Mott transition as an organizing principle for high-temperature superconductivity

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

R3-4 Condensed Matter / Quantum Theory (DTP/DCMMP) | Matière condensée / théorie quantique (DPT/DPMCM) - SUB 307 (cap. 80) (13:30-15:00)

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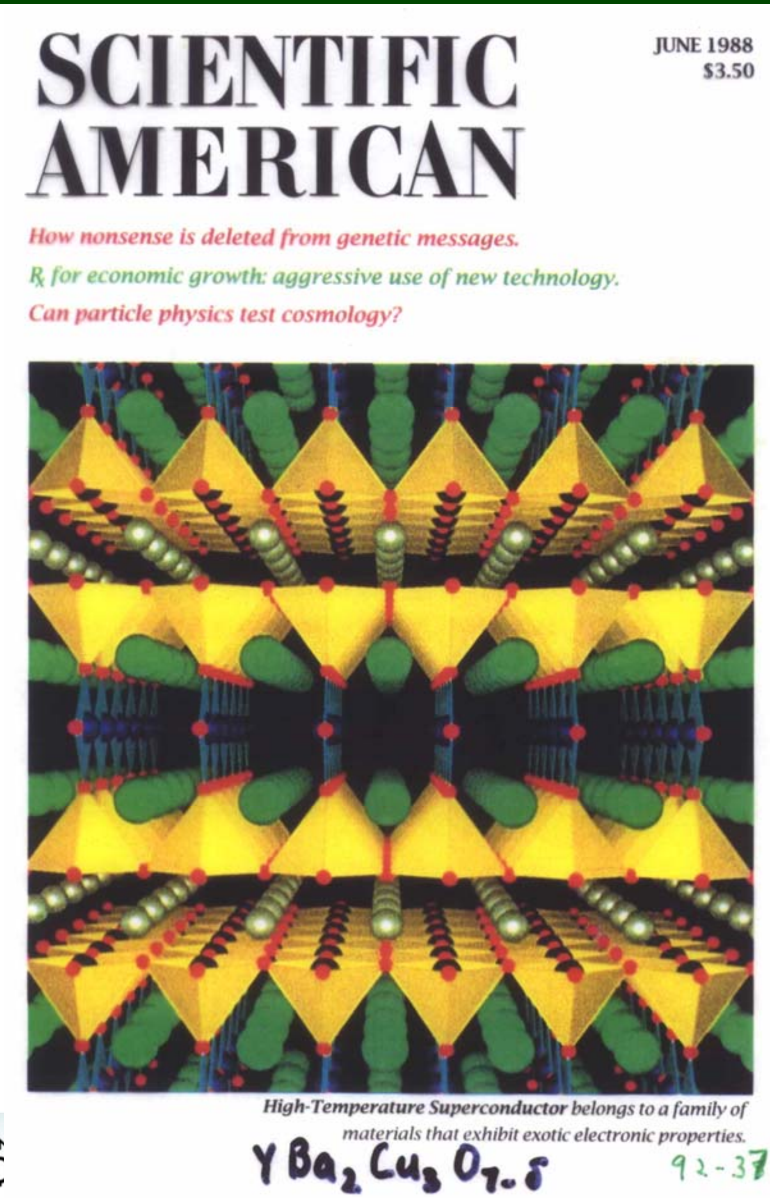
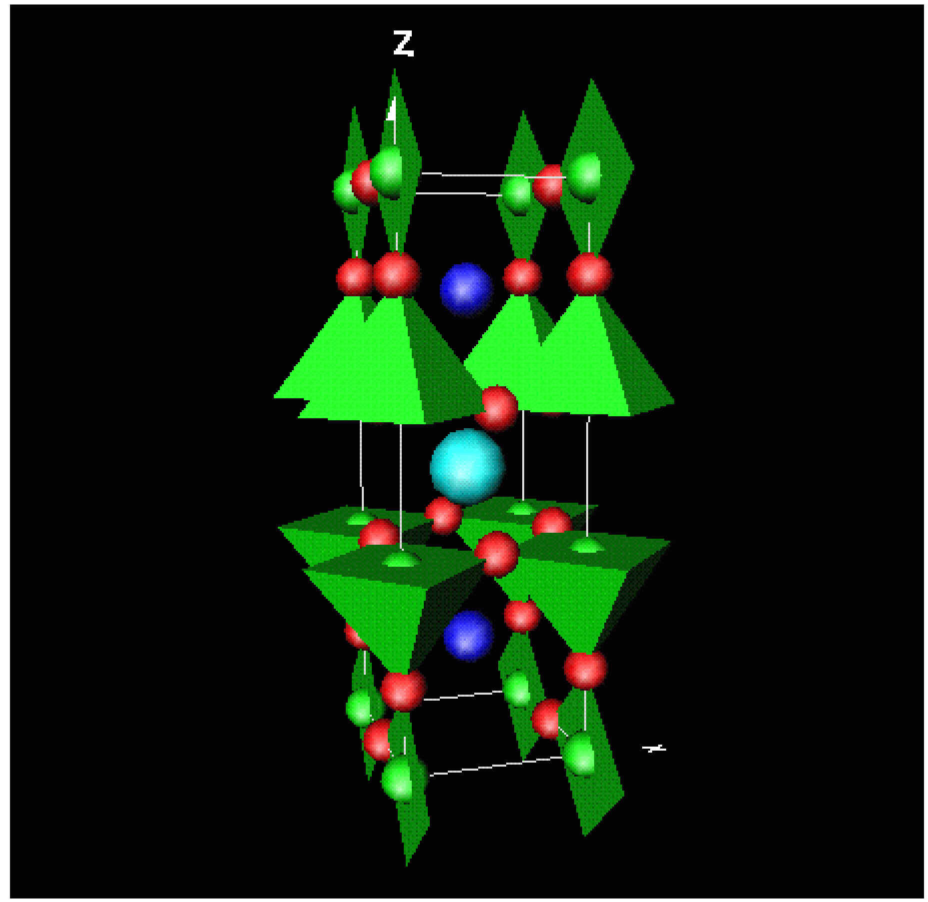
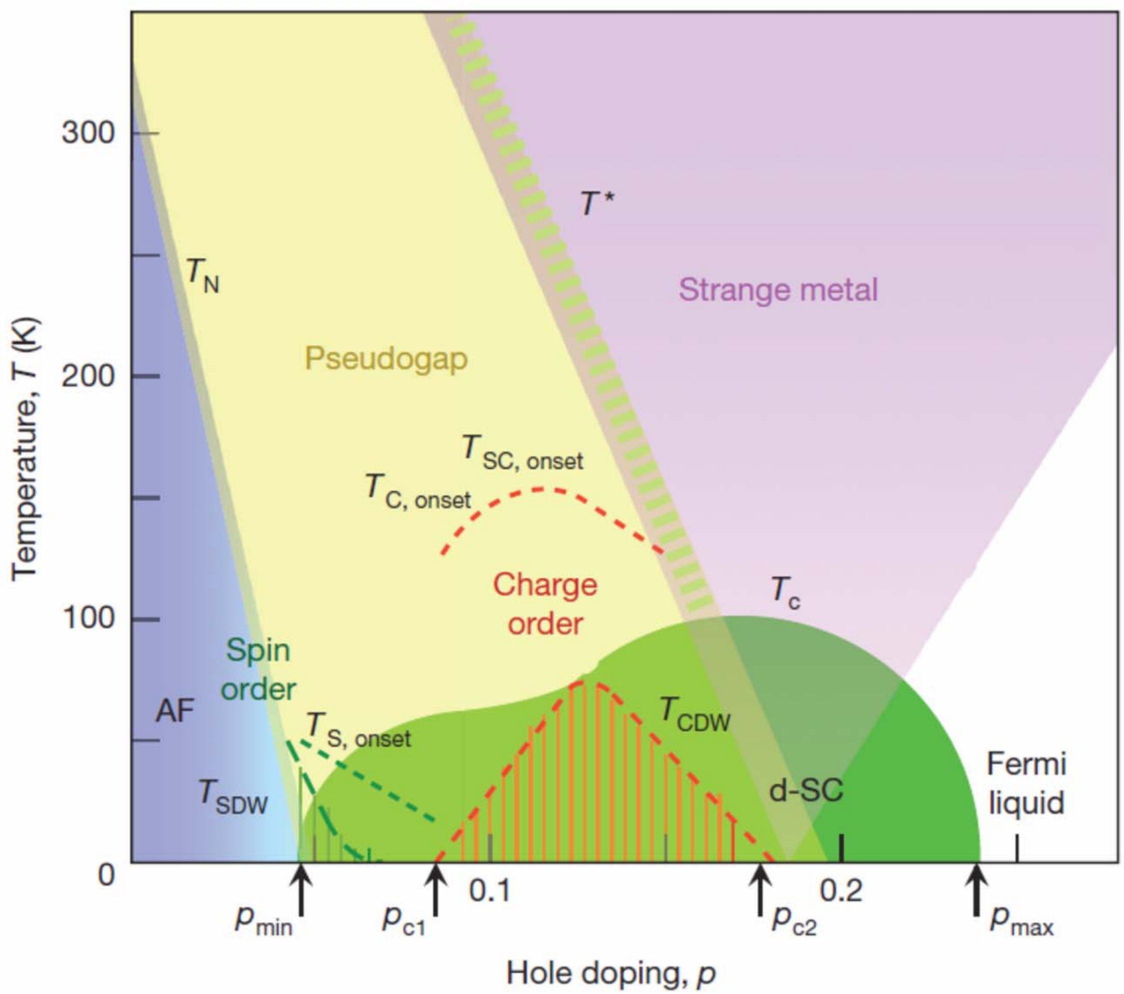
Atomic structure



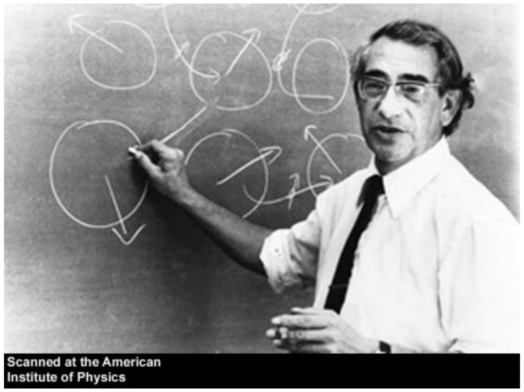


Phase diagram $YBa_2Cu_3O_{7-x}$

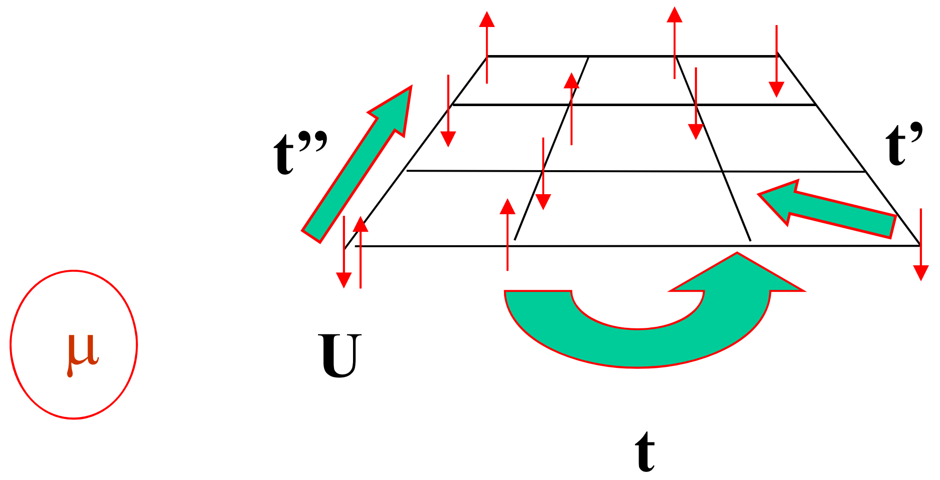


Keimer et al., Nature 518, 179 (2015)

Hubbard model



1931-1980



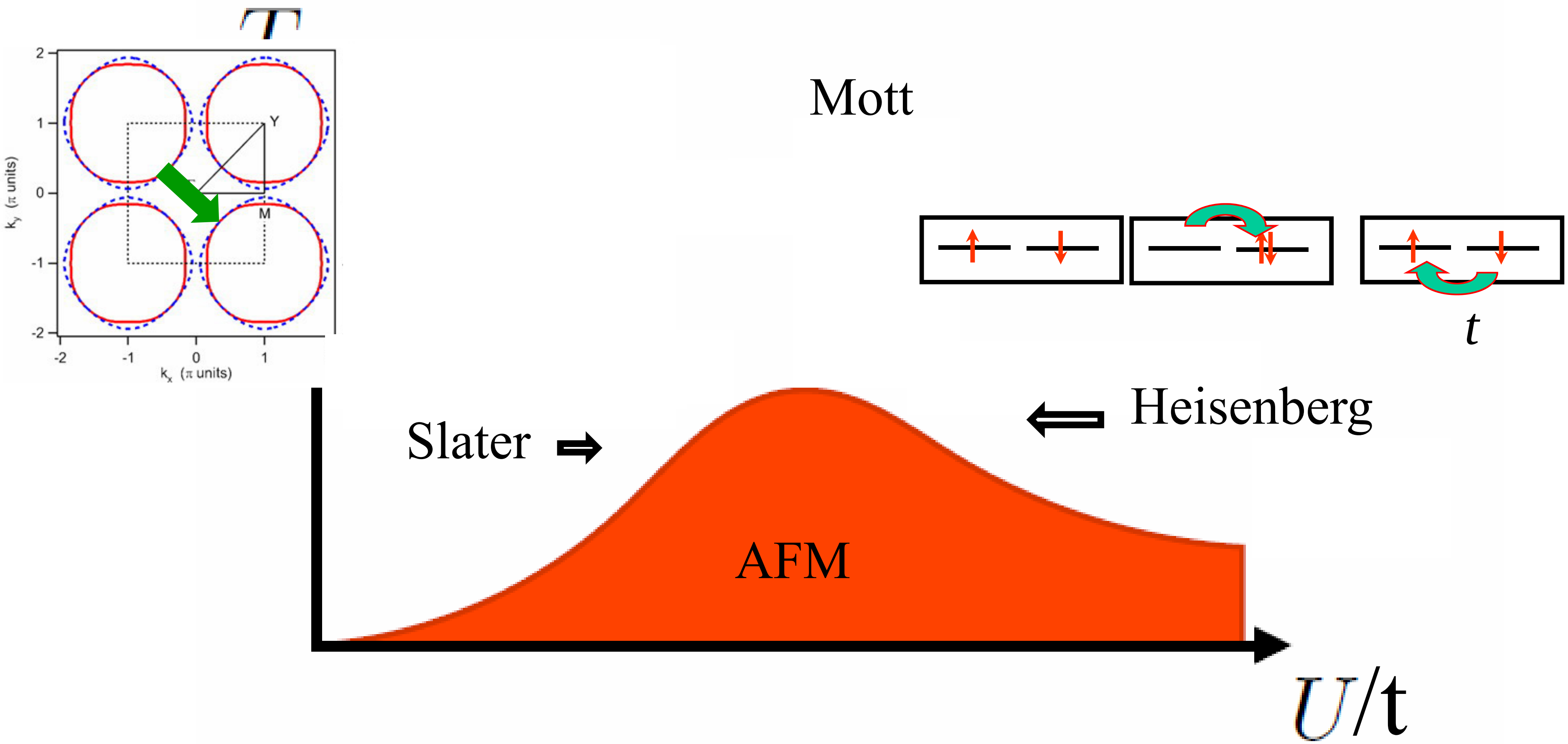
$$H = -\sum_{<ij>\sigma} t_{i,j} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

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

Attn: Charge transfer insulator

Weak vs Strong correlations

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



Method

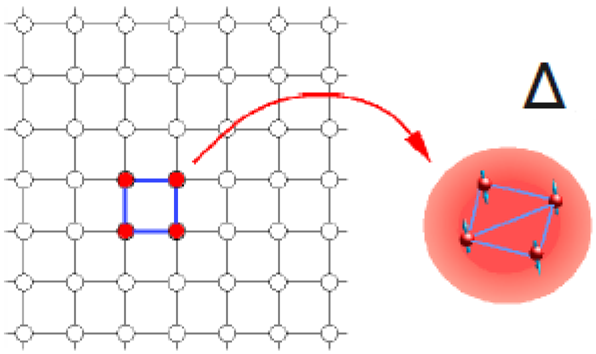
Dynamical Mean Field Theory (+ clusters)

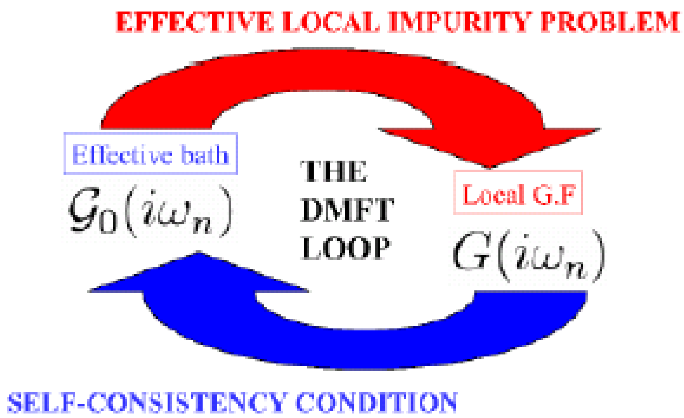
Concept: atomic-like localized correlations consistent with delocalized aspect

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





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

Some groups using these methods for cuprates

- Europe:
  - Georges, Parcollet, Ferrero, Civelli, (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: Weakly vs strongly correlated AFM
- Part II: Strong correlations *h-doped cuprates*

Part I

Weakly vs strongly correlated AFM
CDMFT 2x2

Giovanni Sordi

Lorenzo Fratino

Maxime Charlebois

Patrick Sémon

Mott transition as an organizing principle

Influence of the underlying normal state on the ordered state

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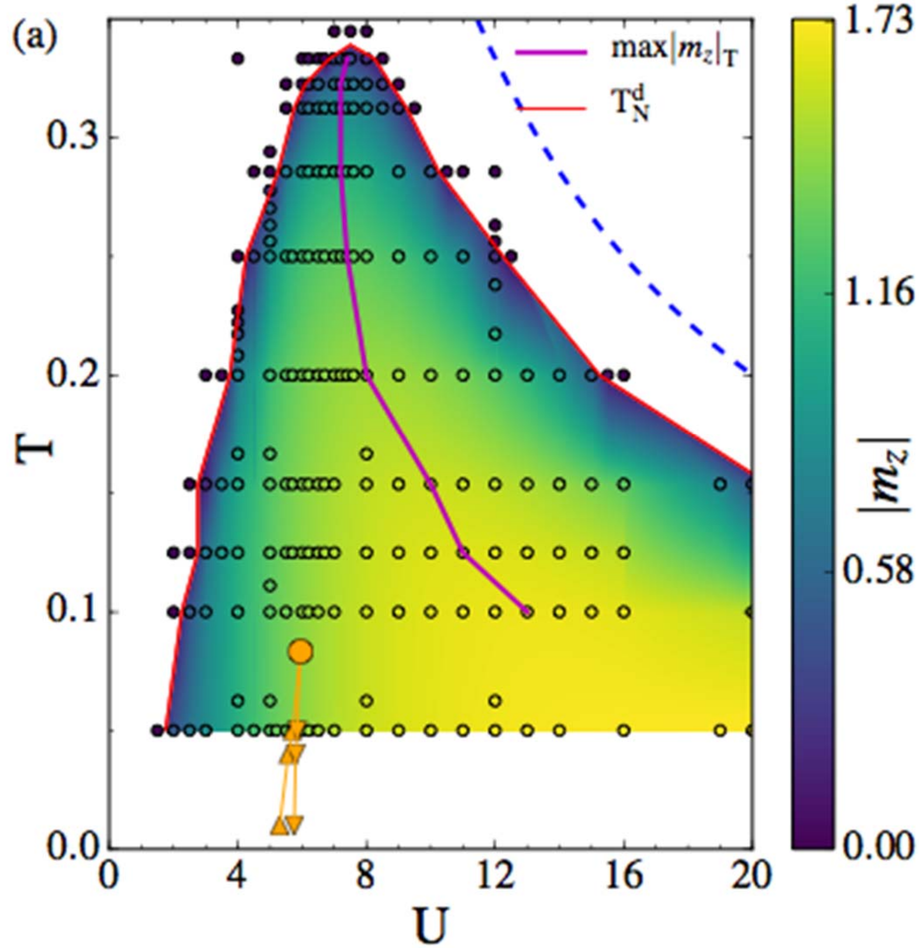
AFM phase diagram $d=2$, $t'=0$



L. Fratino, P. Sémon, M. Charlebois, G. Sordi, AMT Phys. Rev. B **95**, 235109 (2017)

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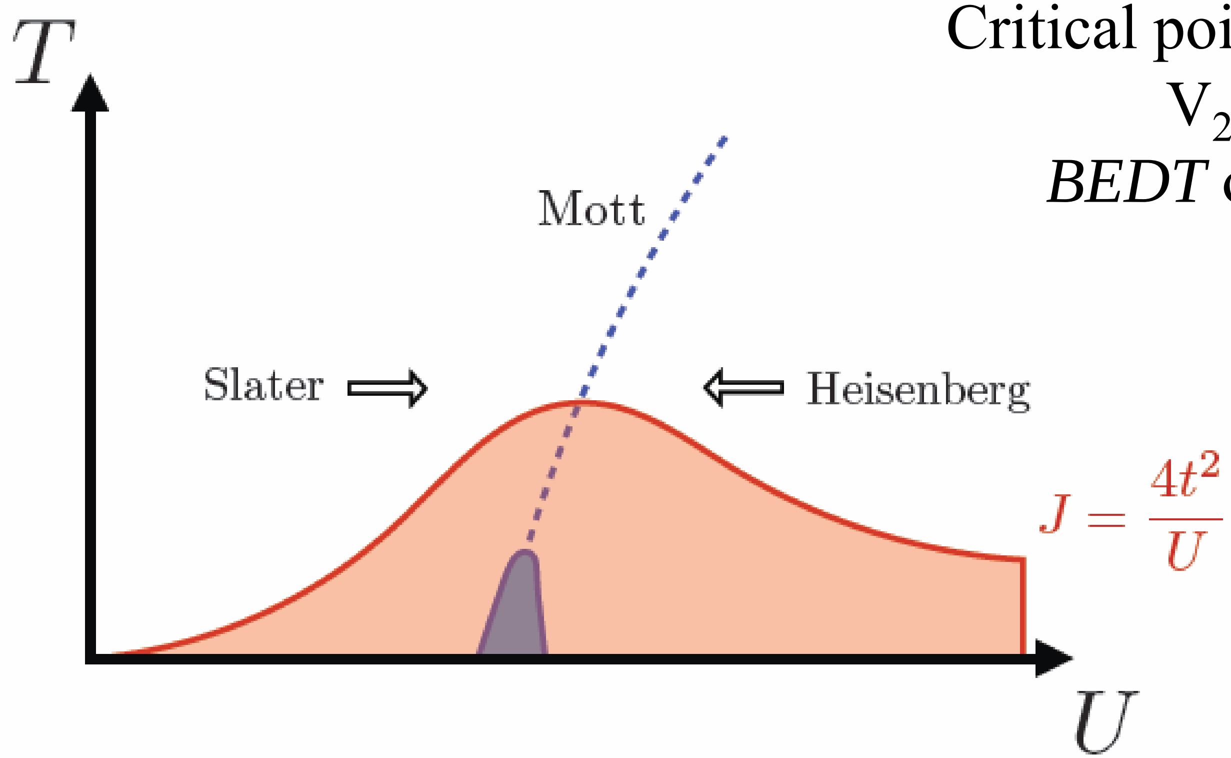
Underlying Mott transition

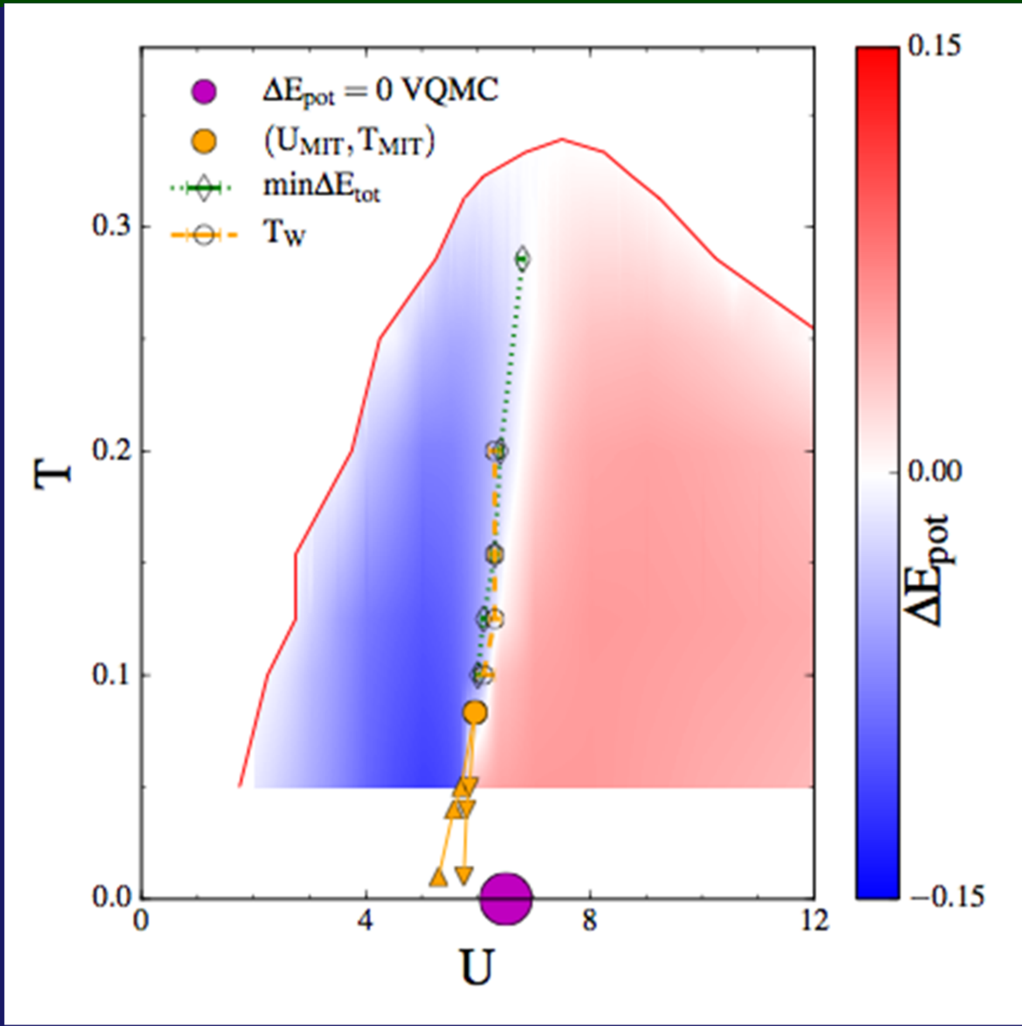
n = 1, d = 2 square lattice

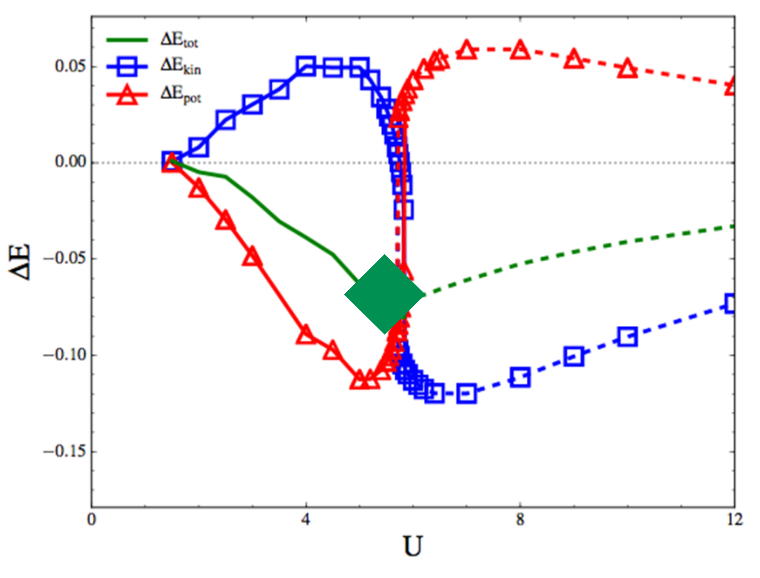


Critical point visible in V_2O_3, *BEDT* organics

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).

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Part II

Strong correlations : CDMFT *h-doped*

Giovanni Sordi

Kristjan Haule

Influence of the Mott transition away from half-filling

Pseudogap in the normal state

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]

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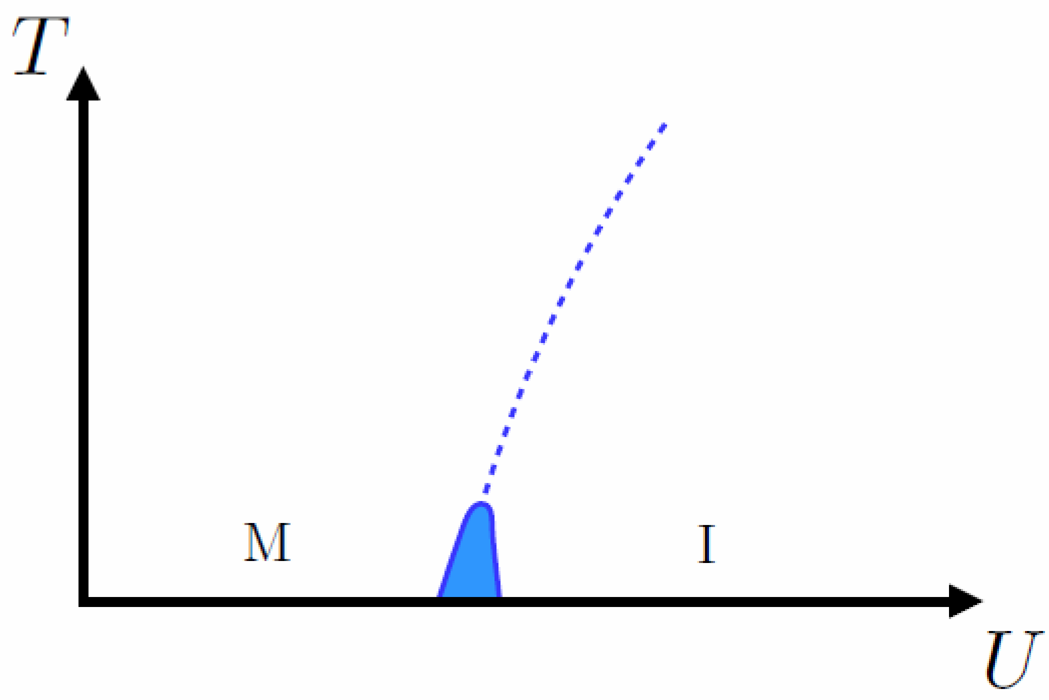
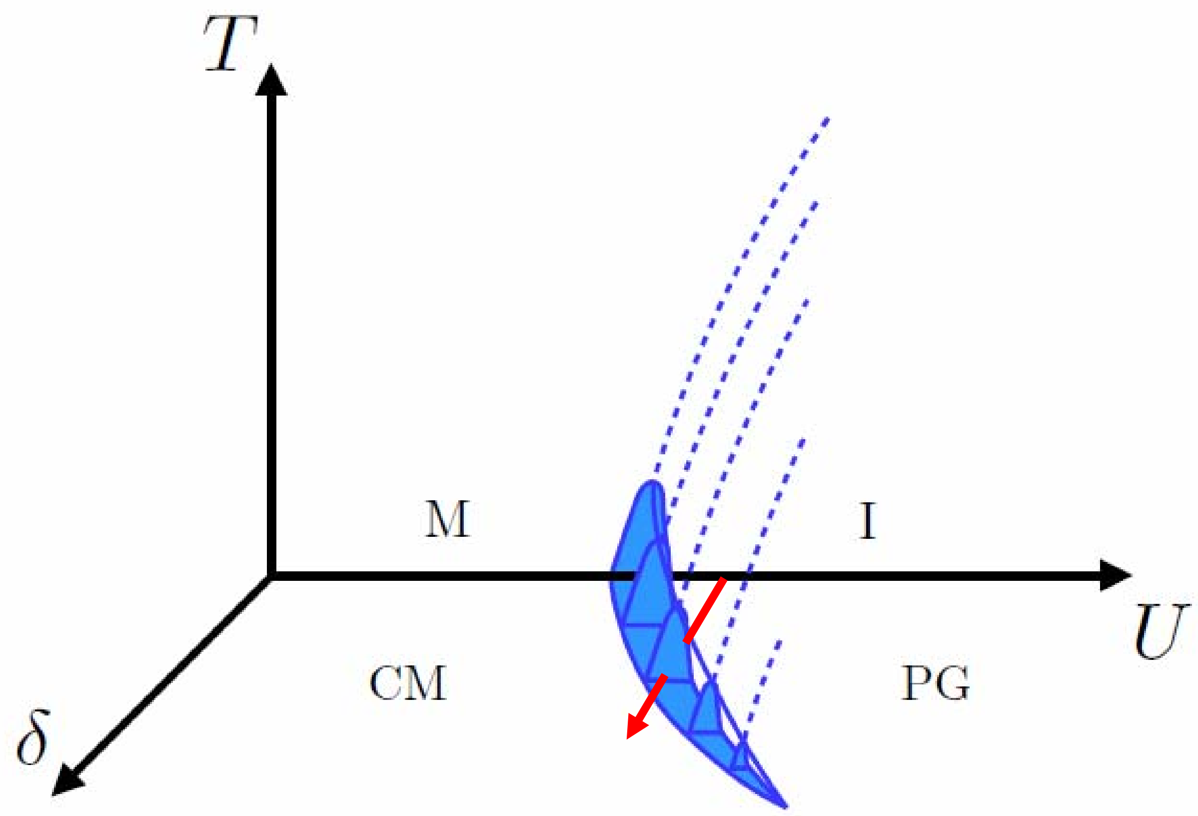
Influence of Mott transition away from half-filling

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

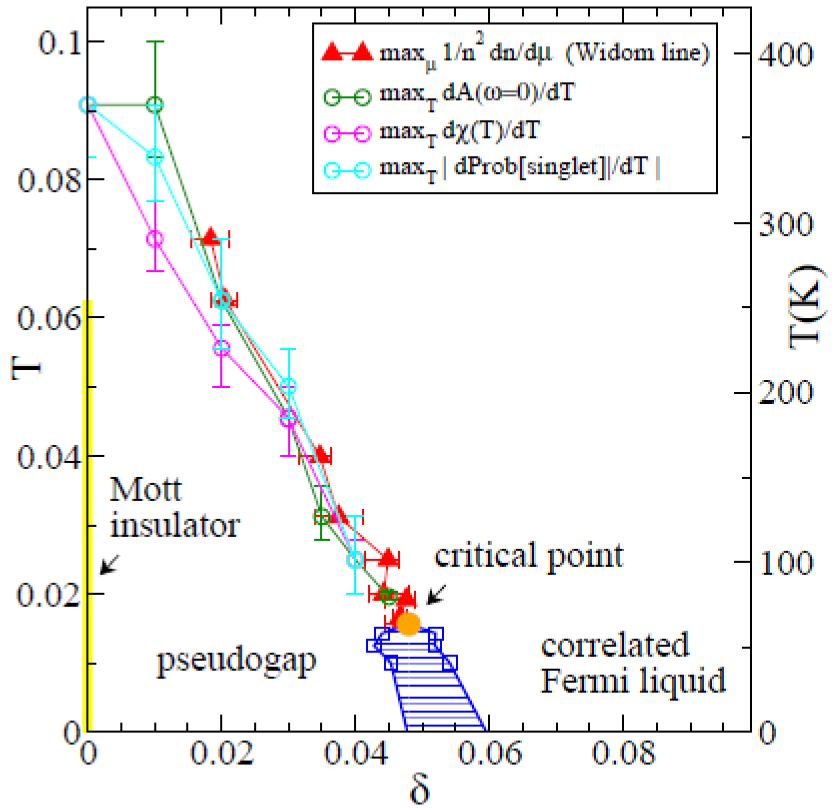


Influence of Mott transition away from half-filling

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

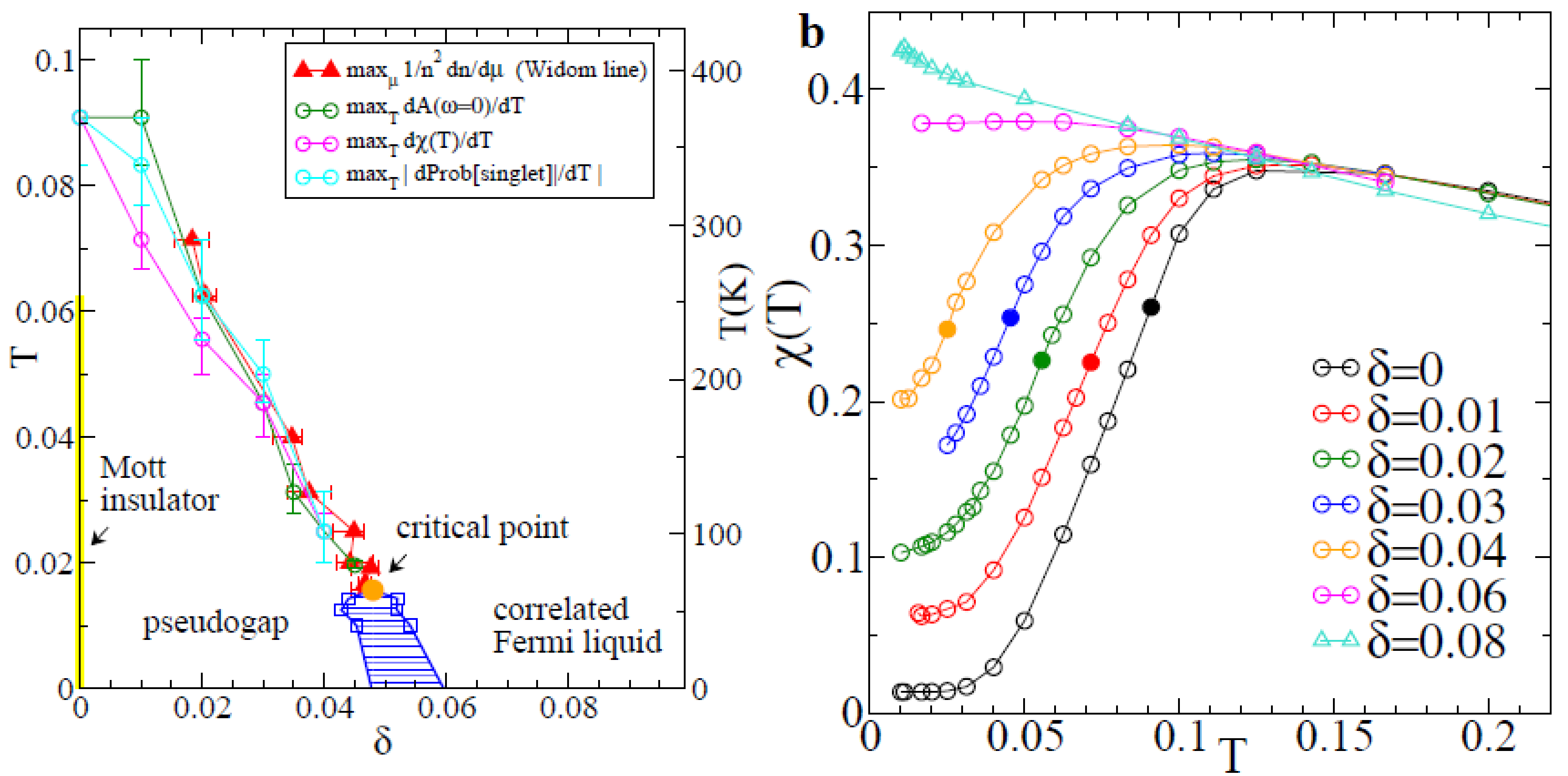


Spin susceptibility



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

Spin susceptibility



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

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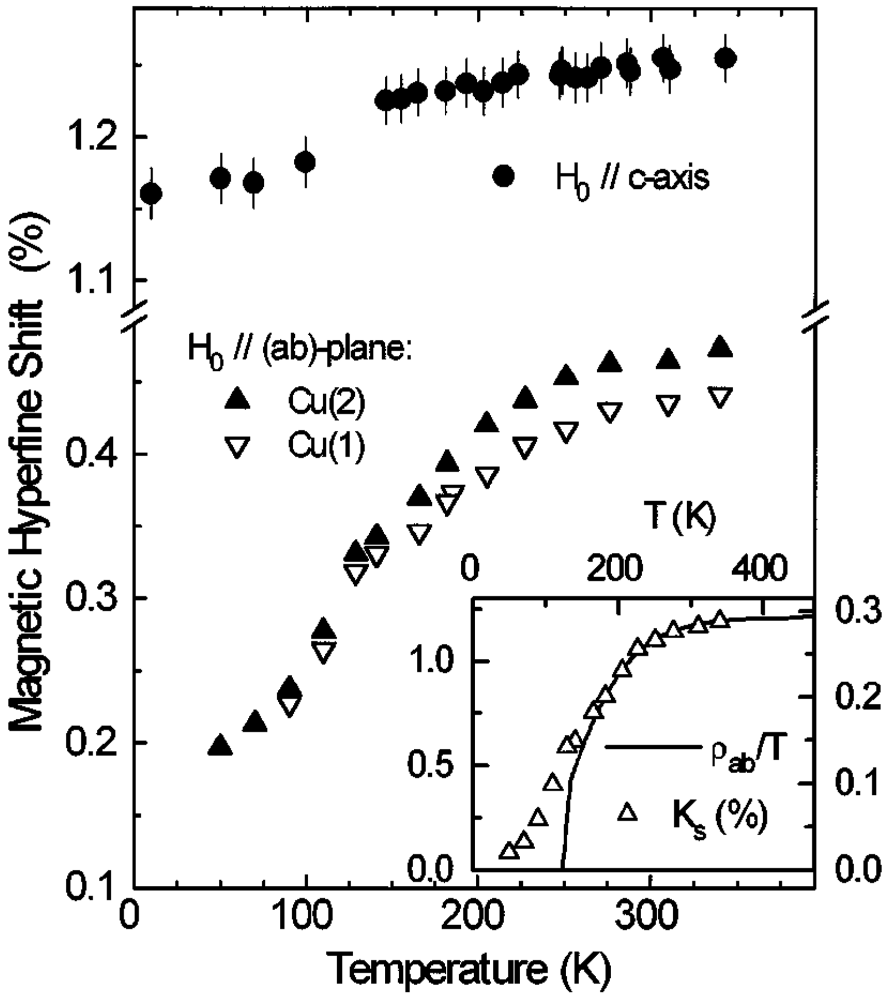
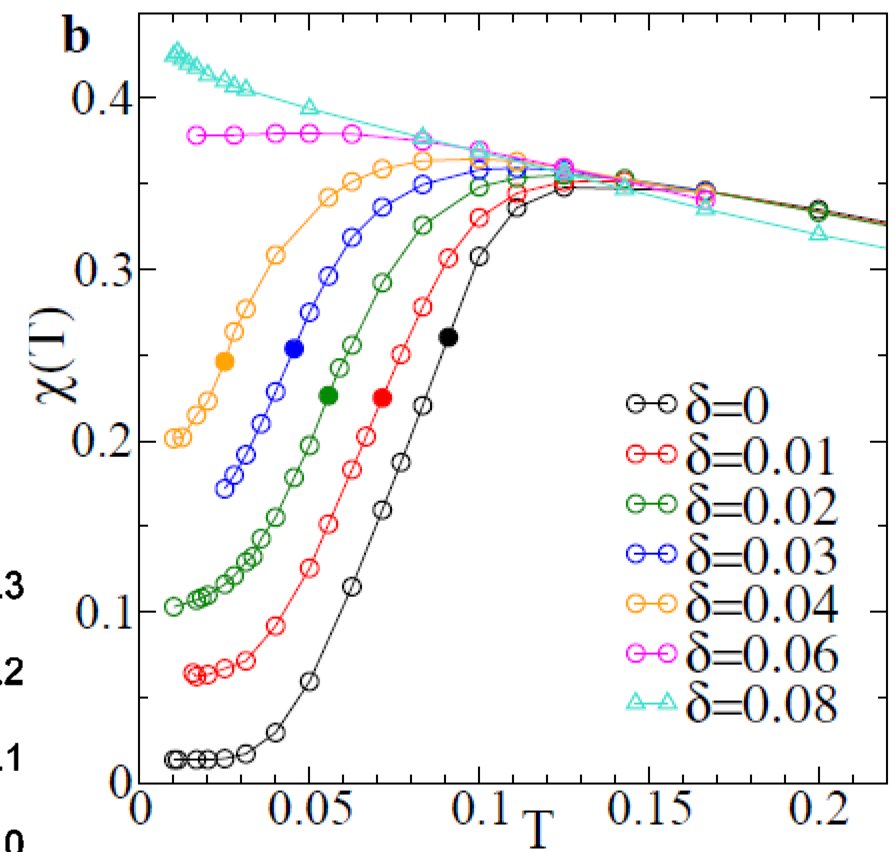
Spin susceptibility





Underdoped Hg1223

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

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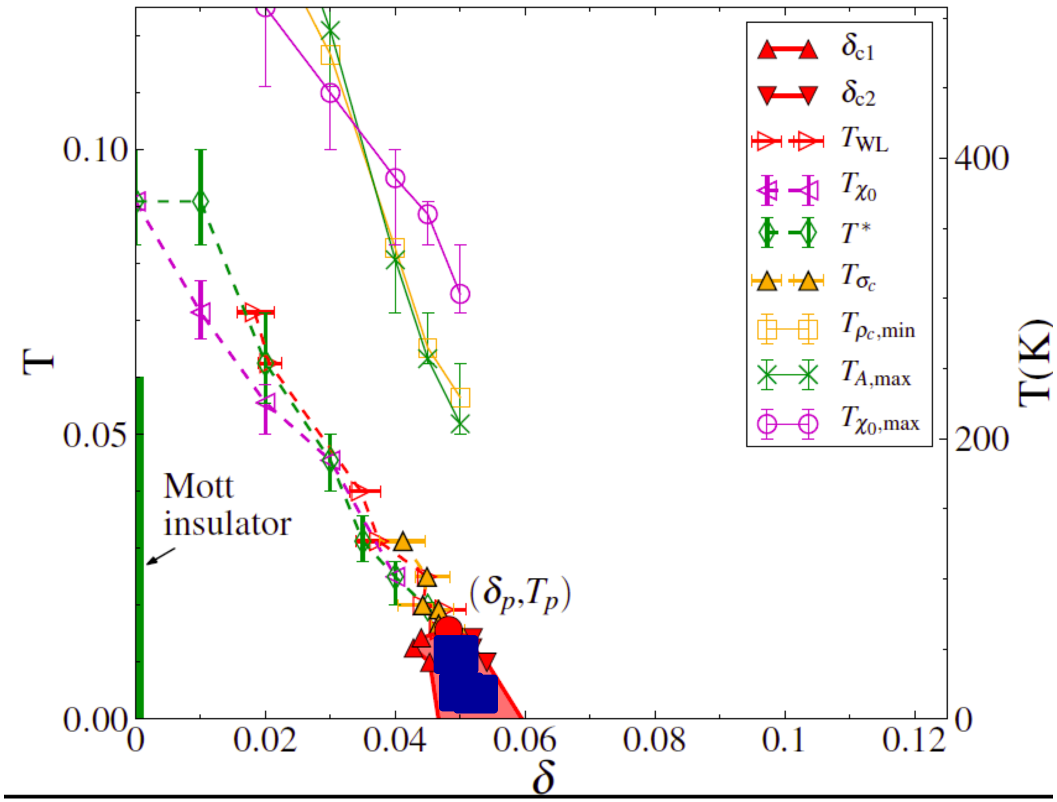
Two crossover lines

Giovanni Sordi

Patrick Sémon



G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)
P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B **89**, 165113/1-6 (2014)

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Results T*

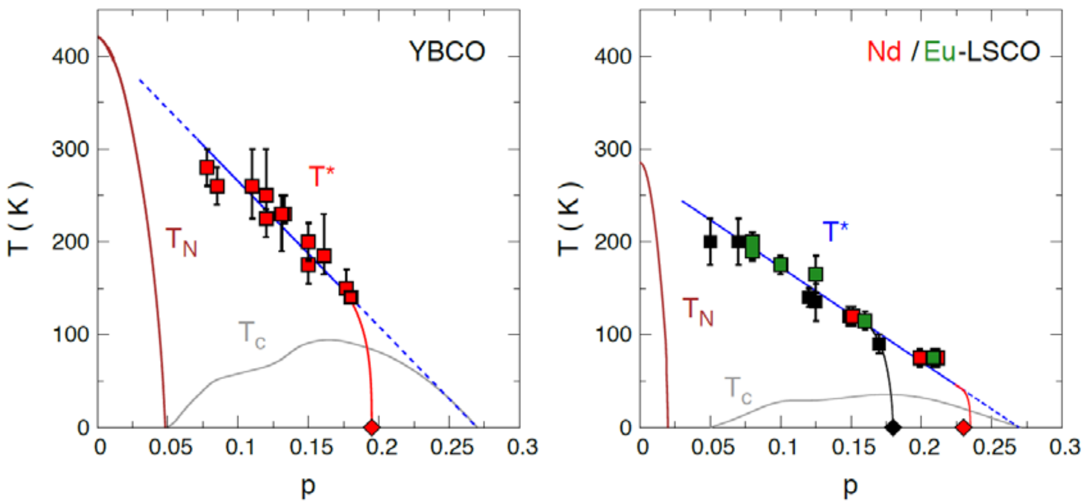
Patrick Sémon

Simon Bergeron

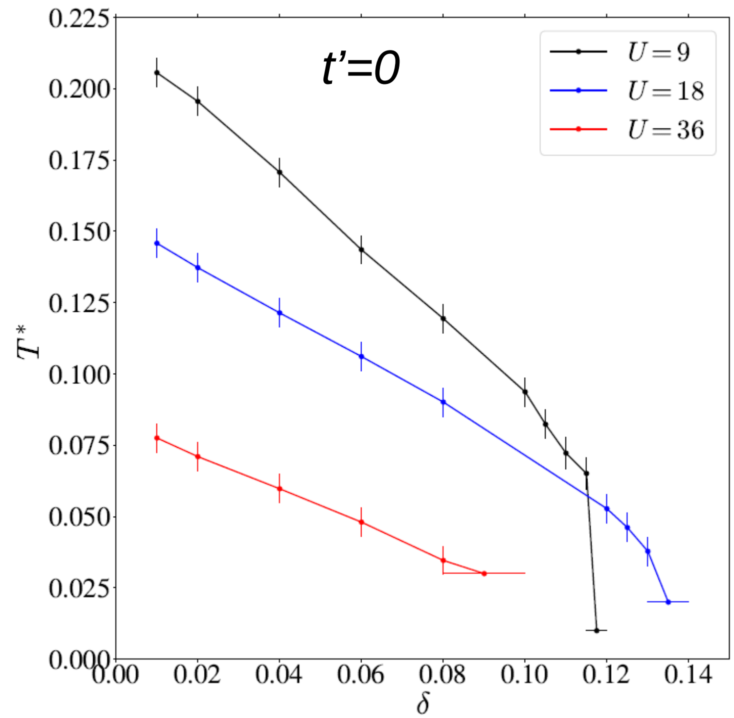
$$k_B T^* \sim J$$

$J = 4t^2/U$

Alexis Reymbaut



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



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

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

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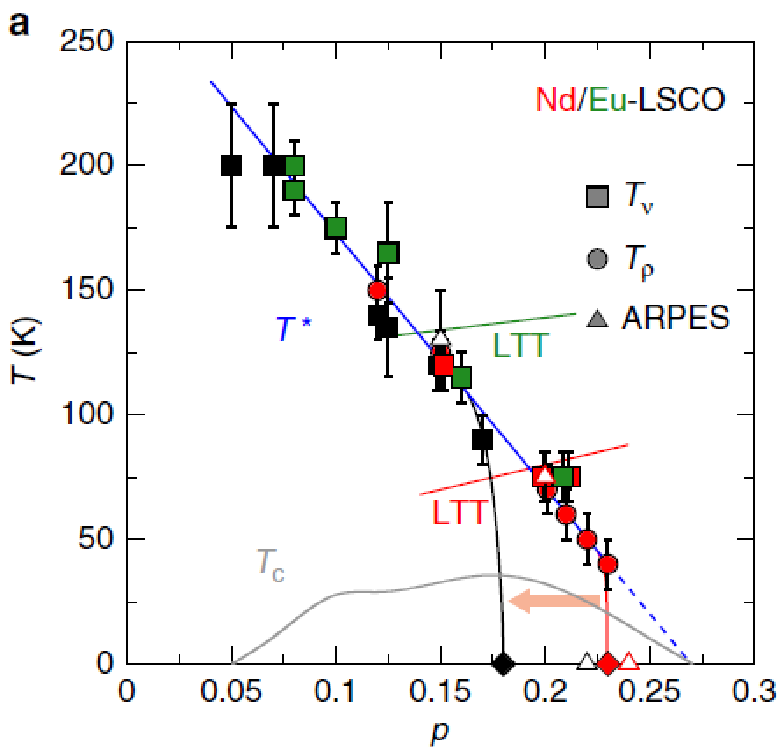
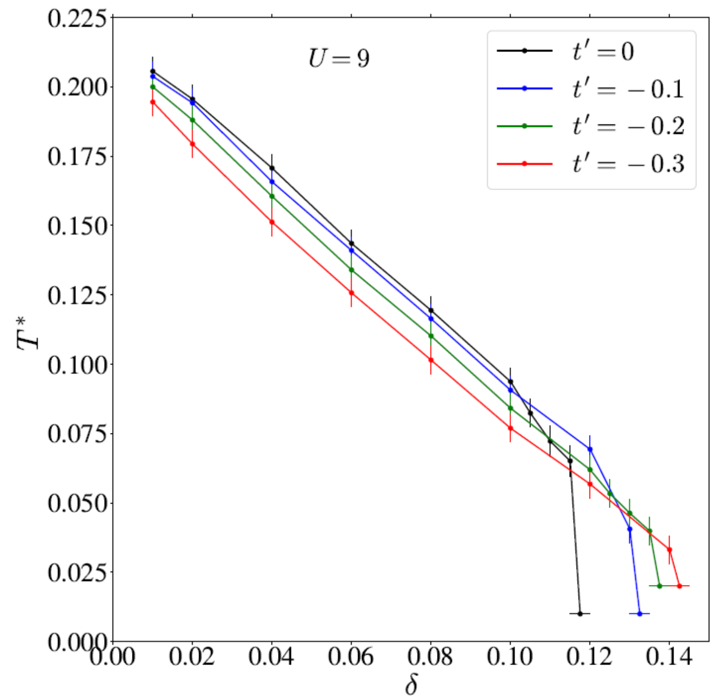
Results : effect of *t'* on *T**



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



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

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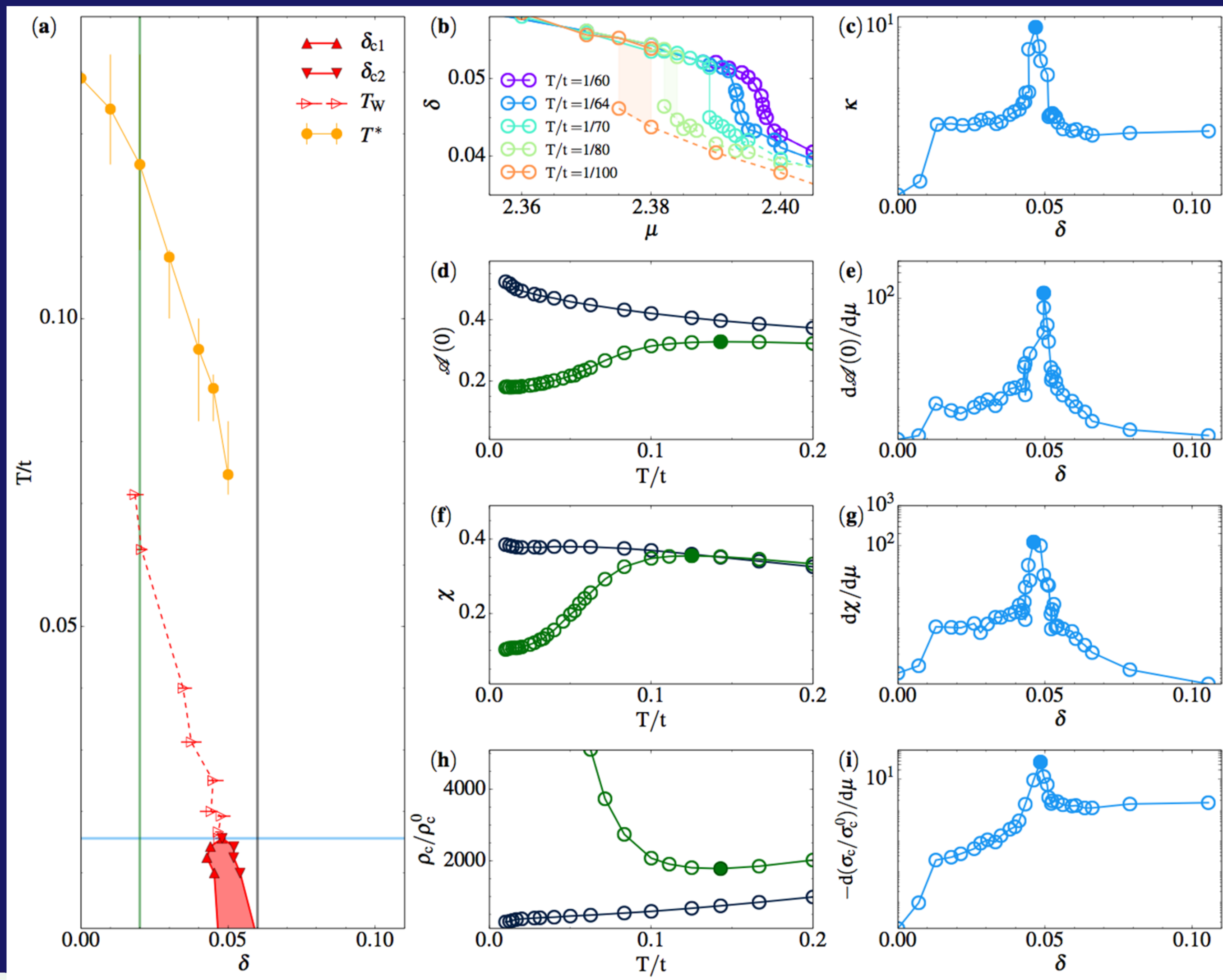
Summary


(a)
T/t
δ
δ_{c1}
δ_{c2}
T_W
T^*
(b)
δ
μ
T/t=1/60
T/t=1/64
T/t=1/70
T/t=1/80
T/t=1/100
(c)
κ
δ
(d)
$\mathscr{A}(0)$
T/t
(e)
$d\mathscr{A}(0)/d\mu$
δ
(f)
χ
T/t
(g)
$d\chi/d\mu$
δ
(h)
ρ_c/ρ_c^0
T/t
(i)
$-d(\sigma_c/\sigma_c^0)/d\mu$
δ

Giovanni Sordi

Patrick Sémon

Lorenzo Fratino

Strongly correlated Superconductivity

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

Fratino et al.

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

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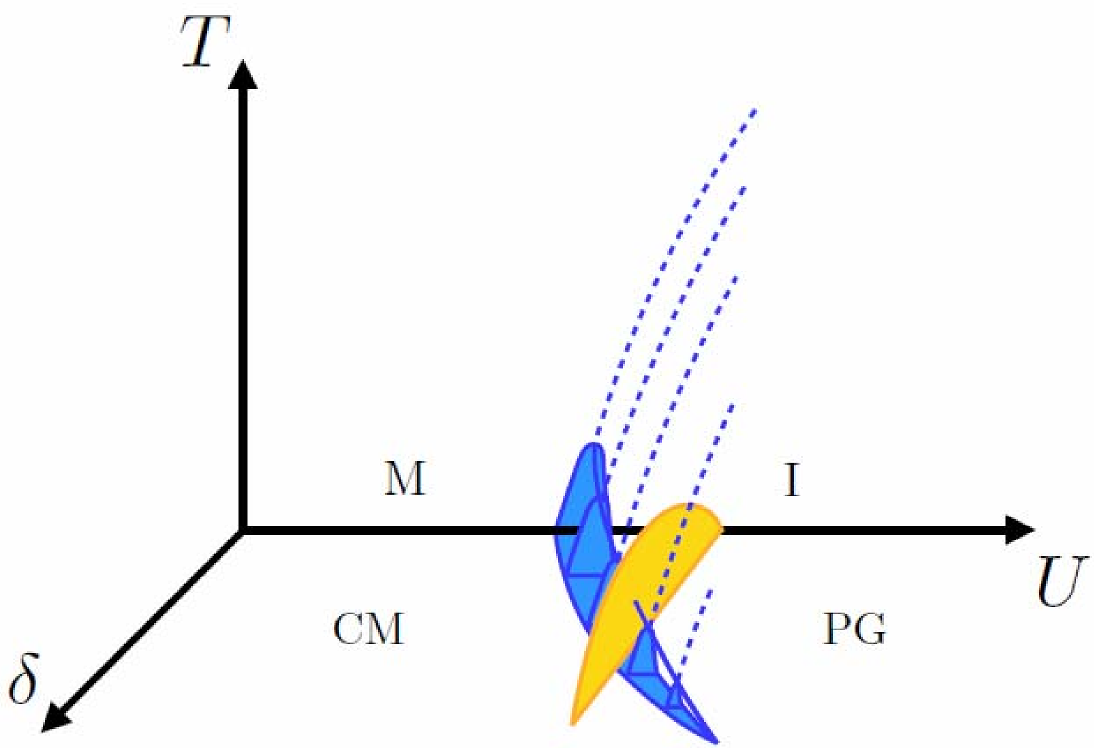
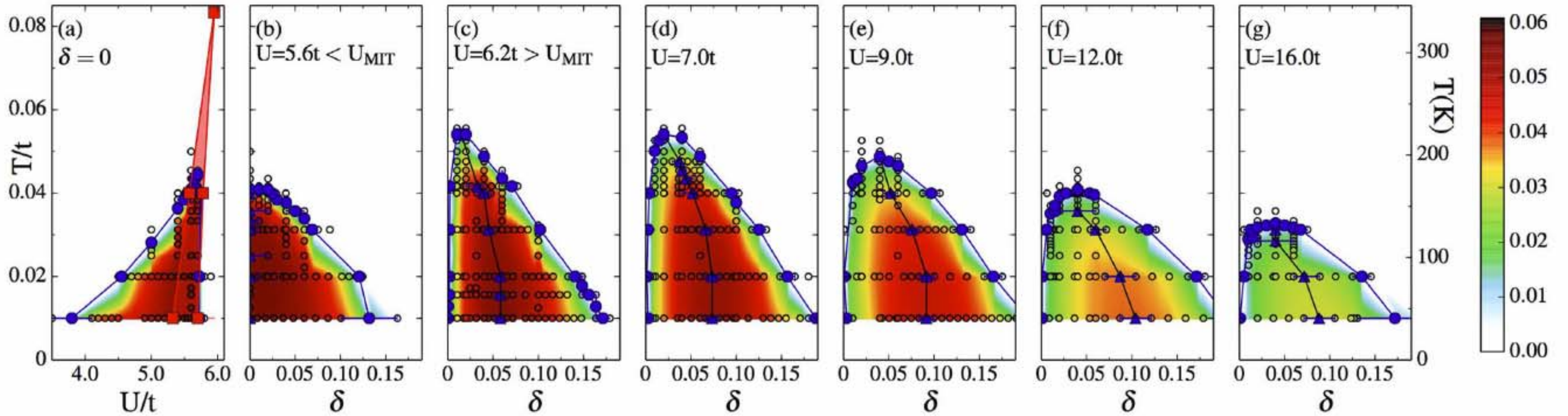
Superconductiviy in Doped Mott insulator

n = 1, d = 2 square lattice

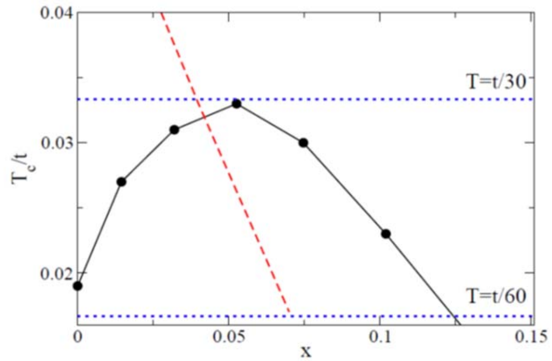


T_c controlled by J

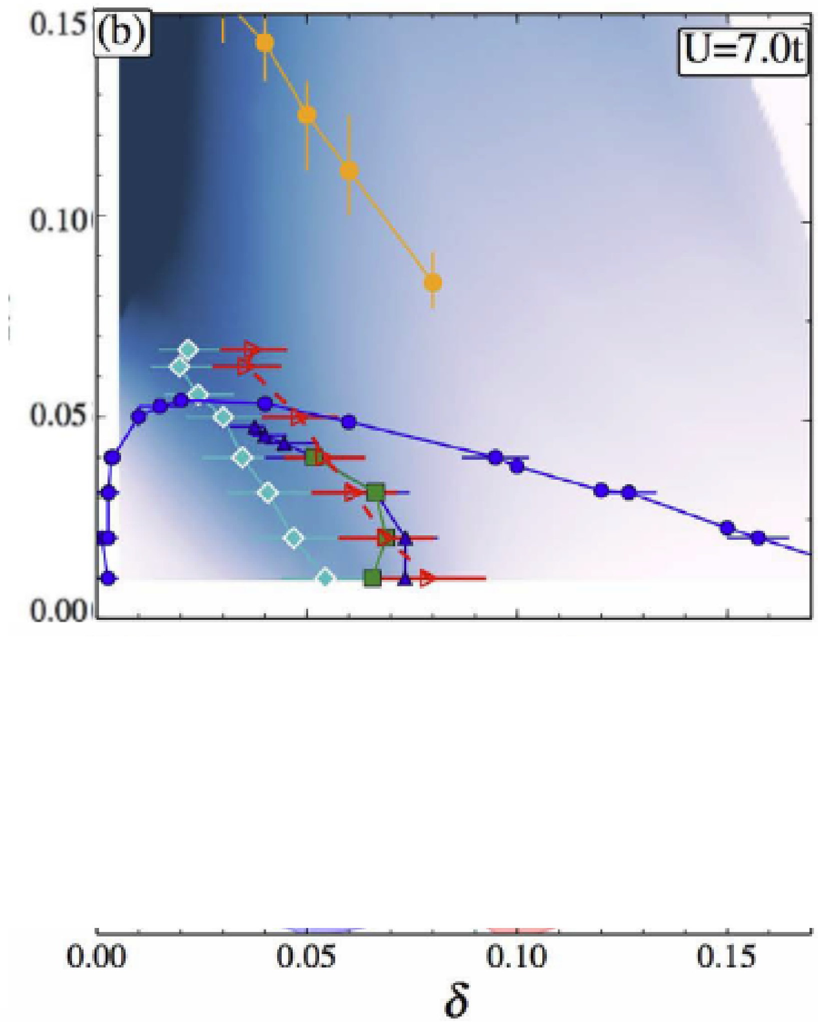


Fratino et al.
Sci. Rep. **6**, 22715

An organizing principle



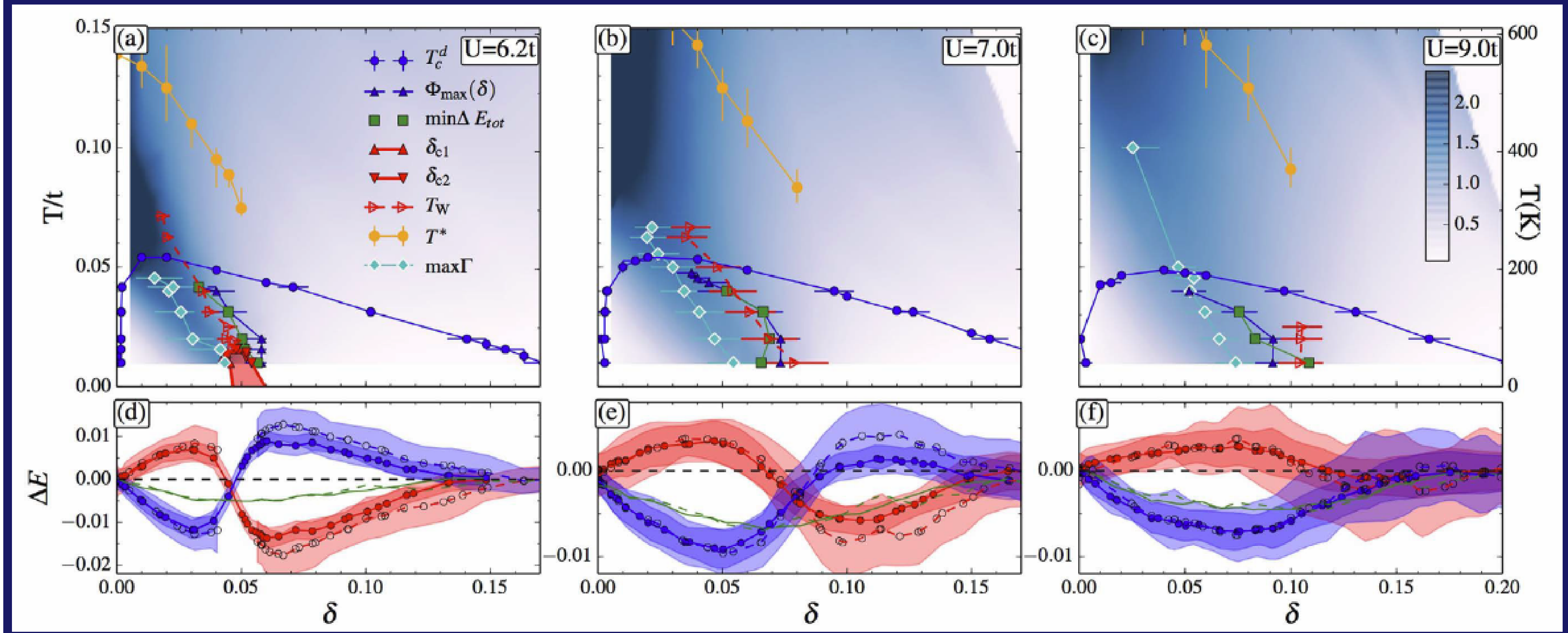
E. Gull and A. J. Millis
Phys. Rev. B 88, 075127



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



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

See also

Jarrell

Gull Millis PRB **90**, 041110(R)

Experiments:

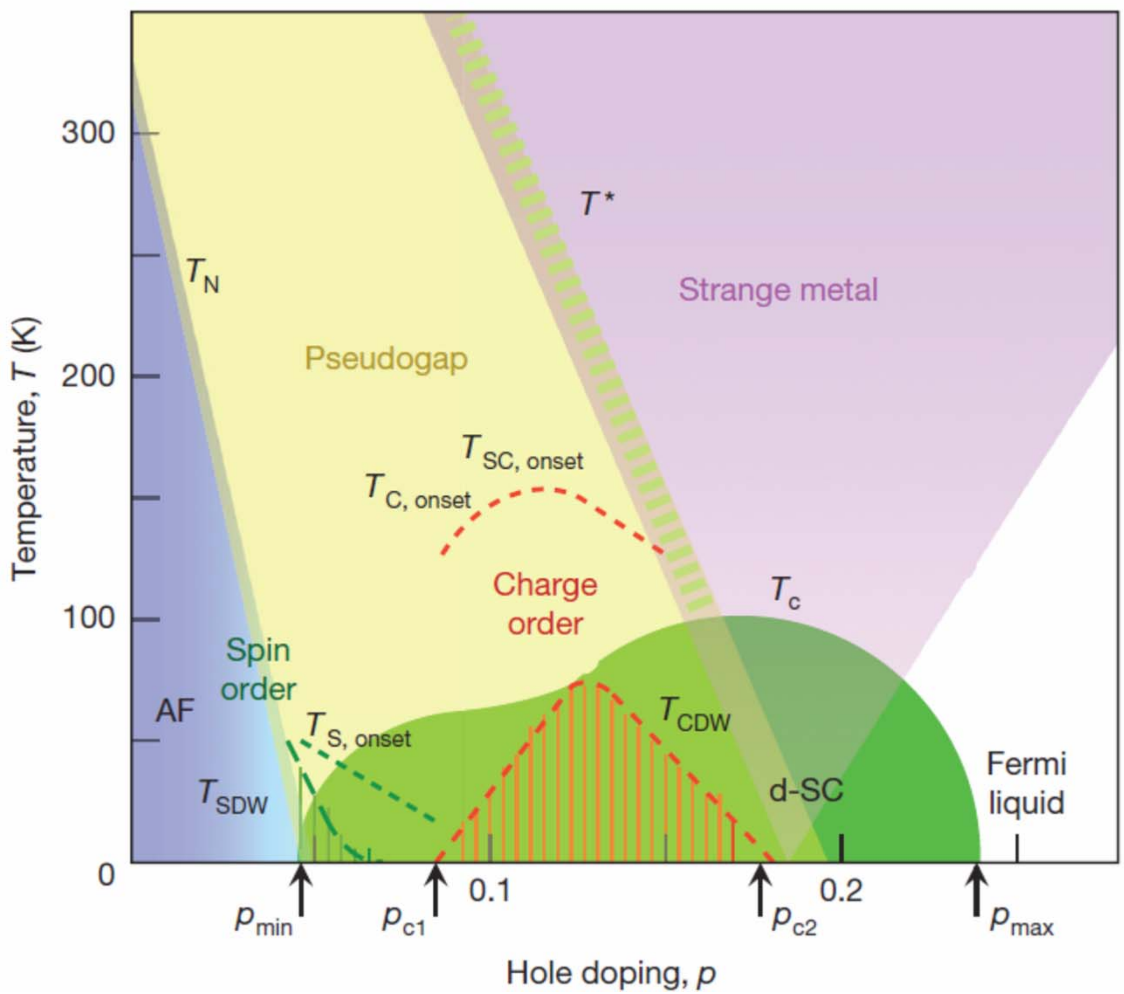
Deutscher et al, PRB 2005;

Molegraaf et al, Science 2002;

Carbone et al, PRB 2006

Giannetti et al, Nat Comm 2014

Phase diagram $YBa_2Cu_3O_{7-x}$



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

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Olivier Simard

Charles-David Hébert

Alexandre Foley

David Sénéchal

What causes T_c to drop?

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

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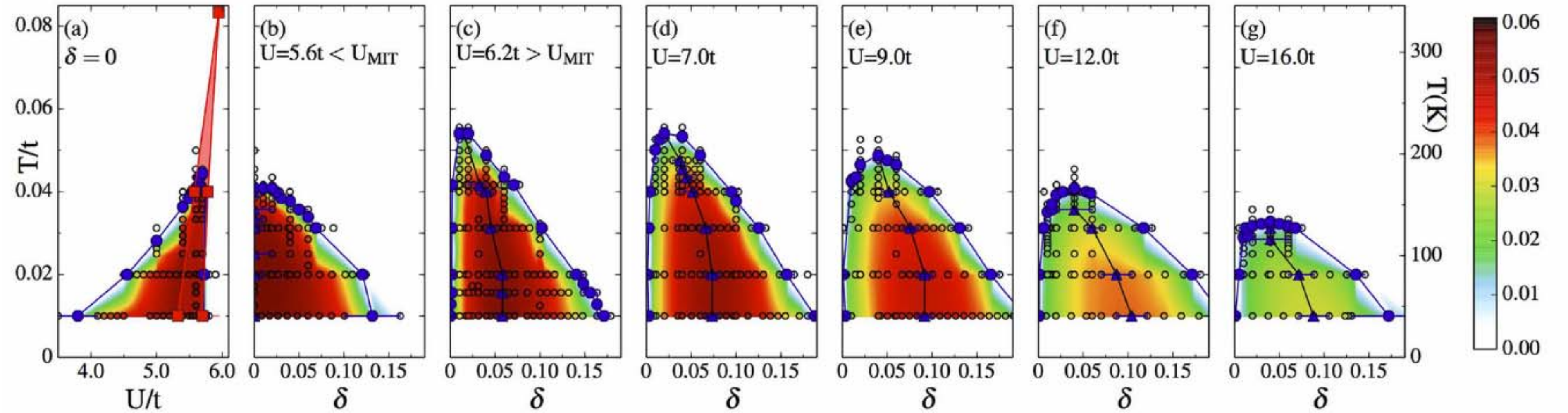
T_c controlled by J



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

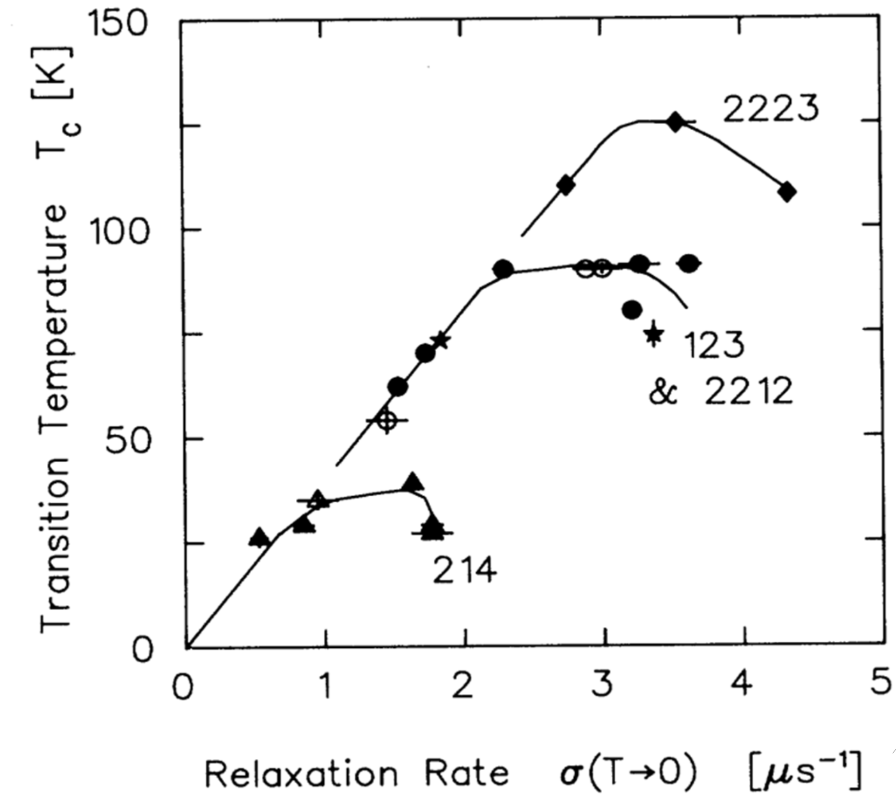
A. Pushp, Parker, … A. Yazdani, Science **364**, 1689 (2009)

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

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

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)

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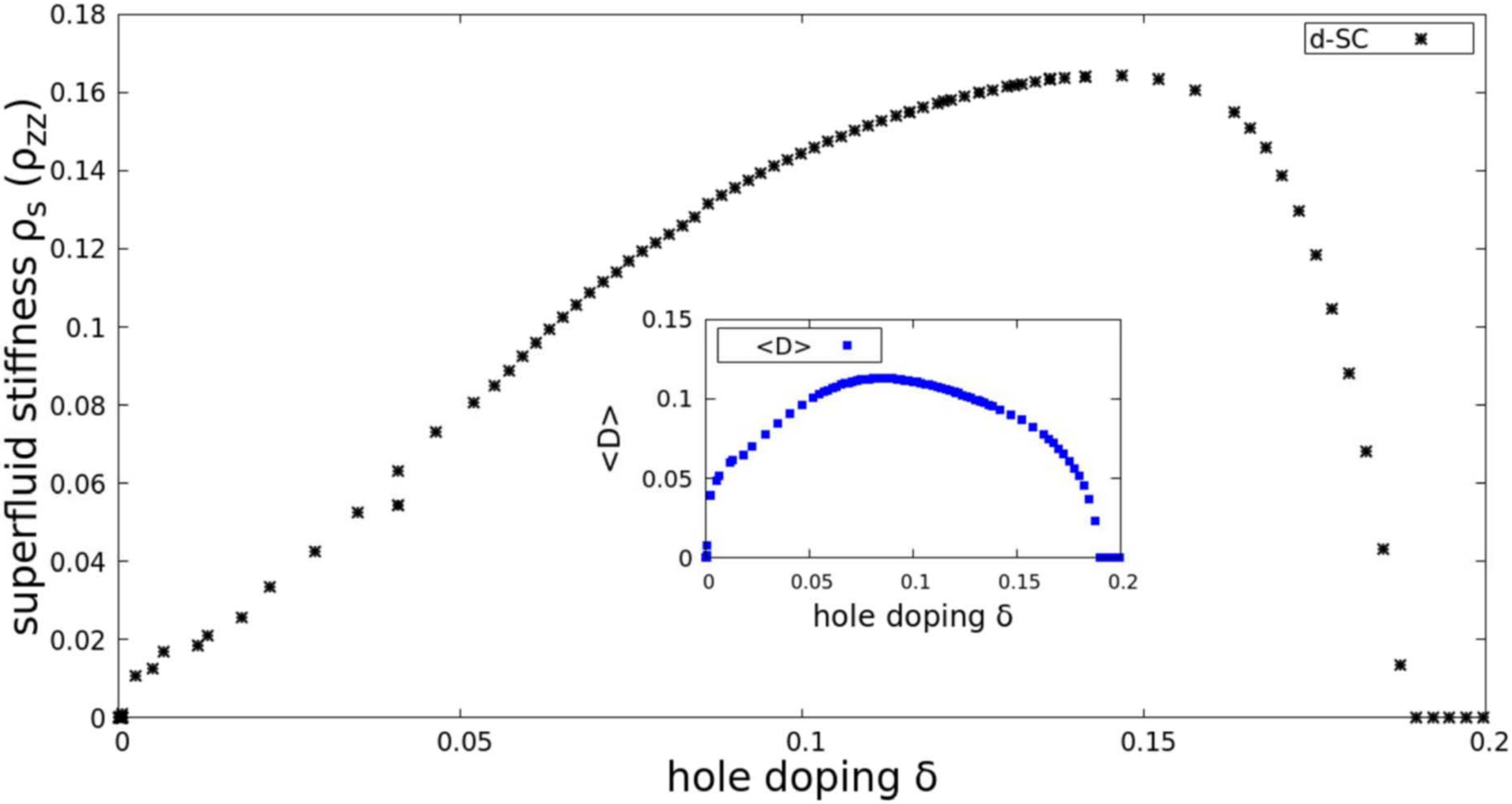
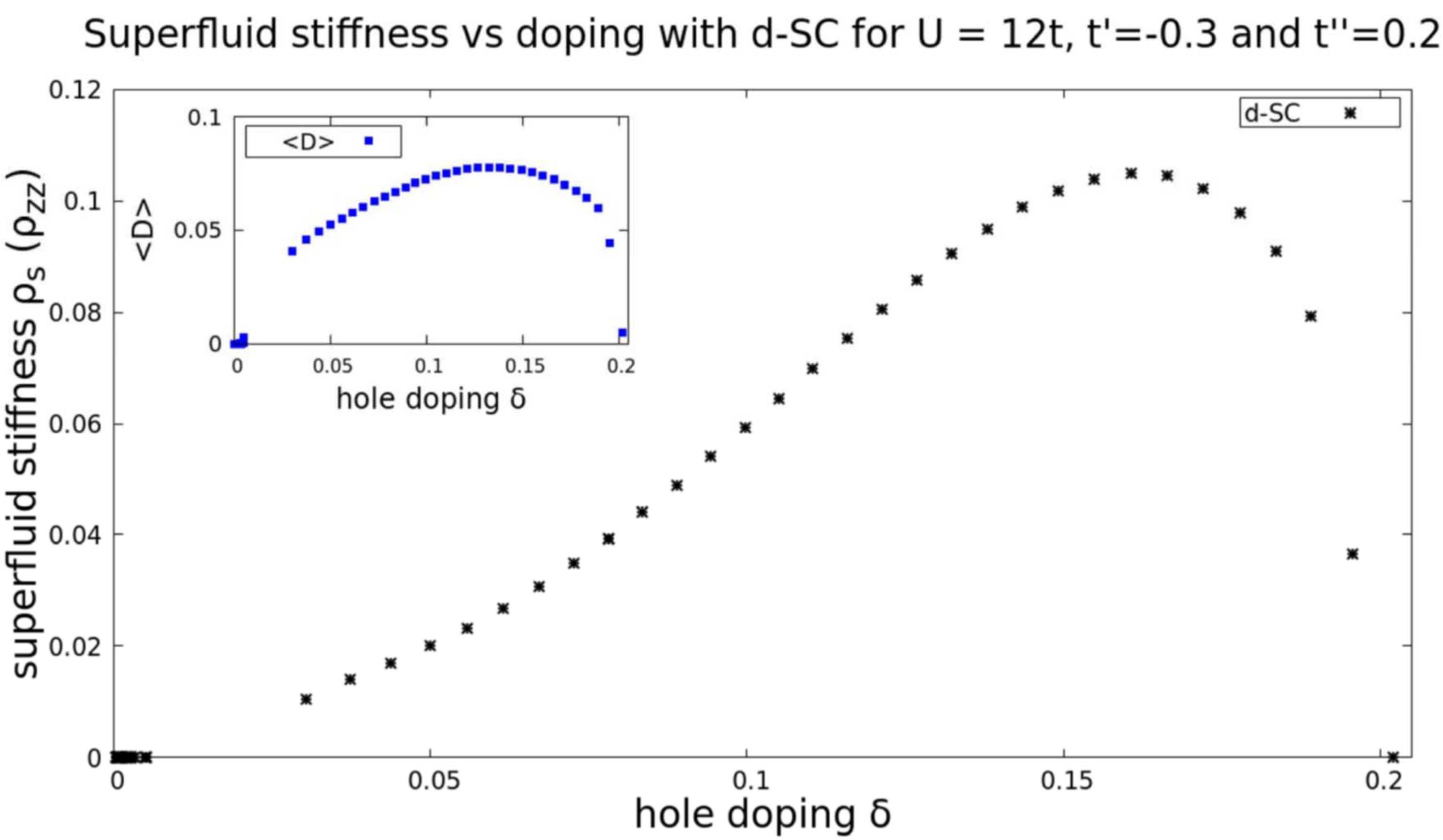
Superfluid stiffness *T=0*

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

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



Superfluid stiffness *T=0*



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

Conclusion

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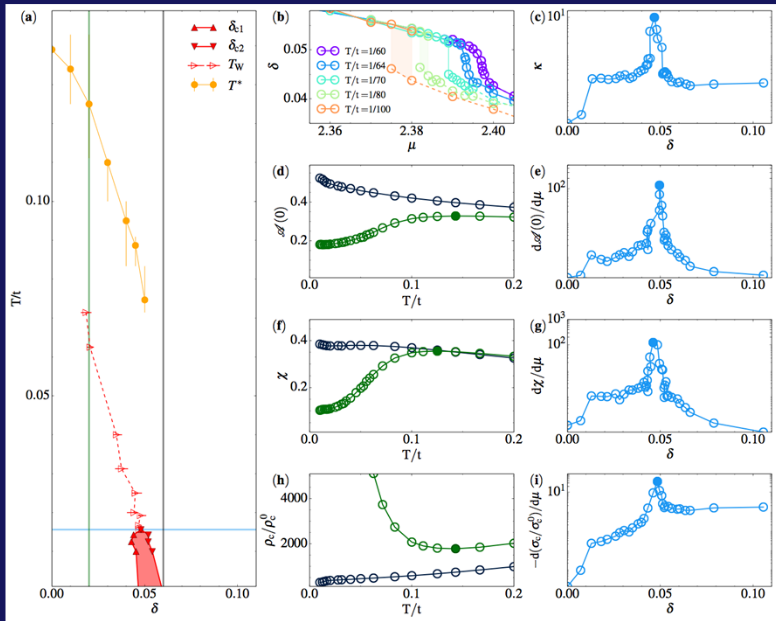

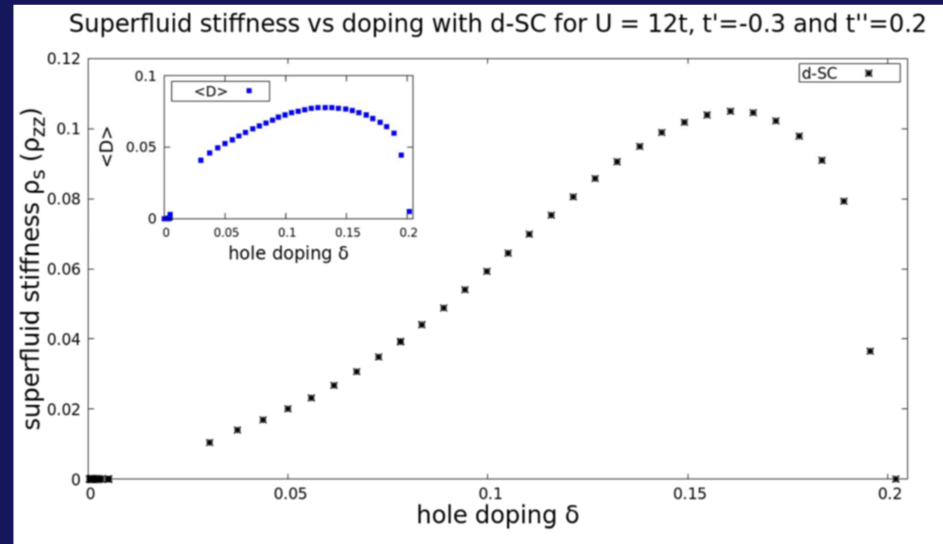

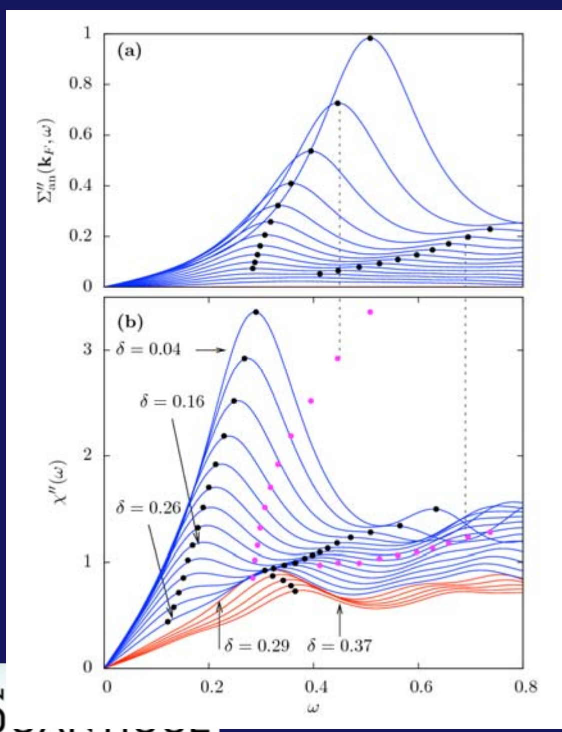

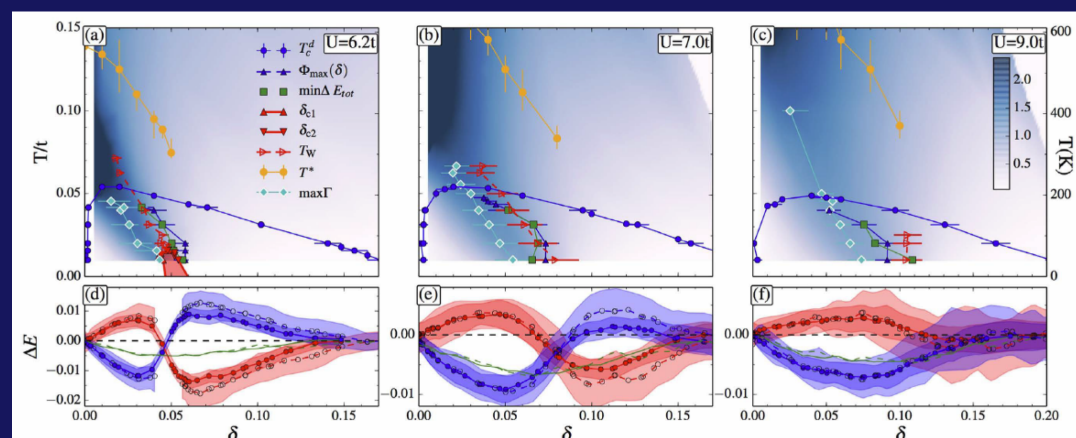

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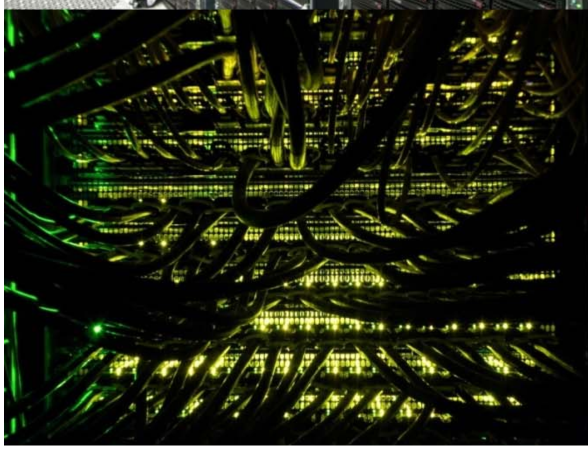
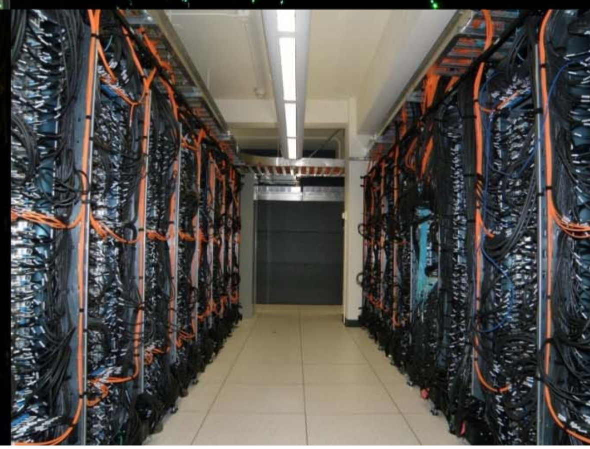
Mammouth





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Le calcul de haute performance
CRÉER LE SAVOIR
ALIMENTER L'INNOVATION
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Merci

Thank you

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