Perspectives on d-wave superconductivity and the pseudogap

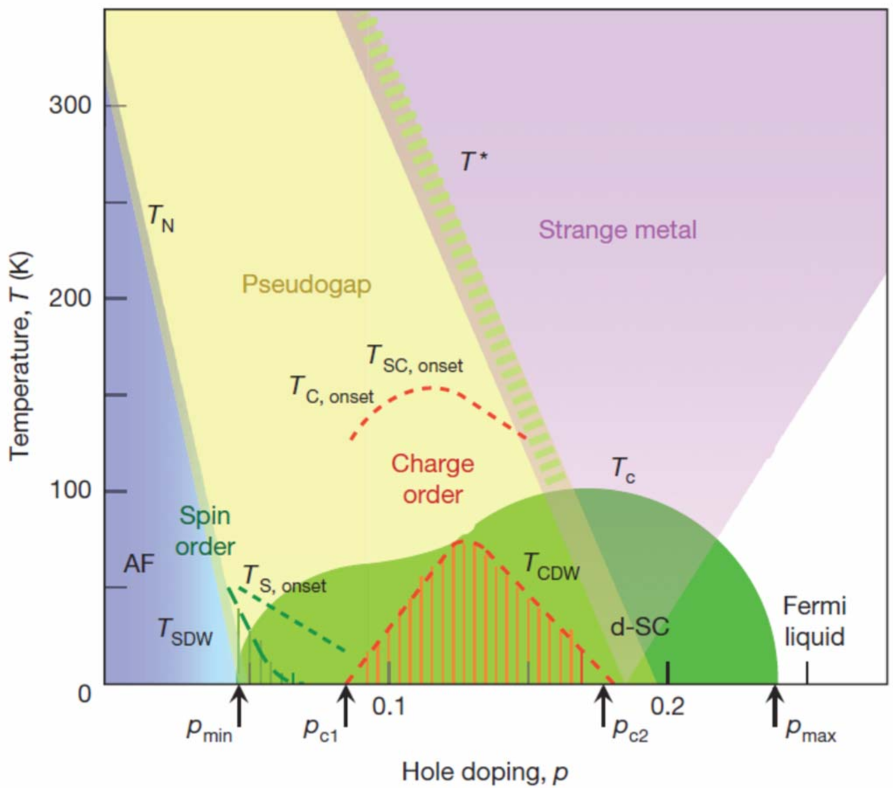
A.-M.S. Tremblay,

CIFAR, Toronto, 19 November 2018

UNIVERSITÉ DE SHERBROOKE

USHERBROOKE.CA/IQ

Phase diagram $YBa_2Cu_3O_{7-x}$



p or δ

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

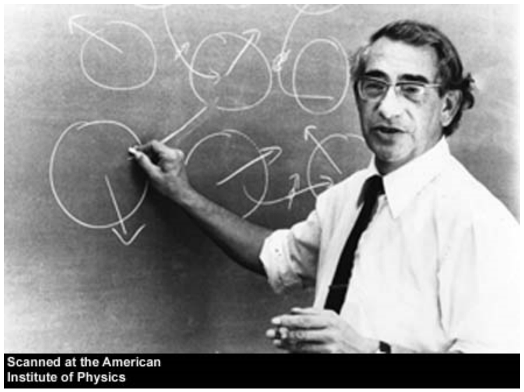
Model

UNIVERSITÉ DE SHERBROOKE

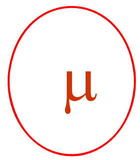
APOGÉE CANADA
FONDS D'EXCELLENCE EN RECHERCHE

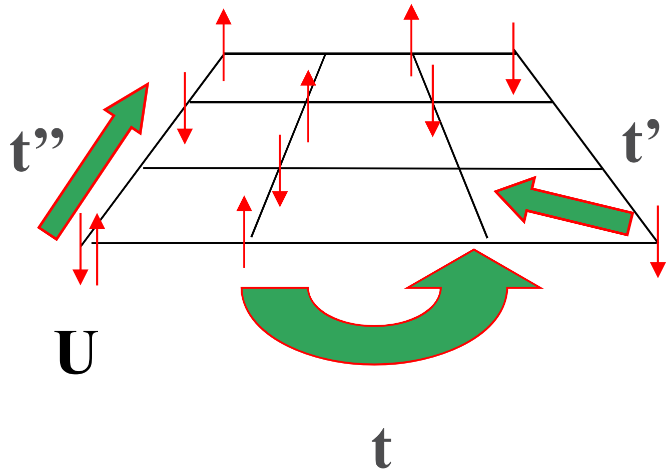
USHERBROOKE.CA/IQ

Hubbard Model



1931-1980





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

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

Traditional mean-field: AFM, no d-wave, very small charge fluctuations

Attn: Charge transfer insulator

Method

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

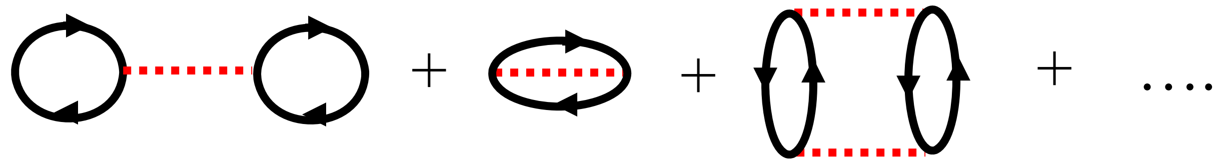
REVIEWS
Maier, Jarrell et al., RMP. (2005)
Kotliar *et al.* RMP (2006)
AMST *et al.* LTP (2006)

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

Dynamical "variational" principle

$$\Omega_{\mathbf{t}}[G] = \Phi[G] - Tr[(G_{0\mathbf{t}}^{-1} - G^{-1})G] + Tr\ln(-G)$$

$$\Phi[G] =$$



$$\frac{\delta\Phi[G]}{\delta G} = \Sigma[G]$$

$$\frac{\delta\Omega_t[G]}{\delta G} = \Sigma[G] - G_{0\mathbf{t}}^{-1} + G^{-1} = 0$$

DMFT

$$\Phi[G] = \sum_i \Phi[G_{ii}(i\omega_n)]$$

Luttinger and Ward 1960, Baym and Kadanoff (1961)

+ 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
- Overall assesment
  - Works well for other correlated cases (BEDT organics)
  - Tools: solvers into modern electronic structure codes (d=3)

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), Scalapino (UCSB)
- Japan
  - Imada (Tokyo) Sakai, Tsunetsugu, Motome

Outline

- The model
- The method

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

Part I

Half-filling

UNIVERSITÉ DE SHERBROOKE

USHERBROOKE.CA/IQ

Giovanni Sordi

Lorenzo Fratino

Maxime Charlebois

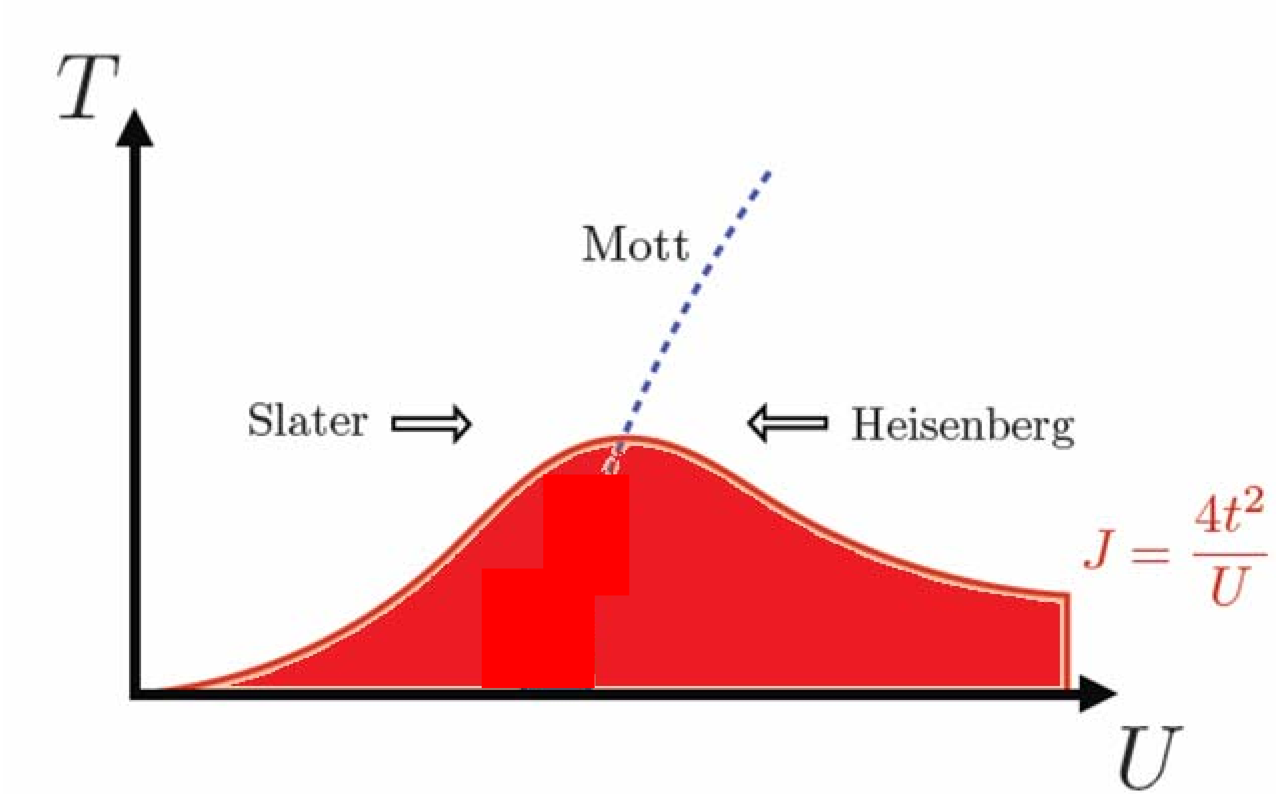
Patrick Sémon

Mott transition and antiferromagnetism

Influence of the underlying normal state
on the ordered state

Underlying Mott transition

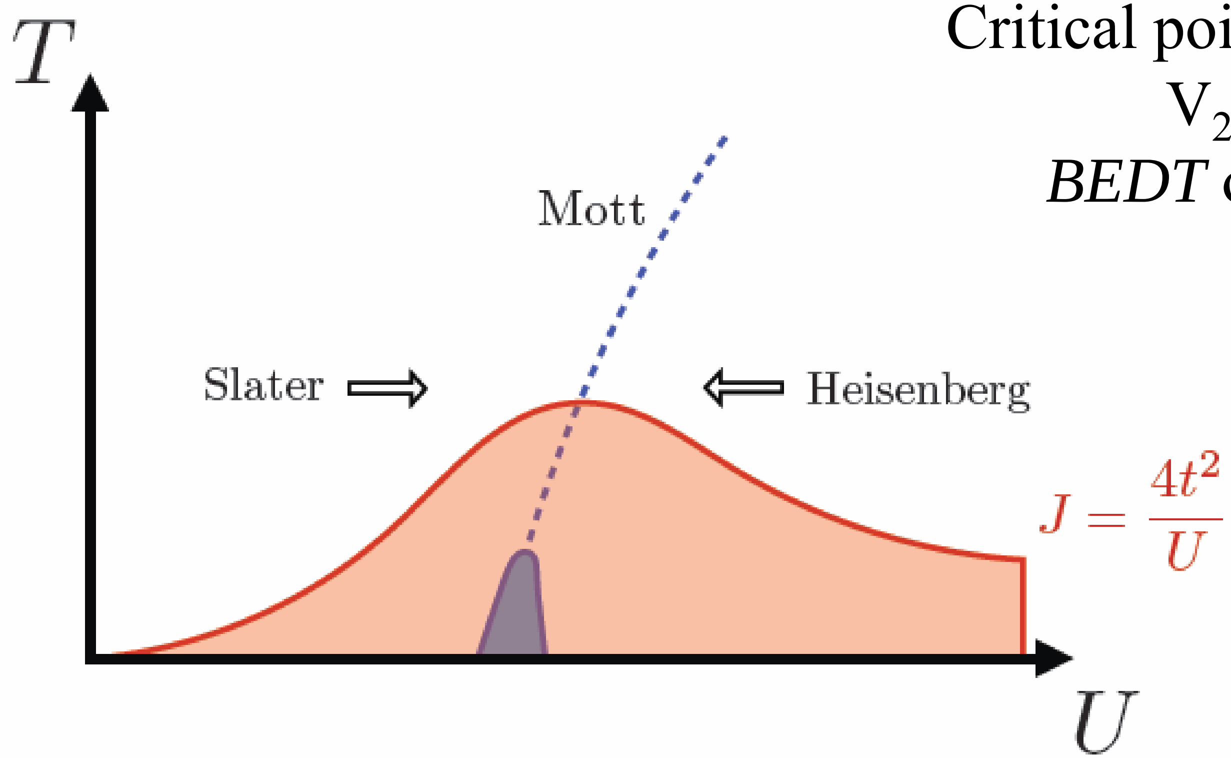
n = 1, d = 3 square lattice



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

Underlying Mott transition

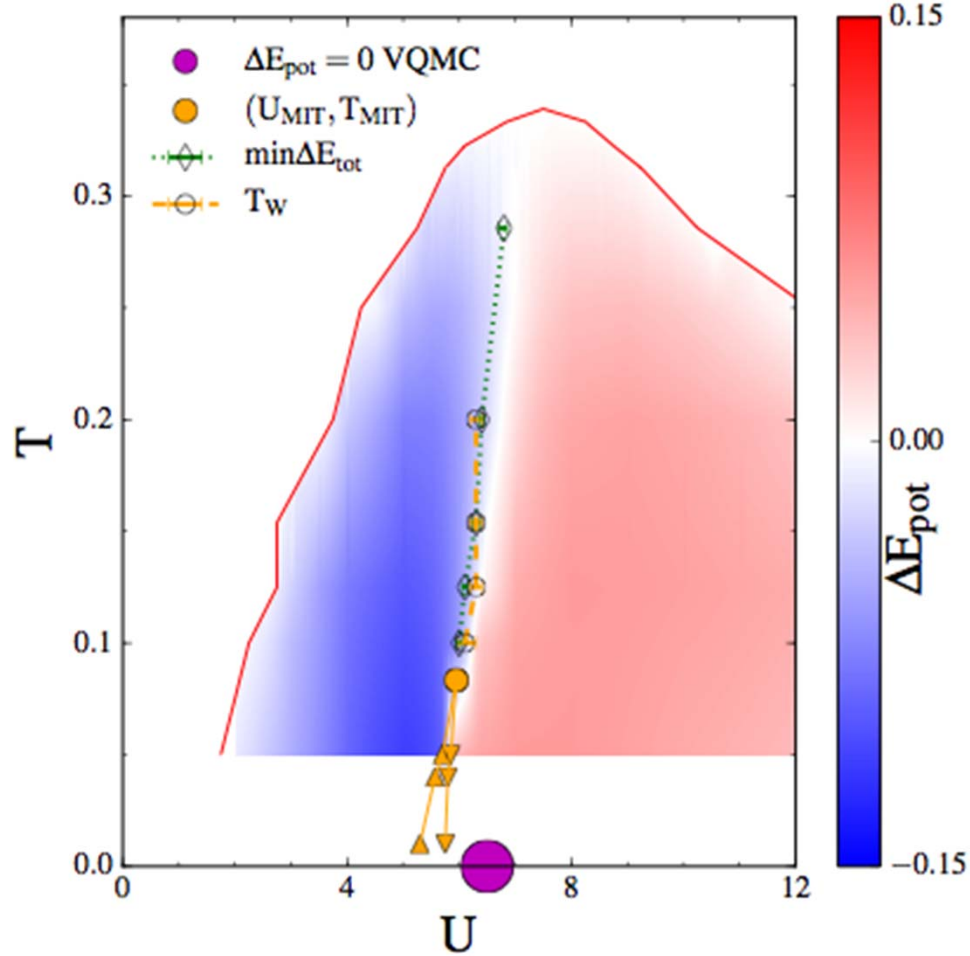
n = *1*, *d* = *2* square lattice



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

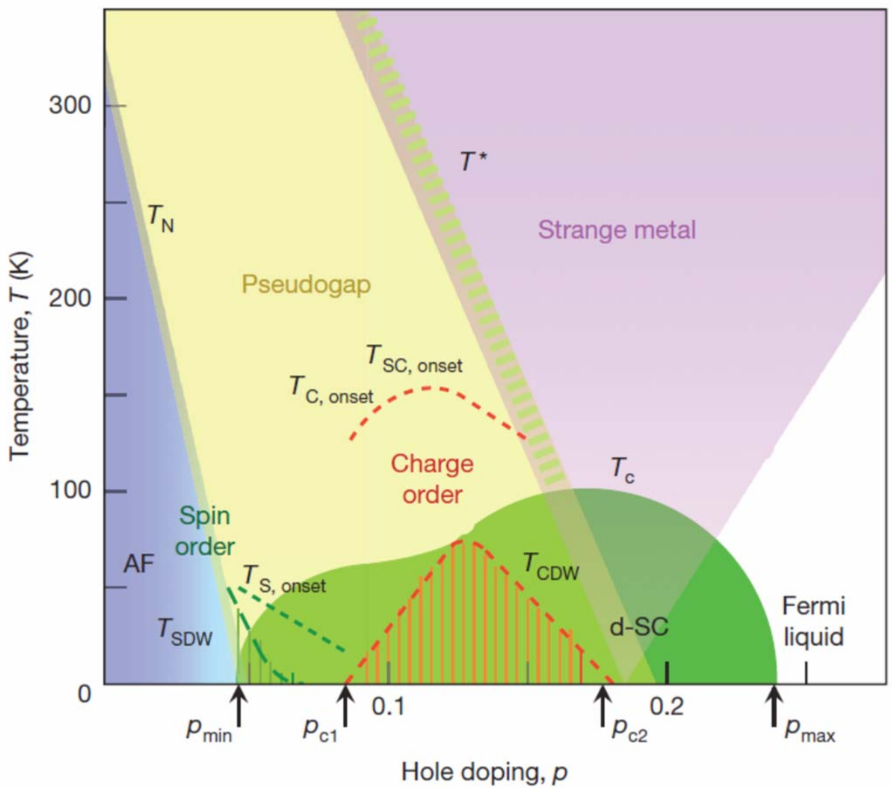


L. F. Tocchio, F. Becca, and S. Sorella, Phys. Rev. B **94**, 195126 (2016).

Part II:

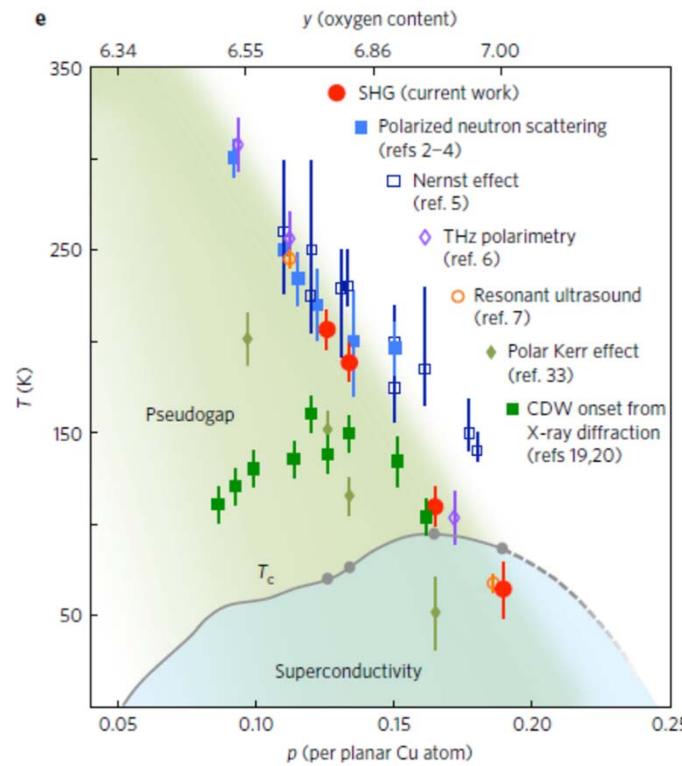
The pseudogap (doped Mott insulator)

Phase diagram $YBa_2Cu_3O_{7-x}$



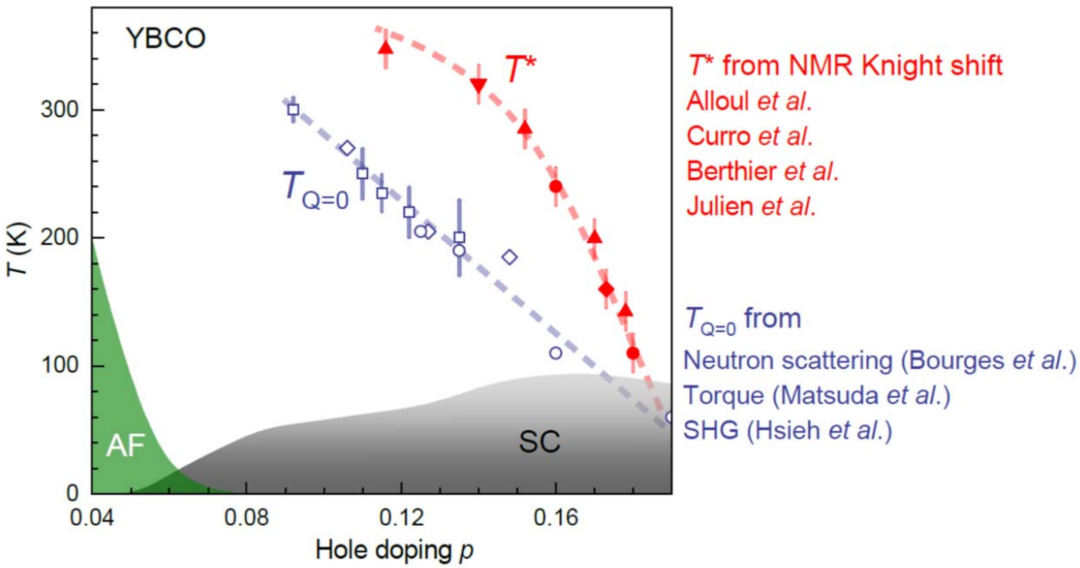
p or δ

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

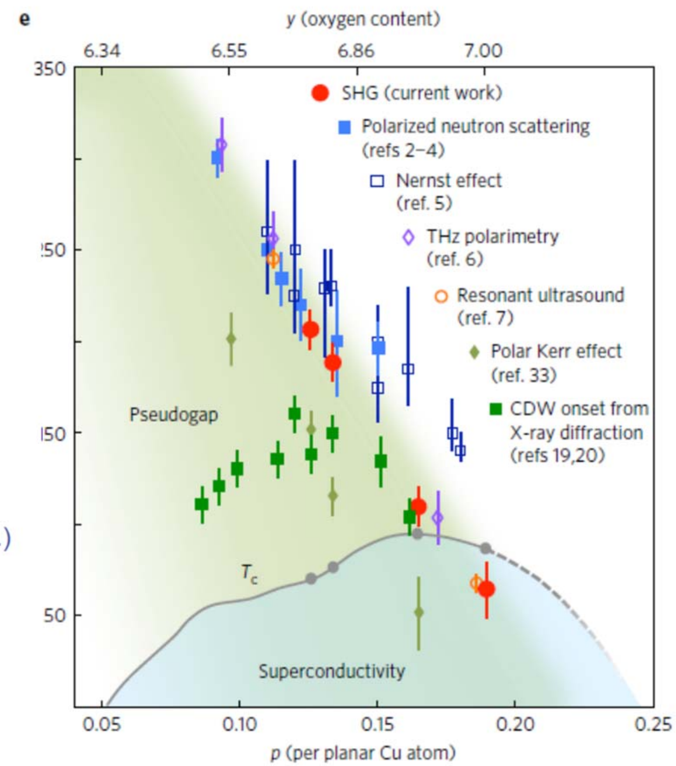


Zhao et al, Nature Physics **13** (2017)

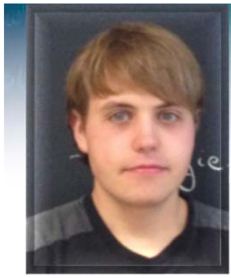
Phase diagram $YBa_2Cu_3O_{7-x}$



Courtesy, M-H. Julien



Zhao et al, Nature Physics **13** (2017)



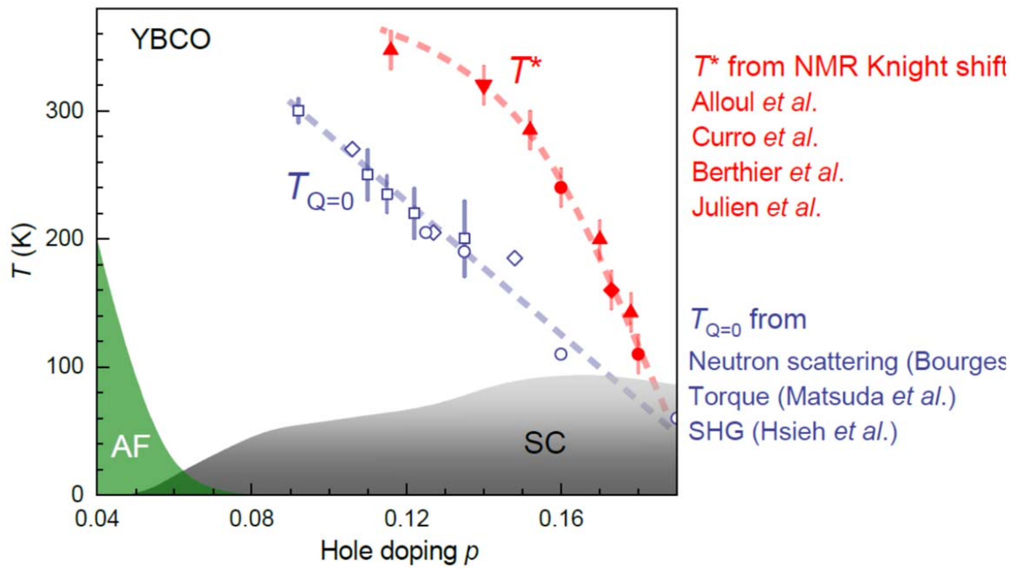
Simon Bergeron

Maxime Charlebois

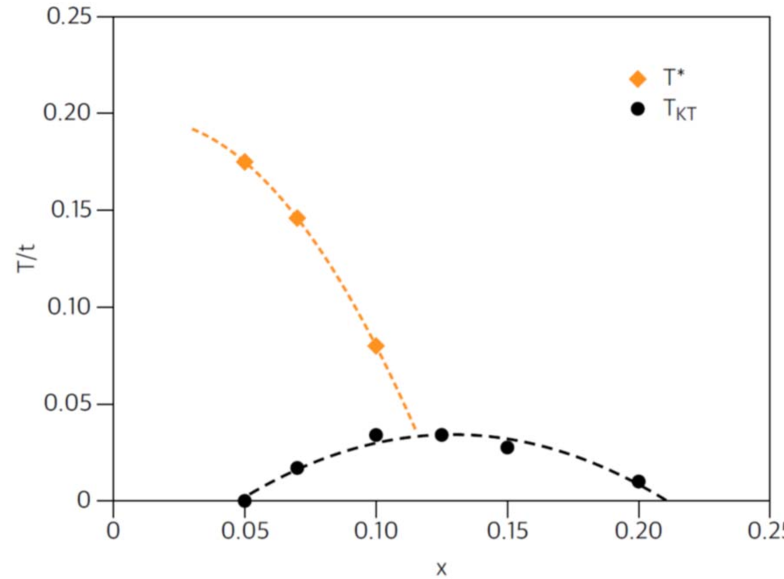
Patrick Sémon

Alexis Reymbaut
Marion Thénault

The pseudogap from the calculated Knight shift



Courtesy, M-H. Julien

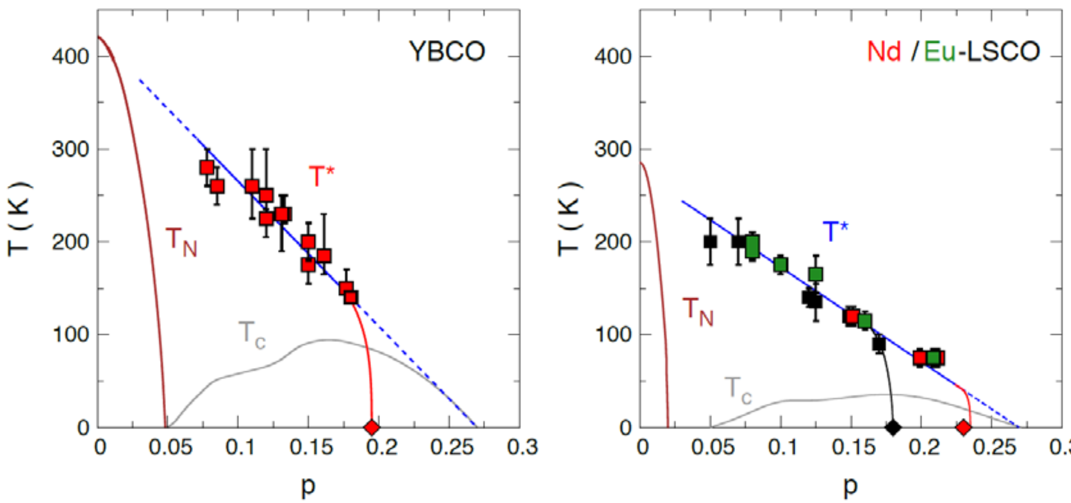


Maier Scalapino, arXiv:1810.10043

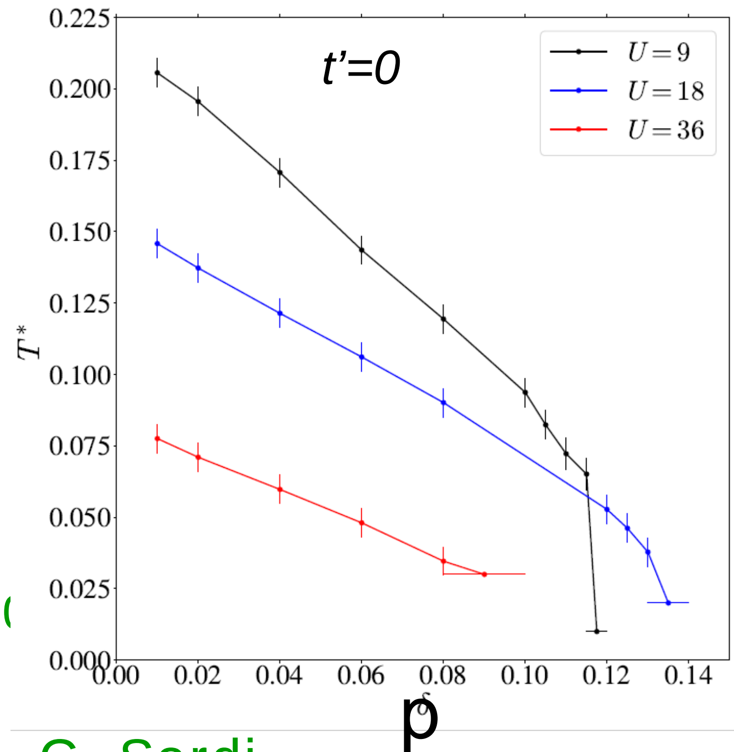
Results T*

$$k_\mathrm{B}T^* \sim J$$

$J = 4t^2/U$



Cyr-Choinières et al. Phys. Rev. B **97**, 0645

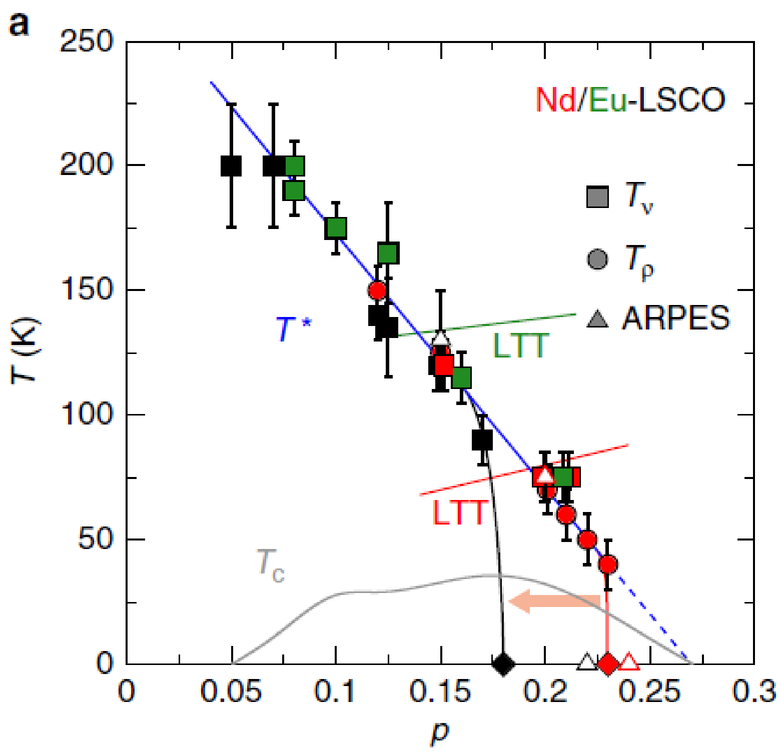


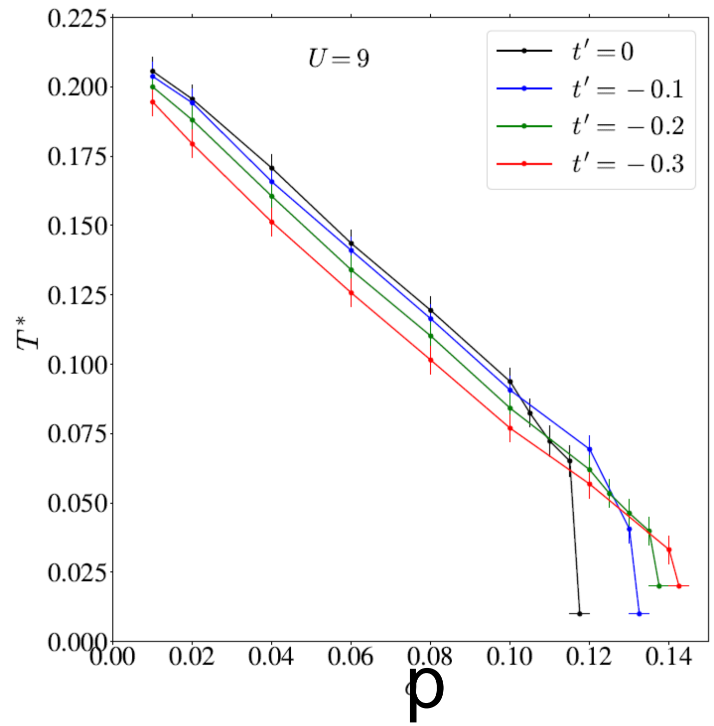
A. Reymbaut, M. Thénault, L. Fratino, G. Sordi, P. Sémon, AMT, unpublished

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**

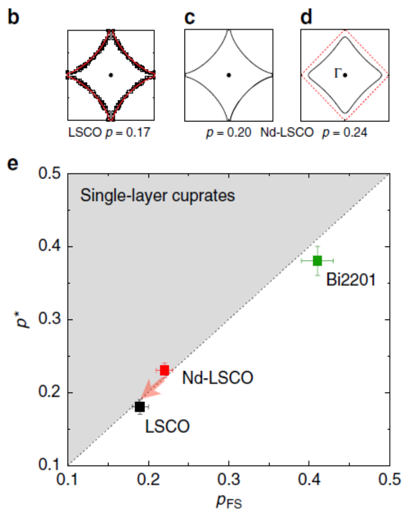




Doiron-Leyraud *et al.*
Nature Comm. **8** 2044

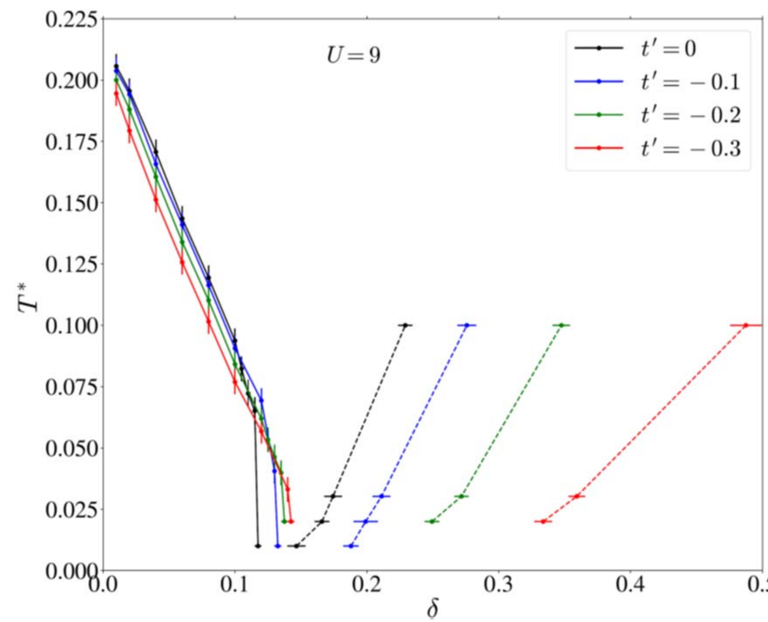
A. Reymbaut, M. Thénault, L. Fratino,
G. Sordi, P. Sémon, AMT, unpublished

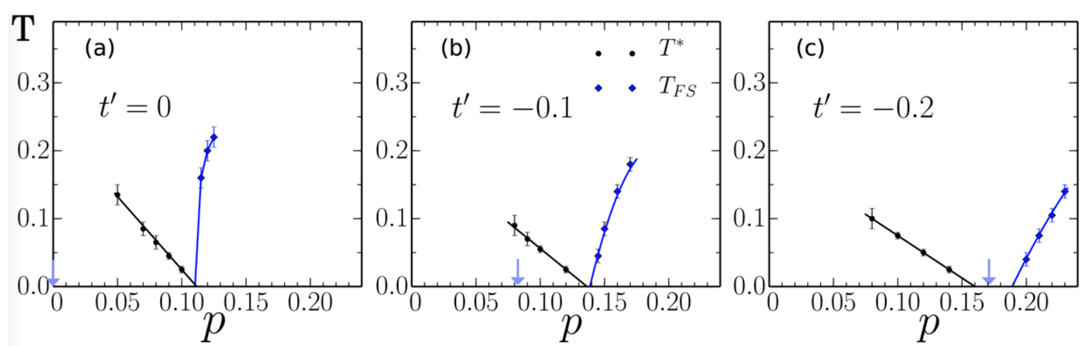
Results: van Hove singularity $\delta^* \leqslant \delta_{vH}$



$p^* < p_{fs}$

Doiron-Leyraud *et al.*
Nature Comm. **8** (2017)



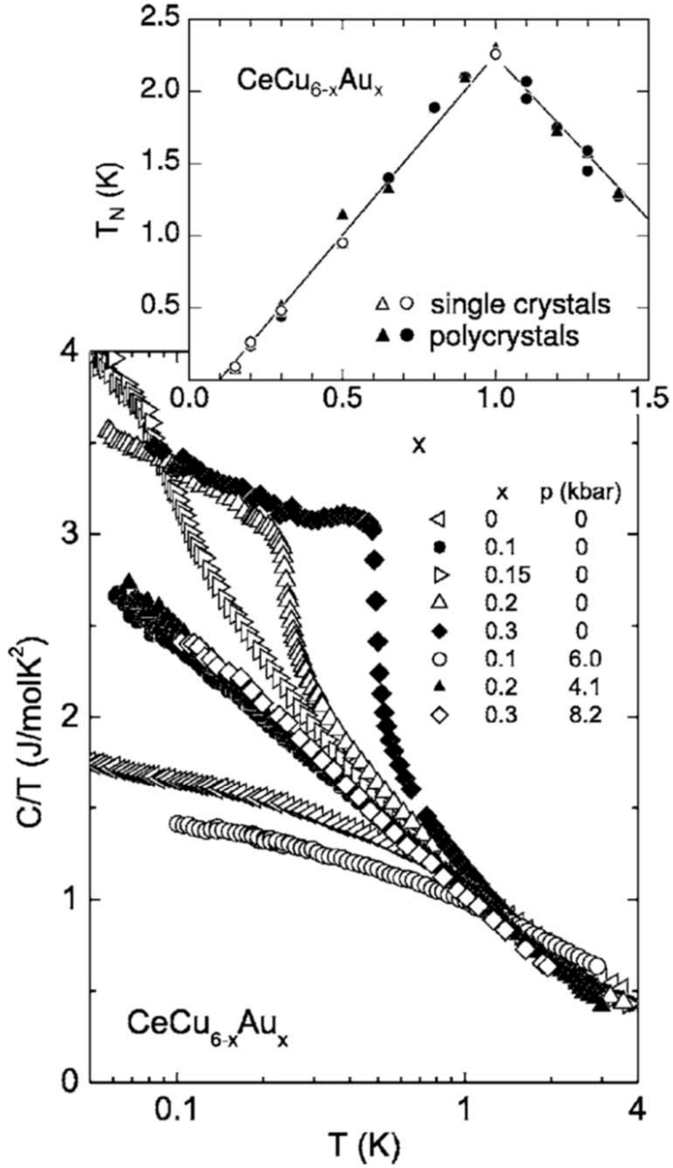


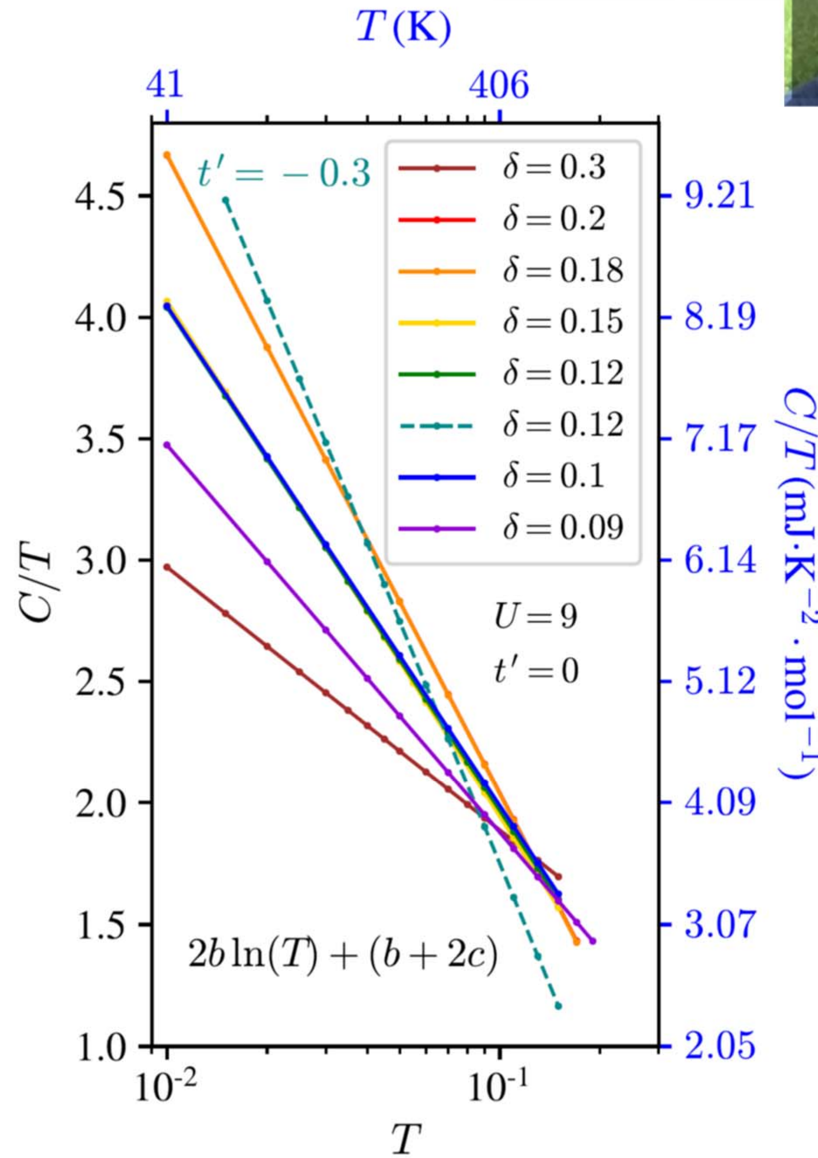
W Wu et al. - arXiv preprint arXiv:1707.06602

Bragança, Sakai, et al. PRL **120**, 067002 (2018)

Quantum critical scaling

Alexis Reymbaut





Hilbert v. Löhneysen Rev. Mod. Phys. **79**, (2007)

S.-X. Yang, *et al.* PRL 106 (2011)

Giovanni Sordi

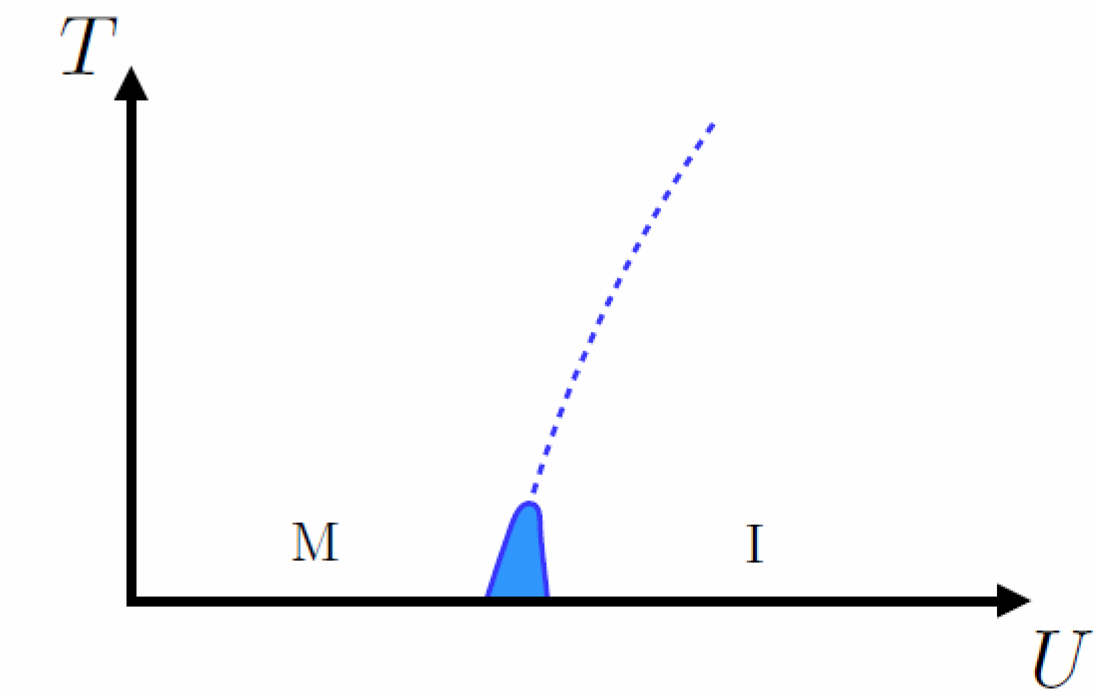
Kristjan Haule

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)

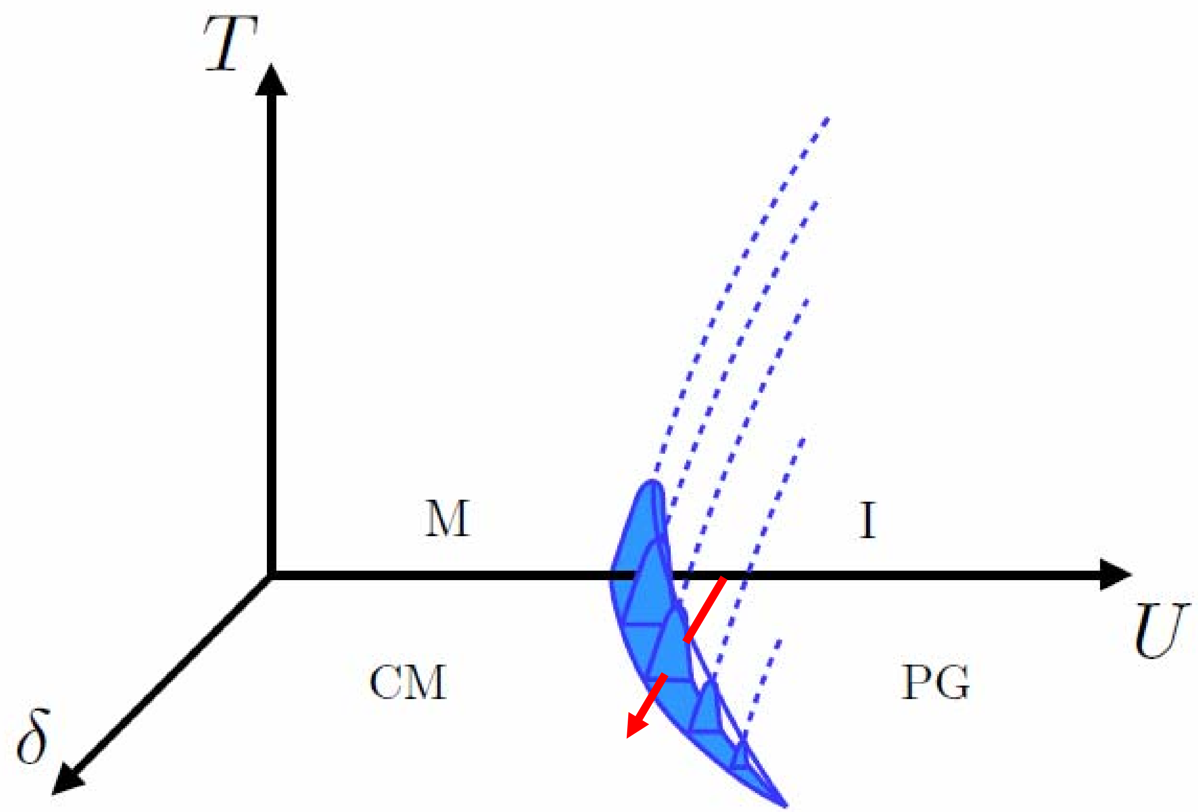
Influence of Mott transition away from half-filling

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



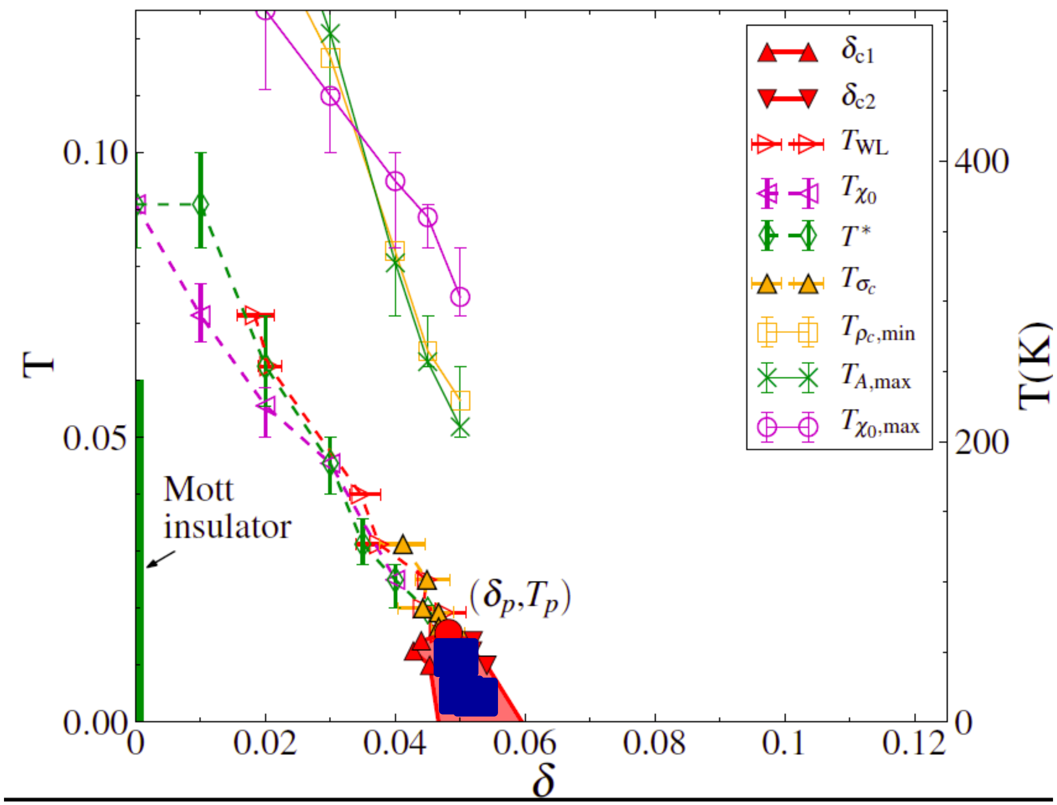
Influence of Mott transition away from half-filling

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



Two crossover lines

Giovanni Sordi

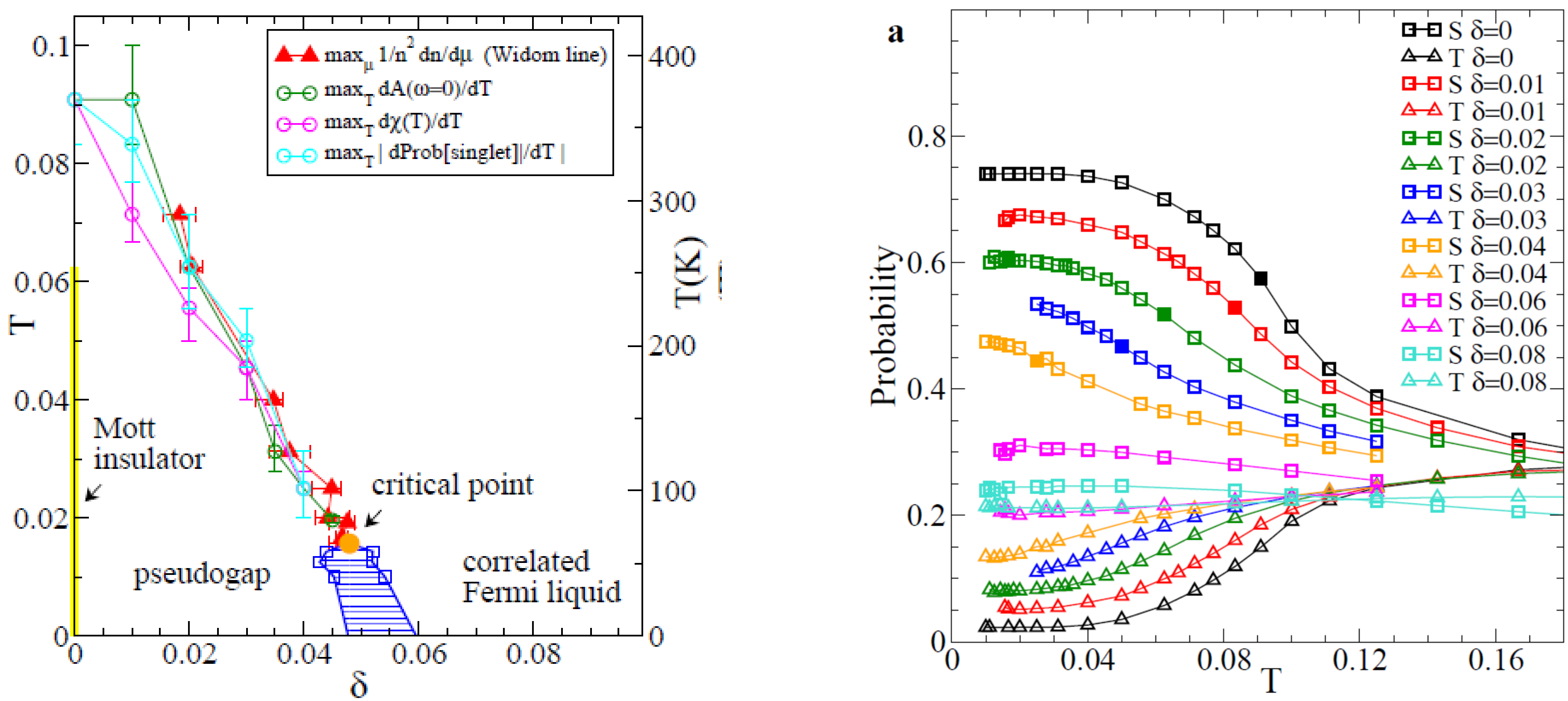


Patrick Sémon

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)

Plaquette eigenstates



See also:

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

Part III:

Strongly correlated superconductivity

UNIVERSITÉ DE SHERBROOKE

USHERBROOKE.CA/IQ


Giovanni Sordi


Patrick Sémon


Lorenzo Fratino

Superconductivity
in a doped Mott insulator

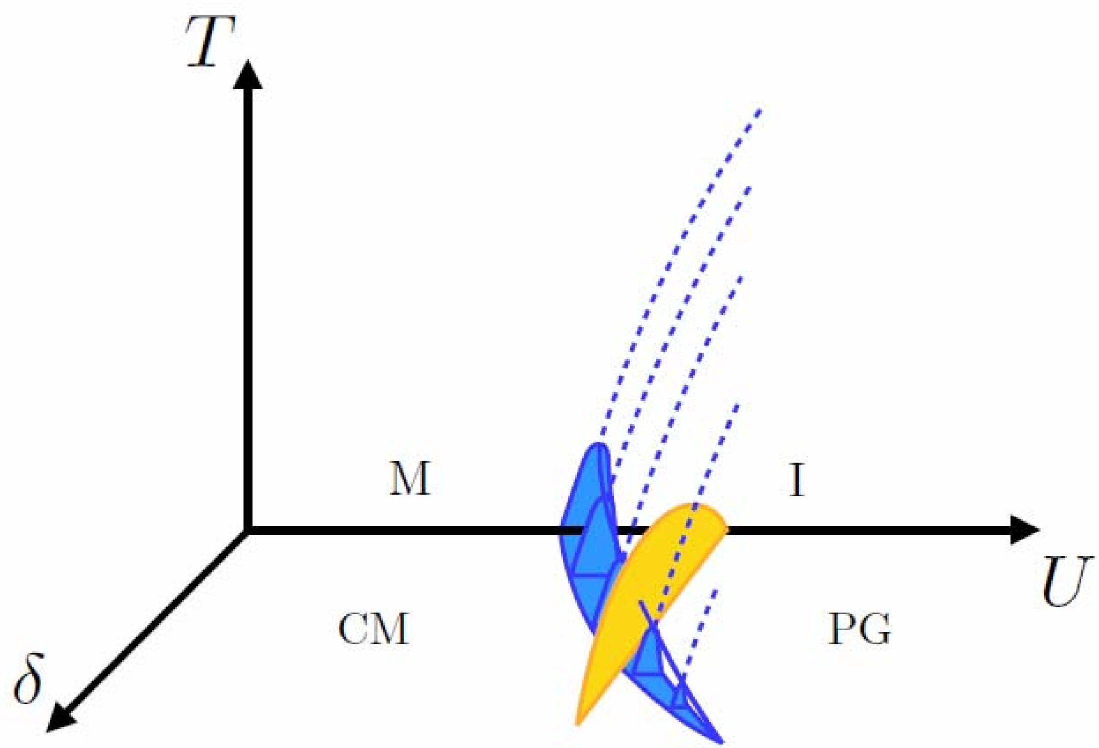
Sordi et al. PRL **108**, 216401 (2012)

Fratino et al.

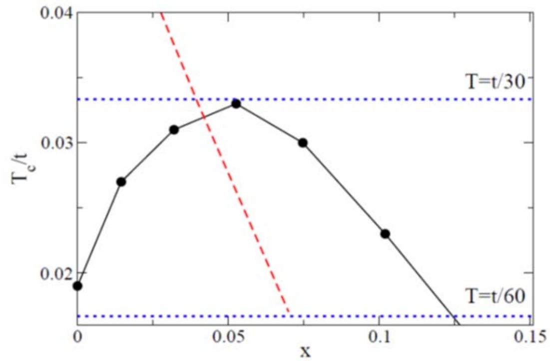
Sci. Rep. **6**, 22715 (2016)

Superconductiviy in Doped Mott insulator

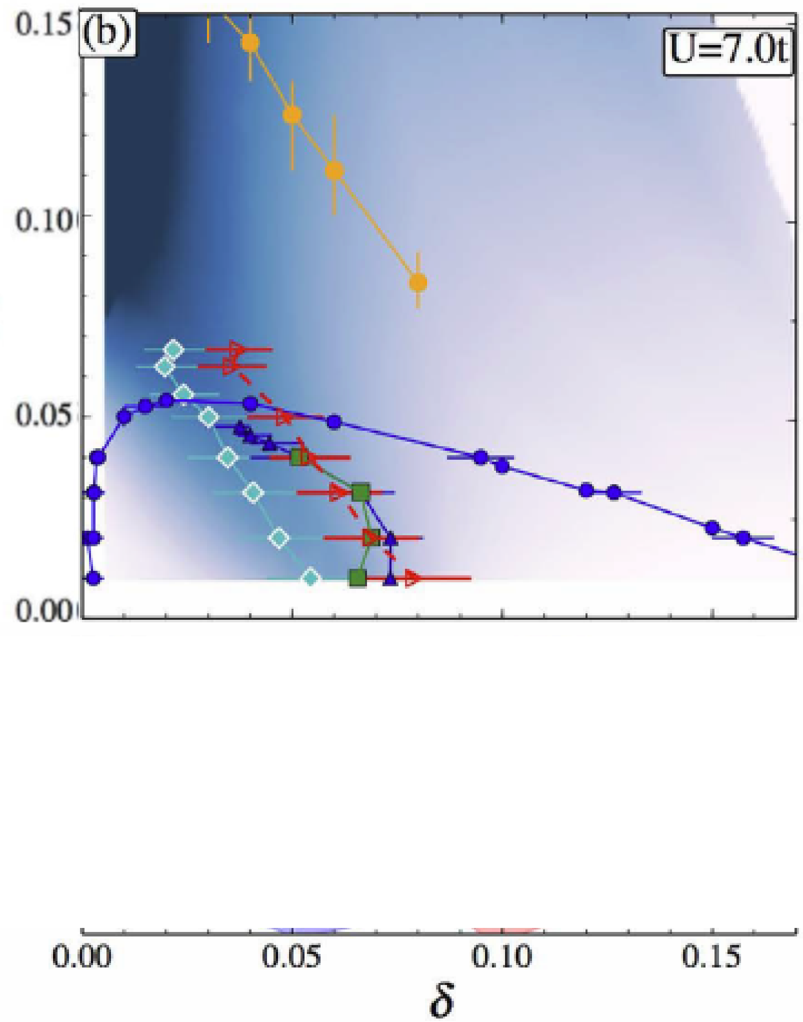
$n = 1, d = 2$ square lattice



An organizing principle



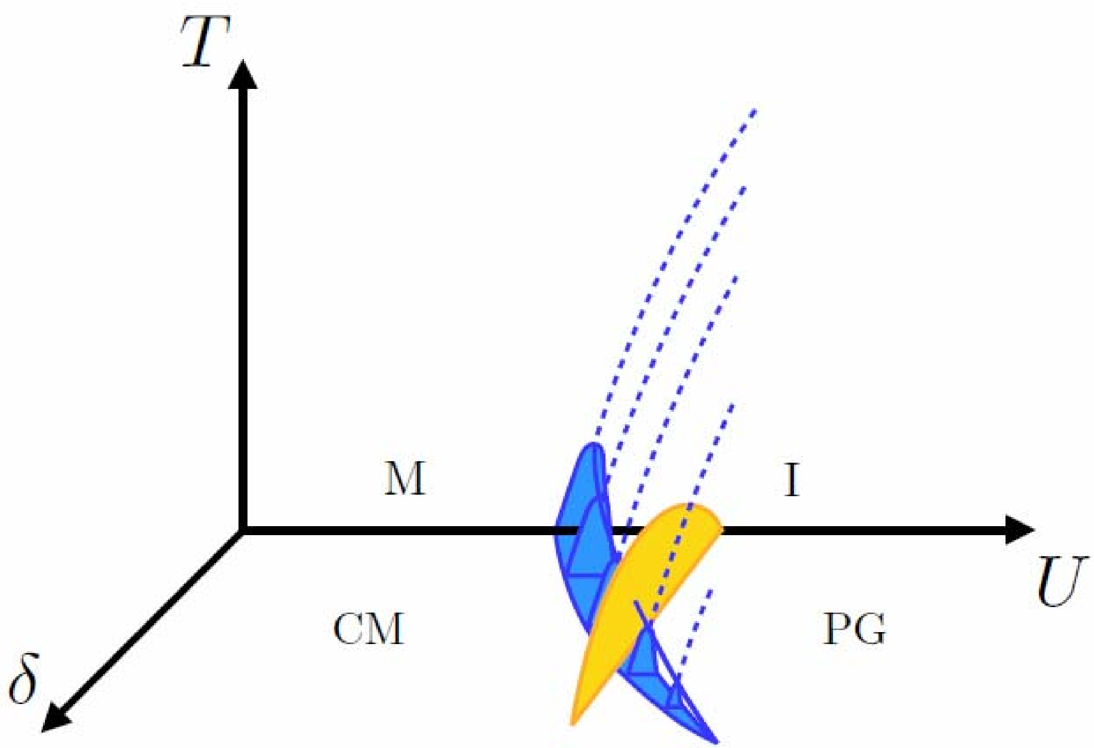
E. Gull and A. J. Millis
Phys. Rev. B 88, 075127



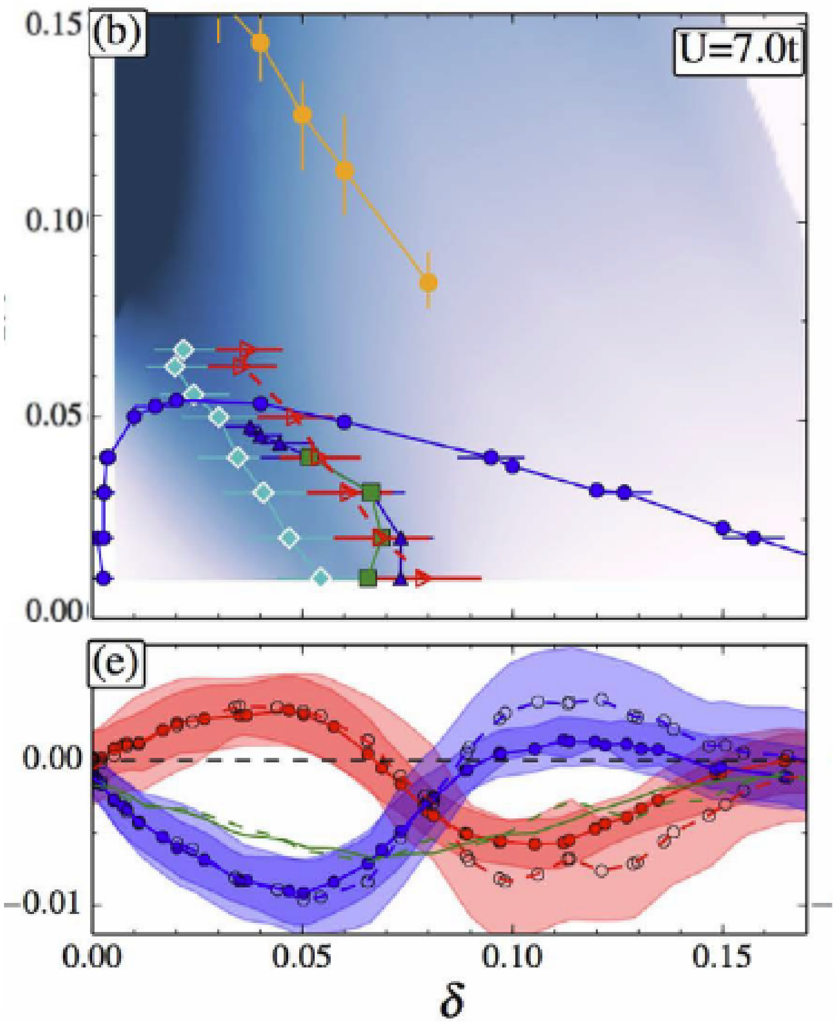
Fratino et al.
Sci. Rep. **6**, 22715

Superconductiviy in Doped Mott insulator

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



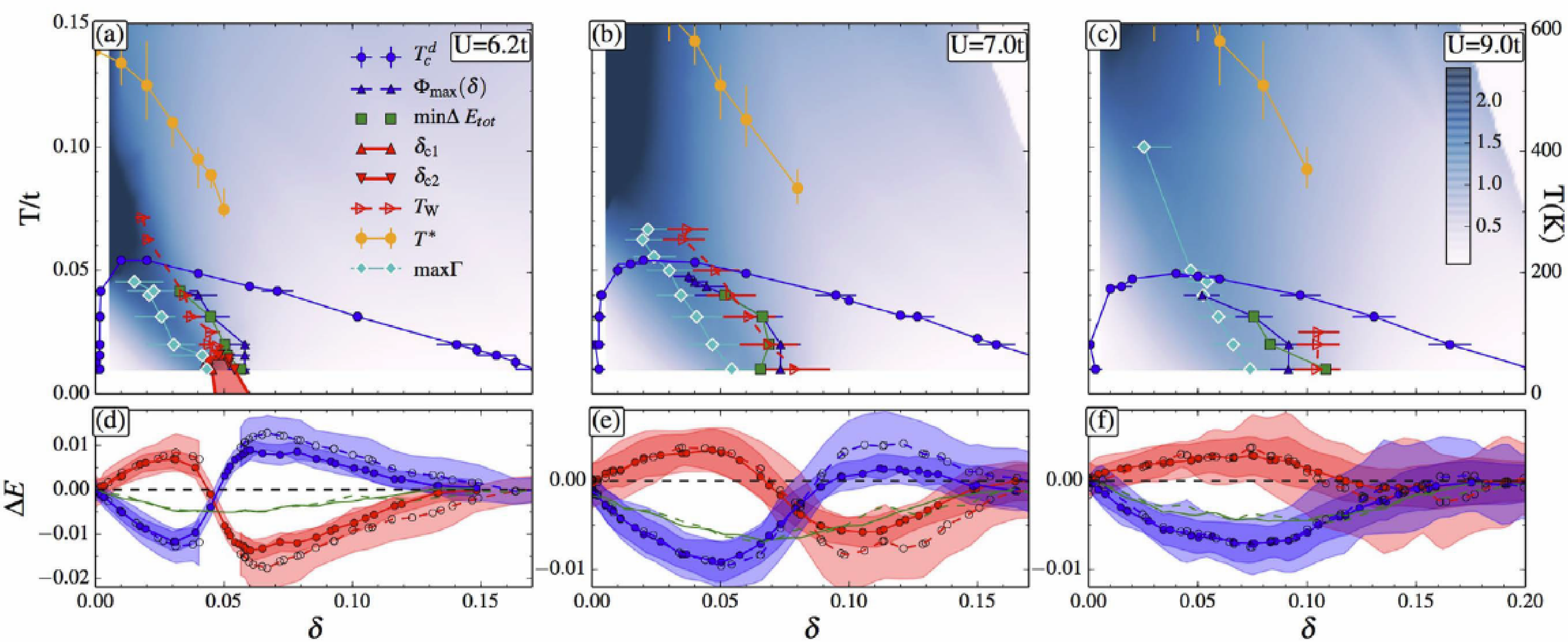
An organizing principle



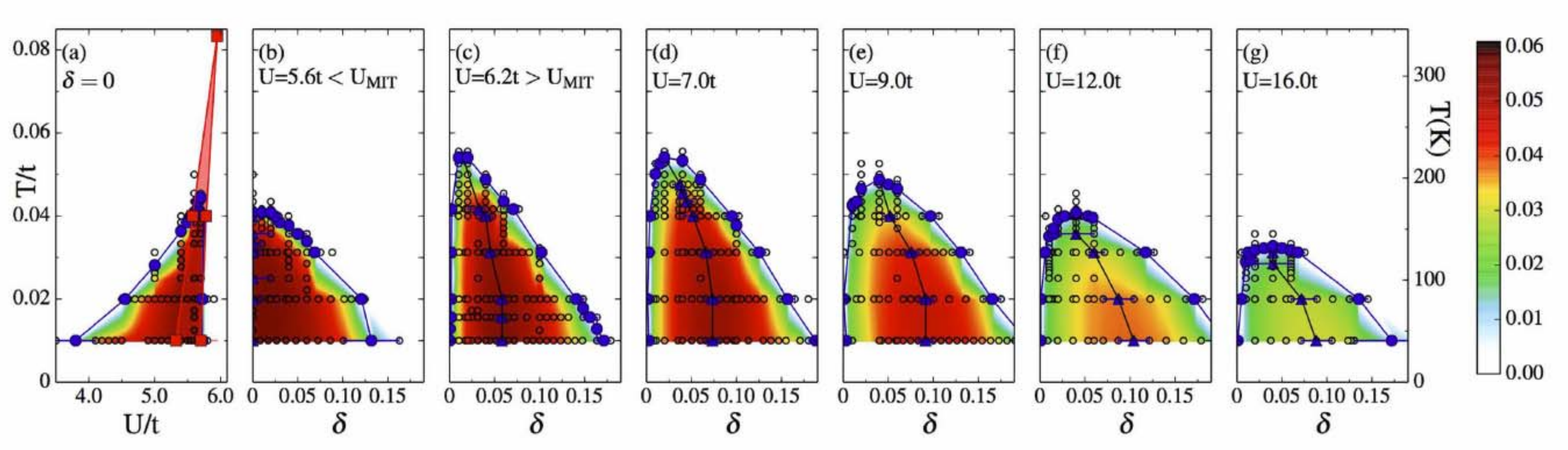
Fratino et al.
Sci. Rep. **6**, 22715

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

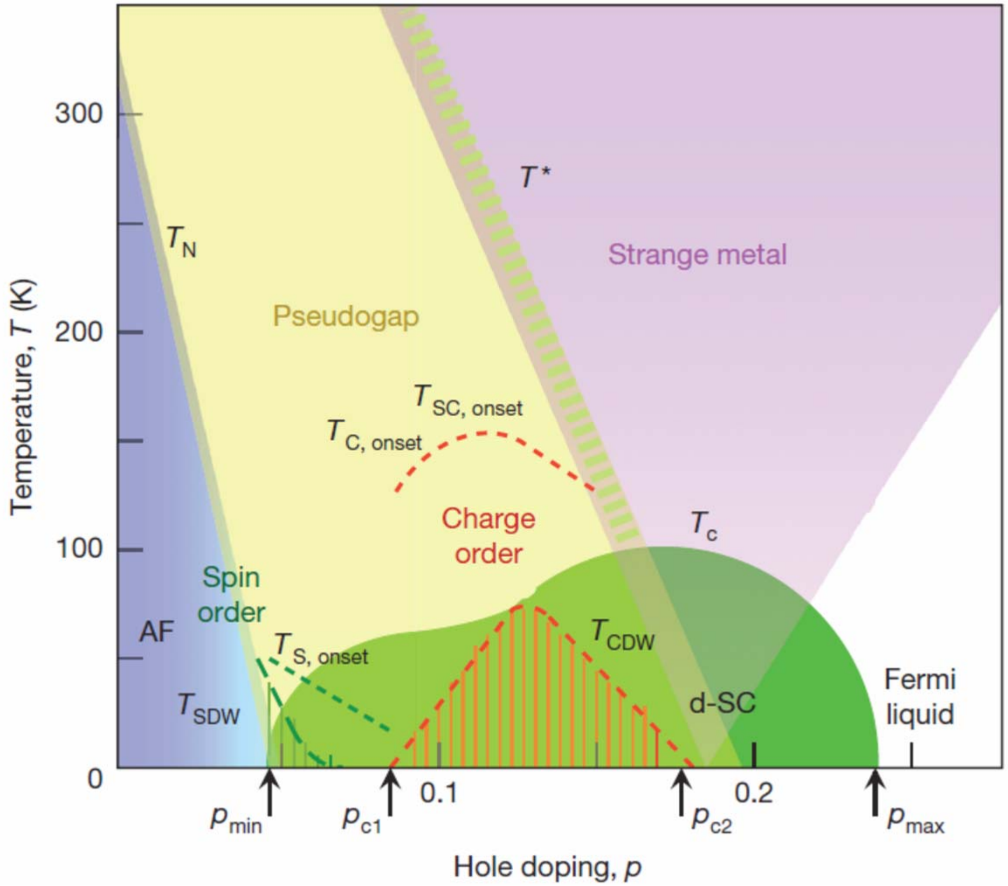
A. Pushp, Parker, … A. Yazdani, Science **364**, 1689 (2009)

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

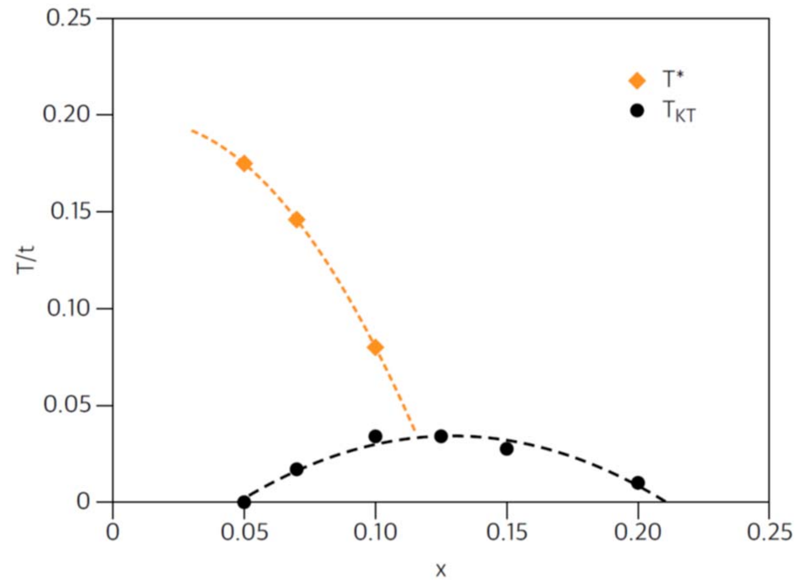
Patrick M. Rourke, et al. Hussey Nature Physics **7,** 455–458 (2011)

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

Phase diagram $YBa_2Cu_3O_{7-x}$



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

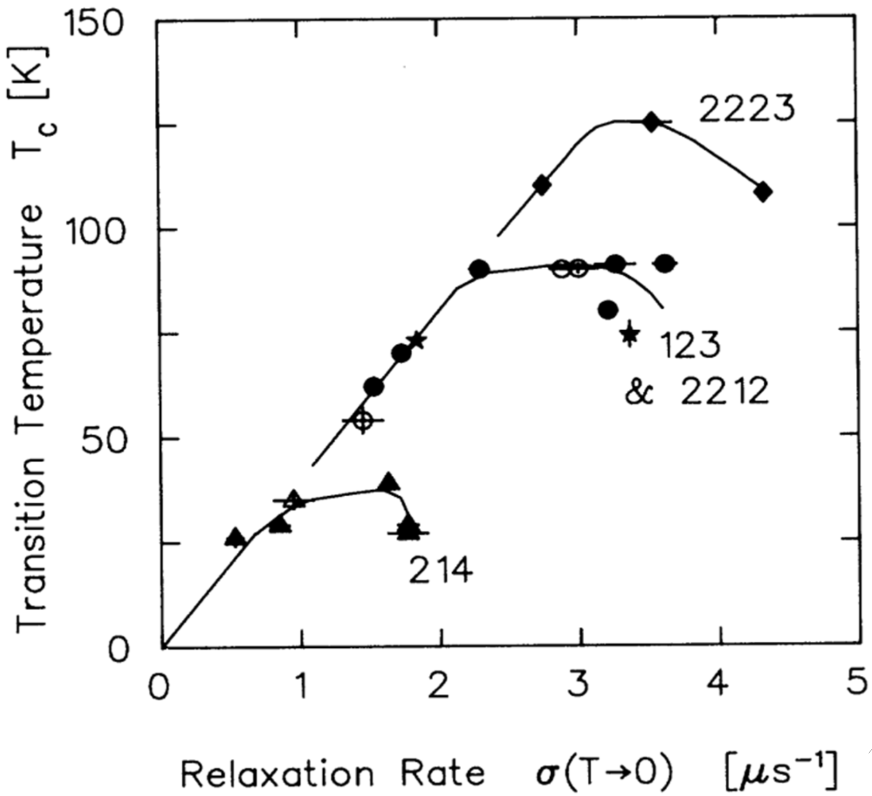


Maier Scalapino, arXiv:1810.10043

U=7, t'=-0,15

What causes T_c to drop?

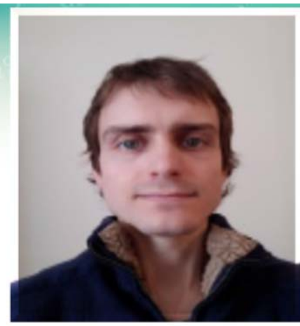
Phase fluctuations? Emery Kivelson Nature **374** (1995)



$\sigma \propto \rho_s$

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


Olivier Simard


Charles-David Hébert

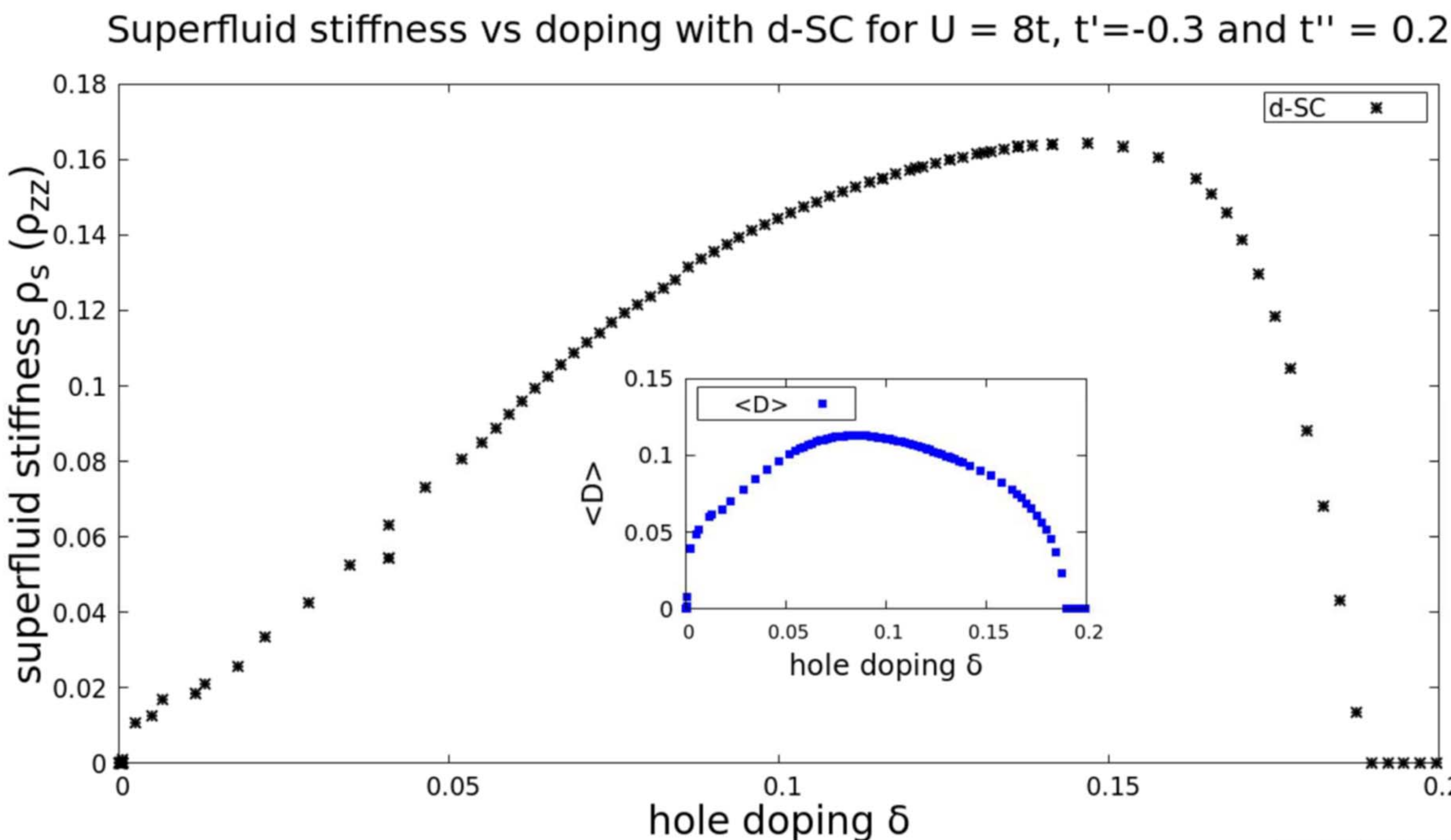

Alexandre Foley


David Sénéchal

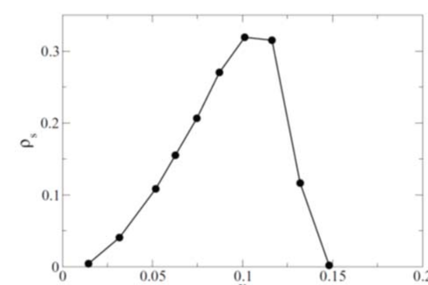
What causes T_c to drop near $n = 1$?

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

Superfluid stiffness *T=0*



Also E. Gull, A.J. Millis, Phys. Rev. B **88**, 075127 (2013), U=6



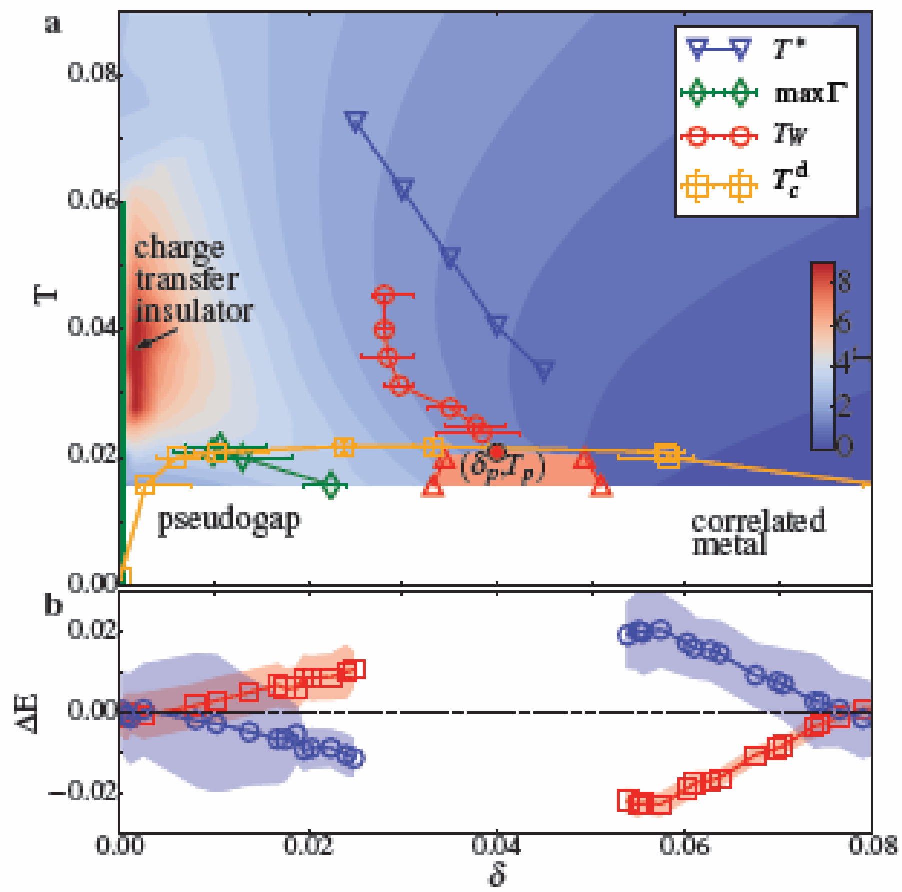
Giovanni Sordi

Lorenzo Fratino

Patrick Sémon

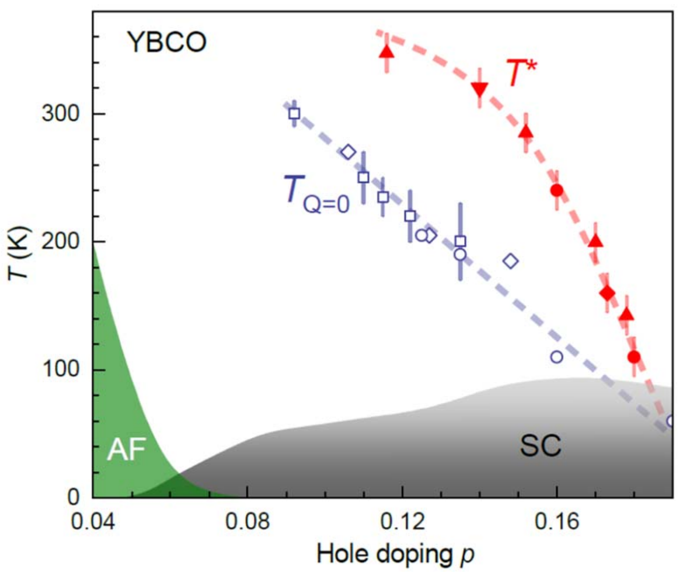
h-doped as charge-transfer insulator

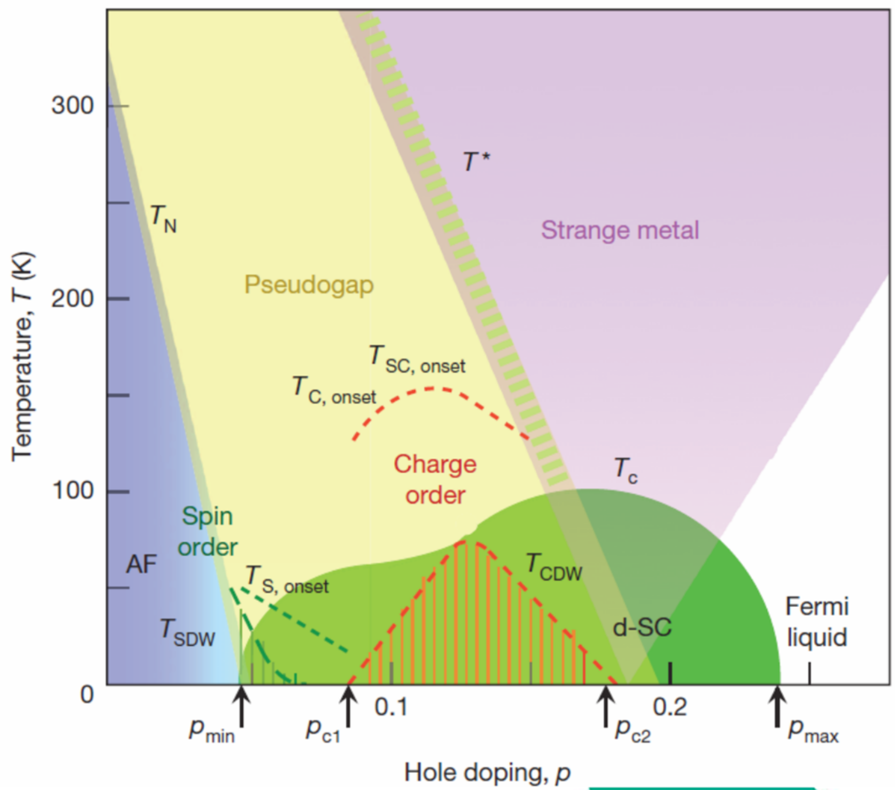
3 bands, charge transfer insulator



Fratino et al. PRB **93**, 245147 (2016)

Conclusion

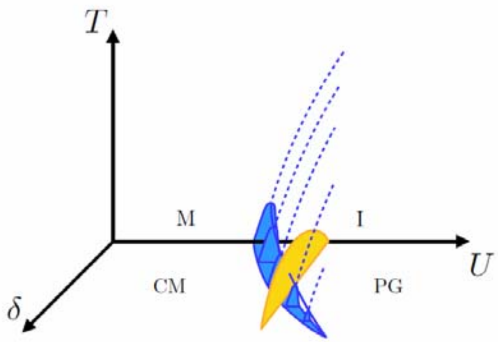


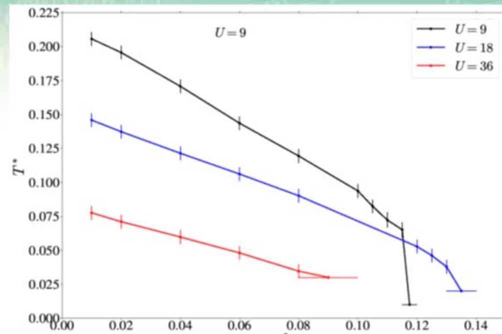


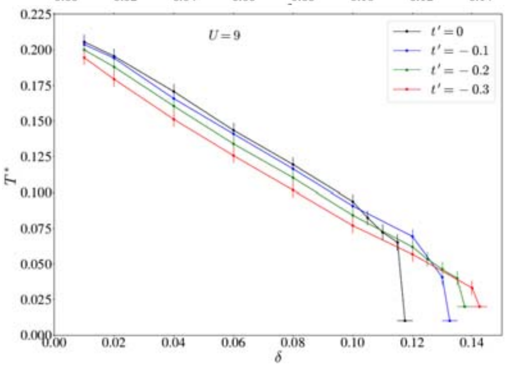
Courtesy, M-H. Julien

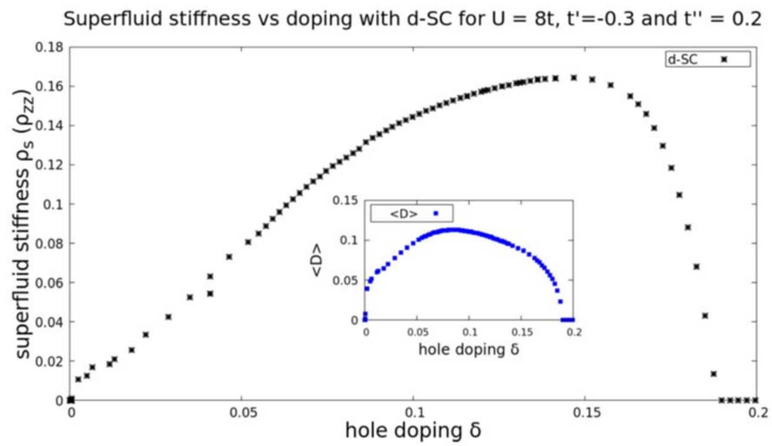
p or δ

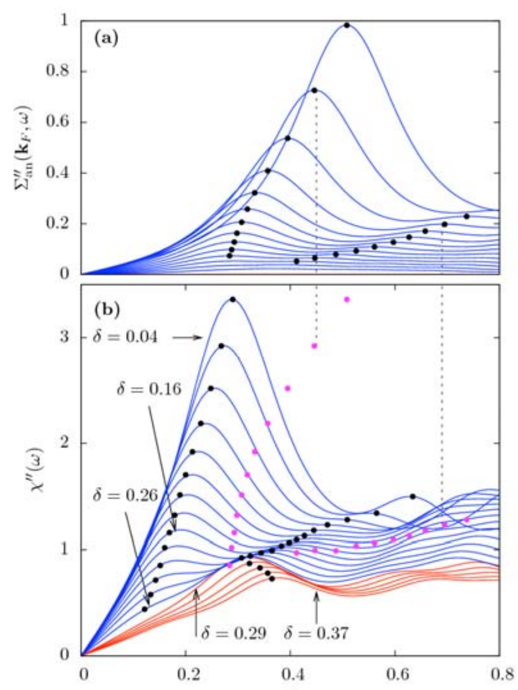
Keimer et al., Nature 518, 179 (2015)

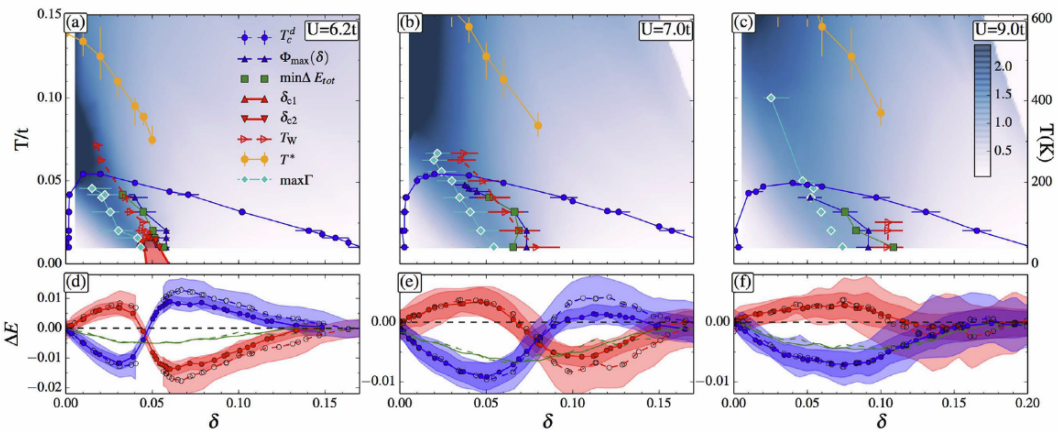

T
M
I
U
δ
CM
PG


U = 9
U = 9
U = 18
U = 36
T*
δ

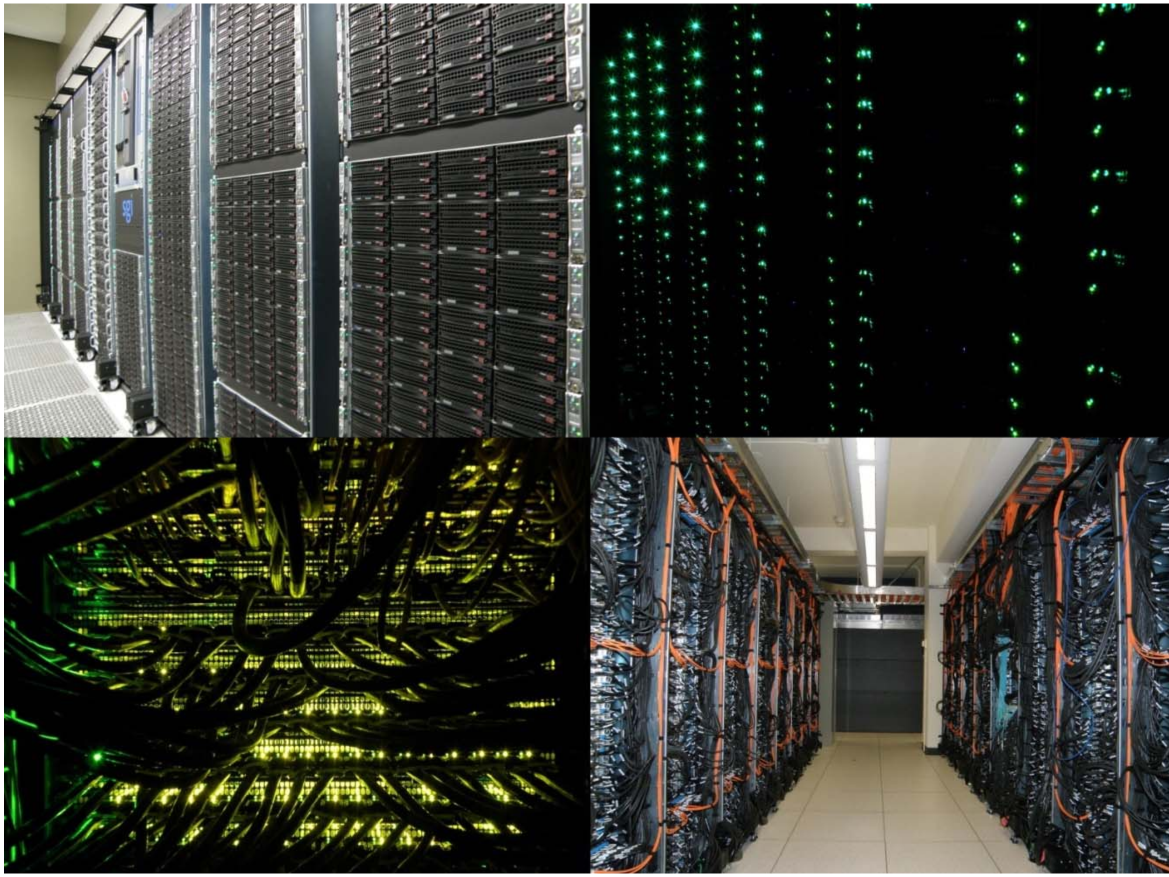

U = 9
t' = 0
t' = − 0.1
t' = − 0.2
t' = − 0.3
T*
δ


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)
Σ''an(kF, ω)
(b)
δ = 0.04
δ = 0.16
δ = 0.26
δ = 0.29
δ = 0.37
χ''(ω)
ω


(a)
U=6.2t
(b)
U=7.0t
(c)
U=9.0t
Tcd
Φmax(δ)
minΔ Etot
δc1
δc2
TW
T*
maxΓ
T/t
T(K)
(d)
(e)
(f)
ΔE
δ

Mammouth



Éducation, Loisir et Sport Québec

Canada Foundation for Innovation
Fondation canadienne pour l'innovation

compute • calcul CANADA

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

UNIVERSITÉ DE SHERBROOKE

USHERBROOKE.CA/IQ