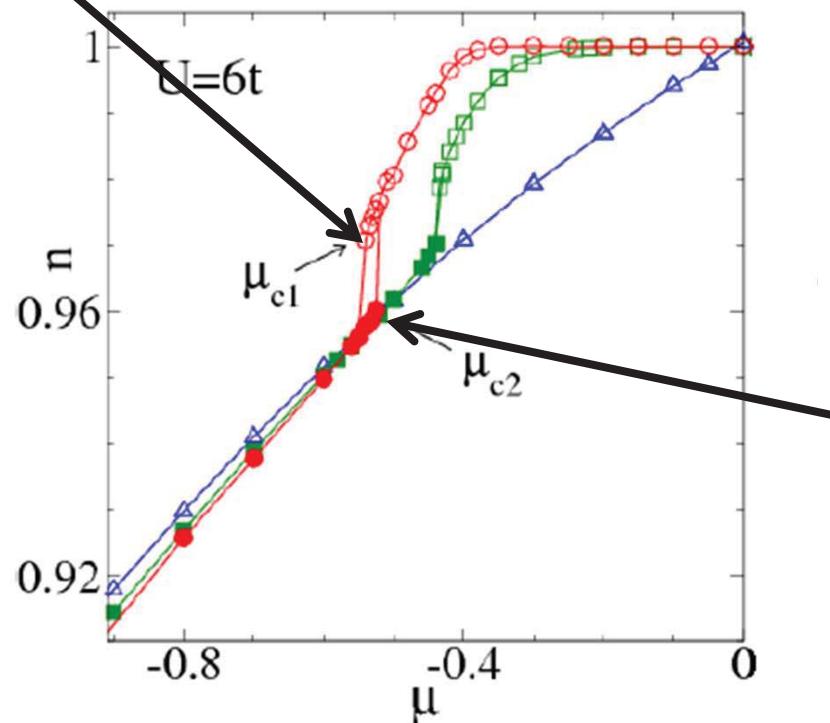


Kristjan Haule

First order transition at finite doping

Spinodals

$t' = 0$



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

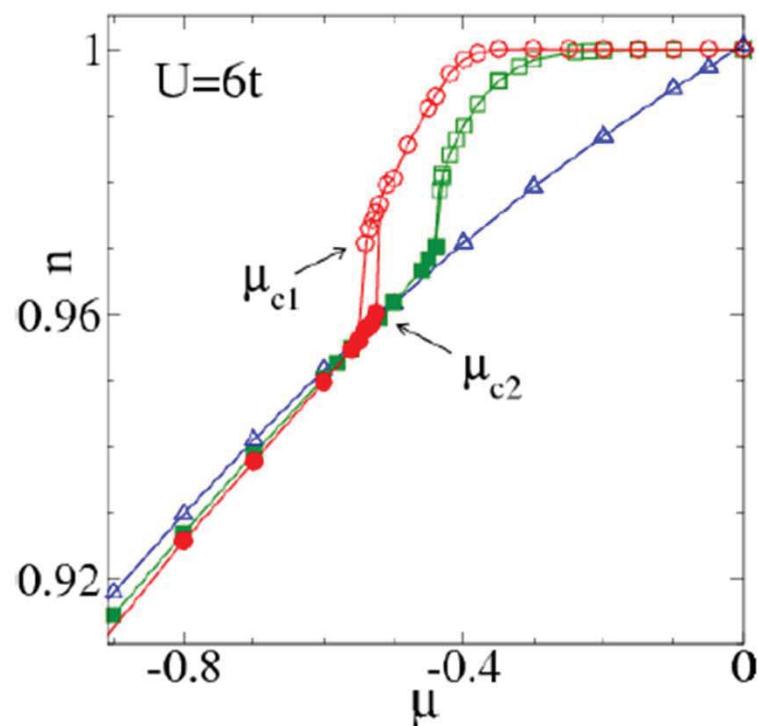
Sordi et al. PRL 2010, PRB 2011



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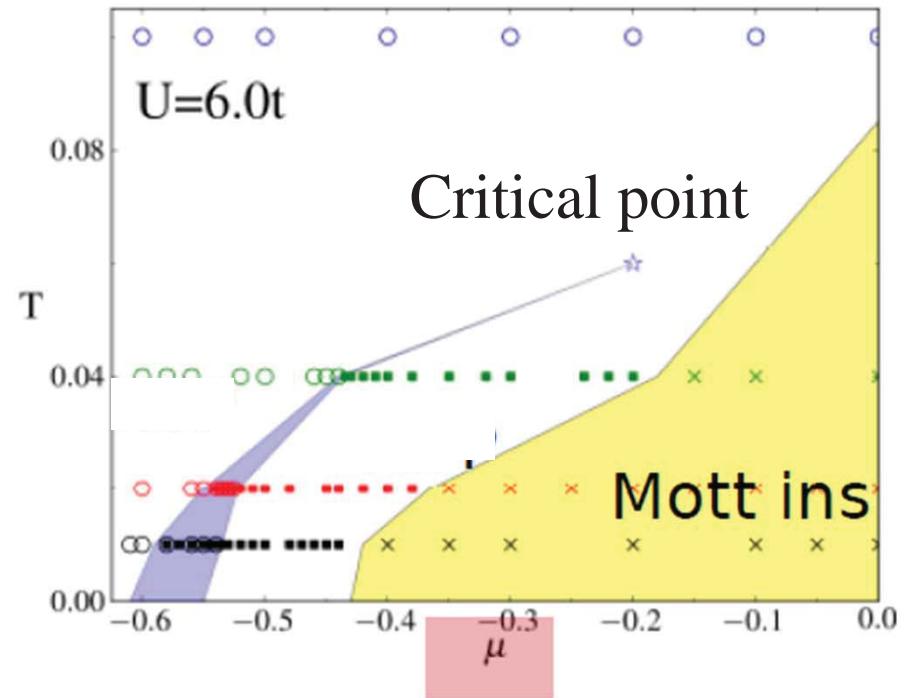
First order transition at finite doping

$$t' = 0$$



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

Sordi et al. PRL 2010, PRB 2011

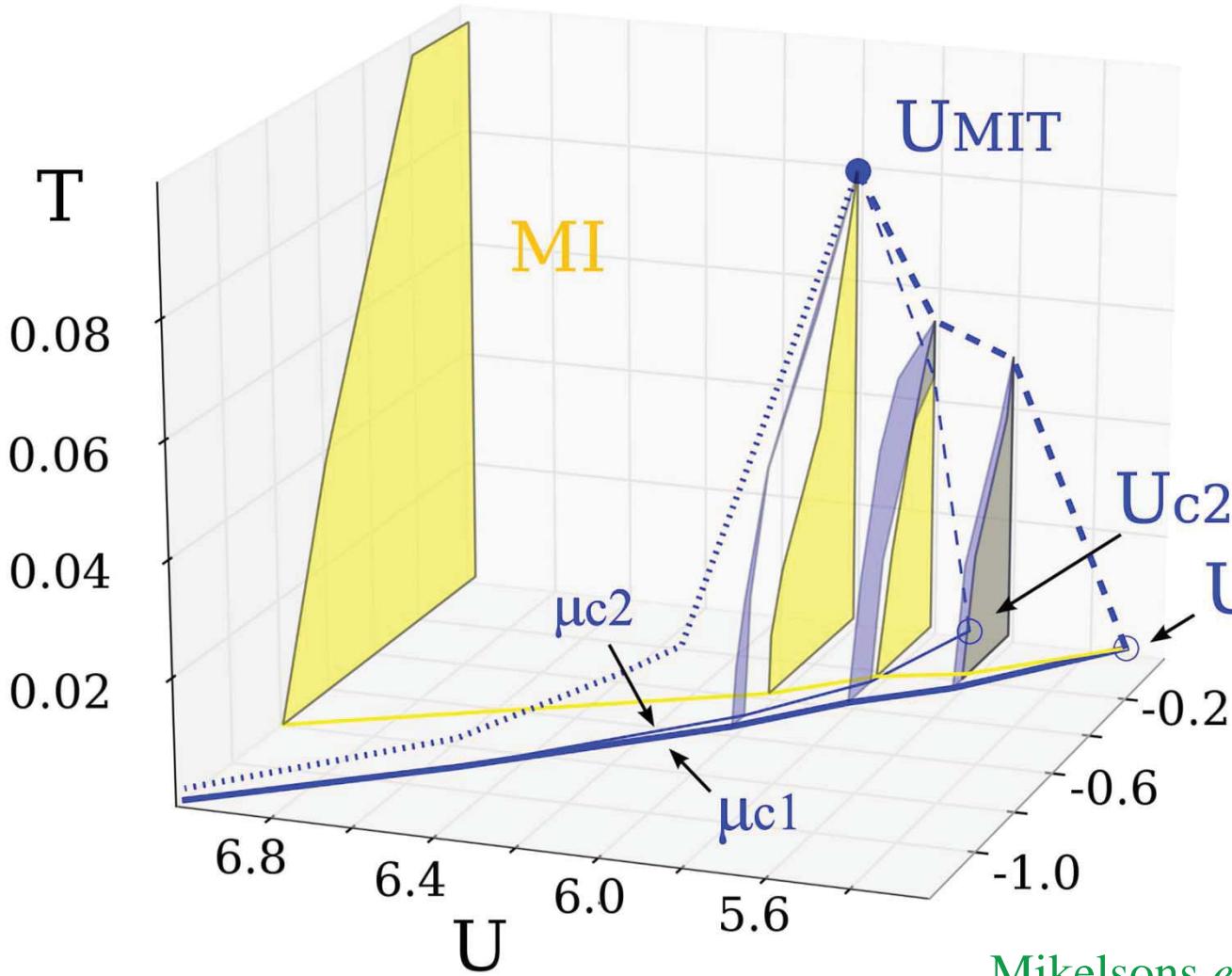


Hysteretic behavior:
fingerprint first order
transition!



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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
 U_{c1} More compressible

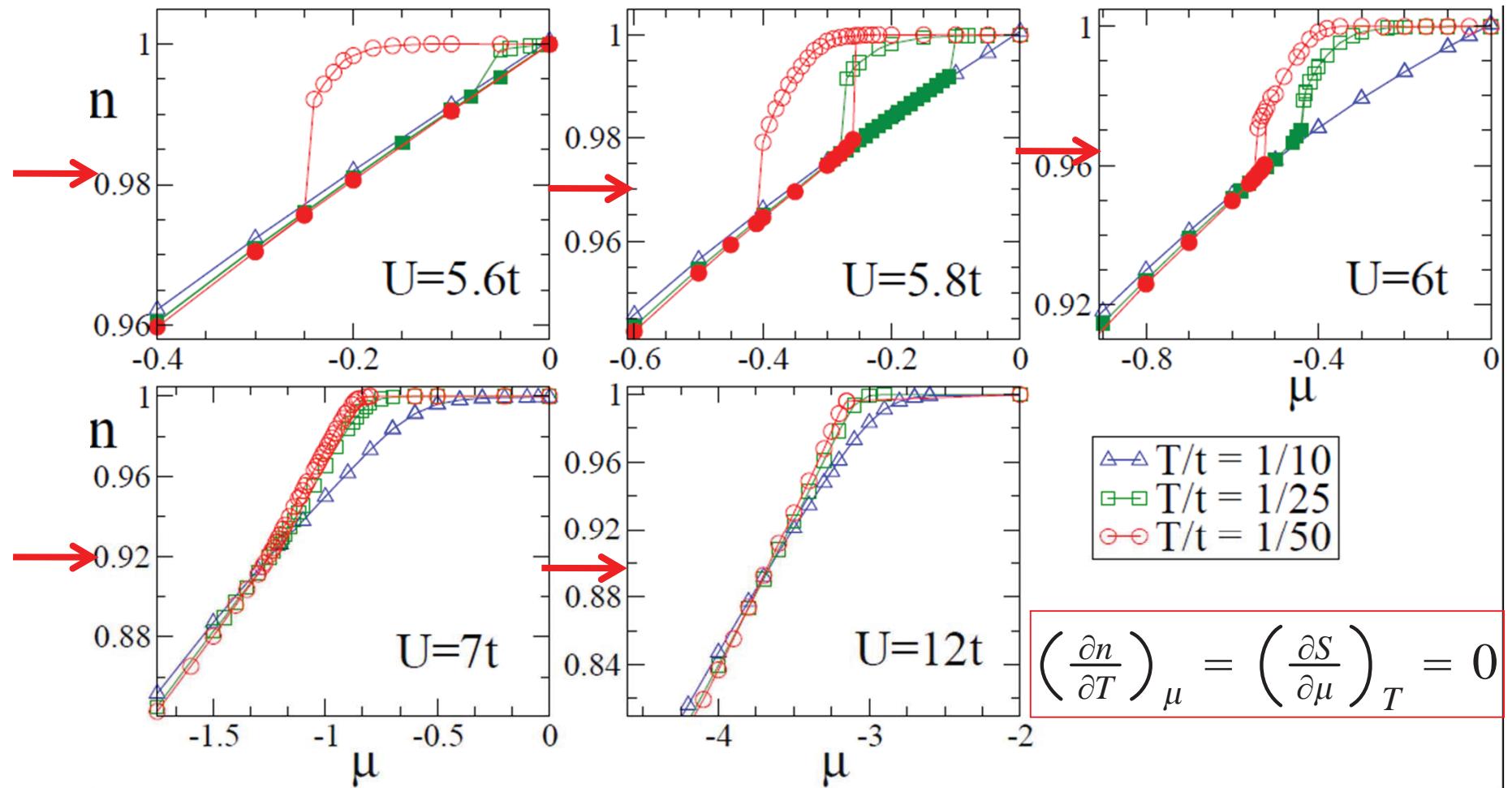
$$\left(\frac{\partial S}{\partial n} \right)_T = 0$$

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



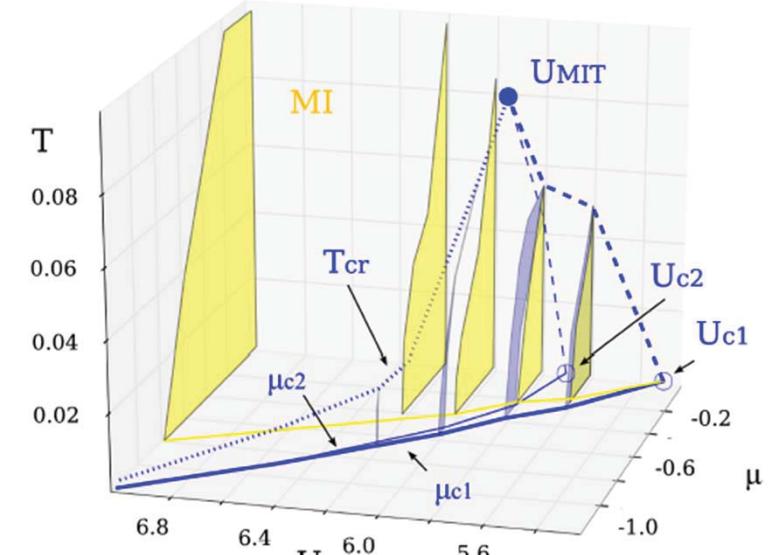
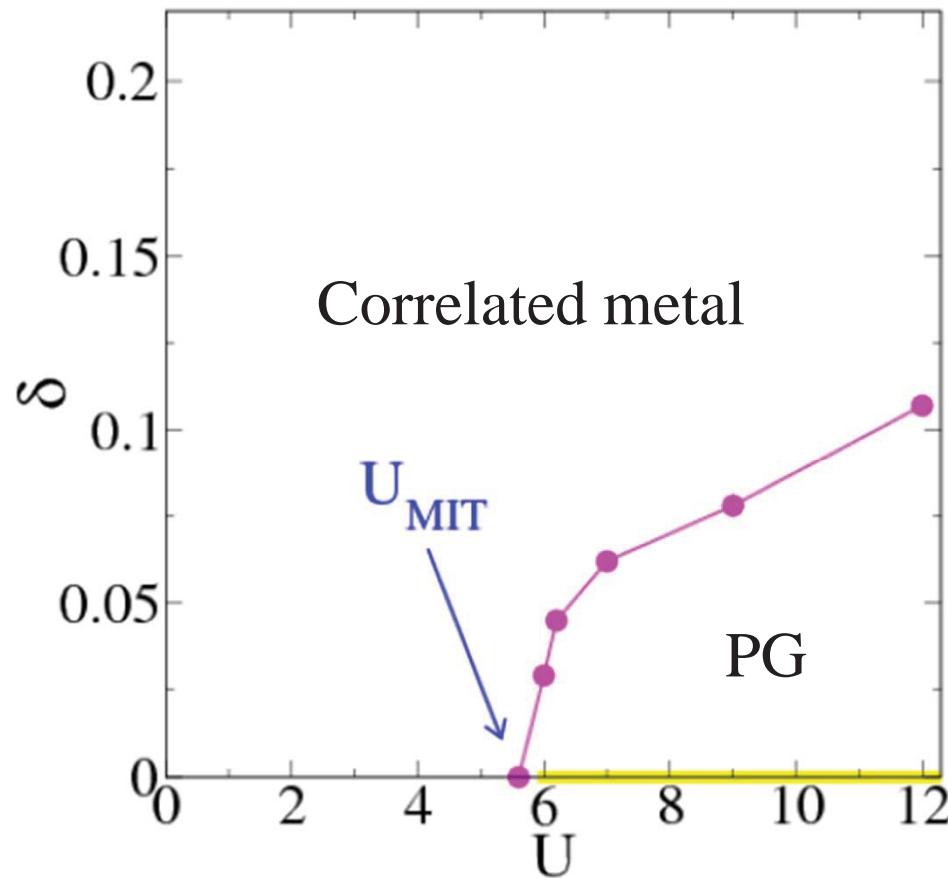
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Critical doping as a function of U increases



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

Doping dependence of critical point as a function of U

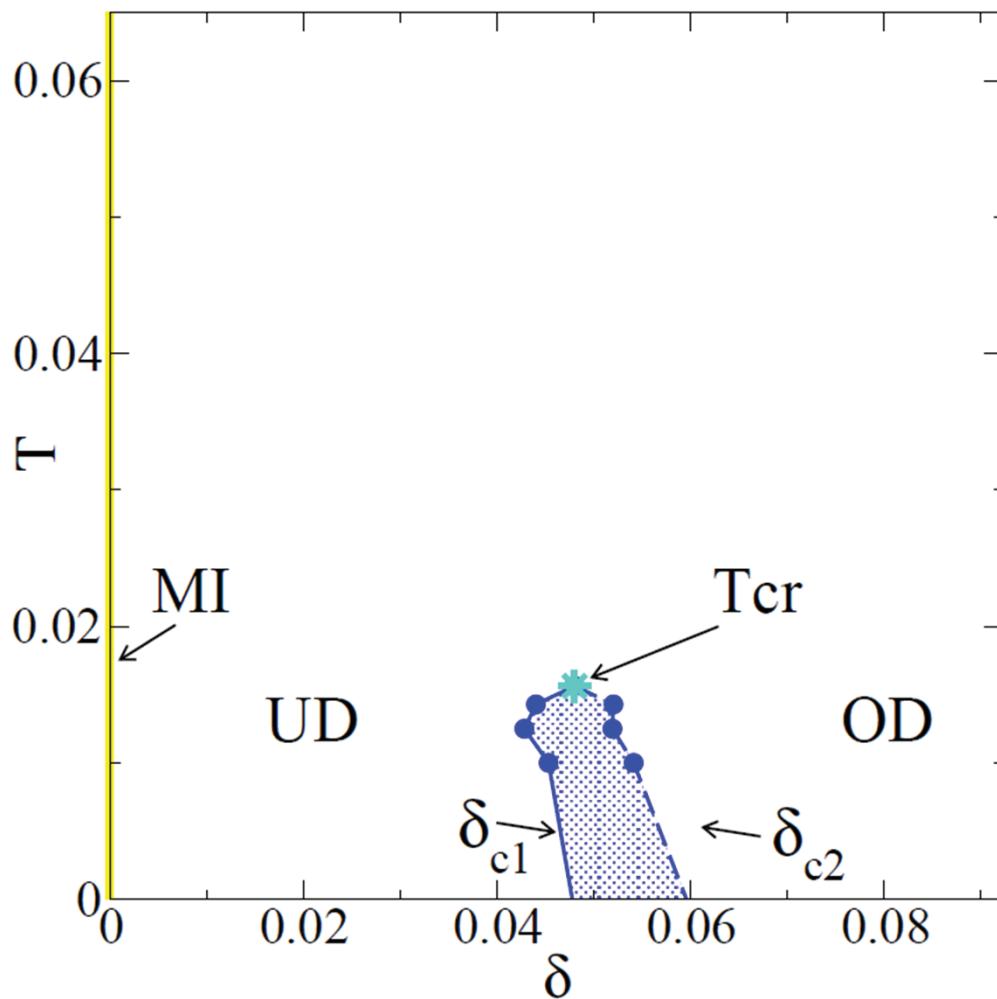


Sordi et al. PRL 2010, PRB 2011



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



$U > U_{MIT}$:

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?



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Giovanni Sordi



Patrick Sémon



Kristjan Haule

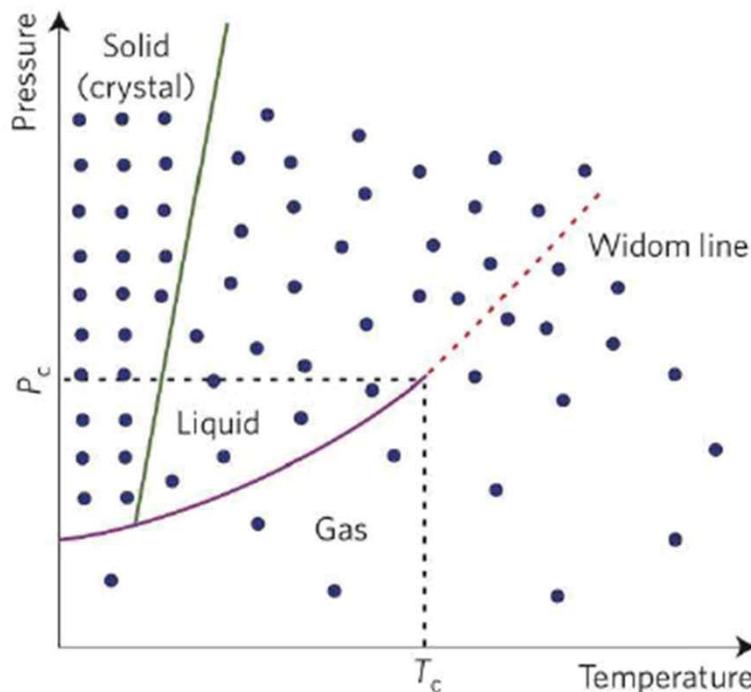
The Widom line ($t' = 0$)

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



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What is the Widom line?



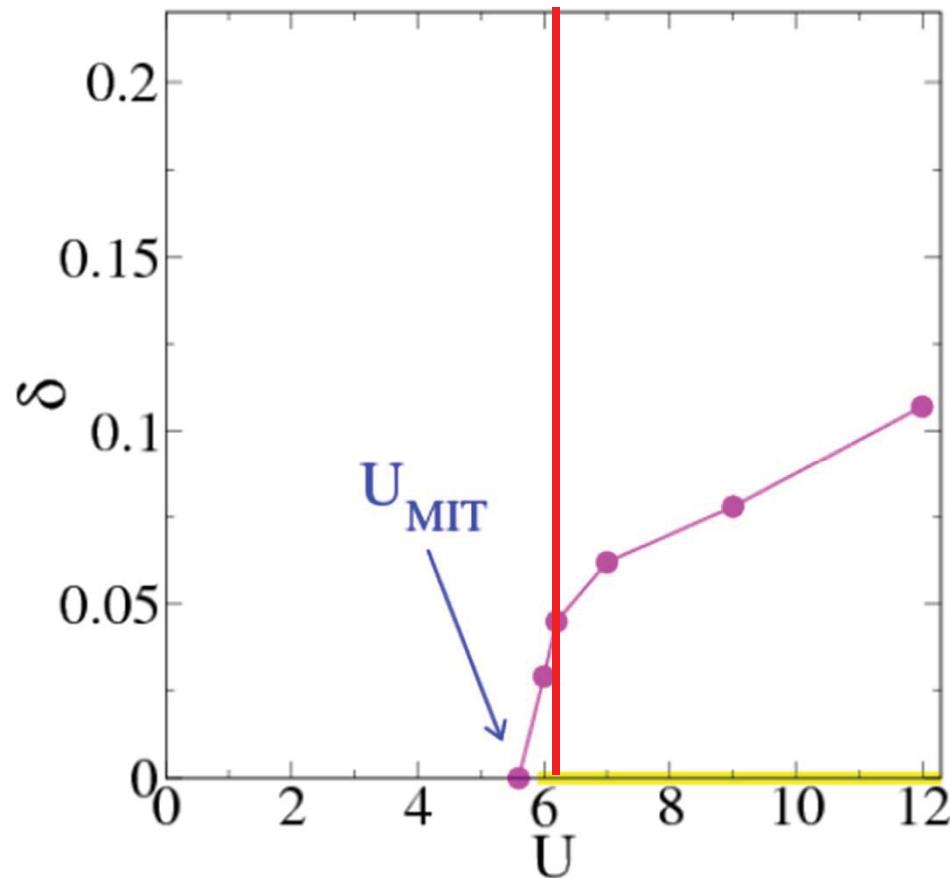
McMillan and Stanley, Nat Phys 2010

- ▶ 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 $T \rightarrow T_p$
- ▶ liquid-gas transition in water: max in isobaric heat capacity C_p , isothermal compressibility, isobaric heat expansion, etc

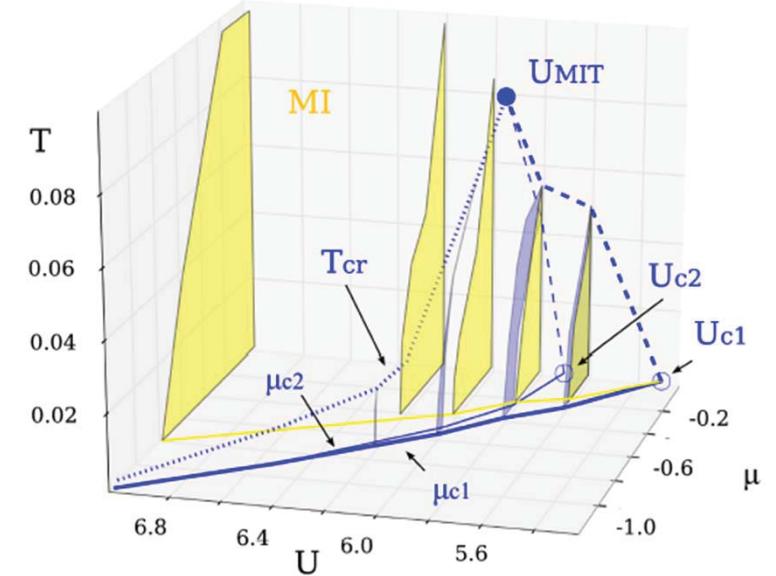
- ▶ **DYNAMIC crossover arises from crossing the Widom line!**
water: Xu et al, PNAS 2005,
Simeoni et al Nat Phys 2010

Link to Mott transition up to optimal doping

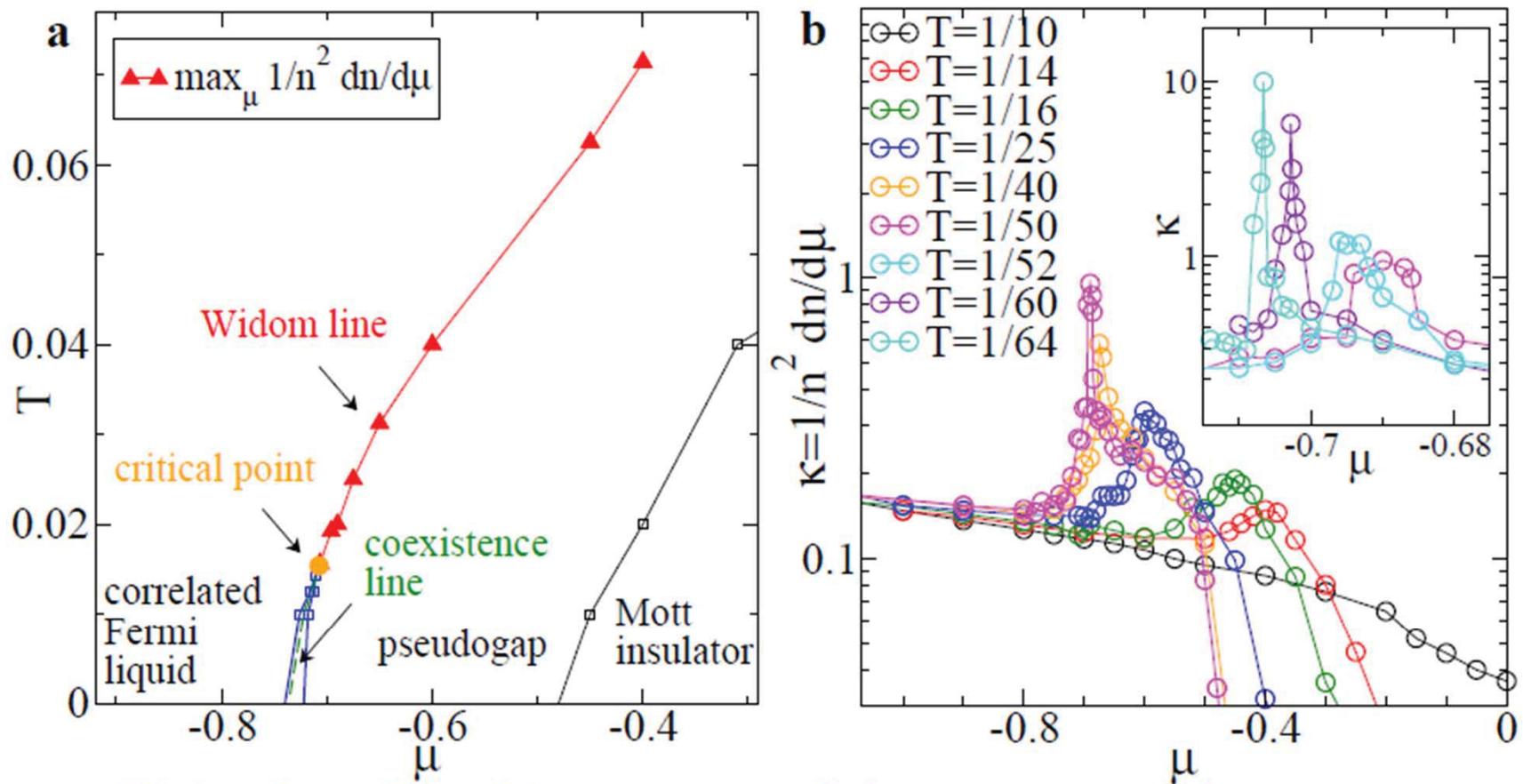
Doping dependence of critical point as a function of U



Smaller D and S



Pseudogap T^* along the Widom line



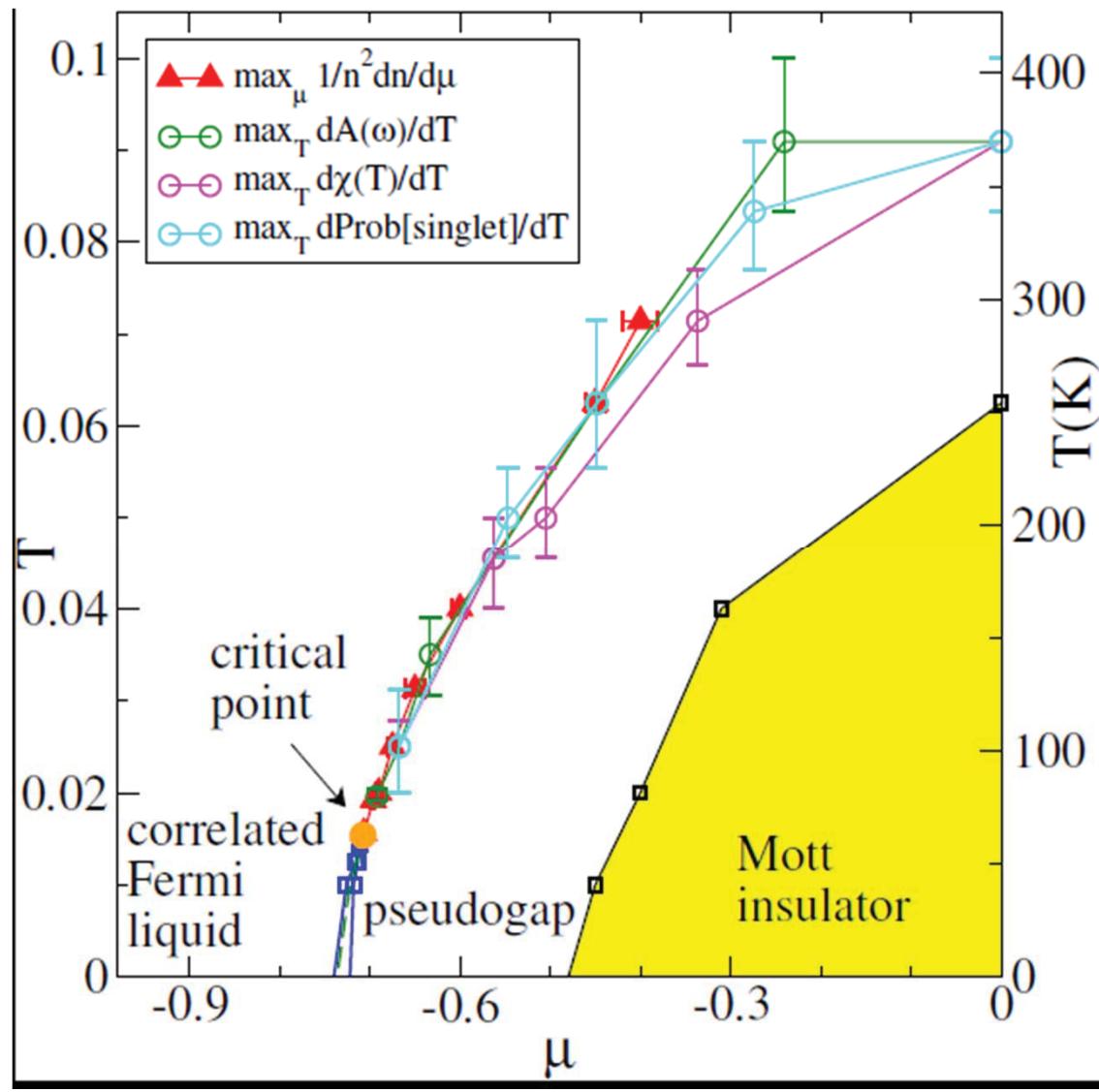
Widom line: defined from maxima of charge compressibility

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

divergence of κ at the (classical) critical point!



Rapid change also in dynamical quantities



Compare a few results for cuprates

Caveats:

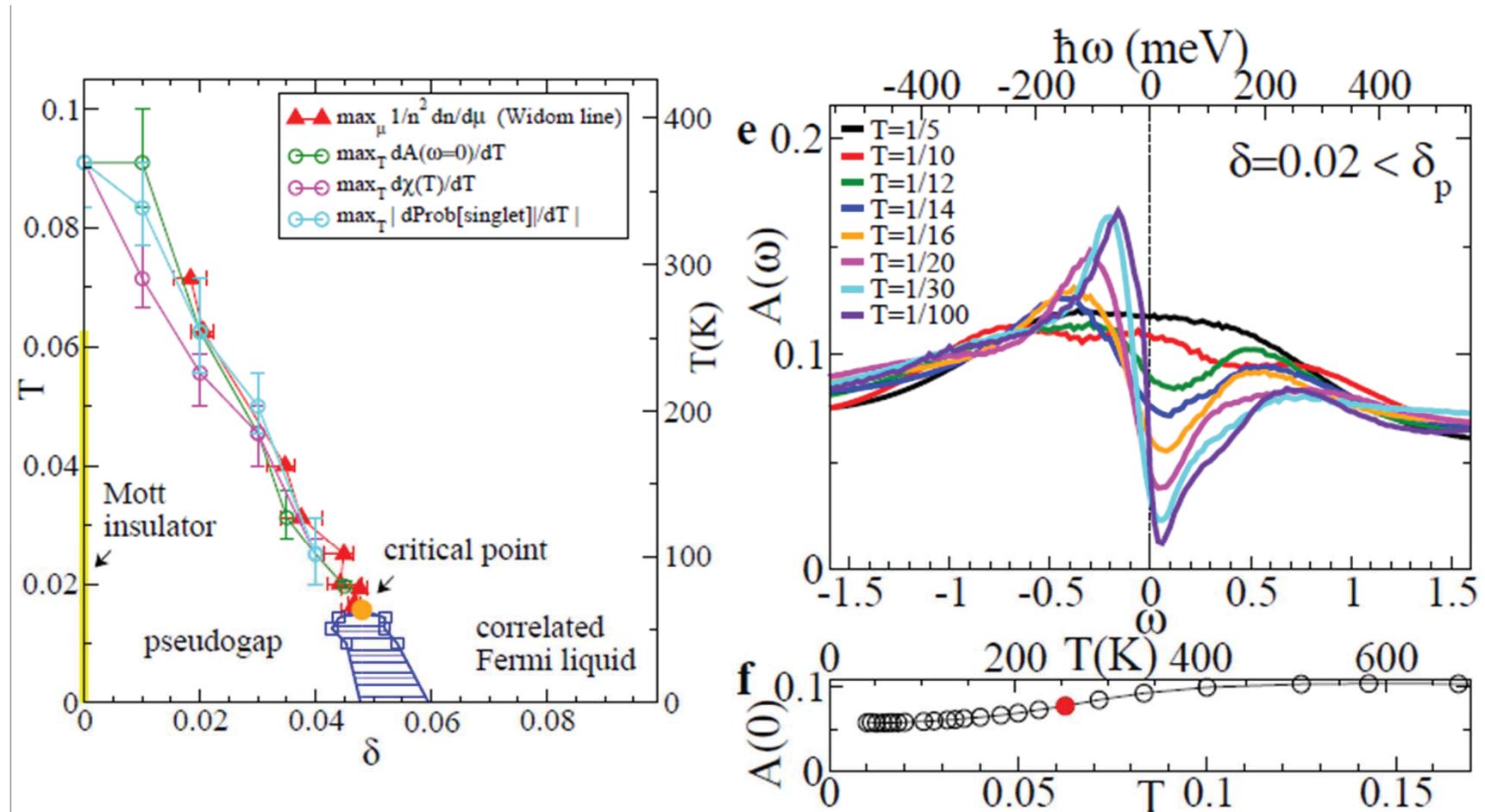
U not large enough

$t' = 0$

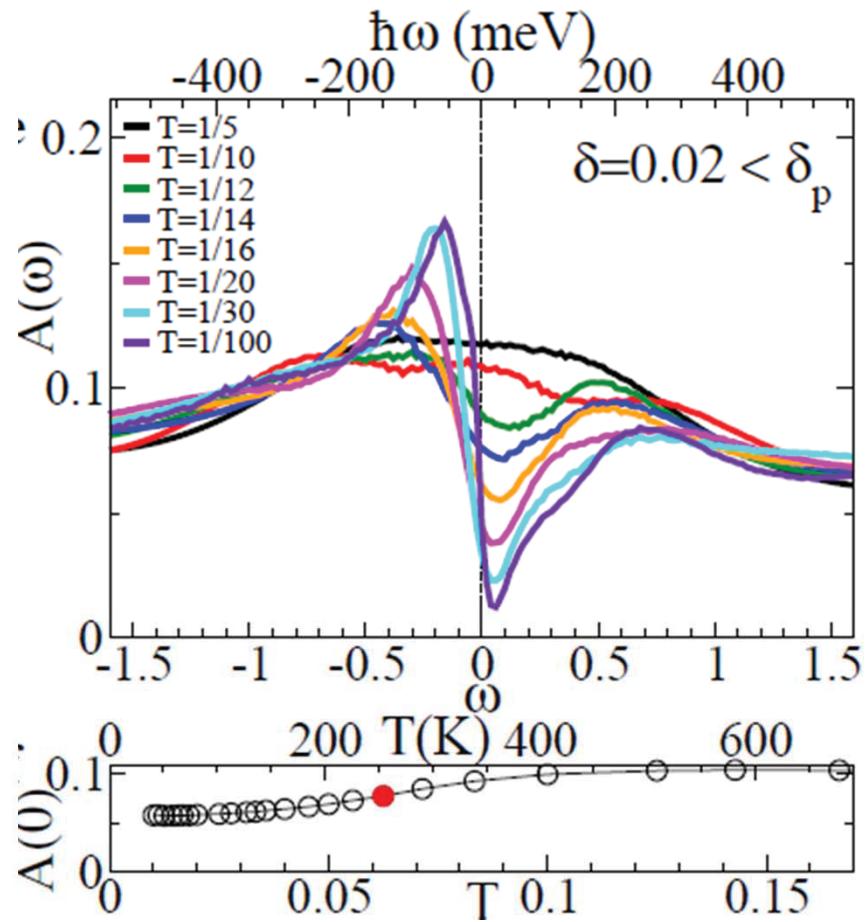
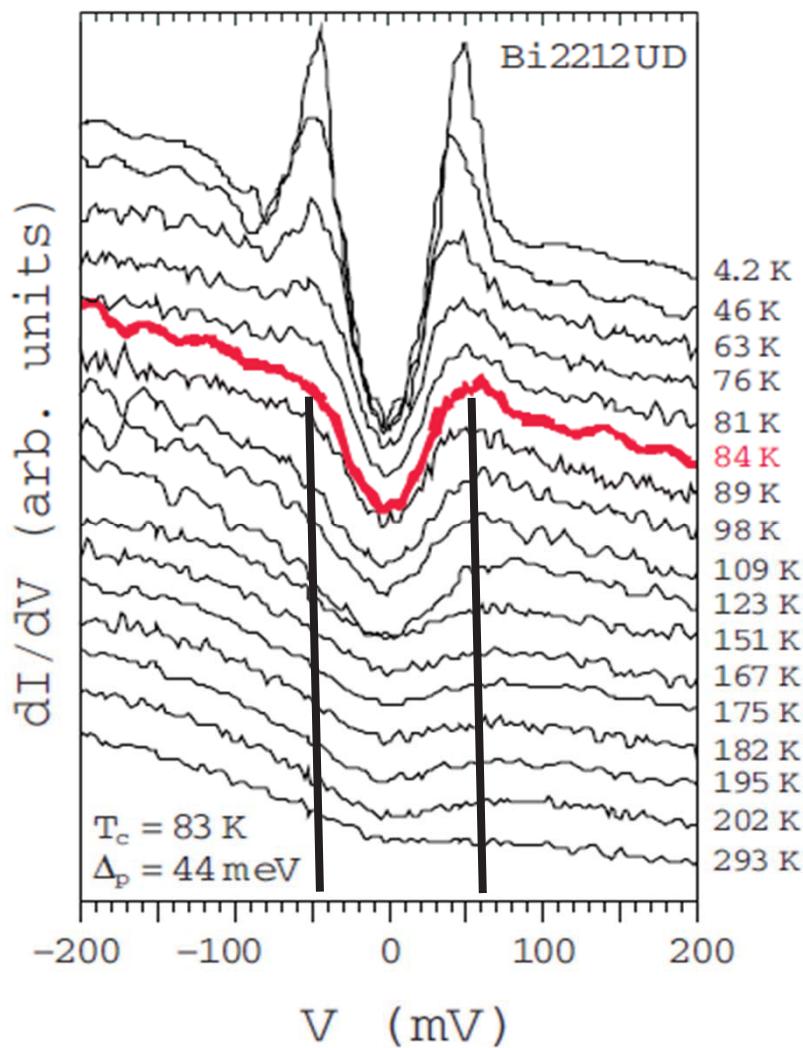


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Density of states



Density of states



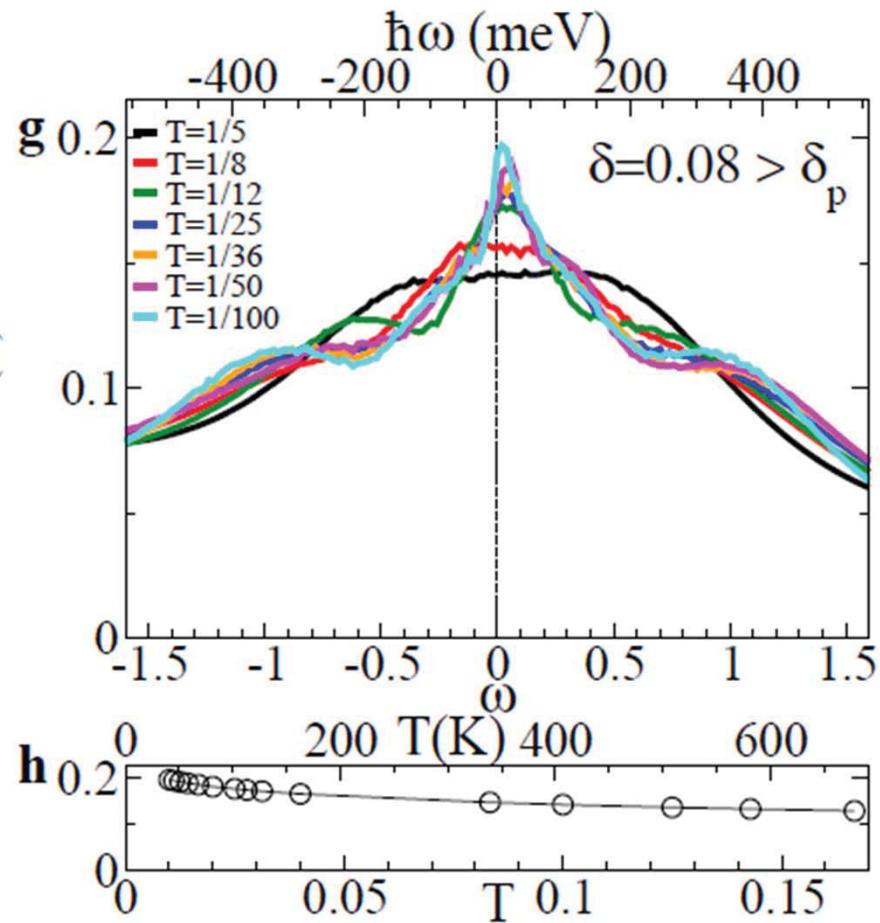
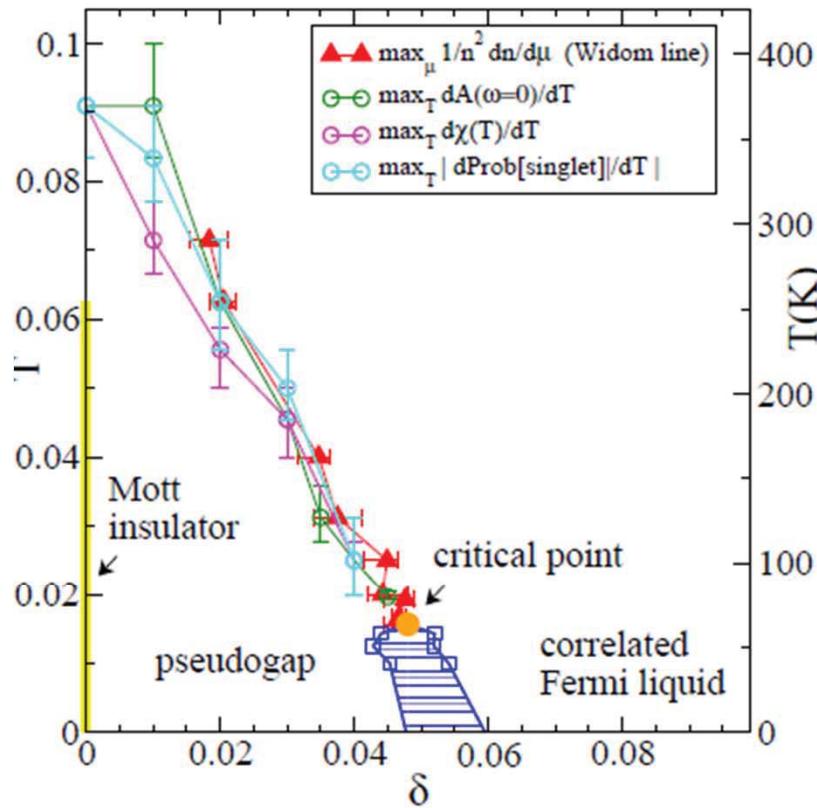
h. Renner, B. Revaz, J.-Y. Genoud,
K. Kadowaki, and Ø. Fischer

PRL 80, 149 (1998)



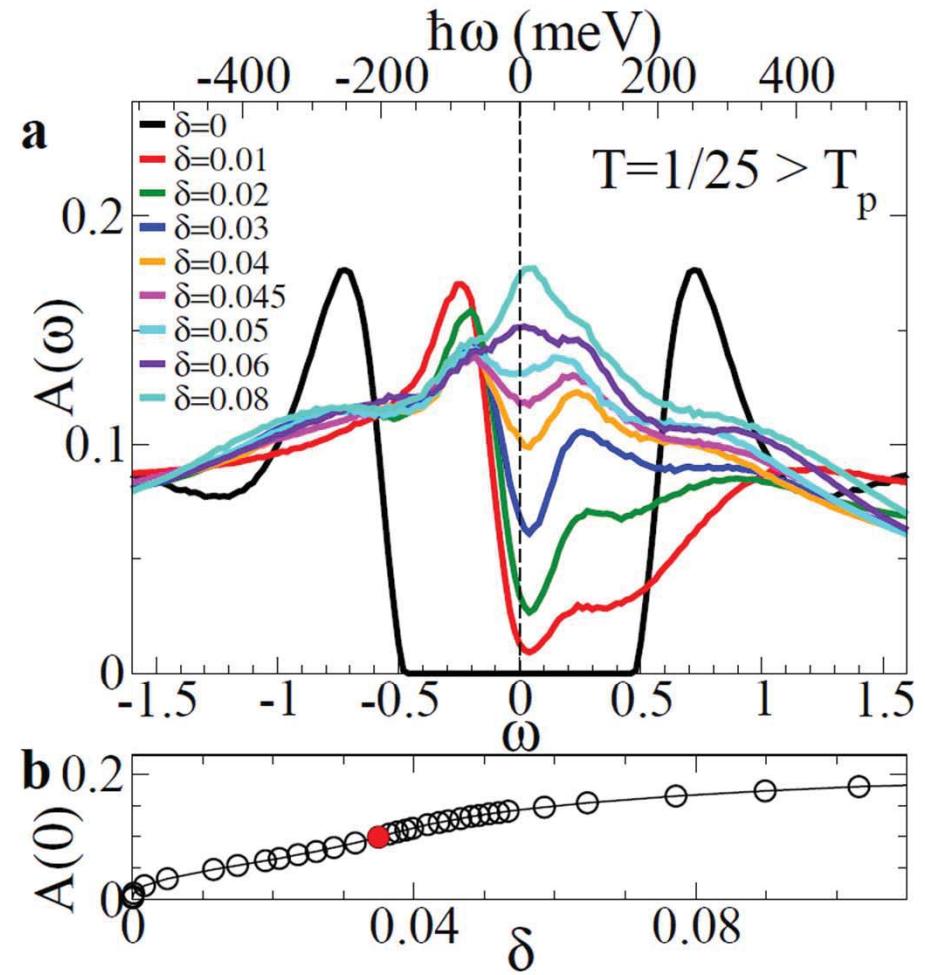
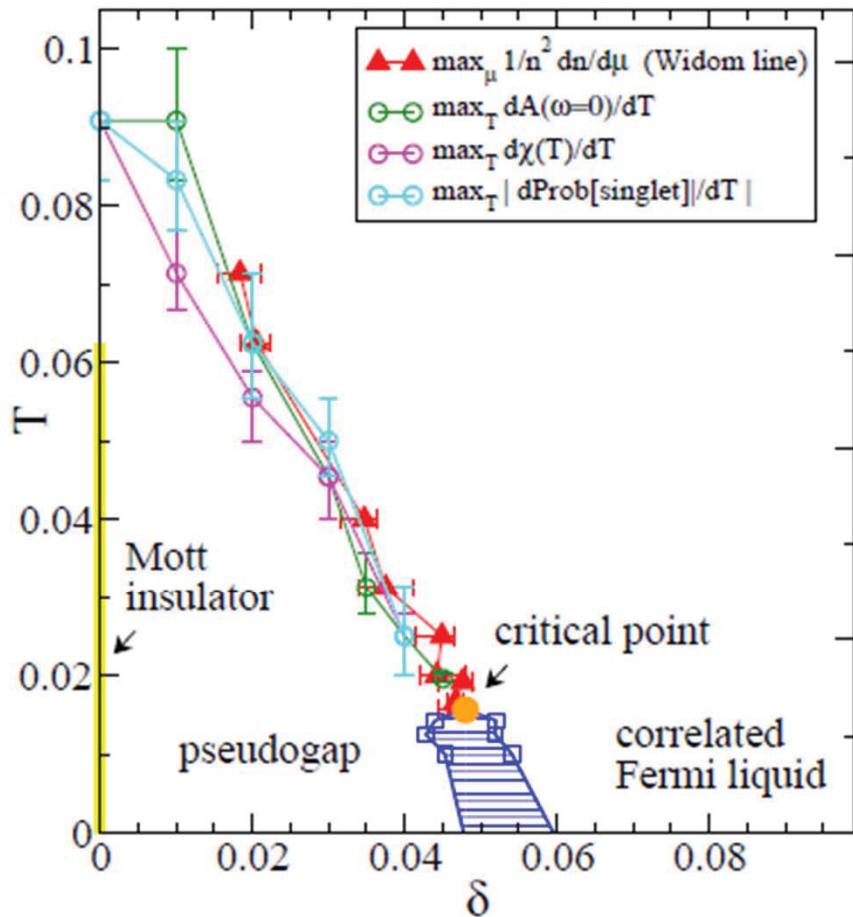
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Density of states

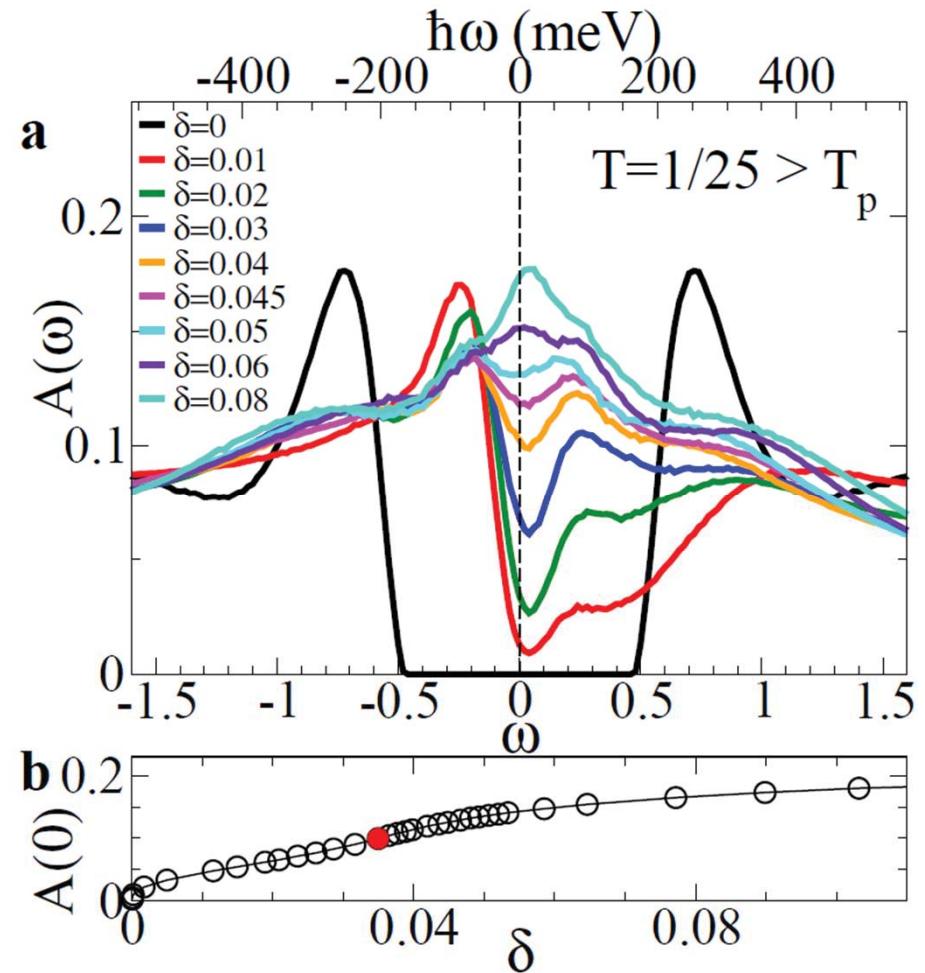
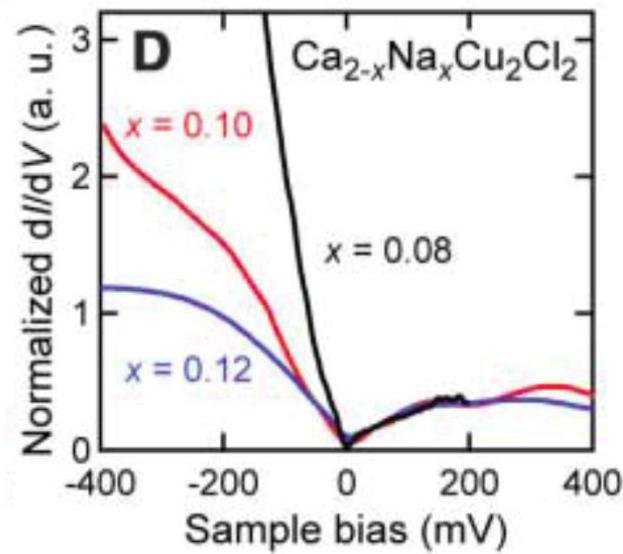


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Density of states

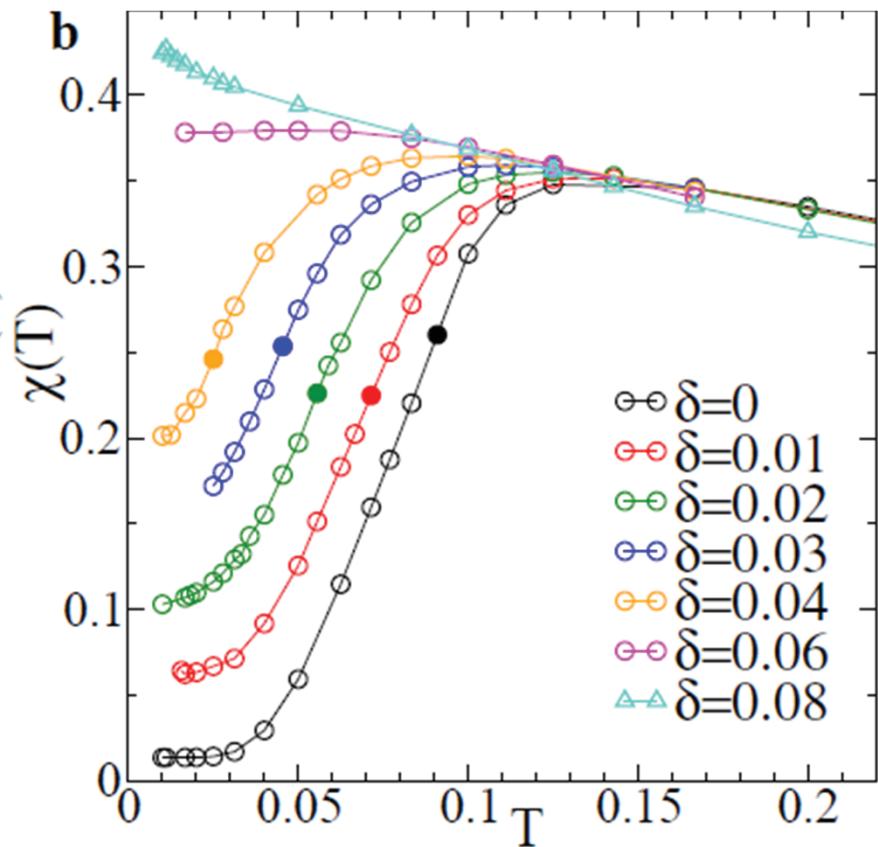
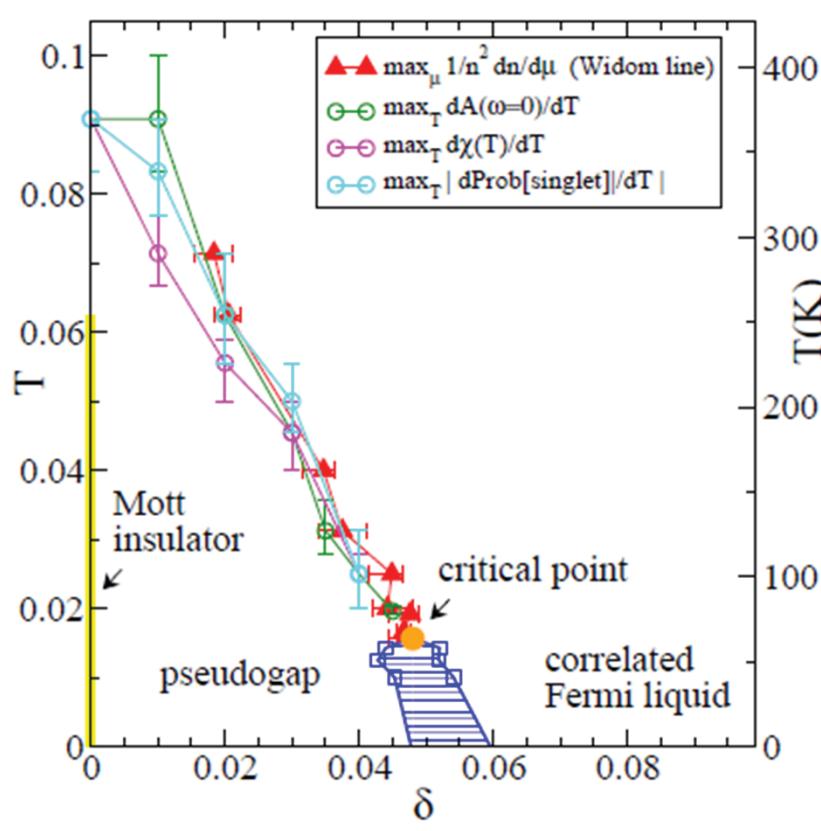


Density of states

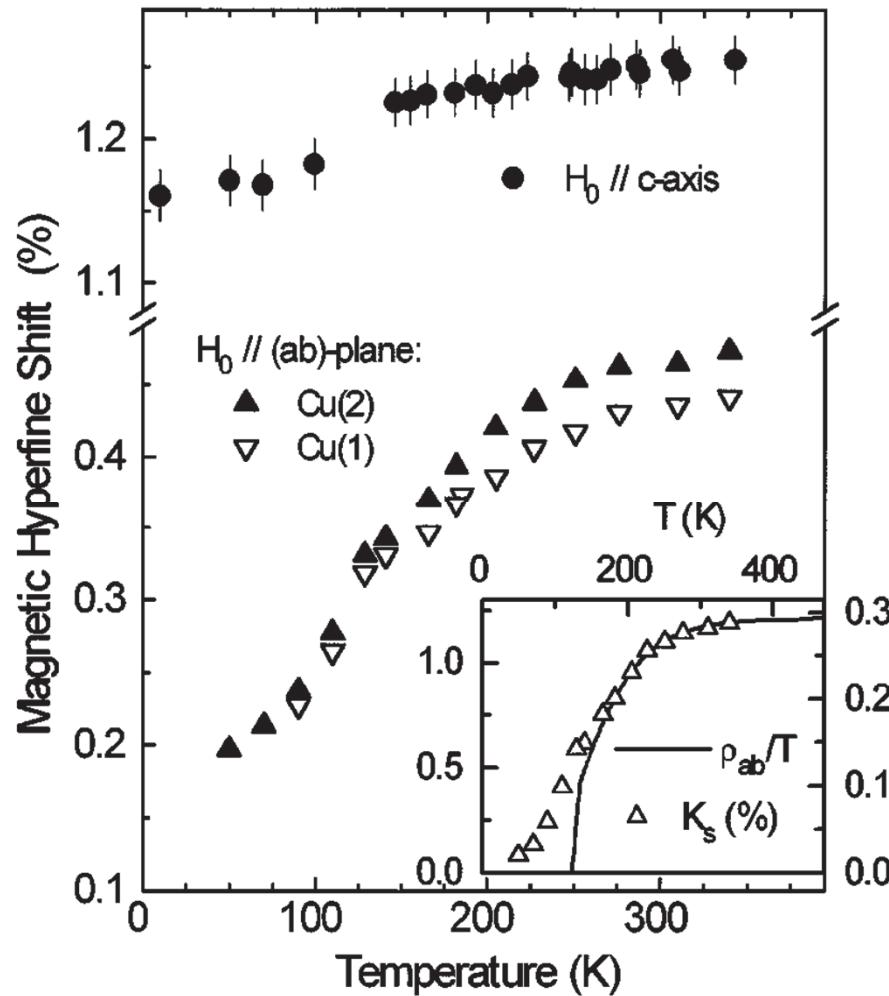


Khosaka et al. *Science* **315**, 1380 (2007);

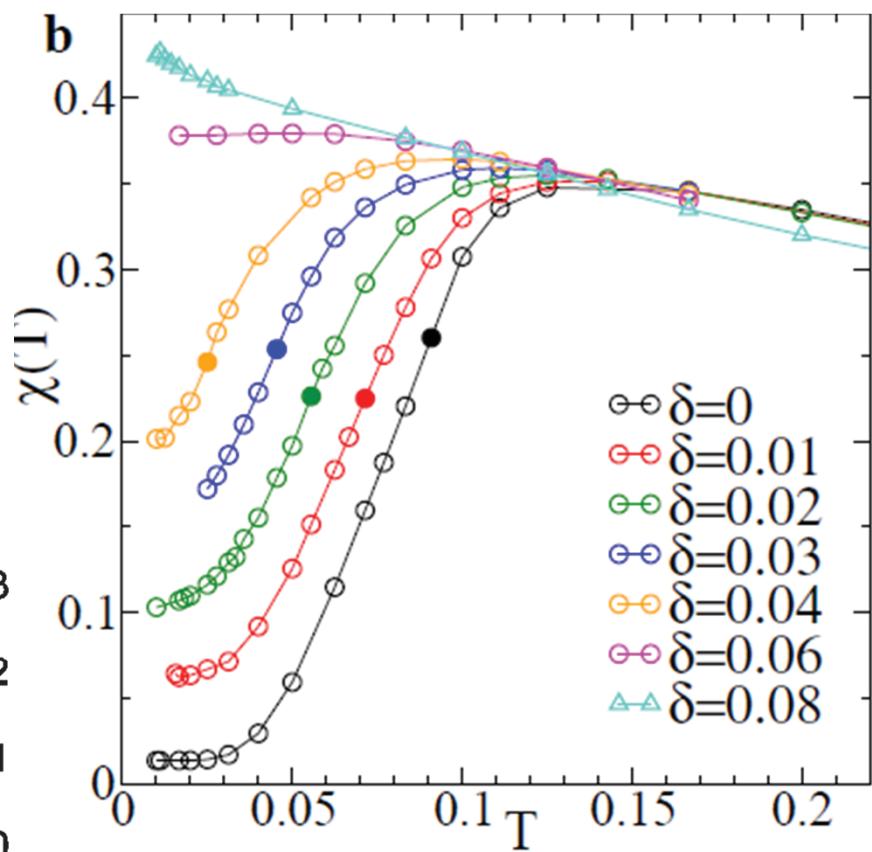
Spin susceptibility



Spin susceptibility



Underdoped Hg1223
Julien et al. PRL 76, 4238 (1996)



What is the minimal model?

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

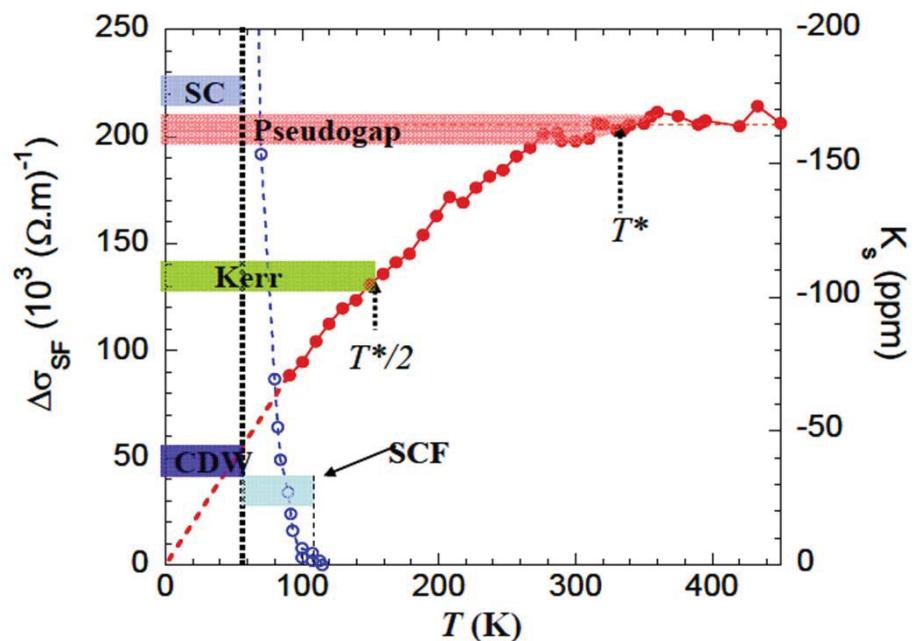


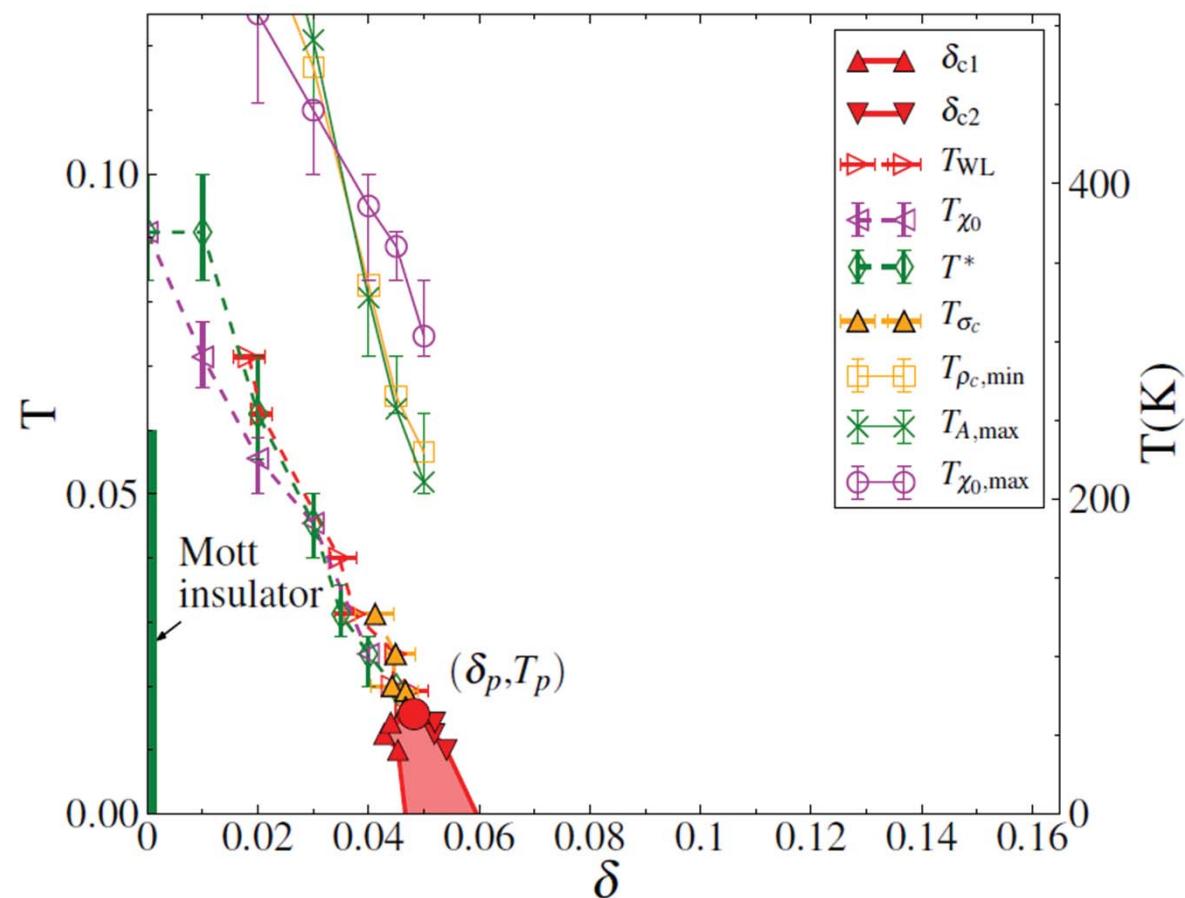
Fig 1 Spin contribution K_s to the ^{89}Y NMR Knight shift [11] for $\text{YBCO}_{6.6}$ permit to define the PG onset T^* . Here K_s is reduced by a factor two at $T \sim T^*/2$. The sharp drop of the SC fluctuation conductivity (SCF) is illustrated (left scale) [23]. We report as well the range over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



Giovanni Sordi



Patrick Sémon



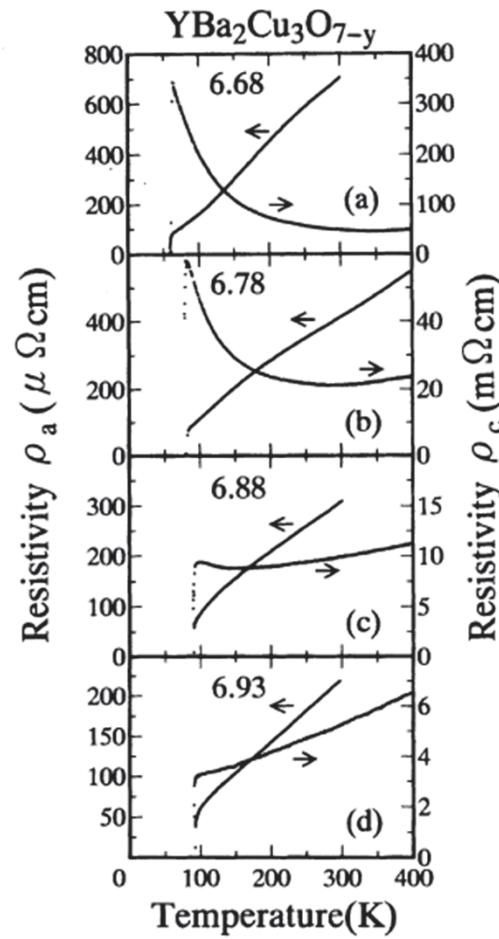
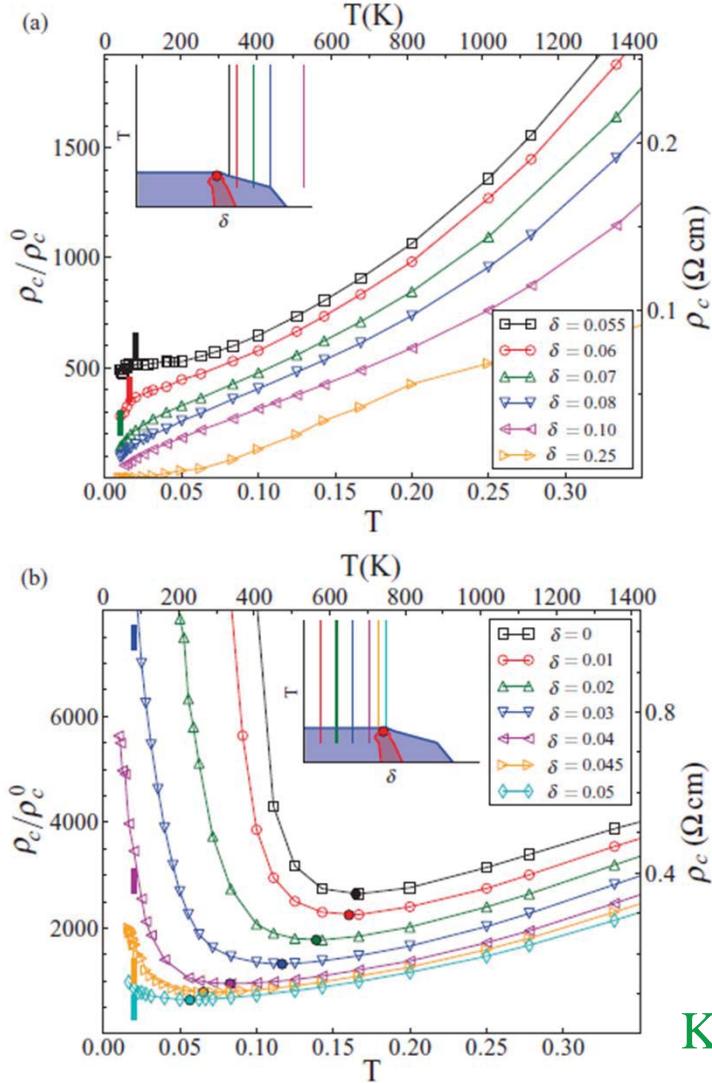
G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)

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



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C-axis resistivity

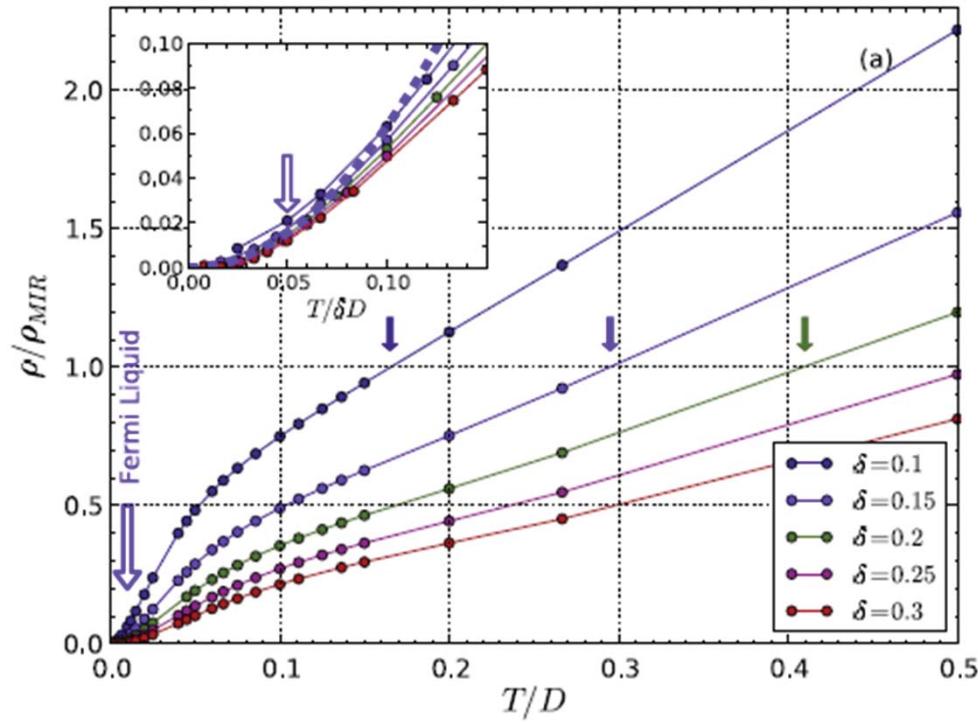


K. Takenaka, K. Mizuhashi, H. Takagi, and S. Uchida,
Phys. Rev.B 50, 6534 (1994).



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Mott-Ioffe-Regel limit



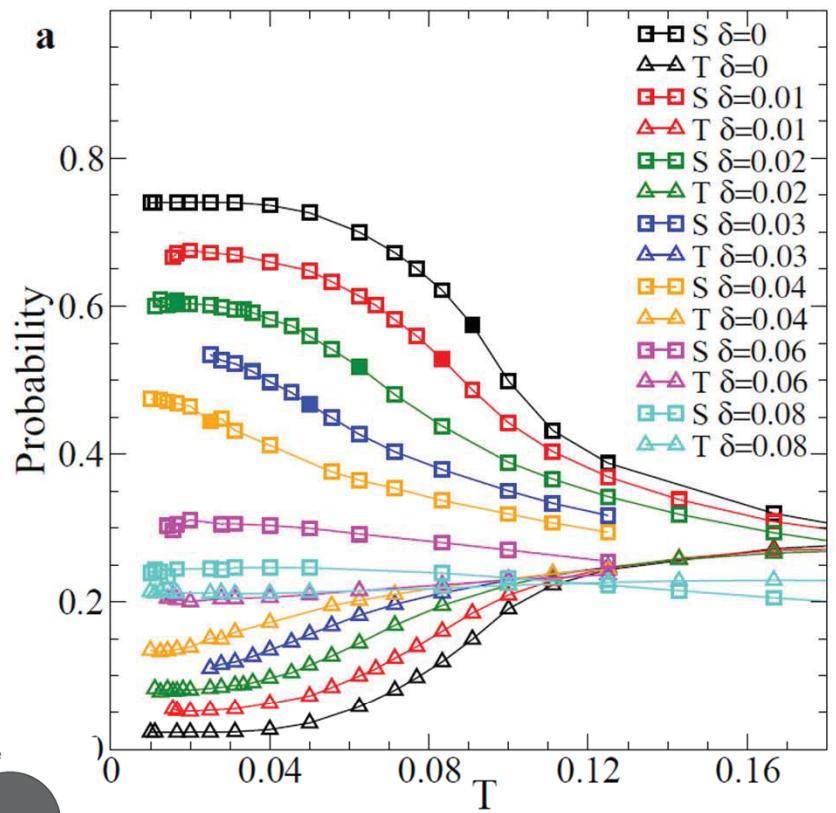
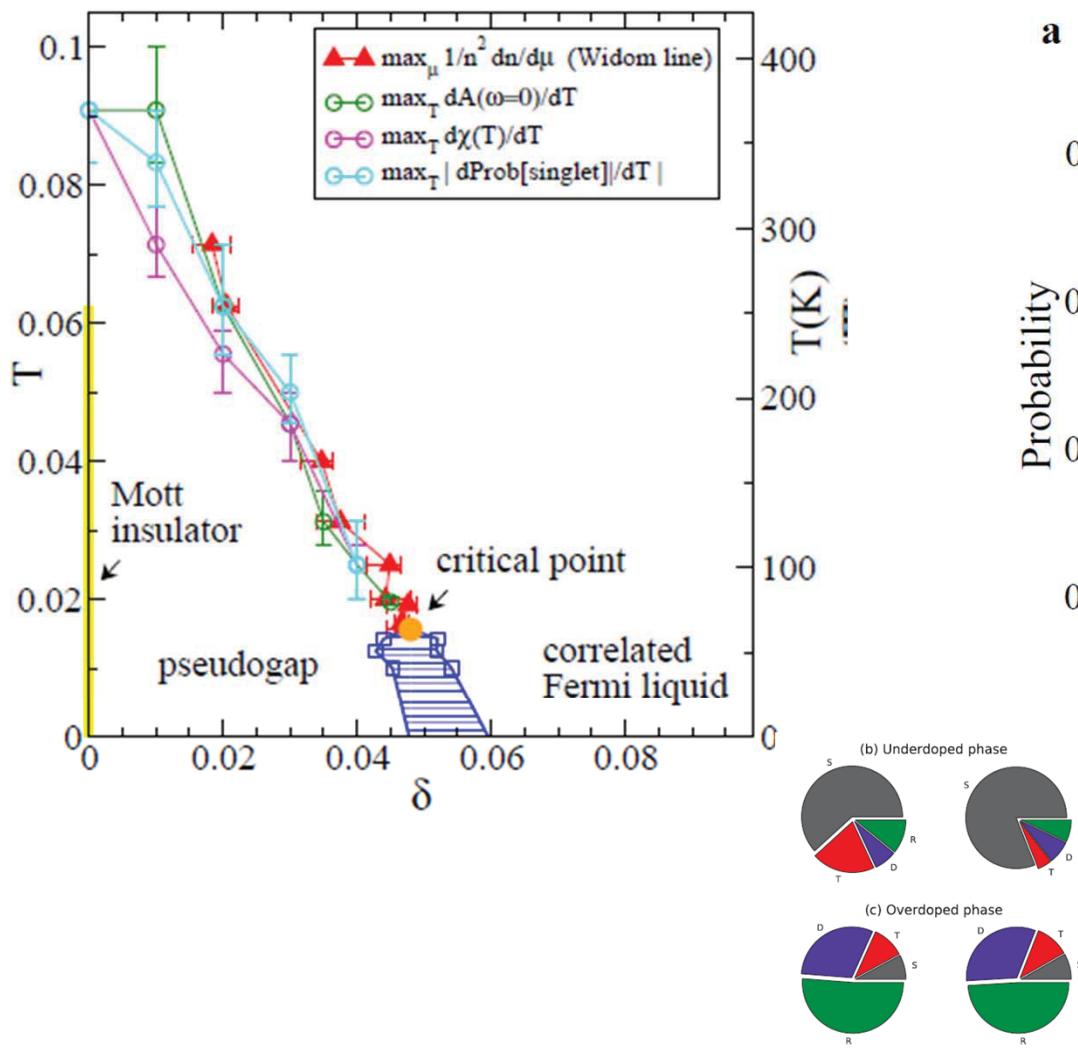
X. Deng, J.j Mravlje, R. Zitko, M. Ferrero, G. Kotliar, and A. Georges
PRL 110, 086401 (2013)

Physics



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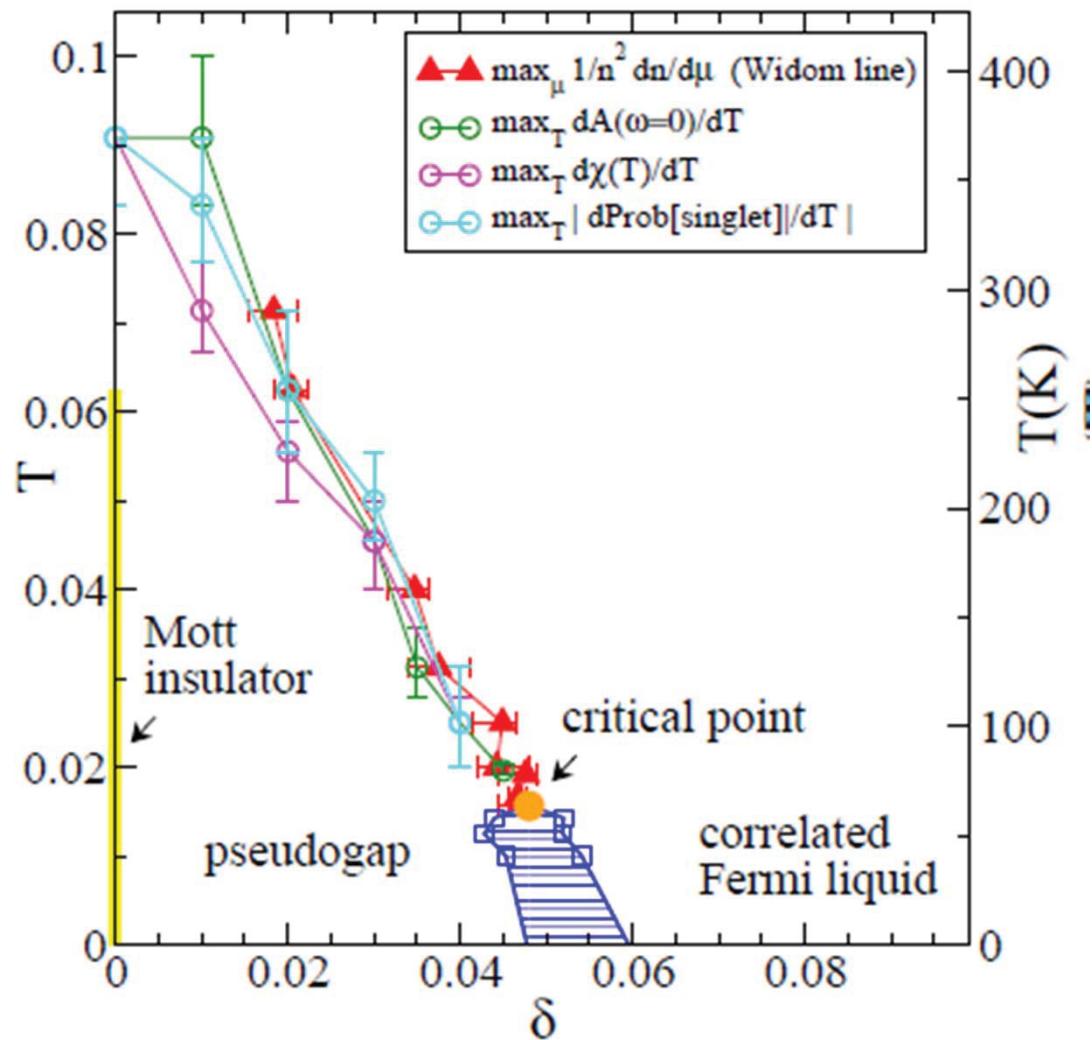
Plaquette eigenstates



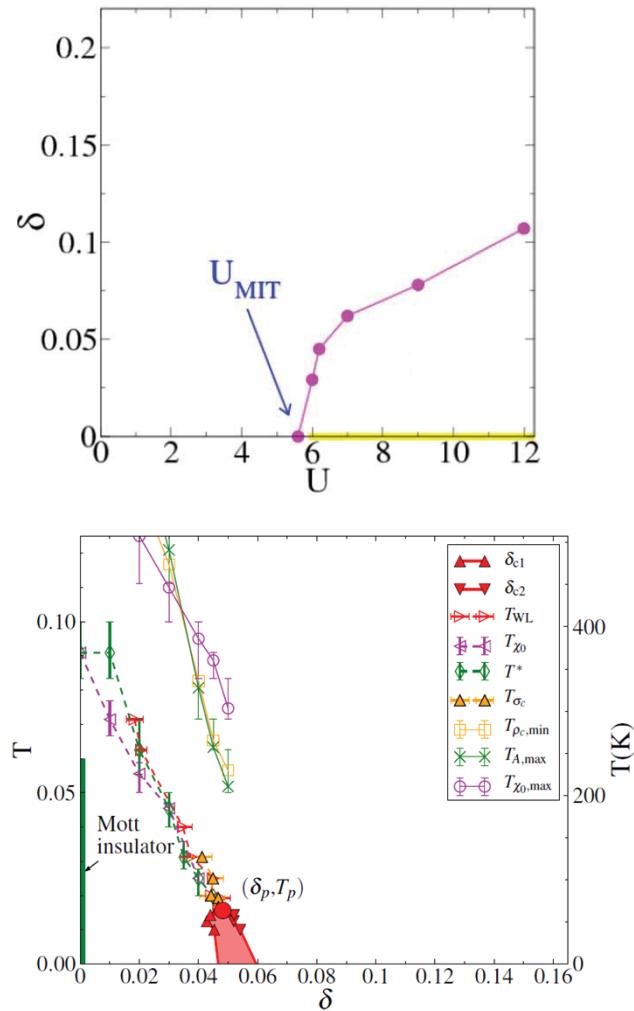
$$T = 1/10, 1/50$$



Pseudogap along the Widom line T_W

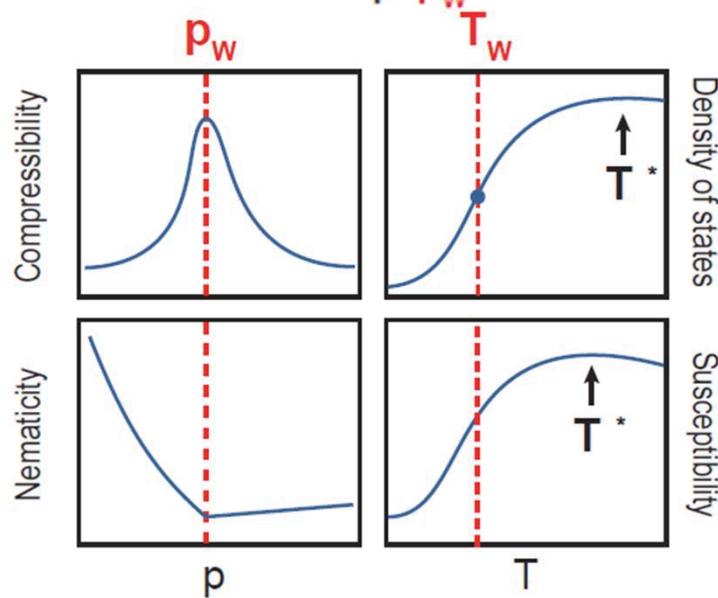
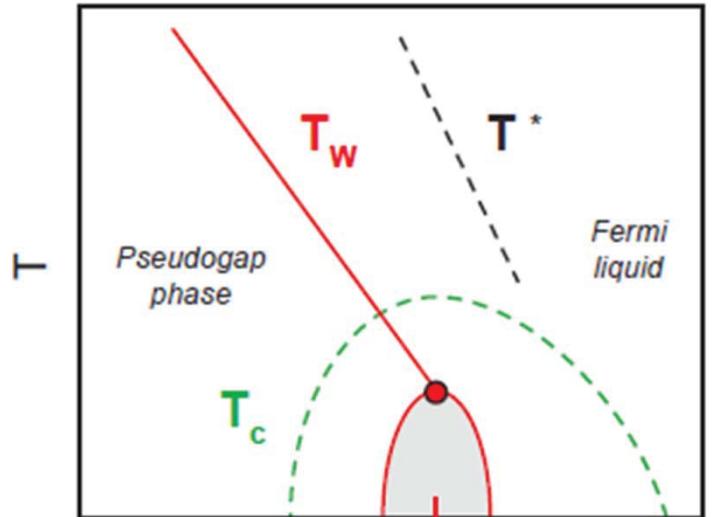


Summary: normal state



- 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?



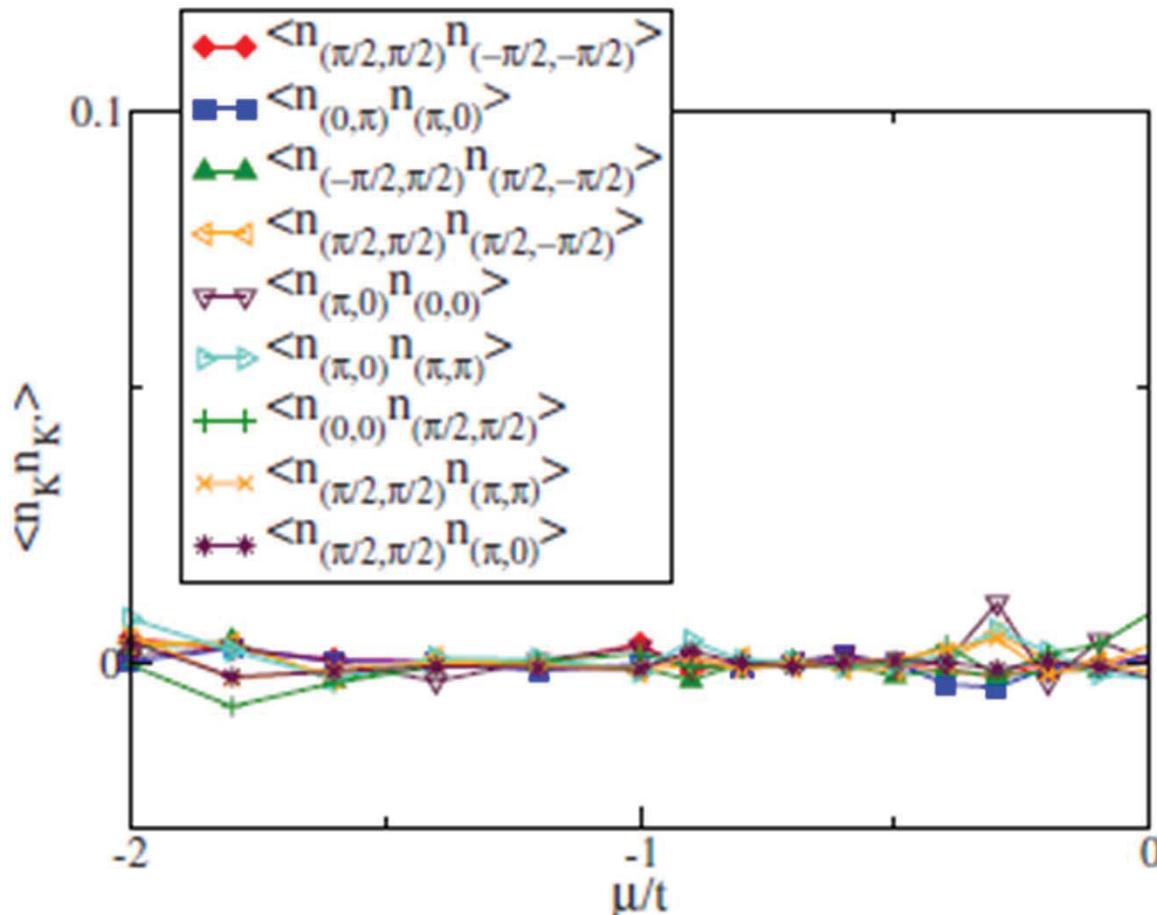
Anisotropy (nematicity)

Normal state and large anisotropy
in an *orthorhombic* crystal



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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

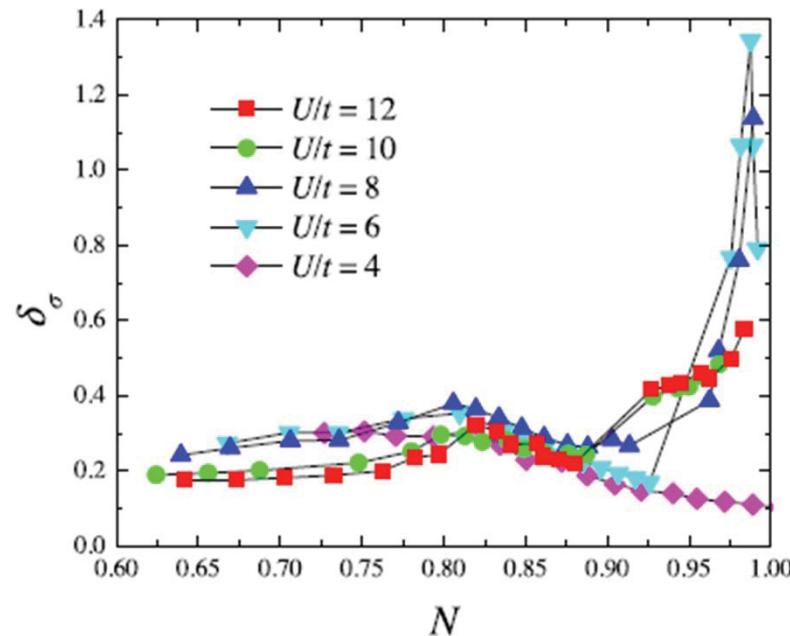
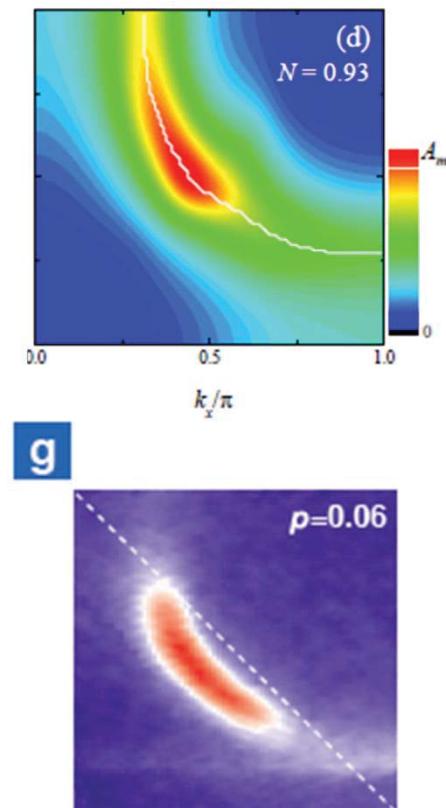


FIG. 3: (Color online) Anisotropy in the CDMFT conductivity $\delta_\sigma = 2 [\sigma_x(0) - \sigma_y(0)] / [\sigma_x(0) + \sigma_y(0)]$ as a function of filling N for various values of U and $\eta = 0.1$, $\delta_0 = 0.04$.



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

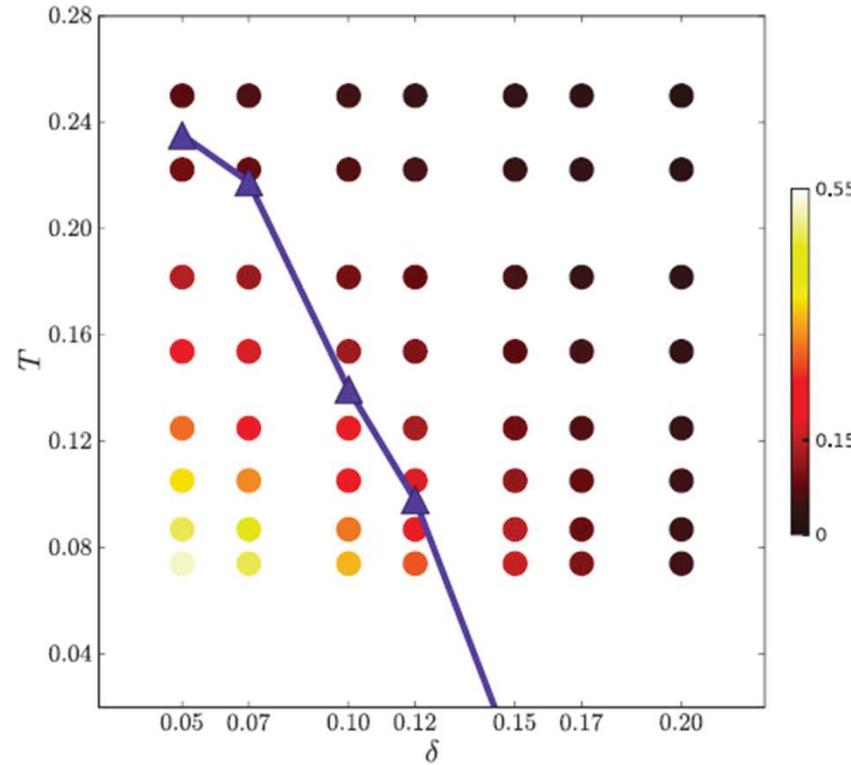
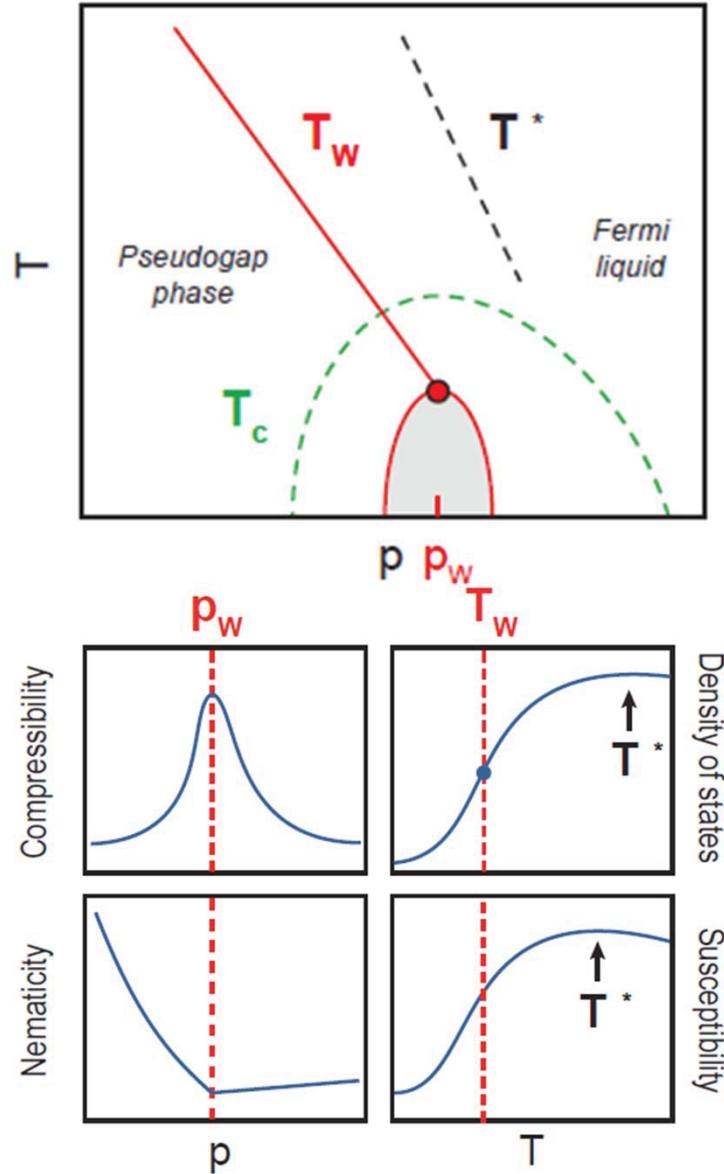


FIG. 3. (Color online) Color map of the anisotropic ratio of the quasiparticle weight σ_Z over the temperature-doping plane, for $U = 6t$. The solid blue curve indicates the pseudogap temperature $T^*(\delta)$ which is obtained as the temperature at which the uniform magnetic susceptibility $\chi_m[q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

$U = 6t$, DCA, 4x4

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

An emergent phenomenon in CDMFT



- 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?



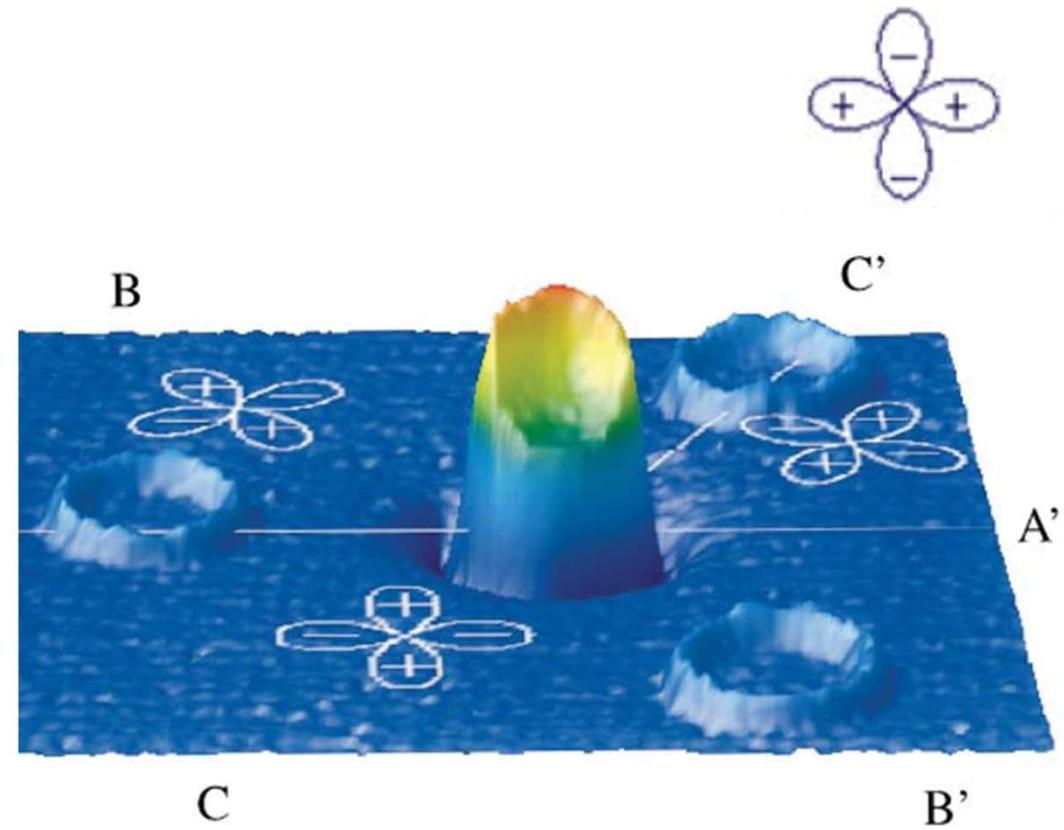
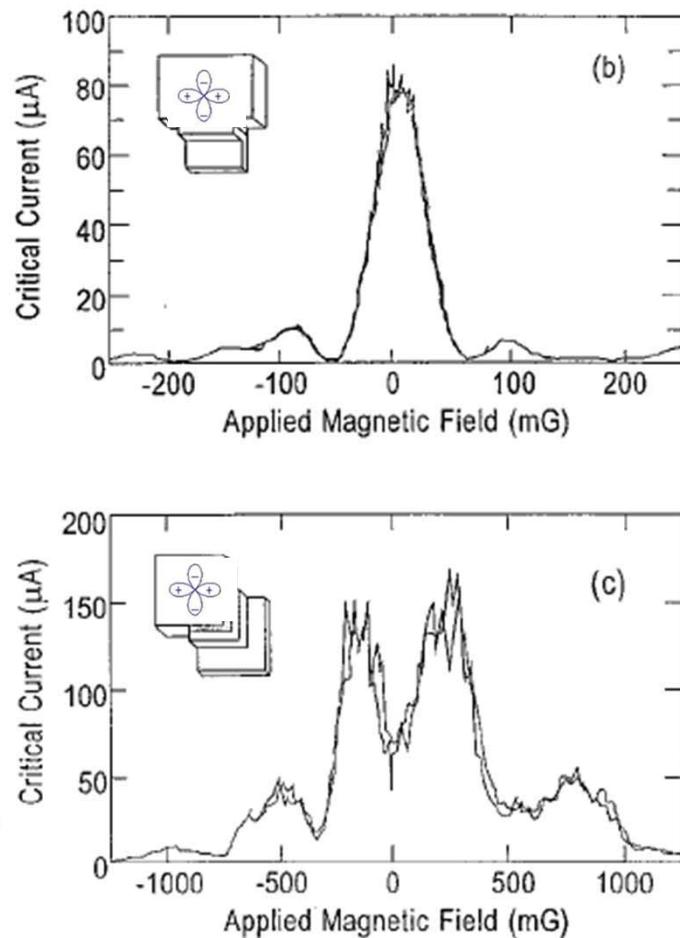
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d-wave superconductivity



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High T_c are d-wave (interference)



Tsuei Kirtley, Rev. Mod. Phys. 2000

Wollman et al. PRL 1993



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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 Mechanisms 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).

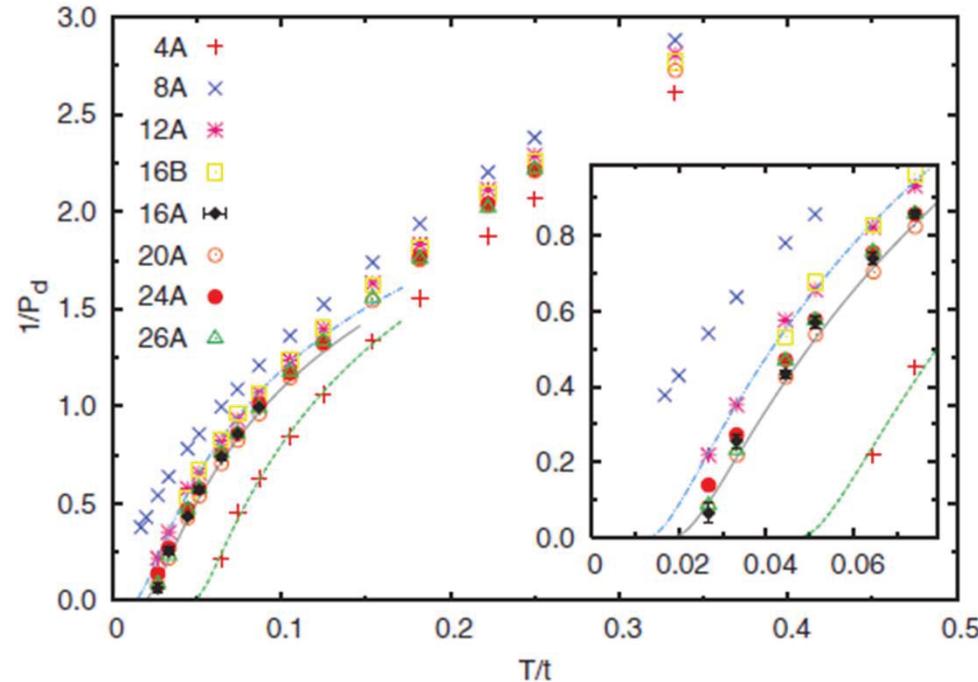
- Slave particles

- 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



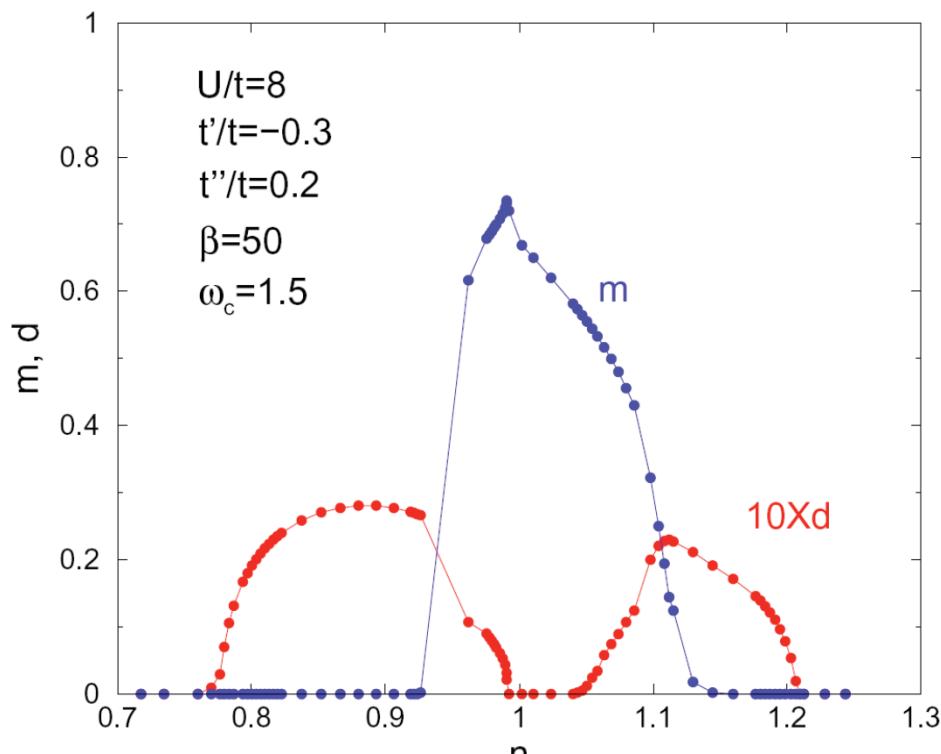
DCA, $U=4$

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



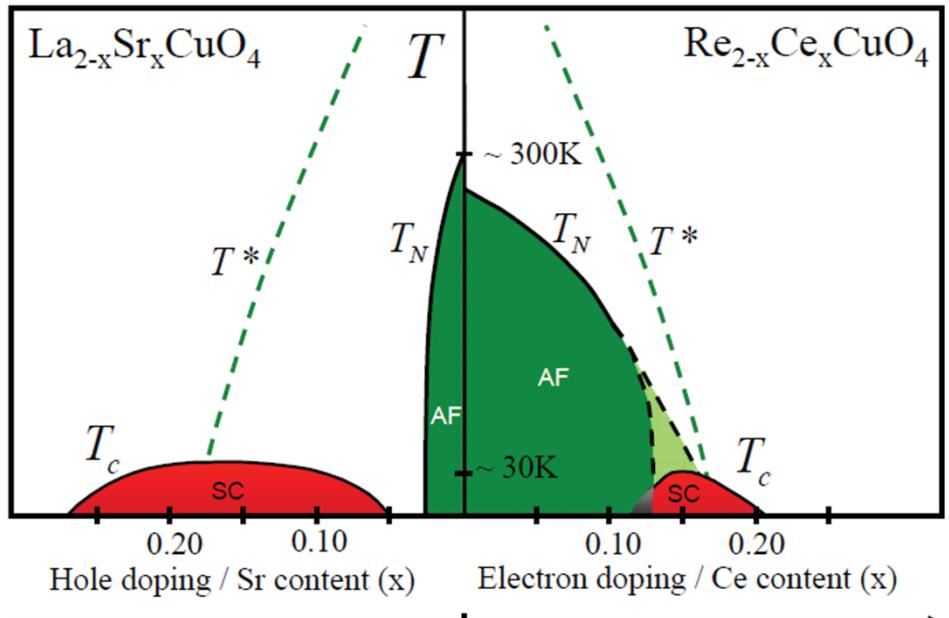
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CDMFT global phase diagram



Kancharla, Kyung, Civelli,
Sénéchal, Kotliar AMST

Phys. Rev. B (2008)
AND Capone, Kotliar PRL (2006)



Armitage, Fournier, Greene, RMP (2009)





Giovanni Sordi



Patrick Sémon



Kristjan Haule

Finite T phase diagram Superconductivity $t' = 0$

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



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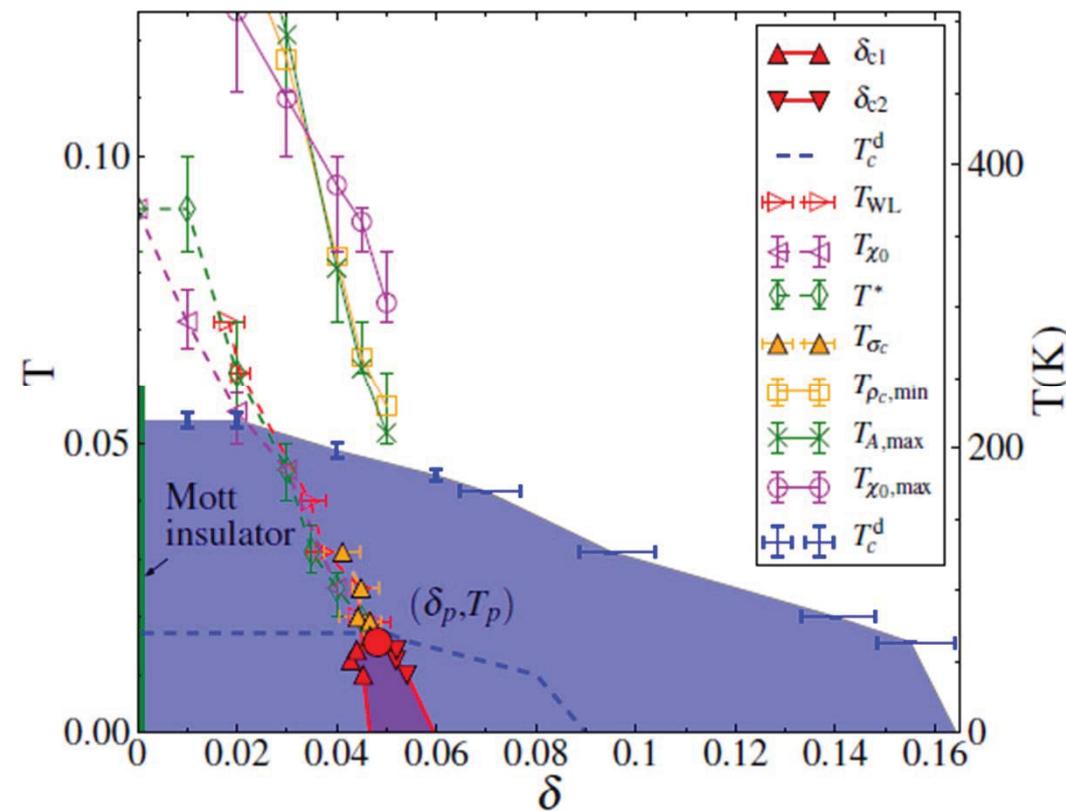


Giovanni Sordi



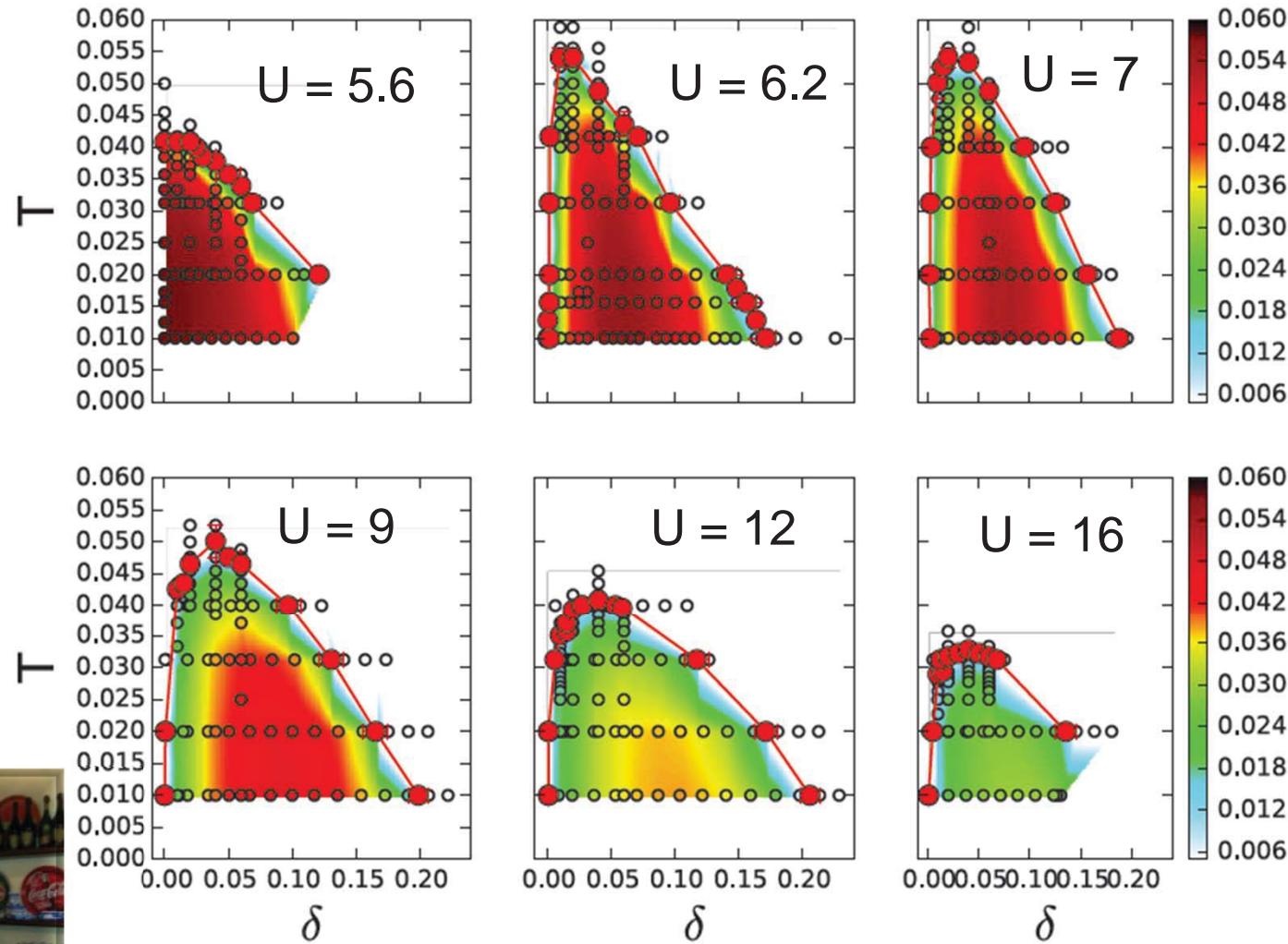
Patrick Sémon

Phase diagram for $U = 6.2 t$



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



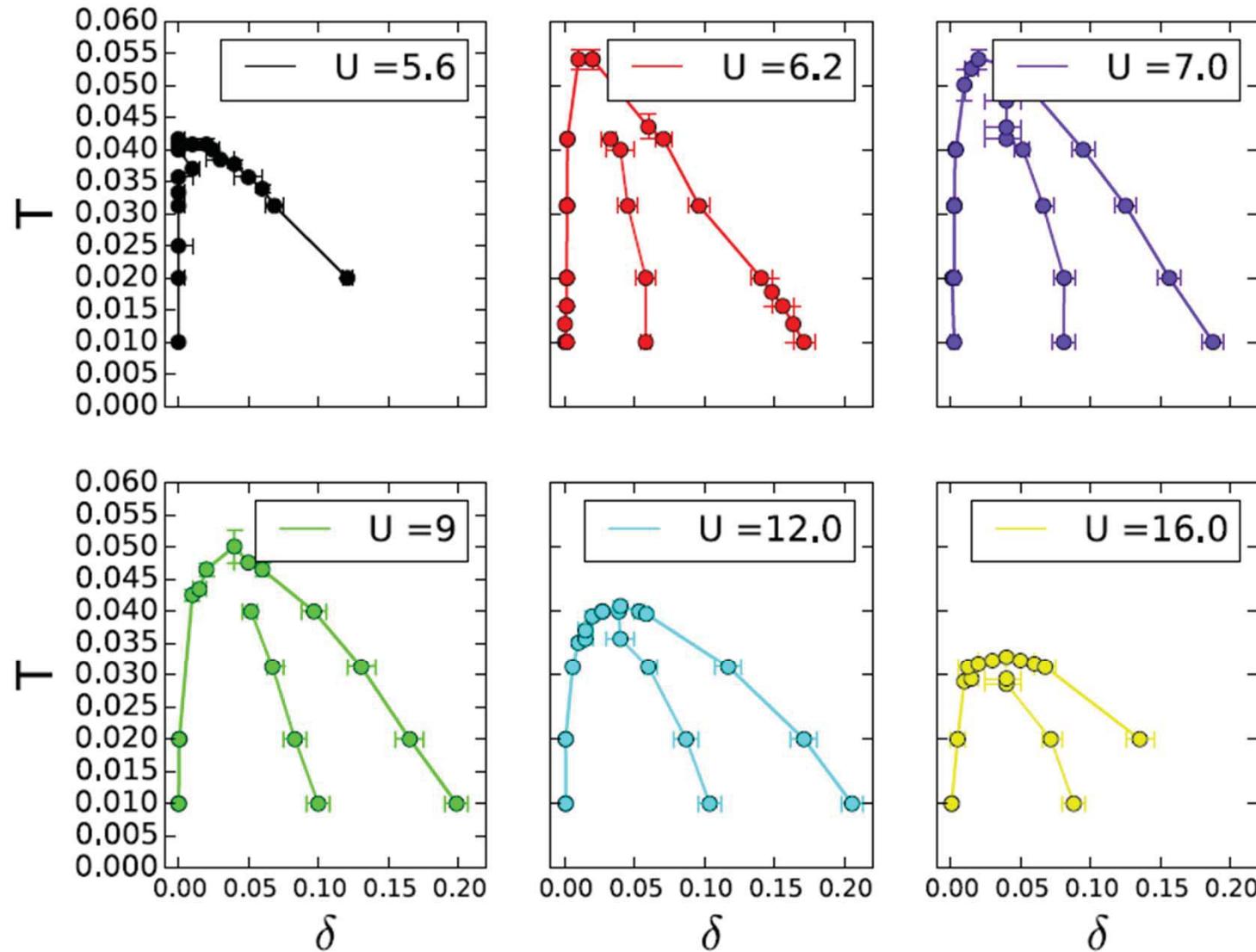
Lorenzo Fratino

L. Fratino, G. Sordi (unpublished)



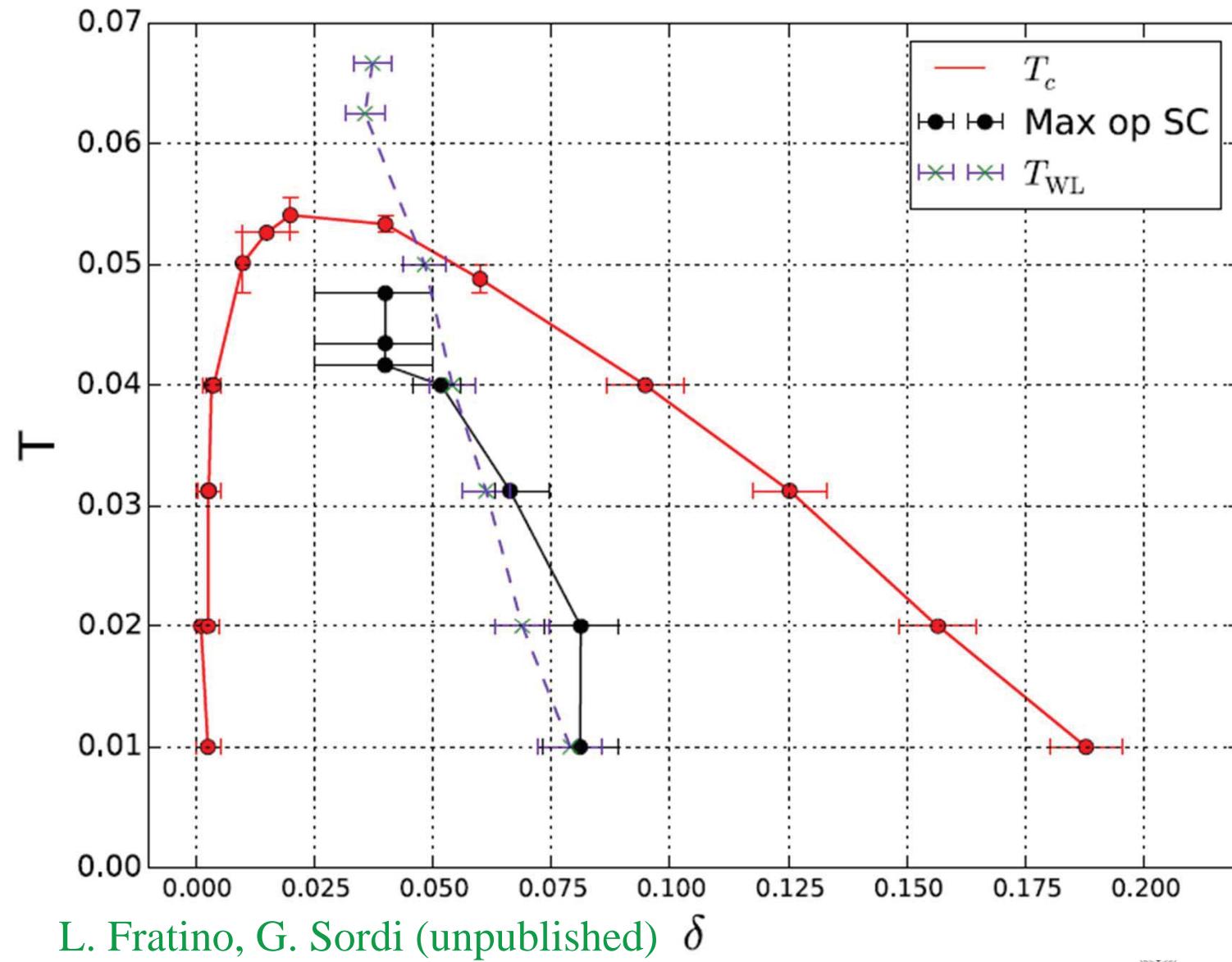
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T_c vs T_{\max} order parameter



L. Fratino, G. Sordi (unpublished)

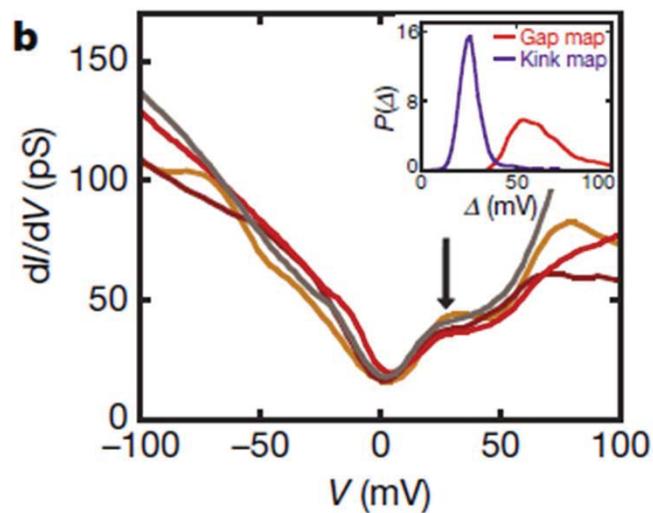
$U=7$, T_W vs T_c vs T_{\max} order parameter



L. Fratino, G. Sordi (unpublished) δ

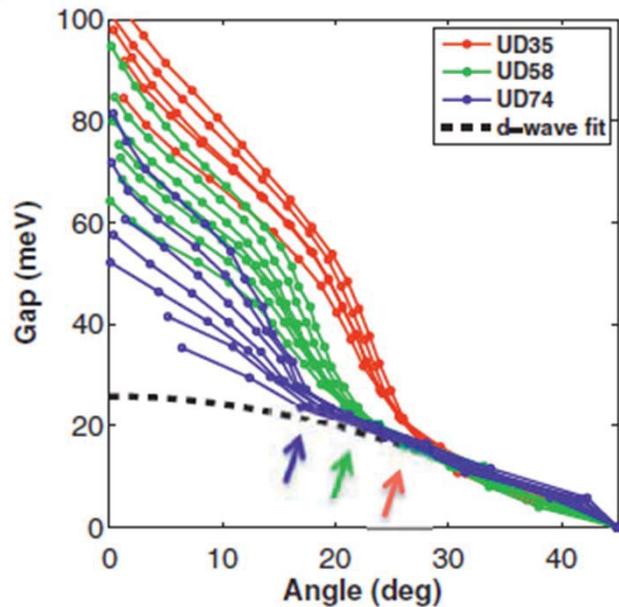
Meaning of T_c^d

- Local pair formation



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

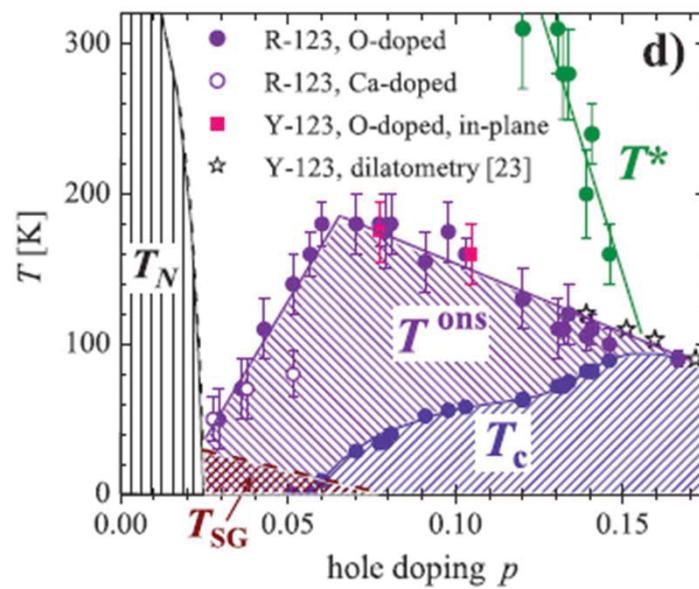
Meaning of T_c^d : Local pair formation



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

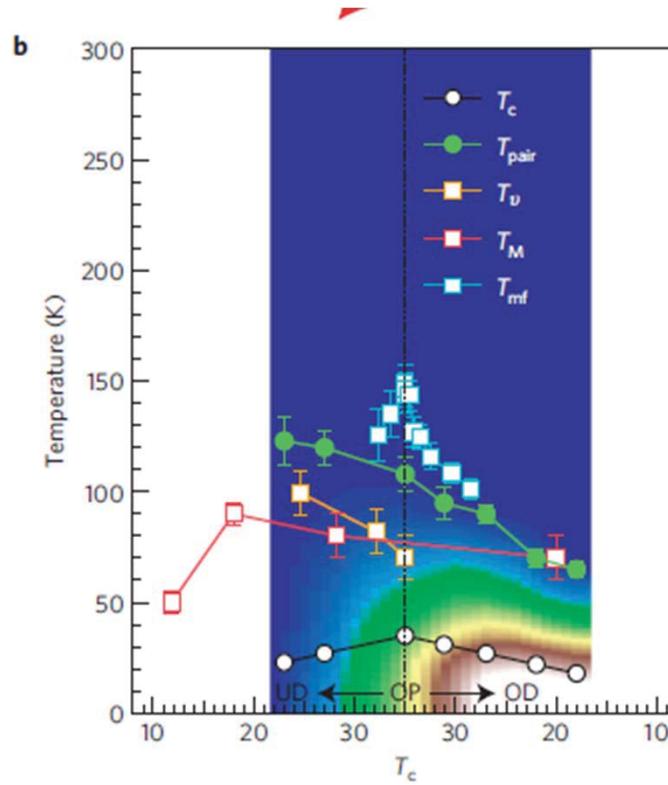


Infrared response

Dubroka et al. PRL 106, 047006 (2011)

T_{pair}

ARPES
Bi2212

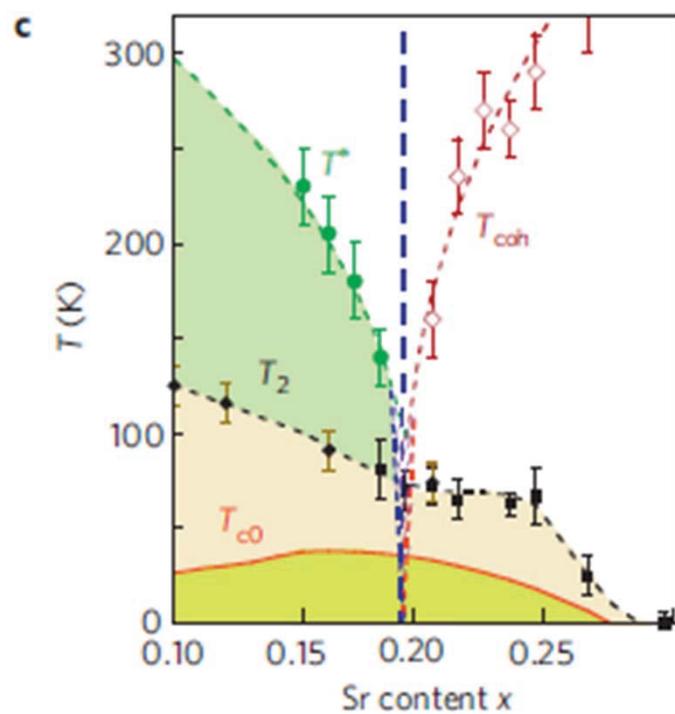


Kondo, Takeshi, et al. Kaminski Nature
Physics 2011, 7, 21-25



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T_2



Magnetoresistance, LSCO
Fluctuating vortices

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

Giant proximity effect

$$\begin{aligned}T_c &= 32 \text{ K} \\T_c &< 5 \text{ K}\end{aligned}$$

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

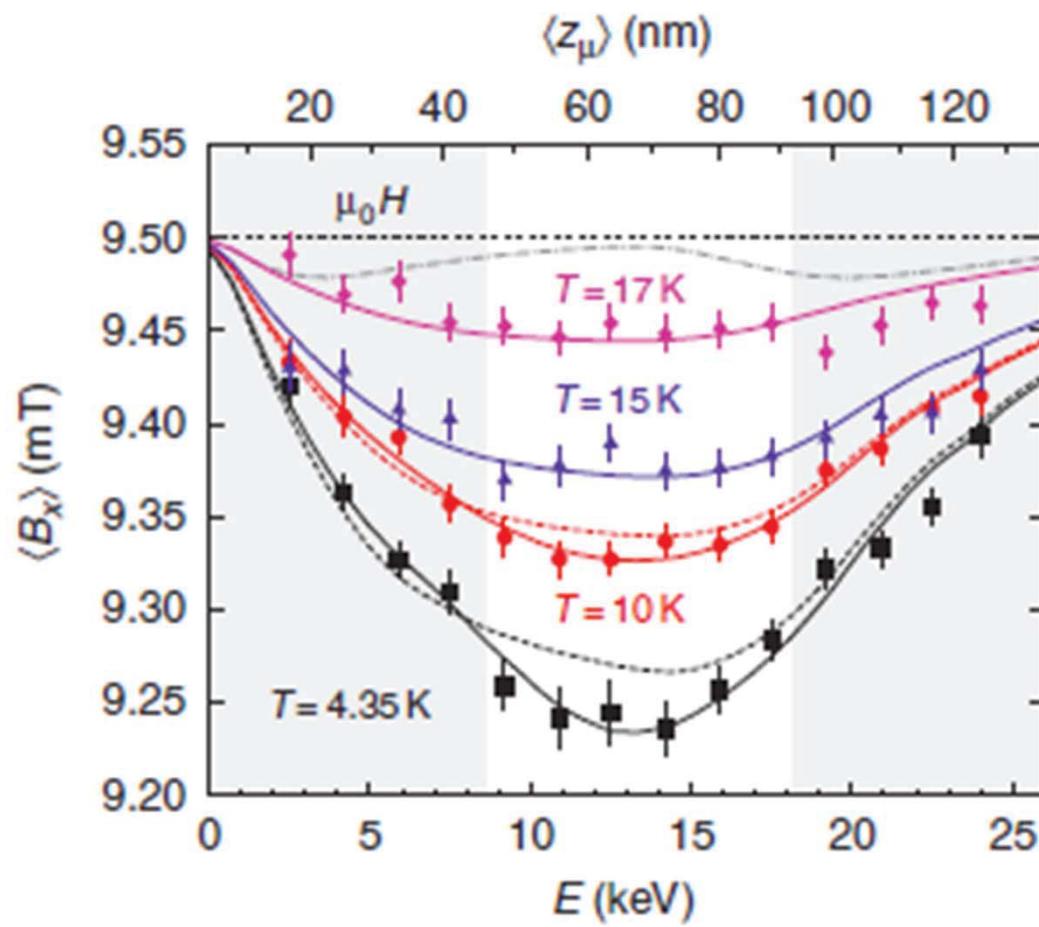


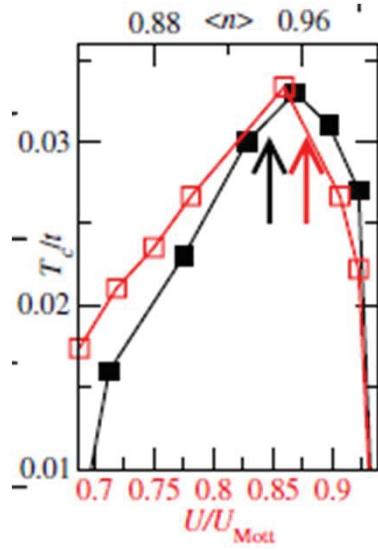
Figure 6 | Depth profile of the local field at different temperatures. The

Actual T_c in underdoped

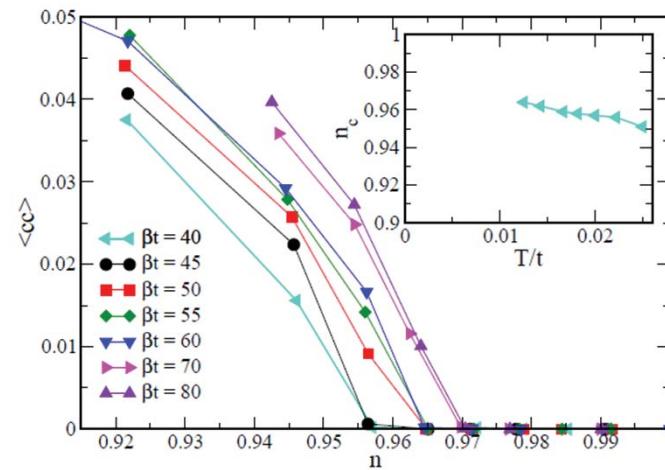
- Quantum and classical phase fluctuations
 - V. J. Emery and S. A. Kivelson, Phys. Rev. Lett. **74**, 3253 (1995).
 - V. J. Emery and S. A. Kivelson, Nature **374**, 474 (1995).
 - D. Podolsky, S. Raghu, and A. Vishwanath, Phys. Rev. Lett. **99**, 117004 (2007).
 - Z. Tesanovic, Nat Phys **4**, 408 (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)



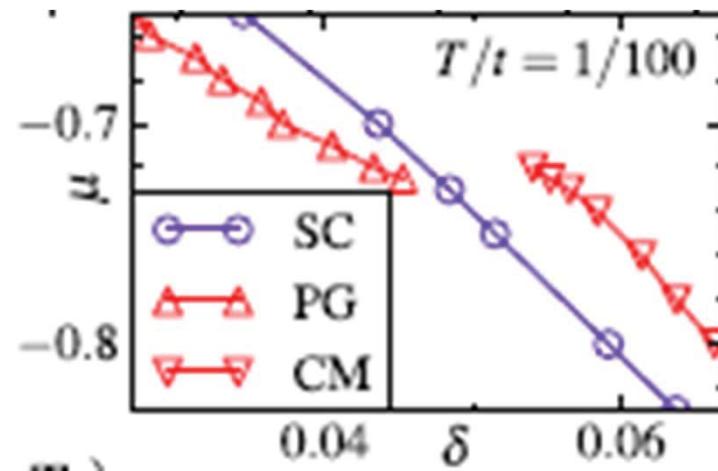
8 site DCA, $U=6t$



8 site DCA, $U=6.5t$

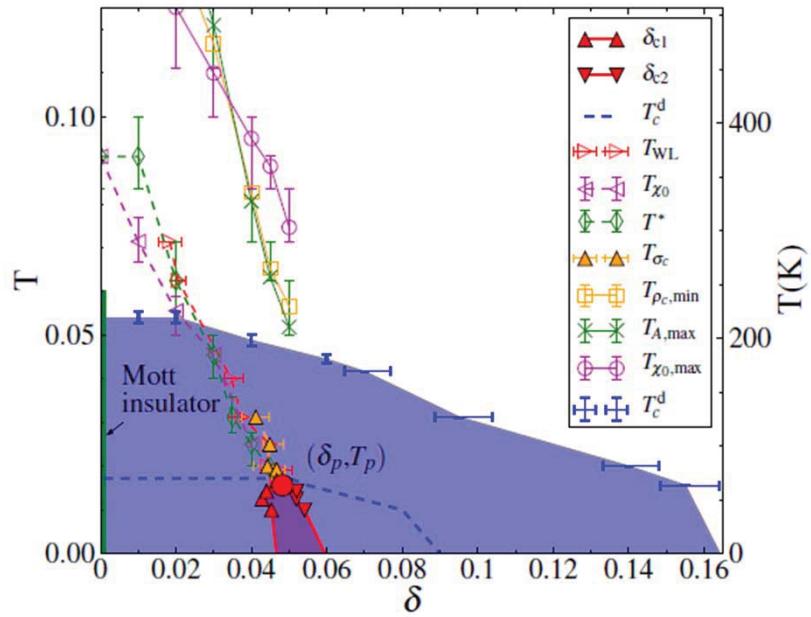
Gull Parcollet Millis,
PRL 110, 216405 (2013)

Fate of the first order transition in SC state



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

Summary

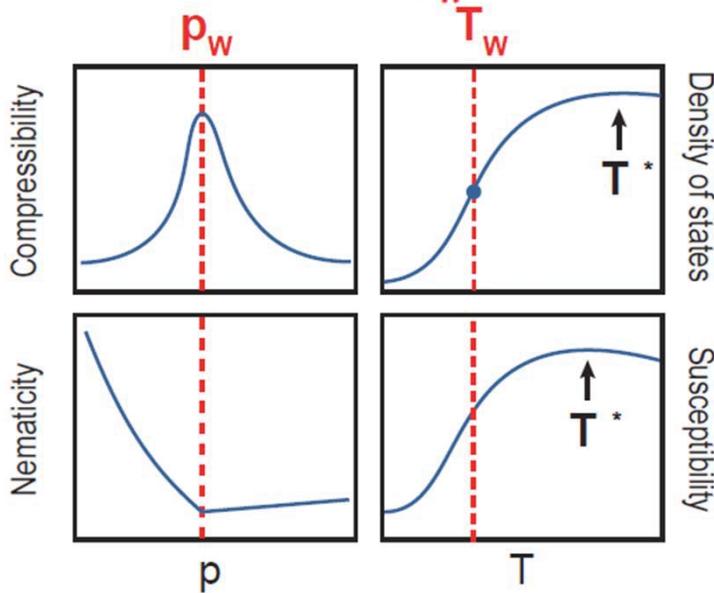
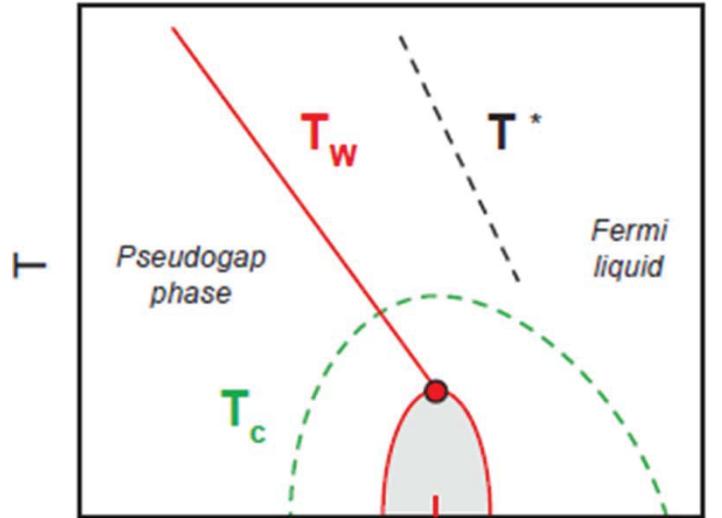


- Below the dome, not QCP (but Mott)
- Maximum near Widom line
- T^* different from T_c^d
- First-order transition destroyed (but traces in the dynamics)
- Actual T_c in underdoped
 - Competing order
 - Long wavelength fluctuations (see O.P.)



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Organizing principle



- Is the pseudogap (PG) a crossover or a phase transition ?
- Relation between CDW and the PG ?
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- 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?



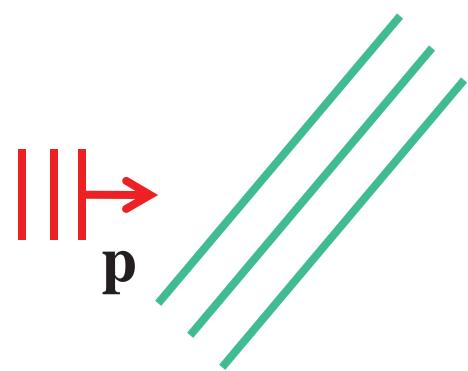


Bio break

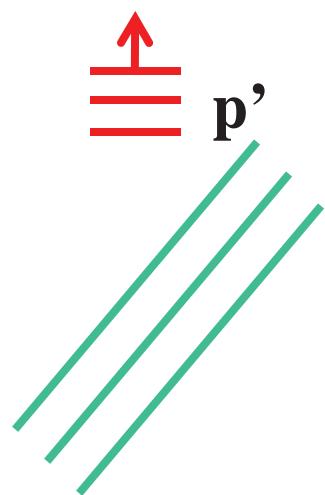


Superconductivity

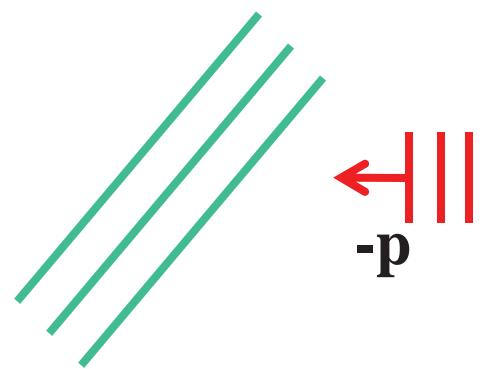
Attraction mechanism in the metallic state



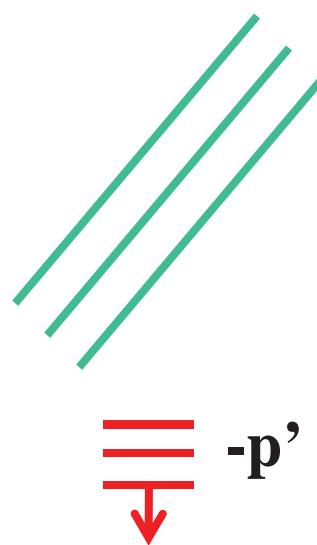
Attraction mechanism in the metallic state



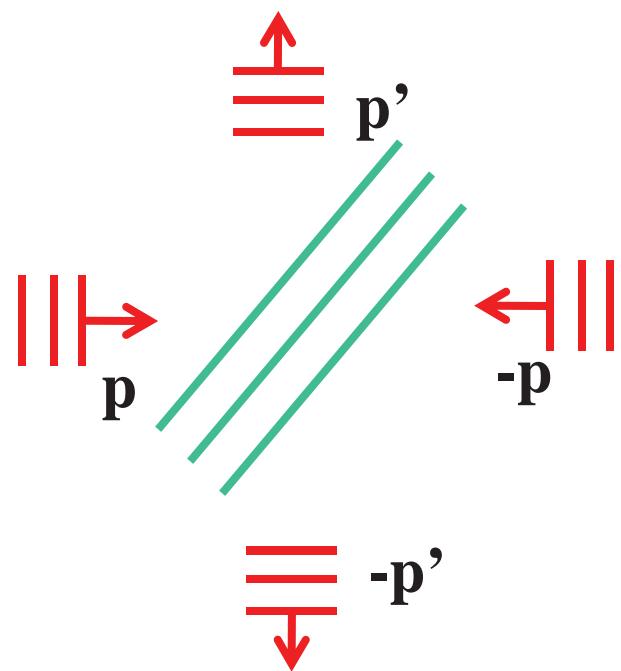
Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



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#1 Cooper pair, #2 Phase coherence

$$E_P = \sum_{\mathbf{p}, \mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \psi_{\mathbf{p}\uparrow, -\mathbf{p}\downarrow} \psi_{\mathbf{p}'\uparrow, -\mathbf{p}'\downarrow}^*$$

$$E_P = \sum_{\mathbf{p}, \mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \left(\langle \psi_{\mathbf{p}\uparrow, -\mathbf{p}\downarrow} \rangle \psi_{\mathbf{p}'\uparrow, -\mathbf{p}'\downarrow}^* + \psi_{\mathbf{p}\uparrow, -\mathbf{p}\downarrow} \langle \psi_{\mathbf{p}'\uparrow, -\mathbf{p}'\downarrow}^* \rangle \right)$$

$$|\text{BCS}(\theta)\rangle = \dots + e^{iN\theta} |N\rangle + e^{i(N+2)\theta} |N+2\rangle + \dots$$



Giovanni Sordi



Patrick Sémon

Superfluid stiffness $T = 0$

8 site cluster DCA $U = 6t$

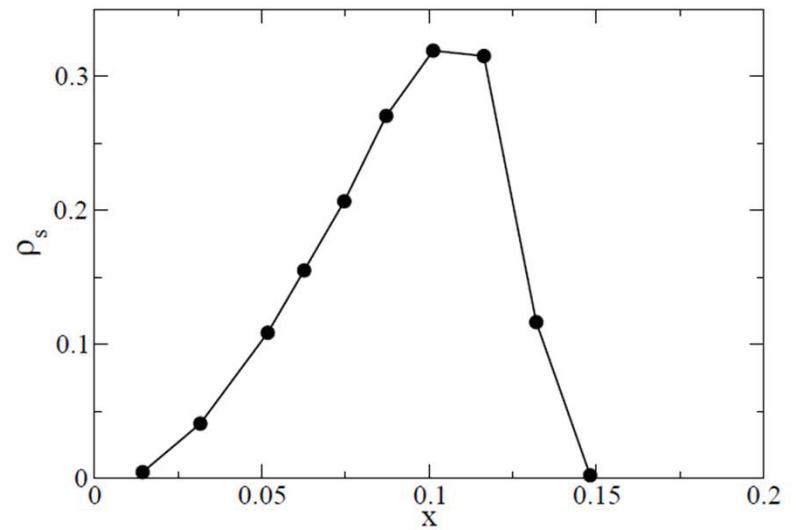
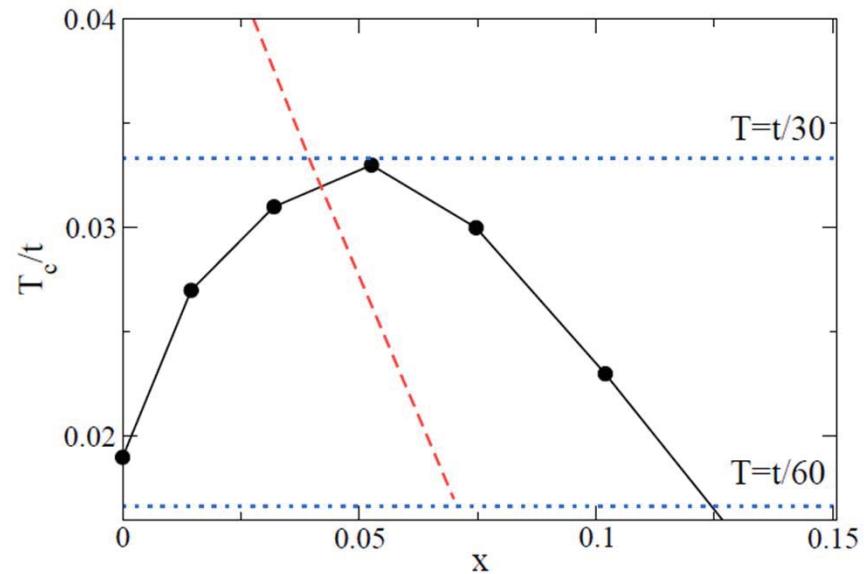
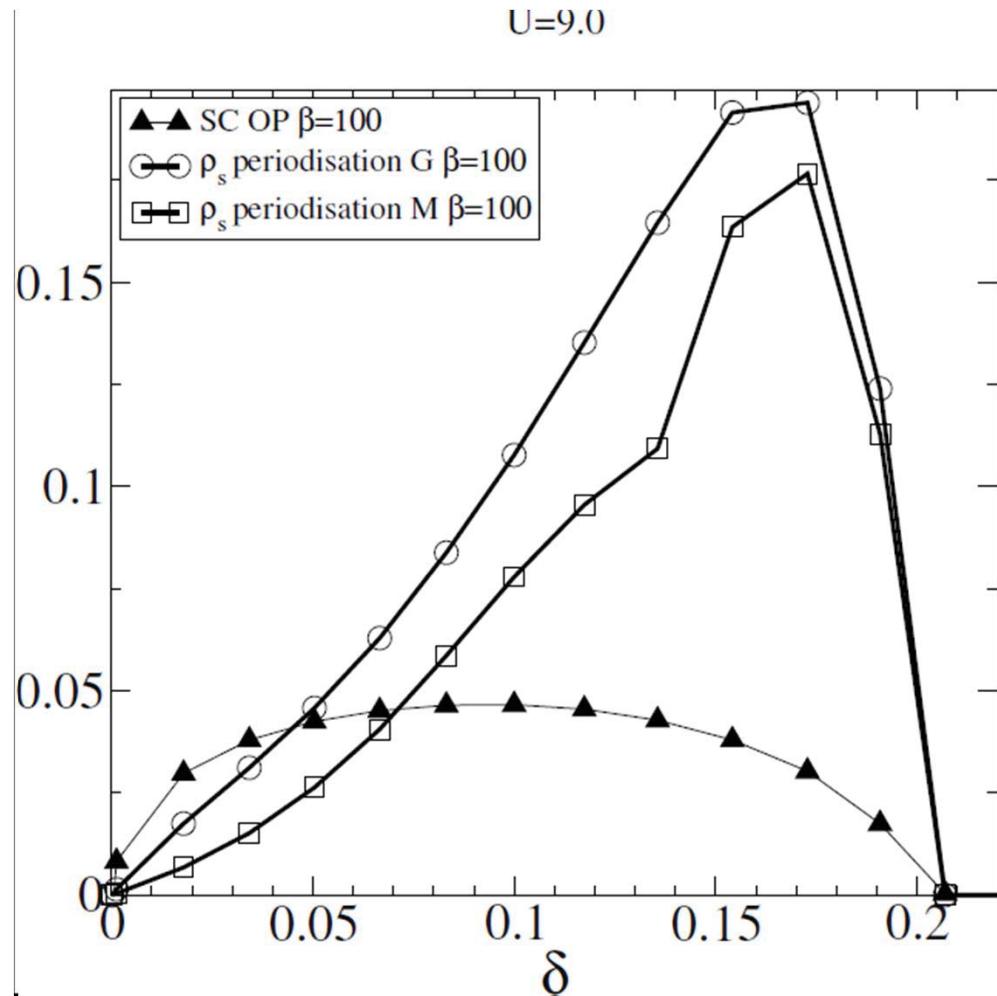


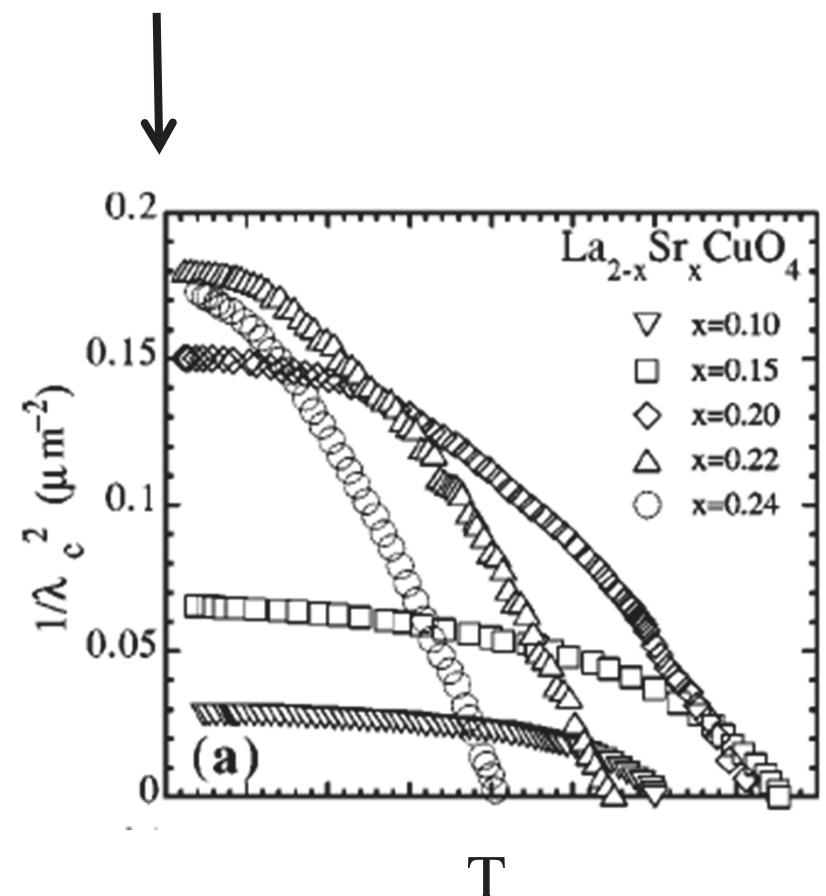
FIG. 8. Superfluid stiffness ρ_s determined in the superconducting state at $T = t/60$ from Eq. 15, as a function of doping.

E. Gull, A.J. Millis,
Phys. Rev. B **88**, 075127 (2013)

c-axis Superfluid stiffness $U = 9t$, $T=1/100$



Sordi, Sémon unpublished

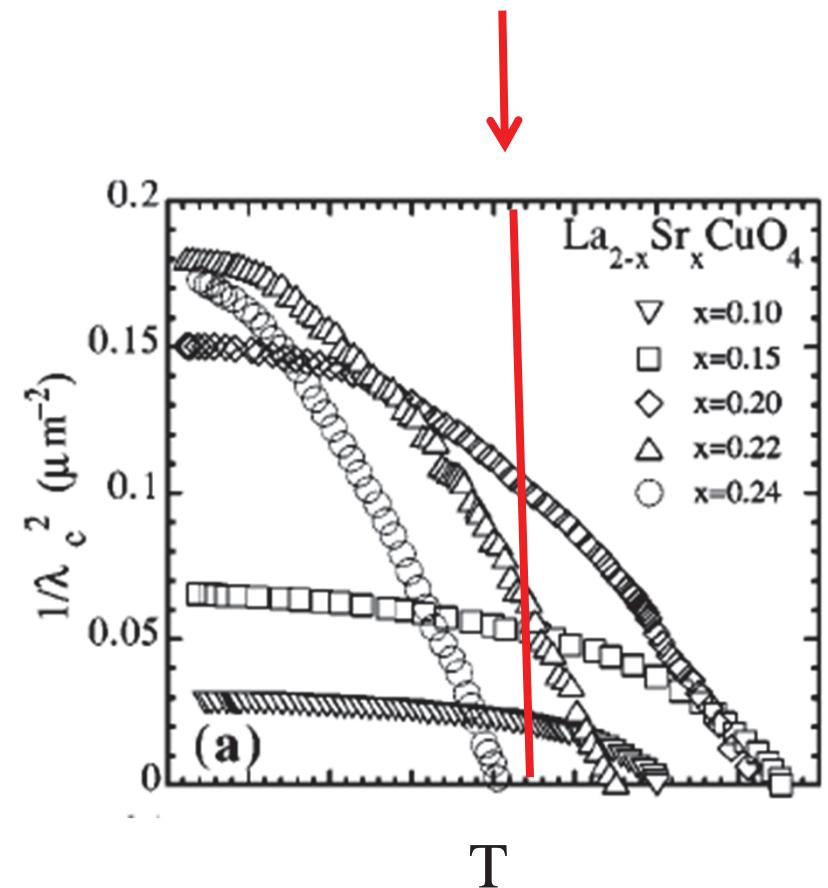
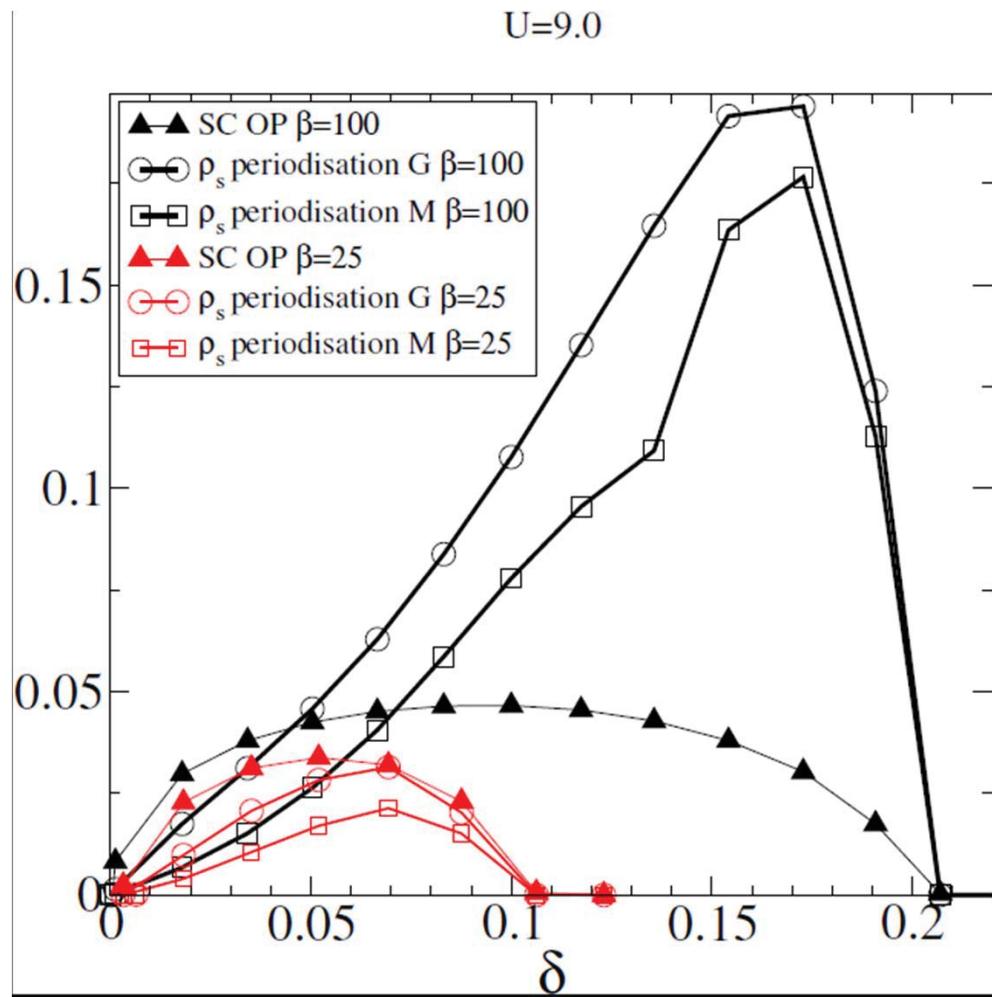


Panagopoulos et al. PRB 2000



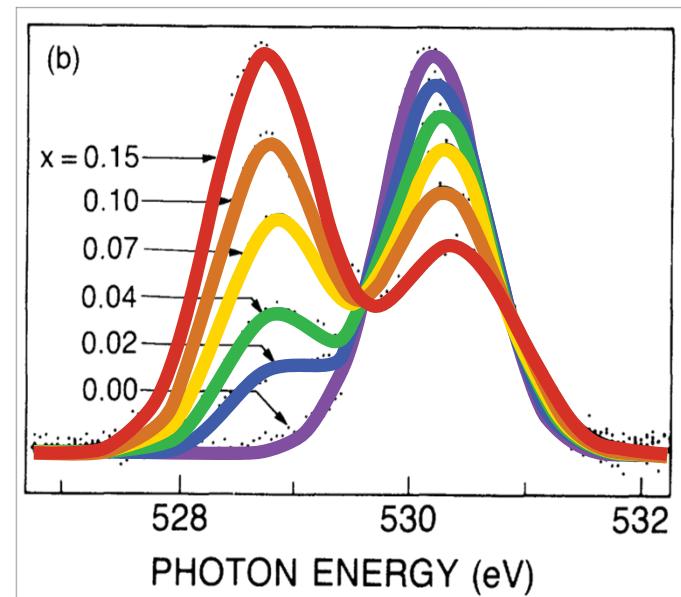
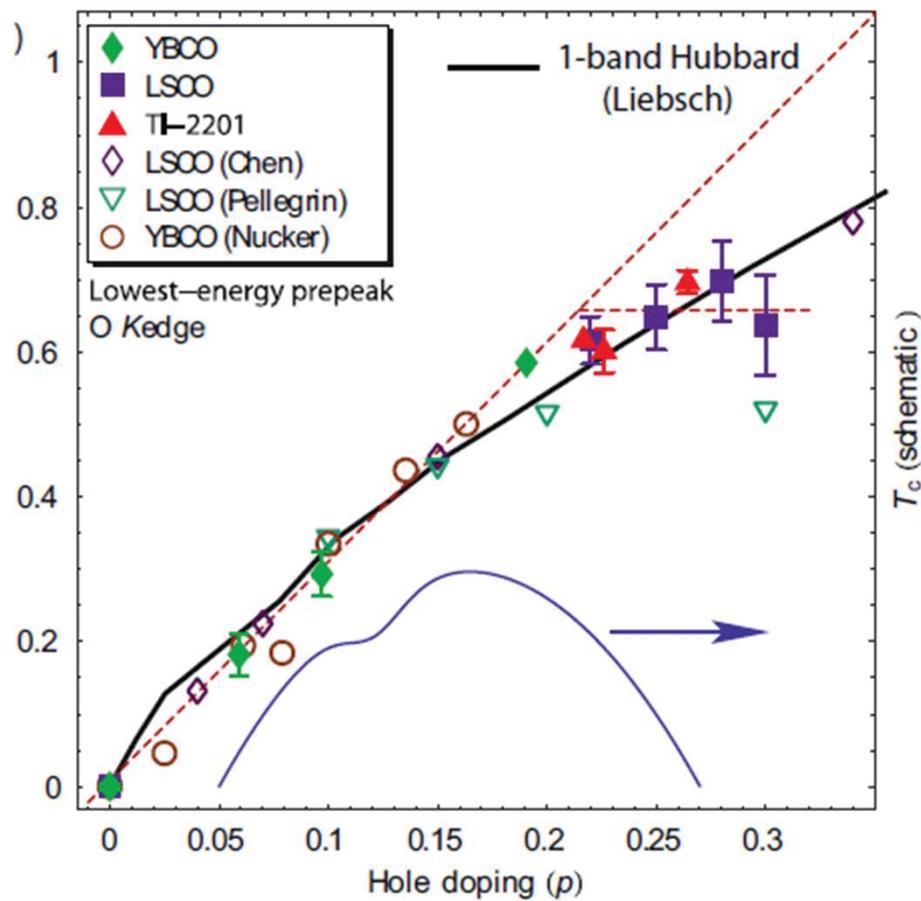
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c-axis Superfluid stiffness $U = 9t$, $T=1/100$



Sordi, Sémon, unpublished

Compare with number of carriers

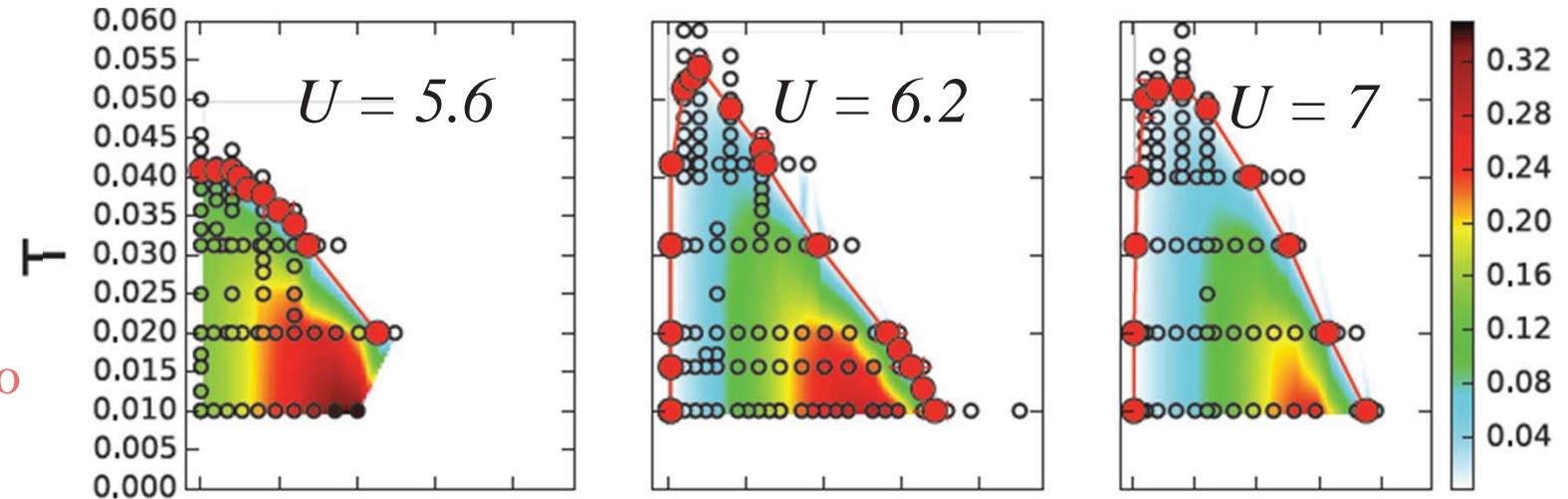


Peets et al. PRL 2009, Phillips and Jarrell, PRL 2010

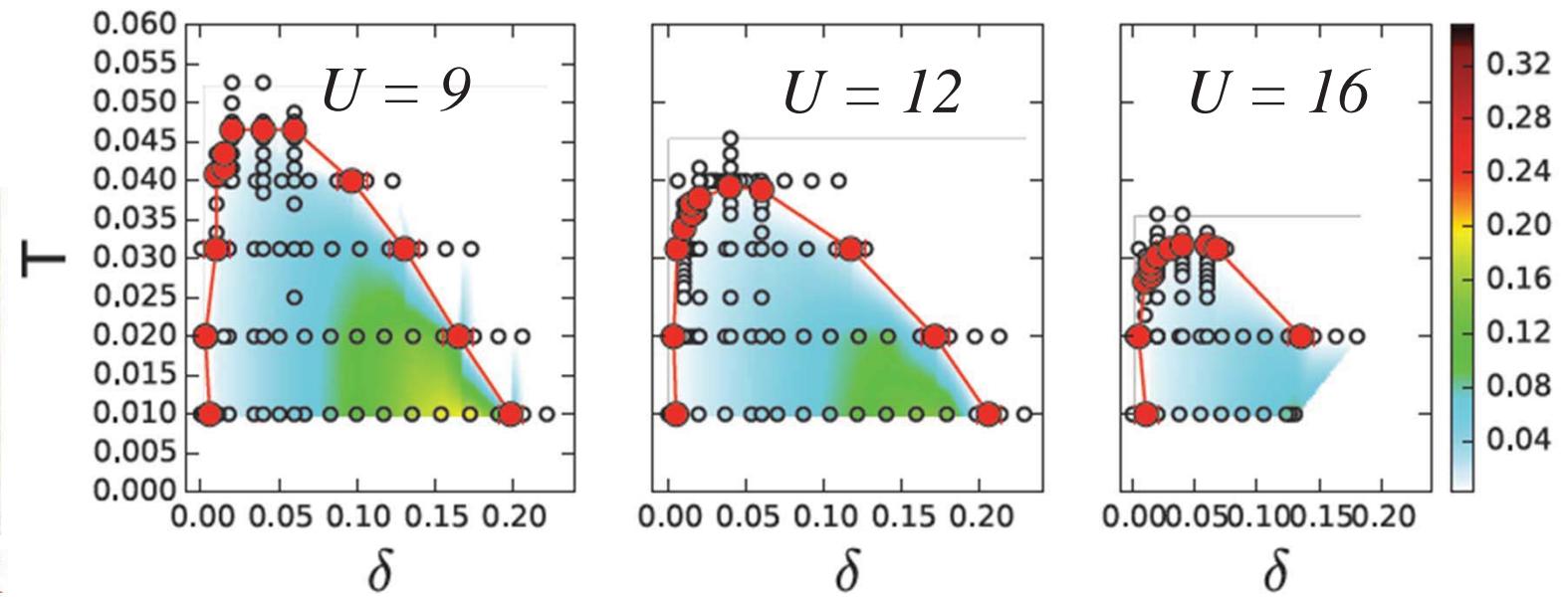
Superfluid stiffness



Lorenzo Fratino

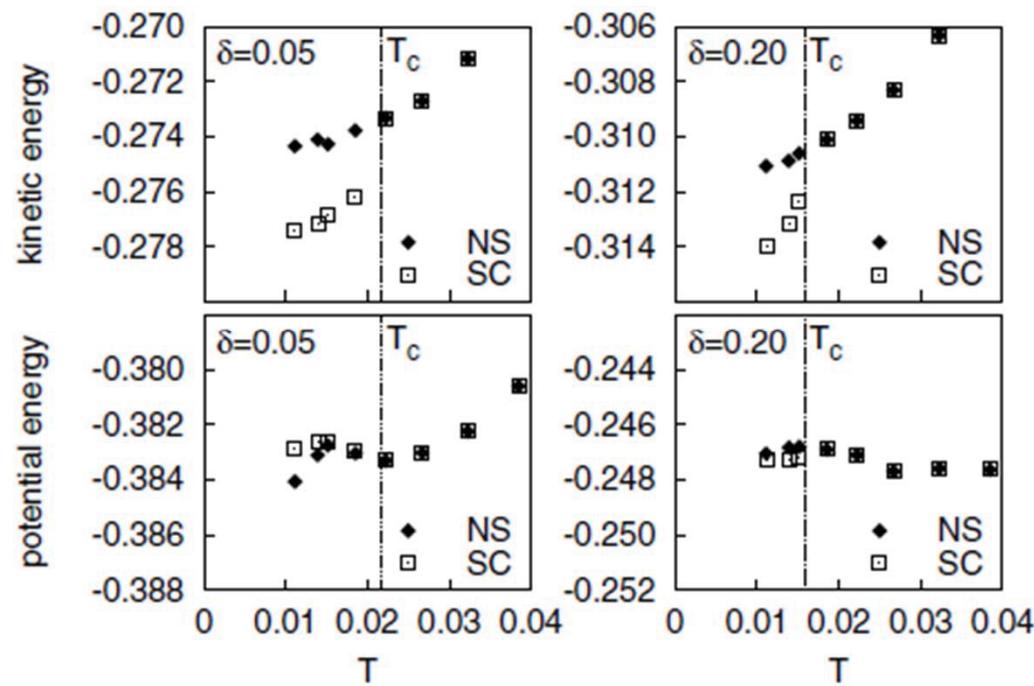


Giovanni Sordi



Condensation energy

Condensation energy

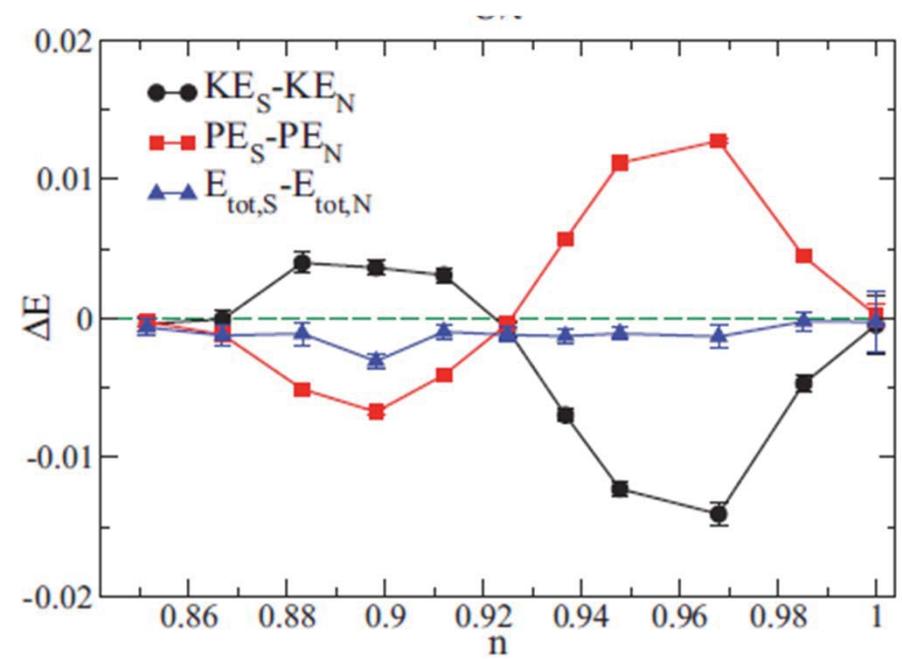
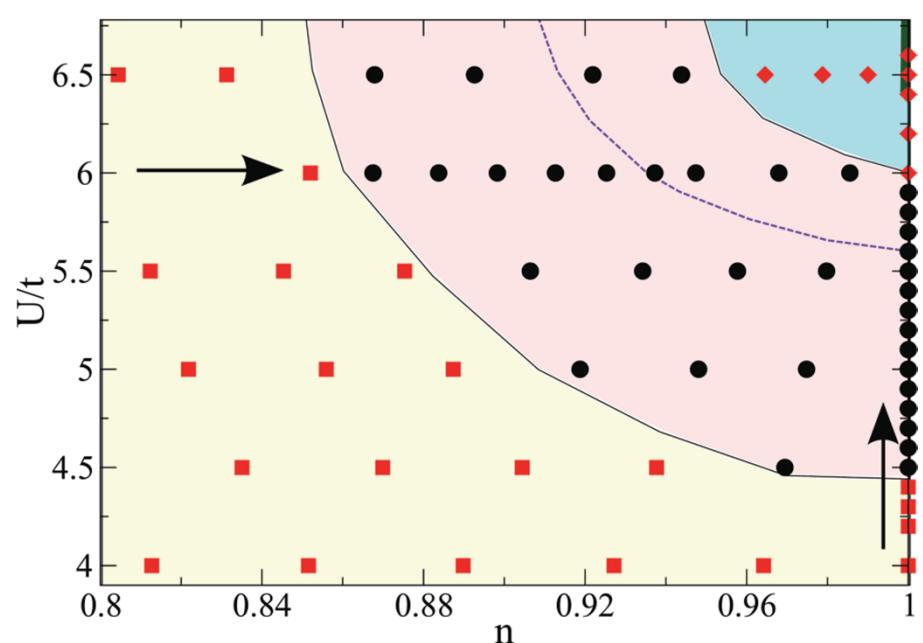


$$U = 8t, 4 \text{ sites} - DCA$$

Th. A. Maier, M. Jarrell, A. Macridin, and C. Slezak
PRL 92, 027005 (2004)

Condensation energy

Experiments: N. Bontemps et al. Annals of Physics 321 (2006) 1547–1558



$$U = 6t, \quad T = 1/60, \quad 8 \text{ sites} - DCA$$

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

K. Haule, G. Kotliar EPL, 77 (2007) 27007

The glue



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Superconductivity in general

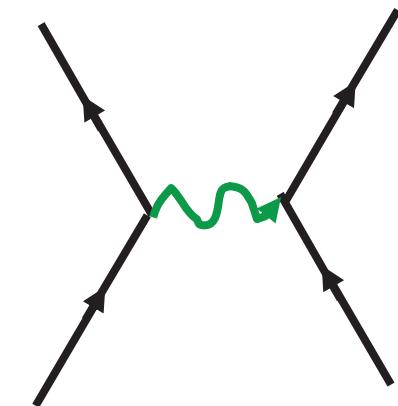
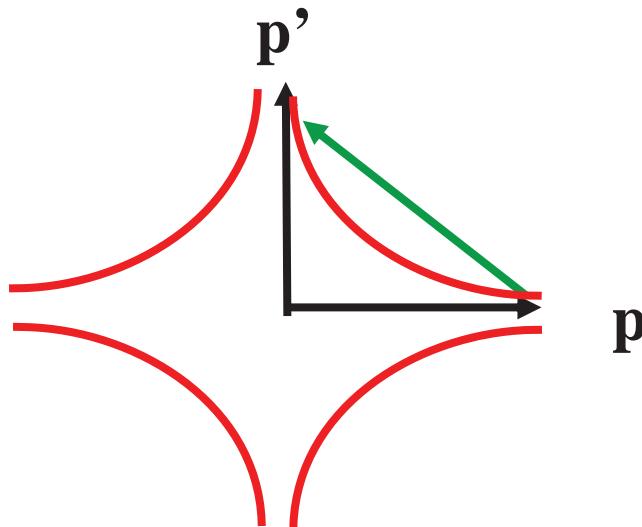
Analog to weakly and strongly
correlated antiferromagnets



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Cartoon « BCS » weak-correlation picture

$$\Delta_{\mathbf{p}} = -\frac{1}{2V} \sum_{\mathbf{p}'} U(\mathbf{p} - \mathbf{p}') \frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}} (1 - 2n(E_{\mathbf{p}'}))$$



Béal–Monod, Bourbonnais, Emery
P.R. B. **34**, 7716 (1986).

D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch
P.R. B **34**, 8190-8192 (1986).

Kohn, Luttinger, P.R.L. **15**, 524 (1965).

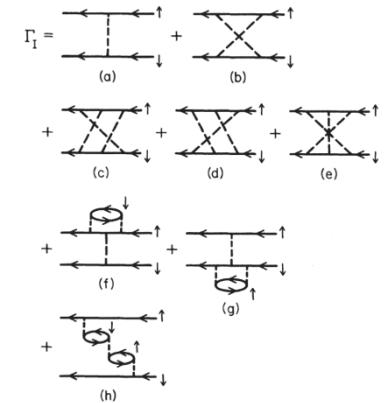
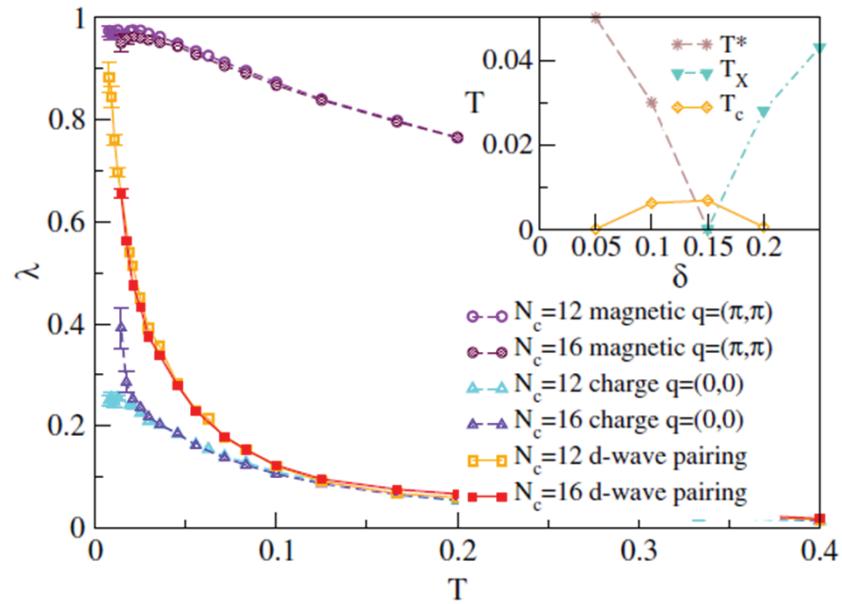
Exchange of spin waves?
Kohn-Luttinger
 T_c with pressure

P.W. Anderson Science 317, 1705 (2007)

Detailed calculations

Bulut, Scalapino, White, PRB 47, 6157 (1993)
 Maier, Jarrell, Scalapino PRL 96, 047005 (2006)

$$\lambda_\alpha \phi_\alpha(p) = -\frac{T}{N} \sum \Gamma_I(p|p') G_\uparrow(p') G_\downarrow(-p') \phi_\alpha(p')$$



DCA, $U=6t$, $N = 12$ and 16 sites

$U = 8t$, the « glue » approximation
does not work so well

E. Khatami, A. Macridin, and M. Jarrell
 Phys. Rev. B **80**, 172505 (2009)

S.-X. Yang, H. Fotso, ... J. Moreno,
 J. Zaanen, and M. Jarrell PRL **106**, 047004 (2011)

A cartoon strong correlation picture

$$J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = J \sum_{\langle i,j \rangle} \left(\frac{1}{2} c_i^\dagger \vec{\sigma} c_i \right) \cdot \left(\frac{1}{2} c_j^\dagger \vec{\sigma} c_j \right)$$

$$d = \langle \hat{d} \rangle = 1/N \sum_{\vec{k}} (\cos k_x - \cos k_y) \langle c_{\vec{k},\uparrow}^\dagger c_{-\vec{k},\downarrow} \rangle$$

$$H_{MF} = \sum_{\vec{k},\sigma} \varepsilon(\vec{k}) c_{\vec{k},\sigma}^\dagger c_{\vec{k},\sigma} - 4Jm\hat{m} - Jd(\hat{d} + \hat{d}^\dagger) + F_0$$

Pitaevskii Brückner:

Pair state orthogonal to repulsive core of Coulomb interaction

P.W. Anderson Science
317, 1705 (2007)

Miyake, Schmitt–Rink, and Varma
P.R. B 34, 6554-6556 (1986)

More sophisticated Slave Boson: Kotliar Liu PRB 1988

d-wave in mean-field

$$\hat{\mathcal{H}}_{modèle t-J} = -t \sum_{\langle i,j \rangle \sigma} \hat{P} \left(\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + c.h \right) \hat{P} + J \sum_{\langle i,j \rangle} \left(\hat{\vec{S}}_i \cdot \hat{\vec{S}}_j - \frac{1}{4} \hat{n}_i \hat{n}_j \right)$$

$$\begin{aligned} J \hat{S}_i^z \hat{S}_j^z &= J(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})(\hat{n}_{j\uparrow} - \hat{n}_{j\downarrow}) \\ &= J(\hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} - \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow})(\hat{c}_{j\uparrow}^\dagger \hat{c}_{j\uparrow} - \hat{c}_{j\downarrow}^\dagger \hat{c}_{j\downarrow}) \\ &= -J(\hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow} \hat{c}_{j\uparrow}^\dagger \hat{c}_{j\uparrow} + \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} \hat{c}_{j\downarrow}^\dagger \hat{c}_{j\downarrow}) + \dots \\ &= -J(\hat{c}_{j\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow} \hat{c}_{j\uparrow} + \hat{c}_{i\uparrow}^\dagger \hat{c}_{j\downarrow}^\dagger \hat{c}_{j\downarrow} \hat{c}_{i\uparrow}) + \dots \end{aligned}$$

Hartree-Fock :

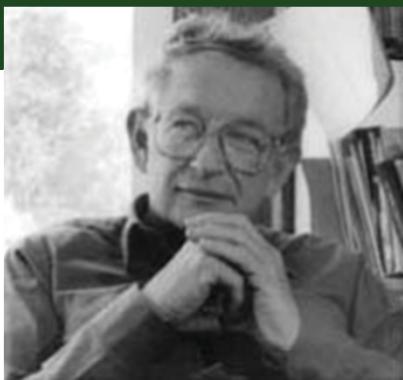
$$d^* = \langle \hat{c}_{j\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \rangle_{\mathcal{H}_{modèle t-J}}$$

$$\langle J \hat{S}_i^z \hat{S}_j^z \rangle = -2J d^* d + \dots$$

Miyake, Schmitt-Rink et Varma, PRB 34, 6554-6556 (1986)

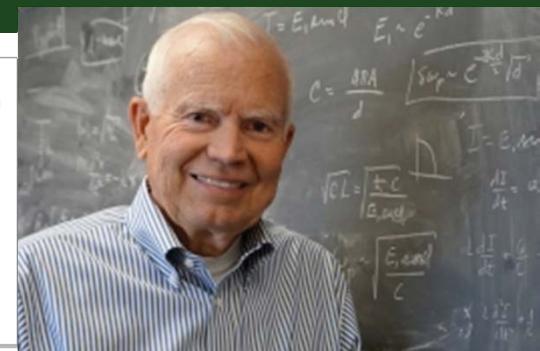
Anderson, Baskaran, Zou et Hsu, PRL 58, 26 (1987)

P.W. Anderson



Raising the question

D.J. Scalapino



Is There Glue in Cuprate Superconductors?

Philip W. Anderson

Science 316, 1705 (2007);

DOI: 10.1126/science.1140970

Is There Glue in Cuprate Superconductors?

Philip W. Anderson

Many theories about electron pairing in cuprate superconductors may be on the wrong track.

Science e-letter, 5 and 10 Dec. 2007

Retardation

$$V_{el-ph}^{eff}(\vec{q}, \omega) = \frac{e^2}{4\pi\epsilon_0(q^2 + k_{TF}^2)} \left[1 + \frac{\omega_{ph}^2(\vec{q})}{\omega^2 - \omega_{ph}^2(\vec{q})} \right]$$



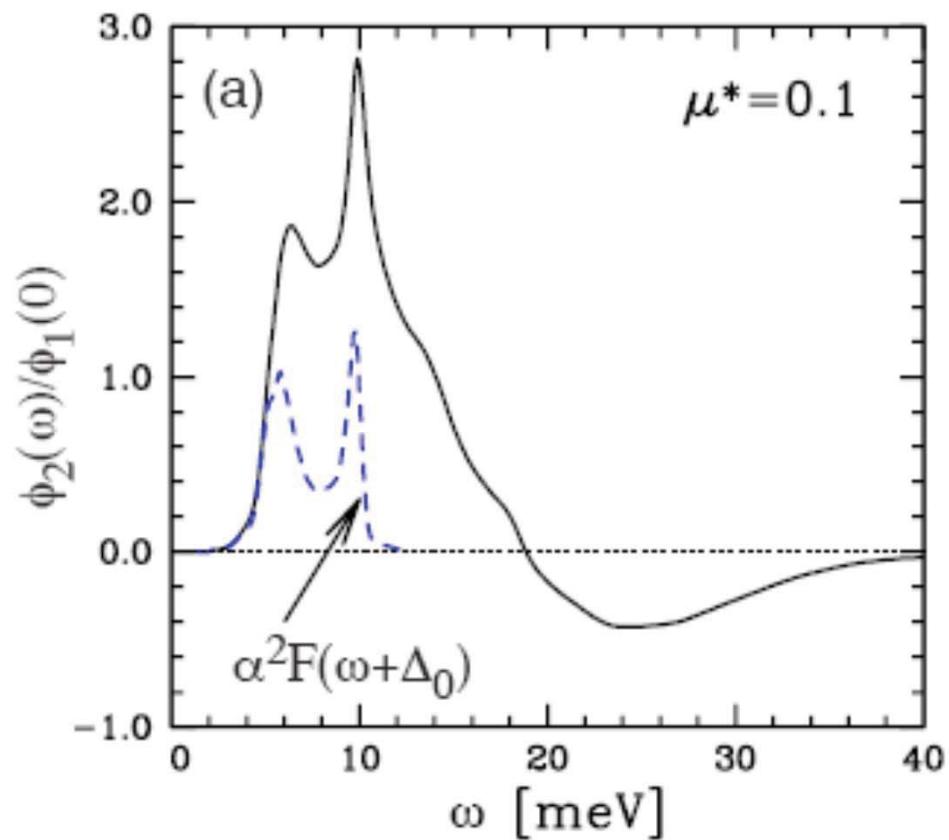
"We have a mammoth and an elephant in our refrigerator—do we care much if there is also a mouse?"



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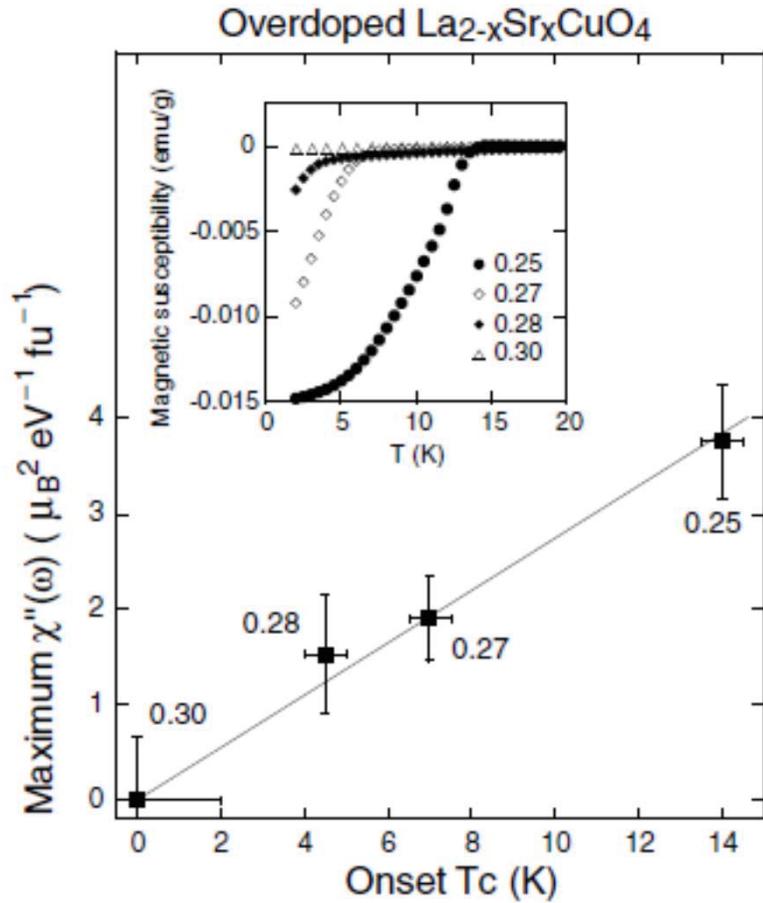
$\text{Im } \Sigma_{\text{an}}$ and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

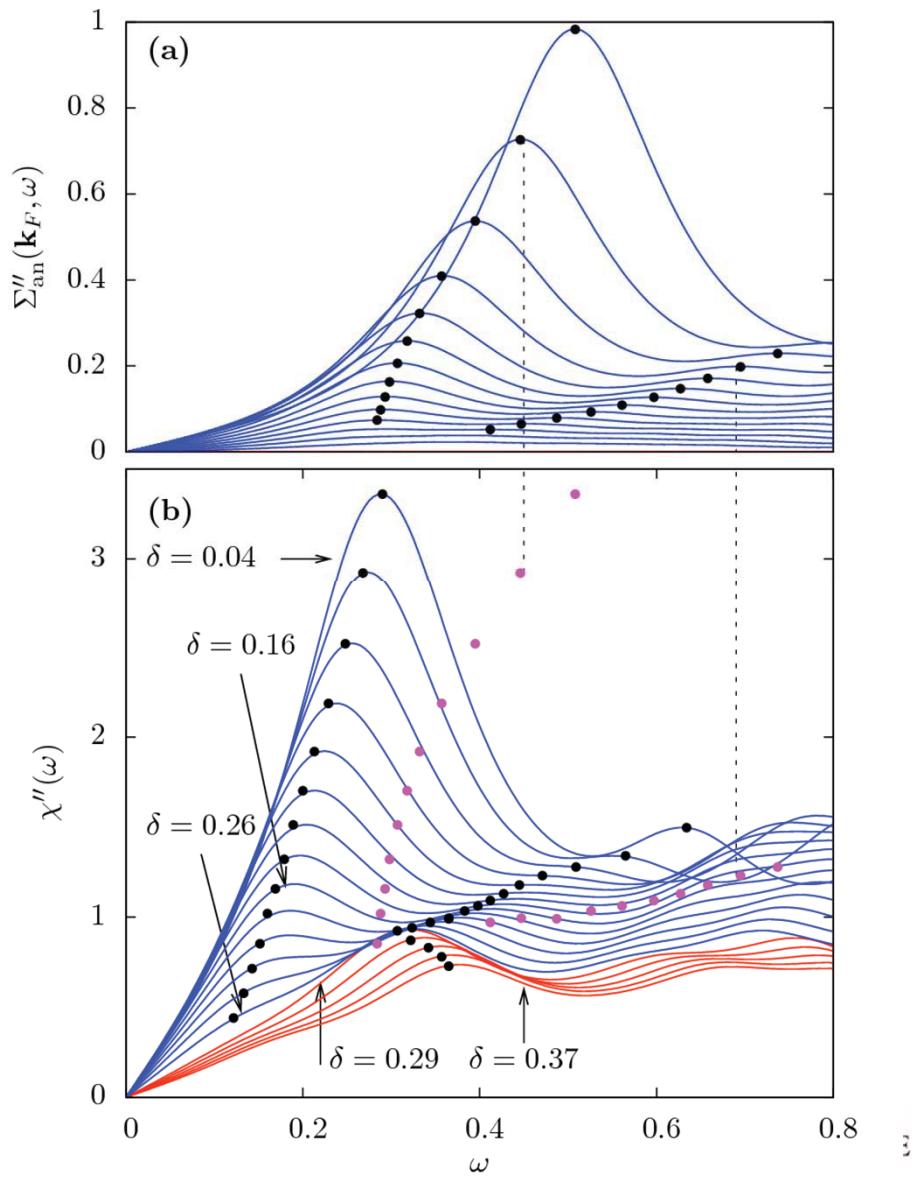


The glue

Kyung, Sénéchal, Tremblay, Phys. Rev. B
80, 205109 (2009)



Wakimoto ... Birgeneau
PRL (2004)



The glue and neutrons

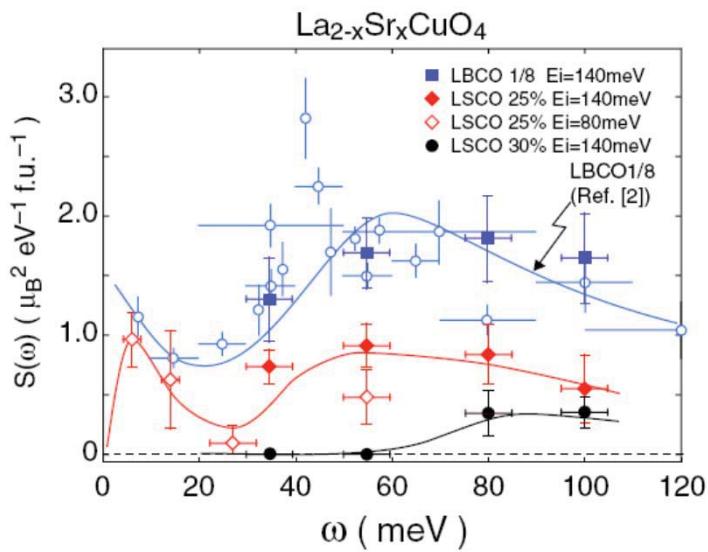
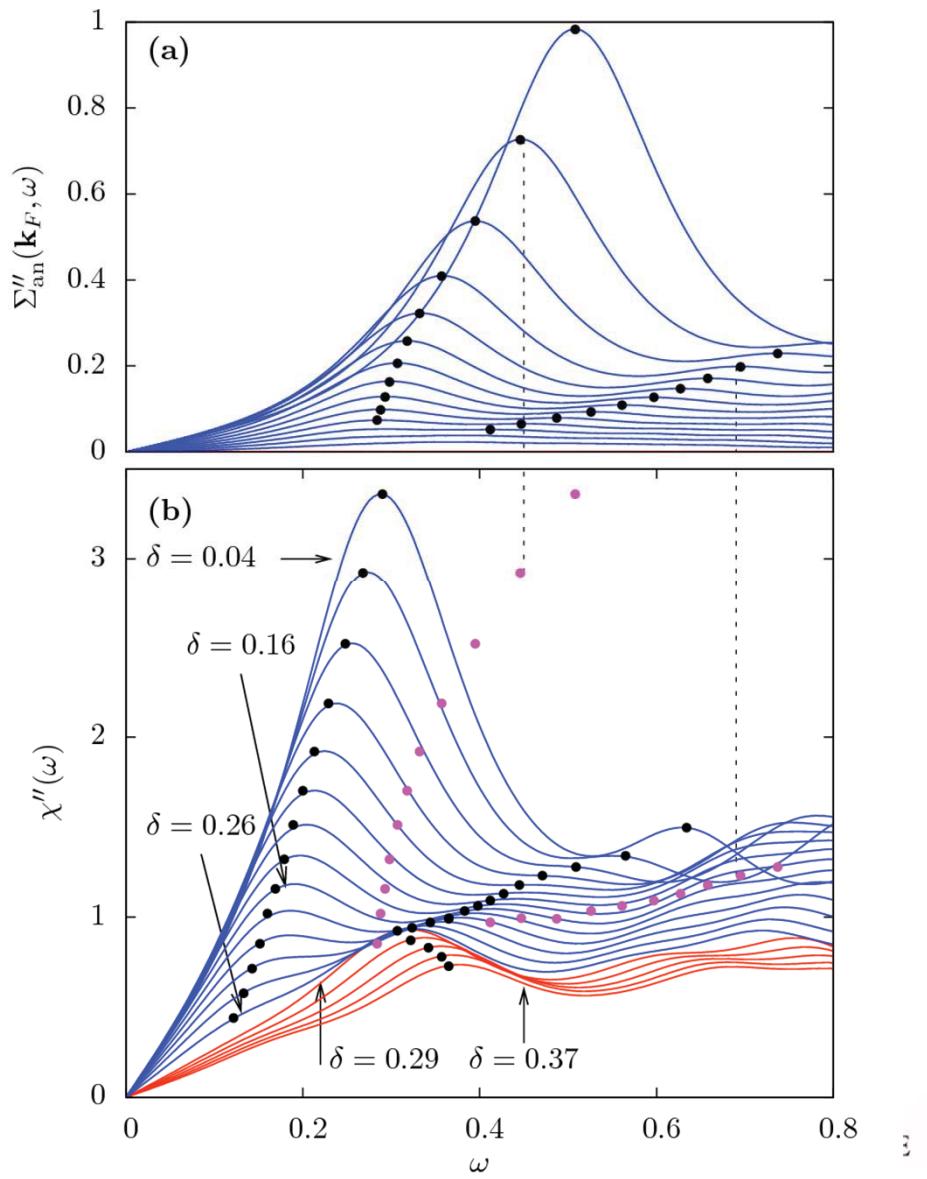


FIG. 3 (color online). \mathbf{Q} -integrated dynamic structure factor $S(\omega)$ which is derived from the wide- H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i = 140$ meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO 1/8 (open circles) from [2]. The solid lines following data of LSCO $x = 0.25$ and 0.30 are guides to the eyes.

Wakimoto ... Birgeneau PRL (2007);
PRL (2004)



The glue in CDMFT and DCA

Th. Maier, D. Poilblanc, D.J. Scalapino, PRL (2008)

M. Civelli, PRL **103**, 136402 (2009)

M. Civelli PRB **79**, 195113 (2009)

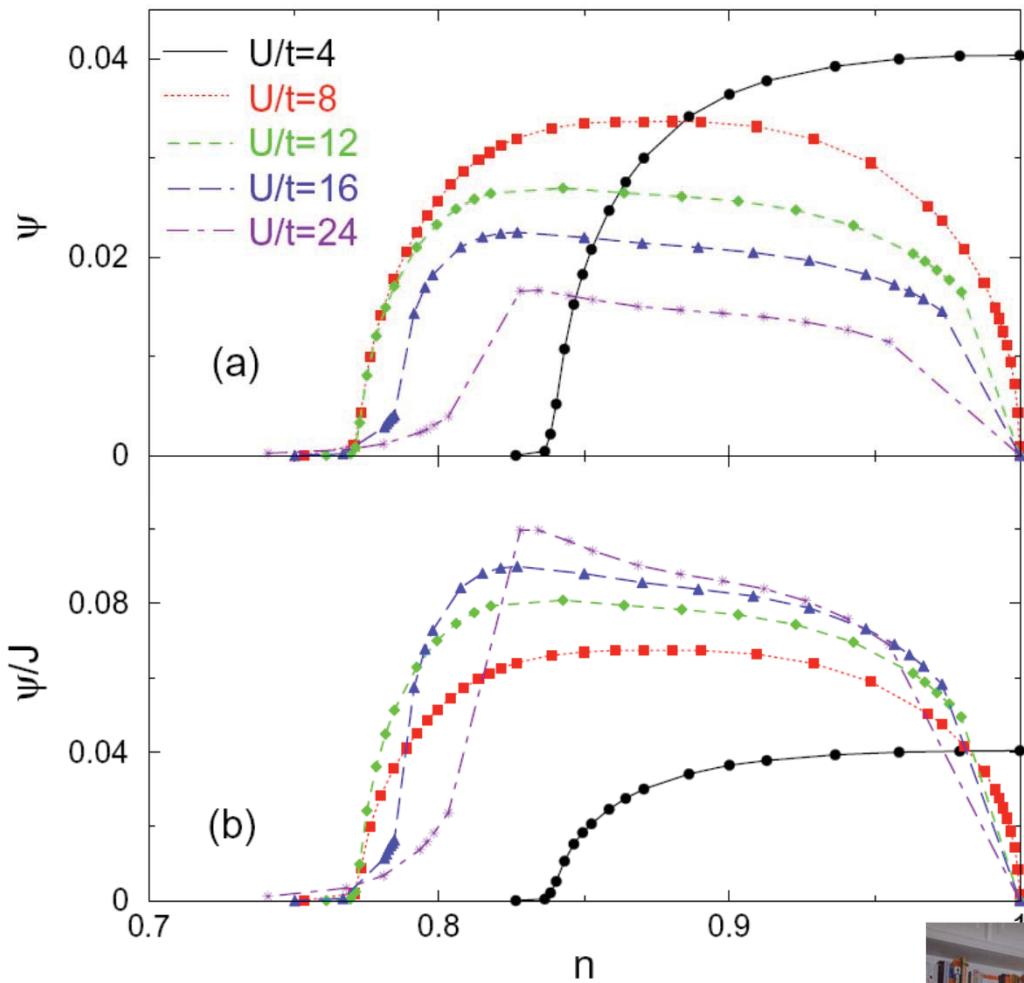
E. Gull, A. J. Millis PRB 90, 041110(R) (2014)

S. Sakai, M. Civelli, M. Imada arXiv:1411.4365

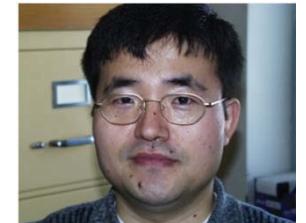


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Dome vs Mott (CDMFT)

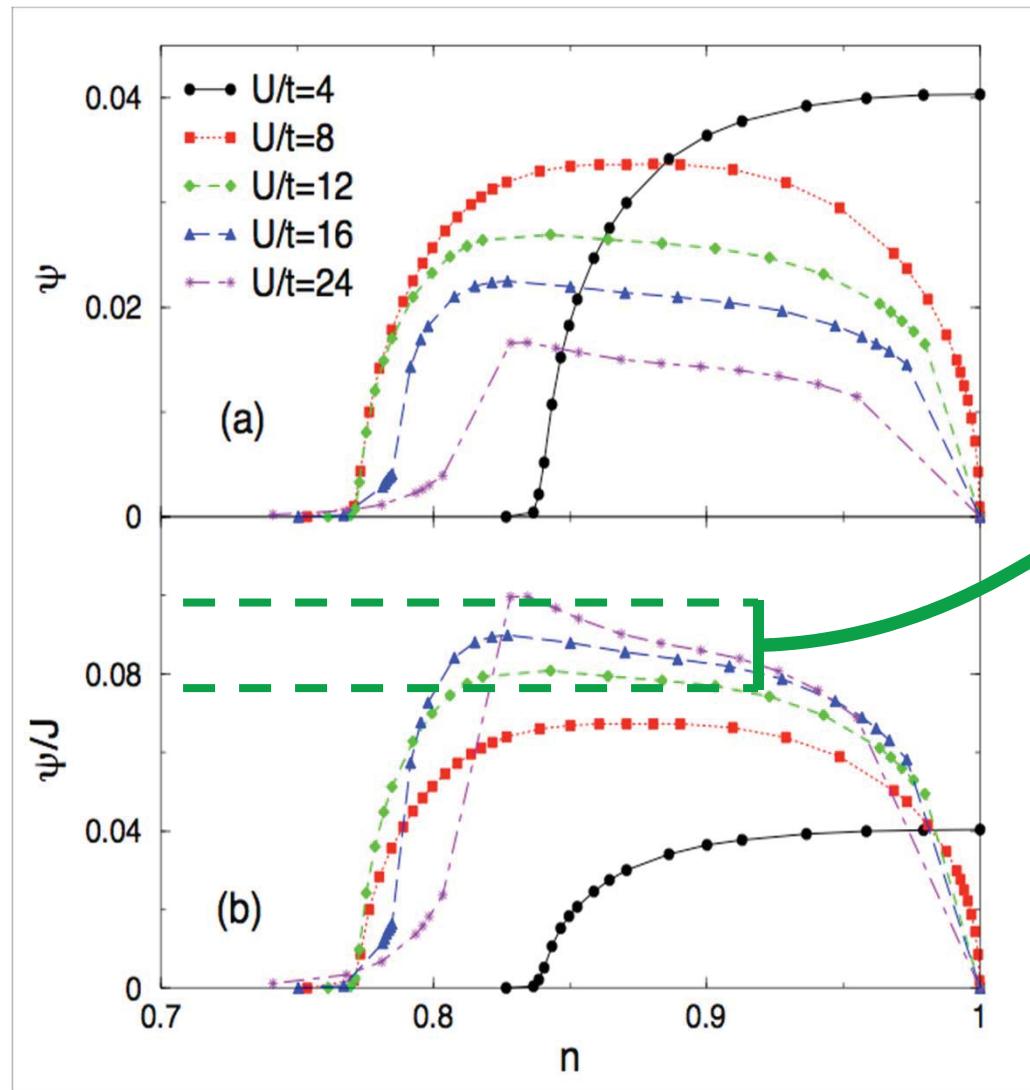


Kancharla, Kyung, Civelli,
Sénéchal, Kotliar AMST
Phys. Rev. B (2008)



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Strength of pairing: cuprates



$$J = \frac{4t^2}{U}$$

The
superconducting
order parameter
scales like J





Frequencies important for pairing



Bumsoo Kyung

Anomalous Green function

$$[\mathcal{F}_{an}(t)]_{lm} = -i\theta(t) \langle \{\hat{c}_{l\uparrow}(t), \hat{c}_{m\downarrow}(0)\} \rangle_{\mathcal{H}_{AIM}}$$

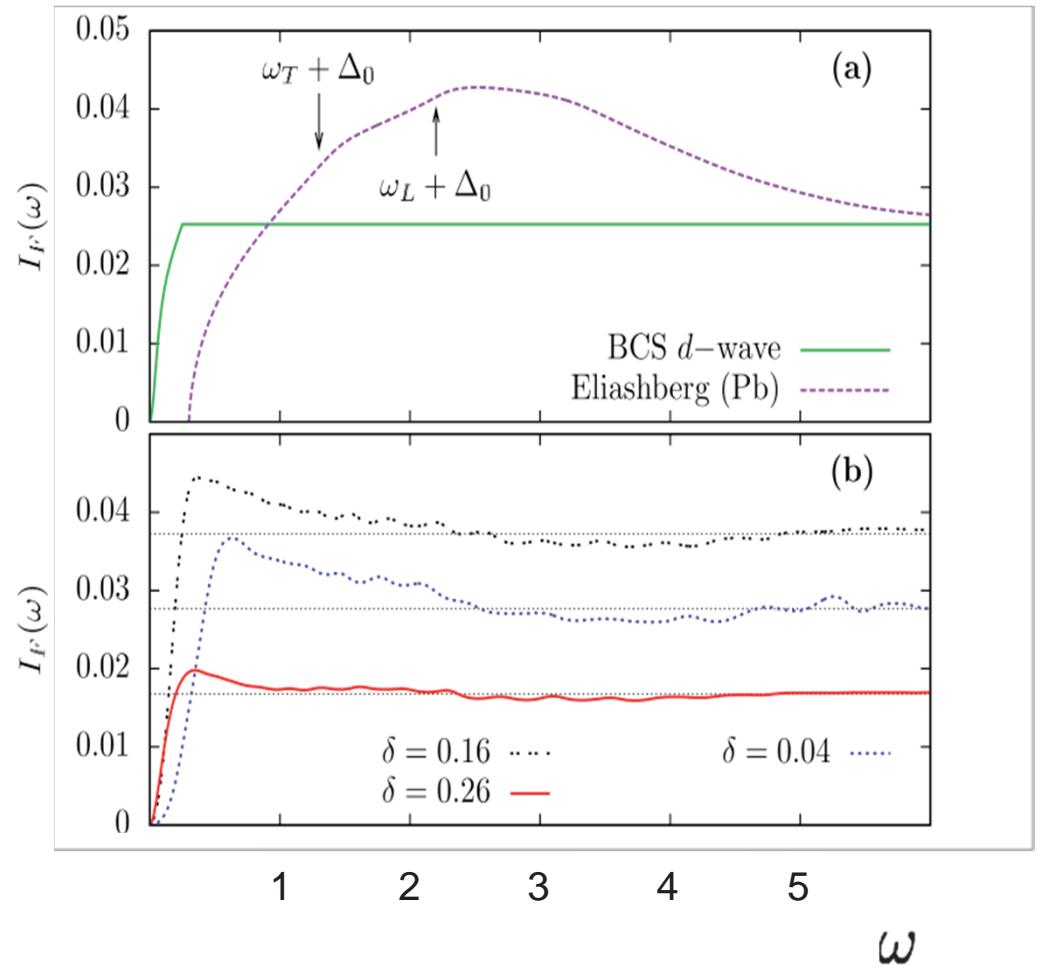
Anomalous spectral function

$$[\mathcal{A}_{an}(\omega)]_{lm} = -\frac{1}{\pi} \text{Im} [\mathcal{F}_{an}(\omega)]_{lm}$$

Cumulative order parameter:

$$I_{\mathcal{F}}(\omega) = - \int_0^{\omega} \frac{d\omega'}{\pi} \text{Im} [\mathcal{F}_{an}(\omega')]_{lm}$$

$$I_{\mathcal{F}}(\omega) \xrightarrow{\omega \rightarrow +\infty} \langle \hat{c}_{l\uparrow} \hat{c}_{m\downarrow} \rangle_{\mathcal{H}_{AIM}}$$



Scalapino, Schrieffer, Wilkins,
Phys. Rev. **148** (1966)



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Resilience to near-neighbor repulsion V (Scalapino)

$$\hat{\mathcal{H}}_{Hubbard} = - \sum_{\langle i,j \rangle_{1,2,3}} \left(t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + c.h \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + V \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j - \mu \sum_{i\sigma} \hat{n}_{i\sigma}$$

YBa₂Cu₃O₇ : $t = 1$ $t' = -0.3$ $t'' = 0.2$

We expect superconductivity to disappear when:

$V > \frac{U^2}{W}$ **In weakly correlated case**
 $U/W < 1$

$V > J$ **In mean-field strongly correlated case**

In cuprates:

$$V = 400 \text{ meV}$$

$$J = 130 \text{ meV}$$

$$U_c = V_c / [1 + N(0)V_c \ln(E_F/\omega_c)] \quad \text{Anderson-Morel}$$

S. Onari, R. Arita, K. Kuroki et H. Aoki, PRB **70**, 094523 (2004)

S. Raghu, E. Berg, A. V. Chubukov et S. A. Kivelson, PRB **85**, 024516 (2012)

S. Sorella, et al. Phys. Rev. Lett. **88**, 117002 (2002)

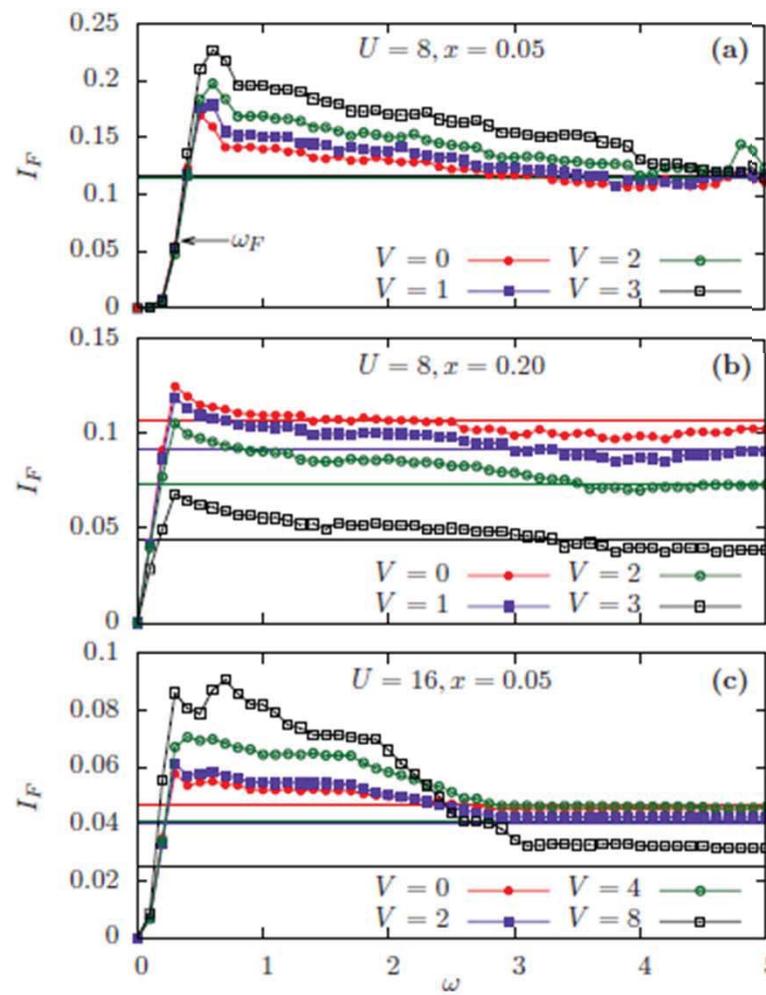
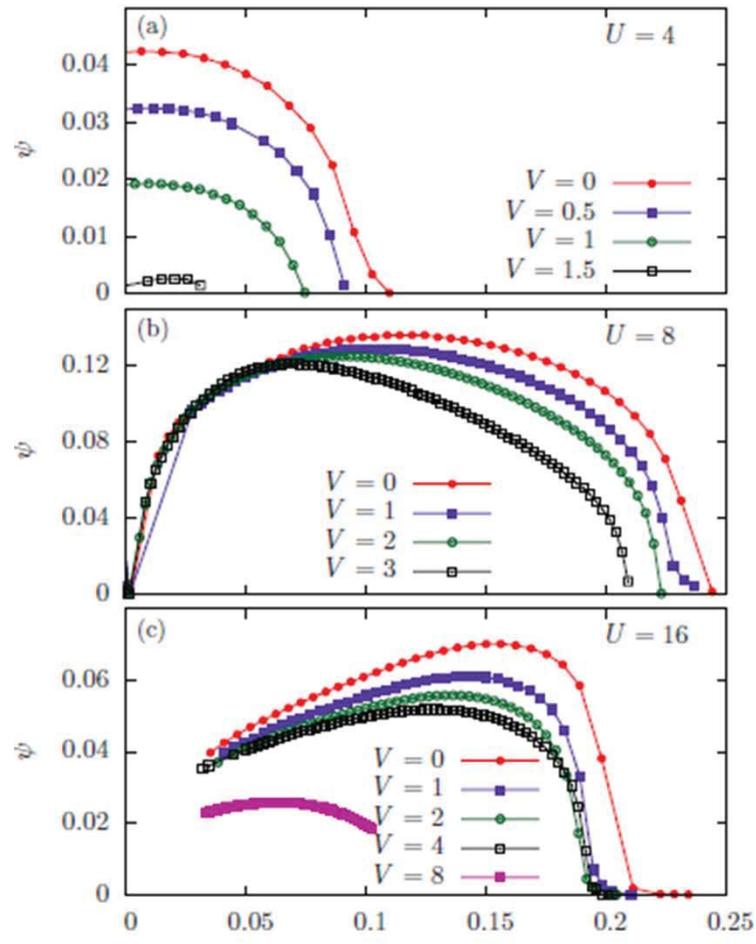


Resilience to near-neighbor repulsion



David Sénéchal

Alexandre Day



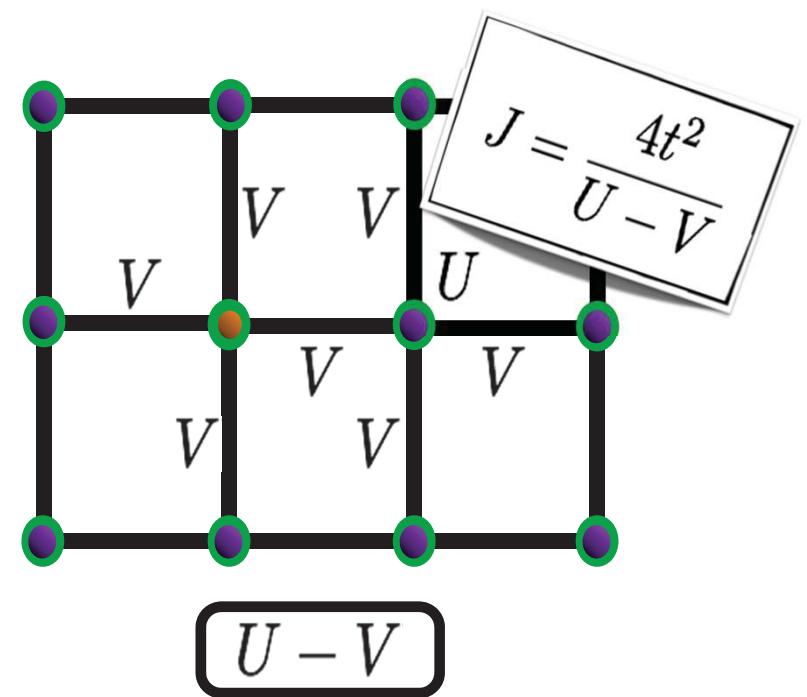
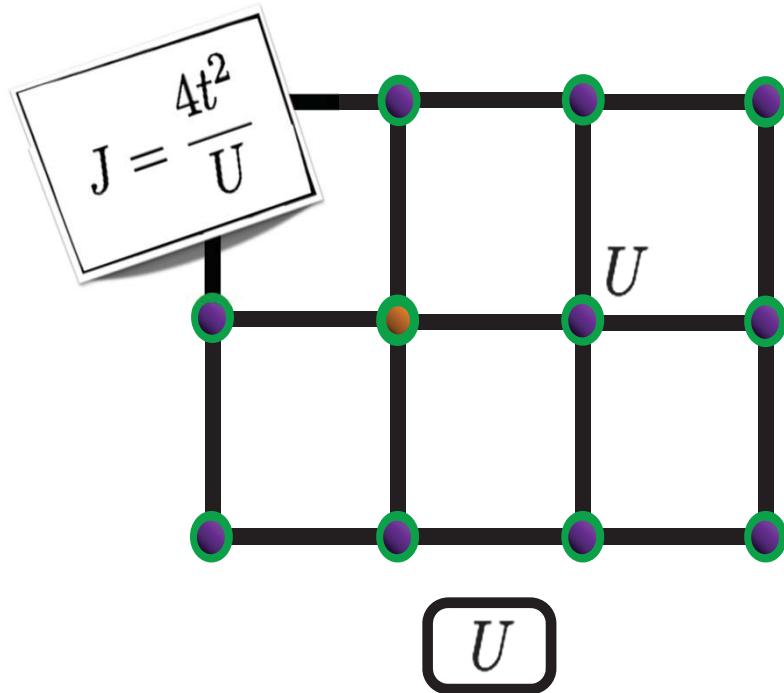
Vincent Bouliane

Sénéchal, Day, Bouliane, AMST PRB ^x 87, 075123 (2013)



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V also increases J



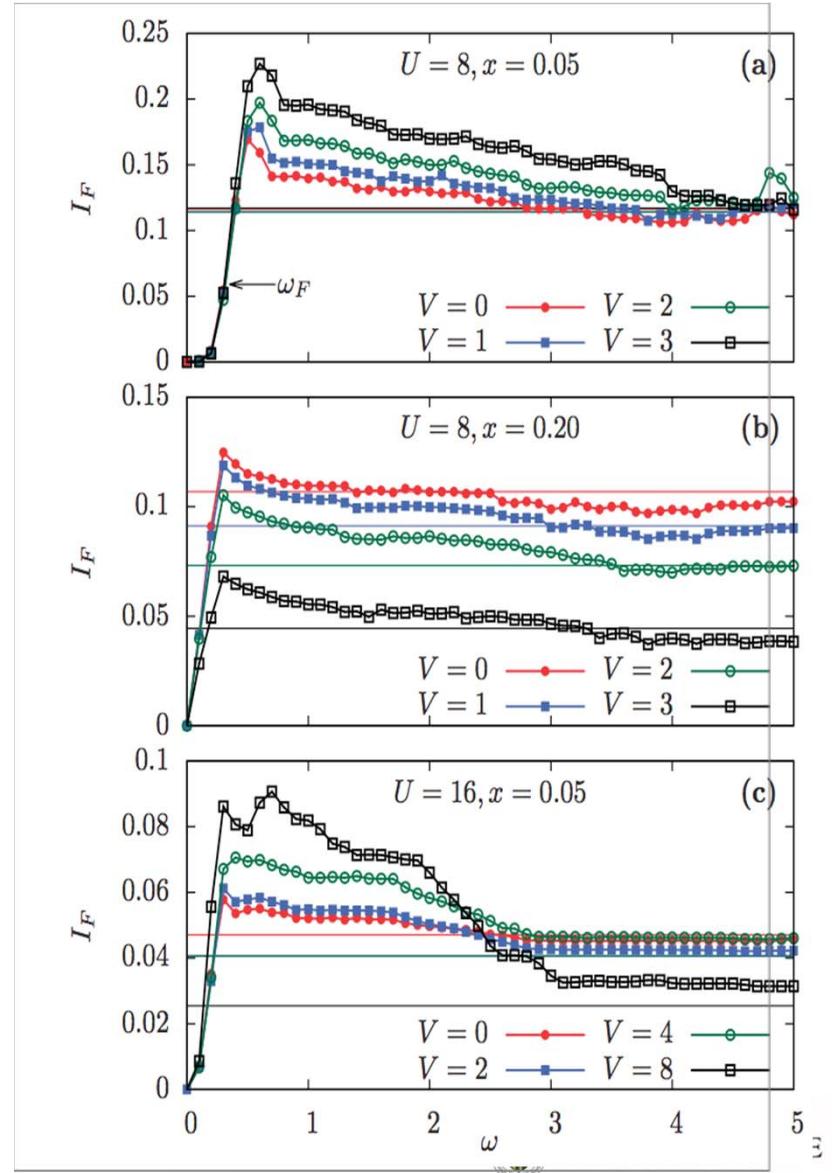
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Binding aspects of V

$$J = \frac{4t^2}{U - V}$$

**J increases with V
explaining better pairing at
low frequency**

**But V also induces more
repulsion at high frequency,
explaining the negative
impact at high frequency on
binding**



Two gaps in underdoped regime of cuprates

Le Tacon *et al.* Nature Physics 2, 537 - 543 (2006)

....

Sakai et al. PRL 111, 107001 (2013)



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David Sénéchal

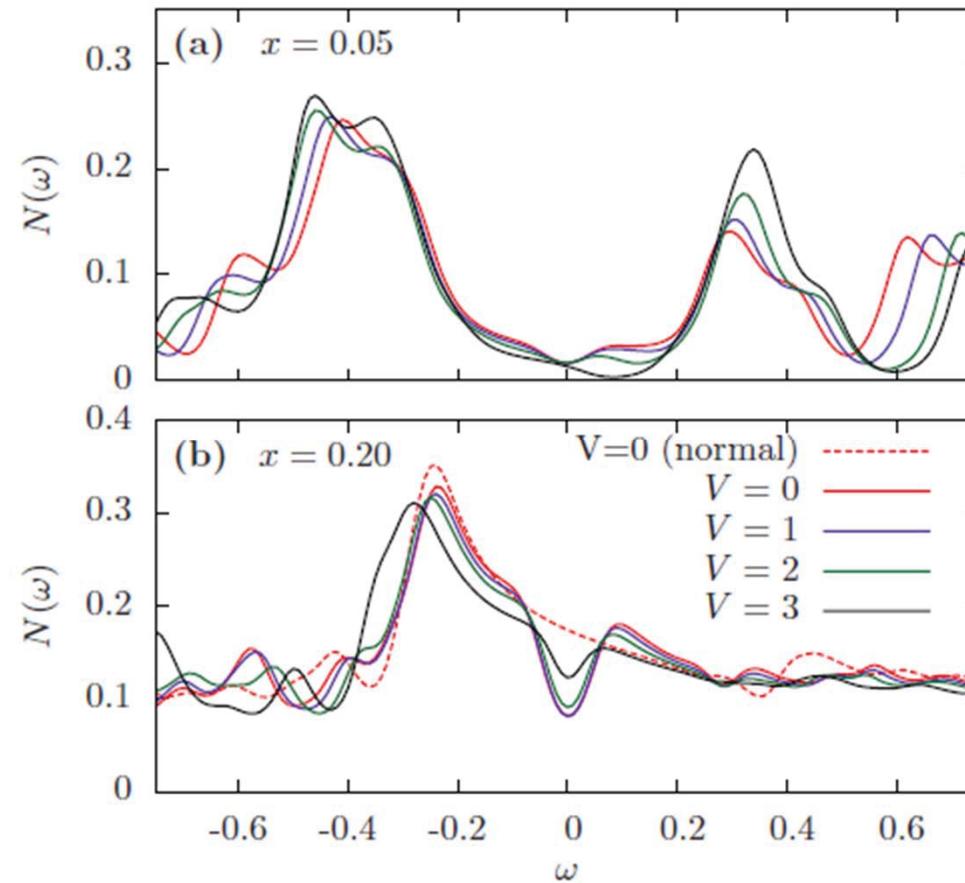


Alexandre Day



Vincent Bouliane

$$U = 8t$$

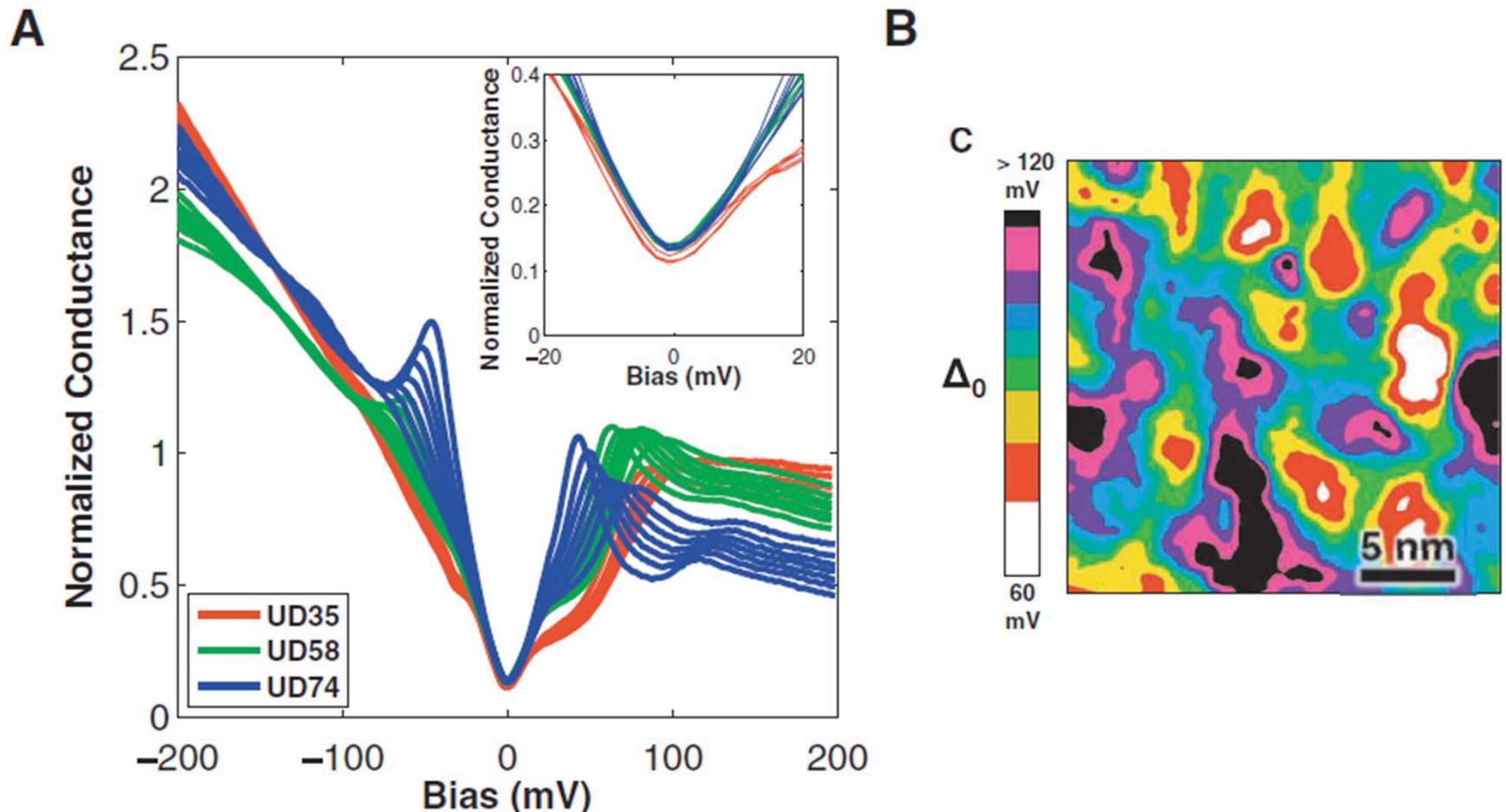


Sénéchal, Day, Bouliane, AMST PRB **87**, 075123 (2013)



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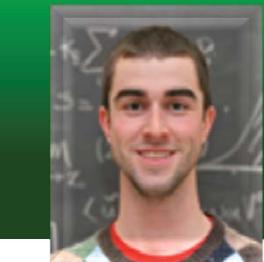
Superconducting gap in STM



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



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Simon Verret

Experiment vs Theory, STM



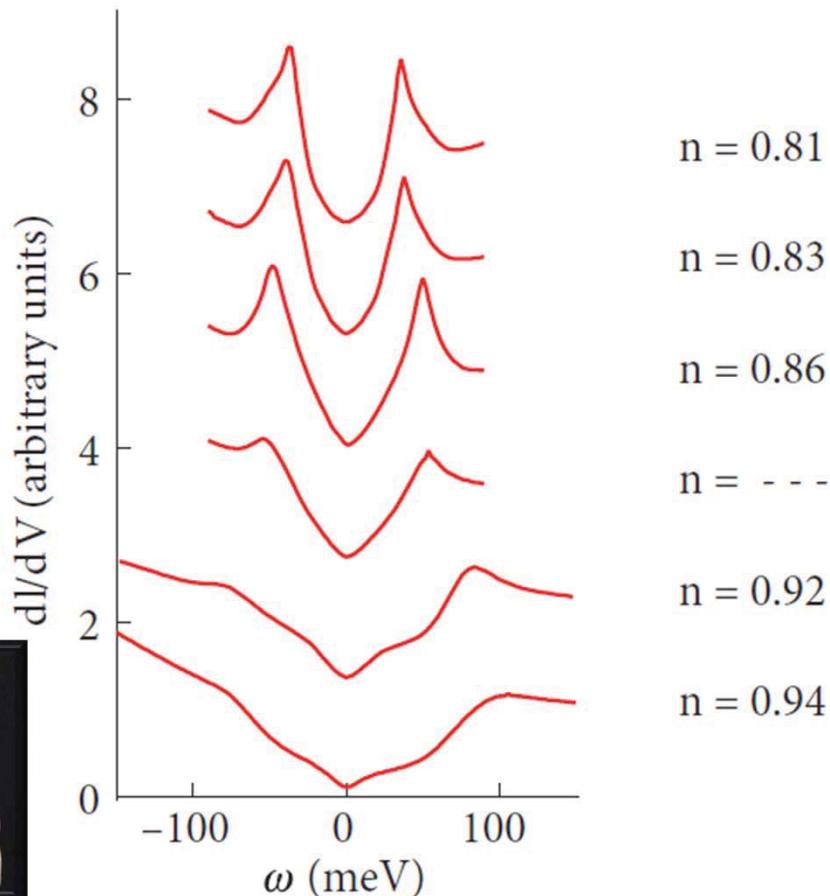
Jyotirmoy Roy

STM data

Kohsaka *et al.*, Nature **454** 1072 (2008)

CDMFT

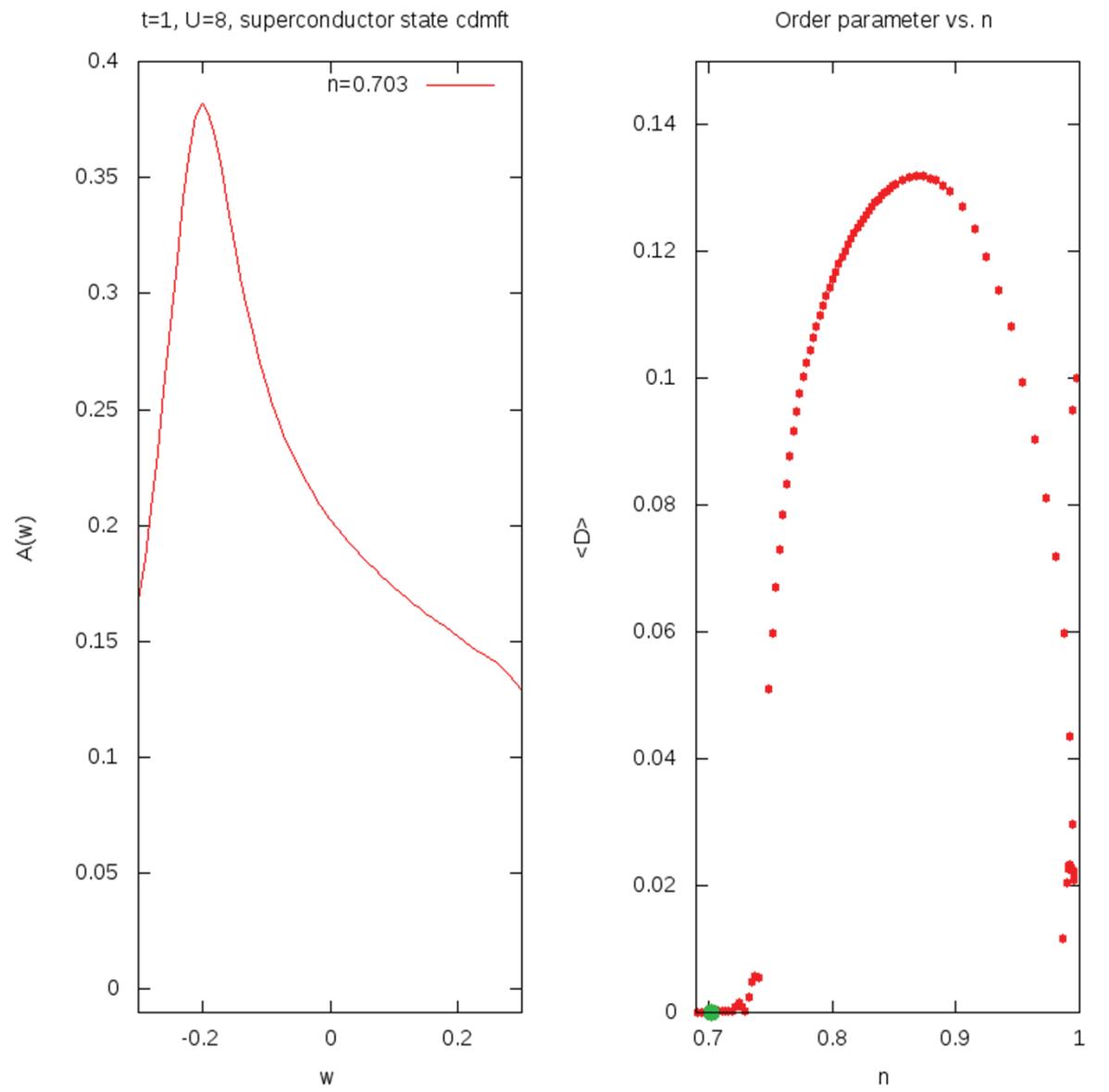
Unpublished



David Sénéchal

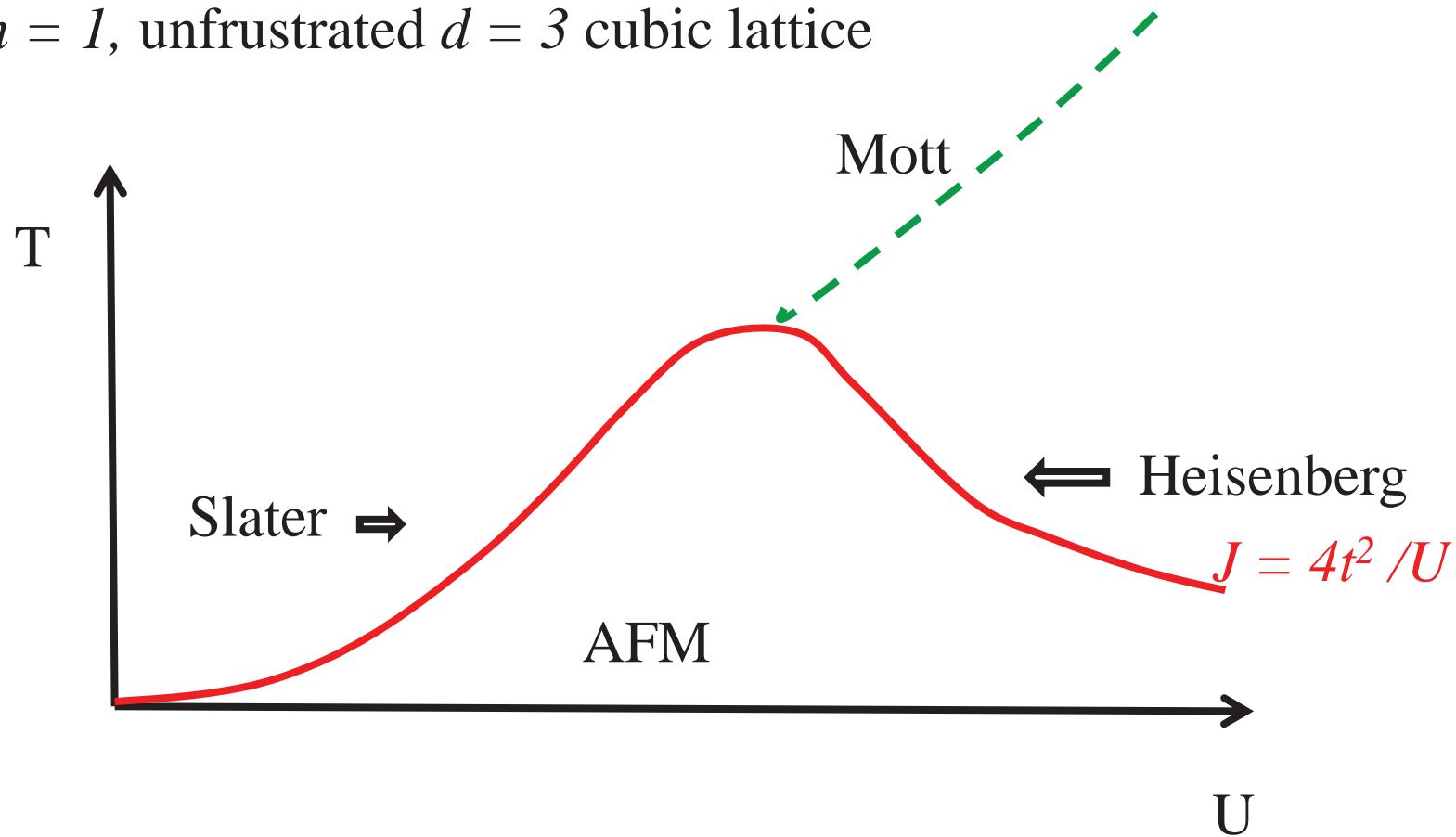
Evolution of SC gap and pseudogap with n

$t' = -0.3 t$
 $t'' = 0.2 t$
 $U=8t$



Local moment and Mott transition

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



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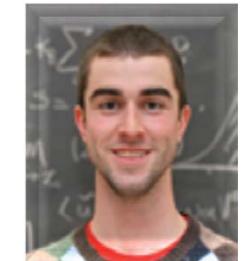
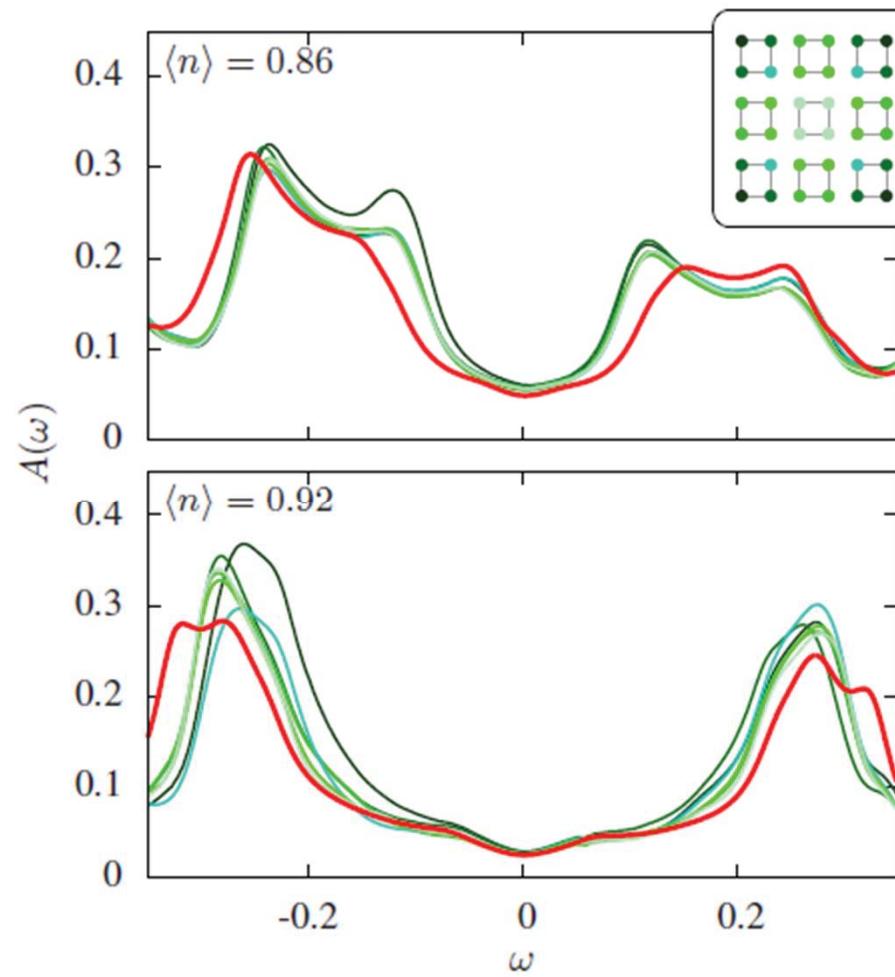
Effect of disorder



Alexandre Prémont
Foley



David Sénéchal



Simon Verret

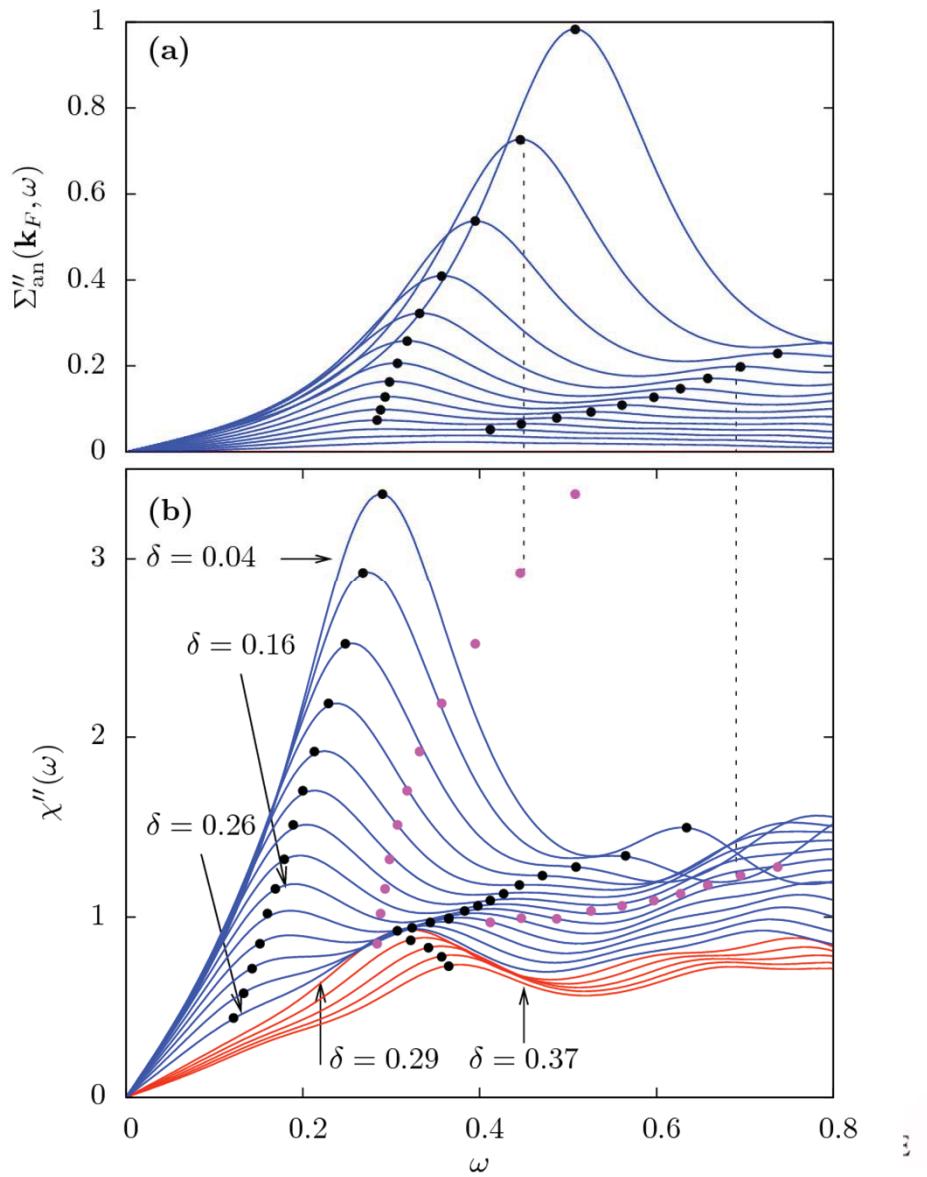
unpublished



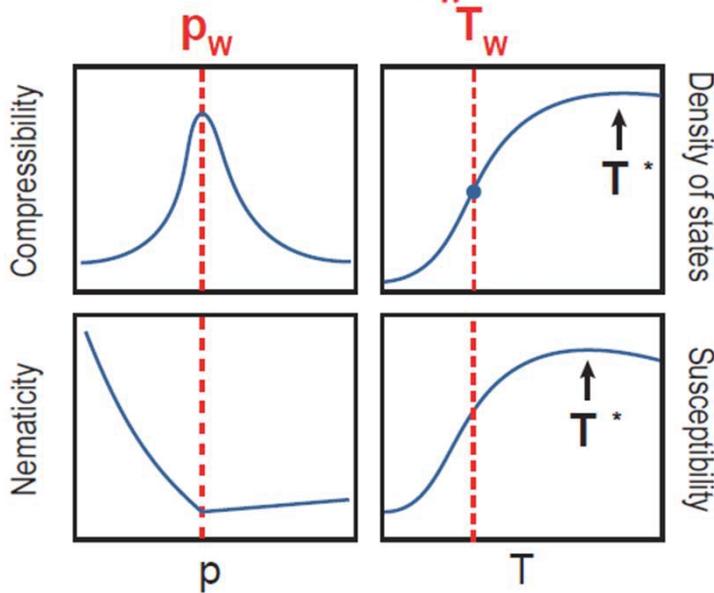
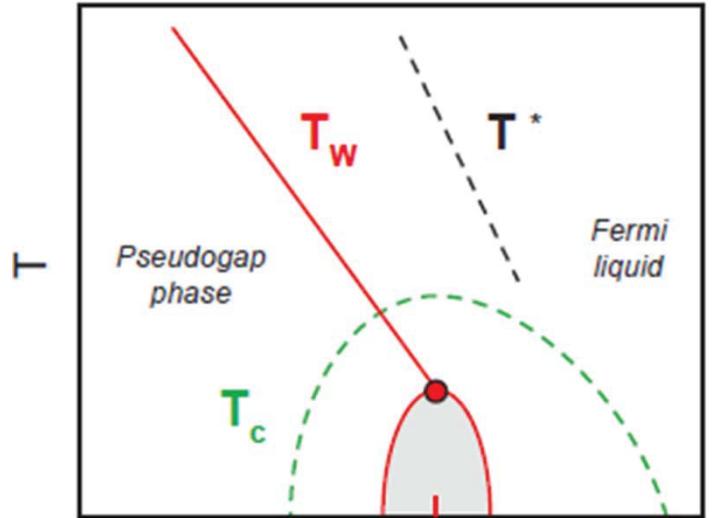
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Summary

- There is retardation
- Strongly and weakly correlated SC differ
 - Penetration depth
 - Resilience to V



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 a dome of SC ?
- Why superconducting ?
- Does a one-band model capture the key physics ?
- AFM QCP important?
- Lessons from other SC?



Main collaborators



Giovanni Sordi



Kristjan Haule



David Sénéchal



Bumsoo Kyung



Alexandre Day



Vincent Bouliane



Patrick Sémon



Lorenzo Fratino



Simon Verret



Jyotirmoy Roy



Gabriel Kotliar



Marcello Civelli

Sarma Kancharla Massimo Capone



GABRIEL KOTLIAR
UNIVERSITÉ DE SHERBROOKE



A.-M.S. Tremblay

“Strongly correlated superconductivity”

Chapt. 10 : *Emergent Phenomena in Correlated Matter Modeling and Simulation*, Vol. 3, E. Pavarini, E. Koch, and U. Schollwöck (eds.)

Verlag des Forschungszentrum Jülich, 2013