Superconductivity in Doped Mott Insulators: A Dynamical Mean Field Perspective

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A. Foley, Charles-David Hébert, A. Reymbaut, D. Sénéchal
O. Simard, G. Sordi, Patrick Sémon, M. Thénault

M2S Beijing, 23 August 2018
Th-S50 Mott Physics-2
Room 6, 14h00-15h55

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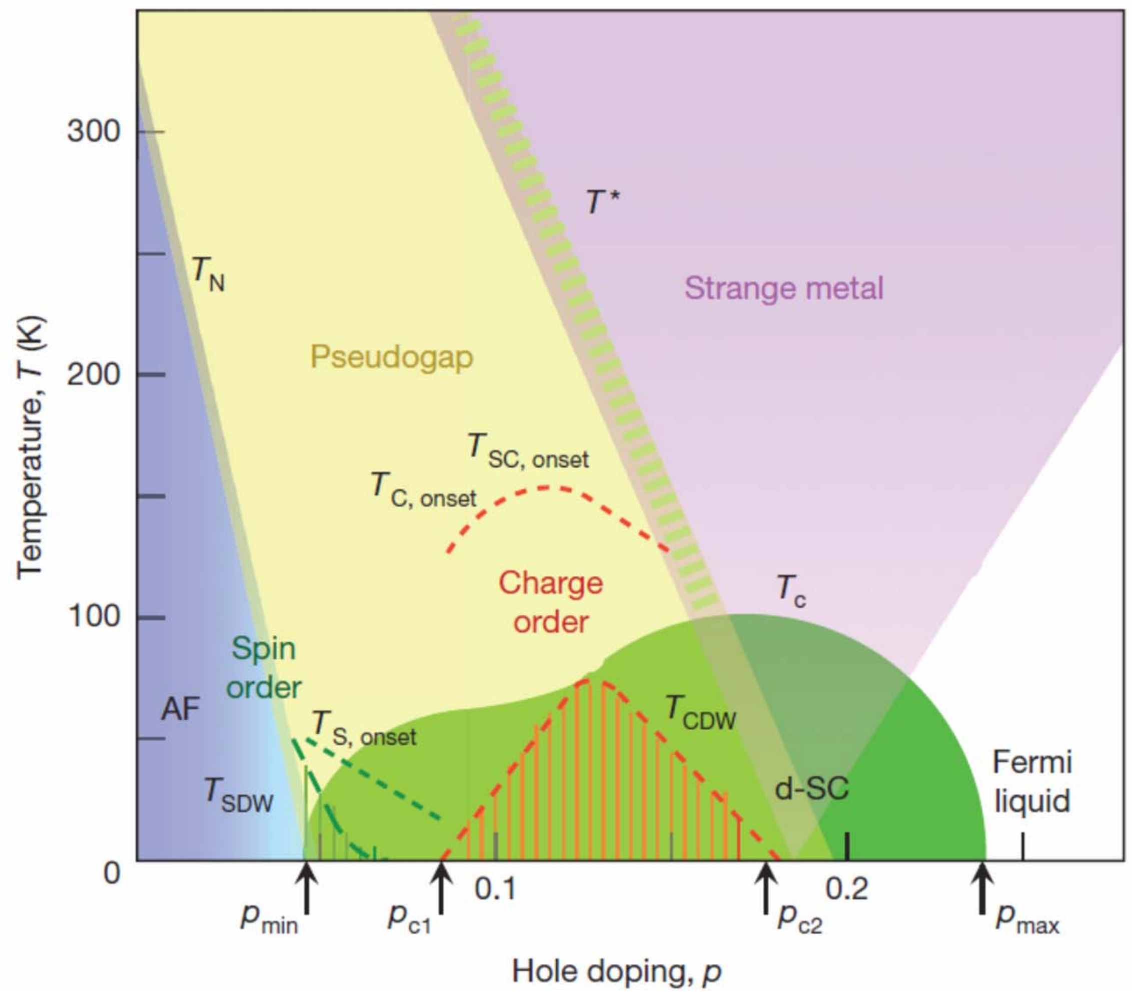
Phase diagram $YBa_2Cu_3O_{7-x}$



p or δ

Keimer et al., Nature 518, 179 (2015)

Model

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APOGÉE CANADA
FONDS D'EXCELLENCE EN RECHERCHE

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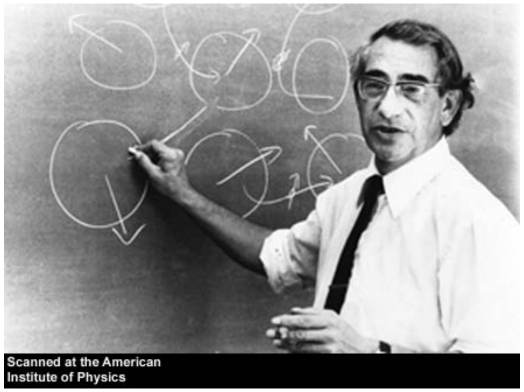
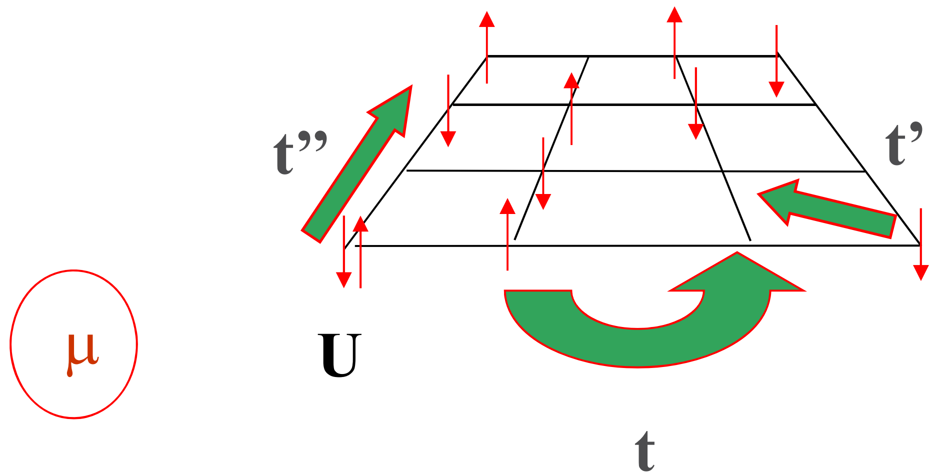
Hubbard Model



1931-1980



$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

$$t = 1,\ k_B = 1,\ \hbar = 1$$

Attn: Charge transfer insulator

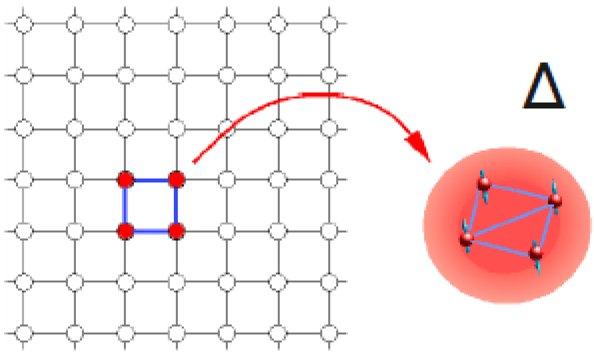
Method

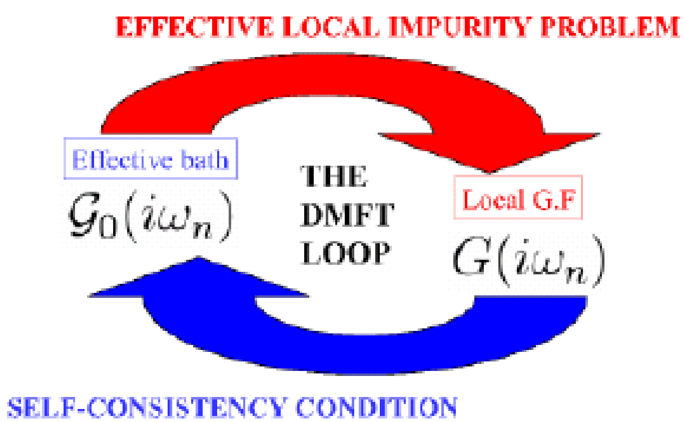
- Dynamical Mean Field Theory
  – clusters
- Concept: atomic-like localized correlations consistent with delocalized aspect

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

Hettler *et al*, PRB 1998
Lichtenstein *et al.*,PRB 2000
Kotliar *et al.*, PRB 2000
M. Potthoff, EJP 2003

Cellular DMFT + CT-QMC





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

+ and -

- Long range order:
  - No mean-field factorization on the cluster
  - Symmetry breaking allowed in the bath (mean-field)
- Included exactly:
  - Short-range dynamical and spatial correlations
- Missing:
  - Long wavelength p-h and p-p fluctuations

Some groups using these methods for cuprates

- Europe:
  - Georges, Parcollet, Ferrero, Civelli, Wu (Paris)
  - Lichtenstein, Potthoff, (Hamburg) Aichhorn (Graz), Liebsch (Jülich) de Medici (Grenoble) Capone (Italy)
- USA:
  - Gull (Michigan) Millis (Columbia)
  - Kotliar, Haule (Rutgers)
  - Jarrell (Louisiana)
  - Maier, Okamoto (Oakridge)
- Japan
  - Imada (Tokyo) Sakai, Tsunetsugu, Motome

Outline

- The model
- The method

- Part I: Half-filling (Mott insulator)
- Part II: The pseudogap (doped Mott insulator)
- Part III: Strongly correlated superconductivity

Part I

Half-filling

Giovanni Sordi

Lorenzo Fratino

Maxime Charlebois

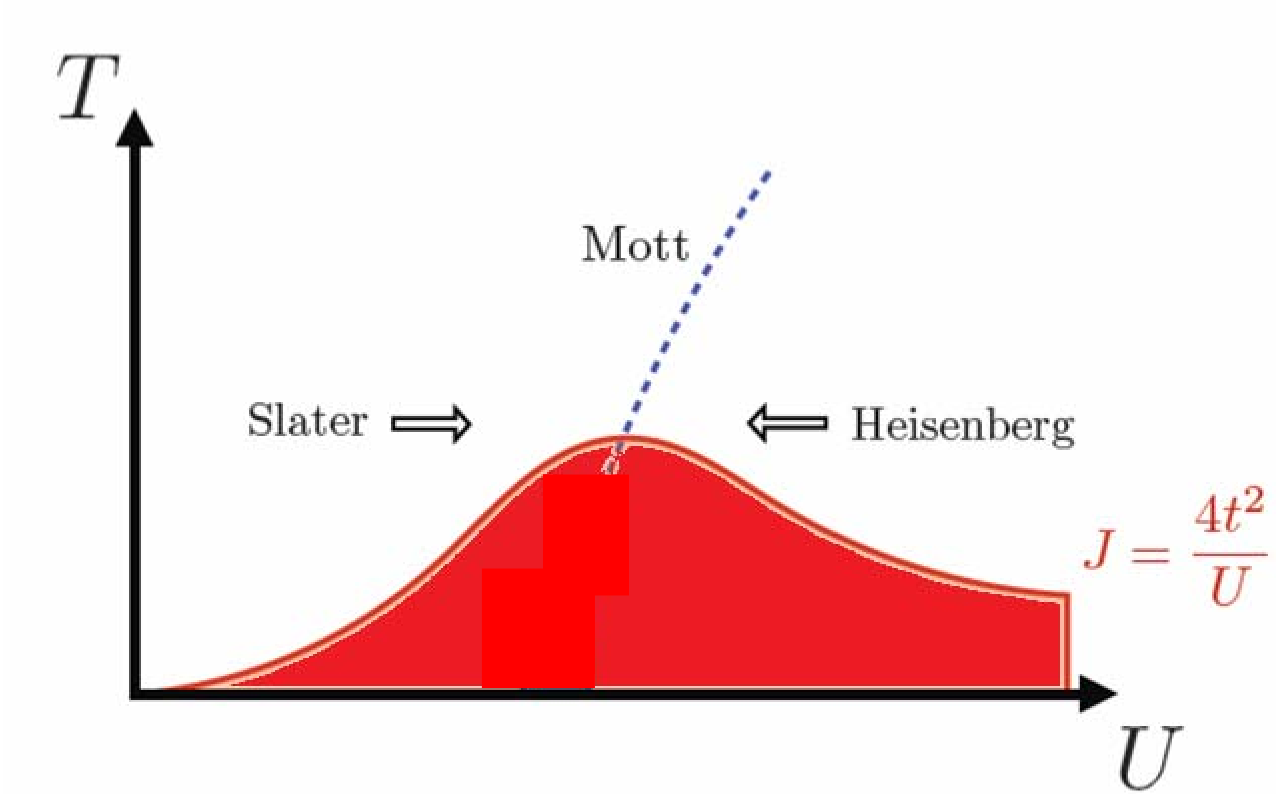
Patrick Sémon

Mott transition and antiferromagnetism

Influence of the underlying normal state
on the ordered state

Underlying Mott transition

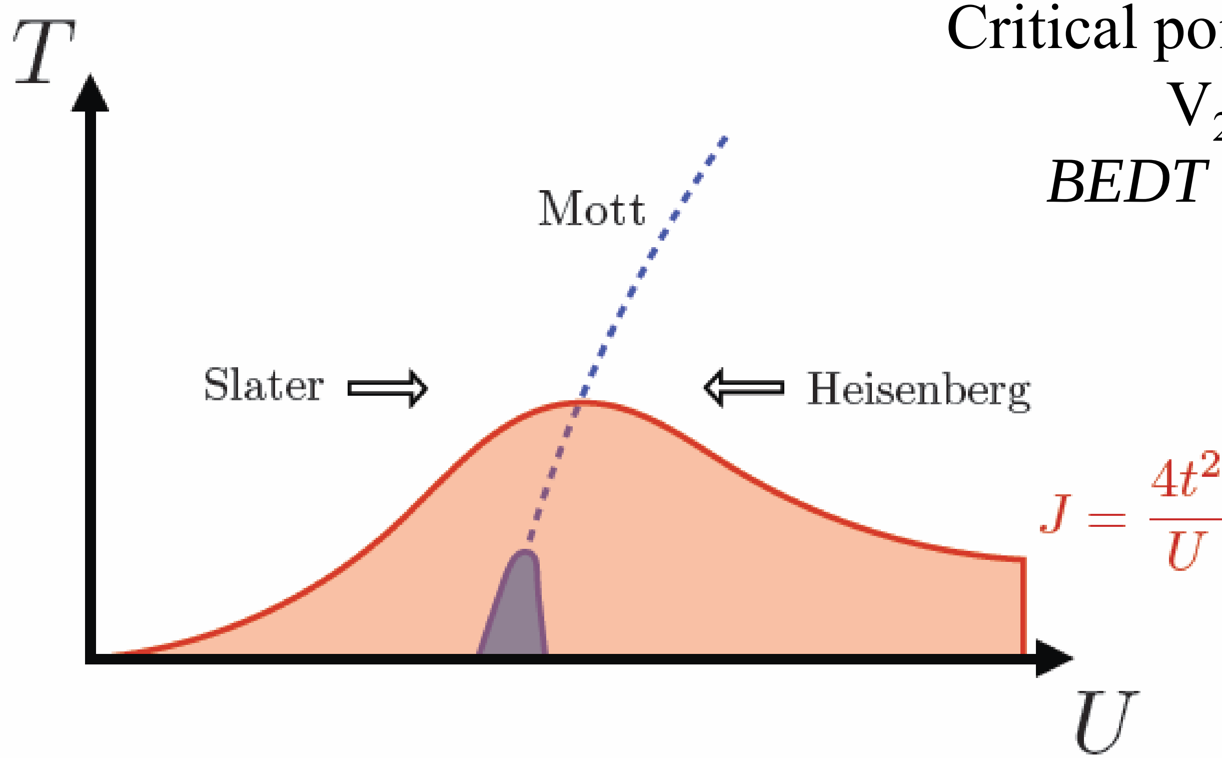
n = 1, d = 2 square lattice



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

Underlying Mott transition

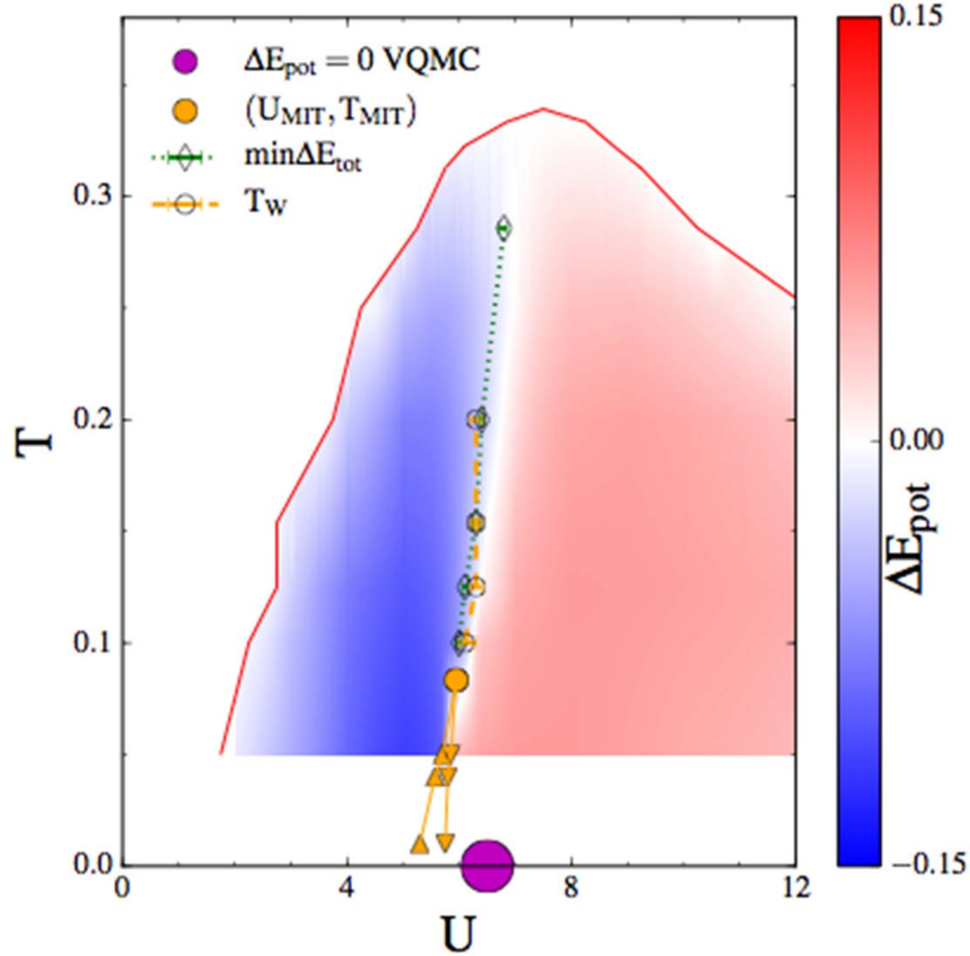
$n = 1$, $d = 2$ square lattice



Critical point visible in
V_2O_3,
BEDT organics

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

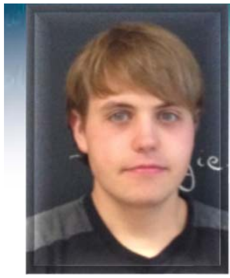
Change in mechanism for stability of the AFM



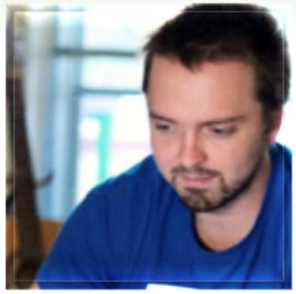
L. F. Tocchio, F. Becca, and S. Sorella, Phys. Rev. B **94**, 195126 (2016).

Part II:

The pseudogap (doped Mott insulator)



Simon Bergeron

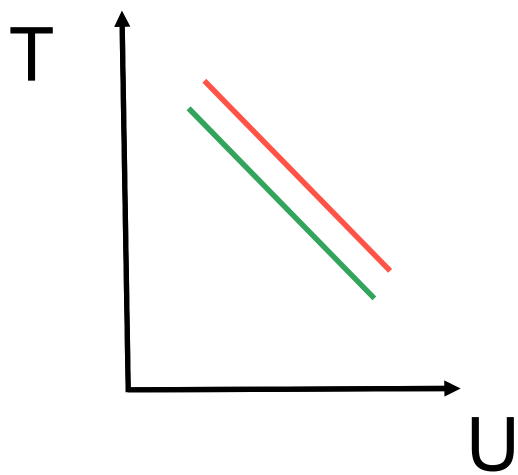


Maxime Charlebois

Patrick Sémon

Alexis Reymbaut

The pseudogap from the calculated Knight shift

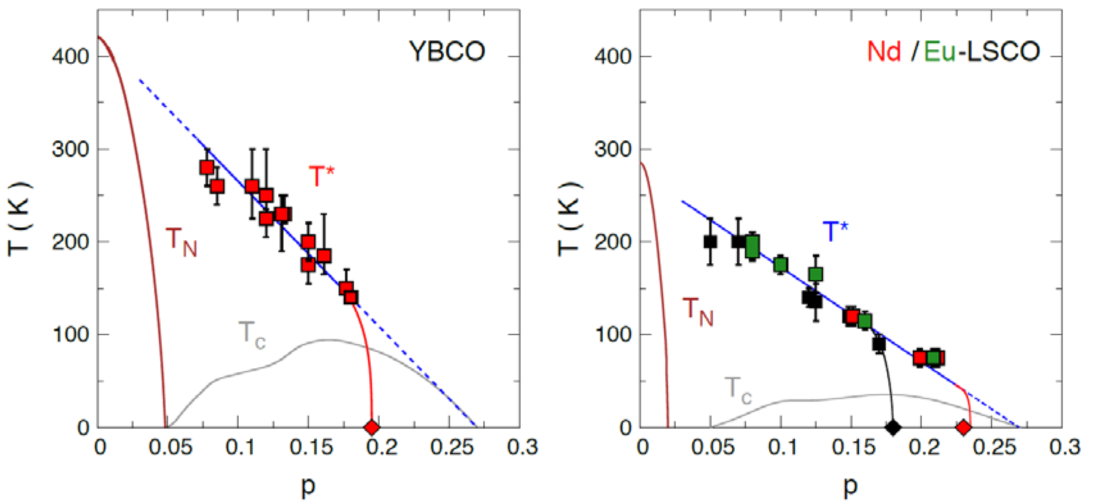


Marion Thénault

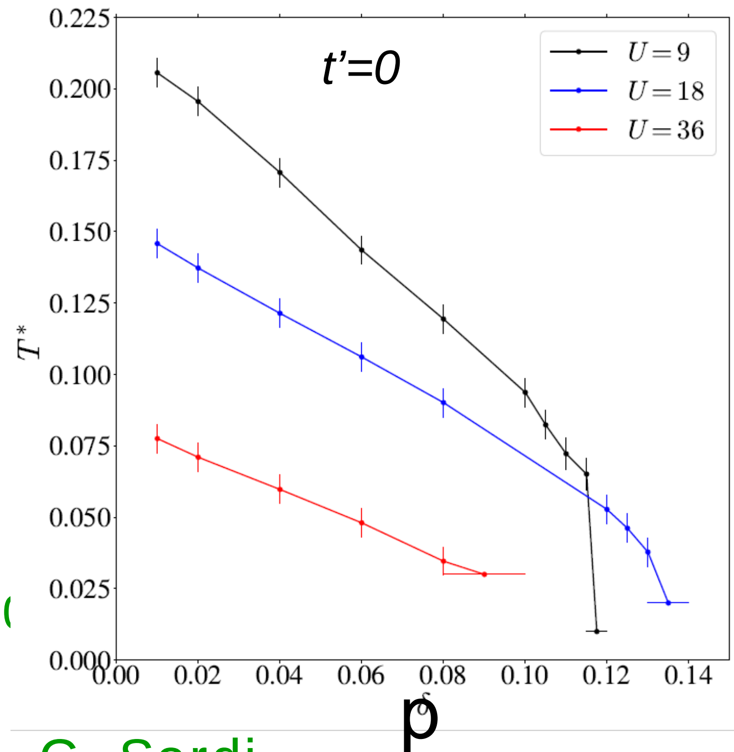
Results T*

$$k_B T^* \sim J$$

$J = 4t^2/U$



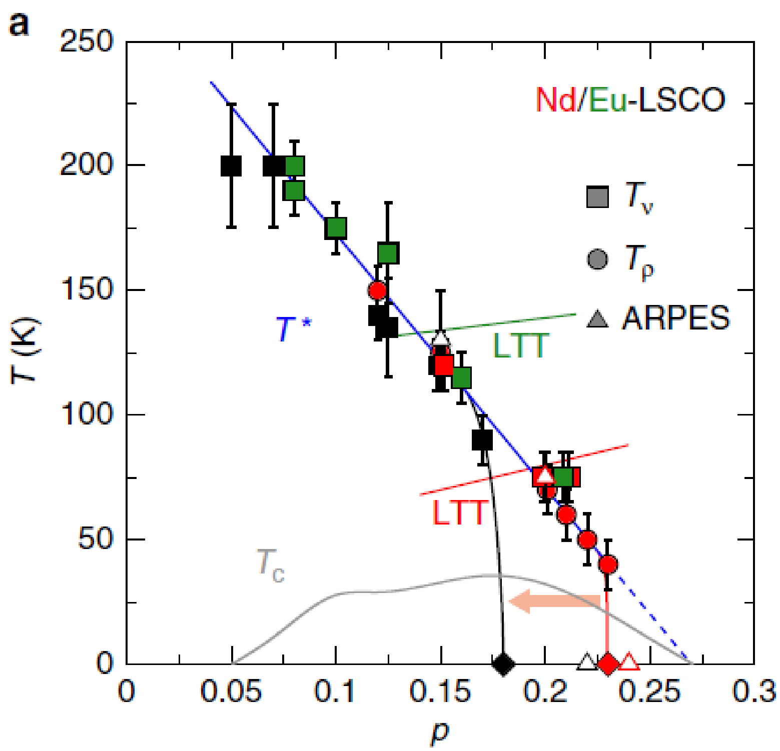
Cyr-Choinières et al. Phys. Rev. B **97**, 06450

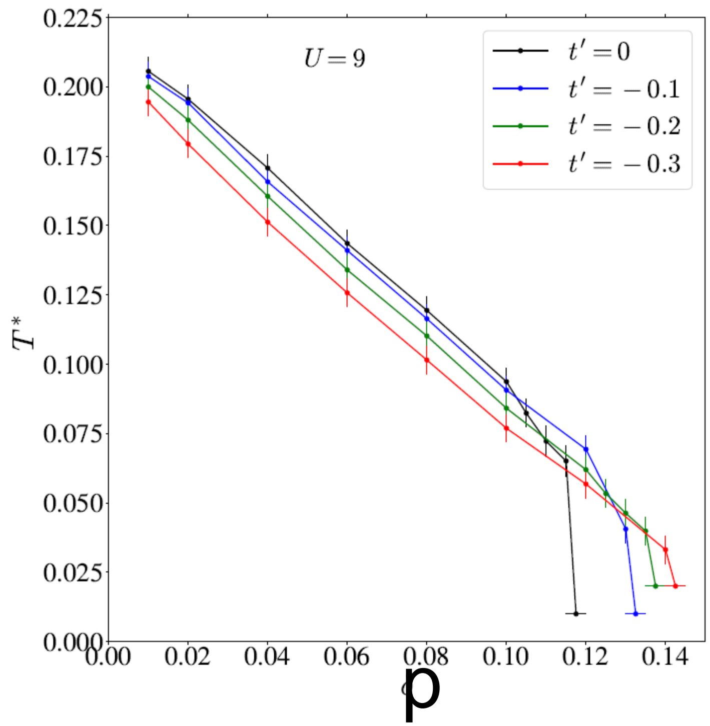


A. Reymbaut, M. Thénault, L. Fratino, G. Sordi,
P. Sémon, AMT, unpublished

W Wu, A Georges, M Ferrero - arXiv preprint arXiv:1707.06602
Bragança, Sakai, Aguiar, Civelli, PRL **120**, 067002 (2018)

Results : effect of *t'* on *T**

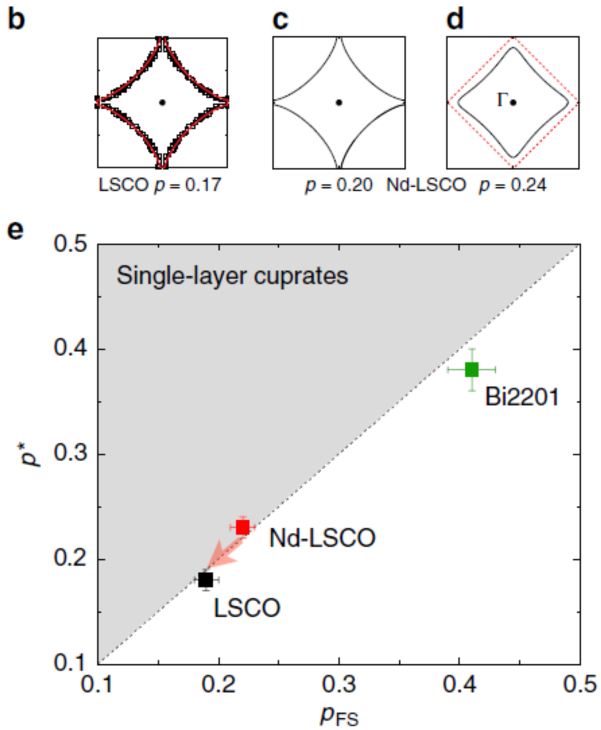


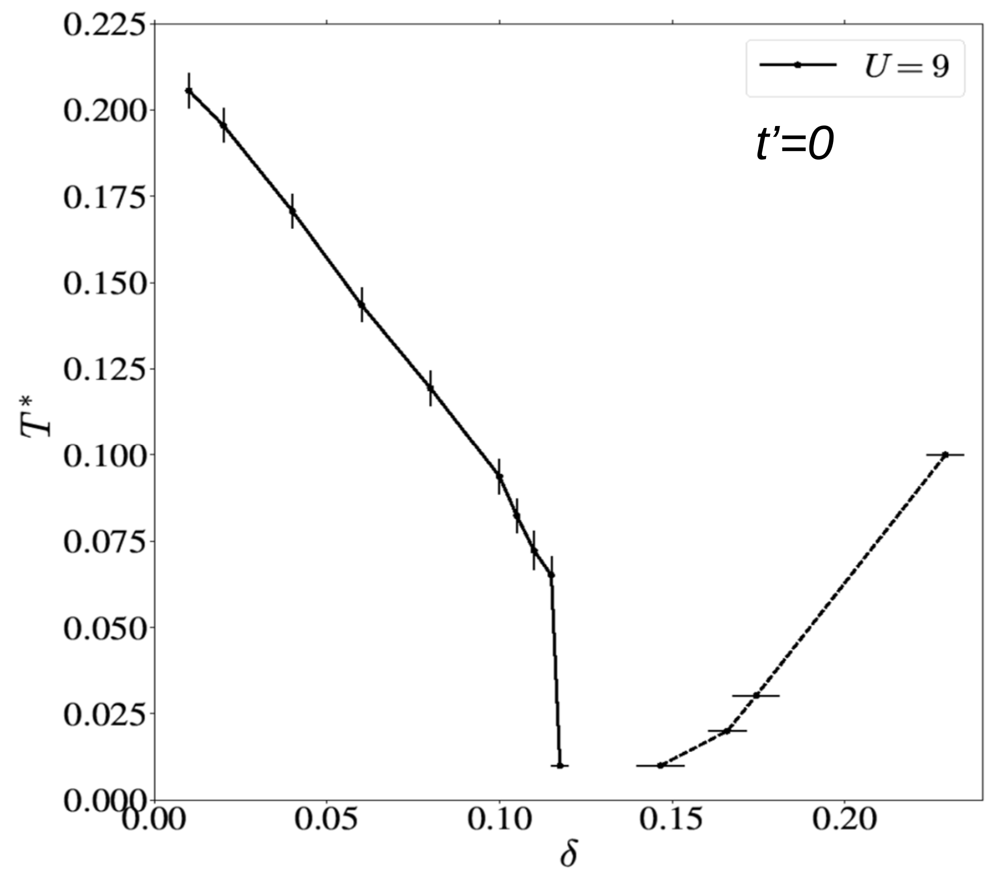


Doiron-Leyraud *et al.*
Nature Comm. **8** 2044

A. Reymbaut, M. Thénault, L. Fratino, G. Sordi, P. Sémon, AMT, unpublished

Results: van Hove singularity





$p^* < p_{fs}$

$p^* \quad p_{fs}$

Giovanni Sordi

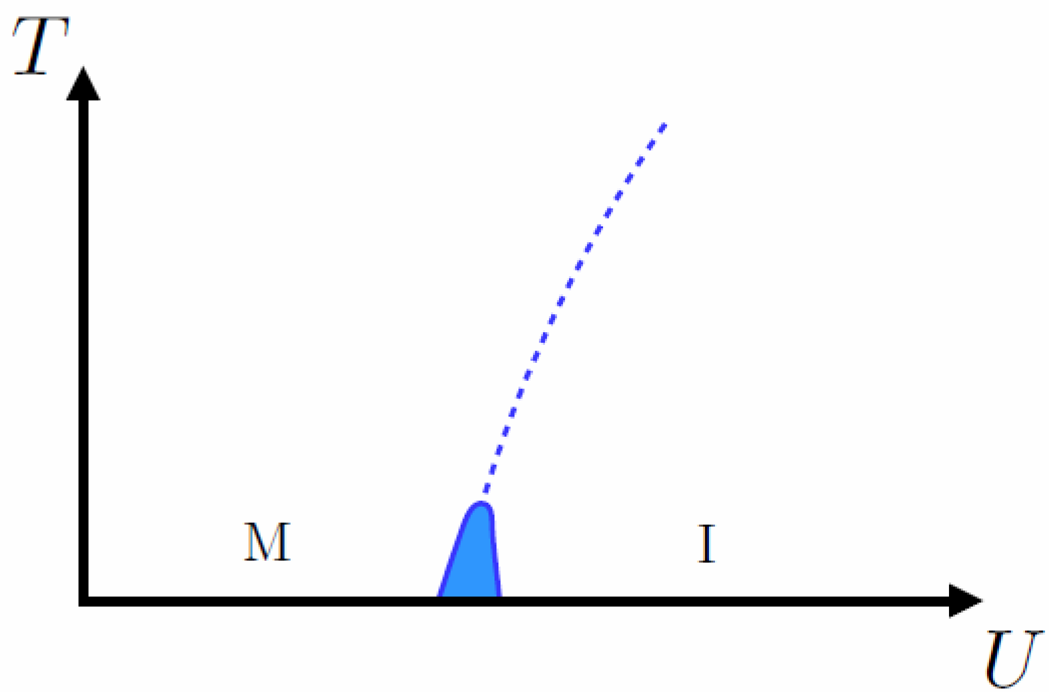
Kristjan Haule

Pseudogap from the influence of the Mott transition away from half-filling

Sordi et al., PRL 104, 226402 (2010)
Sordi et al., PRB 84, 075161 (2011)
Fratino et al., PRB 93, 245147 (2016) [Emery model]
Sordi et al., Sci. Rep. 2 547 (2012);
Sordi et al., PRB 87, 041101(R) (2013)
Fratino et al., PRB 93, 245147 (2016) [Emery model]

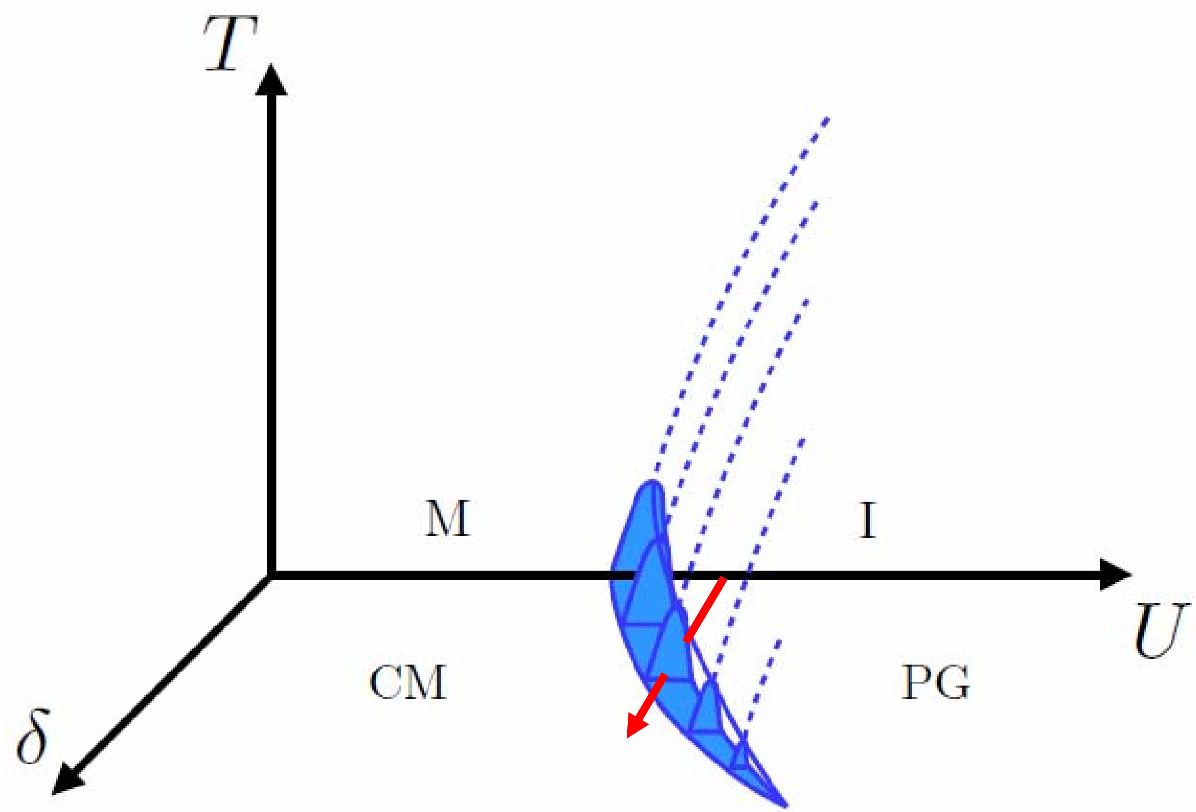
Influence of Mott transition away from half-filling

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



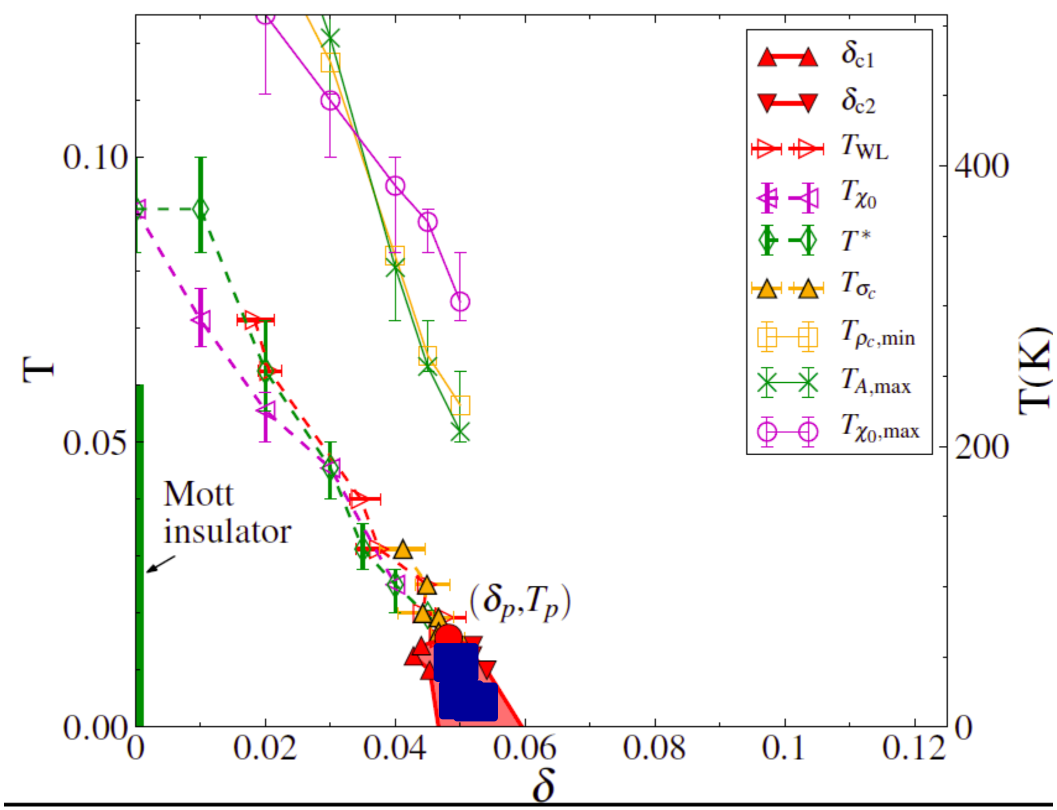
Influence of Mott transition away from half-filling

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



Two crossover lines

Giovanni Sordi

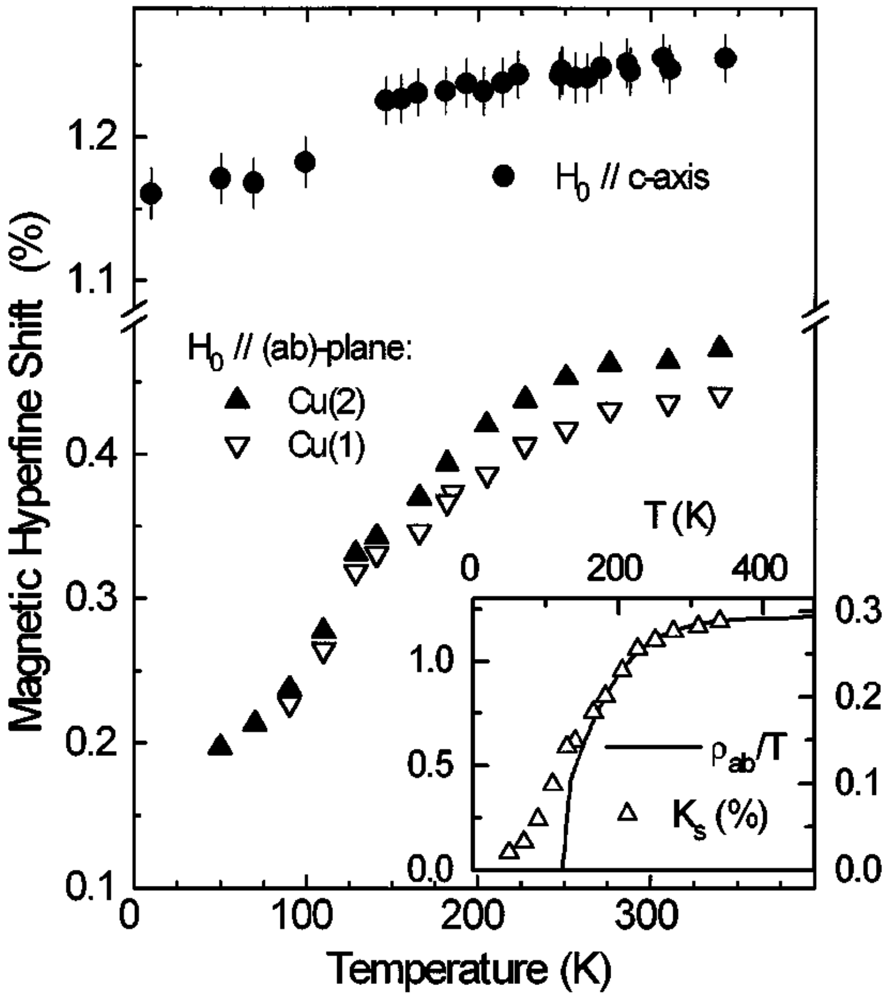


Patrick Sémon

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

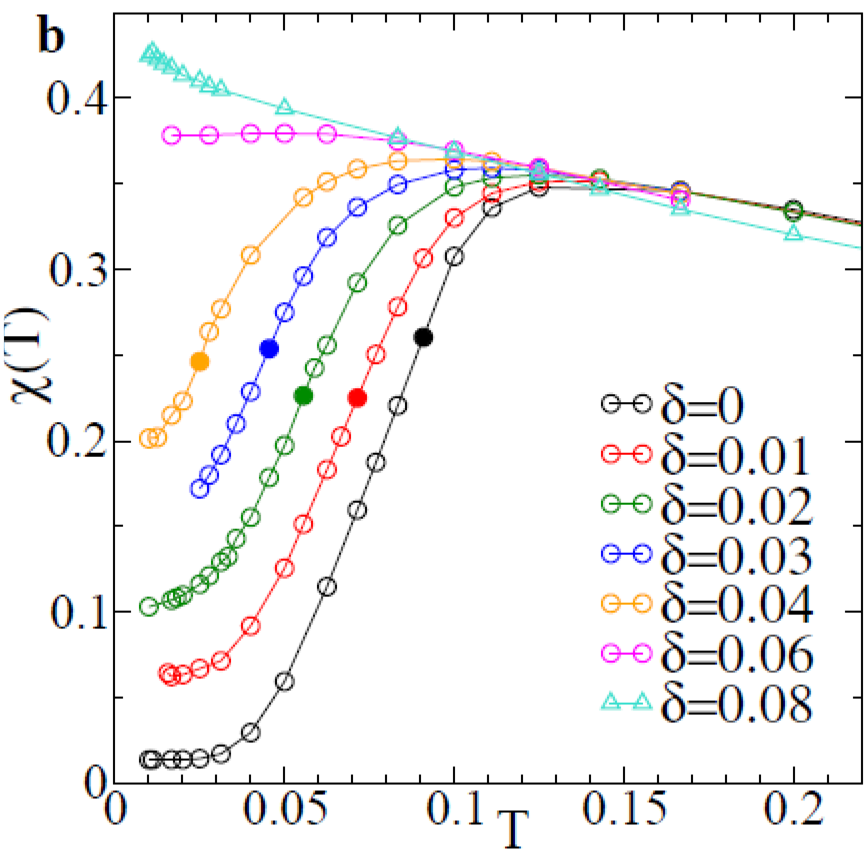
P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B **89**, 165113/1-6 (2014)

Spin susceptibility



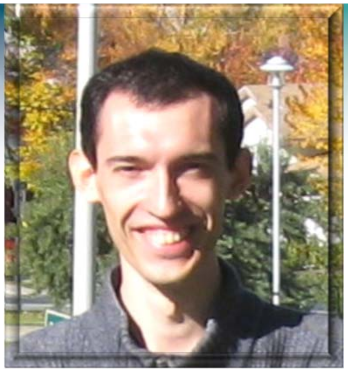
Underdoped Hg1223

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



Part III:

Strongly correlated superconductivity



Giovanni Sordi

Patrick Sémon

Lorenzo Fratino

Superconductivity in a doped Mott insulator

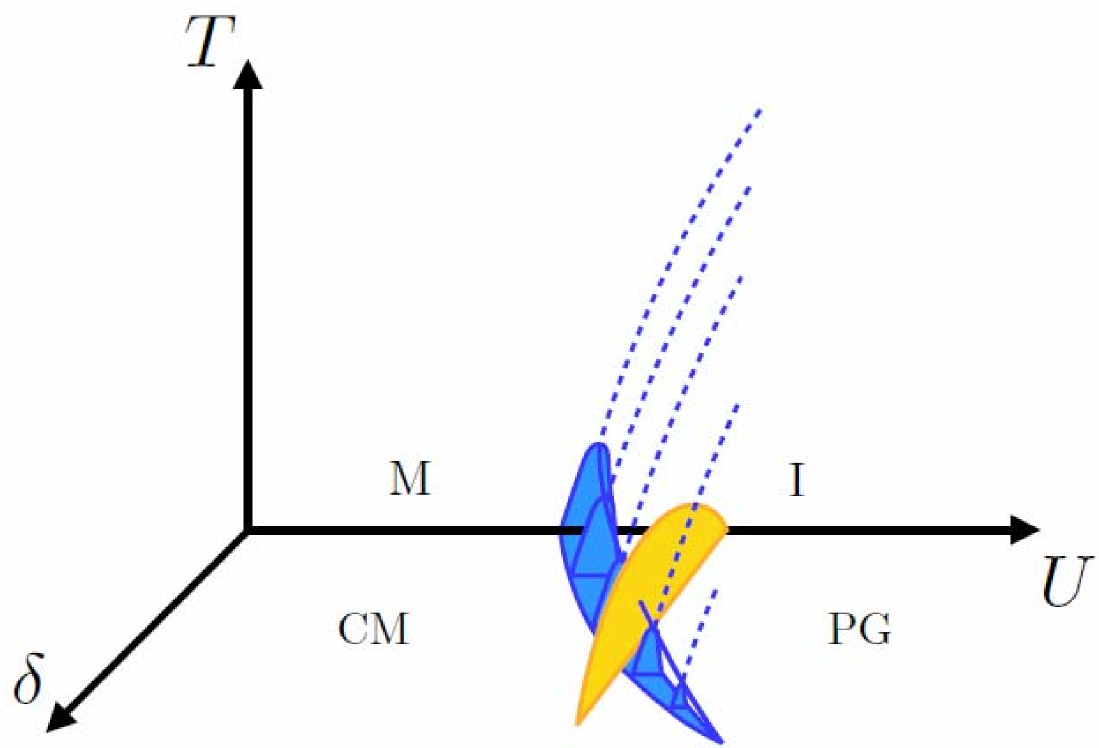
Sordi et al. PRL **108**, 216401 (2012)

Fratino et al.

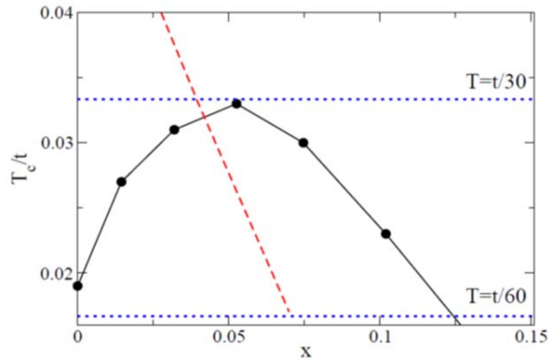
Sci. Rep. **6**, 22715 (2016)

Superconductiviy in Doped Mott insulator

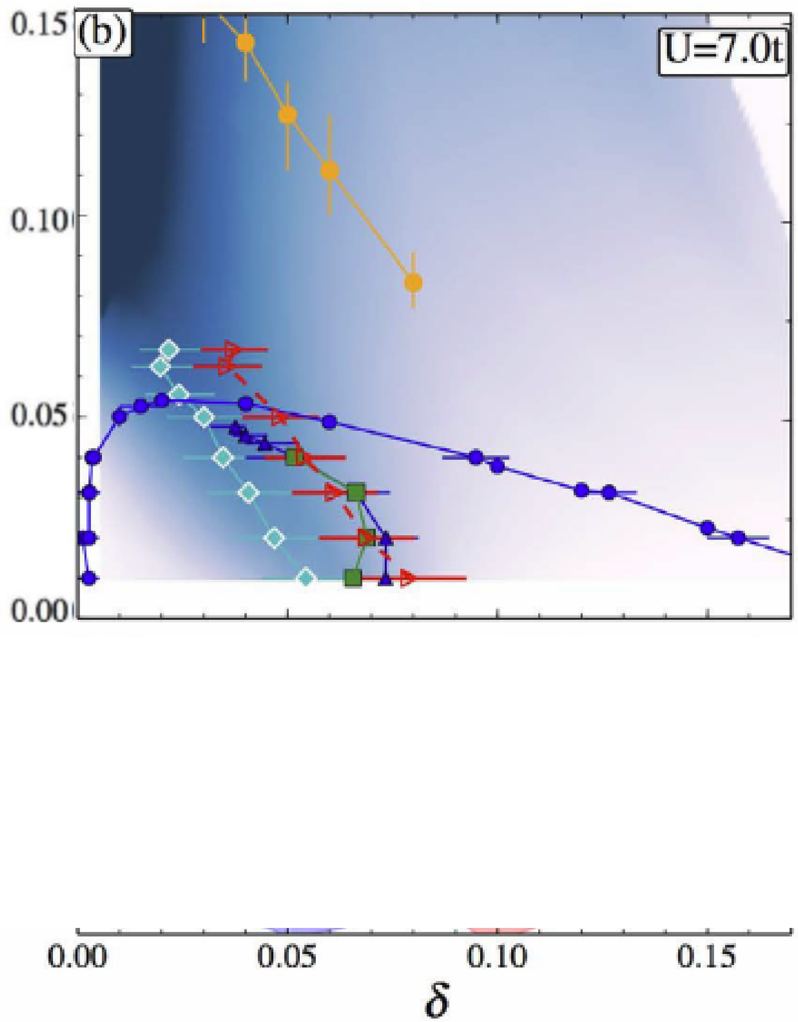
$n = 1, d = 2$ square lattice



An organizing principle



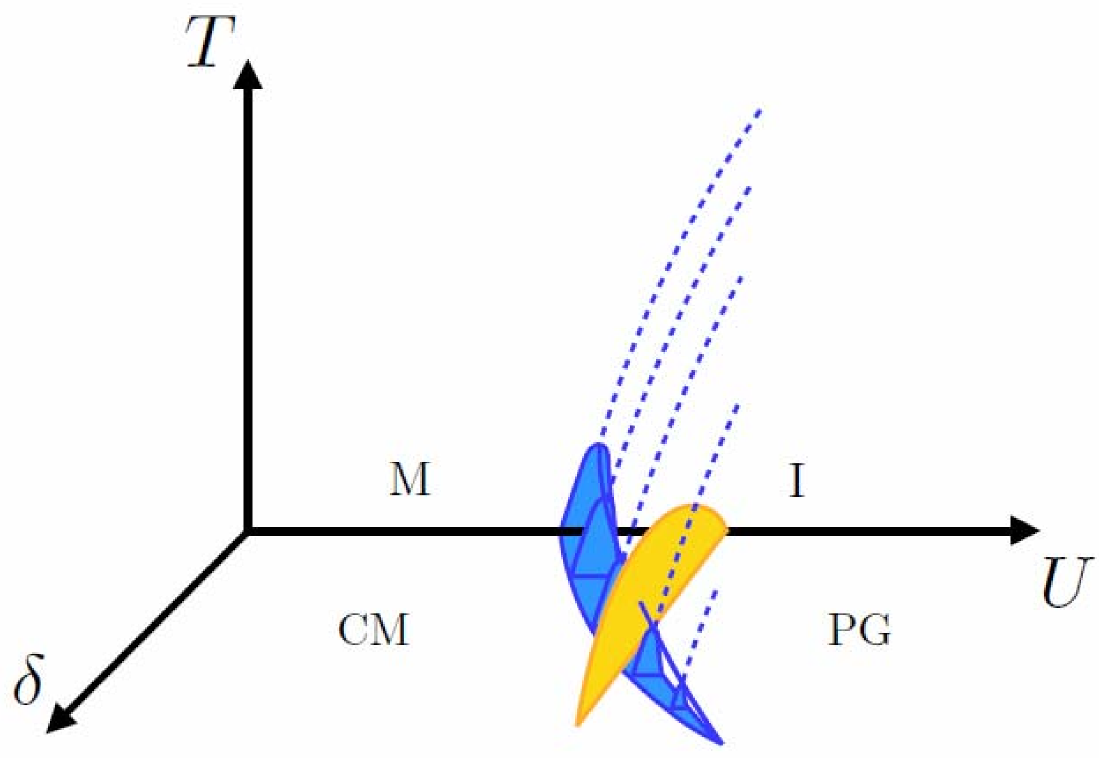
E. Gull and A. J. Millis
Phys. Rev. B 88, 075127



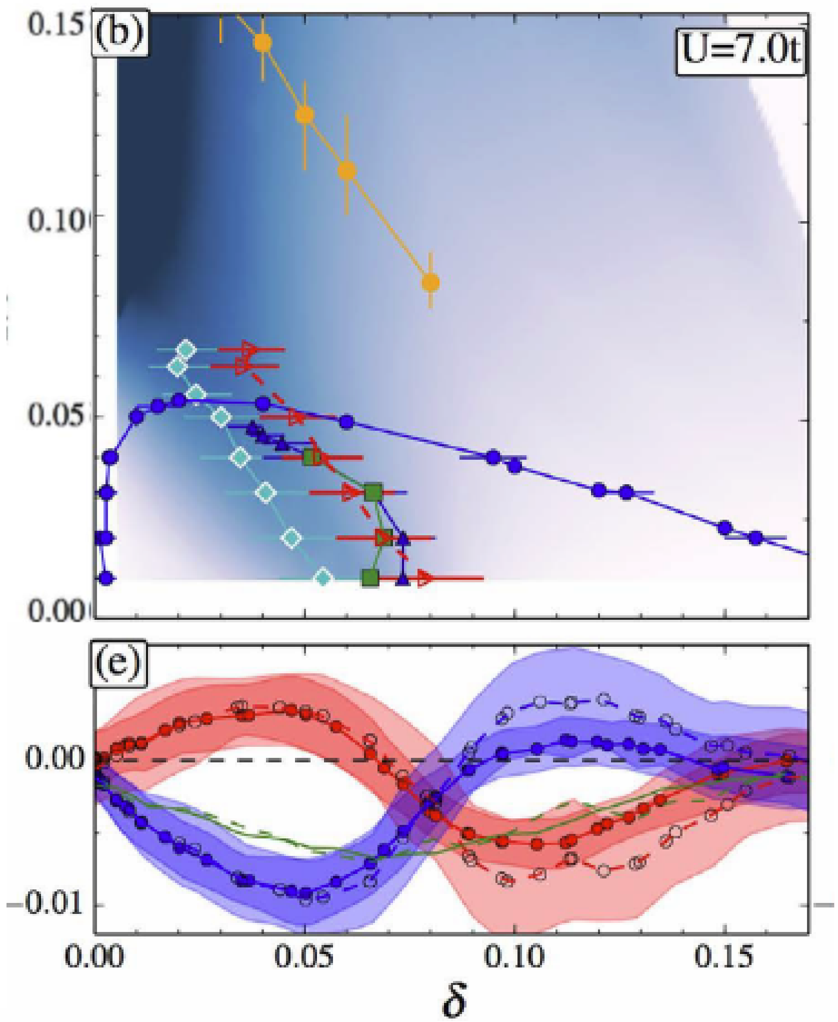
Fratino et al.
Sci. Rep. **6**, 22715

Superconductiviy in Doped Mott insulator

$n = 1, d = 2$ square lattice



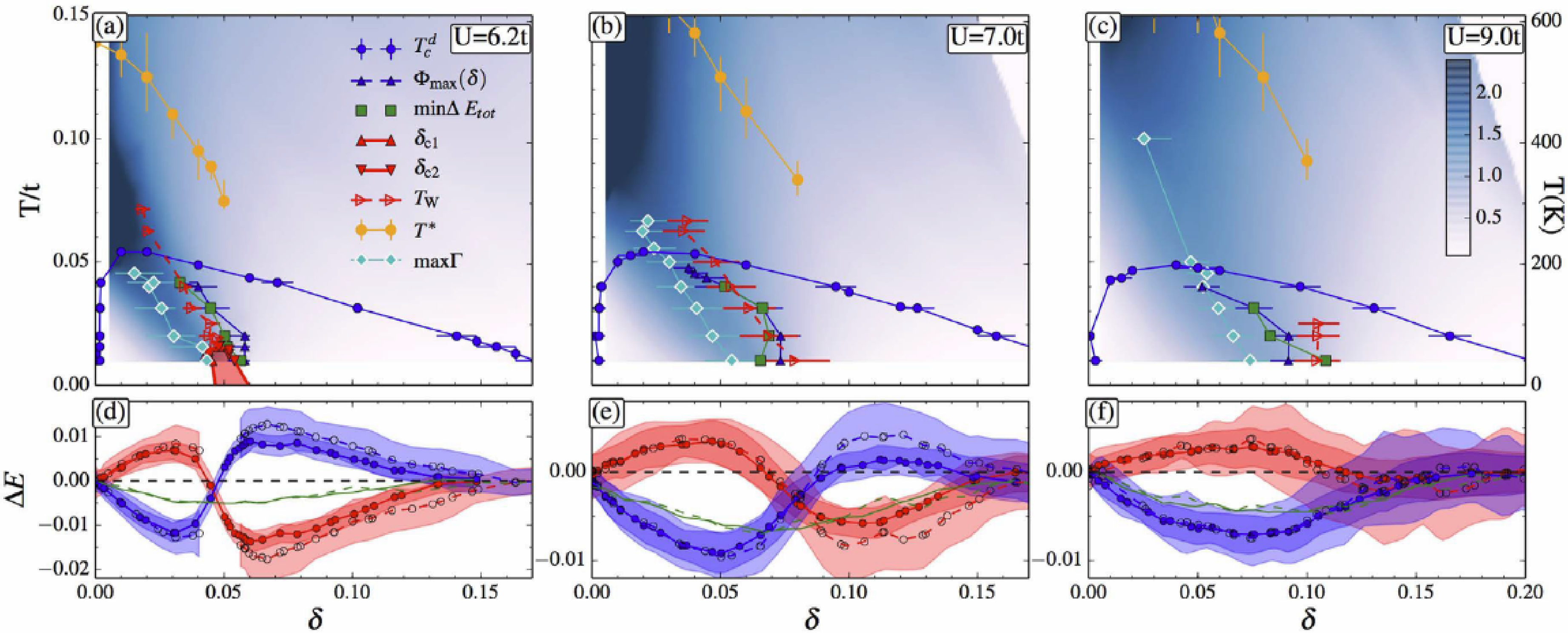
An organizing principle



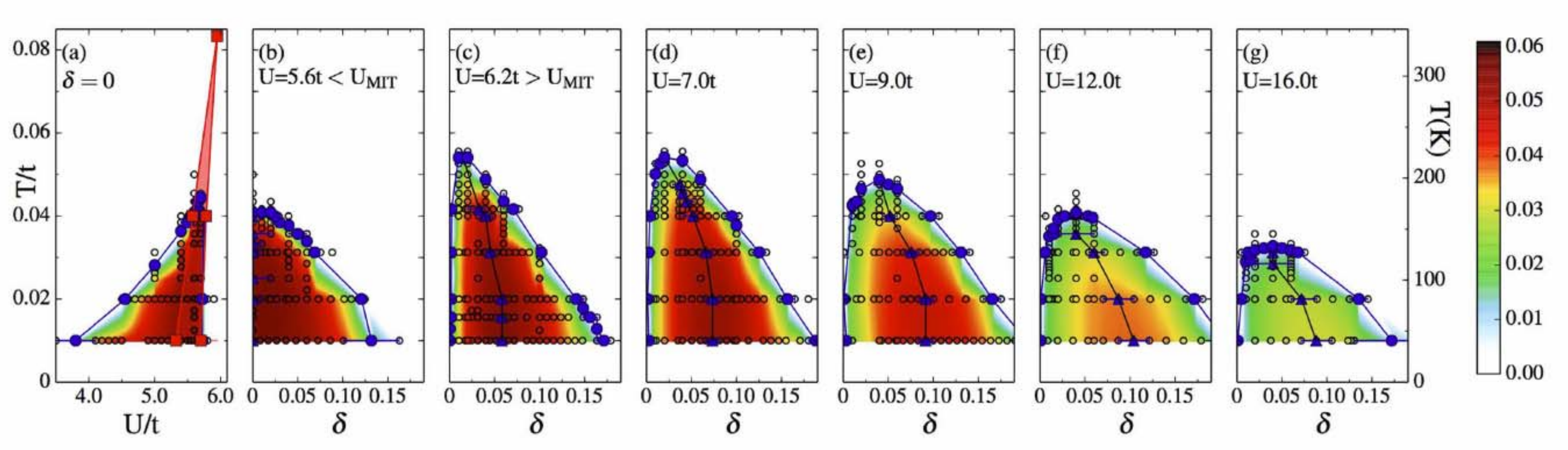
Fratino et al.
Sci. Rep. **6**, 22715

Theory, see also Jarrel PRL (2004), Gull Millis PRB (2014)
Experiments: Bontemps, Santander-Syro Van der Marel …

An organizing principle



T_c controlled by J



Fratino et al.
Sci. Rep. **6**, 22715

Some experiments that suggest $T_c < T_{pair} < T^*$

T. Kondo *et al*. PRL **111** (2013)

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

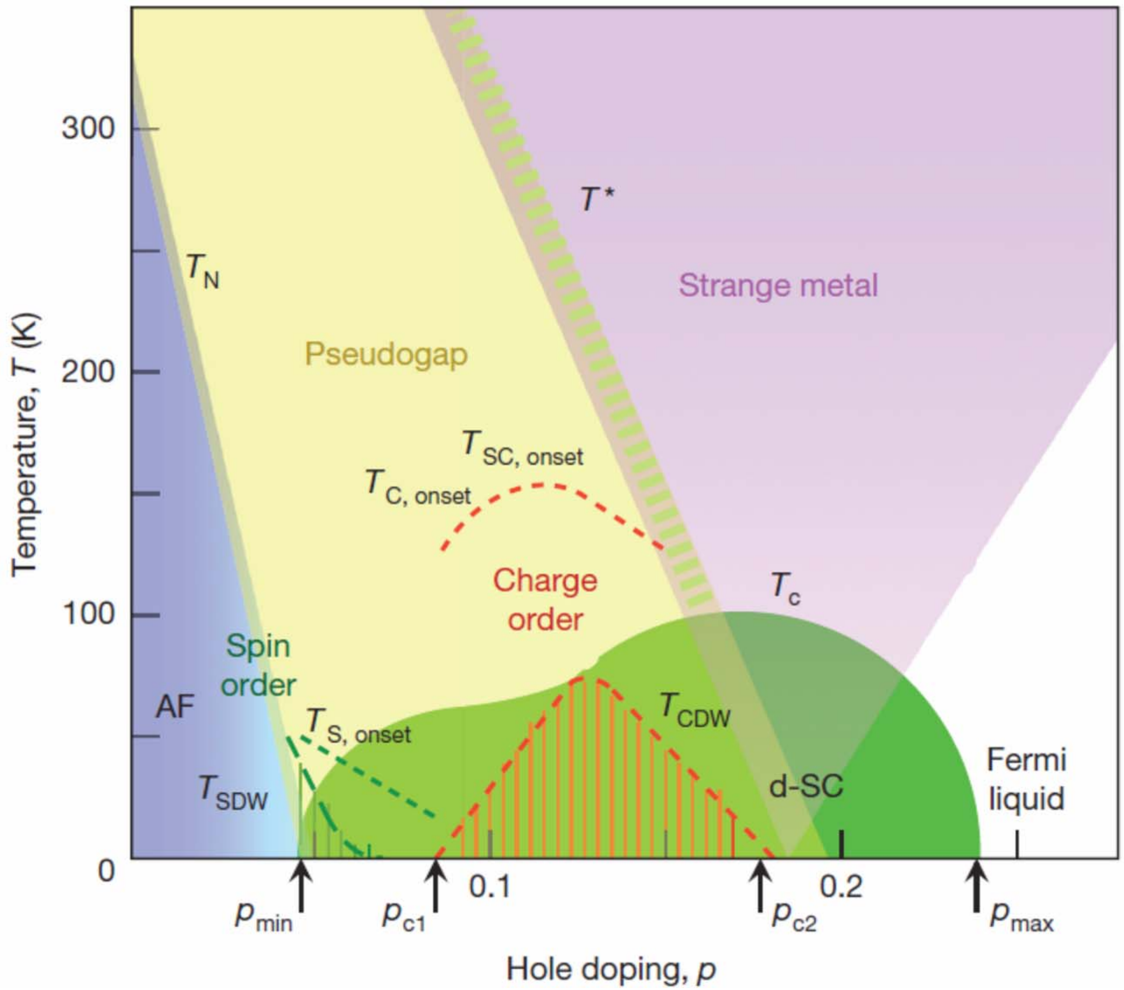
A. Pushp, Parker, … A. Yazdani, Science **364**, 1689 (2009)

Lee …Tajima (Osaka) https://arxiv.org/pdf/1612.08830

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

Lee et al. J. Phys. Soc. Jpn. 86, 023701 (2017)

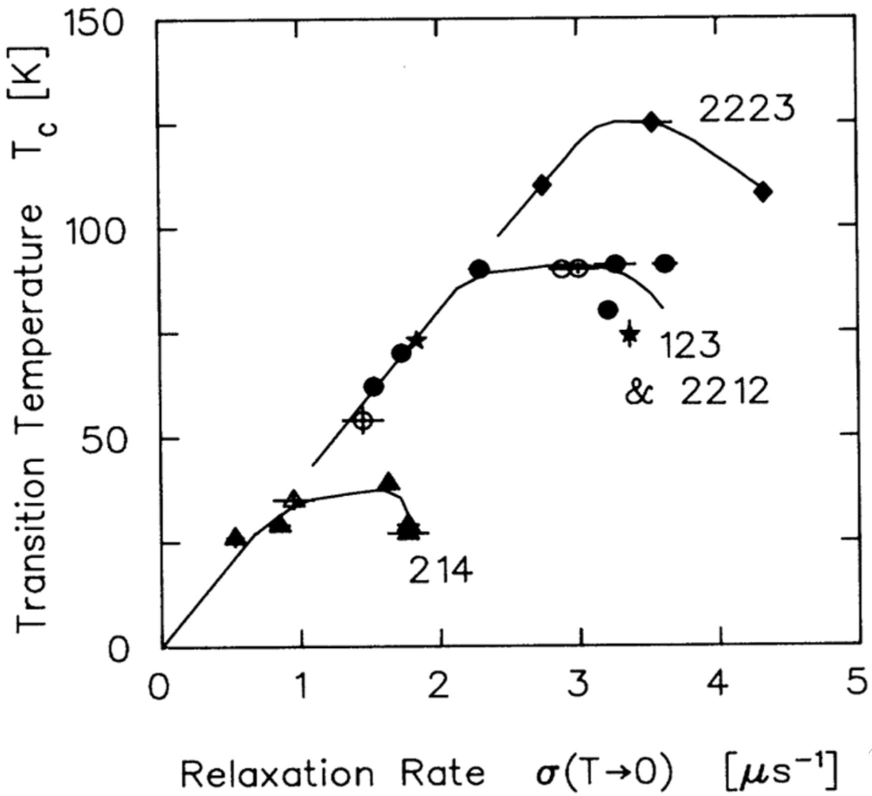
Phase diagram $YBa_2Cu_3O_{7-x}$



Keimer et al., Nature 518, 179 (2015)

What causes T_c to drop?

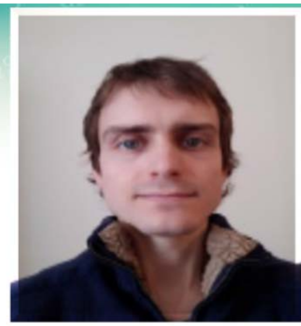
Phase fluctuations? Emery Kivelson Nature **374** (1995)



$\sigma \propto \rho_s$

Uemura, Y.J. *et al.*, PRL vol.62, (1989)
Tallon *et al.*, PRB **68**, 180501(R) (2003)

Olivier Simard



Charles-David Hébert

Alexandre Foley

David Sénéchal

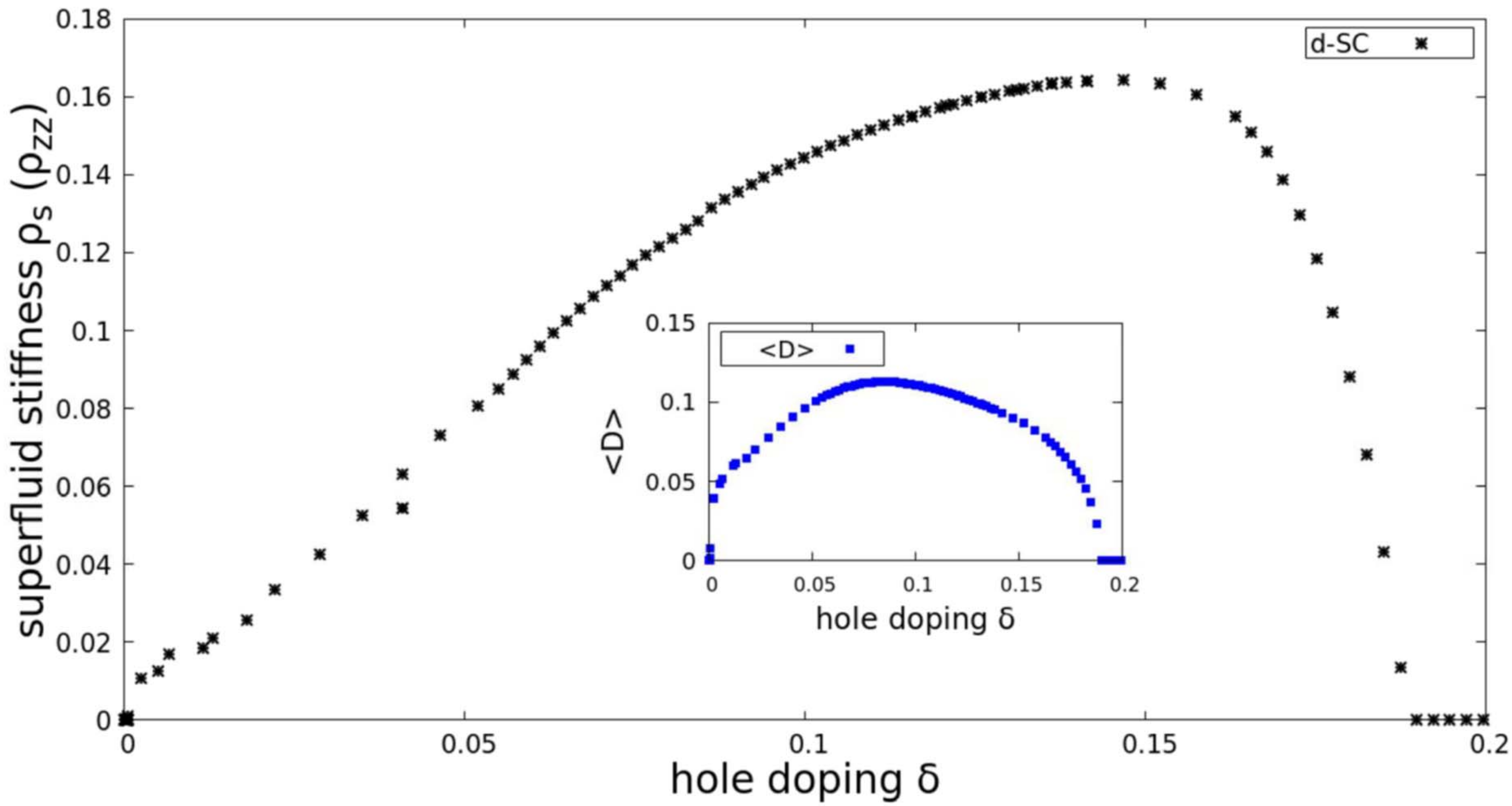
What causes T_c to drop near $n = 1$?

O. Simard, C.-D. Hébert, A. Foley, A.-M.S. Tremblay, D. Sénéchal, unpublished

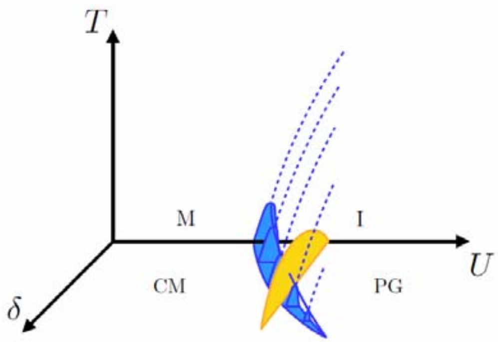
Superfluid stiffness *T=0*

$$\rho_{ab} = \langle \hat{J}_a(\boldsymbol{r},\tau)\,\hat{J}_b(\boldsymbol{r}',\tau')\rangle = \frac{-\beta}{V}\frac{\delta^2\mathcal{F}}{\delta A_a(\boldsymbol{r},\tau)\,\delta A_b(\boldsymbol{r}',\tau')}\bigg|_{\boldsymbol{A}=0}$$

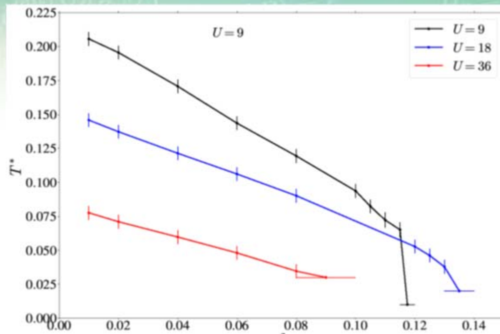
Superfluid stiffness vs doping with d-SC for U = 8t, t'=-0.3 and t'' = 0.2



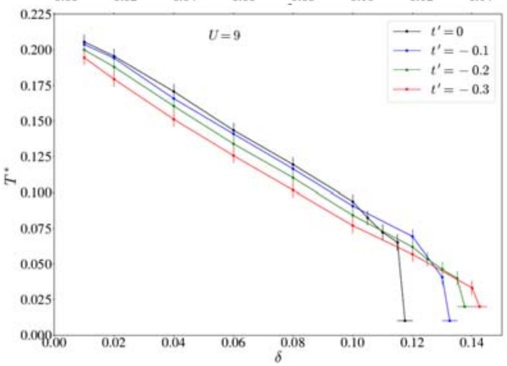
Conclusion



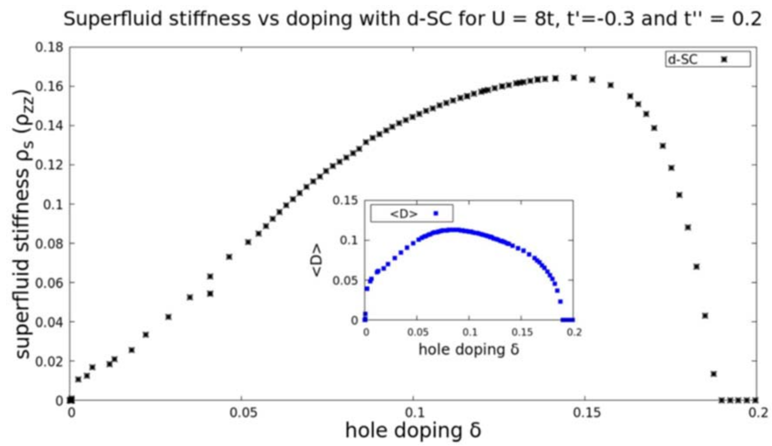
T
M
I
U
CM
PG
δ



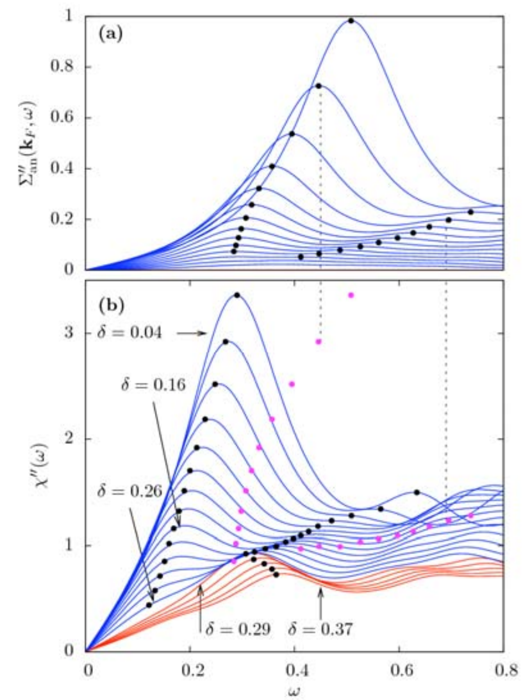
U = 9
U = 9
U = 18
U = 36
T*



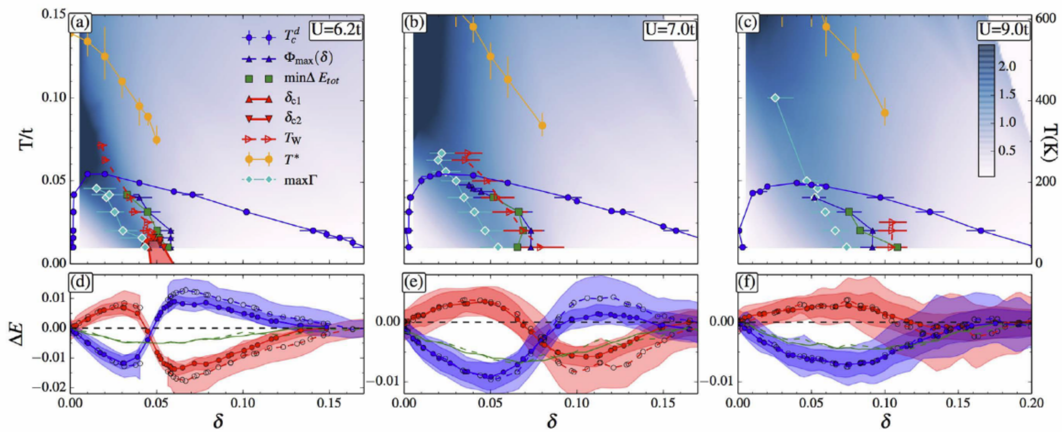
U = 9
t' = 0
t' = − 0.1
t' = − 0.2
t' = − 0.3
T*
δ



Superfluid stiffness vs doping with d-SC for U = 8t, t'=-0.3 and t'' = 0.2
d-SC
superfluid stiffness ρs (ρzz)
hole doping δ
<D>
<D>
hole doping δ

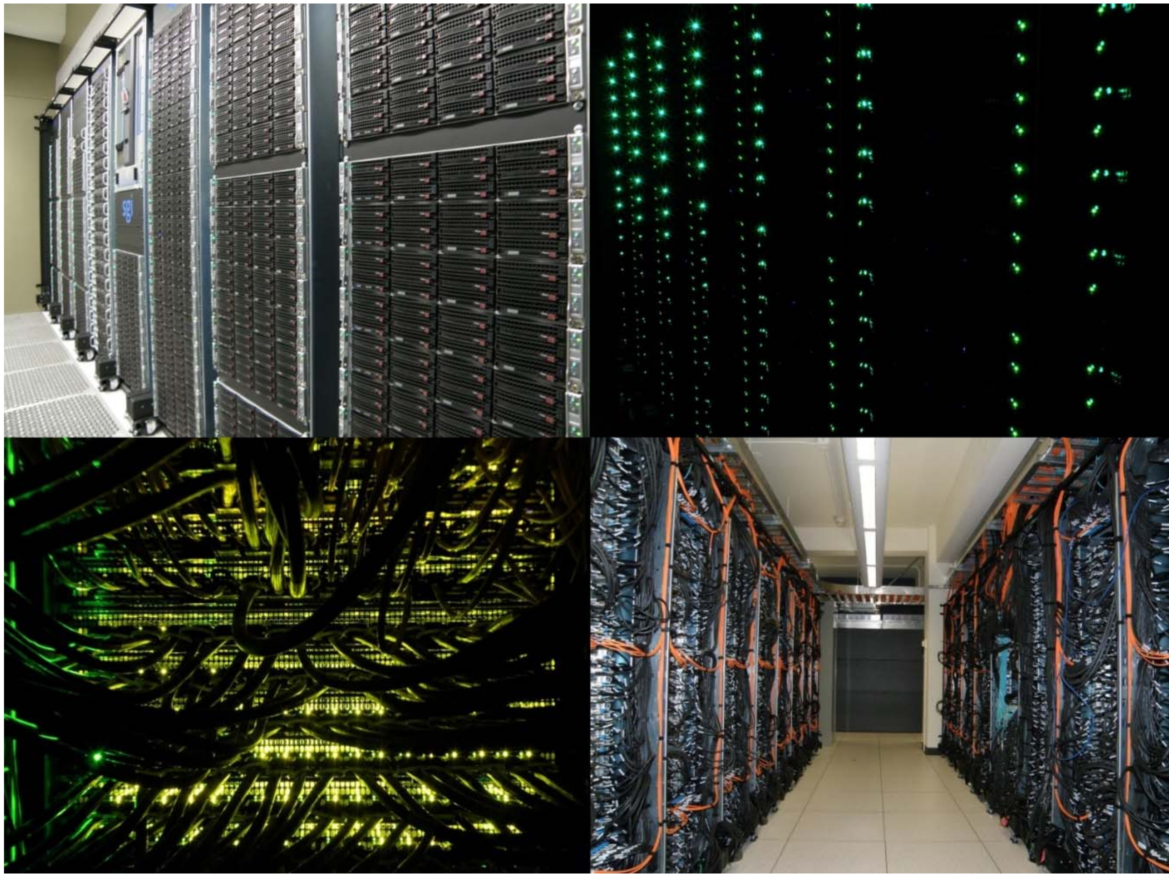


(a)
$\Sigma''_{an}(\mathbf{k}_F, \omega)$
(b)
δ = 0.04
δ = 0.16
δ = 0.26
δ = 0.29
δ = 0.37
$\chi''(\omega)$
ω



(a) U=6.2t
(b) U=7.0t
(c) U=9.0t
T/t
T(K)
T_c^d
$\Phi_{max}(\delta)$
minΔE_{tot}
δ_{c1}
δ_{c2}
T_W
T^*
maxΓ
(d)
(e)
(f)
ΔE
δ

Mammouth



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High Performance Computing
CREATING KNOWLEDGE
DRIVING INNOVATION
BUILDING THE DIGITAL ECONOMY

Le calcul de haute performance
CRÉER LE SAVOIR
ALIMENTER L'INNOVATION
BÂTIR L'ÉCONOMIE NUMÉRIQUE

Calcul Québec

Merci
Thank you

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