Pseudogap and superconductivity in cuprates, a dynamical mean-field perspective

A.-M.S. Tremblay,
S. Bergeron, Maxime Charlebois, L. Fratino,
A. Foley, Charles-David Hébert, A. Reymbaut, D. Sénéchal
O. Simard, G. Sordi, Patrick Sémon, M. Thénault

Ringberg symposium on
Unconventional Superconductivity and Spin Liquids,
14-18 Oct. 2019

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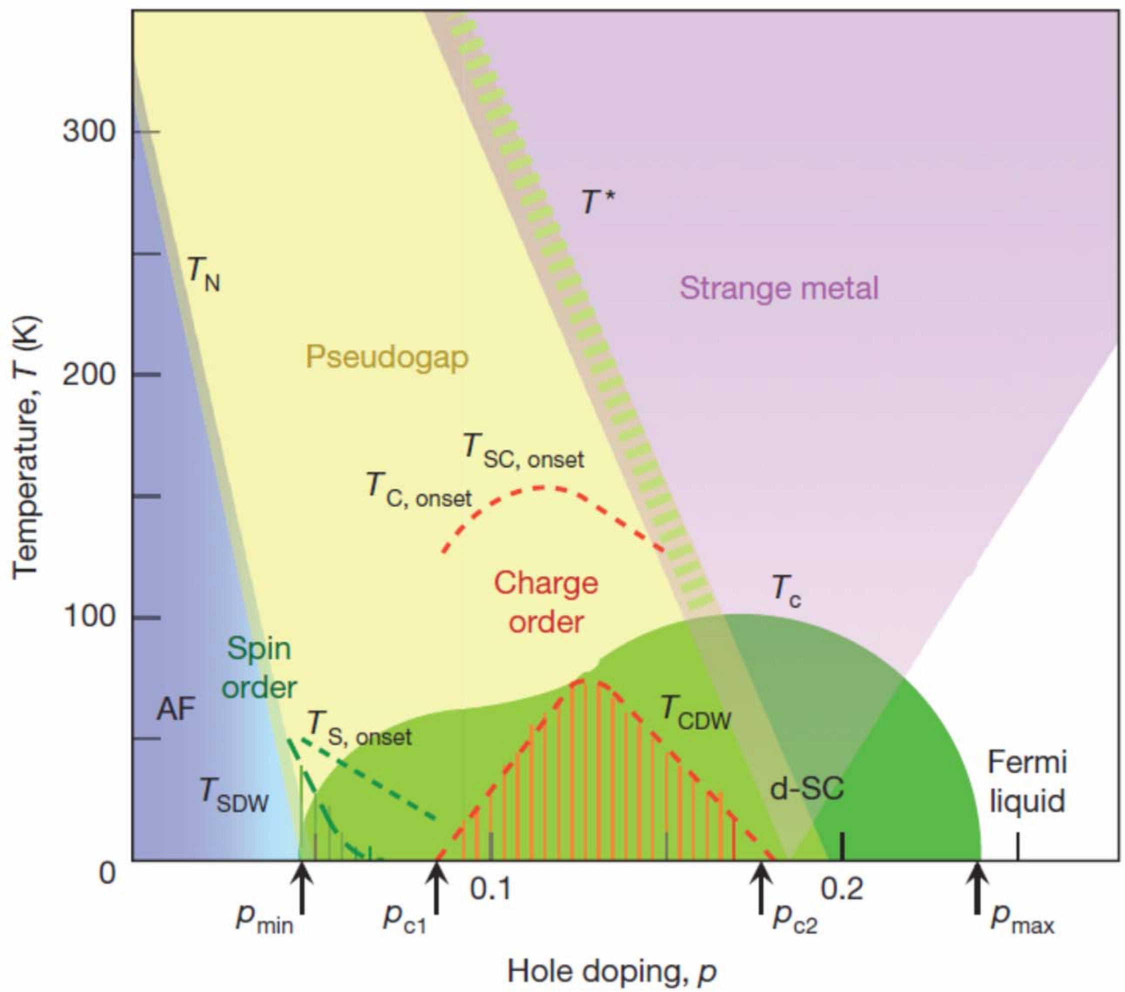
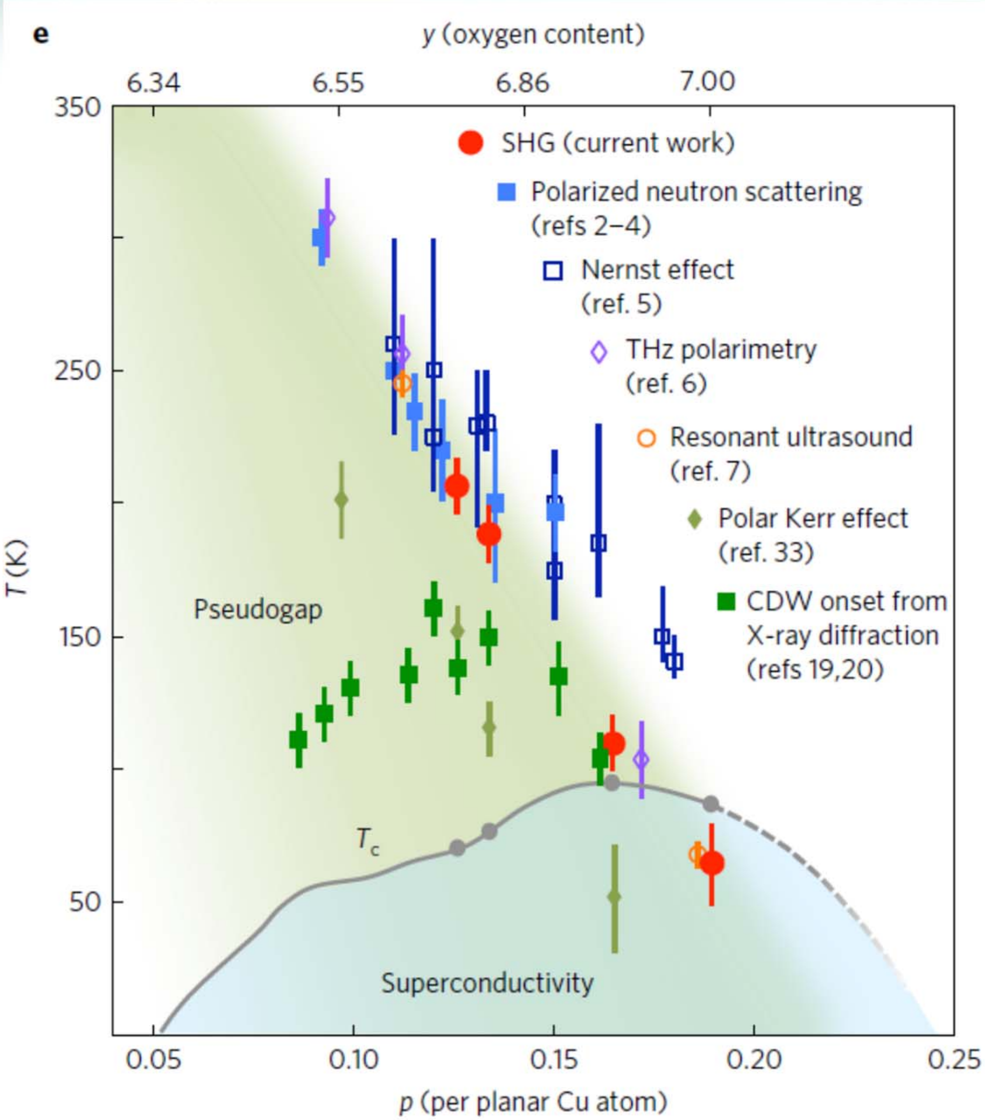
Phase diagram $YBa_2Cu_3O_{7-x}$



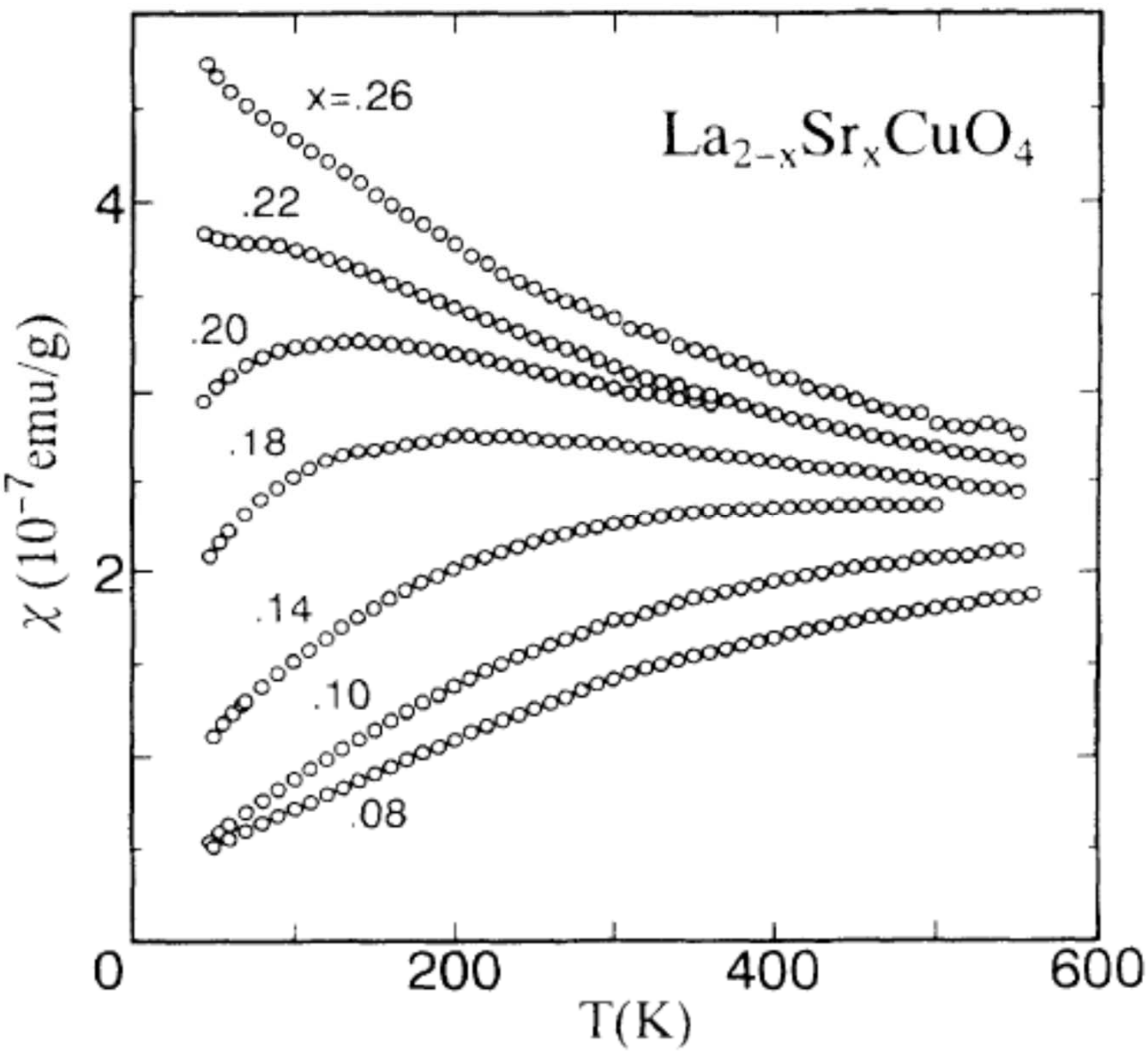
p or δ

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



Zhao *et al.* Nat. Phys. 13, 250 (2017).

Knight shift (Spin susceptibility)



Nakano *et al.* Phys. Rev. B **49**, 16000 (1994)
Alloul *et al* (1989)

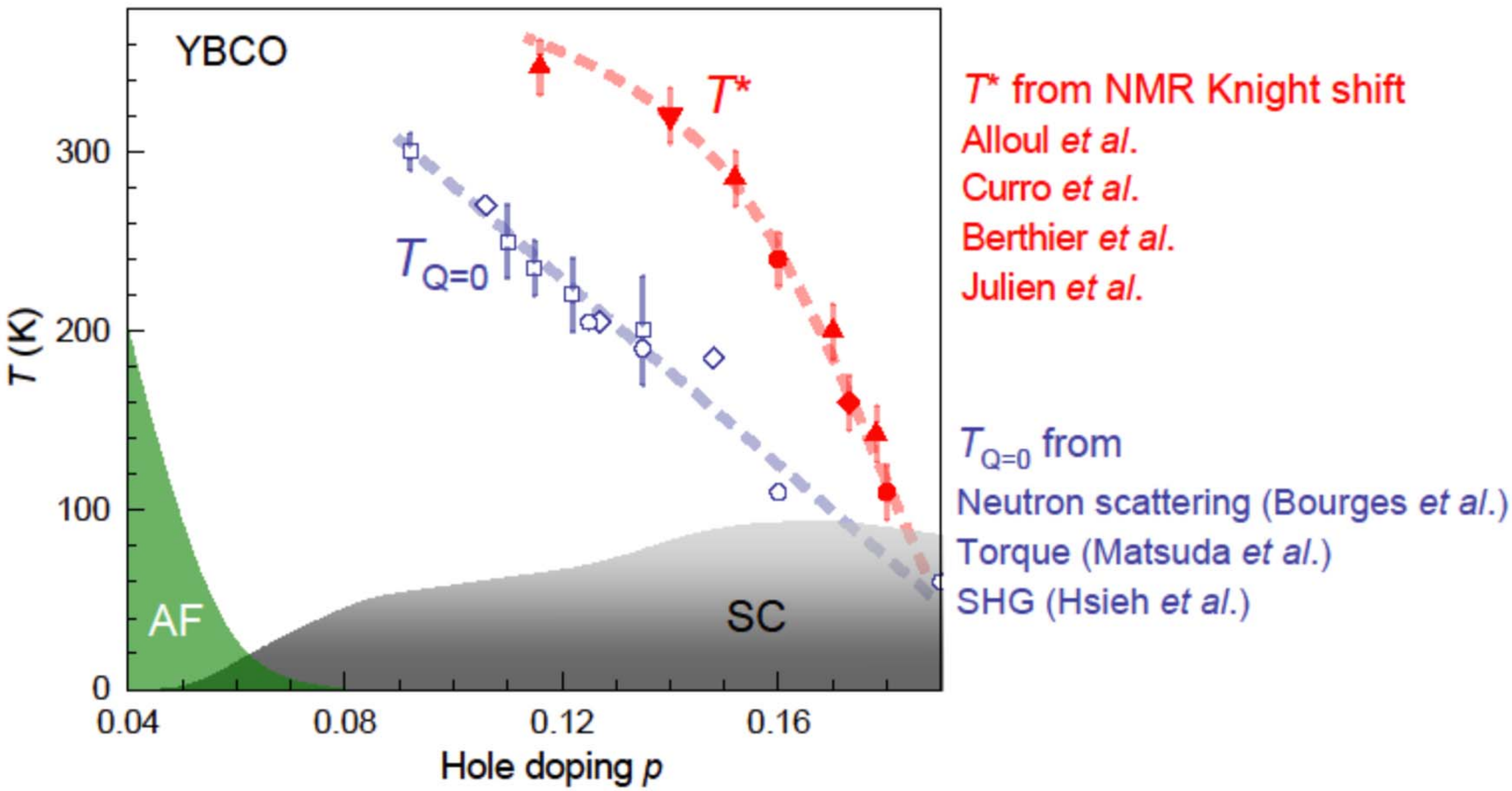


Figure from: Marc-Henri Julien

Model

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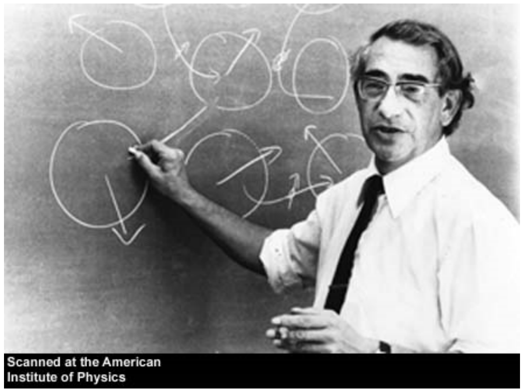
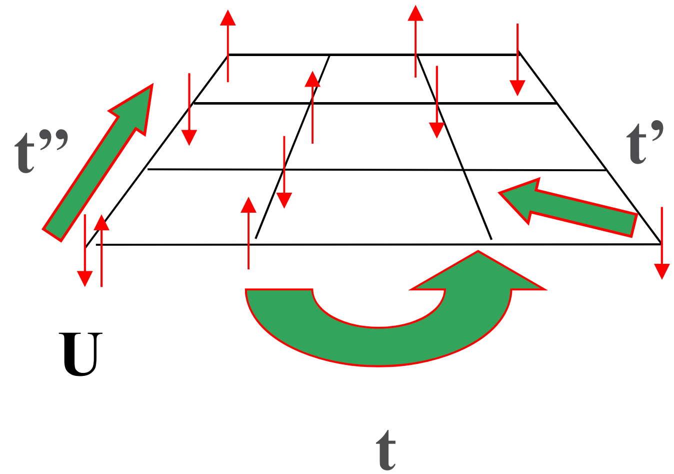
Hubbard model

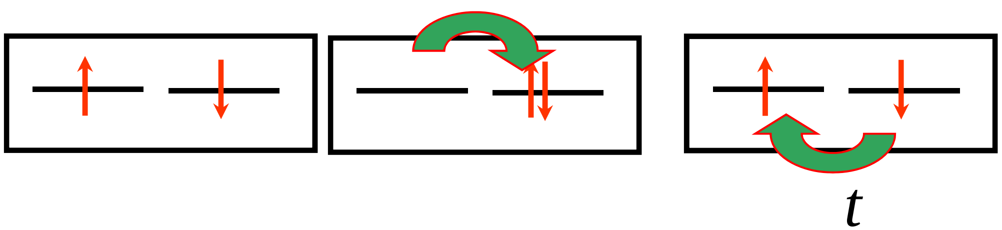


μ



1931-1980

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



Effective model, Heisenberg: $J = 4t^2/U$

Attn: Charge transfer insulator

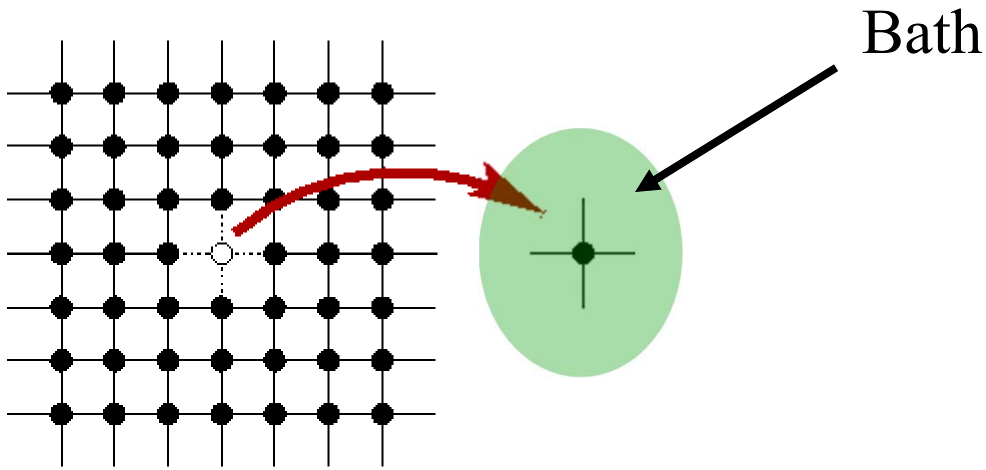
Method

- 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

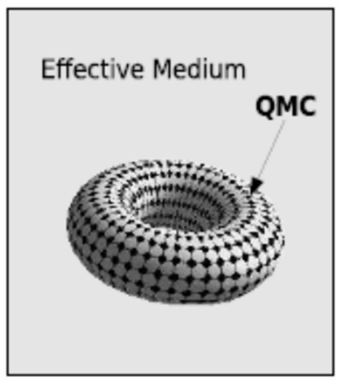
Dynamical Mean-Field Theory.
The beginnings in *d = infinity*



W. Metzner and D. Vollhardt, PRL (1989)
A. Georges and G. Kotliar, PRB (1992)
M. Jarrell PRB (1992)

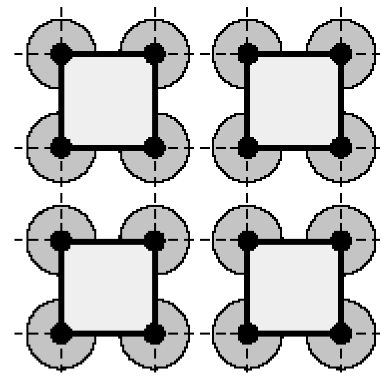
DMFT, (d = *3)*

2d Hubbard: Quantum cluster method

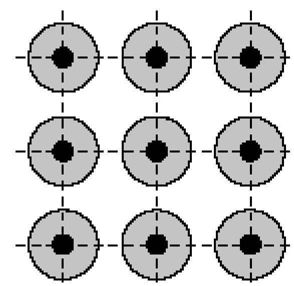


DCA

C-DMFT



DMFT



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

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

+ 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
  - Hence good when the correponding correlation lengths are small

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

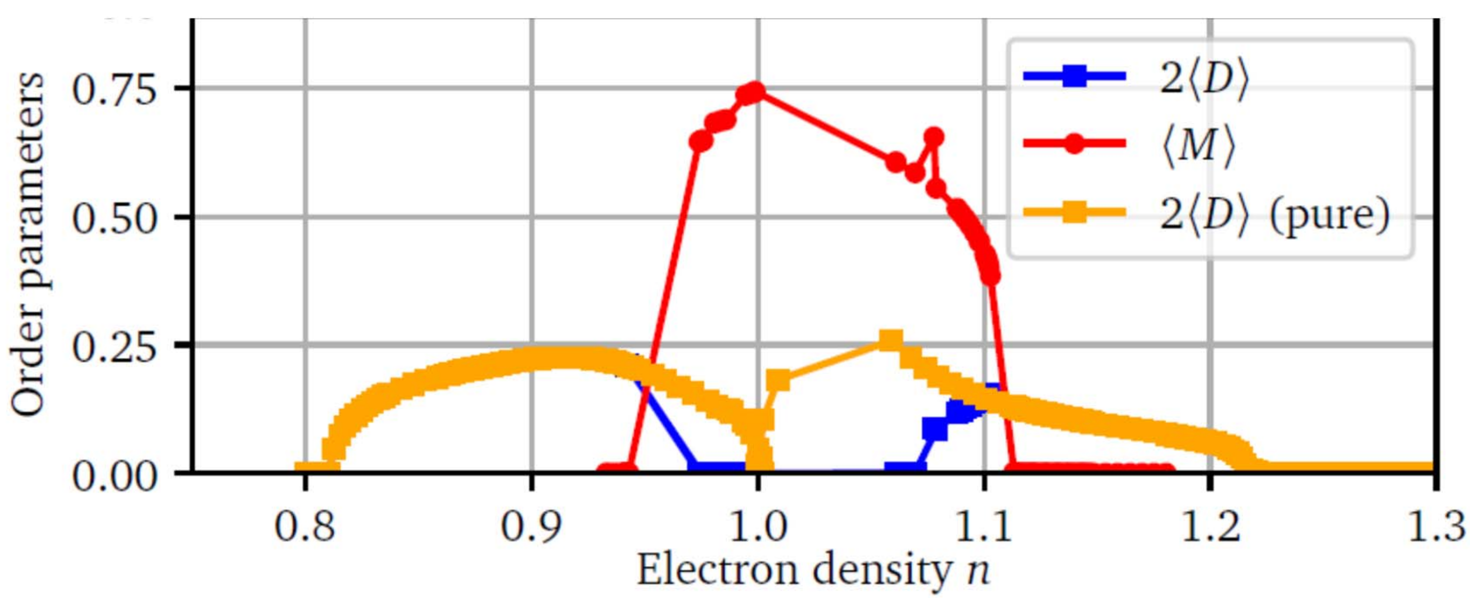
- Part I: $T = 0$ phase diagram
- Part II: The pseudogap from Knight shift
- Part III: Specific heat in the strange metal
- Part IV: Strongly correlated superconductivity
- Part V: Perspective

Part I

$T = 0$ phase diagram

$T = 0$ phase diagram

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

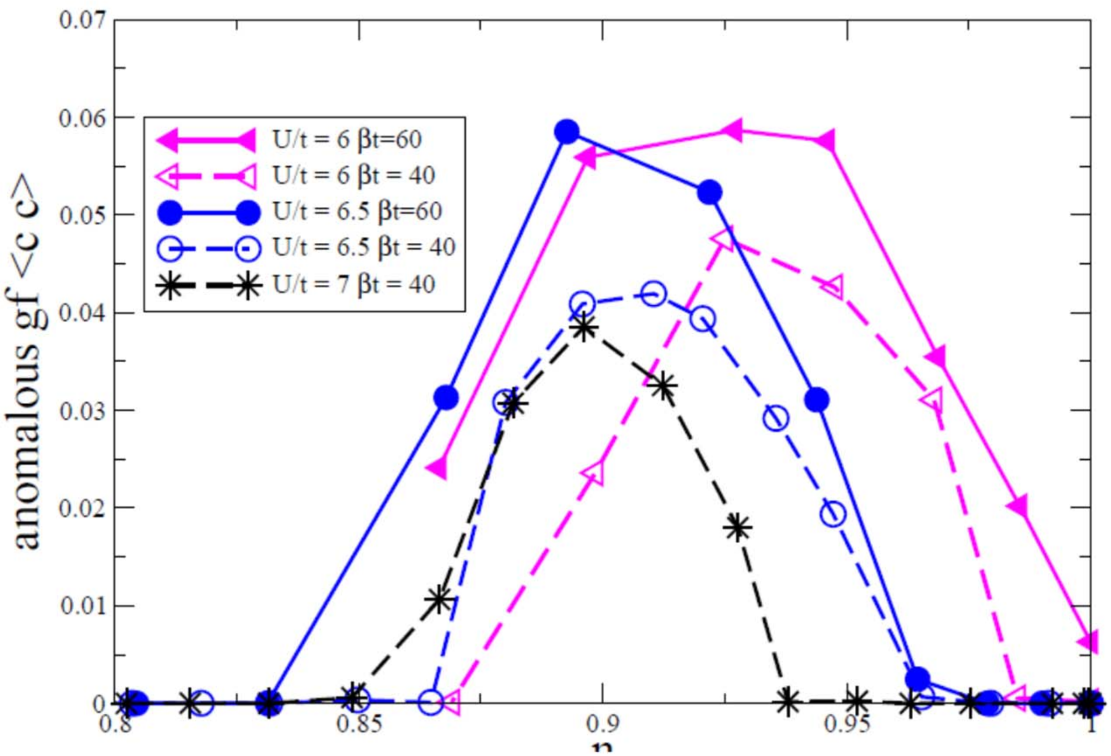


A. Foley *et al.* Phys. Rev. B **99**, 184510 (2019)
S. S. Kancharla, *et al.* Phys. Rev. B **77**, 184516 (2008)
D. Sénéchal, *et al.* Phys. Rev. Lett. **94**, (2005)
M. Jarrell *et al.* EPL **56** 563, (2001)

CDMFT 4 sites

Fall at half-filling without AFM

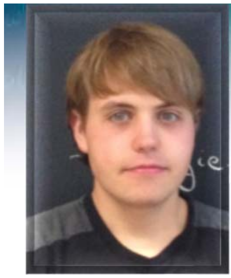
t' = 0   DCA, 8 site



Gull *et al.* Phys. Rev. Lett. **110**, 216405 (2013)

Part II:

The pseudogap



Simon Bergeron

Maxime Charlebois

Patrick Sémon

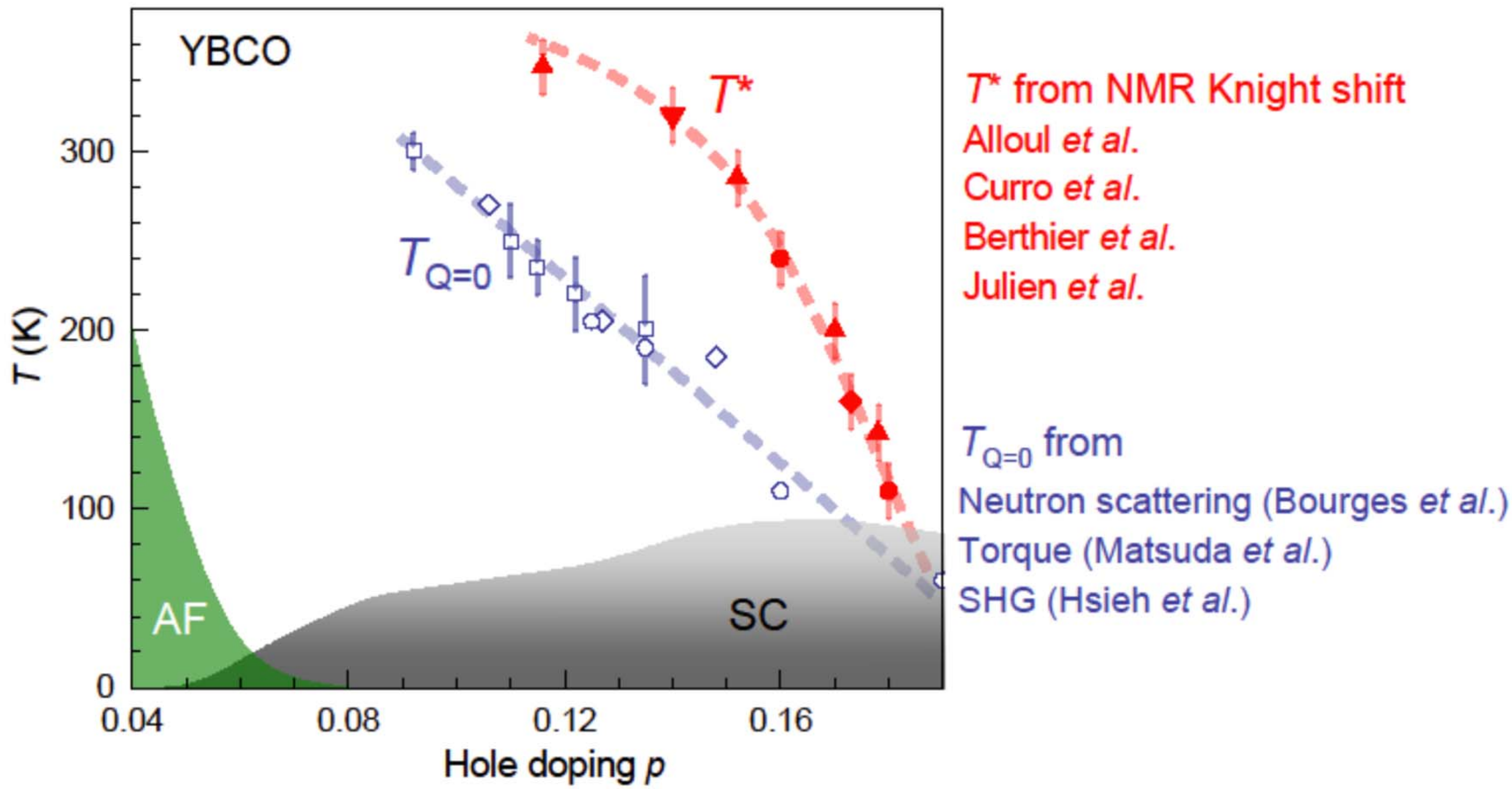
Alexis Reymbaut

R. Garioud

The pseudogap from Knight shift

A. Reymbaut, *et al.* Phys. Rev. Research **1**, 023015 (2019)

Marion Thénault



Thanks: Marc-Henri Julien

Knight shift (Q=0 spin susceptibility)

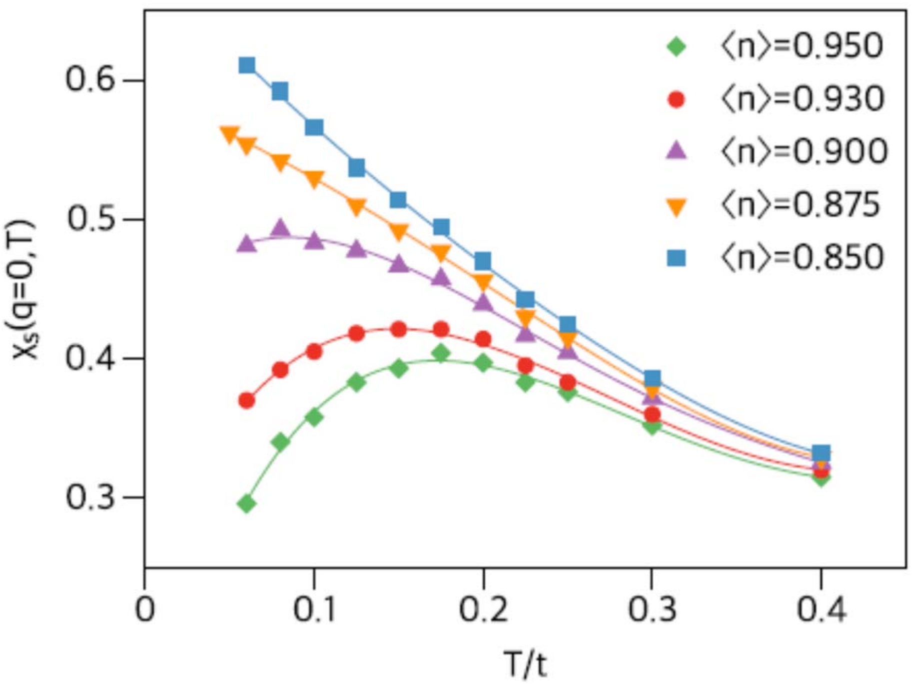
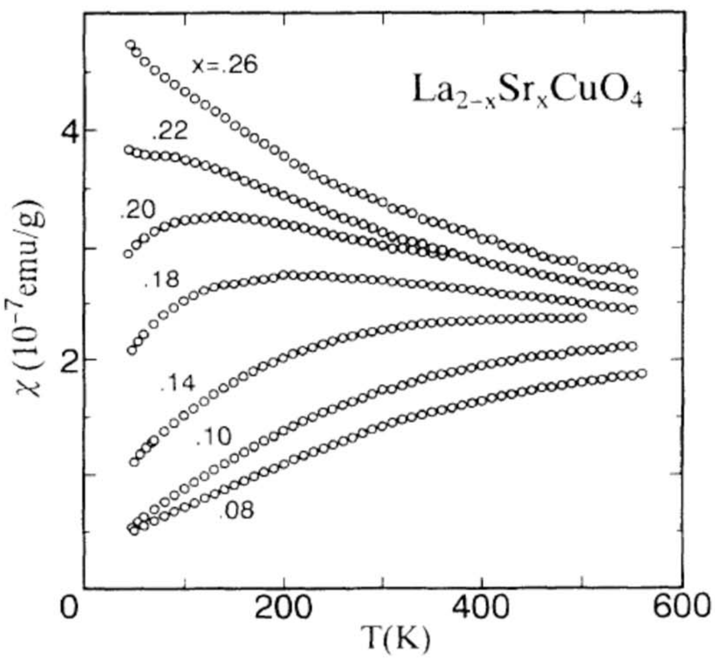


Fig. 3 Temperature and doping dependence of the $q = 0$ spin susceptibility. At the smaller dopings (larger filling $\langle n \rangle$), $\chi_s(T)$ exhibits a peak in the temperature dependence indicating the opening of a PG

DCA 12 sites, *t'=0, U = 7*

T.A. Maier, D.J. Scalapino, npj Quantum Materials (2019)

Comparison



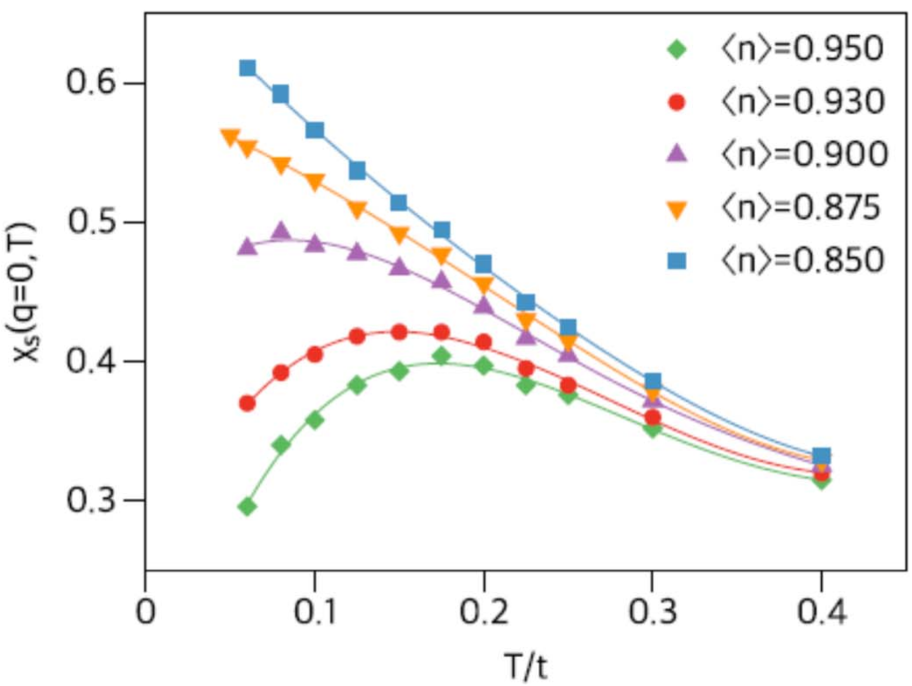
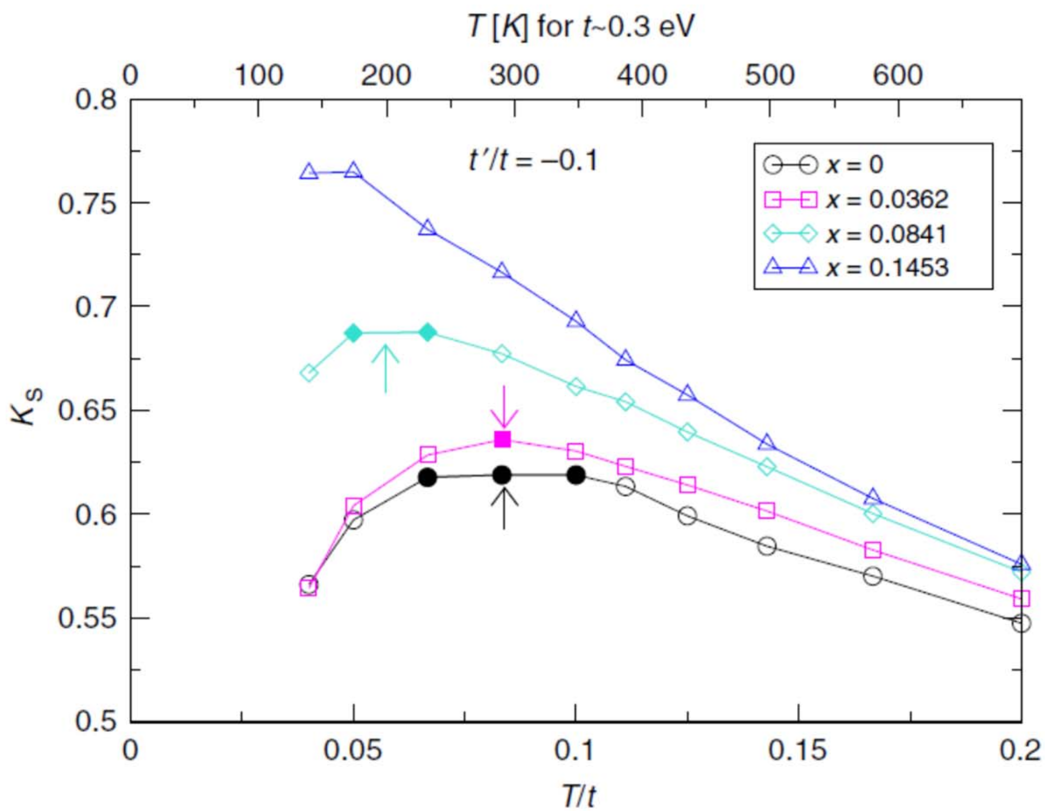


Fig. 3 Temperature and doping dependence of the $q = 0$ spin susceptibility. At the smaller dopings (larger filling $\langle n \rangle$), $\chi_s(T)$ exhibits a peak in the temperature dependence indicating the opening of a PG

Knight shift

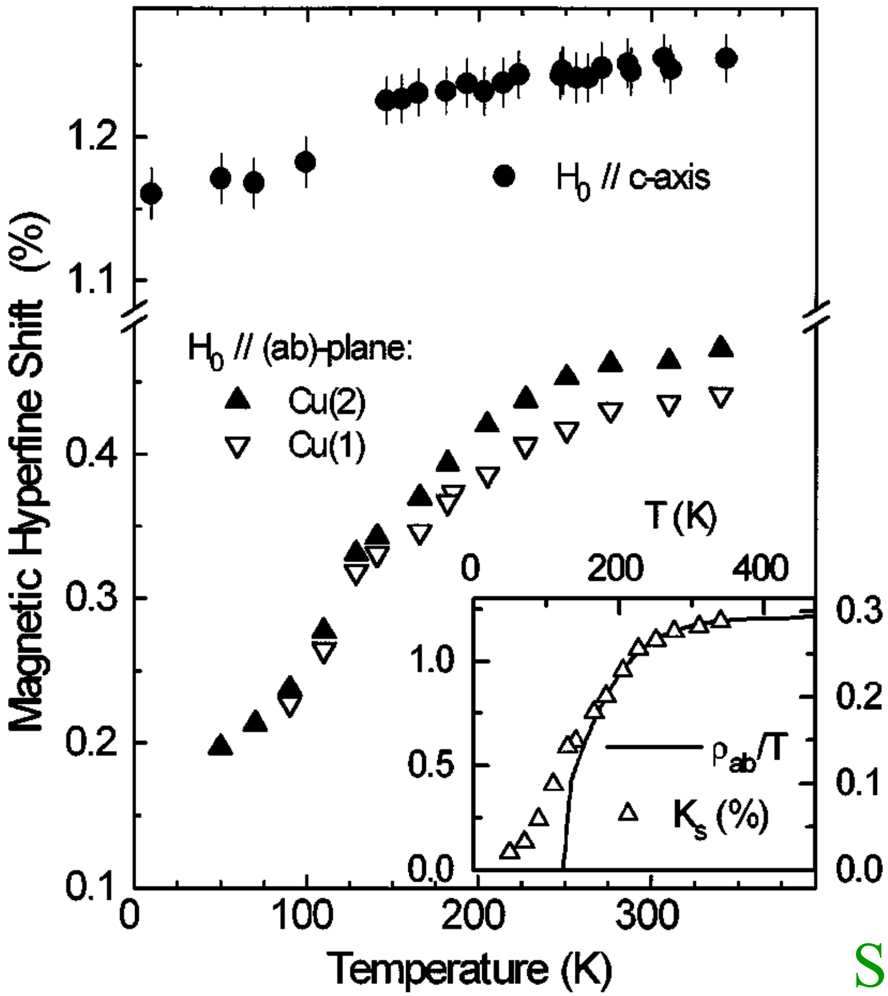


DCA 8 sites, $U = 6$, $t' = -0.1t$

Chen, LeBlanc, Gull, Nature Com. Apr. 2017

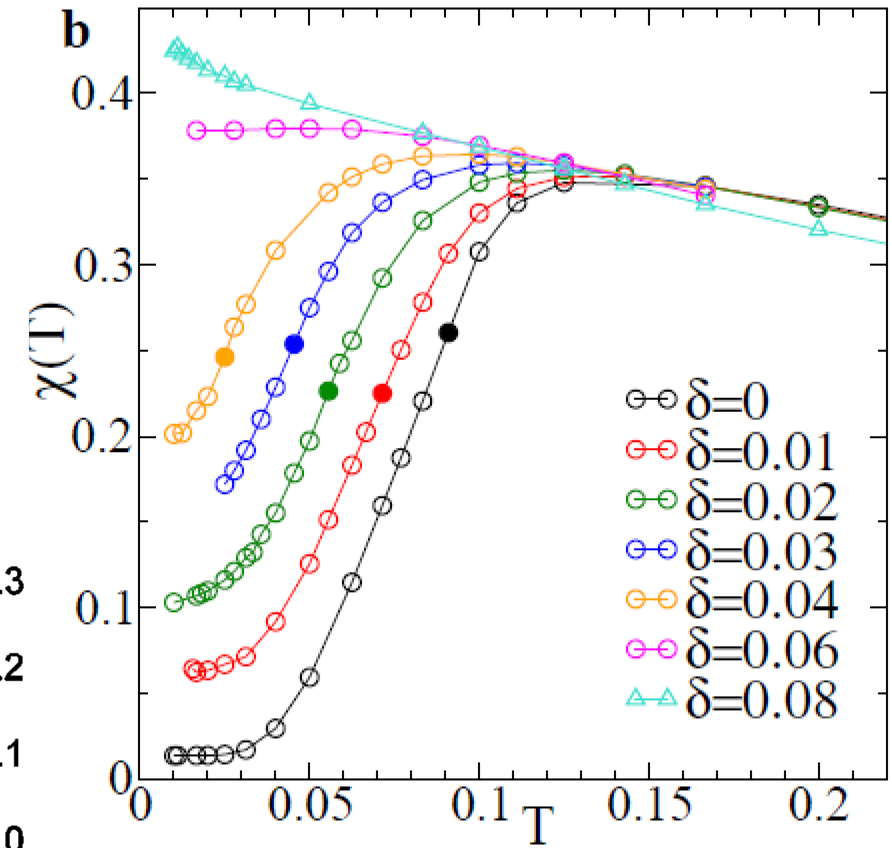
See also Jarrell *et al.* 2001, 2002

Spin susceptibility



Underdoped Hg1223

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

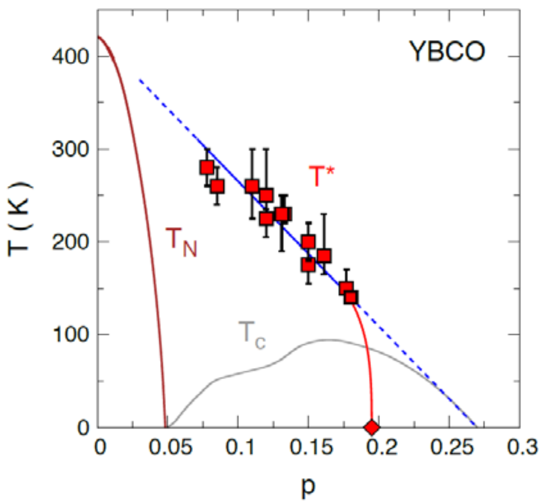


Sordi et al., Sci. Rep. 2 547 (2012);

U = 6.2 , t'=0

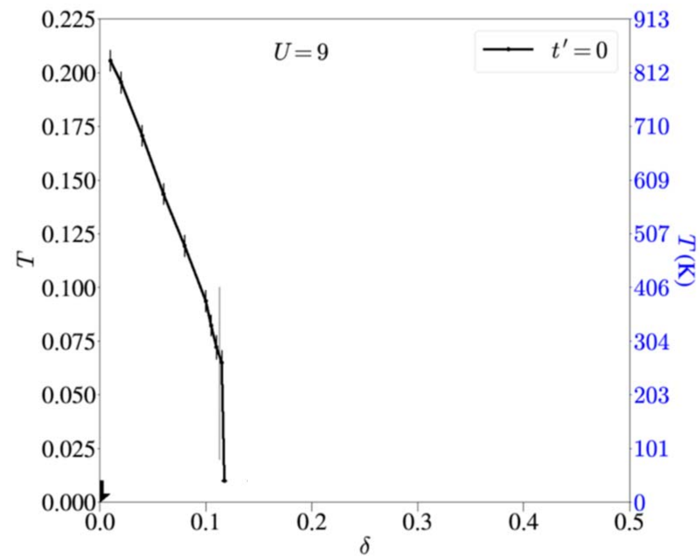
Results *T**

G.Sordi et al. Phys. Rev. B **87**, 041101(R) (2013)



Cyr-Choinières et al. Phys. Rev. B **97**, 064502

t'=0



p

A. Reymbaut, M. Thénault, L. Fratino, G. Sordi, P. Sémon, AMT, Phys. Rev. Research **1**, 023015 (2019)

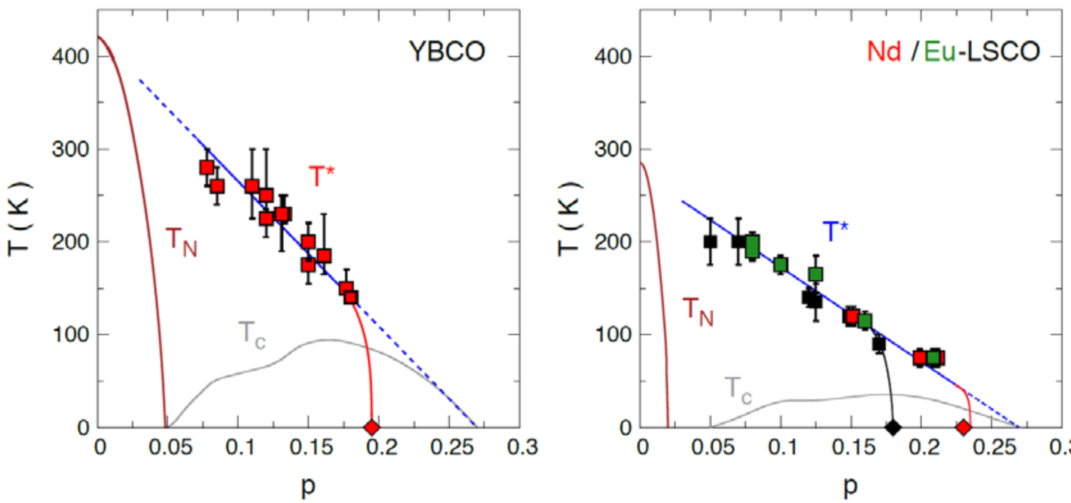
W Wu, A Georges, M Ferrero Phys. Rev. X 8, 021048 (2018).

Bragança, Sakai, Aguiar, Civelli, PRL **120**, 067002 (2018)

Results *T**

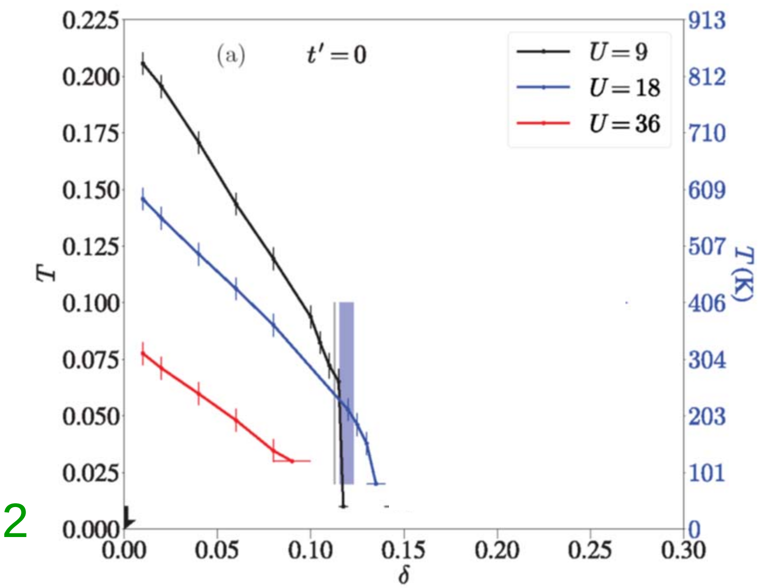
$$\boxed{k_{\mathrm{B}} T^* \sim J}$$

J = 4t²/U



Cyr-Choinières et al. Phys. Rev. B **97**, 064502

t'=0



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A. Reymbaut, M. Thénault, L. Fratino, G. Sordi, P. Sémon, AMT, Phys. Rev. Research **1**, 023015 (2019)

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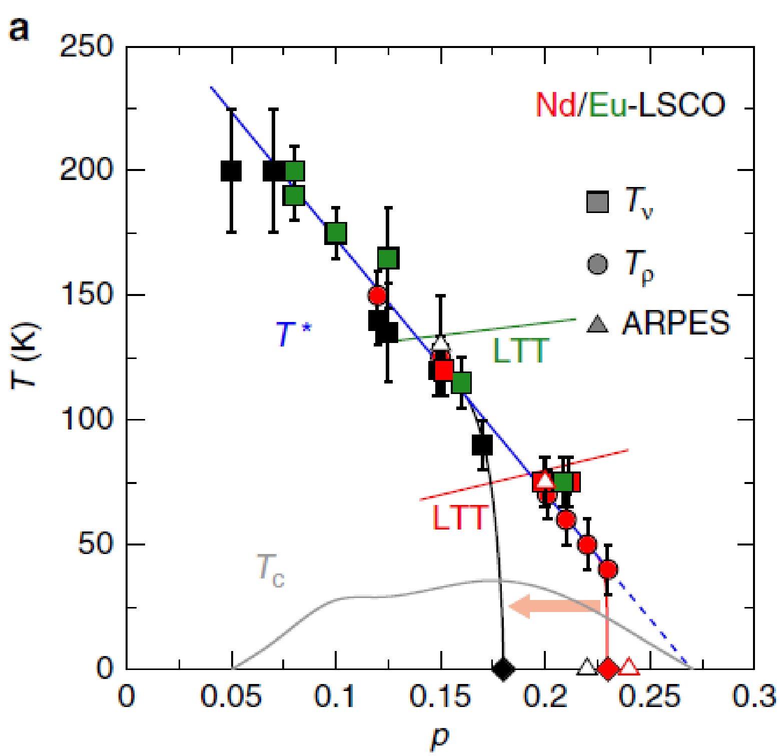
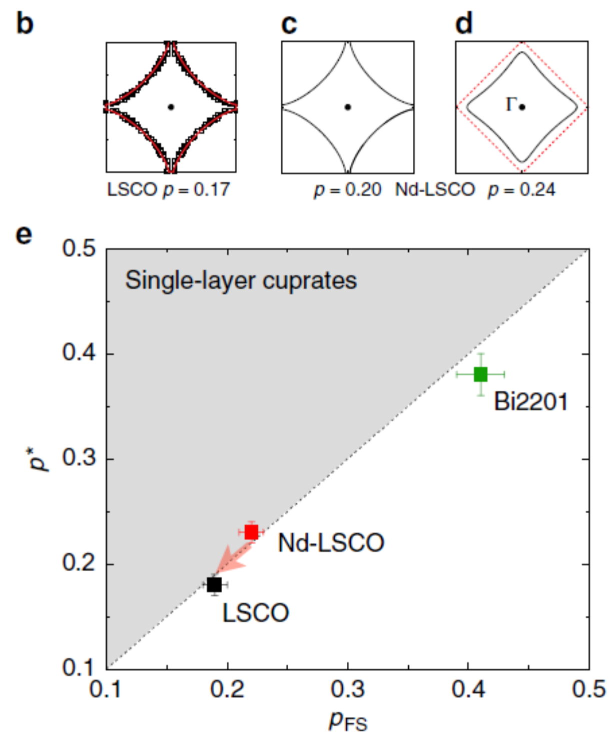
Bragança, Sakai, Aguiar, Civelli, PRL **120**, 067002 (2018)

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



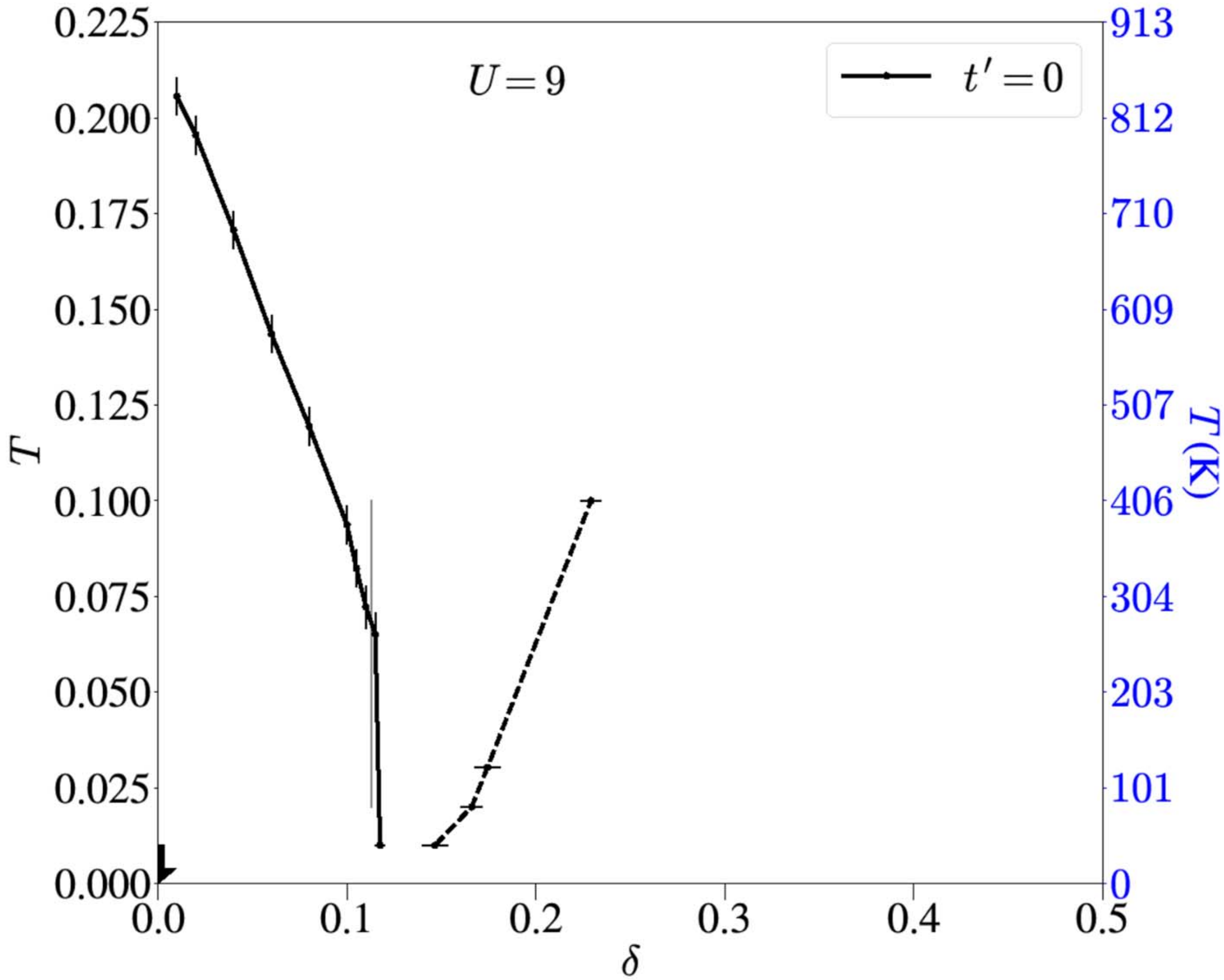
Doiron-Leyraud *et al.*
Nature Comm. **8** 2044



$$p^* < p_{fs}$$

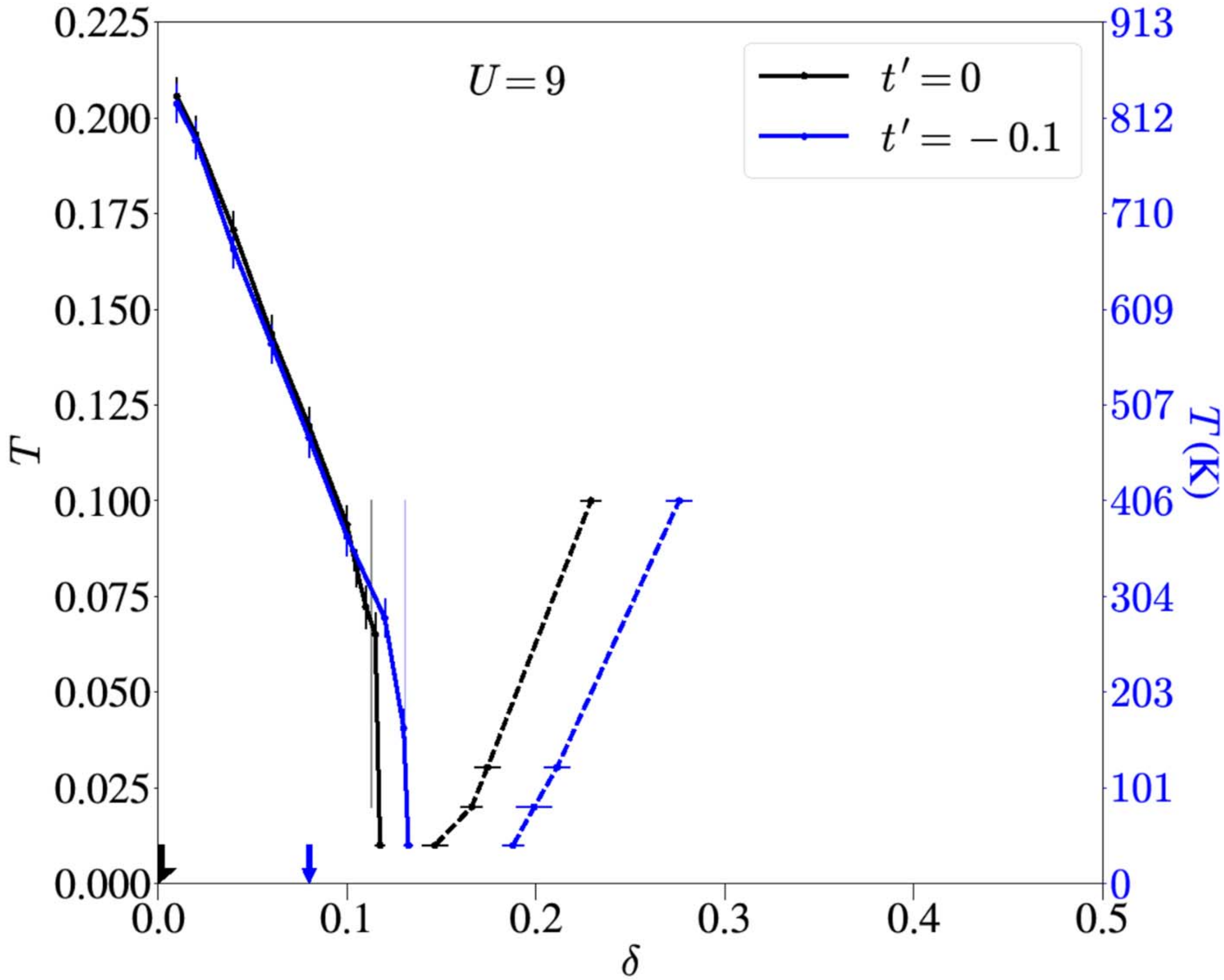
Doiron-Leyraud *et al.*
Nature Comm. **8** 2044

Effect of *t'*



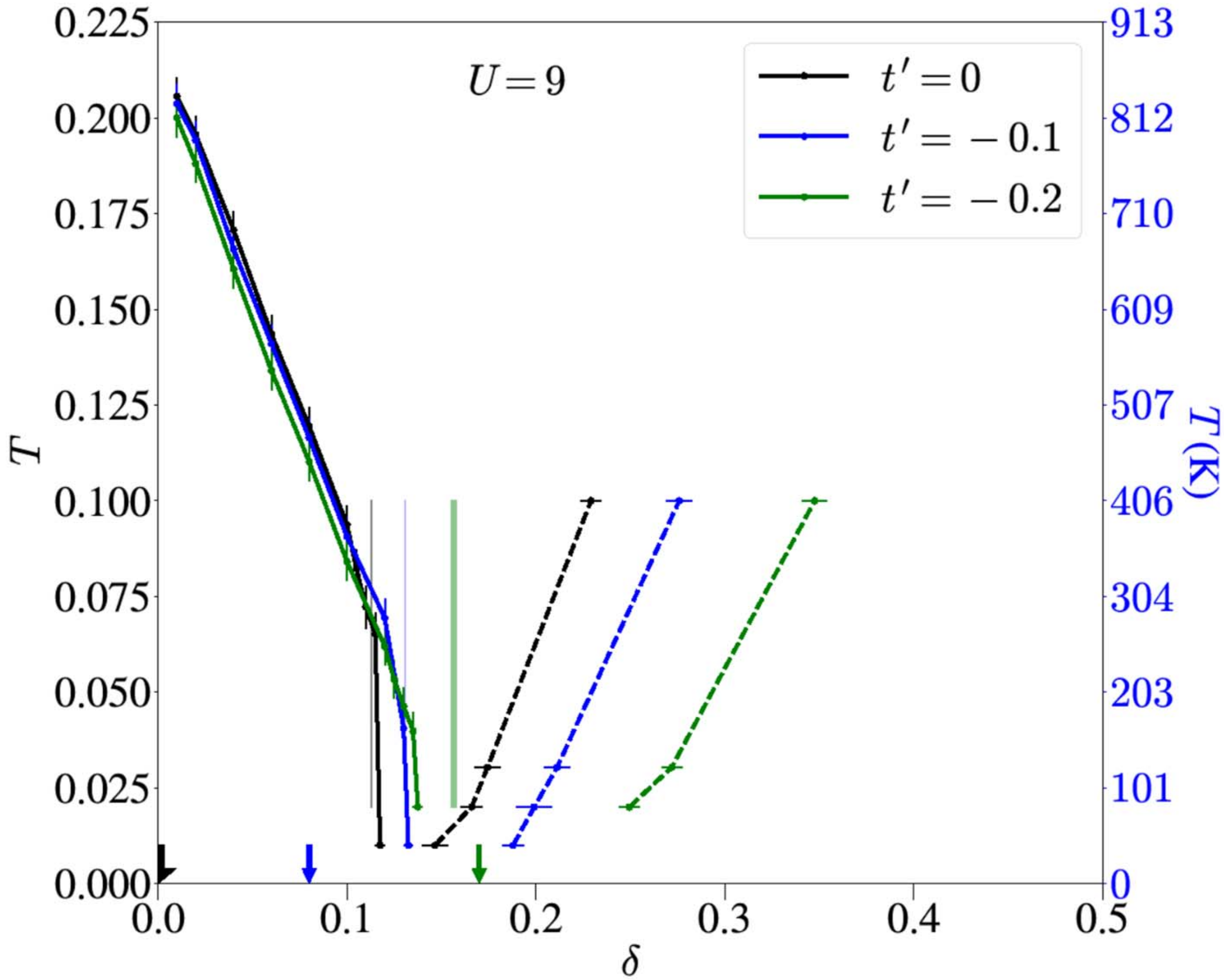
A. Reymbaut *et al.*
Phys. Rev. Research **1**, 023015 (2019)

Effect of *t'*



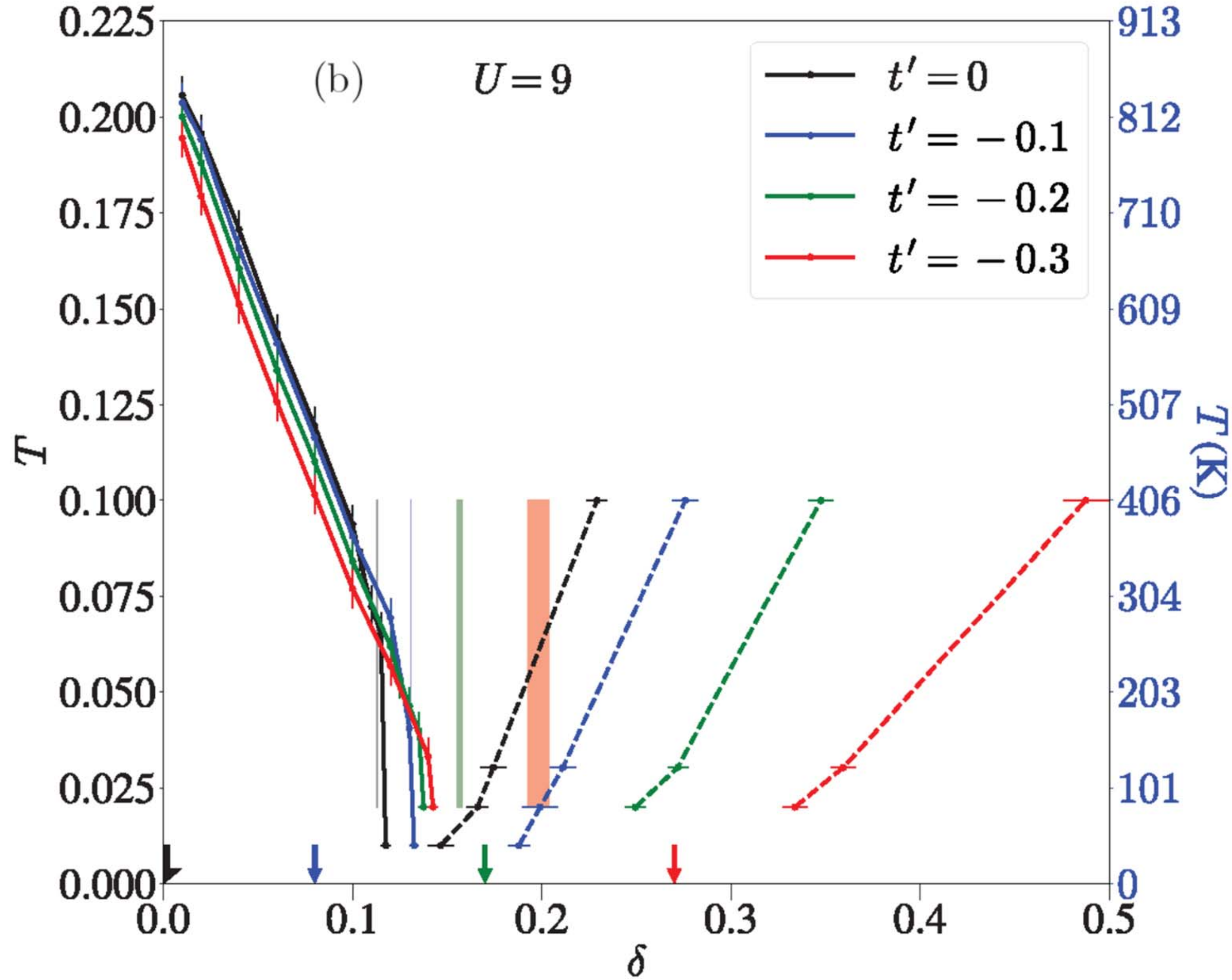
A. Reymbaut *et al.*
Phys. Rev. Research **1**, 023015 (2019)

Effect of *t'*



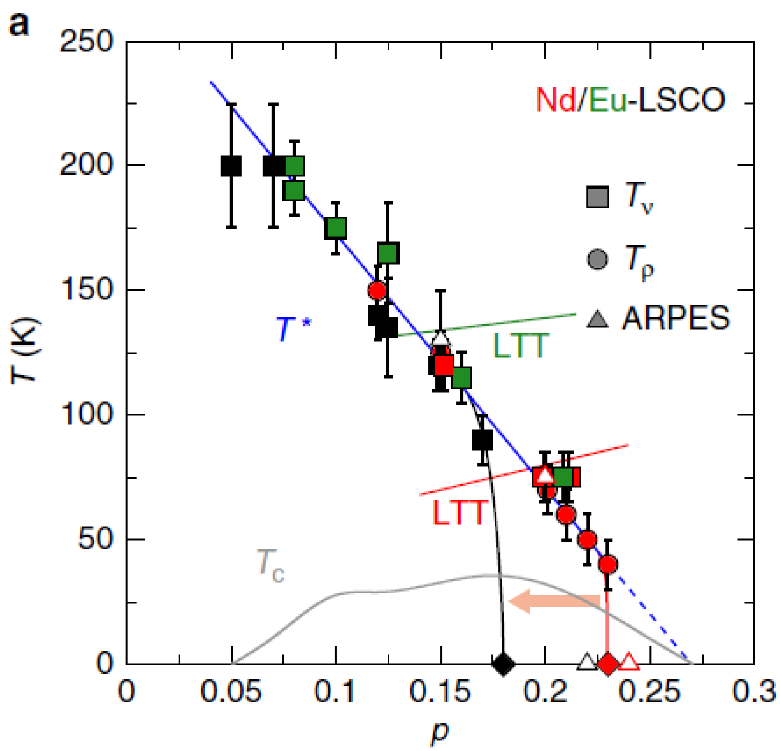
A. Reymbaut *et al.*
Phys. Rev. Research **1**, 023015 (2019)

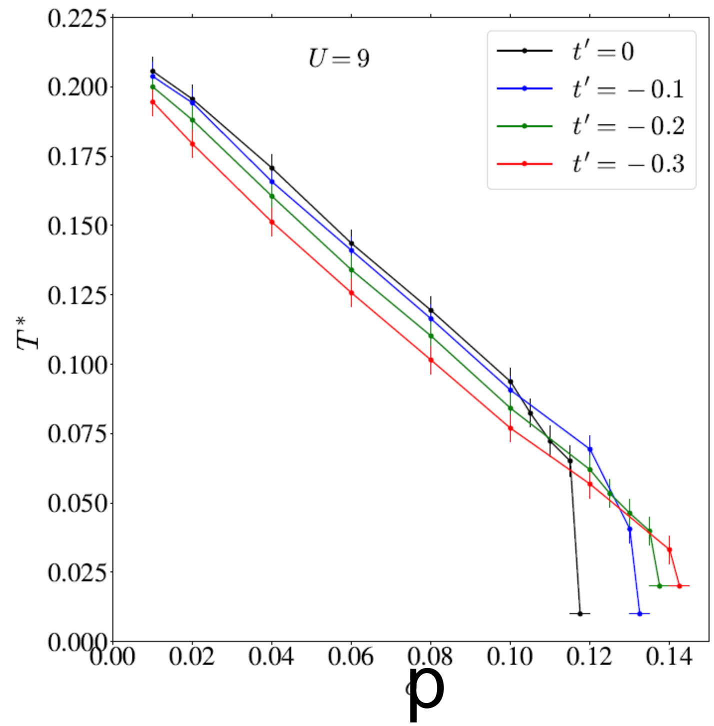
Effect of *t'*



A. Reymbaut *et al.*
Phys. Rev. Research **1**, 023015 (2019)

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

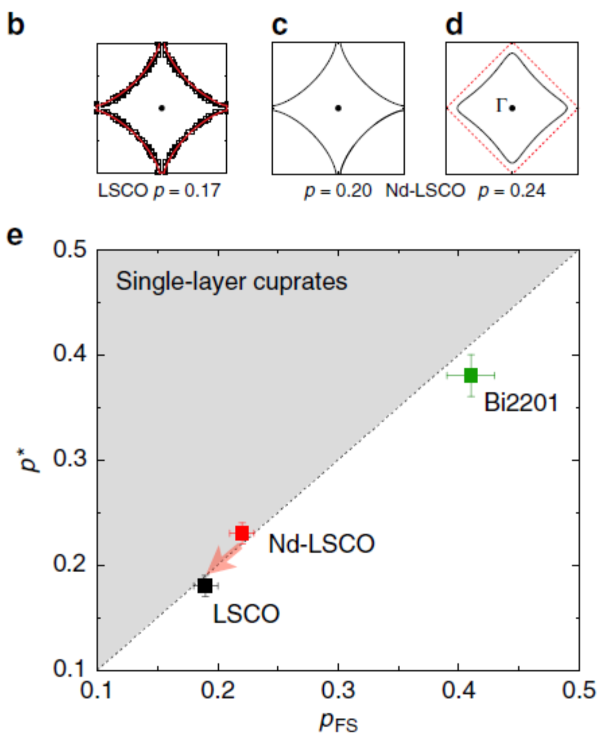




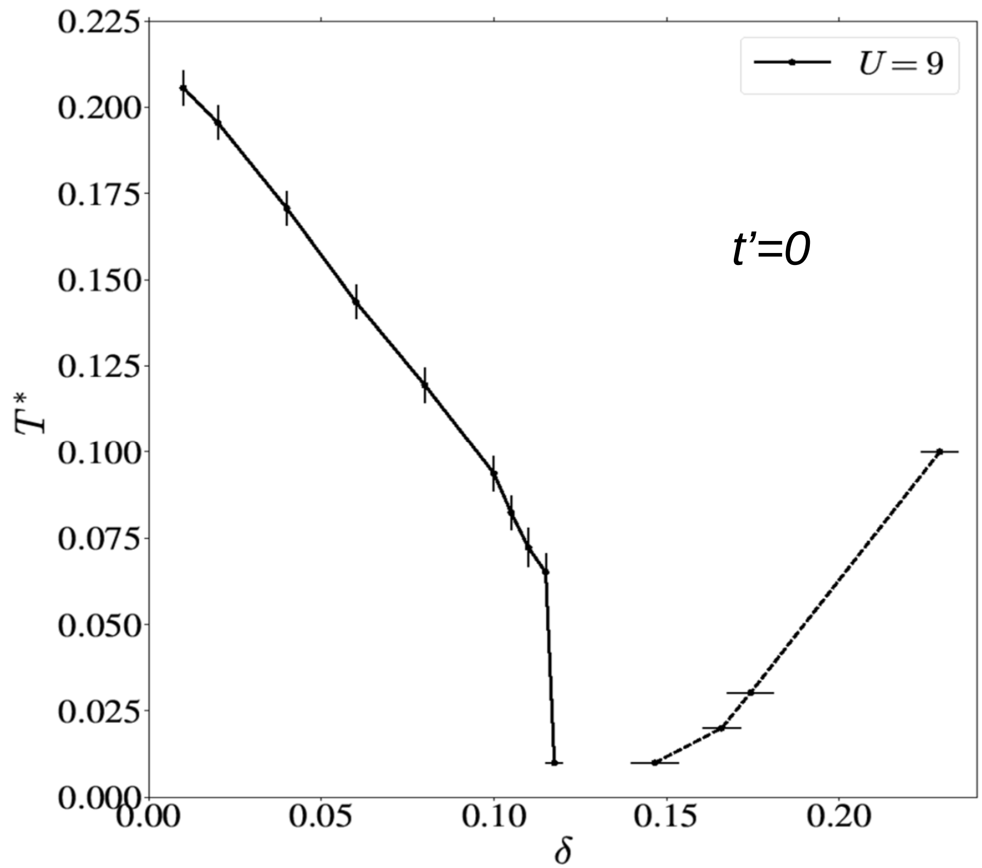
Doiron-Leyraud *et al.*
Nature Comm. **8** 2044

A.Reymbaut, *et al.*
Phys. Rev. Research **1**, 023015 (2019)

Results: van Hove singularity



$p^* < p_{fs}$

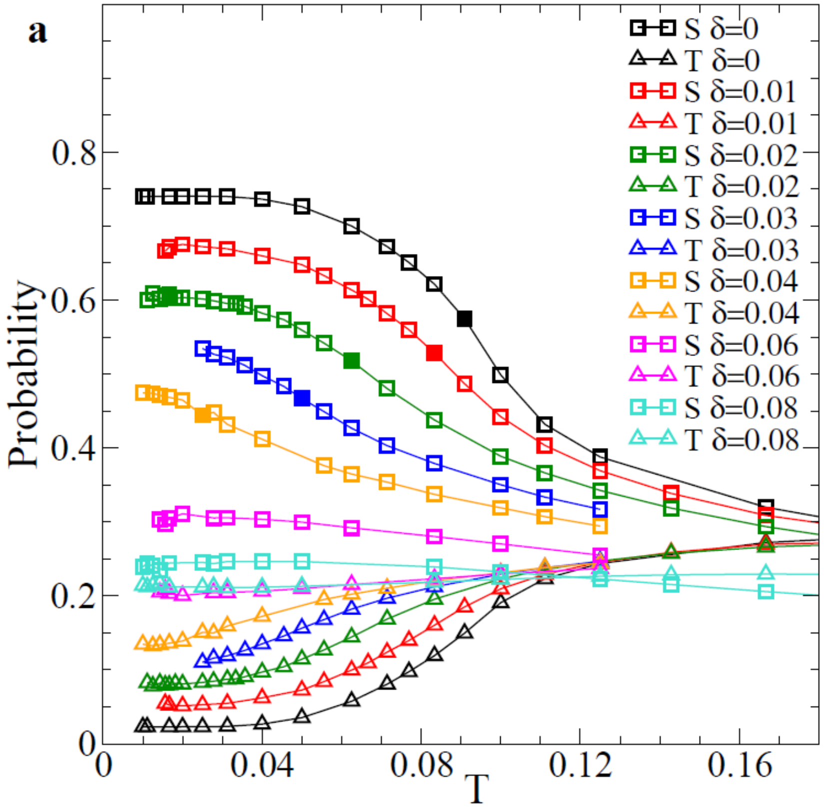


p^* p_{fs}

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

A.Reymbaut, *et al.*
Phys. Rev. Research **1**, 023015 (2019)
Sordi et al., Sci. Rep. 2 547 (2012);

Physics: Plaquette eigenstates



U = 6.2; t' = 0

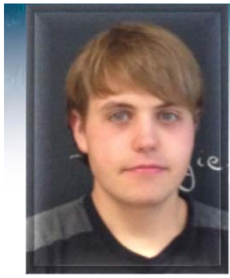
Sordi et al., Sci. Rep. 2 547 (2012);

See also:

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

Part III:

Specific heat in the strange metal phase



Simon Bergeron

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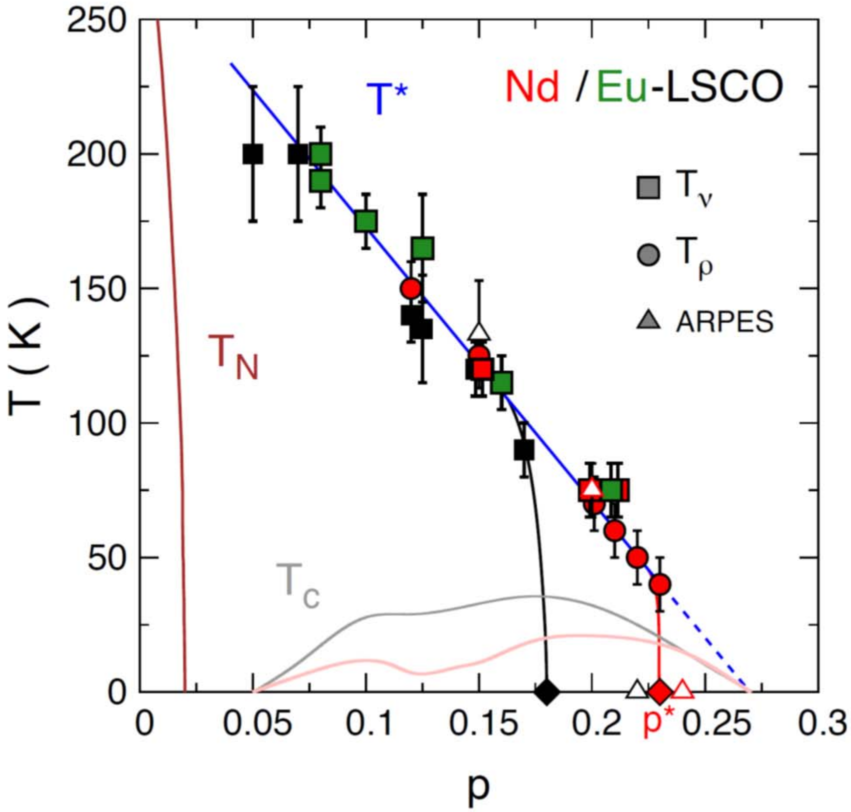
Specific heat in the strange metal phase

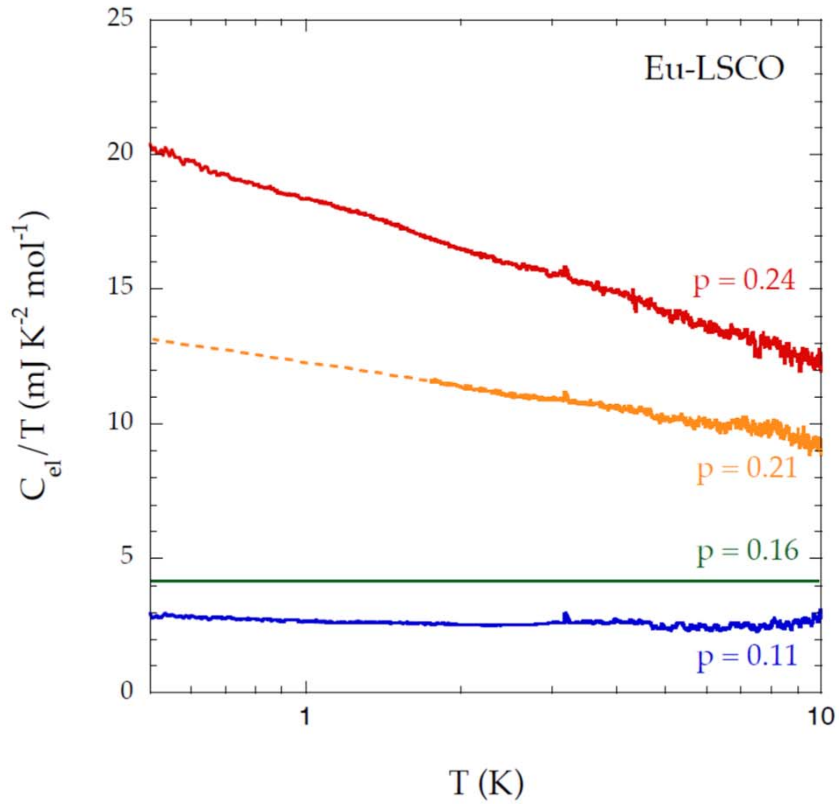
A. Reymbaut, *et al.* Phys. Rev. Research **1**, 023015 (2019)

Marion Thénault

R. Garioud

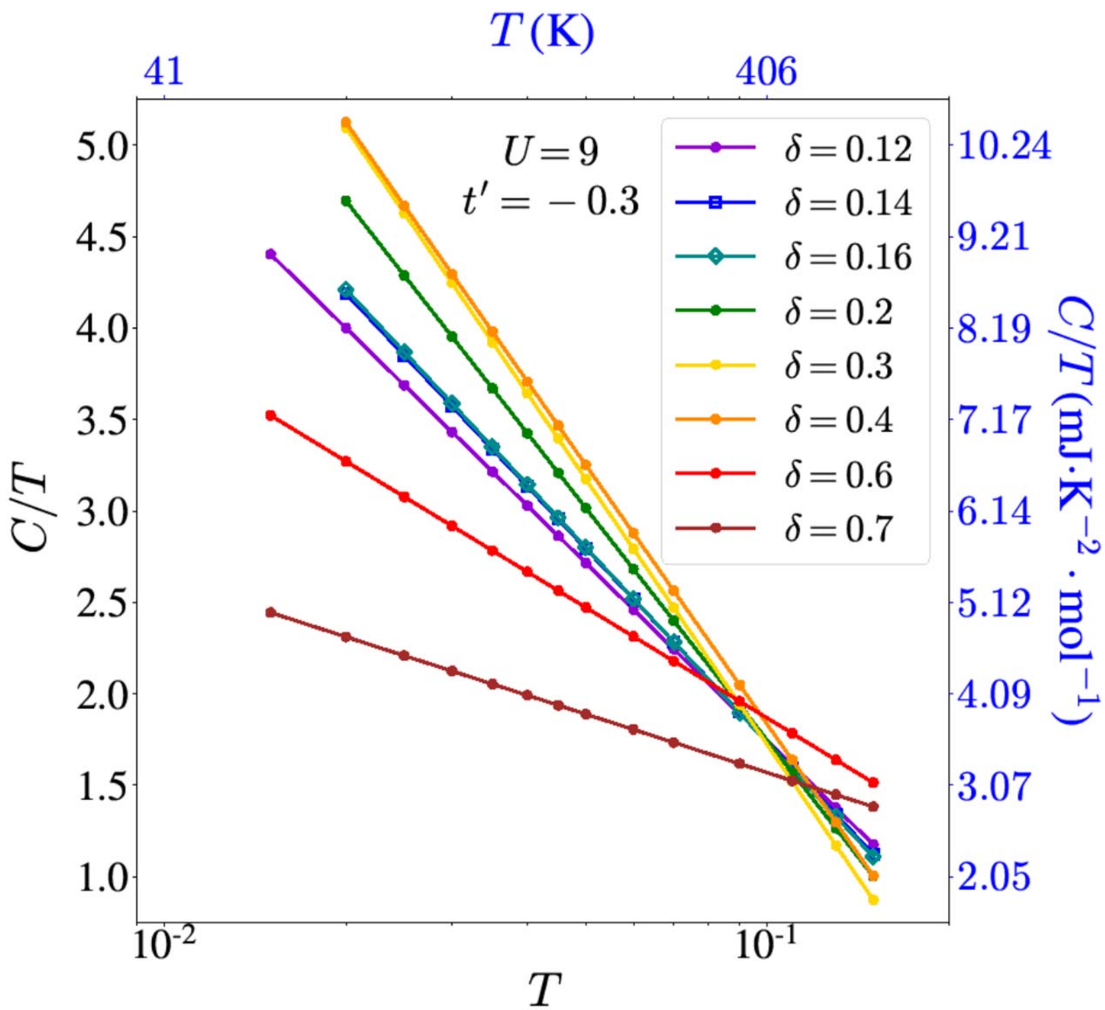
Specific heat in the strange metal phase





B. Michon, C. Girod, Taillefer, Klein, Nature **567**, 218 (2019)

Specific heat in the strange metal phase



Part IV:

Strongly correlated superconductivity

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Giovanni Sordi

Patrick Sémon

Lorenzo Fratino

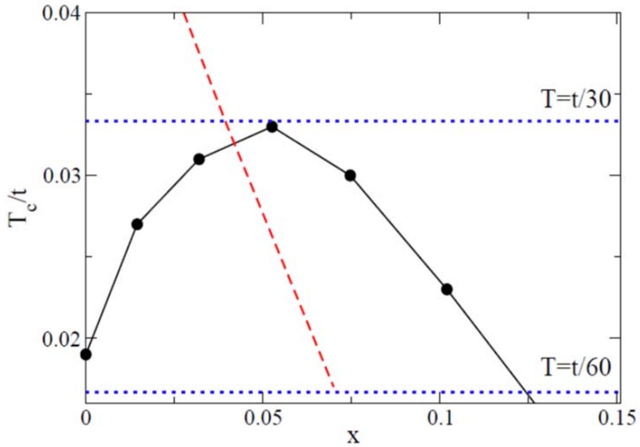
Superconductivity for large *U*

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

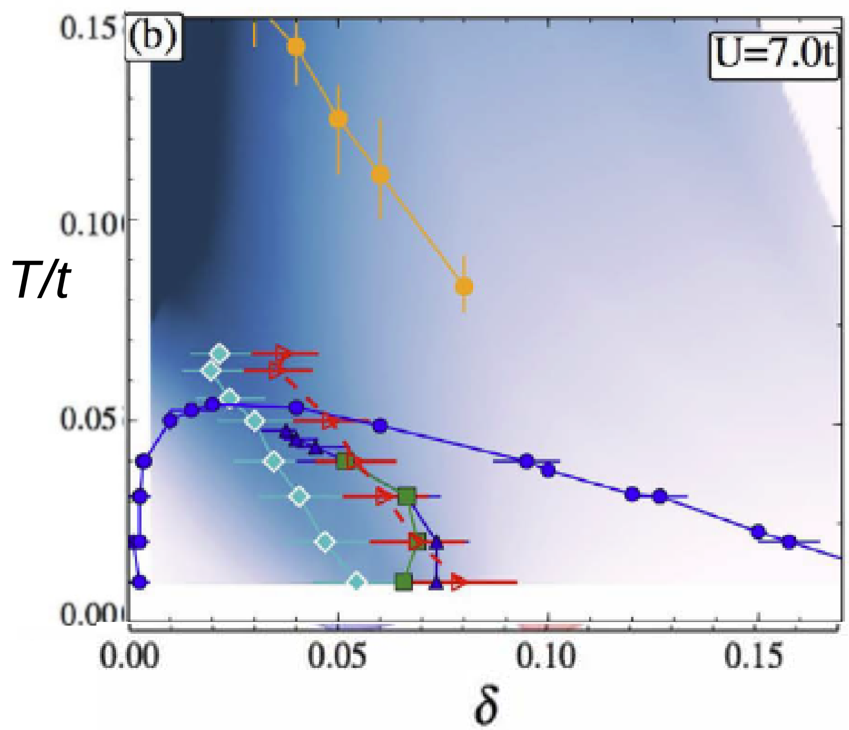
Fratino et al.

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

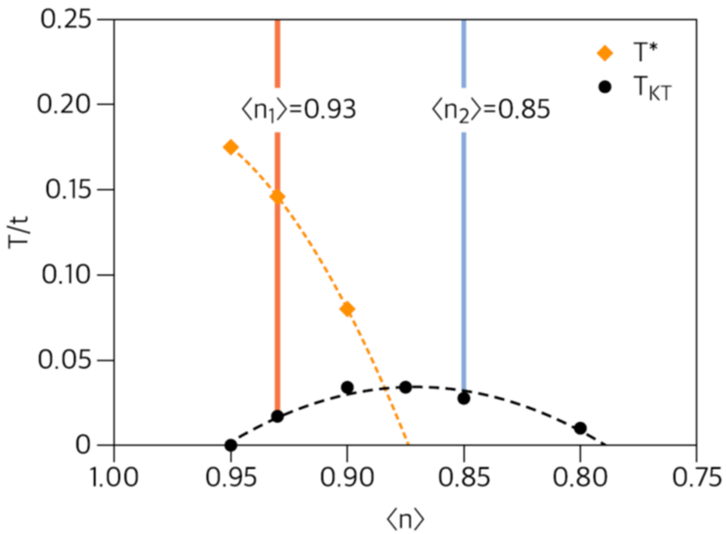
Superconducting transition temperature



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

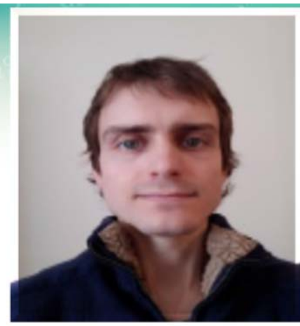


Fratino et al.
Sci. Rep. **6**, 22715



T.A. Maier, D.J. Scalapino, npj Quantum Materials (2019)

Olivier Simard



Charles-David Hébert

Alexandre Foley

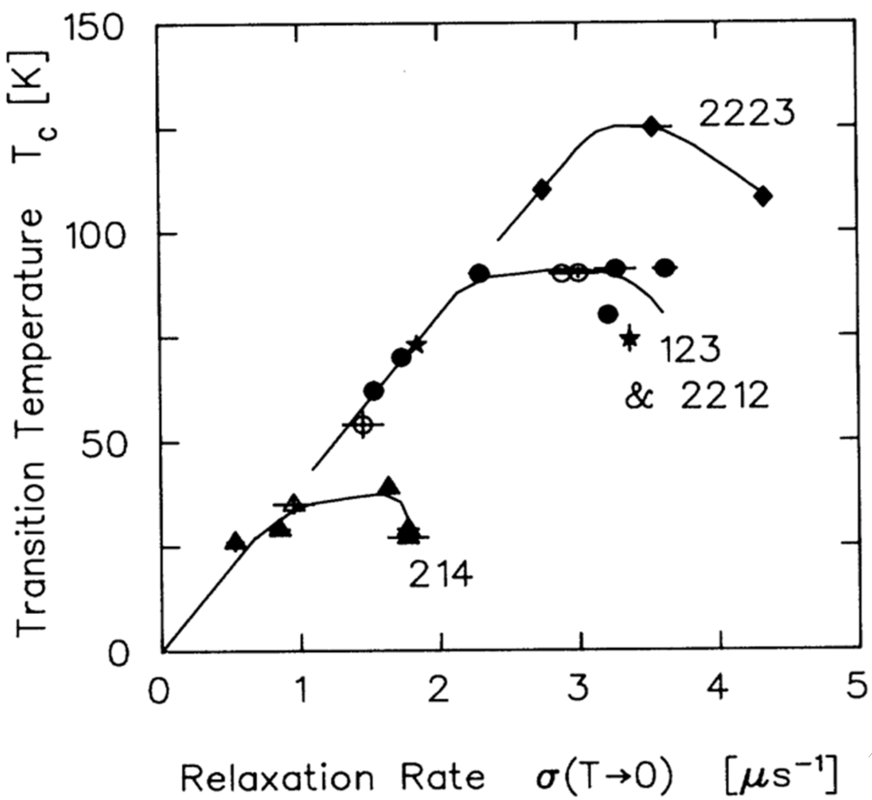
David Sénéchal

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

O. Simard, C.-D. Hébert, A. Foley, A.-M.S. Tremblay, D. Sénéchal, Phys. Rev. B **100**, 094506 (2019)

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)

Superfluid stiffness *T=0*

$$j = -\rho_s A$$

d = 2

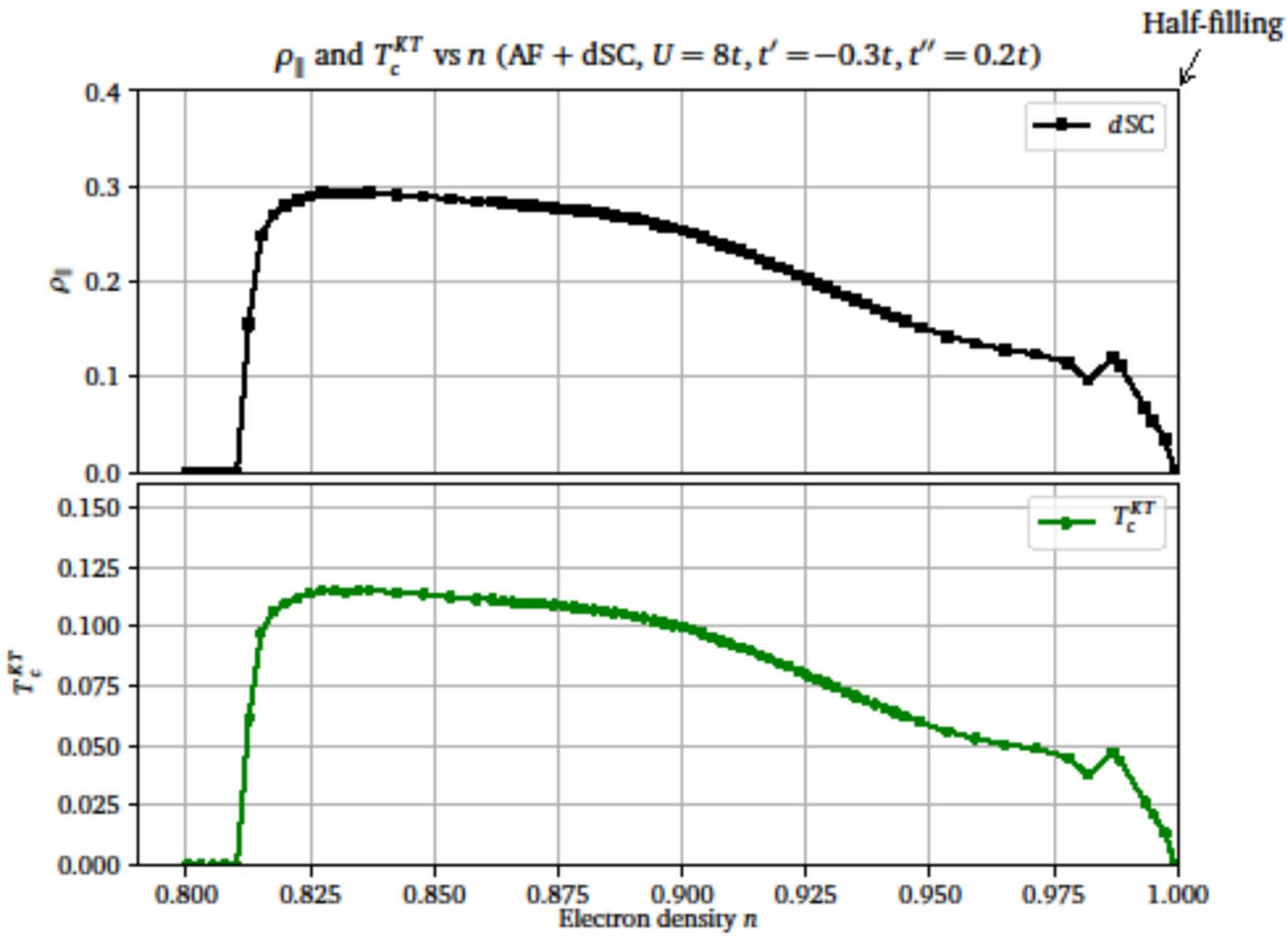
$$\frac{1}{\lambda^2} = \rho_s \mu_0$$

$$T_c^{KT} = \frac{\pi}{8e^2}\rho_s(T_c^{KT})$$

$$T_c^{KT} < \frac{\pi}{8e^2}\rho_s(T_c^{KT} = 0)$$

$$\hbar = 1\,;\; k_B = 1$$

Emery Kivelson, Nature **374**, 434 (1995)
Metzner, Yamase, Phys. Rev. B **100**, 014504 (2019)
Hazra, Verma, and Randeria, Phys. Rev. X **9**, 031049 (2019)

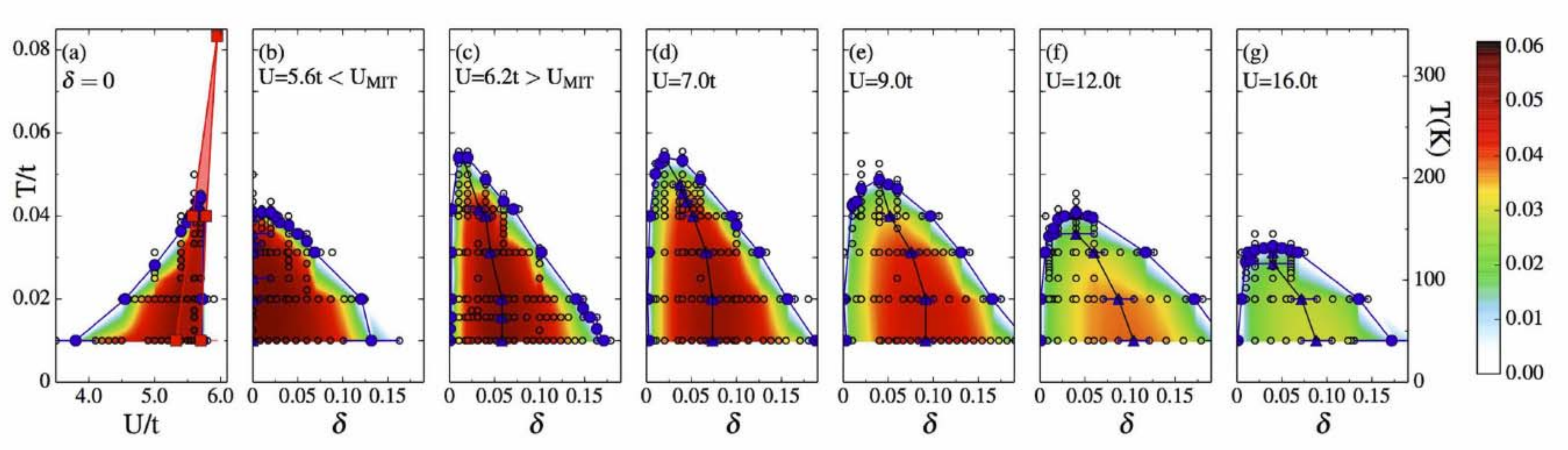


O. Simard, *et al.* Phys. Rev. B **100**, 094506 (2019)

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

What energy scale controls *Tc* ?

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)

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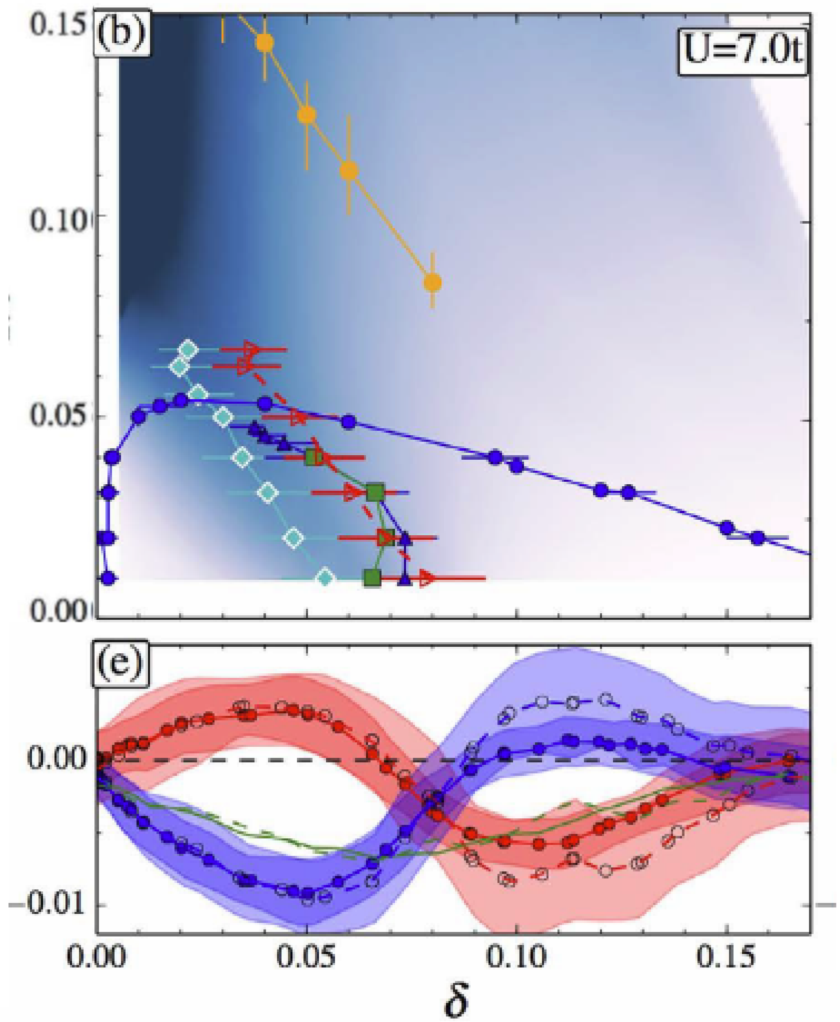
Condensation energy



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

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

Part V:

Perspective

Giovanni Sordi

Kristjan Haule

Influence of the Mott transition away from half-filling

Sordi et al., PRL 104, 226402 (2010)
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Sordi et al., Sci. Rep. 2 547 (2012);
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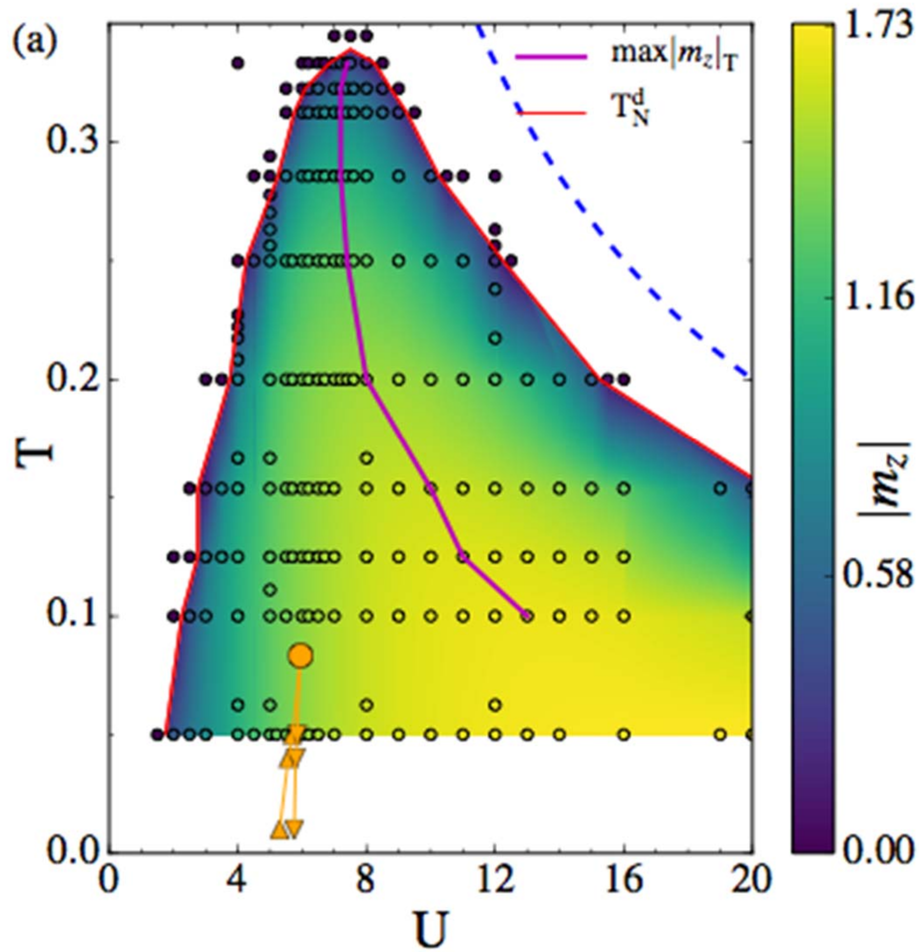
AFM phase diagram d=2, t'=0



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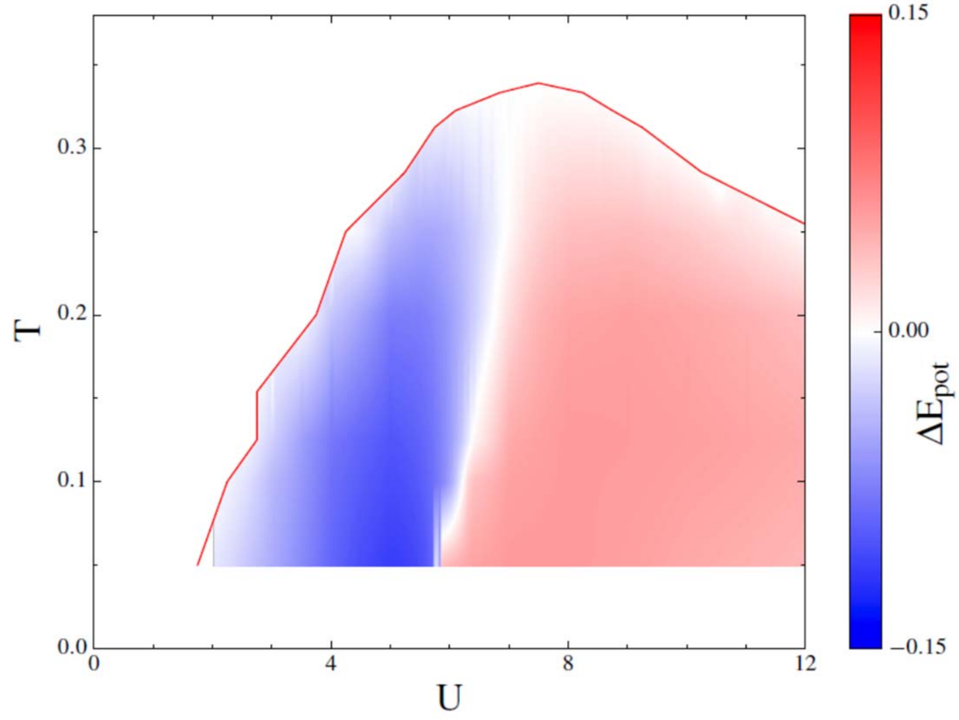
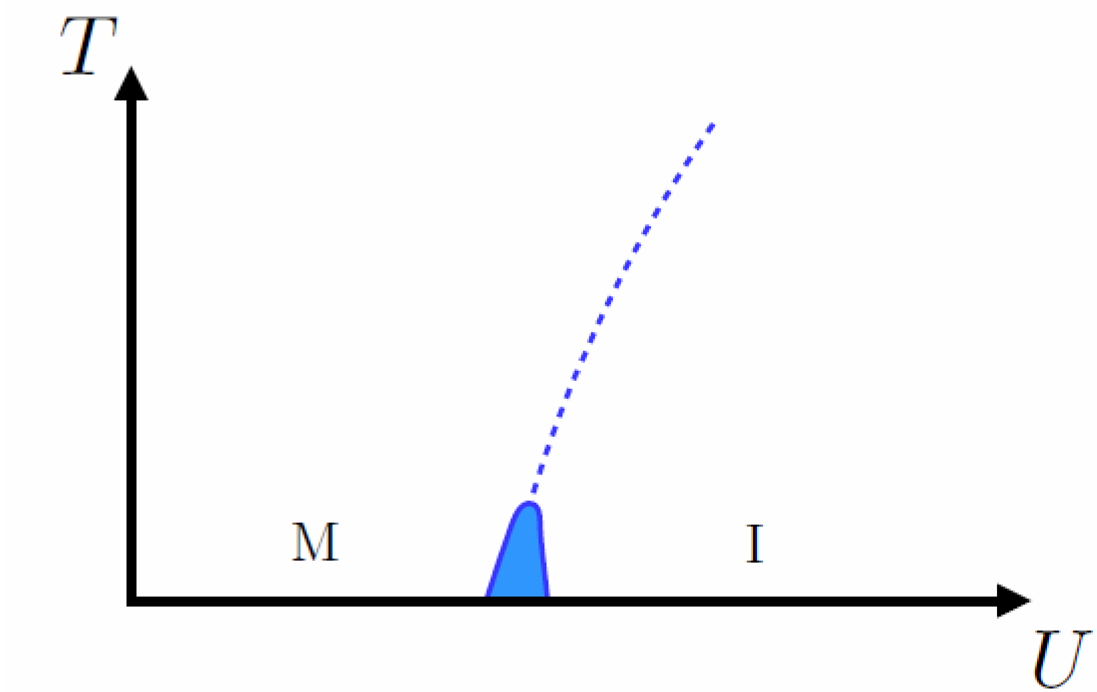
Change in potential energy due to large ξ



L. Fratino,[1] P. Sémon,[2] M. Charlebois,[2] G. Sordi,[1] and A.-M. S. Tremblay[2,3]
arXiv:1702.01821

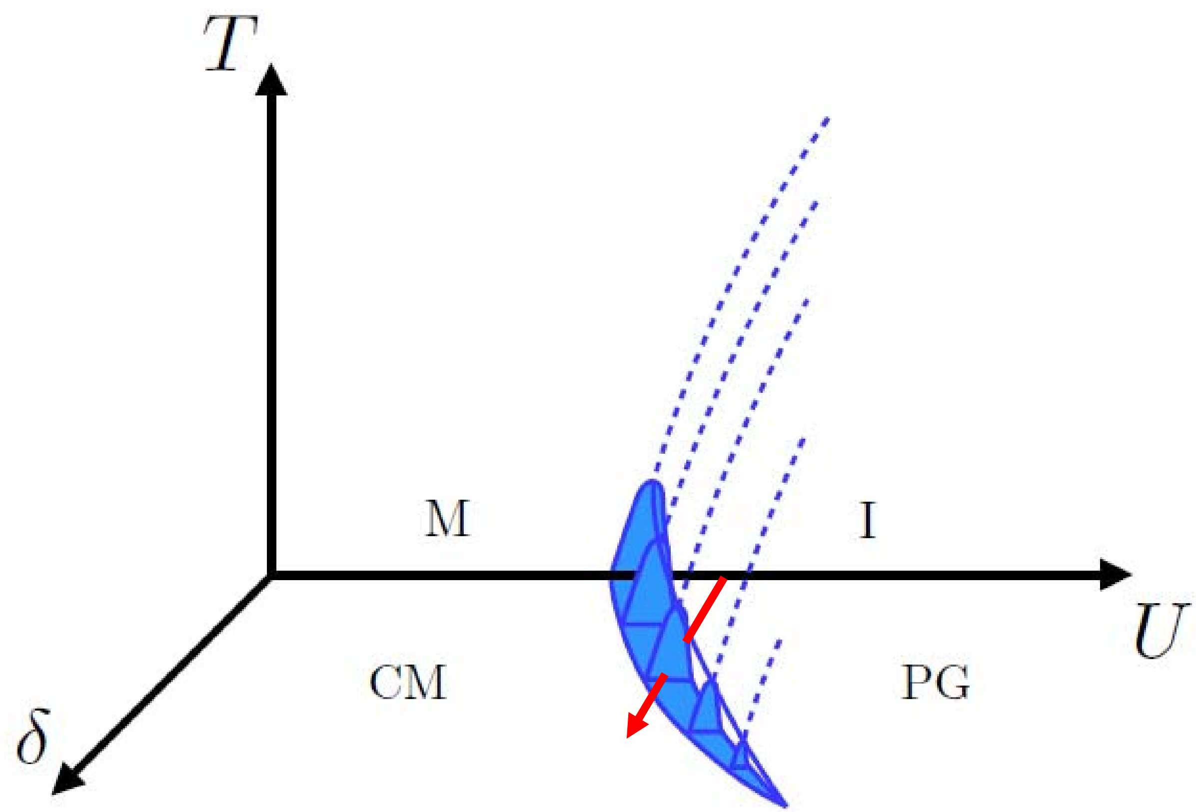
Influence of Mott transition away from half-filling

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



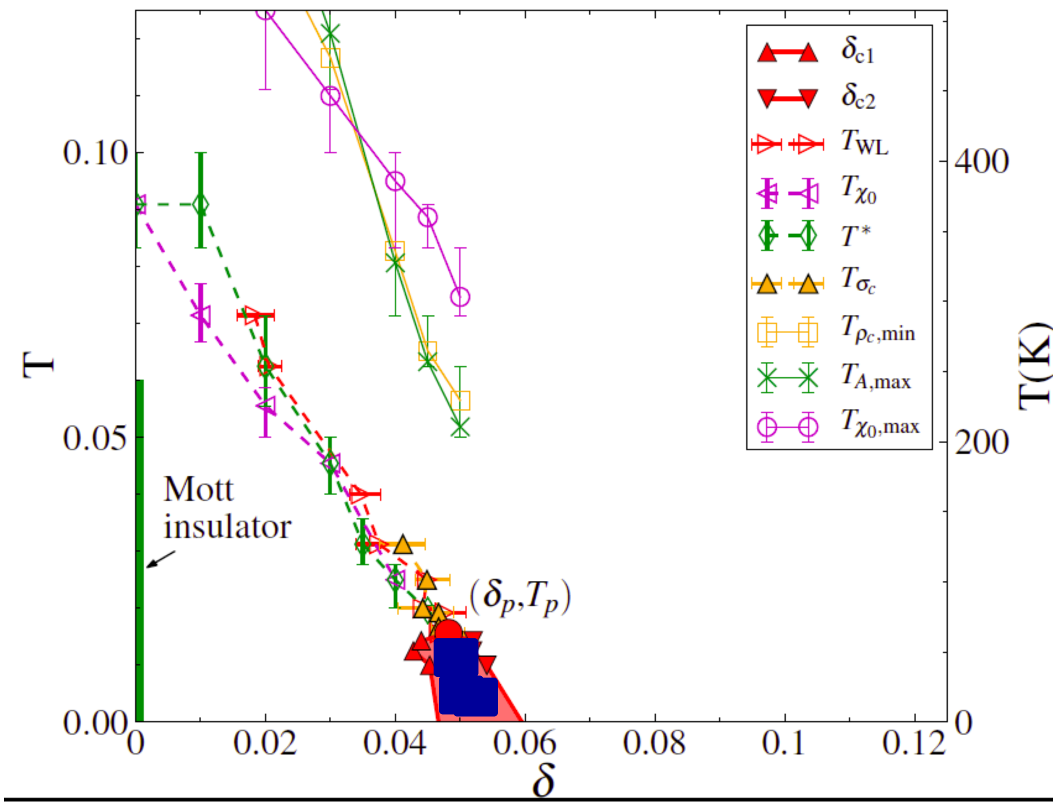
Influence of Mott transition away from half-filling

$n = 1, d = 2$ square lattice



Two crossover lines

Giovanni Sordi



Patrick Sémon

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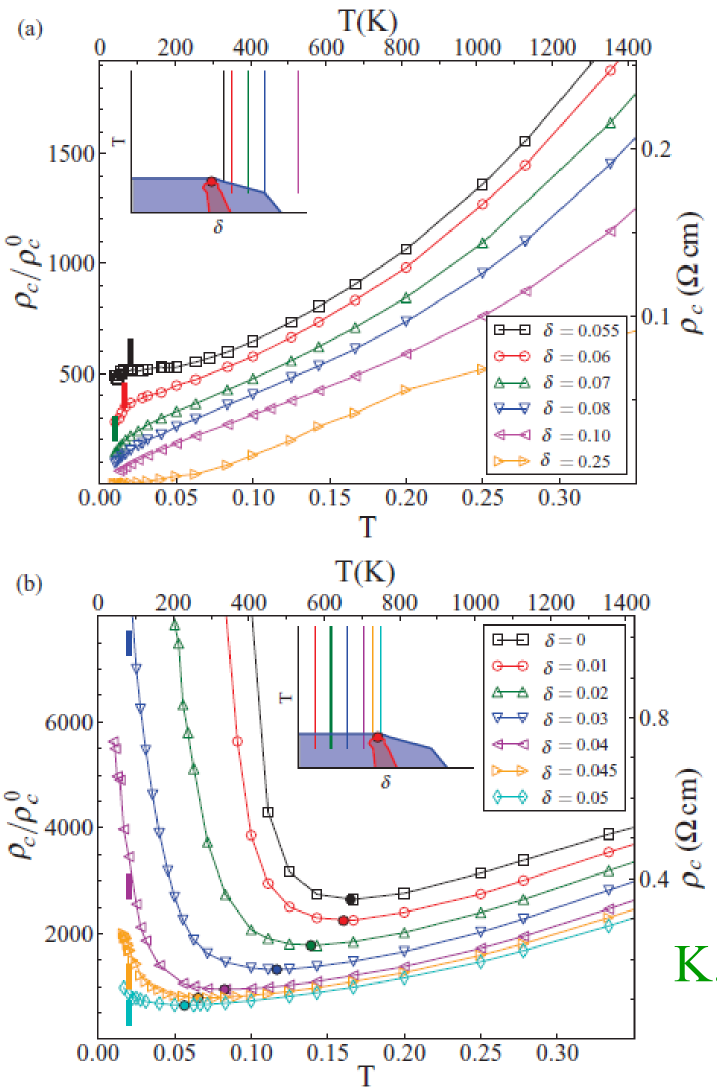
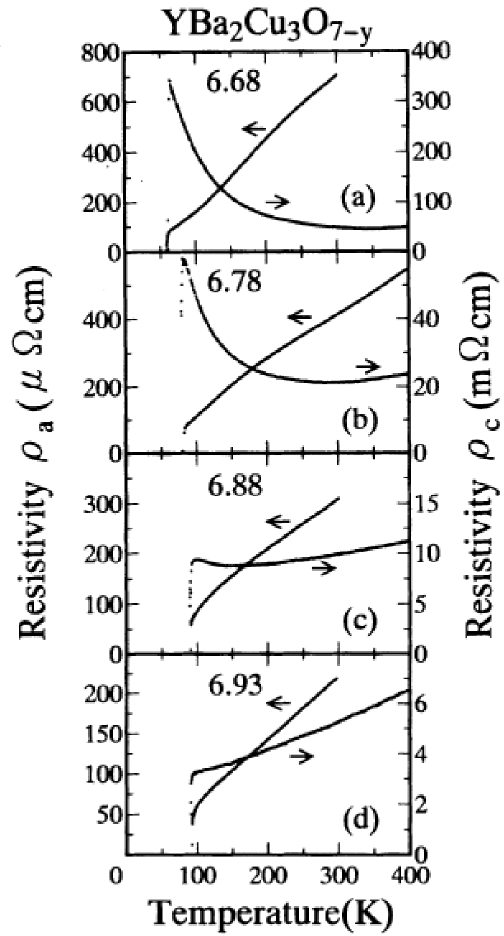
P. Sémon, G. Sordi, *et al.*, Phys. Rev. B **89**, 165113/1-6 (2014)

c-axis resistivity





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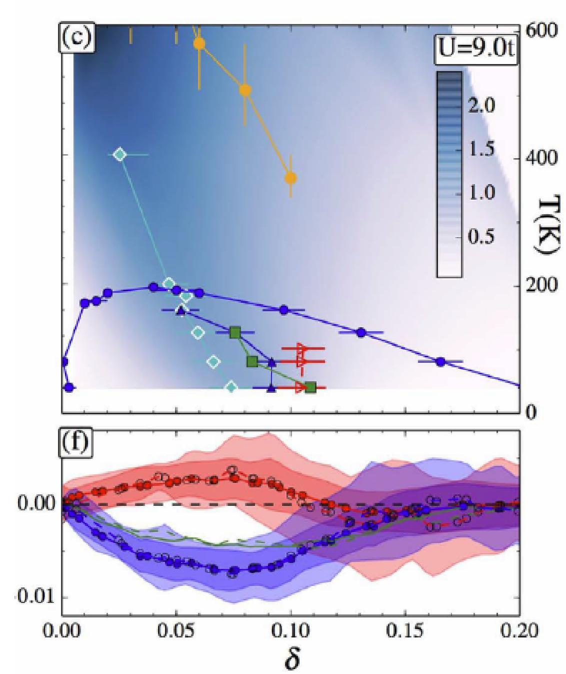
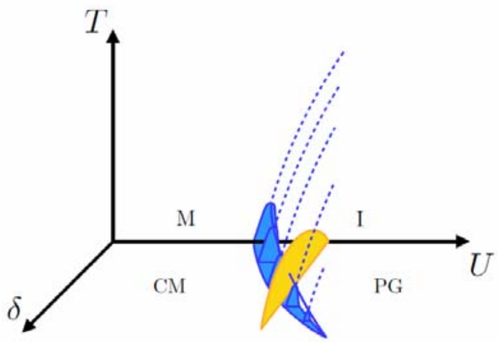
Connecting the finite doping behavior to the Mott transition at half-filling

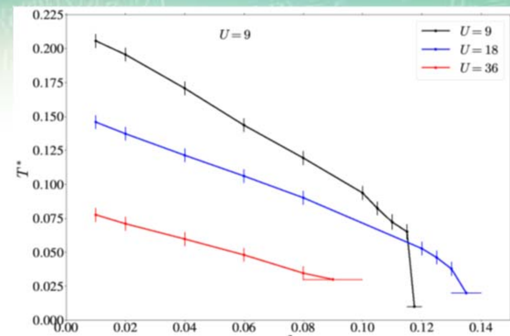


Conclusion

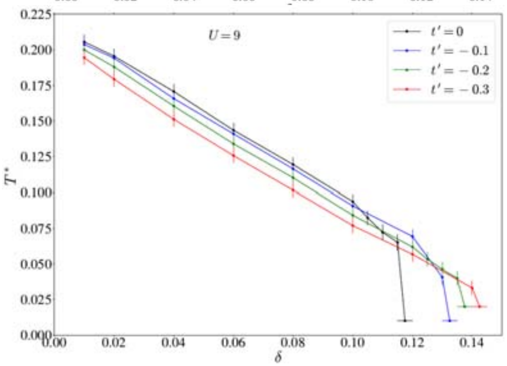
*p** in Hubbard is the end of Mott physics

Mott transition and its finite doping extension is the organizing principle



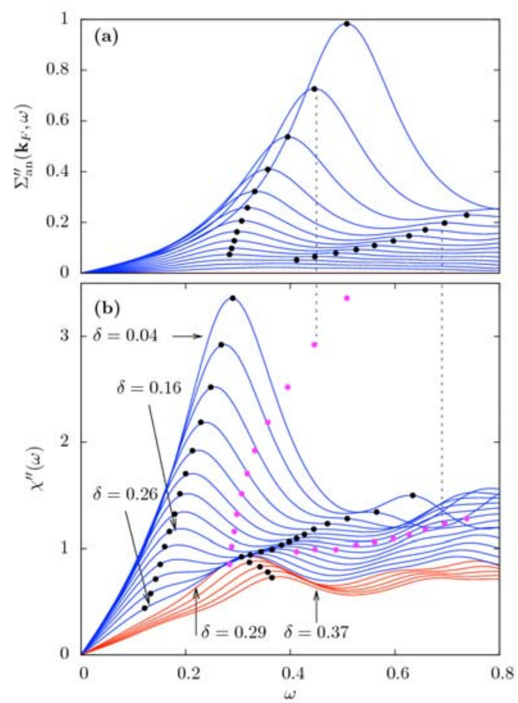


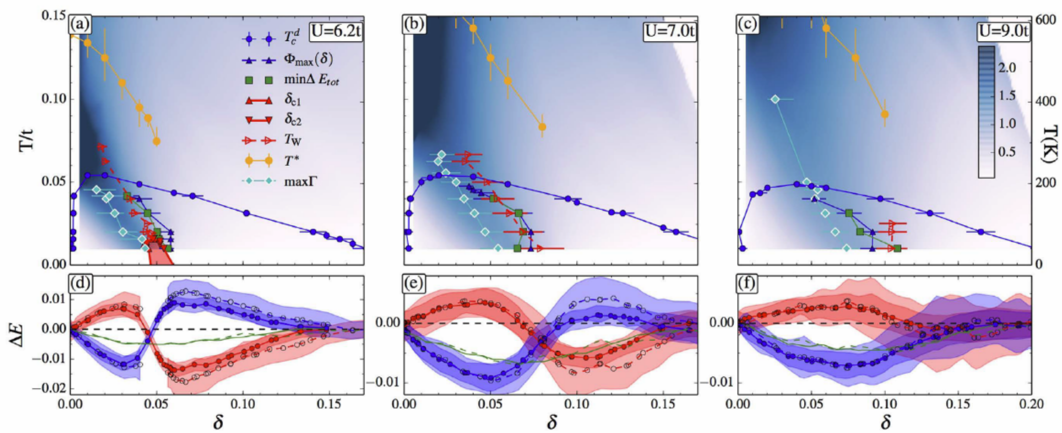
$T^* \sim J$



$p^* < p_{fs}$

Pressure dependence of p^*





$T_c \sim J$

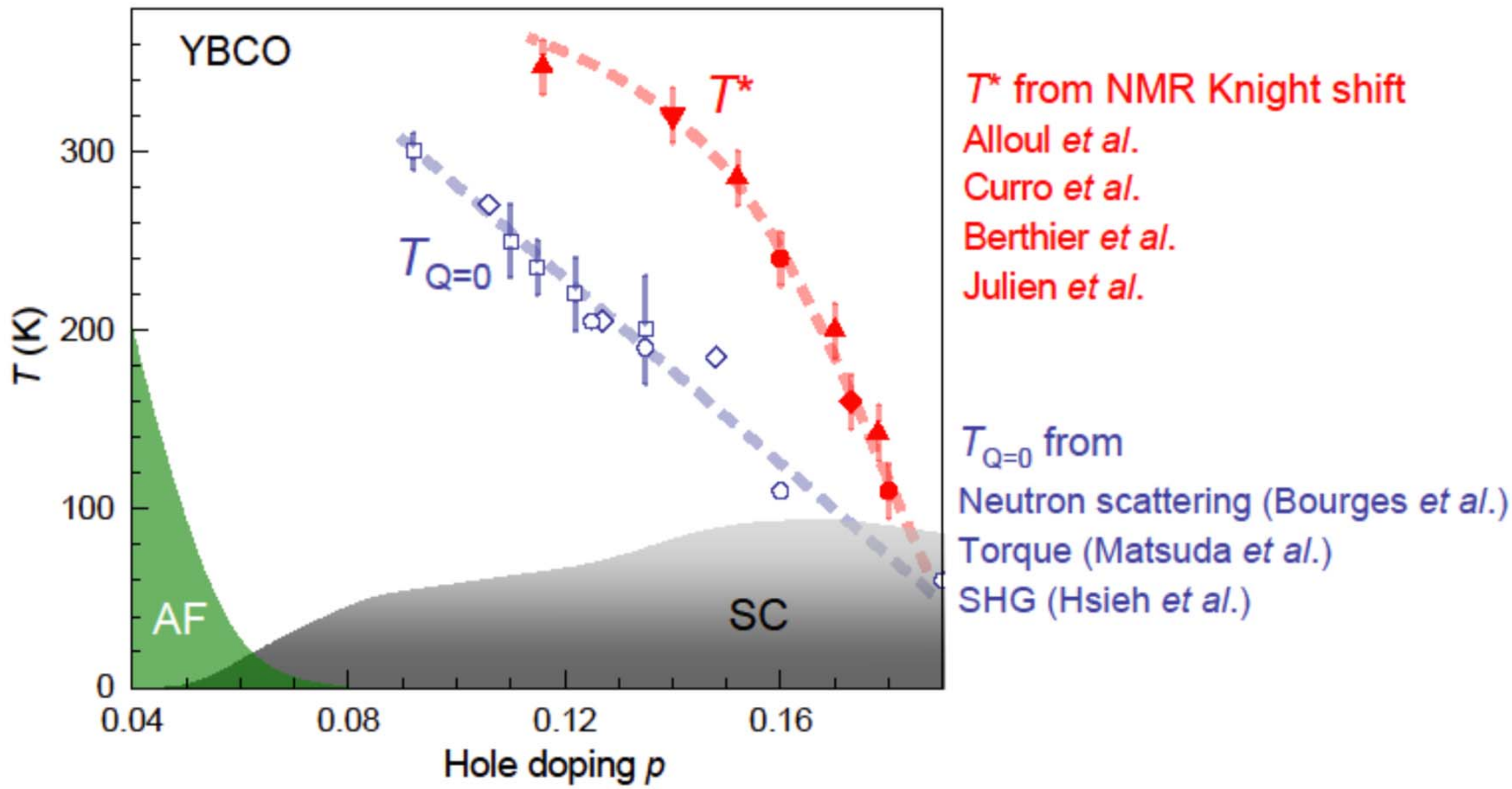
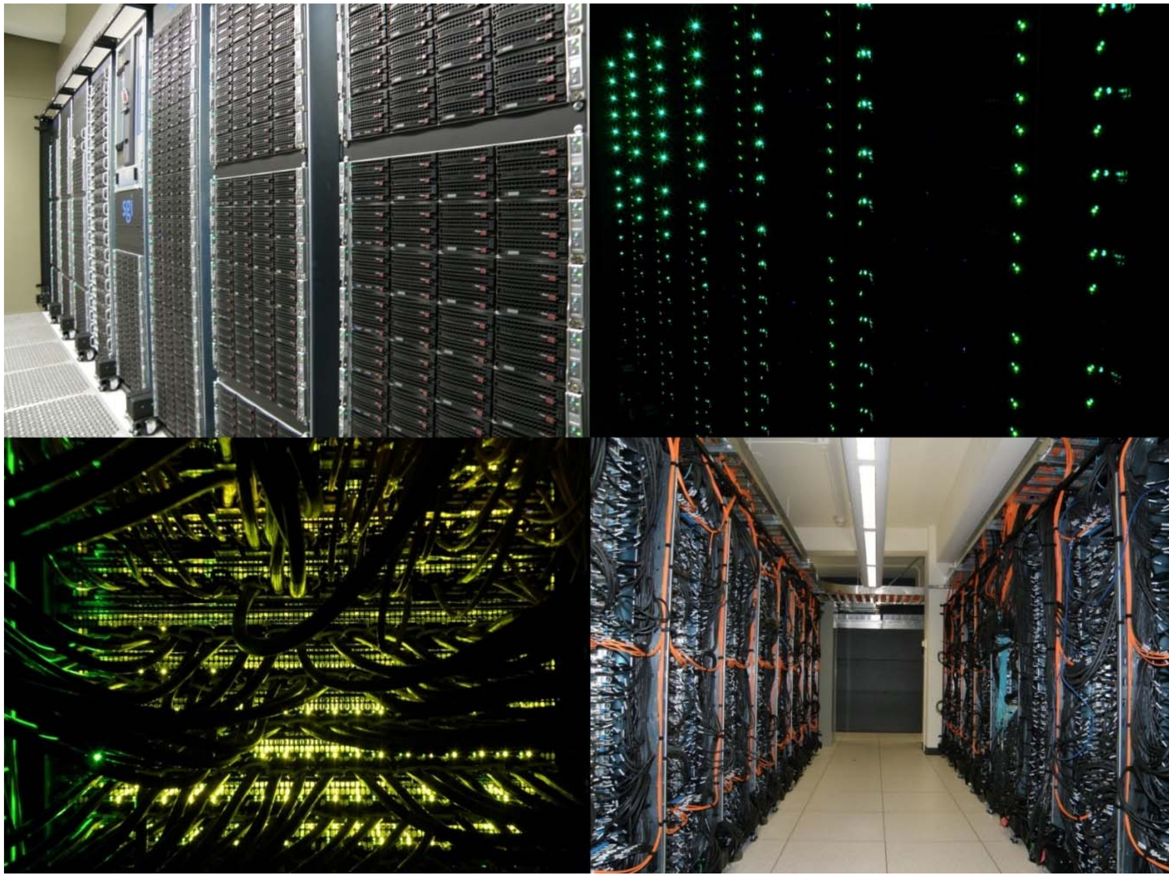


Figure from: Marc-Henri Julien

Mammouth



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Merci
Thank you

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D. Sénéchal

Bumsoo Kyung

The glue

Kyung, Sénéchal, Tremblay, Phys. Rev. B **80,** 205109 (2009)
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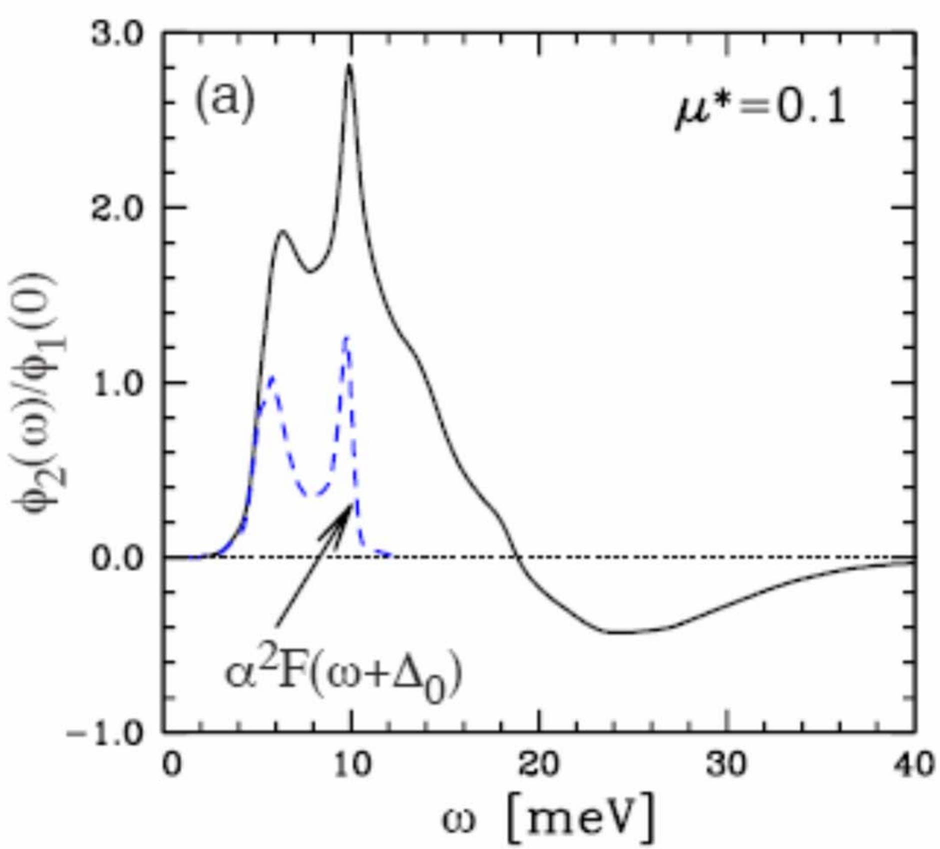
A. Reymbaut *et al*. PRB **94** 155146 (2016)

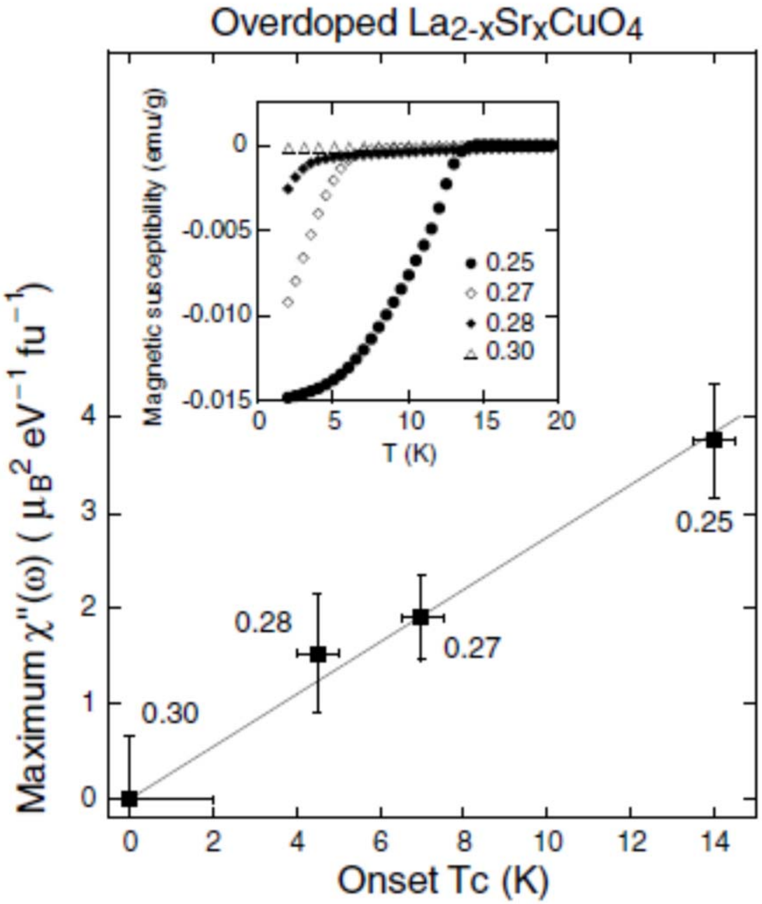
Im Σ_{an} and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

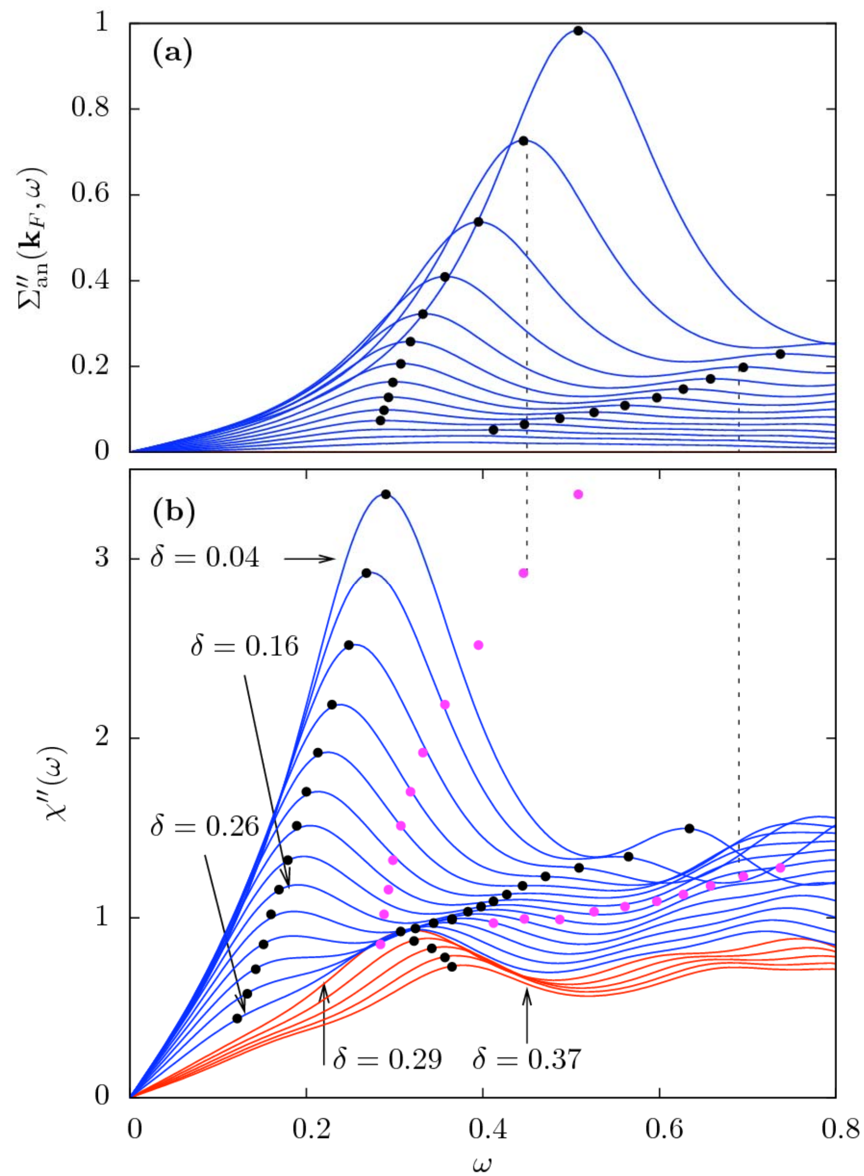


The glue

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



Wakimoto … Birgeneau PRL (2004)



The glue and neutrons

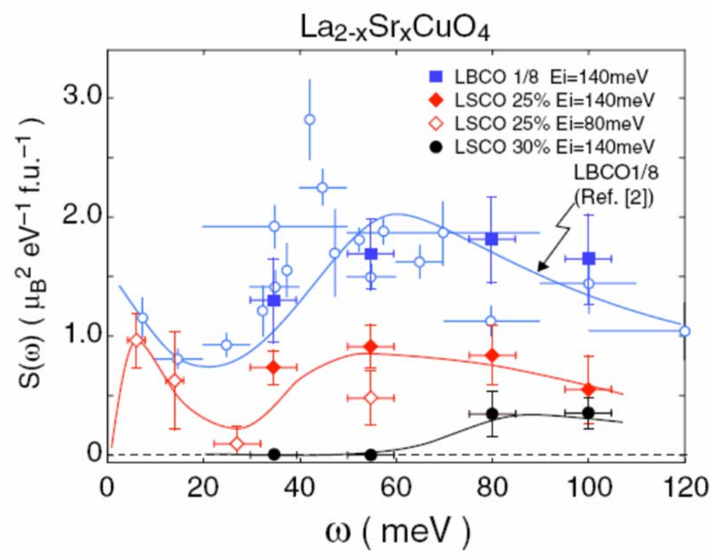


FIG. 3 (color online). **Q**-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i = 140$ meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO 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)