Pseudogap, van Hove Singularity, Maximum in Entropy and Specific Heat for Hole-Doped Mott Insulators

A.-M.S. Tremblay,
A. Reymbaut, S. Bergeron, R. Garioud,
M. Thénault, M. Charlebois, P. Sémon,

APS March Meeting Denver
J56.00007,
3:42 PM, Mile High Ballroom 2C

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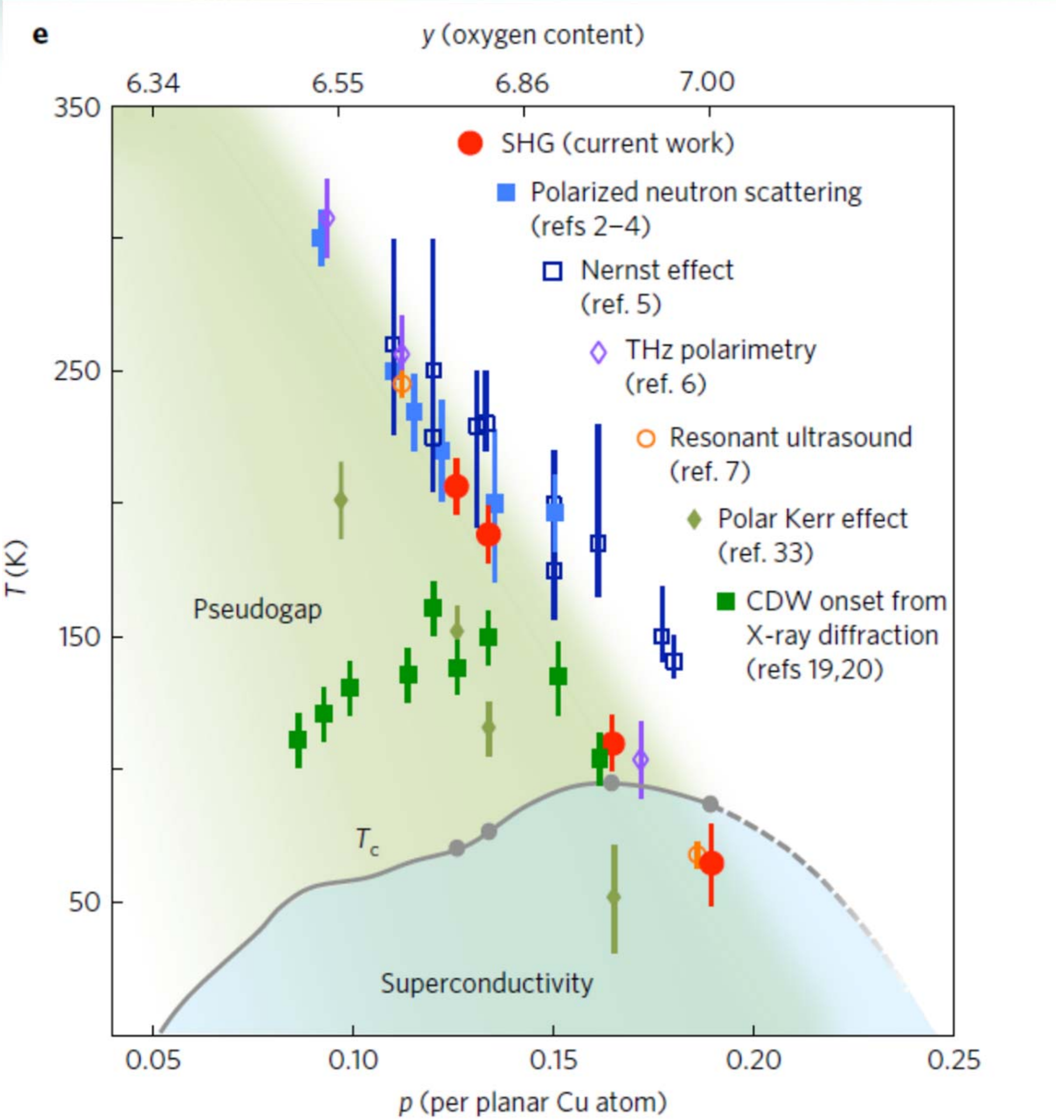
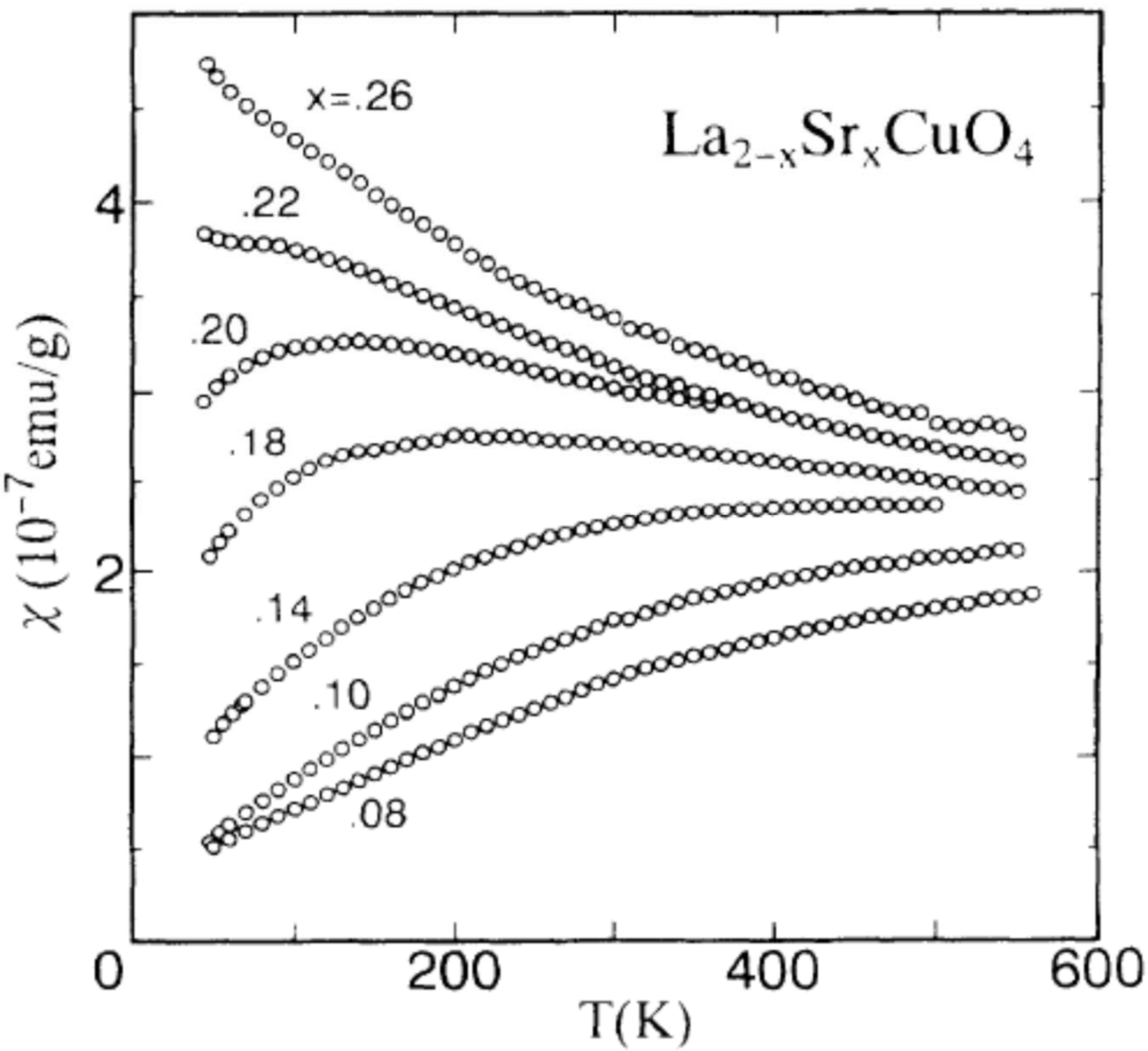


Zhao *et al.* Nat. Phys. 13, 250 (2017).

Spin susceptibility (Knight shift)



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

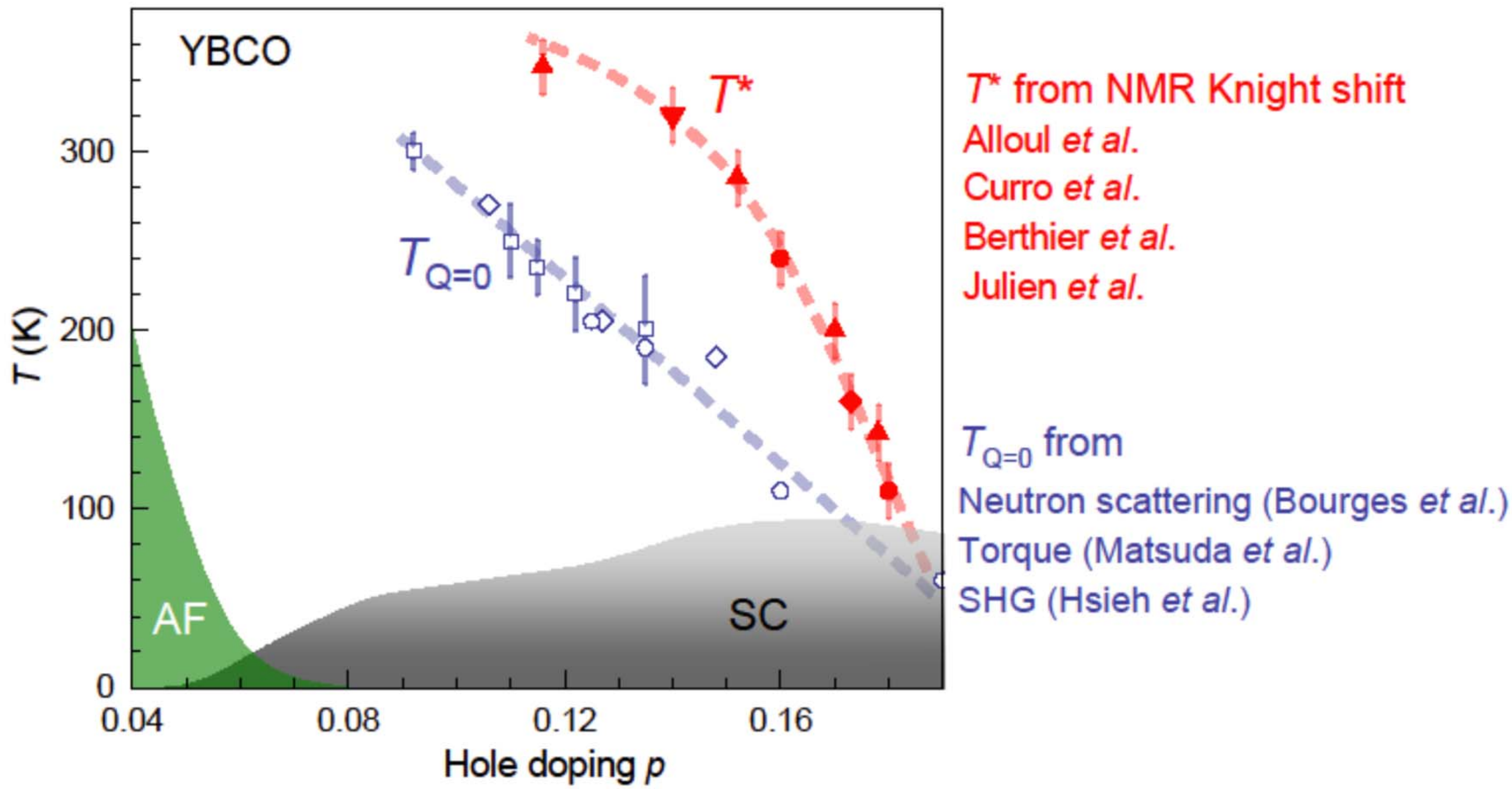


Figure from: Marc-Henri Julien

Model

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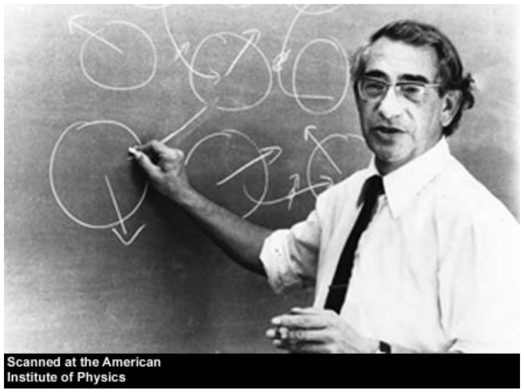
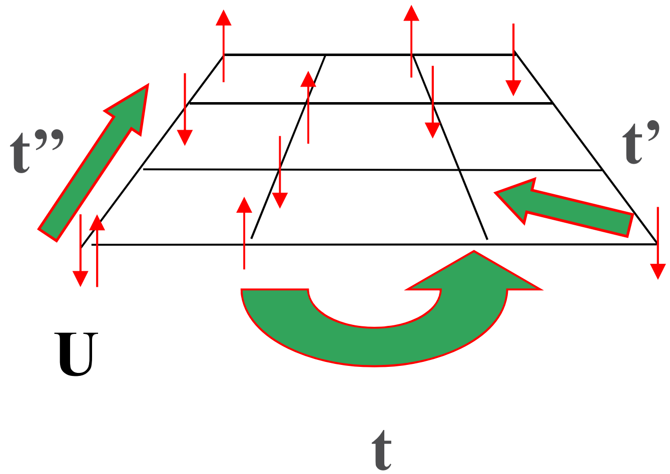
Hubbard model

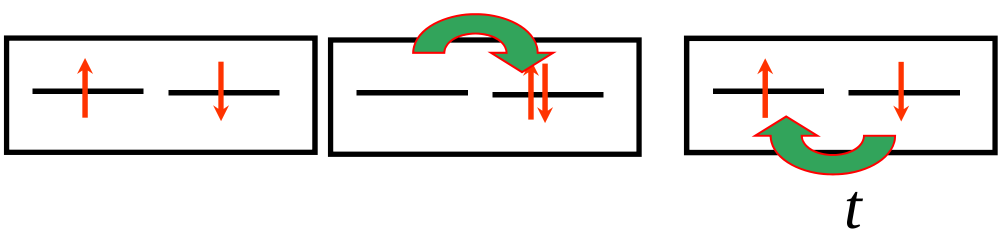


μ



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

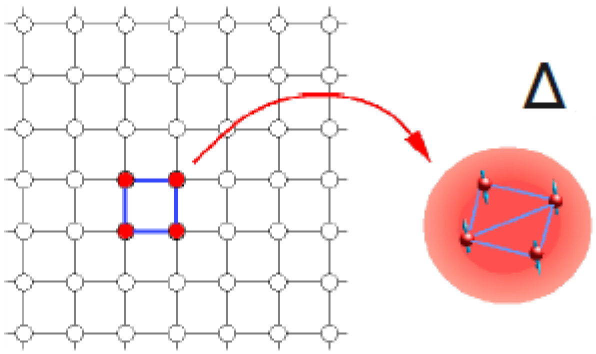
Method

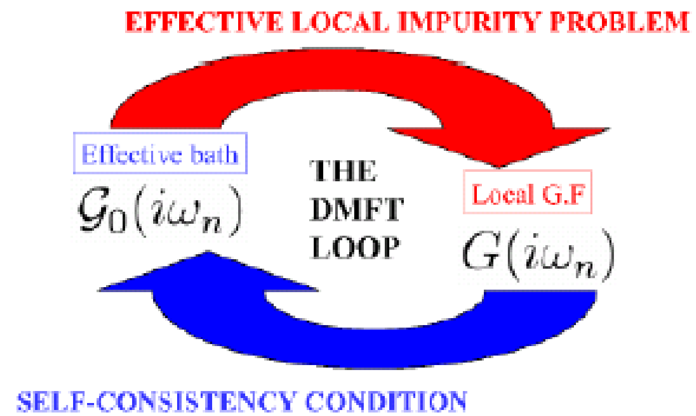
- Dynamical Mean Field Theory
  - clusters
- Concept: atomic-like localized correlations consistent with delocalized aspect

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

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
  - Hence good when the correponding correlation lengths are small

Alexis Reymbaut

Maxime Charlebois

Patrick Sémon

Simon Bergeron

Marion Thénault

R. Garioud

The pseudogap from spin susceptibility

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

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Knight shift (Q=0 spin susceptibility)

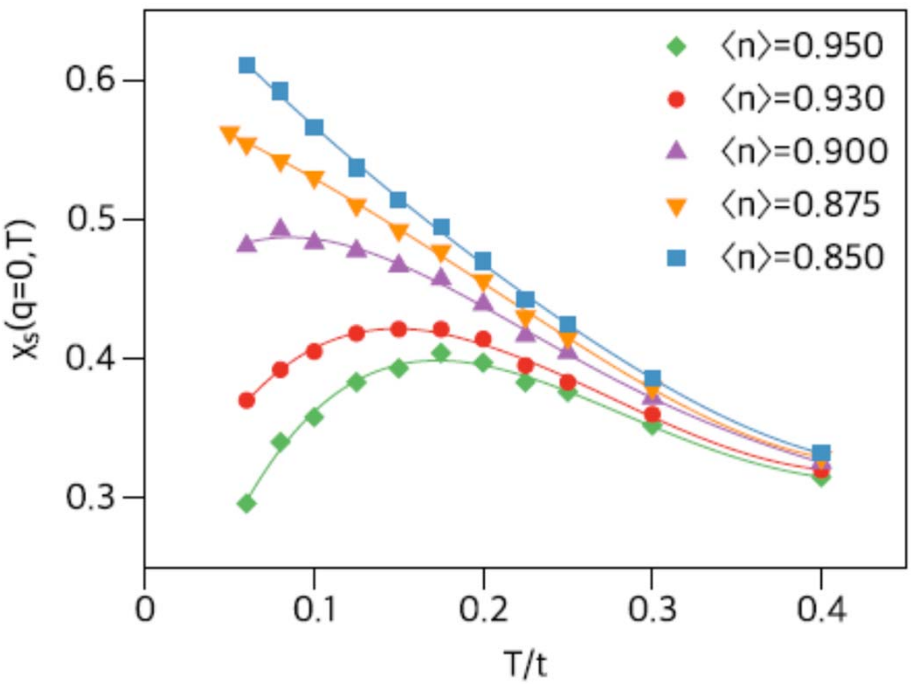
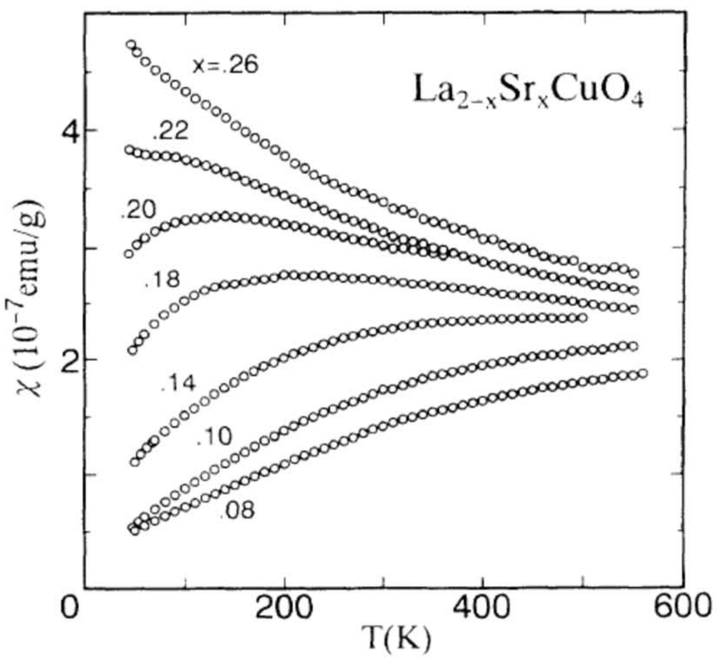


Fig. 3 Temperature and doping dependence of the $q=0$ spin susceptibility. At the smaller dopings (larger filling $\langle n \rangle$), $\chi_s(T)$ exhibits a peak in the temperature dependence indicating the opening of a PG

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

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

Comparison



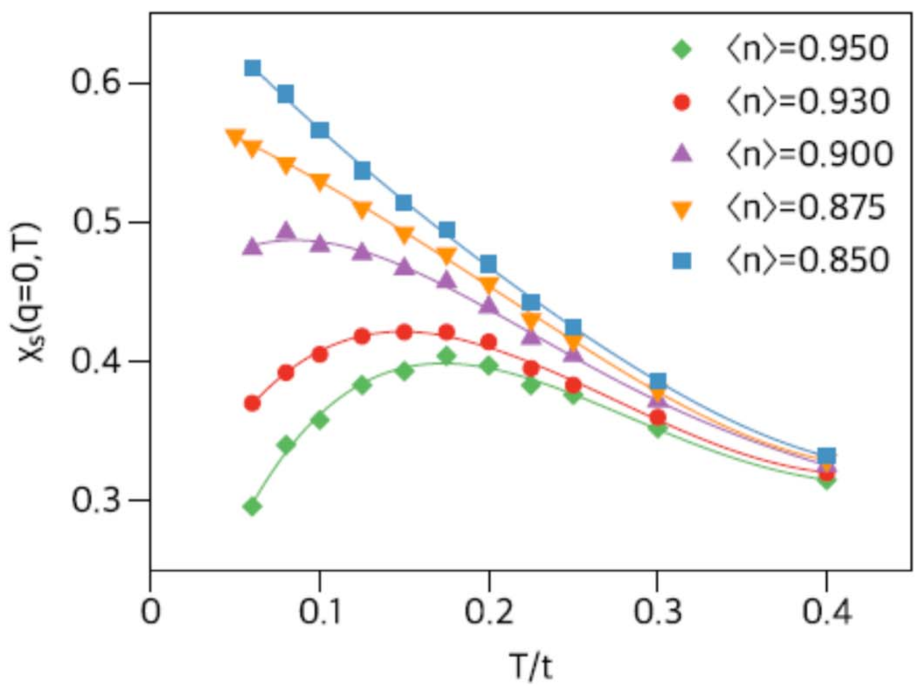
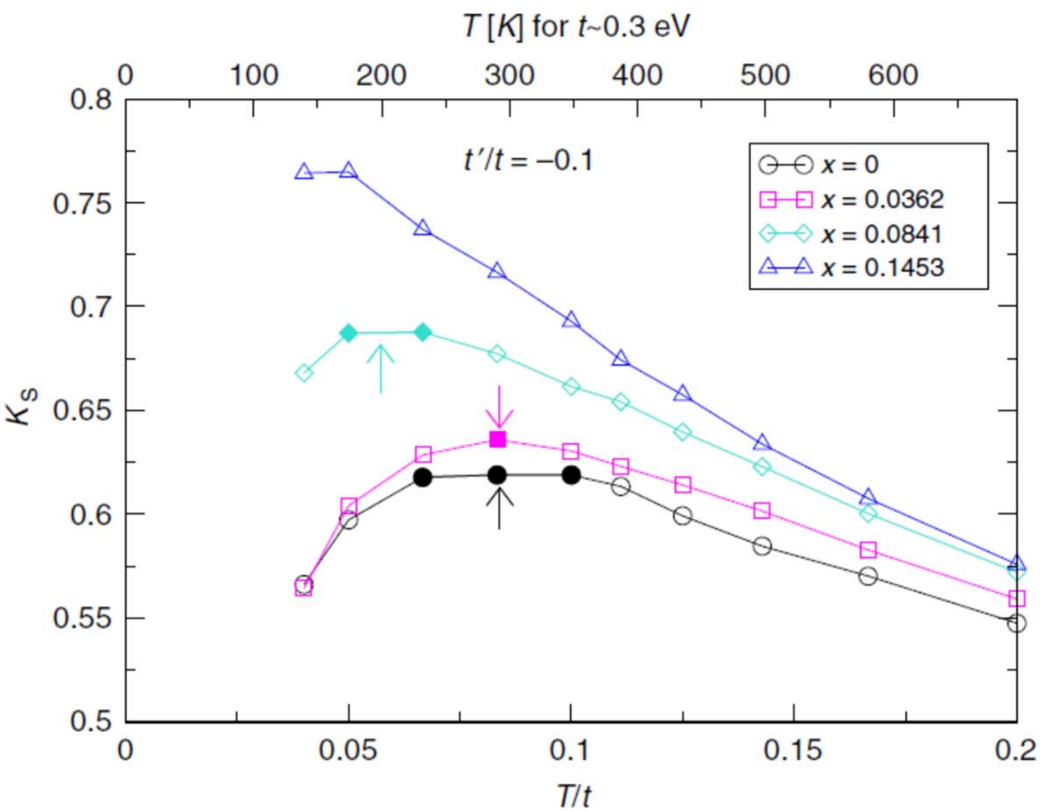


Fig. 3 Temperature and doping dependence of the $q = 0$ spin susceptibility. At the smaller dopings (larger filling $\langle n \rangle$), $\chi_s(T)$ exhibits a peak in the temperature dependence indicating the opening of a PG

Knight shift

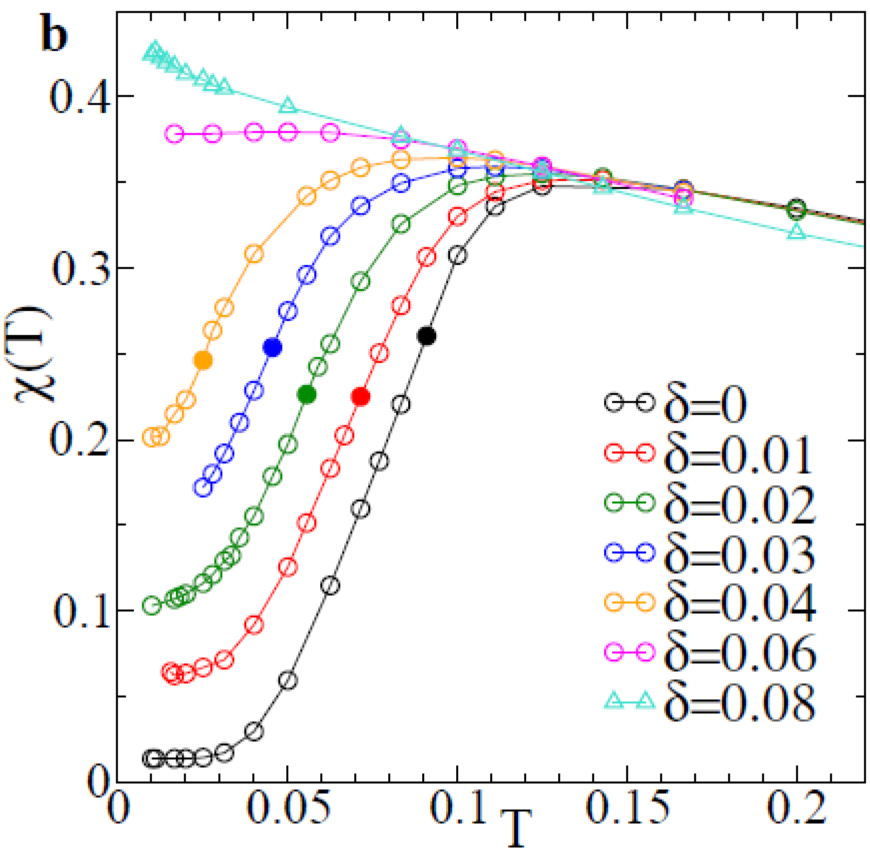


DCA 8 sites, *U = 6, t' = -0.1t*

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

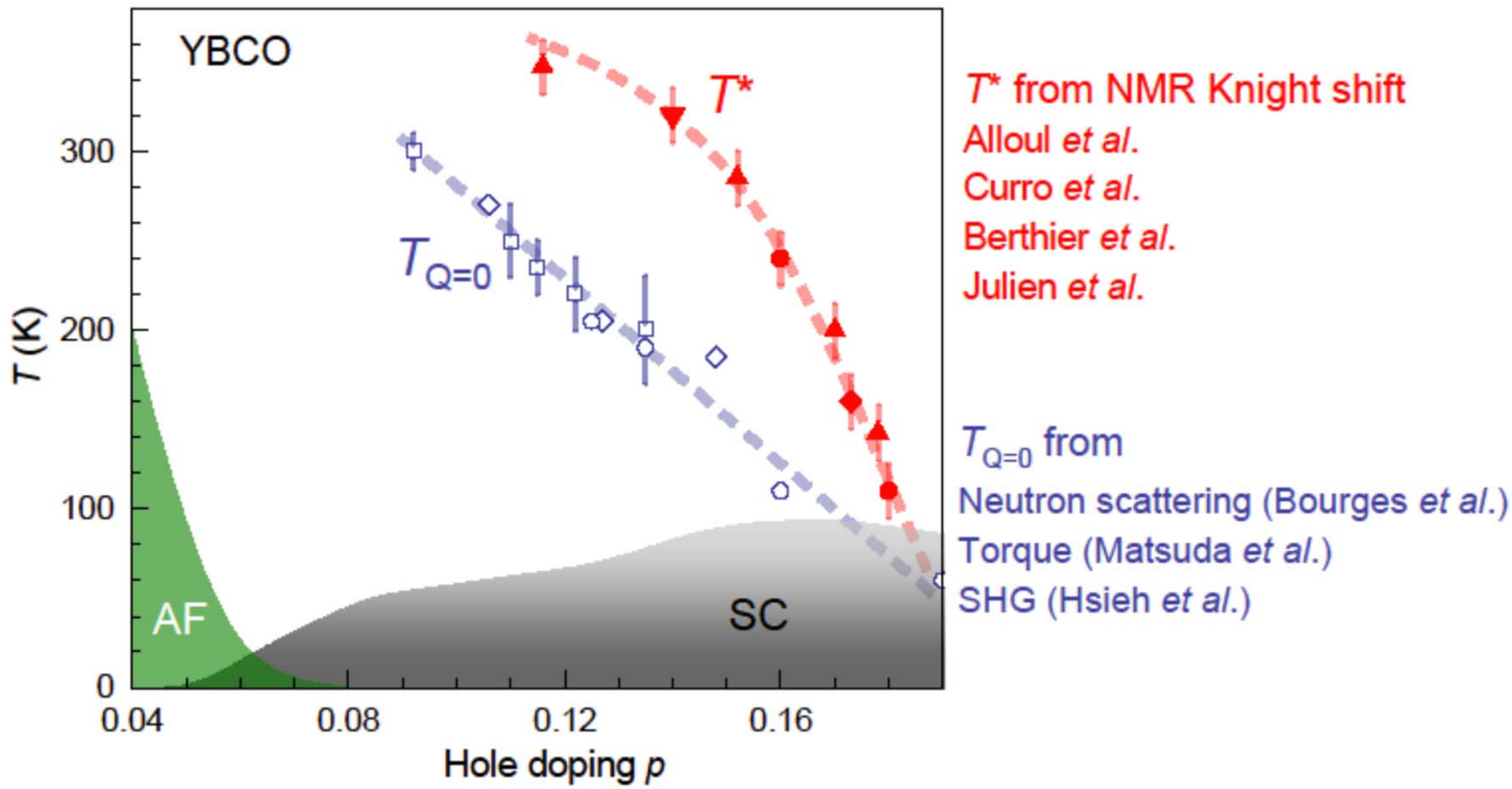
See also Jarrell *et al.* 2001, 2002

Spin susceptibility



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

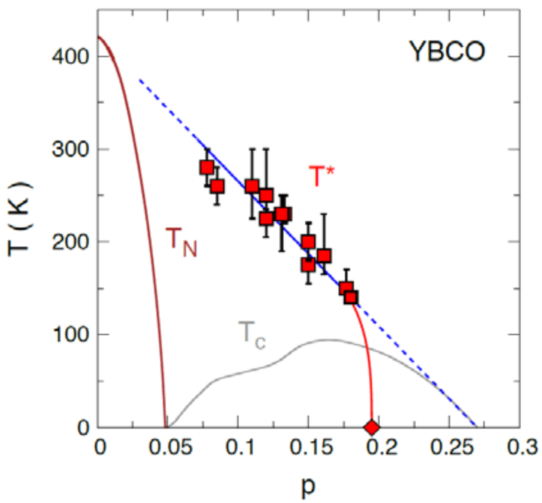
U = 6.2 , t'=0



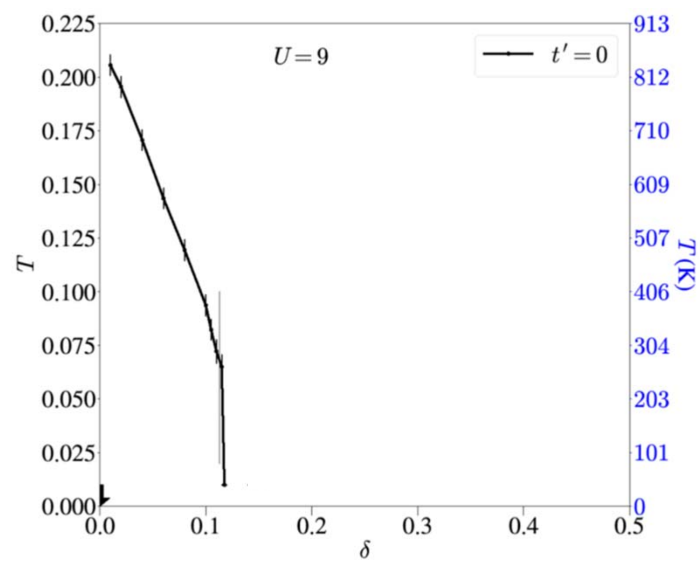
Thanks: Marc-Henri Julien

1. Results T^*

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



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



p

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

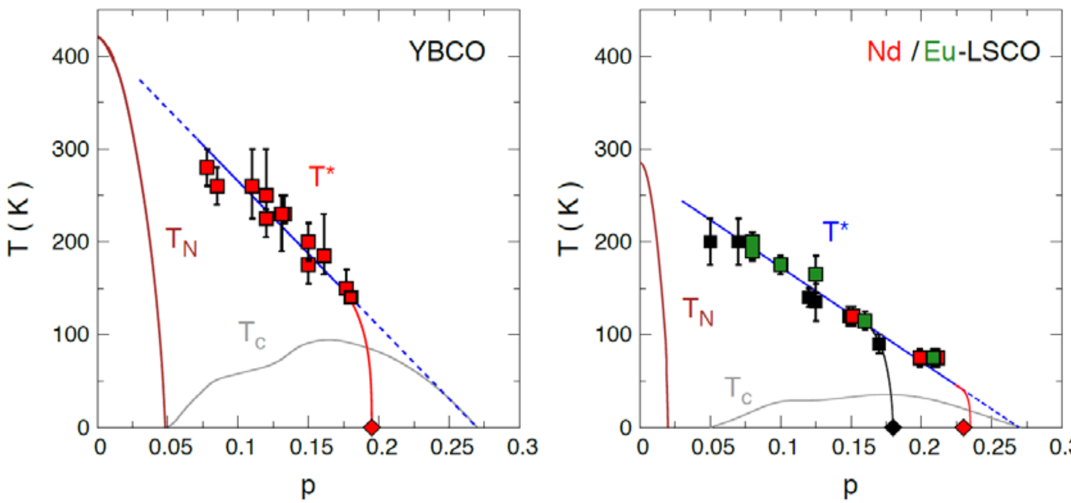
W Wu, A Georges, M Ferrero Phys. Rev. X 8, 021048 (2018).

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

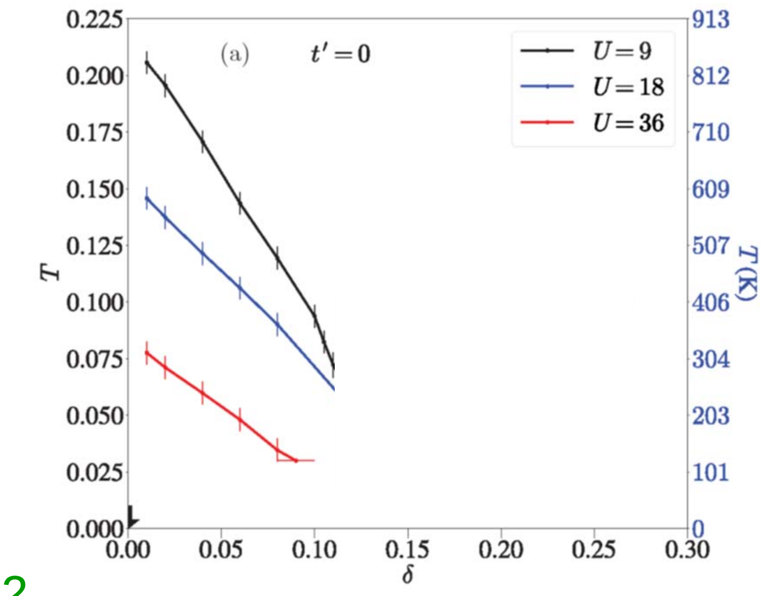
2. Results *T**

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

$J = 4t^2/U$



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



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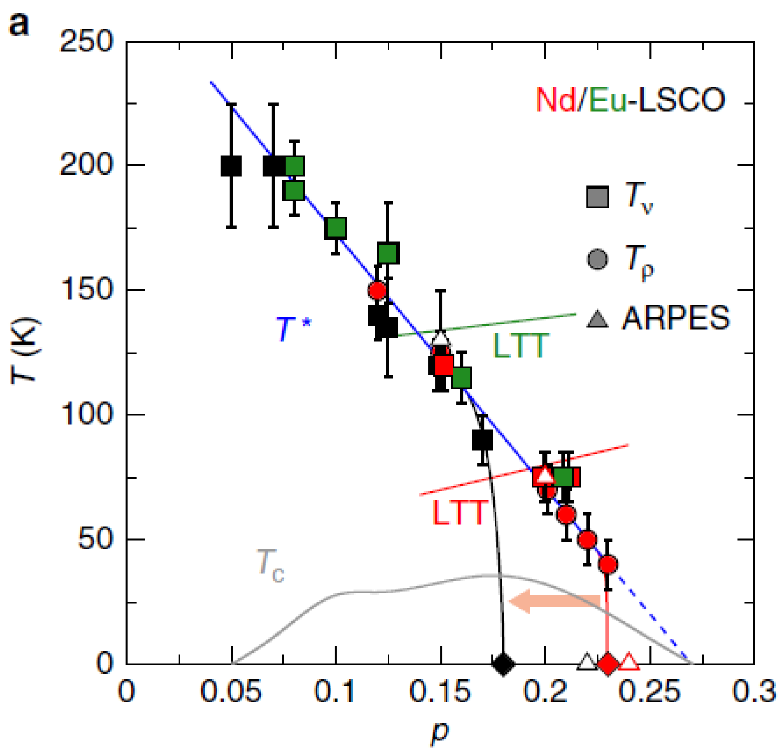
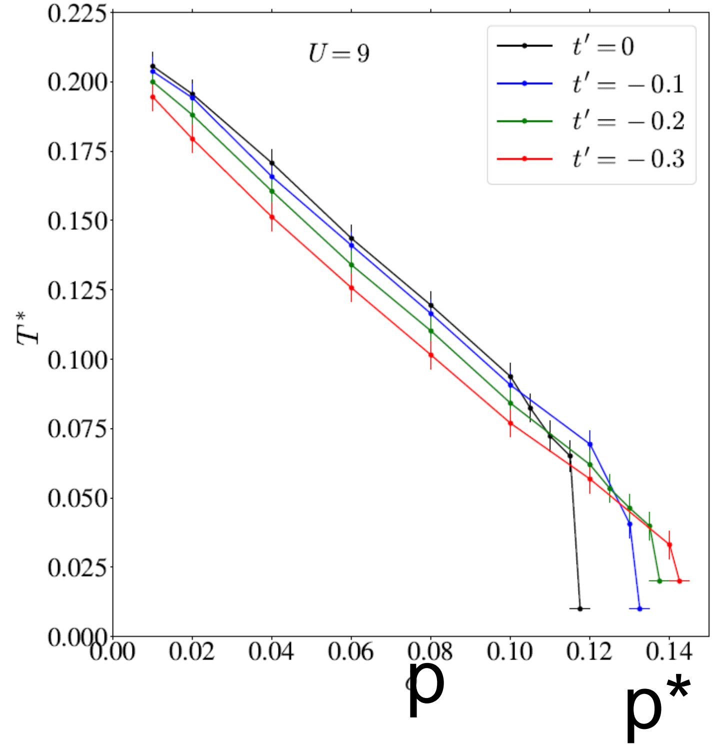
A. Reymbaut, M. Thénault, L. Fratino, G. Sordi, P. Sémon, AMT, Phys. Rev. Research **1**, 023015 (2019)

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

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

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

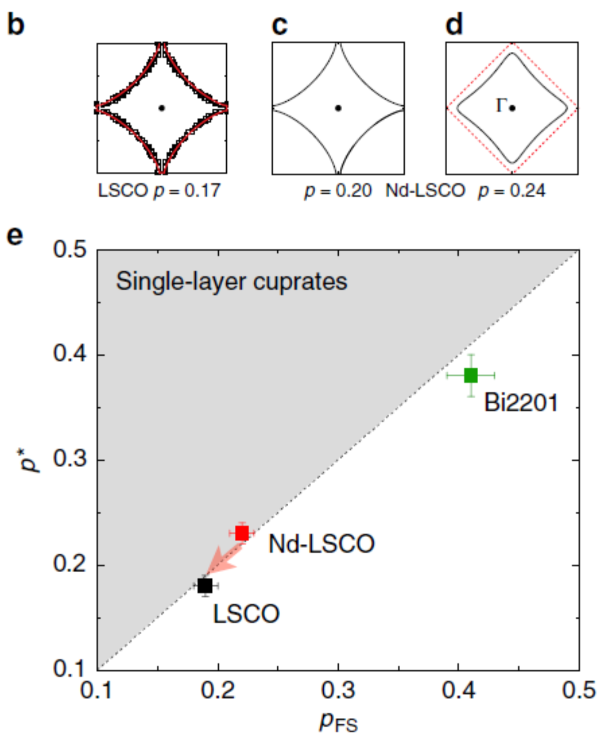


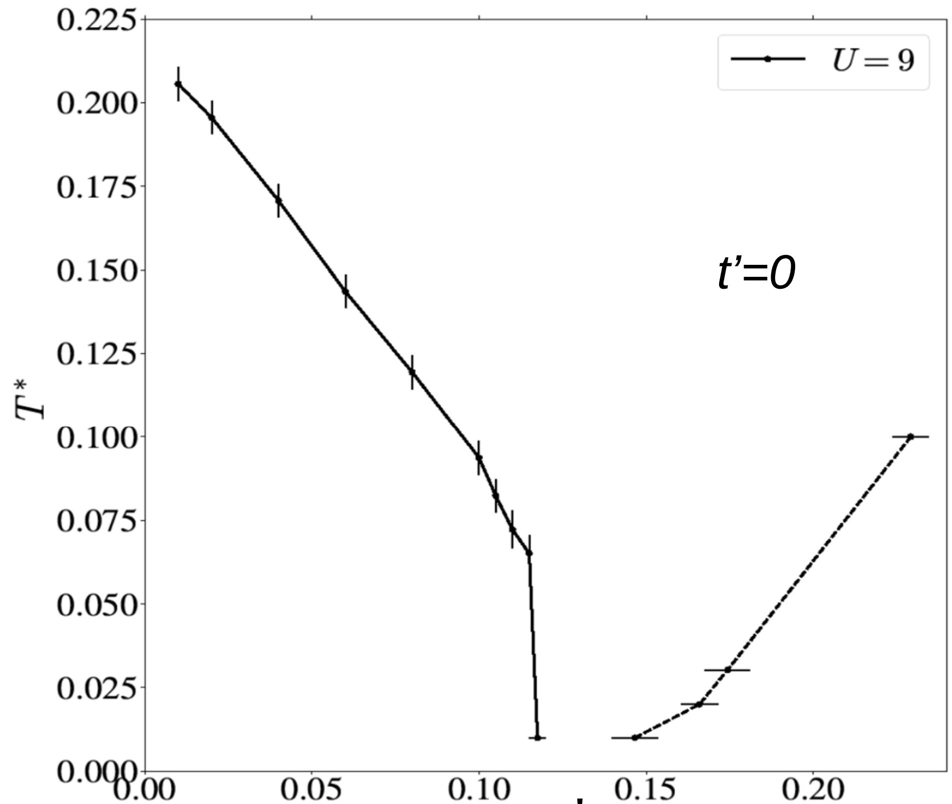


Doiron-Leyraud *et al.*
Nature Comm. **8** 2044

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

4. Results: van Hove singularity





p^* p_{fs}

$p^* < p_{fs}$

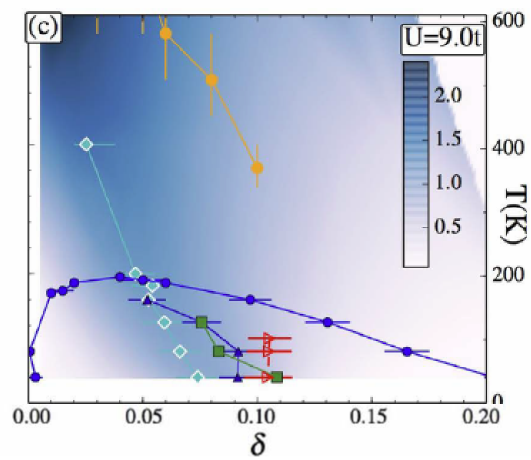
Doiron-Leyraud *et al.*
Nature Comm. **8** 2044

A.Reymbaut, *et al.*
Phys. Rev. Research **1**, 023015 (2019)
Sordi et al., Sci. Rep. 2 547 (2012);
W. Wu, *et al.* PRX **8**, 021048 (2018)
Bragança, *et al.* PRL **120**, 067002 (2018)

Perspective

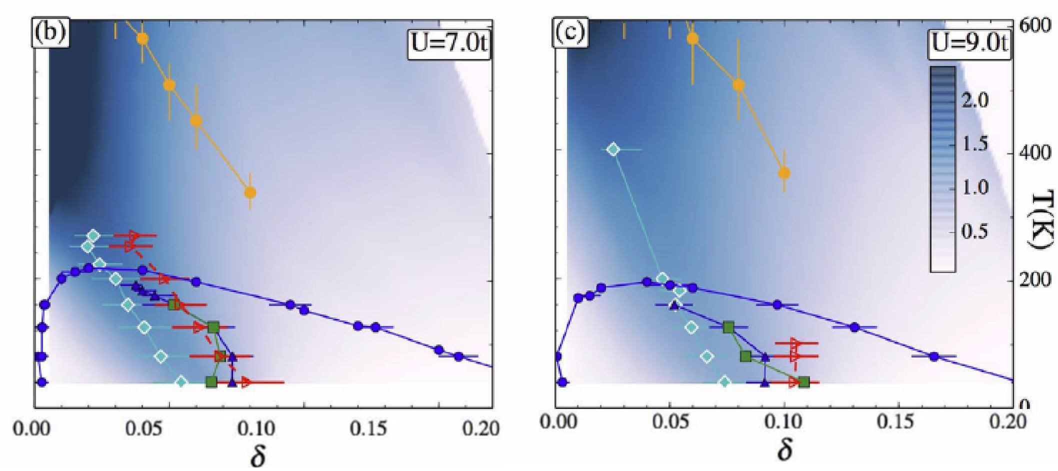
Connecting the finite doping behavior to the Mott transition at half-filling

U = 9



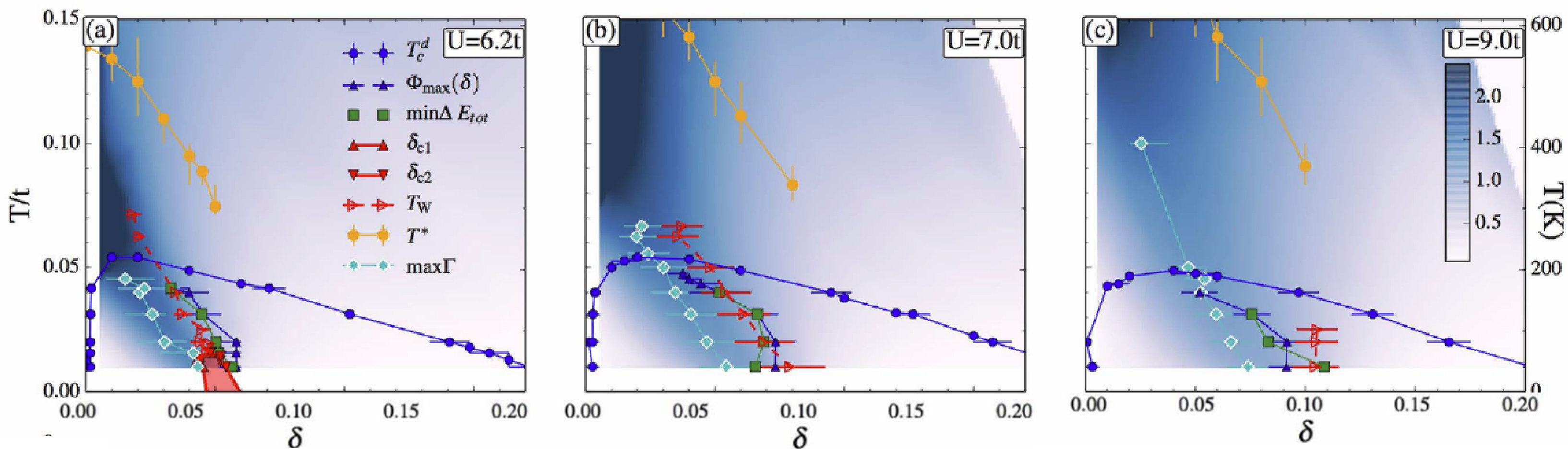
Connecting the finite doping behavior to the Mott transition at half-filling

U = 7 *U* = 9



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

U = 6.2 *U* = 7 *U* = 9



Giovanni Sordi

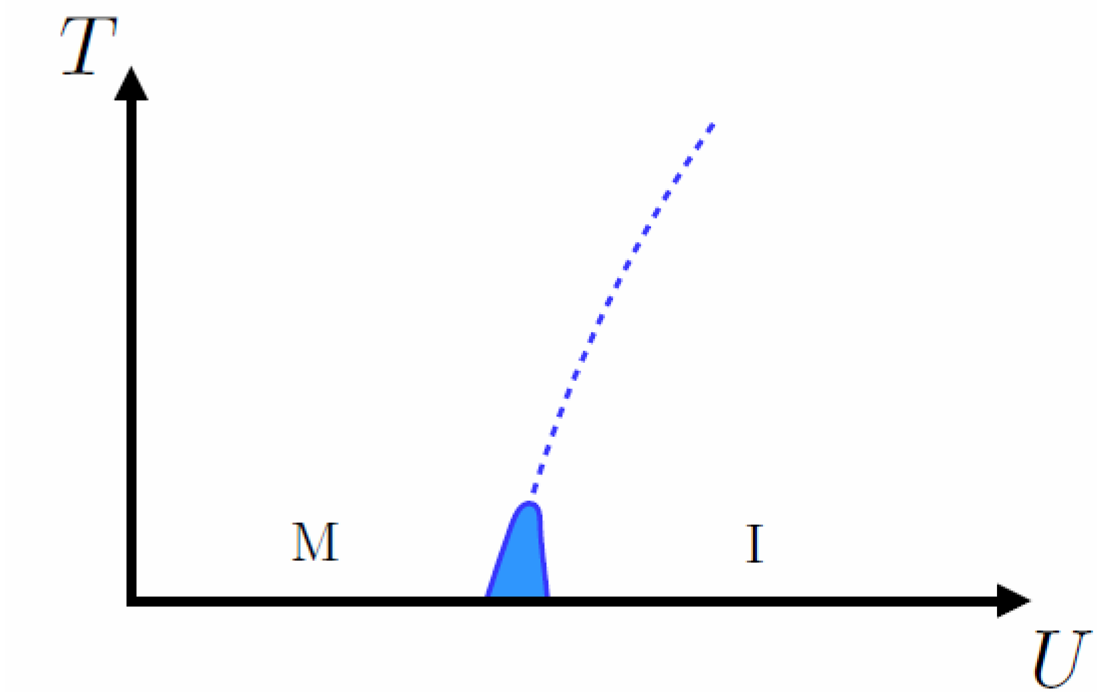
Kristjan Haule

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)

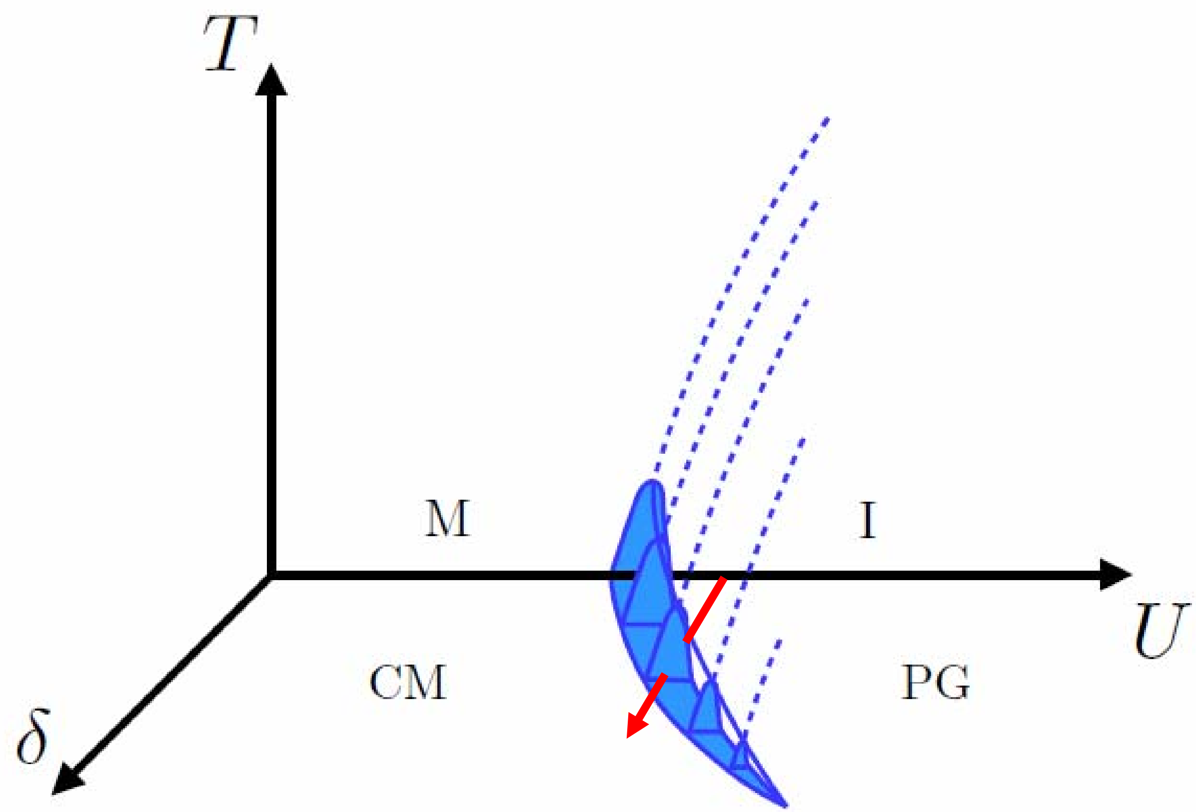
Influence of Mott transition away from half-filling

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



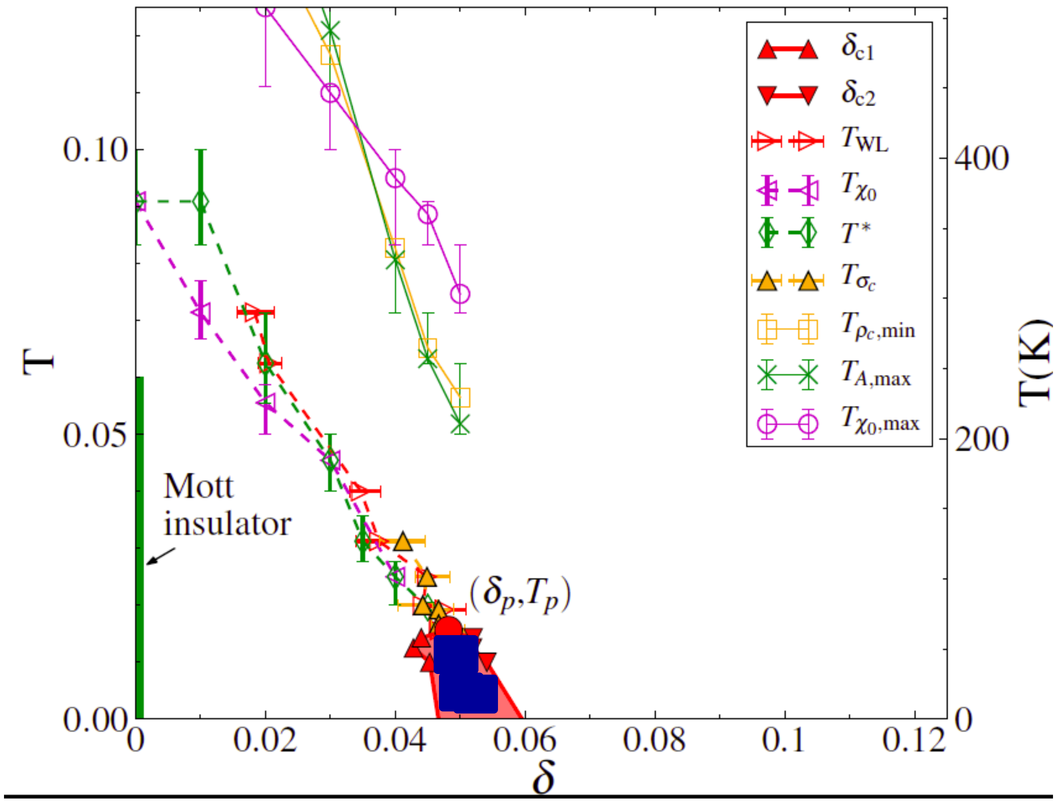
Influence of Mott transition away from half-filling

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



Two crossover lines

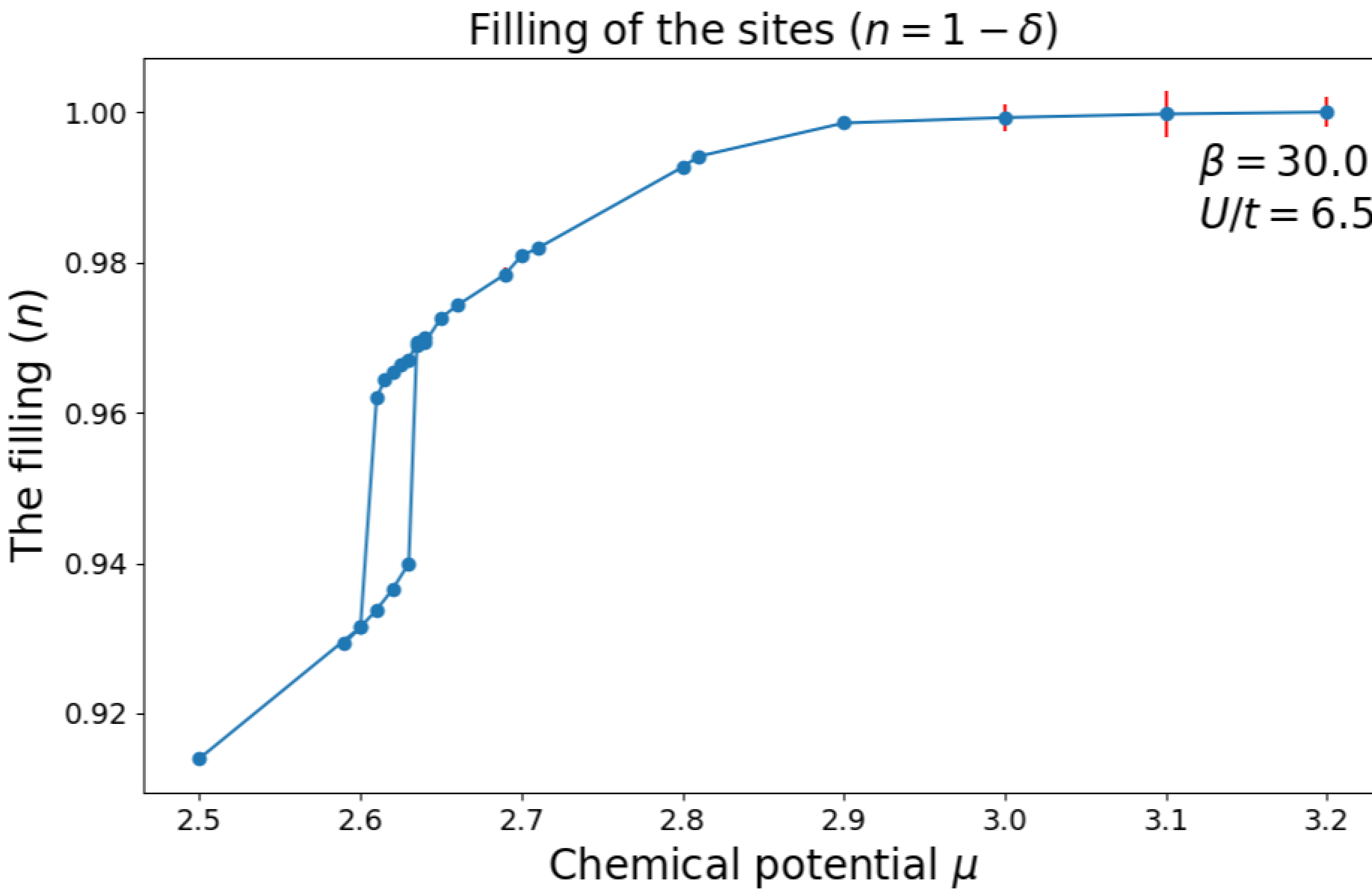
Giovanni Sordi



Patrick Sémon

G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)
G.Sordi et al. Phys. Rev. B 87, 041101(R)/1-5 (2013)
P. Sémon, G. Sordi, *et al.*, Phys. Rev. B **89**, 165113/1-6 (2014)

Anisotropic triangular, 3x2 cluster DCA



Conclusion

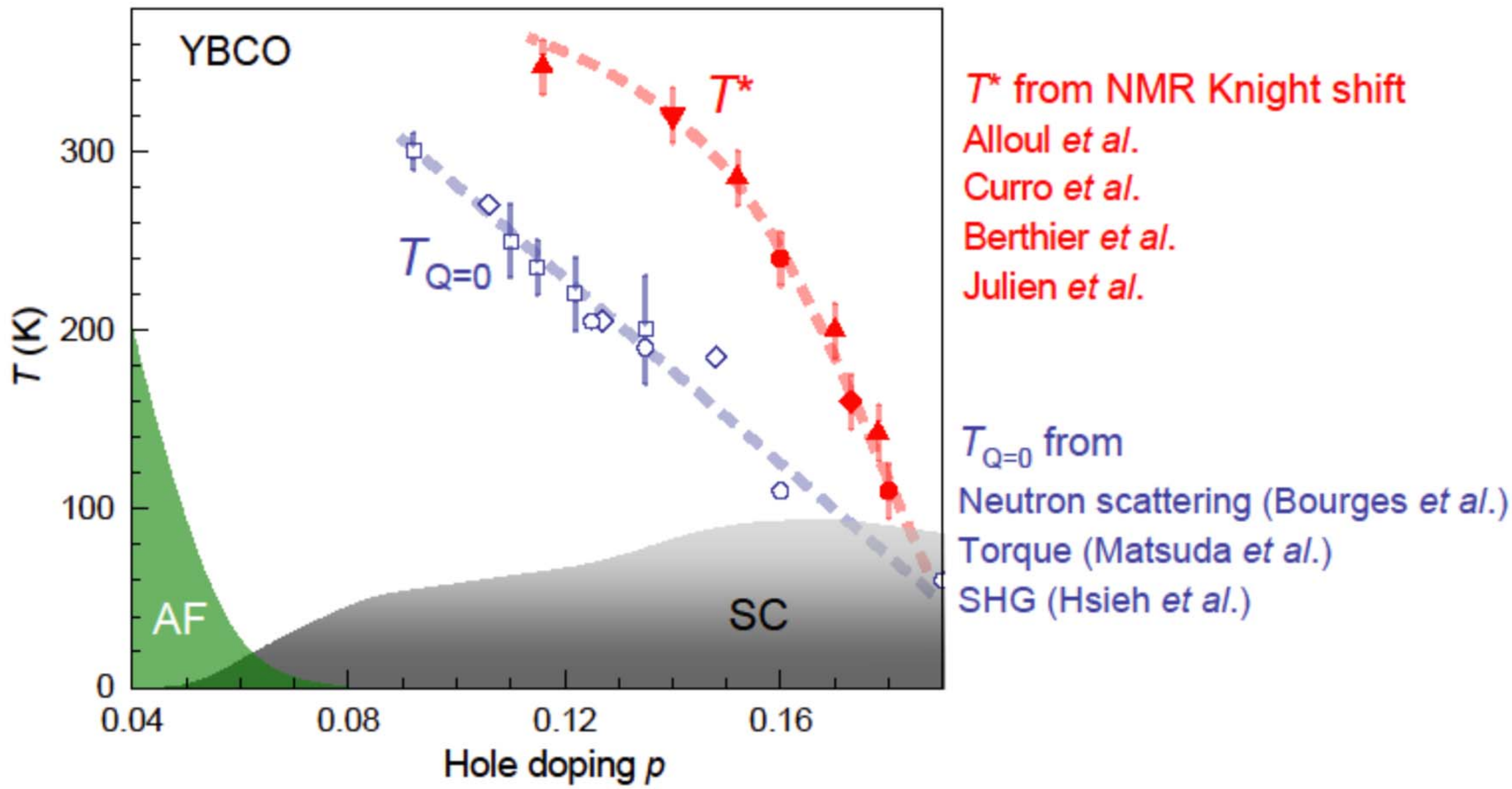
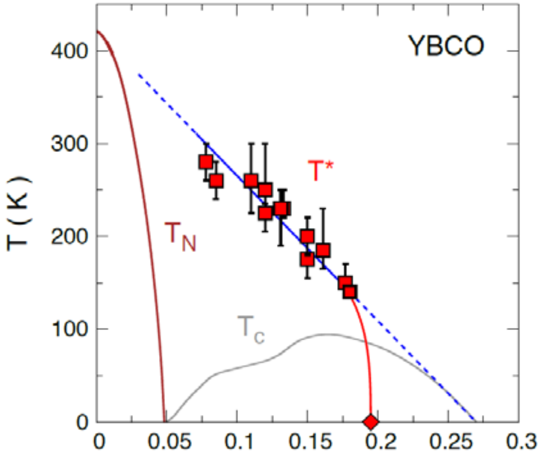
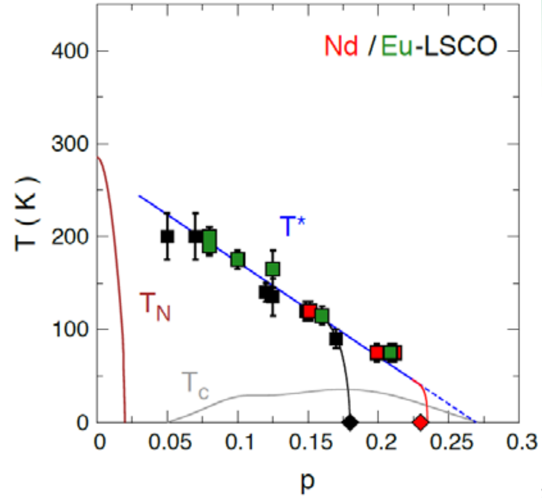
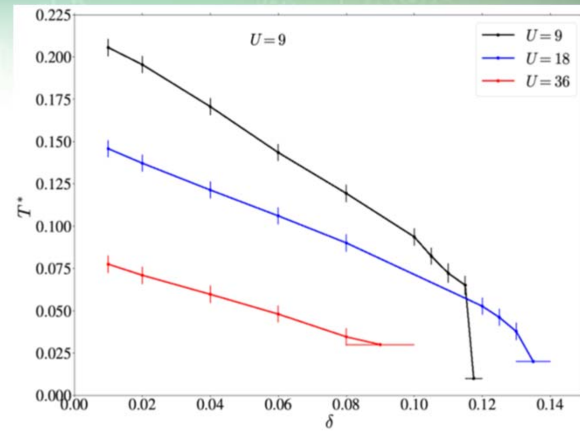


Figure from: Marc-Henri Julien

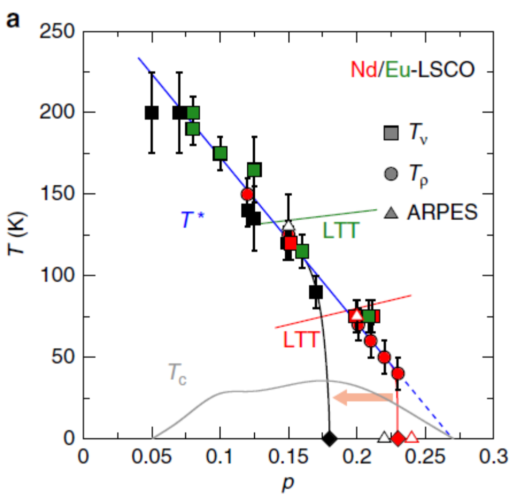


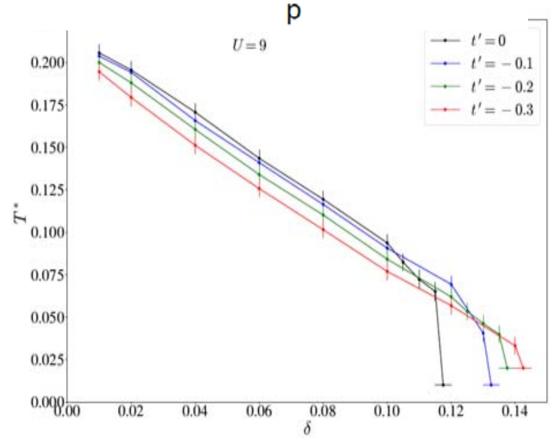




fall

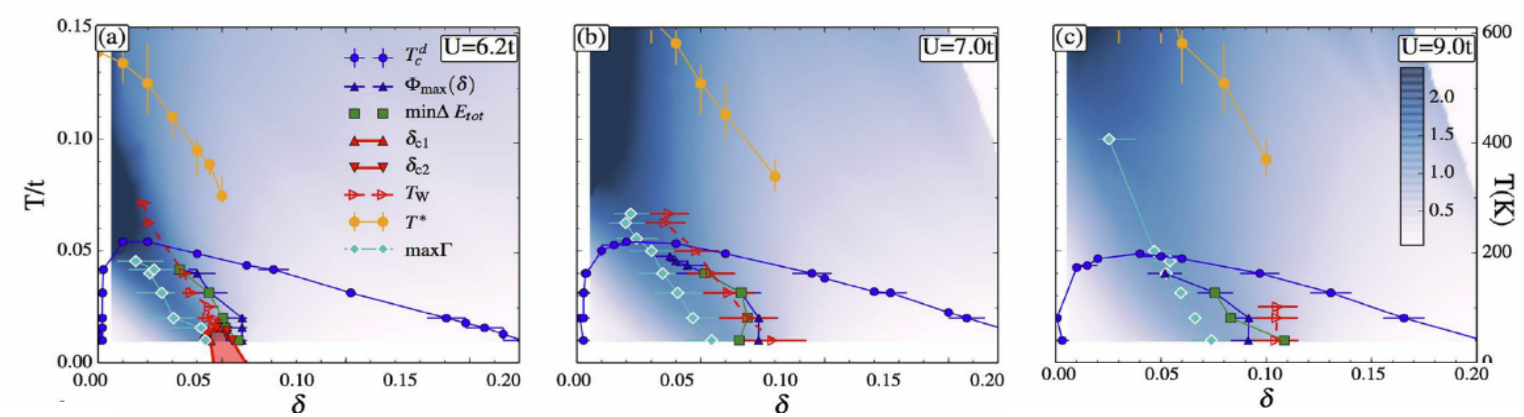
T ~ J*





Pressure dep of p*

p* < p_{fs}

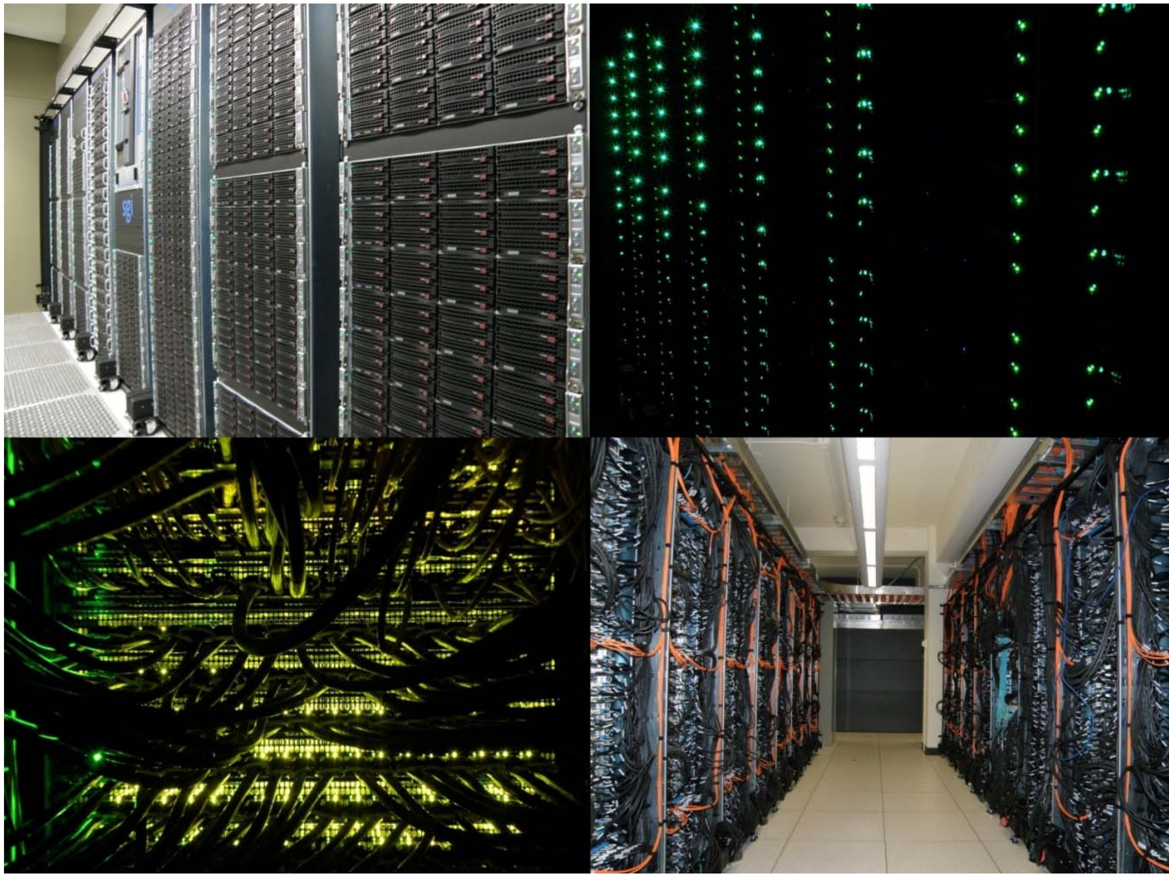


Conclusion

p^* in Hubbard is the end of Mott physics

Mott transition and its finite doping extension is the organizing principle

Mammouth



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Merci
Thank you

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