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Pseudogaps and their relation to superconductivity

*A.-M.S. Tremblay, S. Arya, D. Bergeron,
M. Charlebois, L. Fratino,
P. Sémon, G. Sordi, and A. Venne

CORPES2017 Hiroshima

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CANADIAN INSTITUTE for ADVANCED RESEARCH

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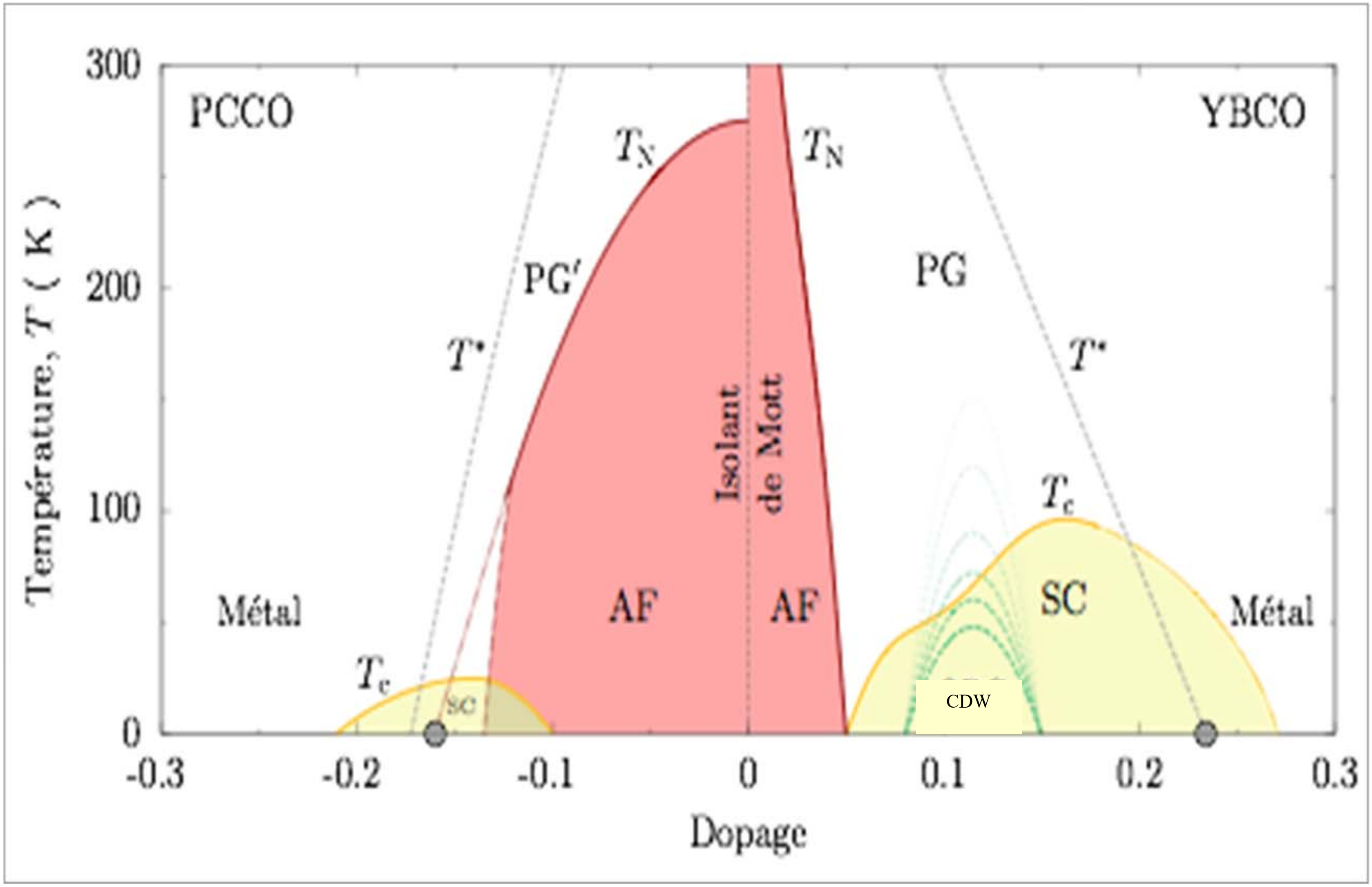
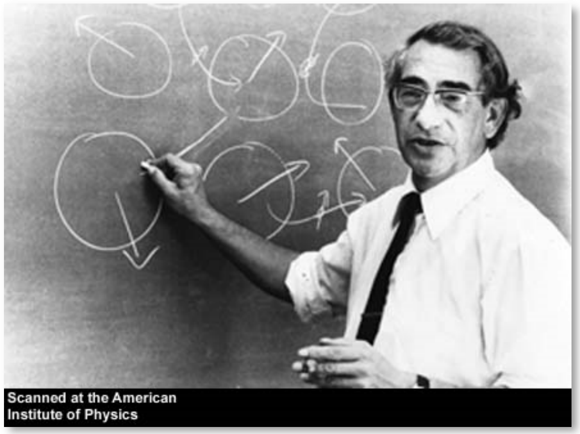
VERITATEM IN CHARITATE

Our road map

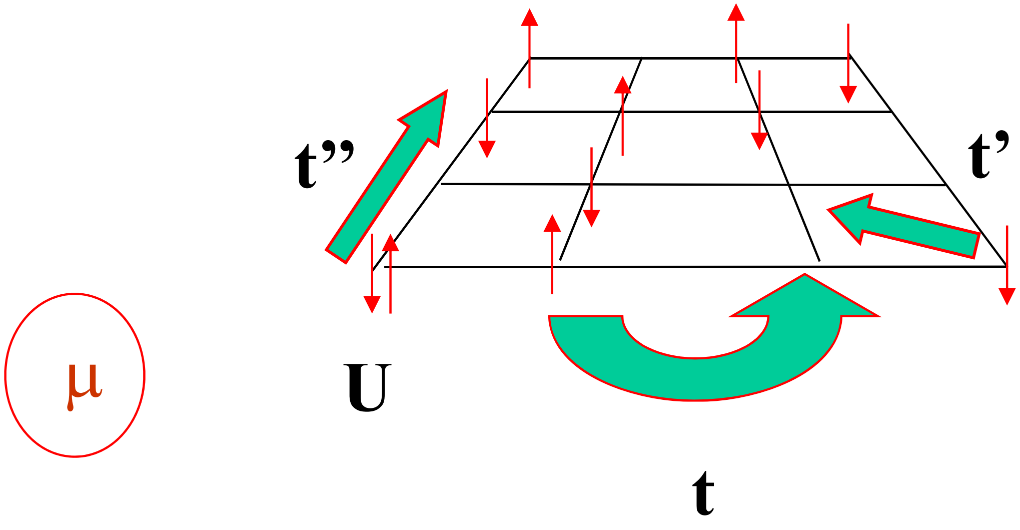
Thèse de Francis Laliberté,
Université de Sherbrooke



Hubbard model



1931-1980



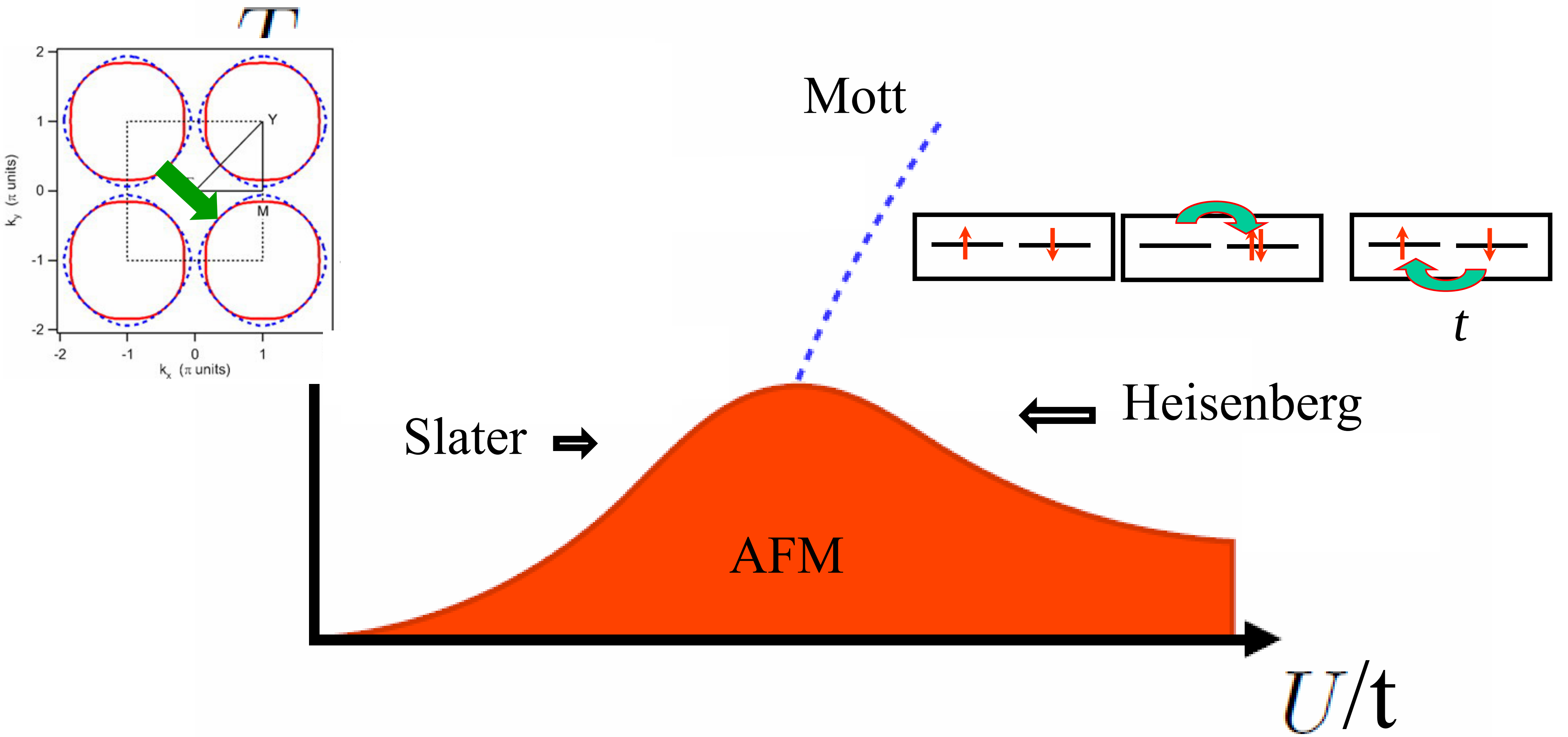
$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}\right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

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

Attn: Charge transfer insulator

Weak vs Strong correlations

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



Method 1

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)

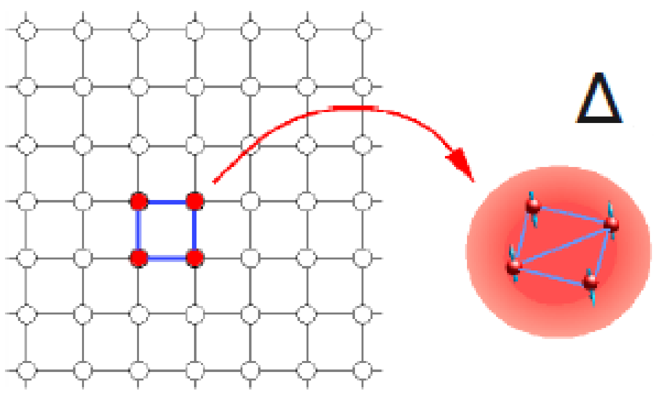
Hettler *et al*, PRB 1998

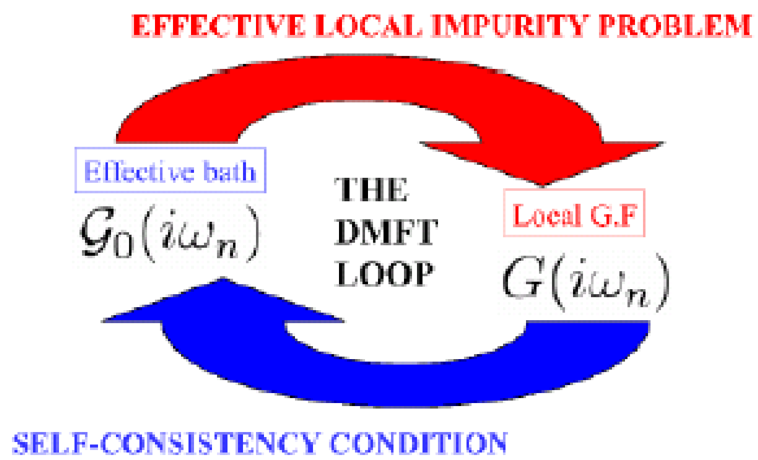
Lichtenstein *et al.*, PRB 2000

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 III: Weaker correlations *e-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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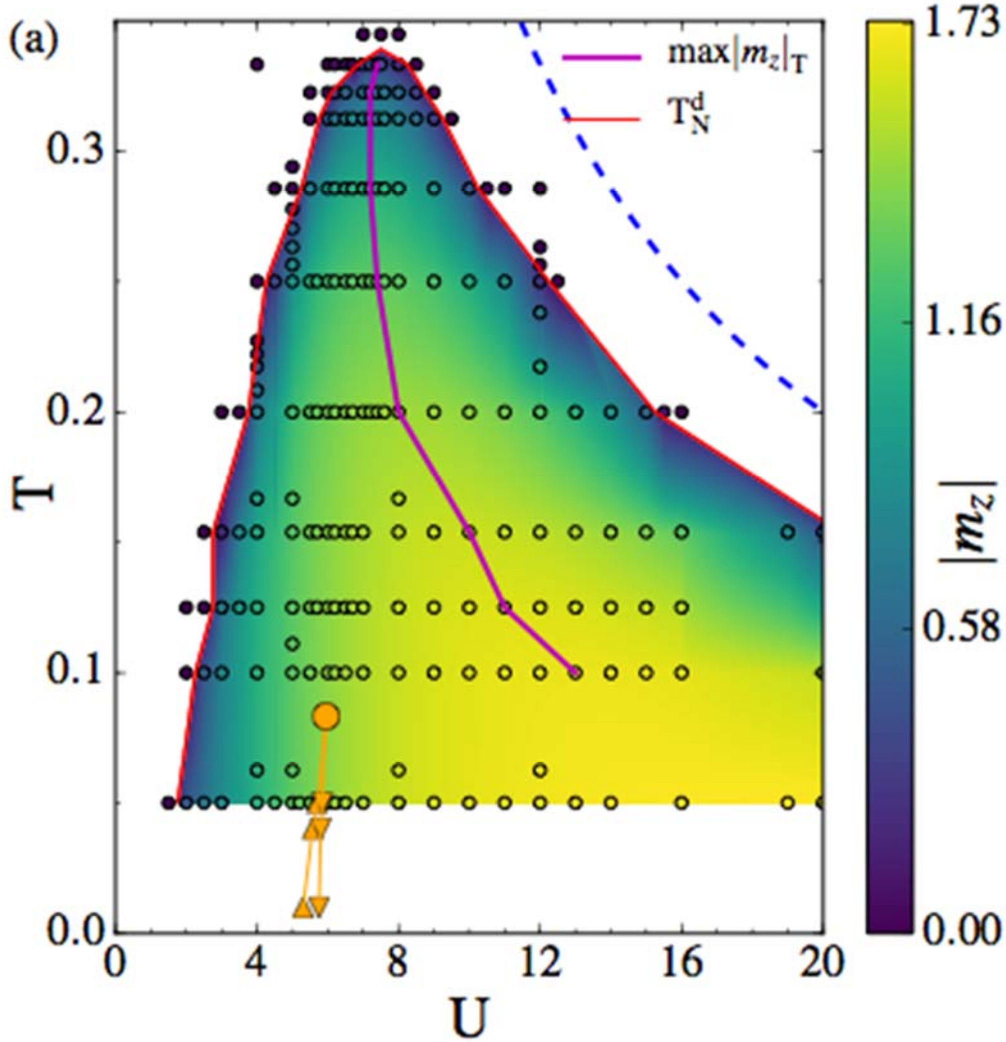
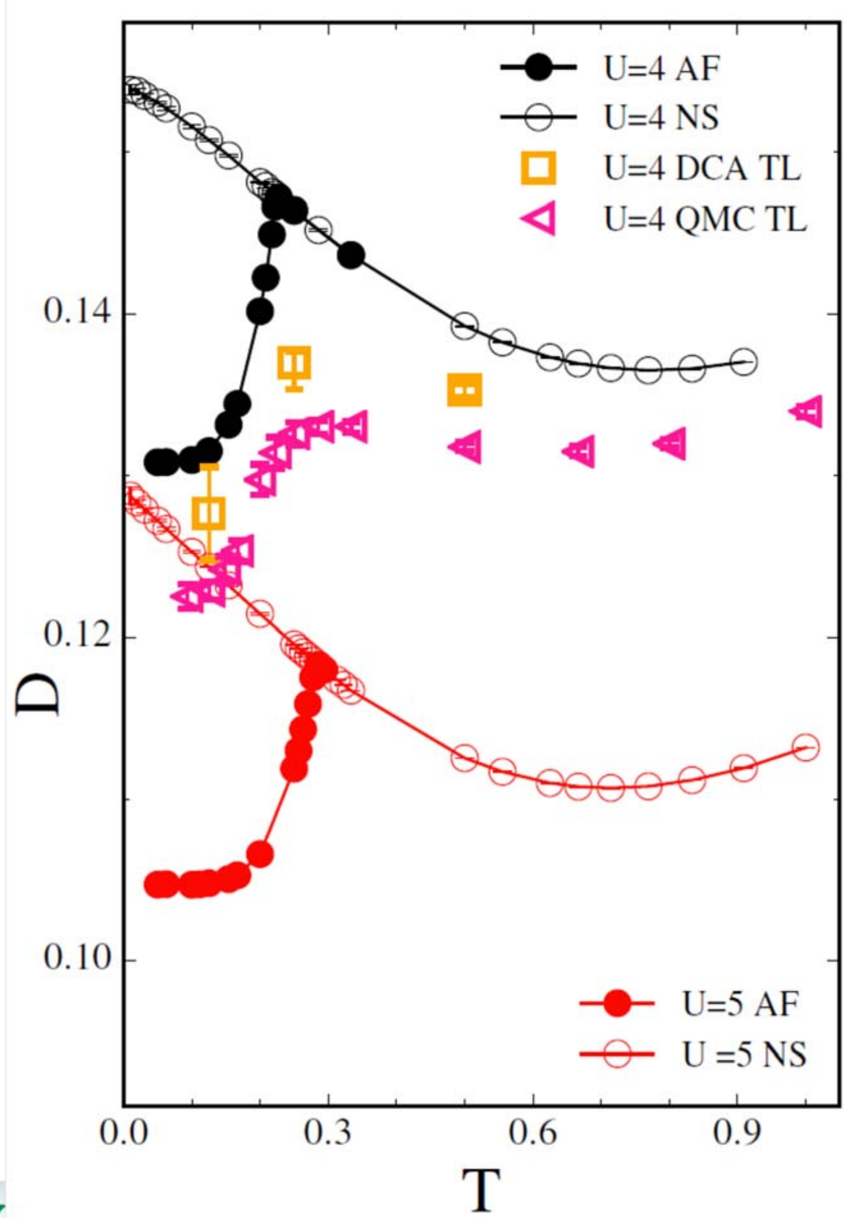
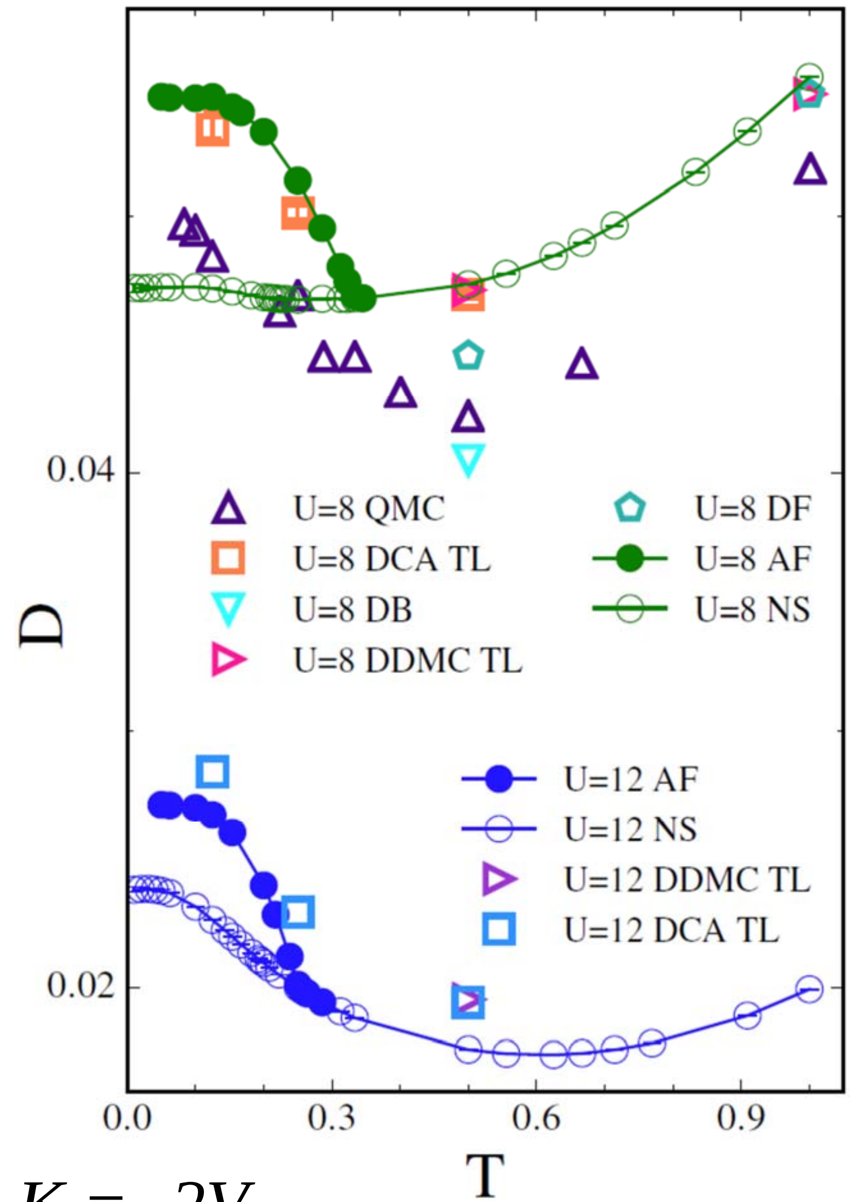
AFM phase diagram *d=2, t'=0*



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

Double occupancy at weak and strong interactions: benchmarks





$K = -2V$

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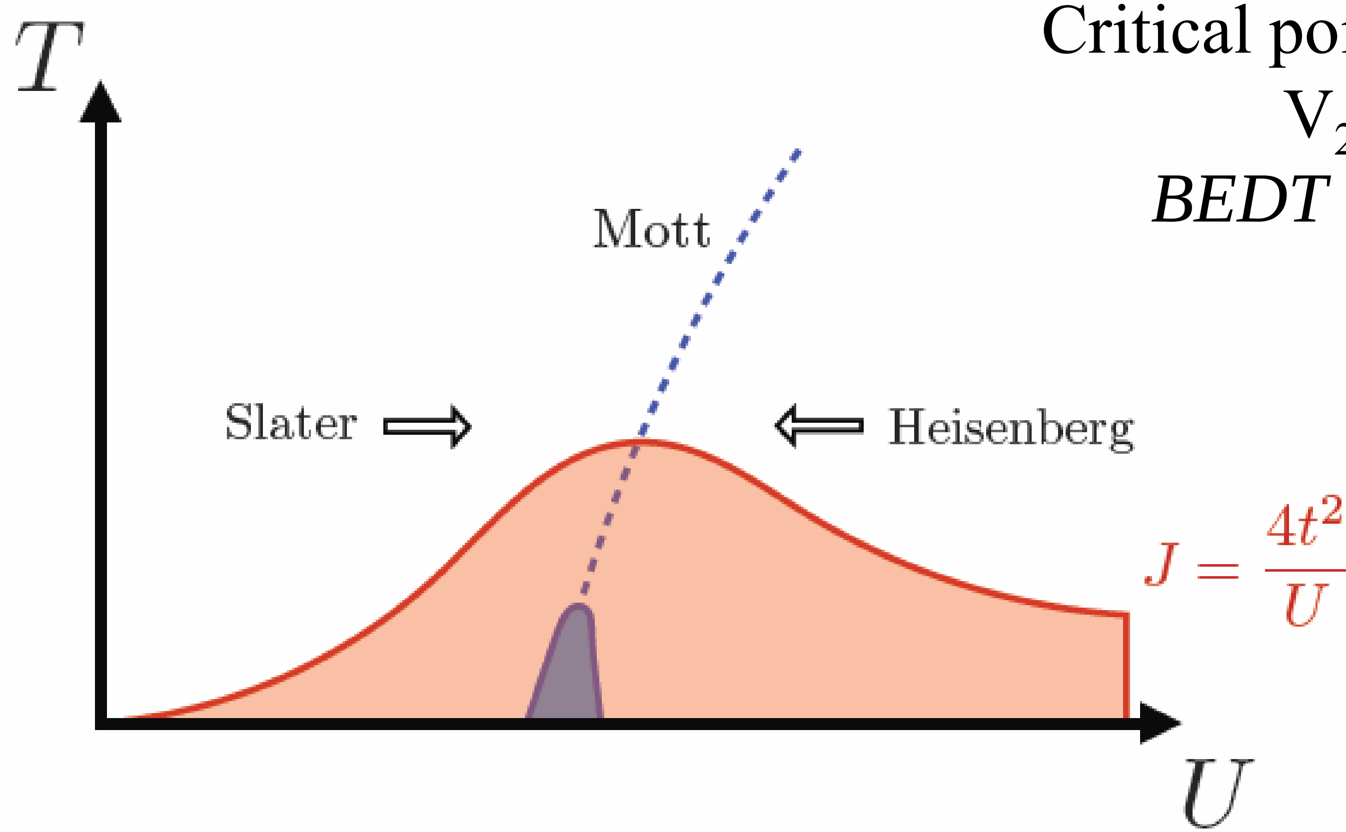
Underlying Mott transition

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*

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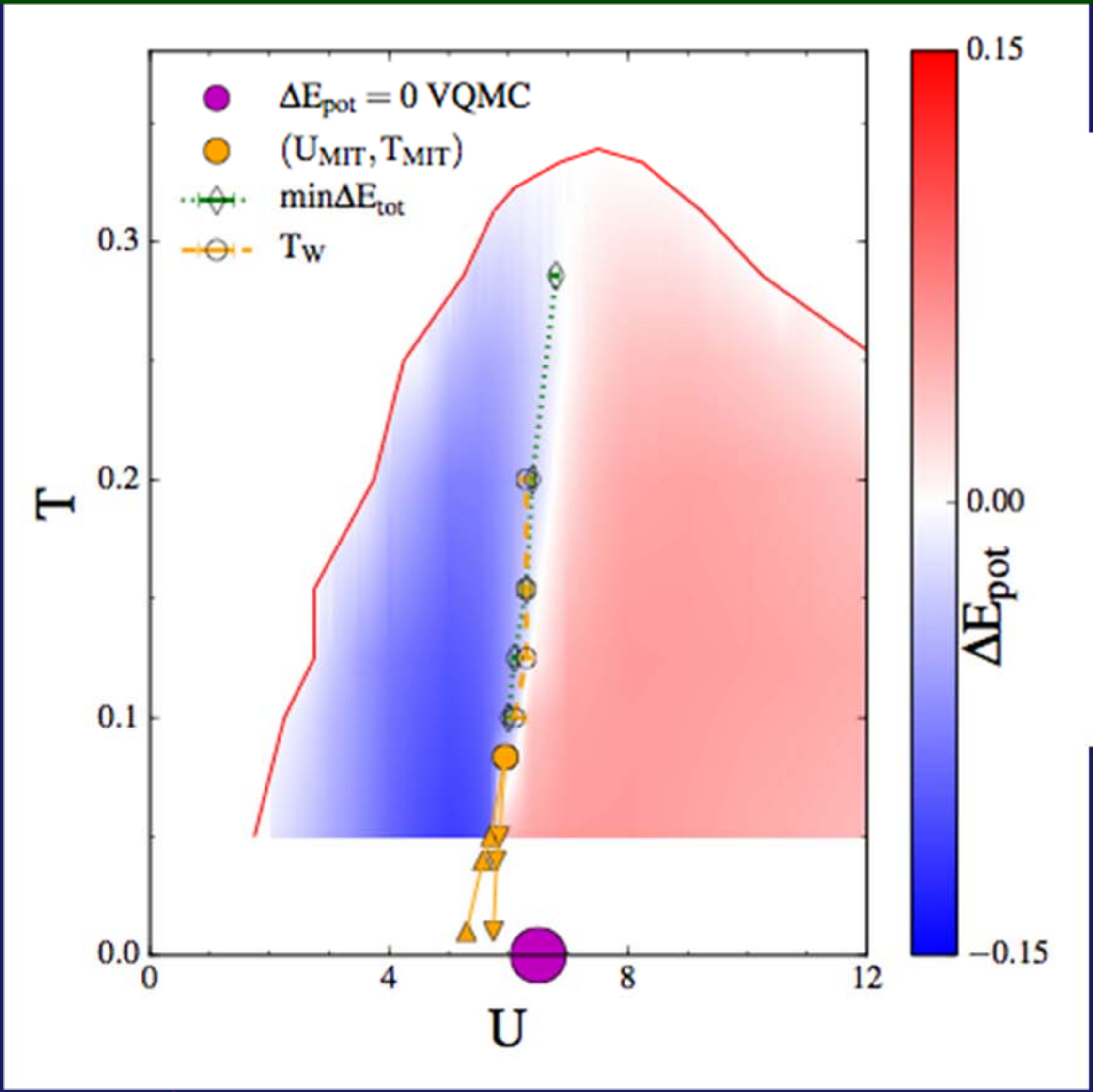
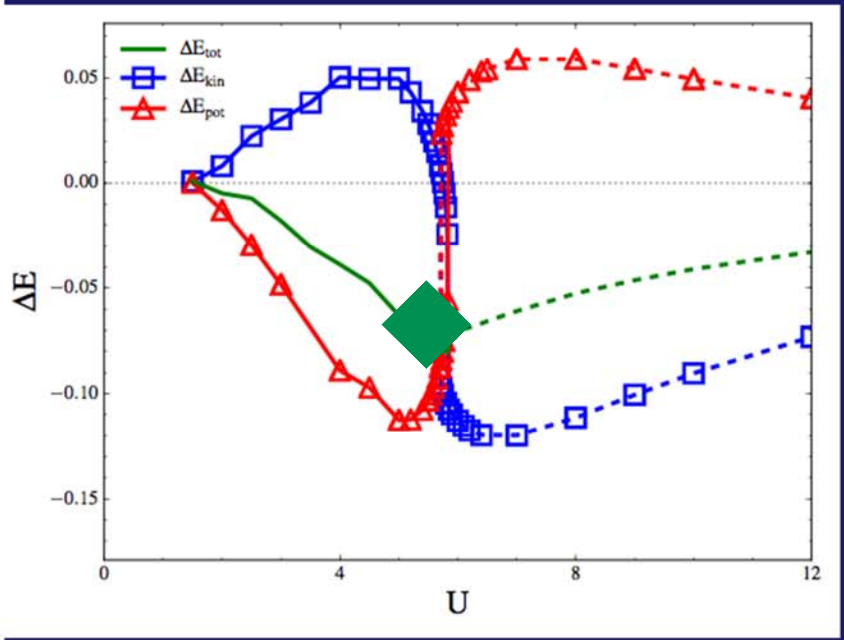
Change in mechanism for stability of the AFM





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

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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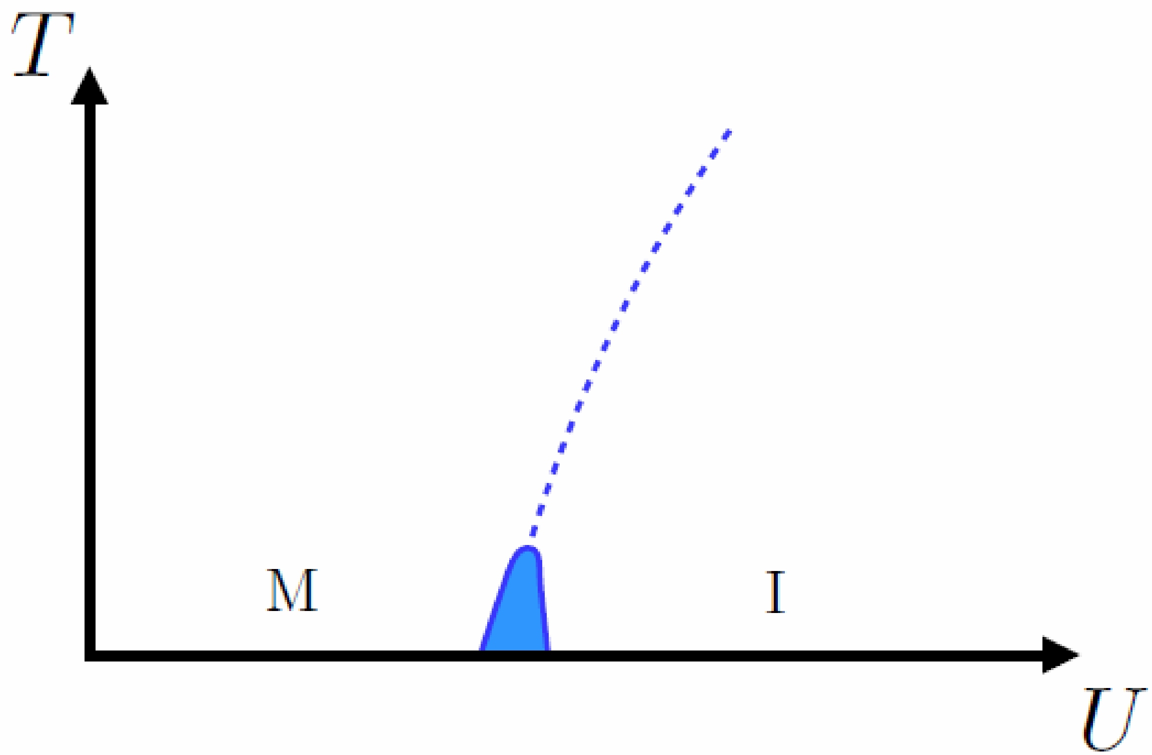
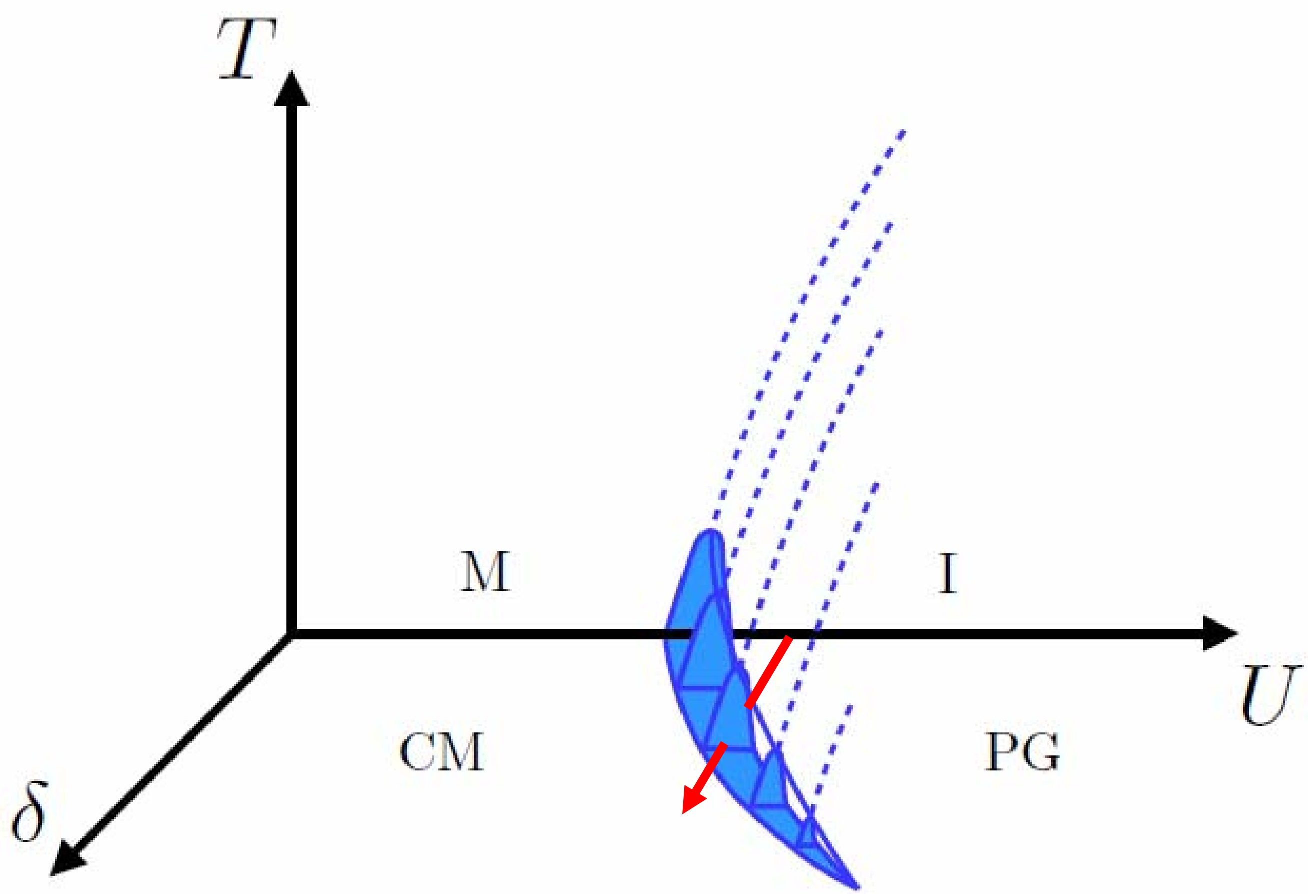
Influence of Mott transition away from half-filling

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

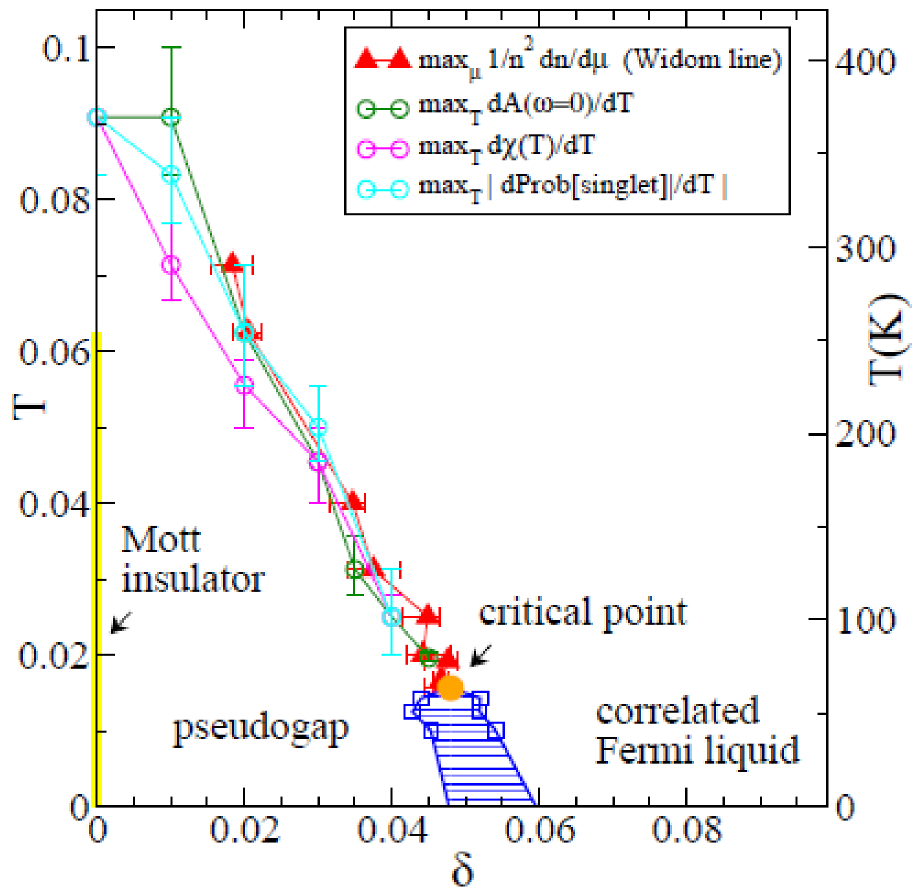


Influence of Mott transition away from half-filling

n = 1, d = 2 square lattice

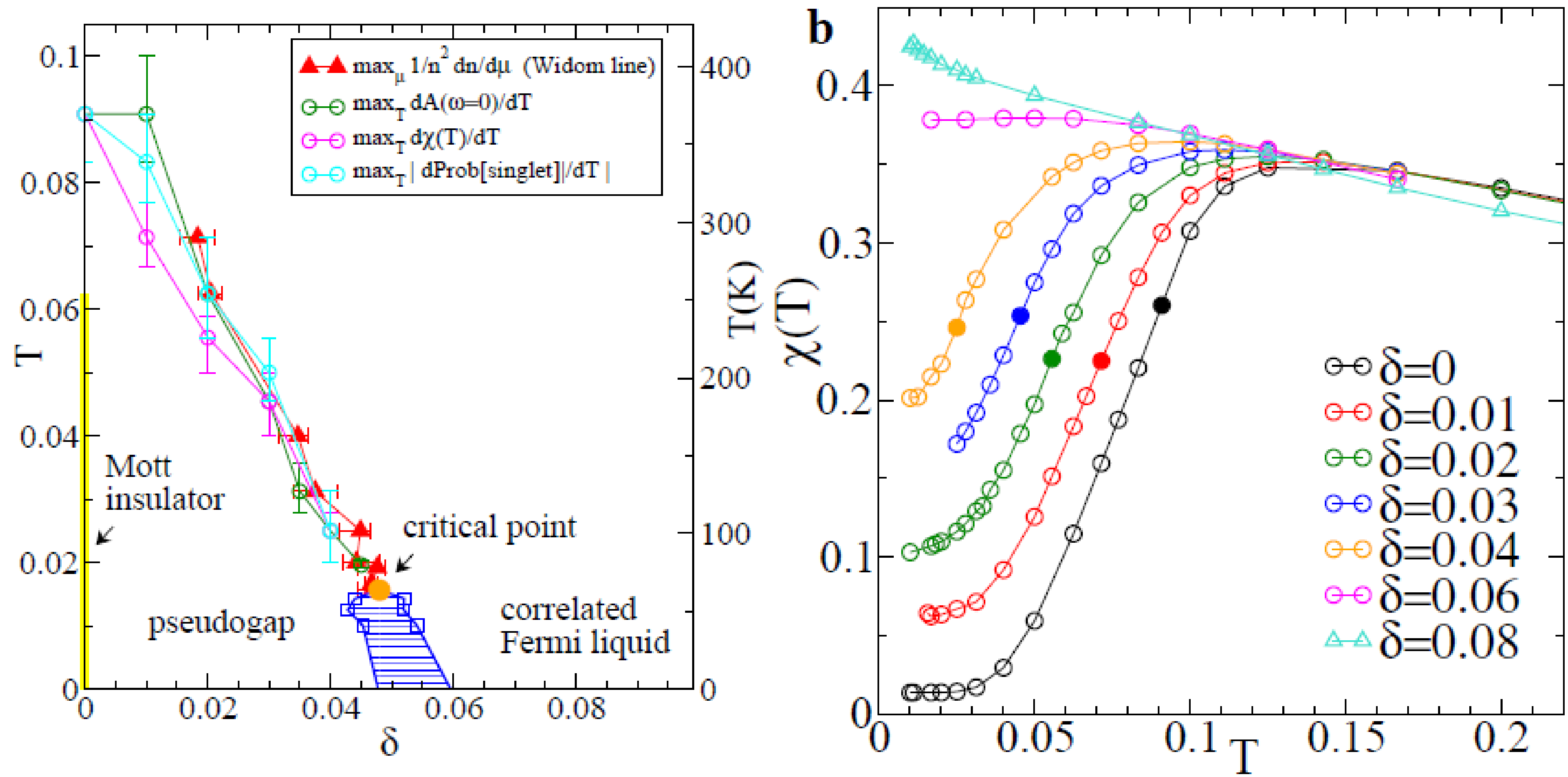


Spin susceptibility



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

Spin susceptibility



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

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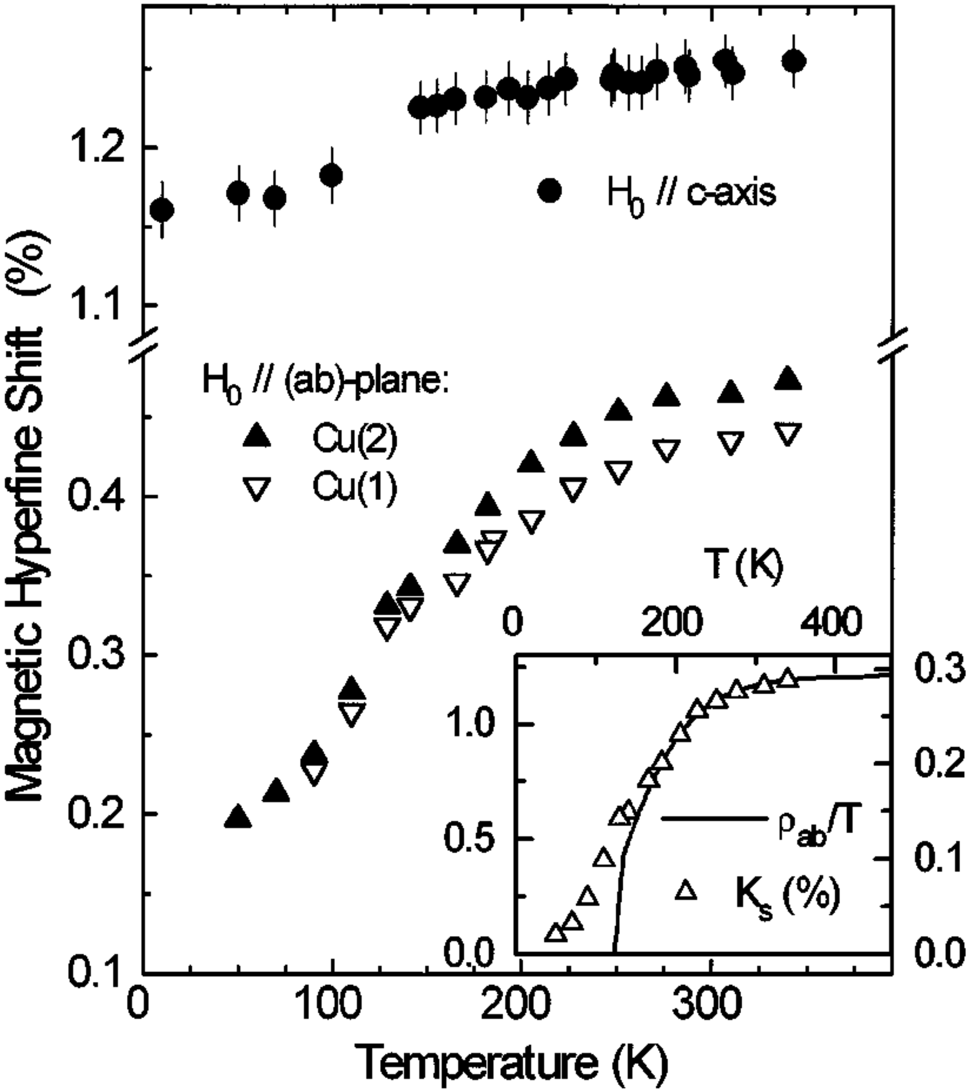
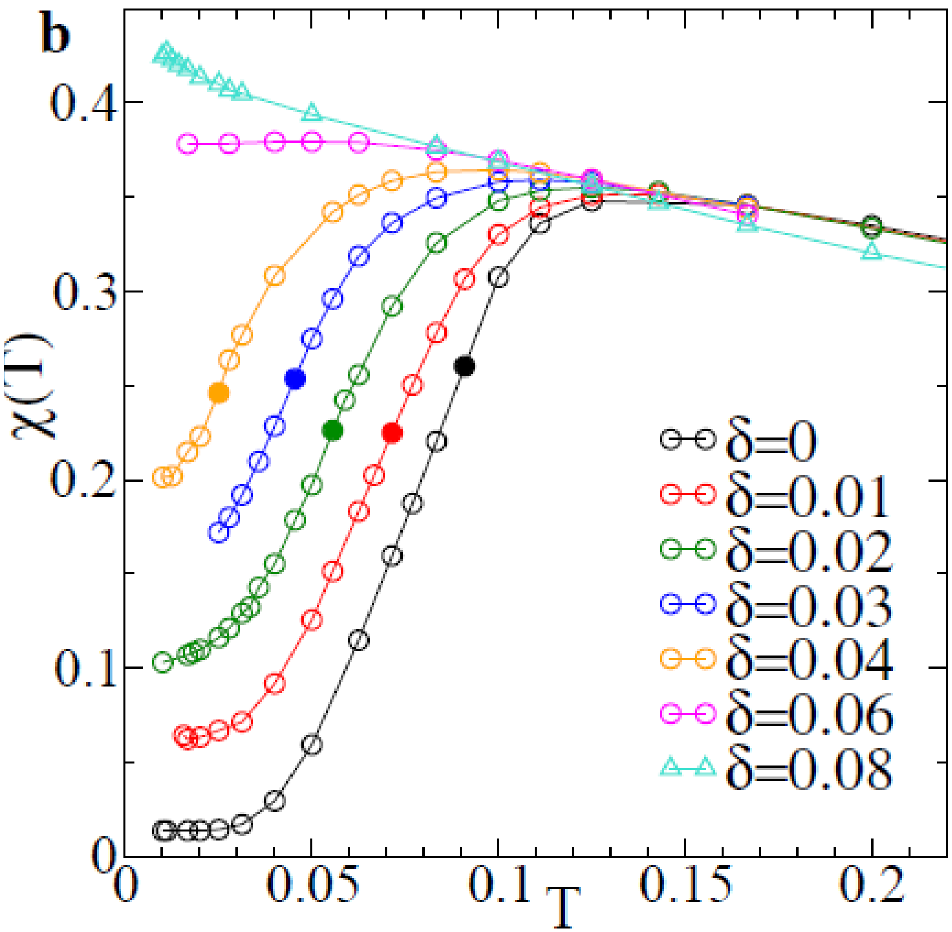
Spin susceptibility



Underdoped Hg1223

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



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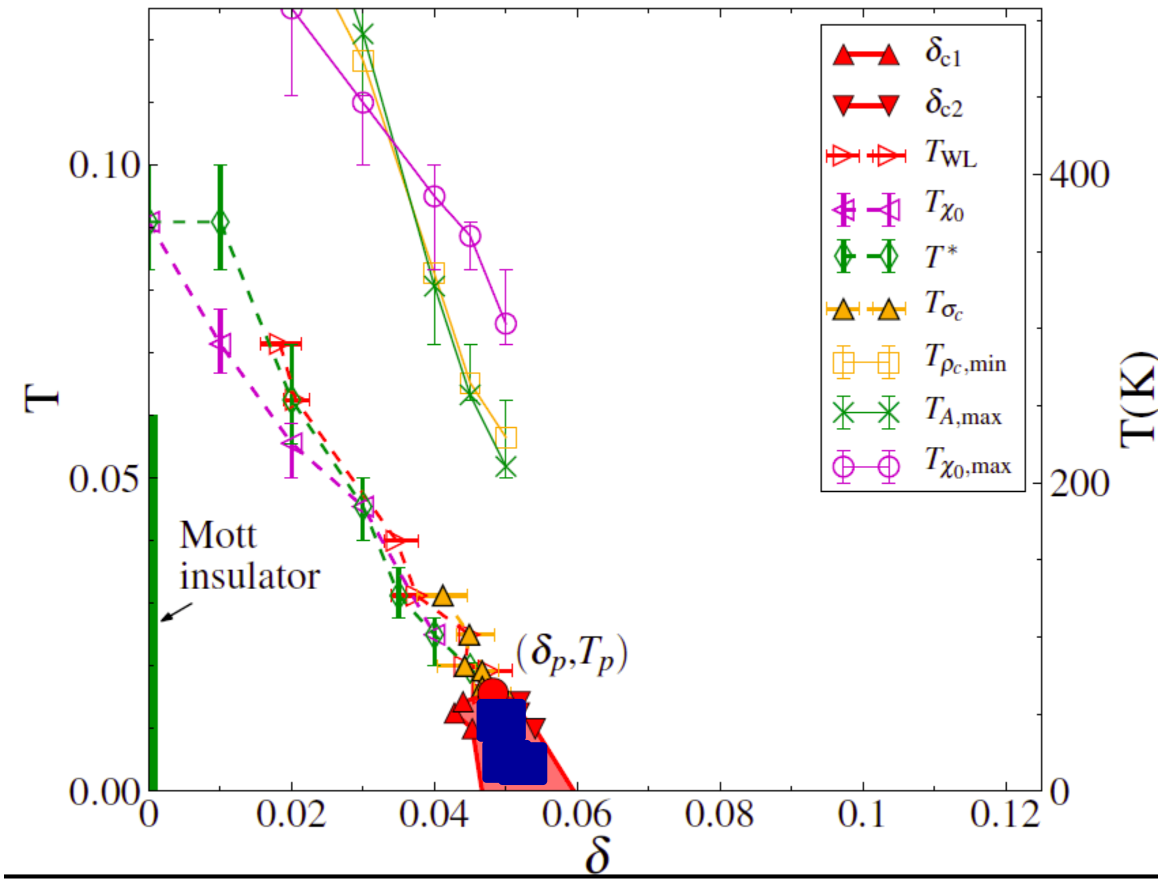
Two crossover lines

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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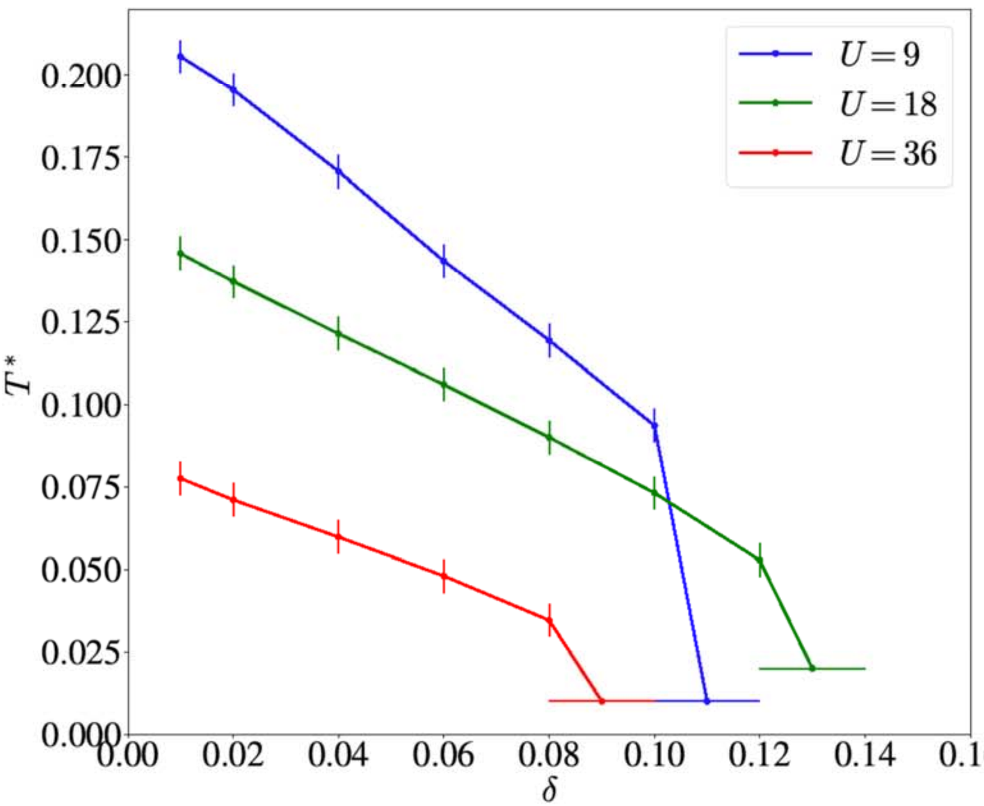
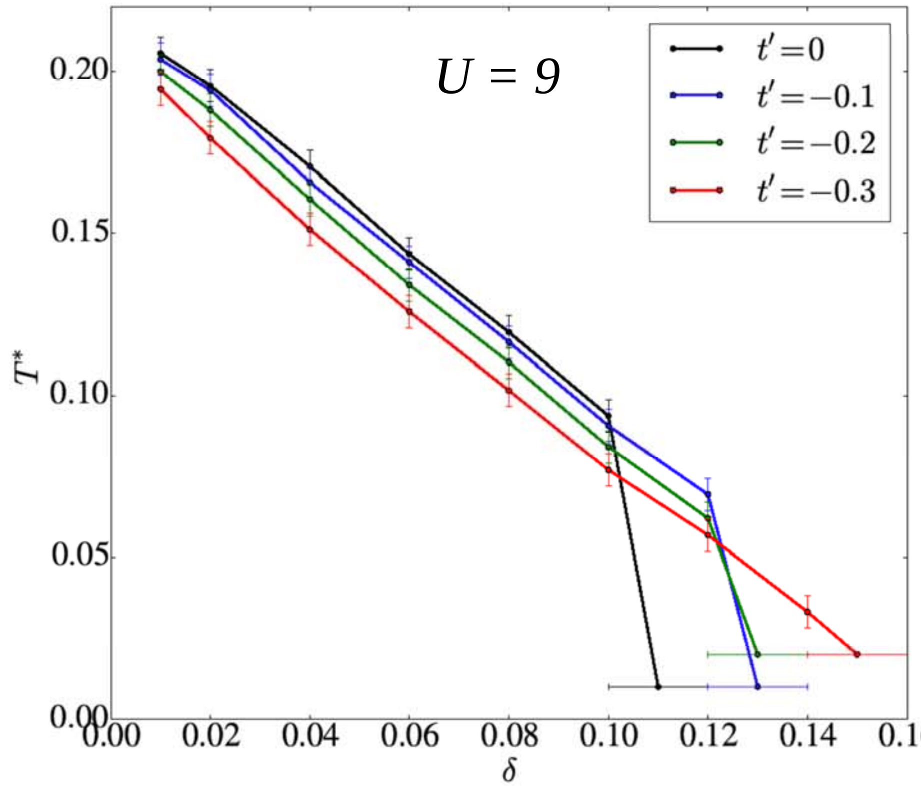
Scaling with J and with t'

$J = 4t^2 /U$

Alexis Reymba





A. Reymbaut, Marion, A. Fratino, G. Sordi, P. Sémon, AMT, unpublished

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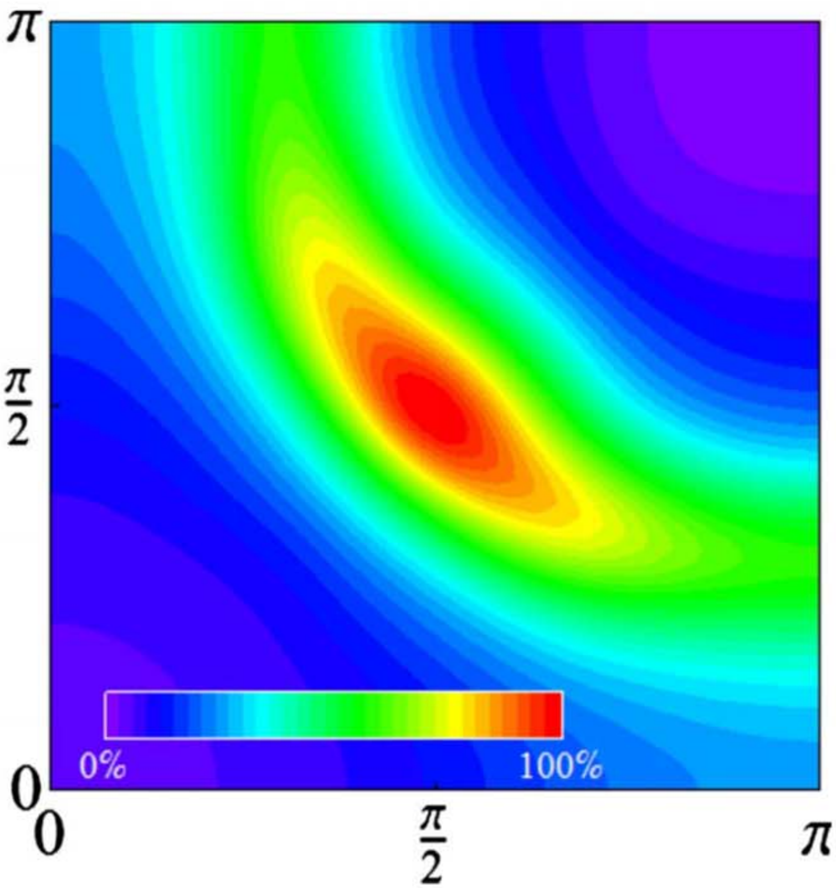
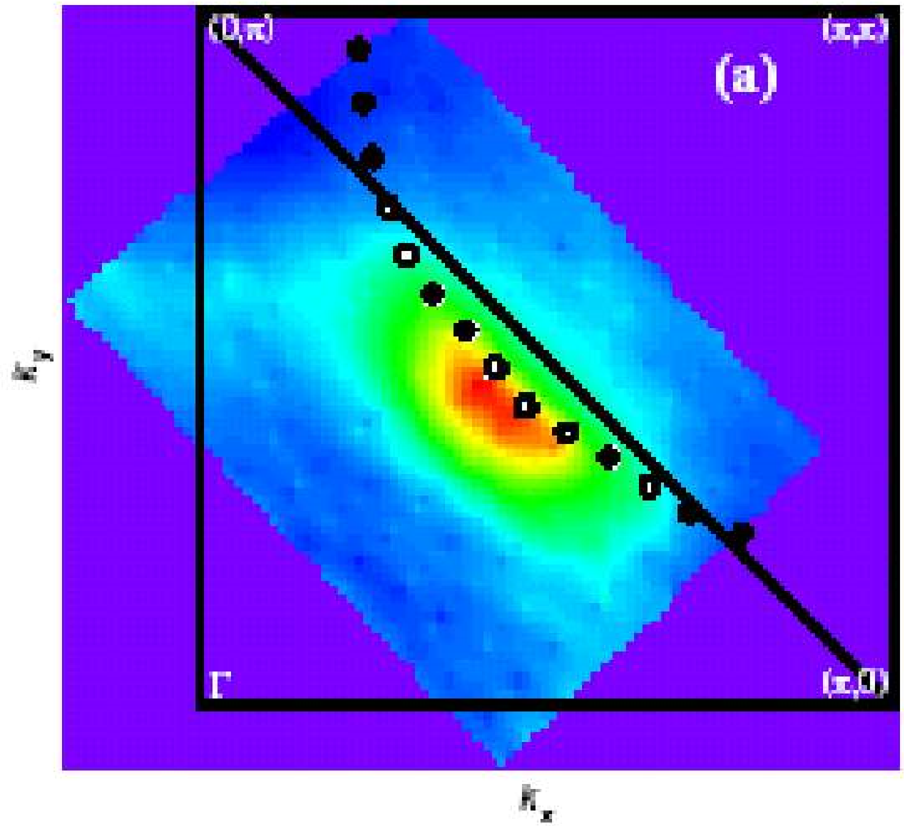
ARPES



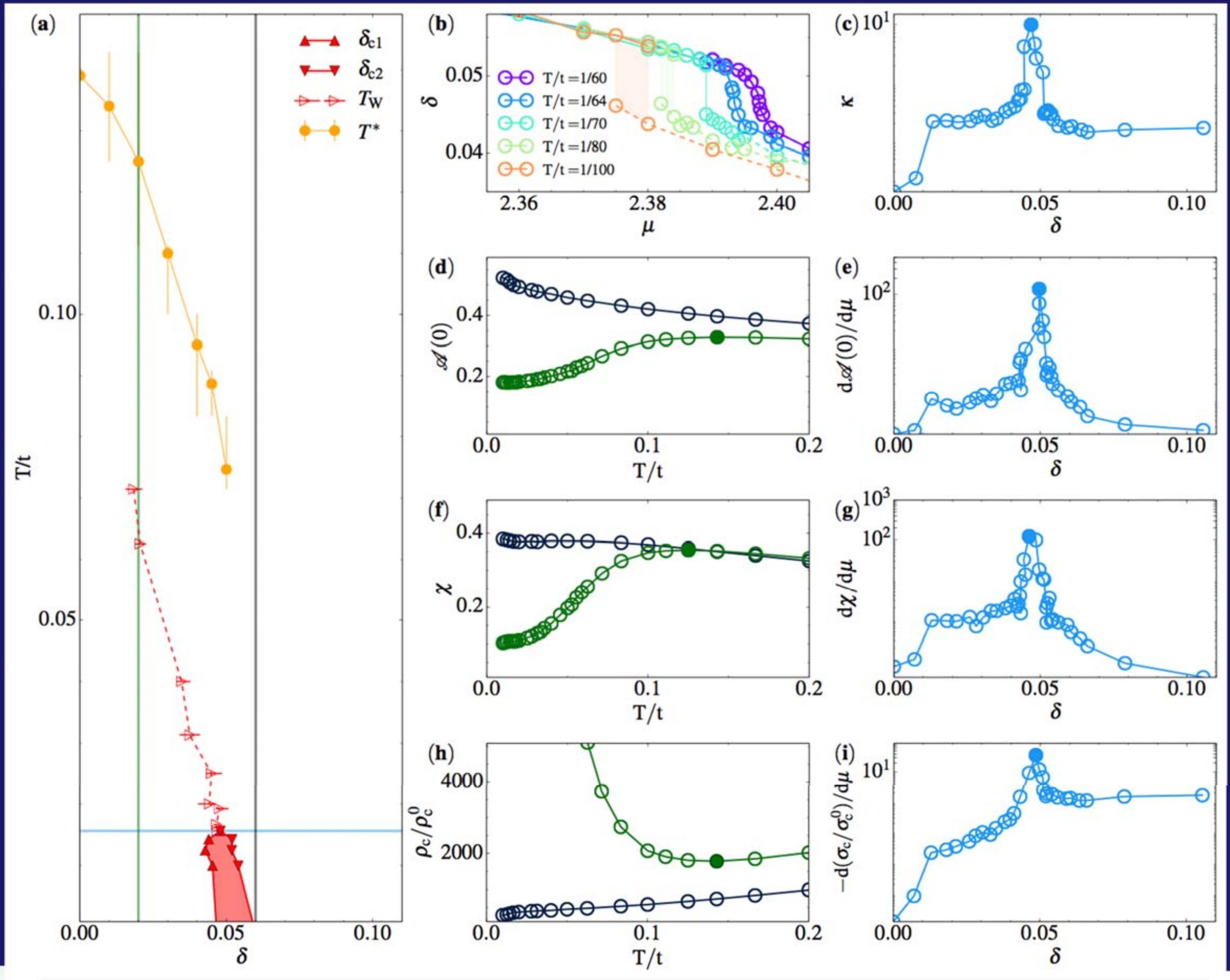
Kancharla *et al.* PRB **77** (2008)

Hole-doped, 10%



F. Ronning et al. Jan. 2002, $Ca_{2-x}Na_xCuO_2Cl_2$

Summary



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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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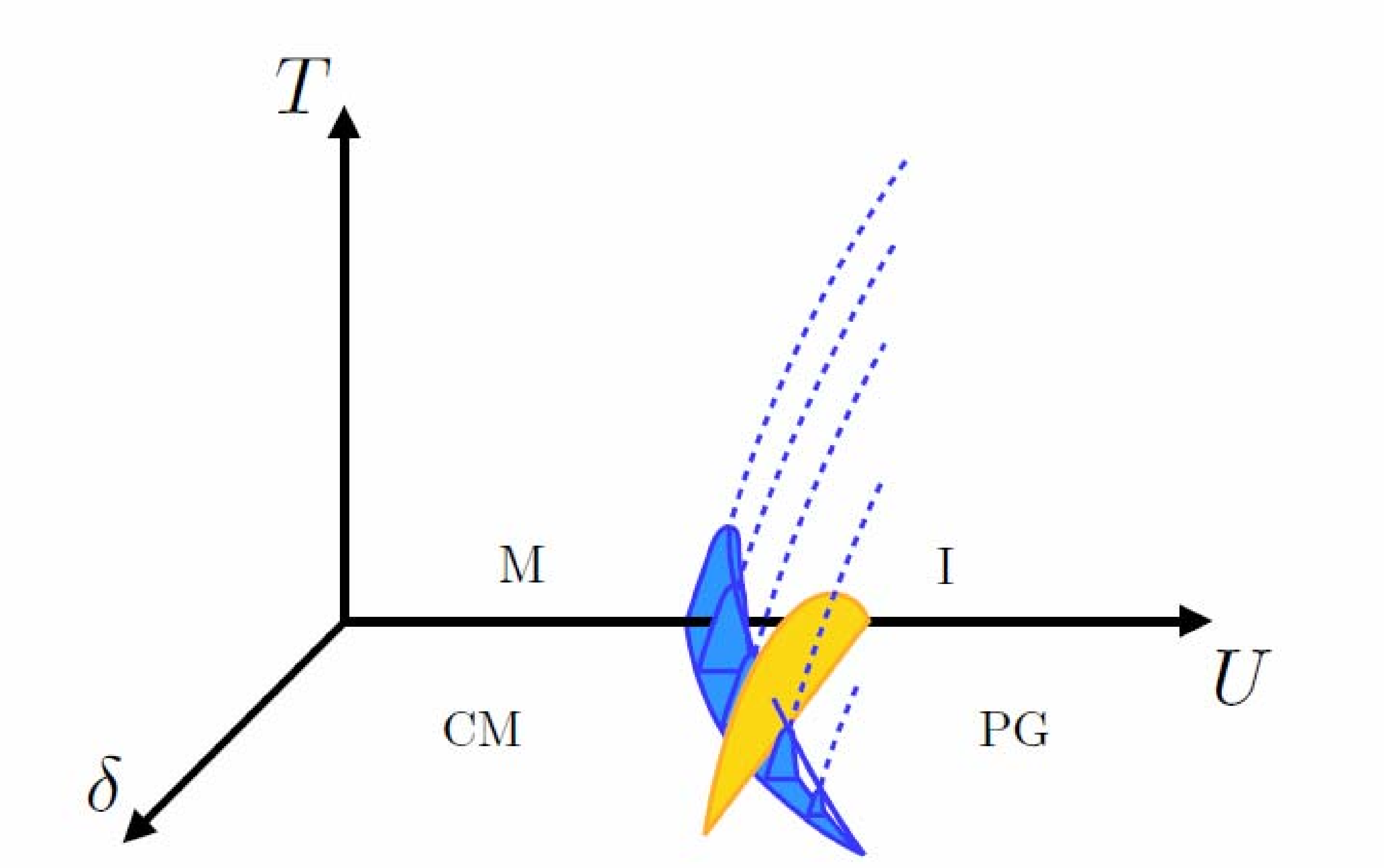
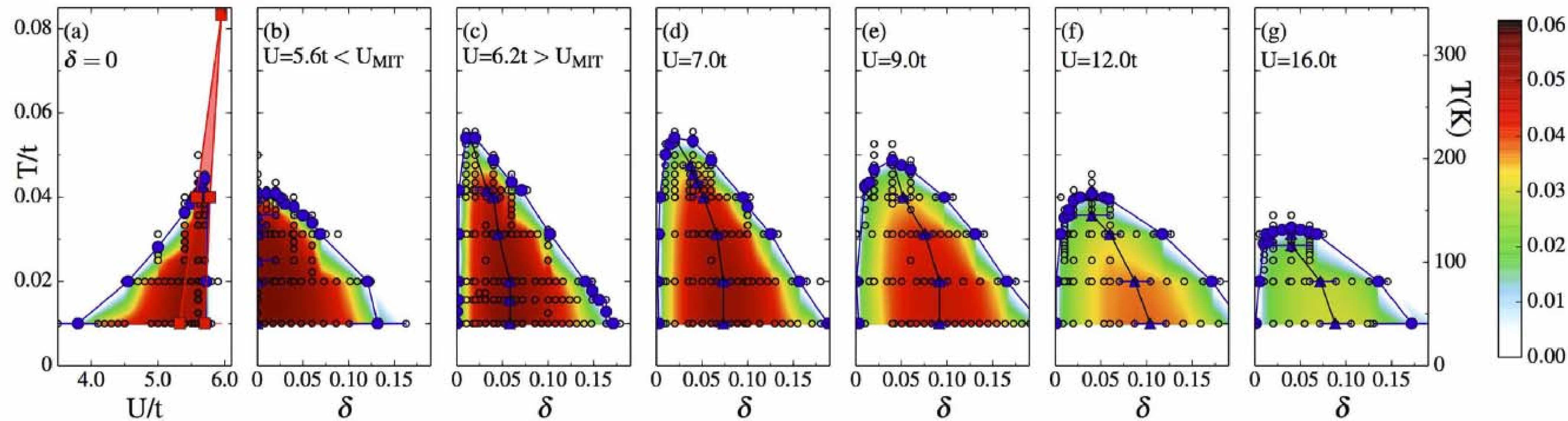
Superconductiviy in Doped Mott insulator

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



T_c controlled by J



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

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

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

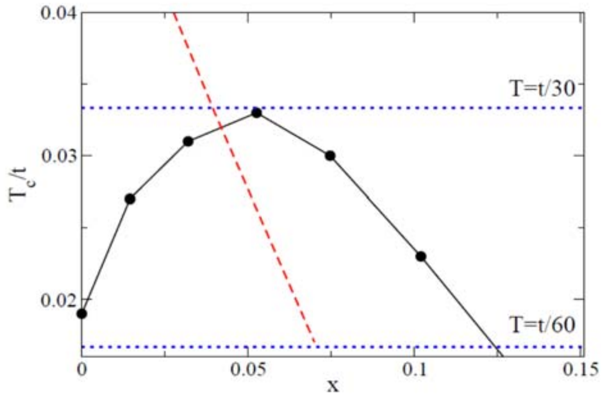
Kondo, Takeshi, et al. Kaminski Nature Physics 2011, ***7***, 21-25

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

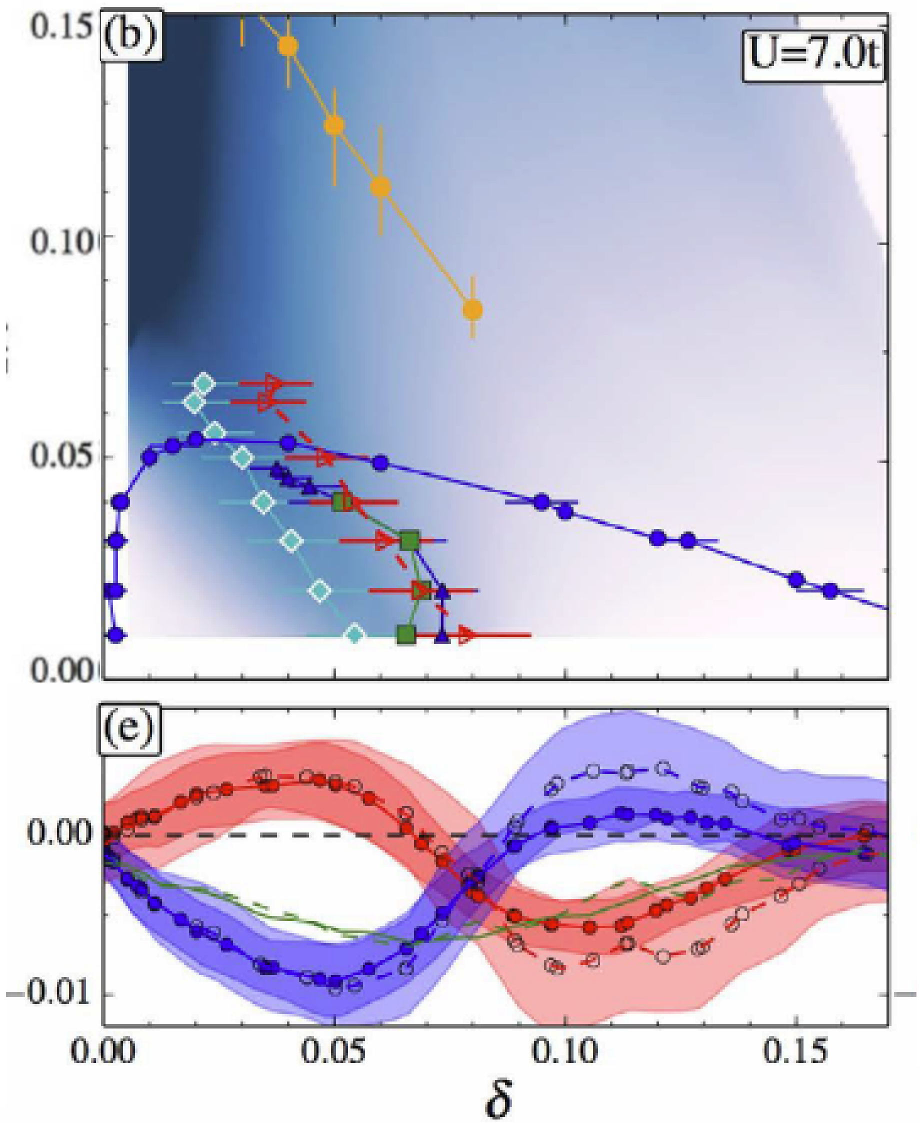
Lee …Tajima (Osaka) https://arxiv.org/pdf/1612.08830

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

An organizing principle



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

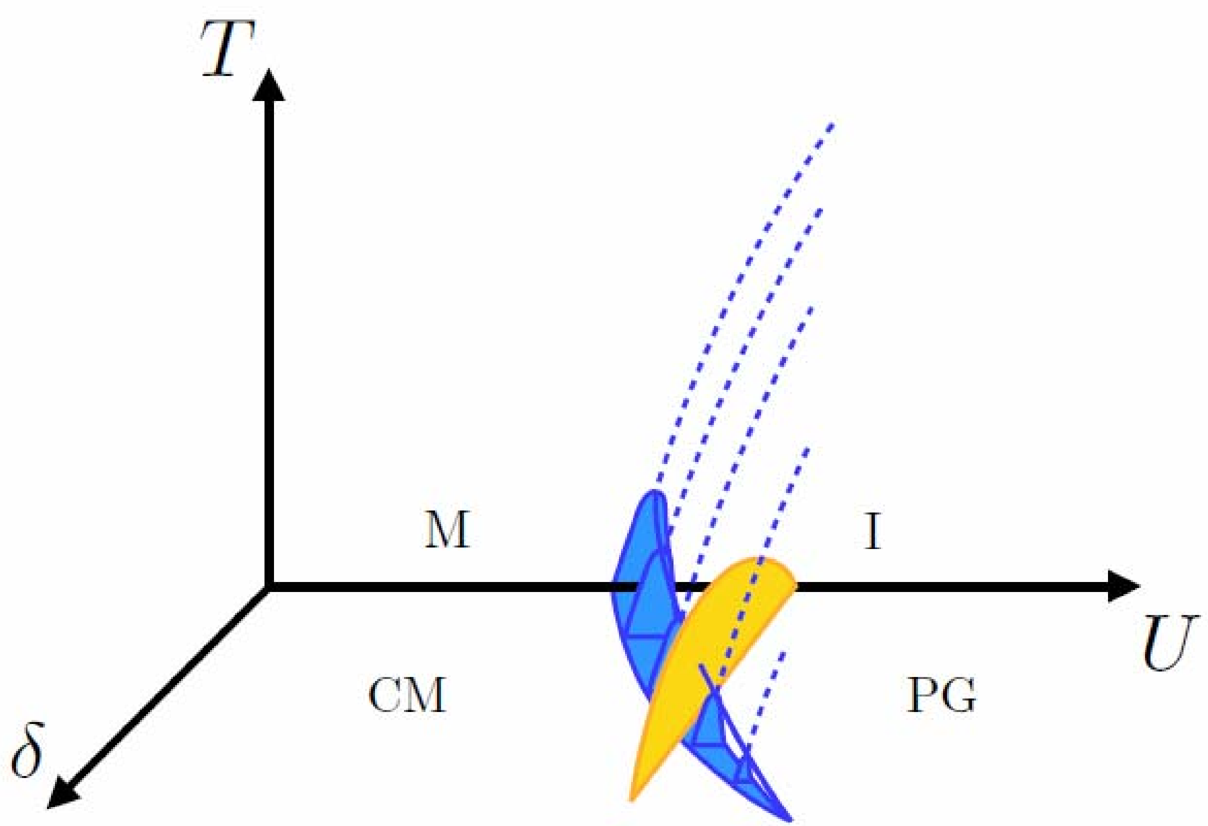


Fratino et al.
Sci. Rep. **6**, 22715

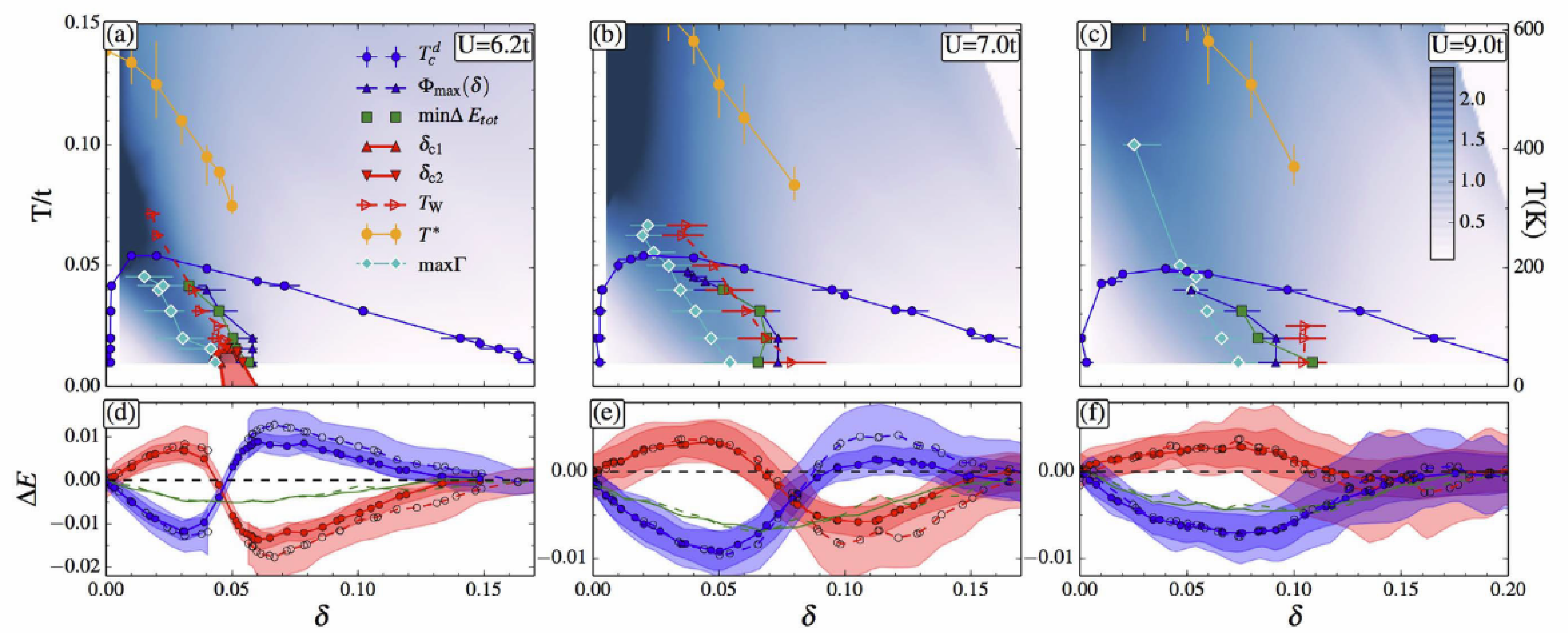
Theory, see also Jarrel PRL (2004), Gull Millis PRB (2014)
Experiments: Bontemps, Santander-Syro Van der Marel …

Superconductiviy in Doped Mott insulator

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



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

Part III

Intermediate correlations : TPSC *e-doped*

Dominic Bergeron

Bumsoo Kyung

V. Hankevych

A.-M. Daré

Pseudogap in the normal state *e-doped*

A. Subromanian

A. Venne

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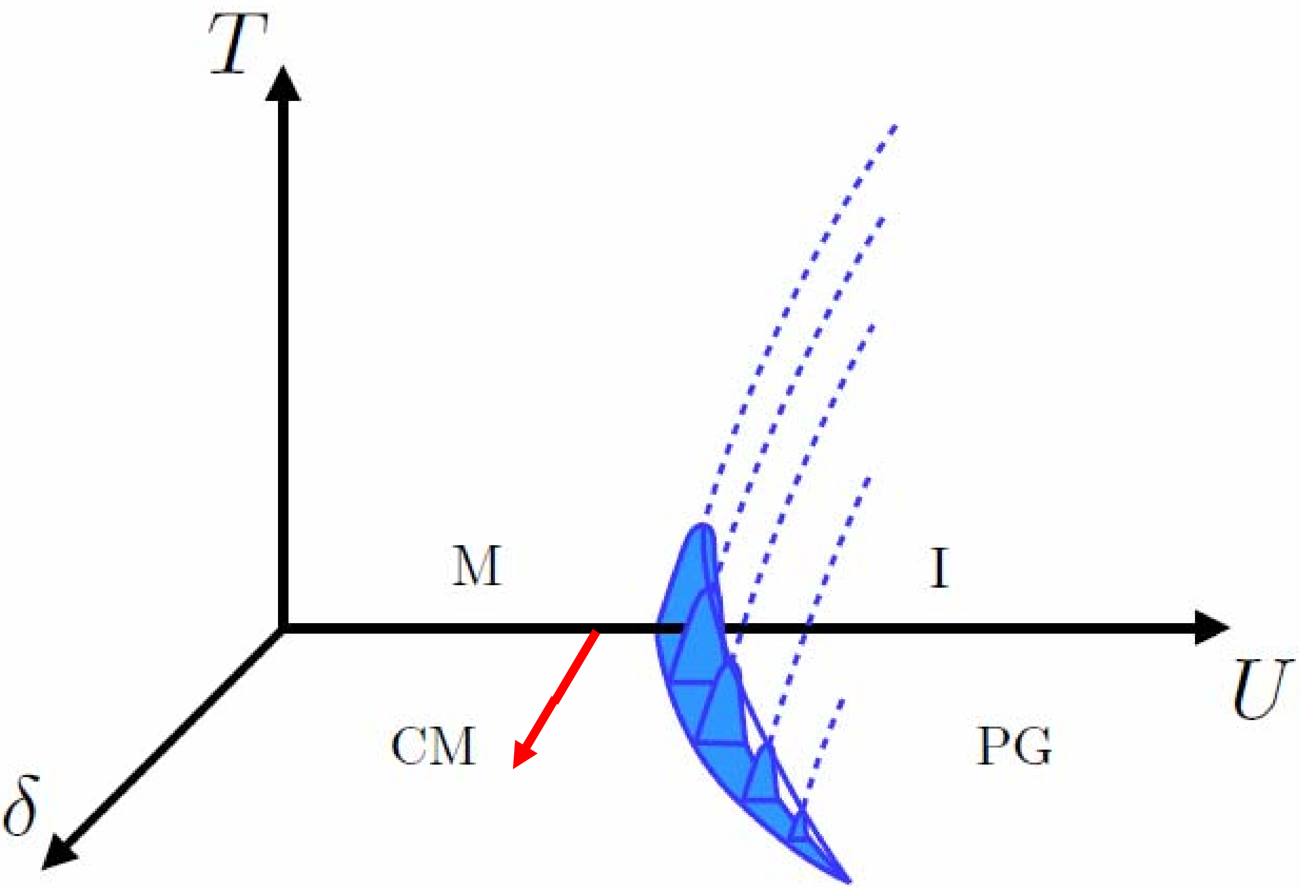
Influence of Mott transition away from half-filling

n = 1, d = 2 square lattice



Method 2 : Small to intermediate *U/t*

Two-particle self-consistent

Vilk, AMT J. Phys. I France, **7**, 1309 (1997);
REVIEW:
AMT *Theoretical methods for strongly correlated electrons*
Ed. F. Mancini *et al*. Springer 2011
Mahan, *Many-Particle Physics* 3rd edition

Yury Vilk

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TPSC: general ideas

- Approach
  - Non perturbative: Drop diagrams
  - Impose constraints and sum rules
    - Conservation laws
    - Pauli principle ($\langle n_\sigma^2 \rangle = \langle n_\sigma \rangle$)
    - Local moment and local density sum-rules
- Get for free:
    - Mermin-Wagner theorem
    - Kanamori-Brückner screening
    - Consistency between one- and two-particle

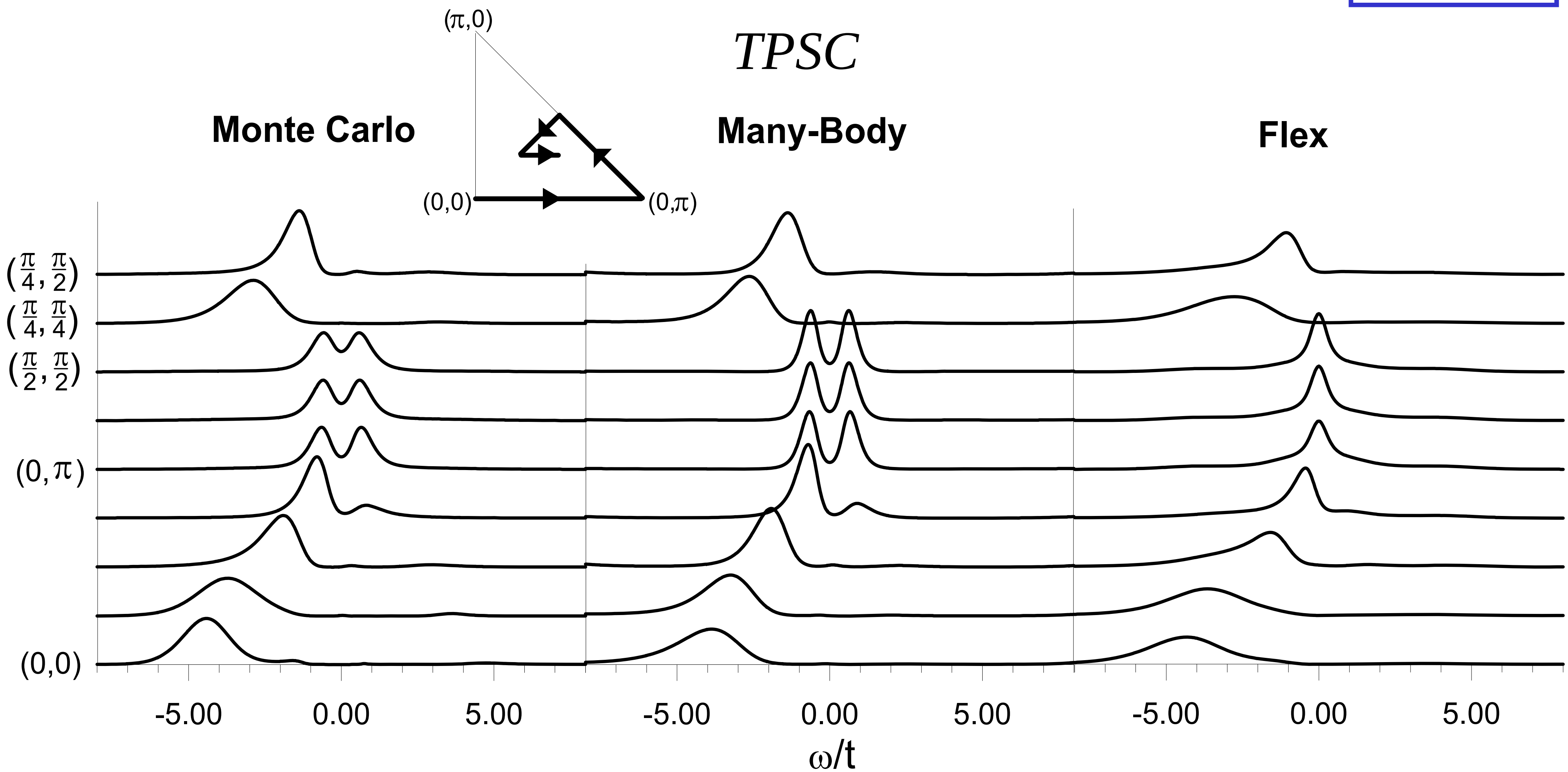
$$\Sigma G = U \langle n_\sigma \, n_{-\sigma} \rangle$$

Vilk, AMT J. Phys. I France, **7**, 1309 (1997);
Theoretical methods for strongly correlated electrons also (Mahan, 3rd)

Benchmarks

$U = +4$
$\beta = 5$

TPSC



Calc. + QMC: Moukouri et al. P.R. B 61, 7887 (2000).

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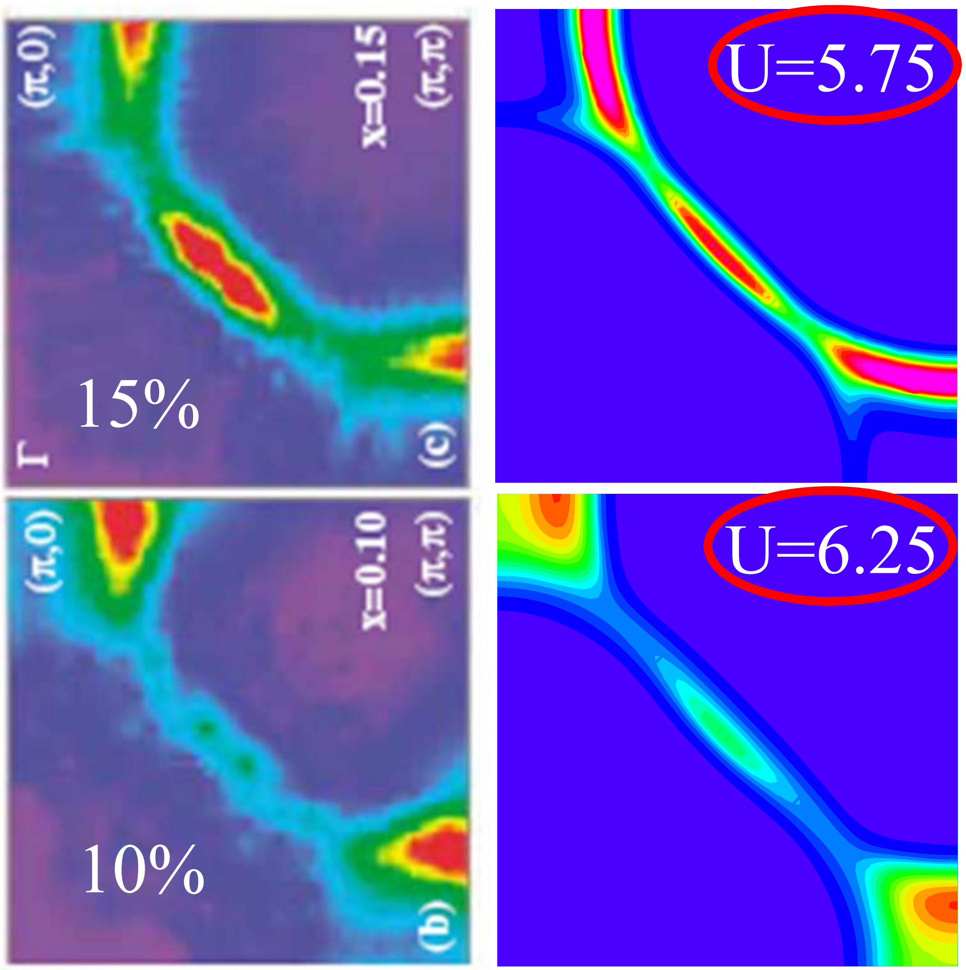
Fermi surface plots

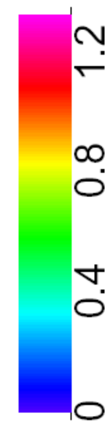
Hankevych, Kyung, A.-M.S.T., PRL, sept. 2004

t'=-0.175t, t"=0.05t
t=350 meV, T=200 K



Hubbard repulsion U has to…

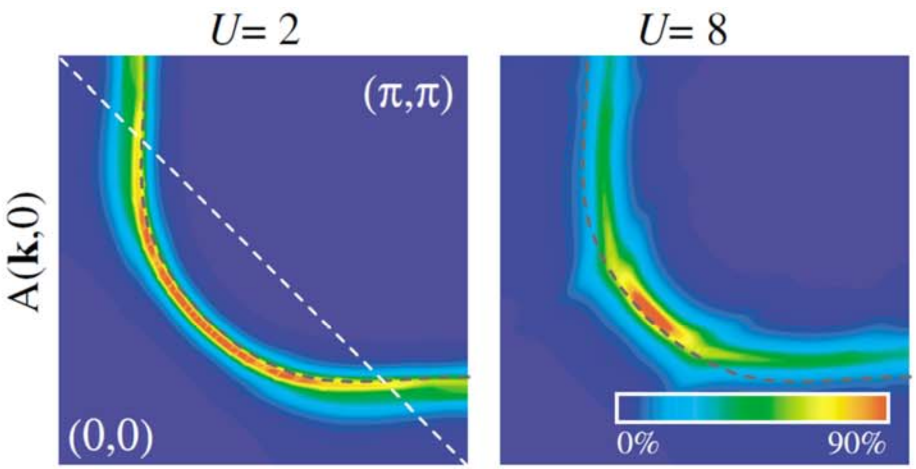
be not too large

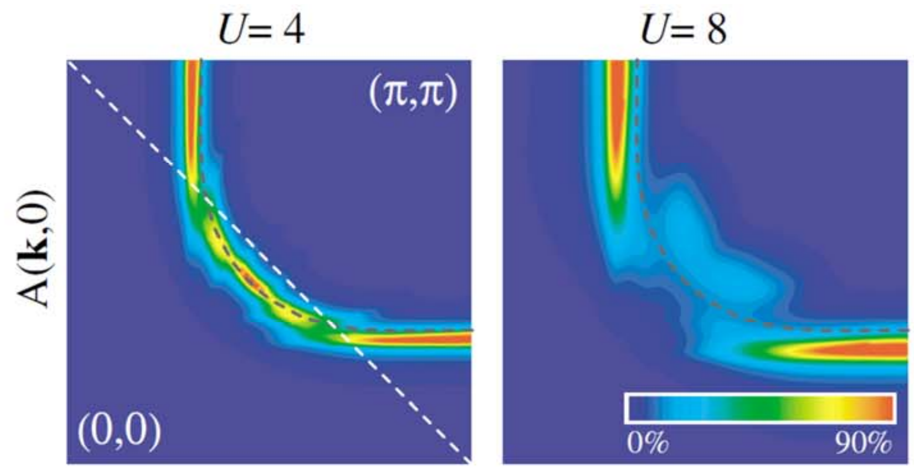


increase for
smaller doping

B.Kyung *et al.*,PRB **68**, 174502 (2003)

U/t smaller, at least near optimal doping





h-doped

e-doped

D. Sénéchal

Sénéchal, AMT, PRL (2004)
Weber, Haule, Kotliar, PRB (2010)

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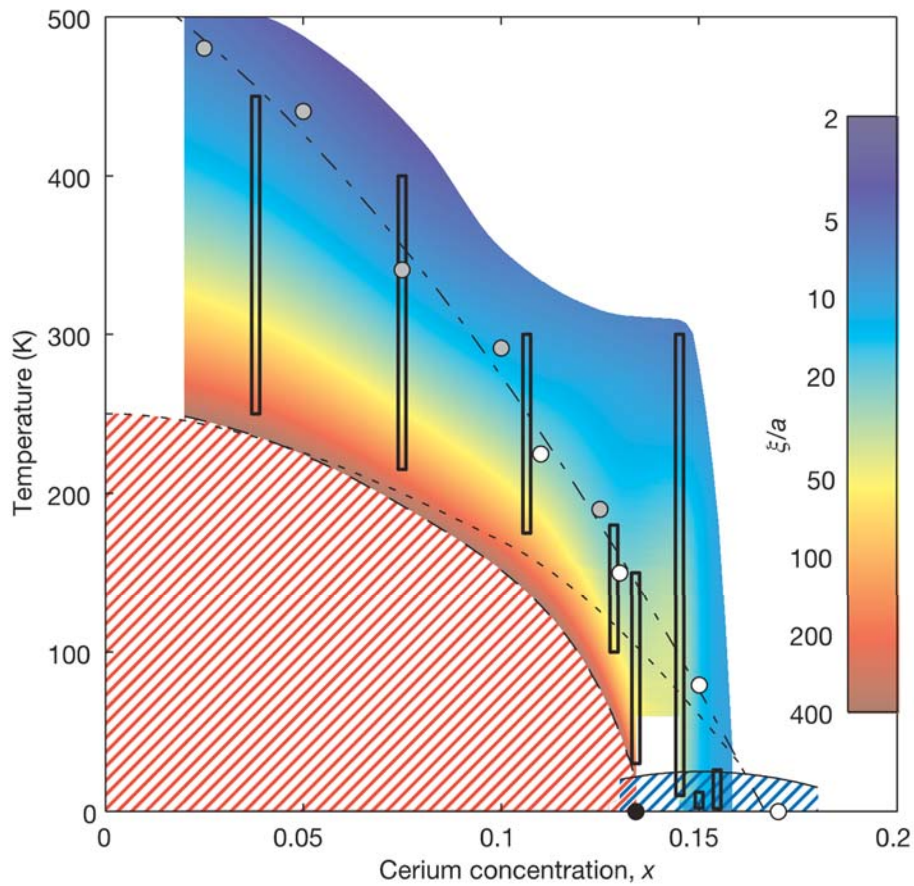
e-doped pseudogap

E. M. Motoyama et al.. Nature 445, 186–189 (2007).



Vilk criterion $\xi^{*} = 2.6(2)\,\xi_{th}$.

Thermal de Broglie wavelength

$$\Delta\varepsilon \sim k_B T$$

$$\nabla_{\mathbf{k}}\varepsilon \; \Delta k \sim k_B T$$

$$\xi_{th} \sim \frac{v_F}{T}$$

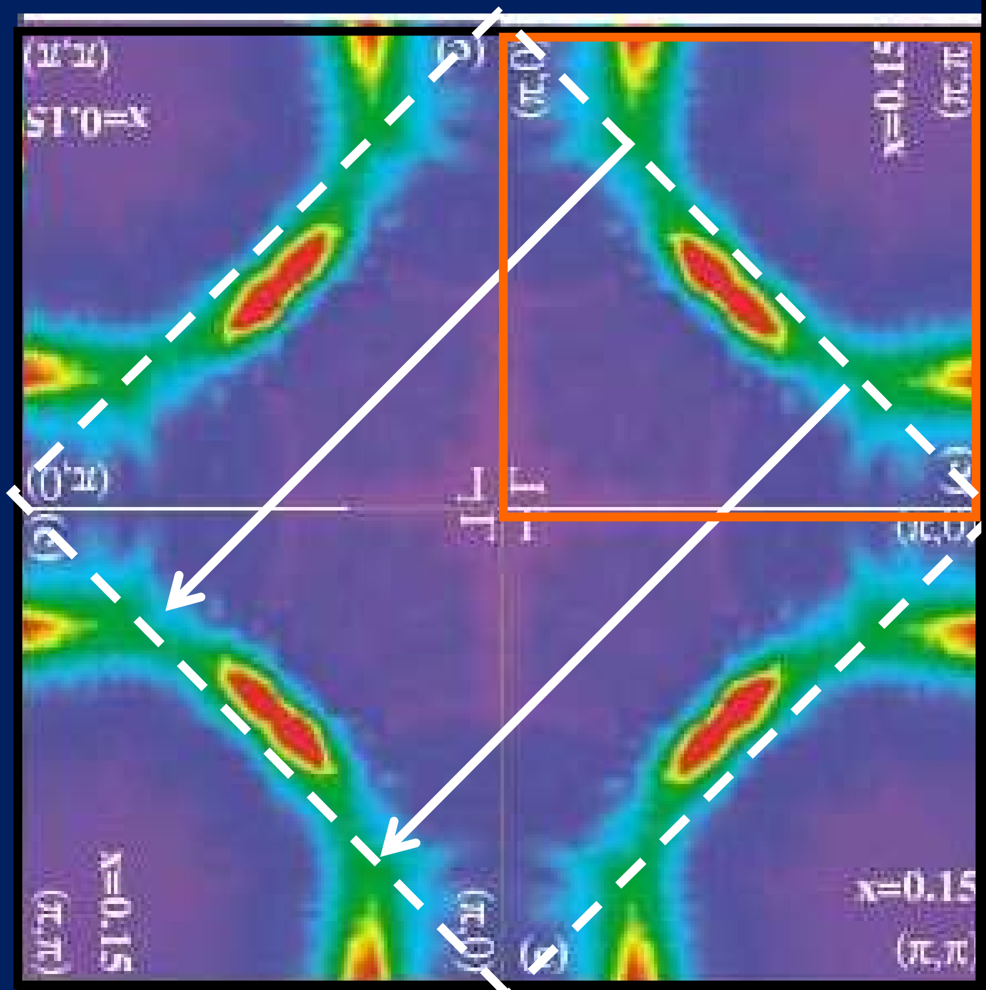
$$\Delta k \sim \frac{k_B T}{\hbar v_F}$$

$$\frac{2\pi}{\xi_{th}} \sim \frac{k_B T}{\hbar v_F}$$

Hot spots from AFM quasi-static scattering

Mermin-Wagner

$d = 2$

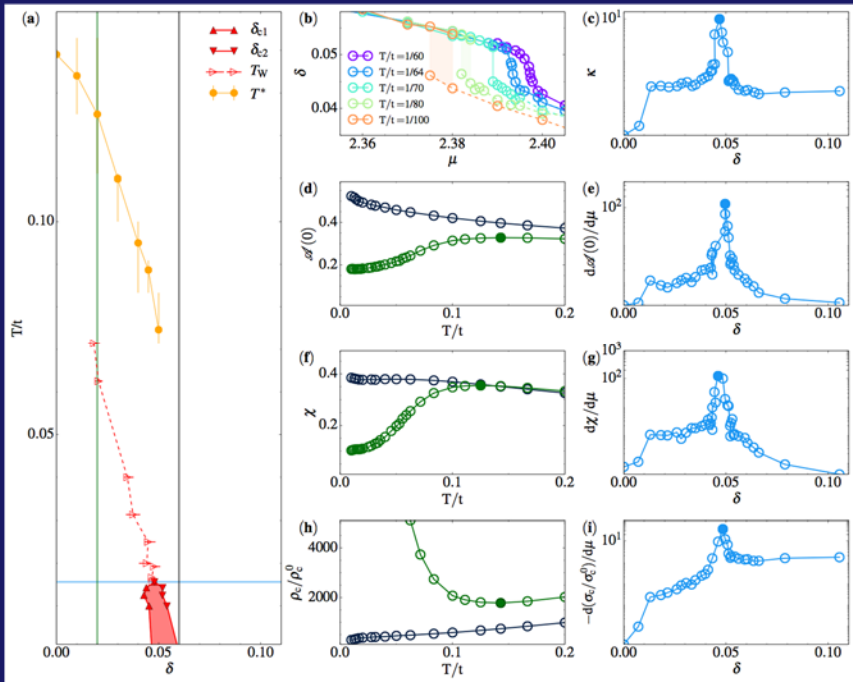


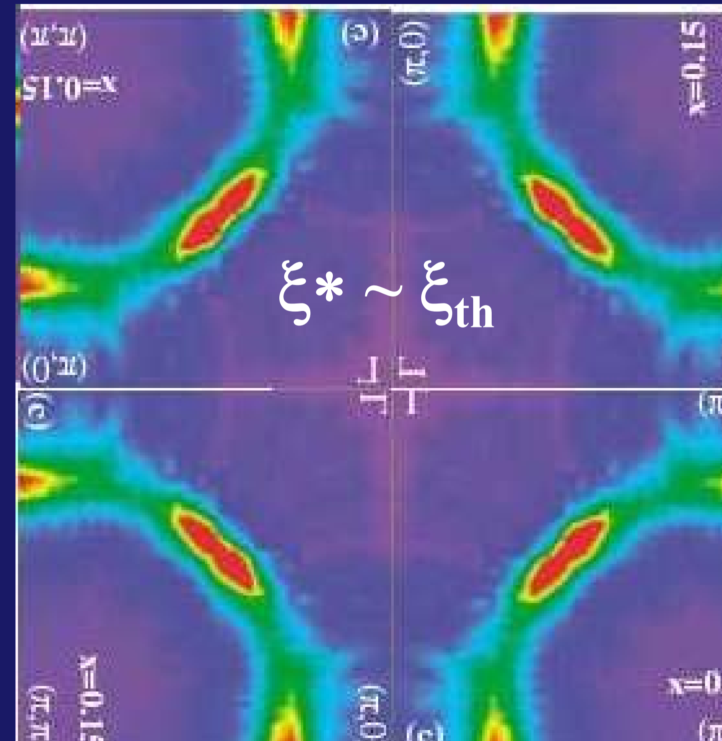
$\xi^* \sim \xi_{th}$

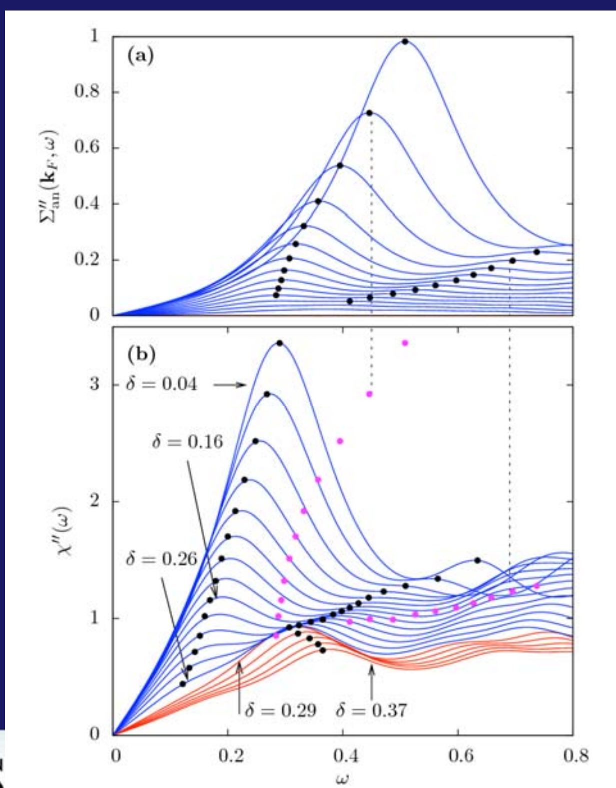
Vilk, AMT (1997)
Kyung, *et al.*
PRL, 2004

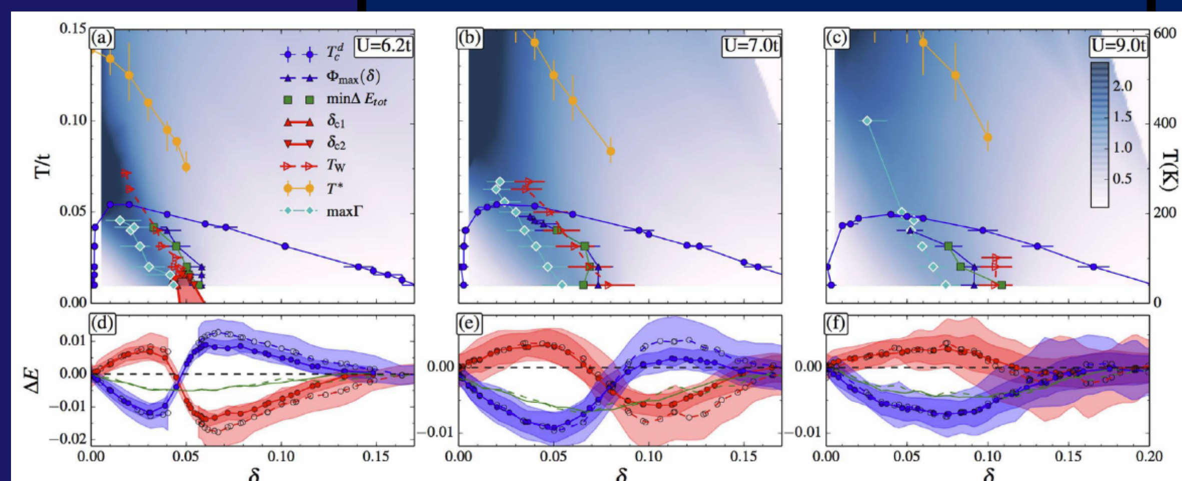
Armitage et al. PRL 2001

Conclusion









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BÂTIR L'ÉCONOMIE NUMÉRIQUE

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+

IQ Postdoctoral Research Fellow

The Institut quantique welcomes Sébastien Jezouin. He will join us on July 1st.

Supervising Professor: Bertrand Reulet

Research Subjects: quantum computing, experimental

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CFREF – Major grant

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Review: A.-M.S.T. arXiv: 1310.1481

Arigato

Merci

Thank you

A.-M.S. Tremblay

"Strongly correlated superconductivity"

Chapt. 10 : *Emergent Phenomena in Correlated Matter Modeling and Simulation*, *Vol. 3*, E. Pavarini, E. Koch, and U. Schollwöck (eds.)

Verlag des Forschungszentrum Jülich, 2013

D. Sénéchal

Bumsoo Kyung

The glue

Kyung, Sénéchal, Tremblay, Phys. Rev. B **80,** 205109 (2009)
Sénéchal, Day, Bouliane, AMST, Phys. Rev. B **87**, 075123 (2013)
A. Reymbaut *et al*. PRB **94** 155146 (2016)

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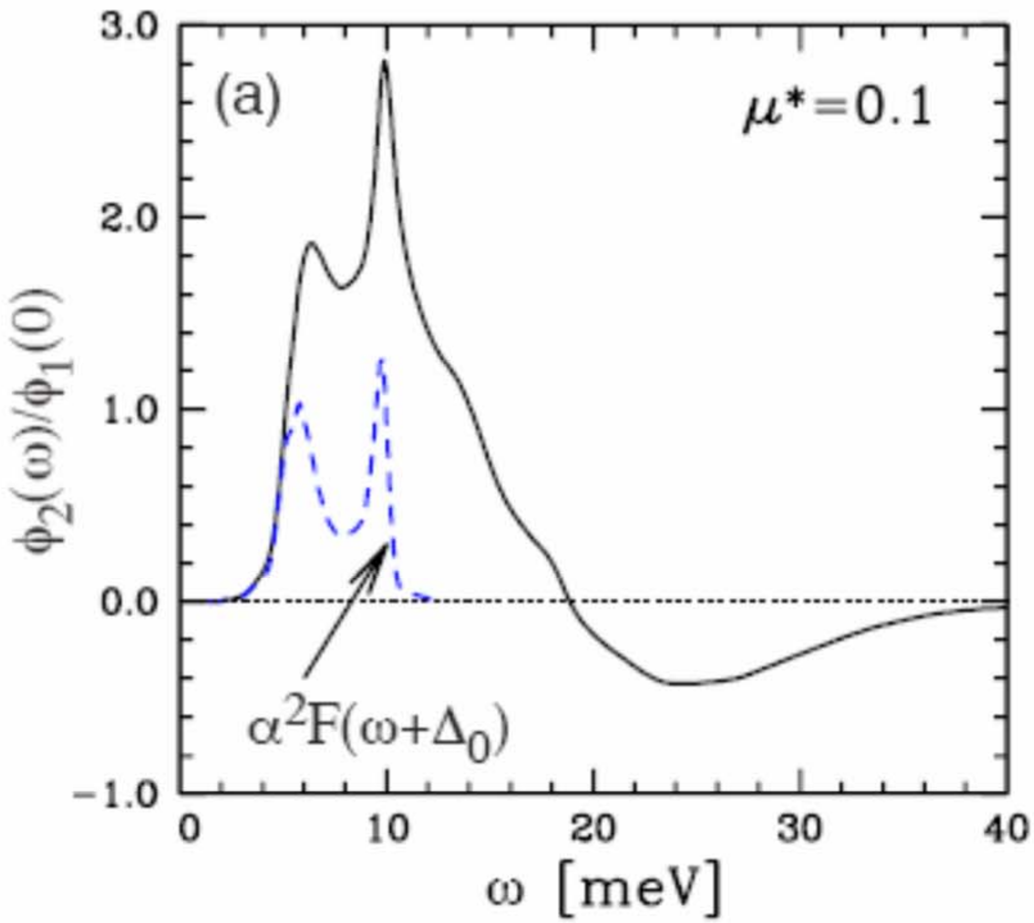
Im Σ_{an} and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)



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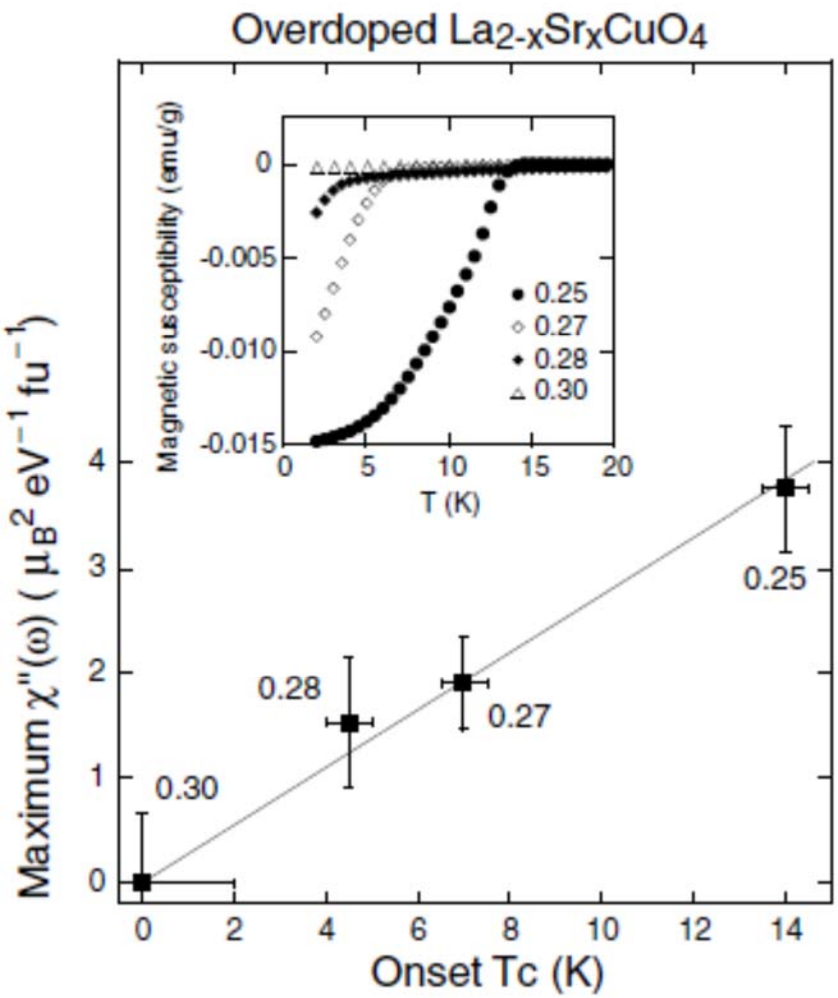
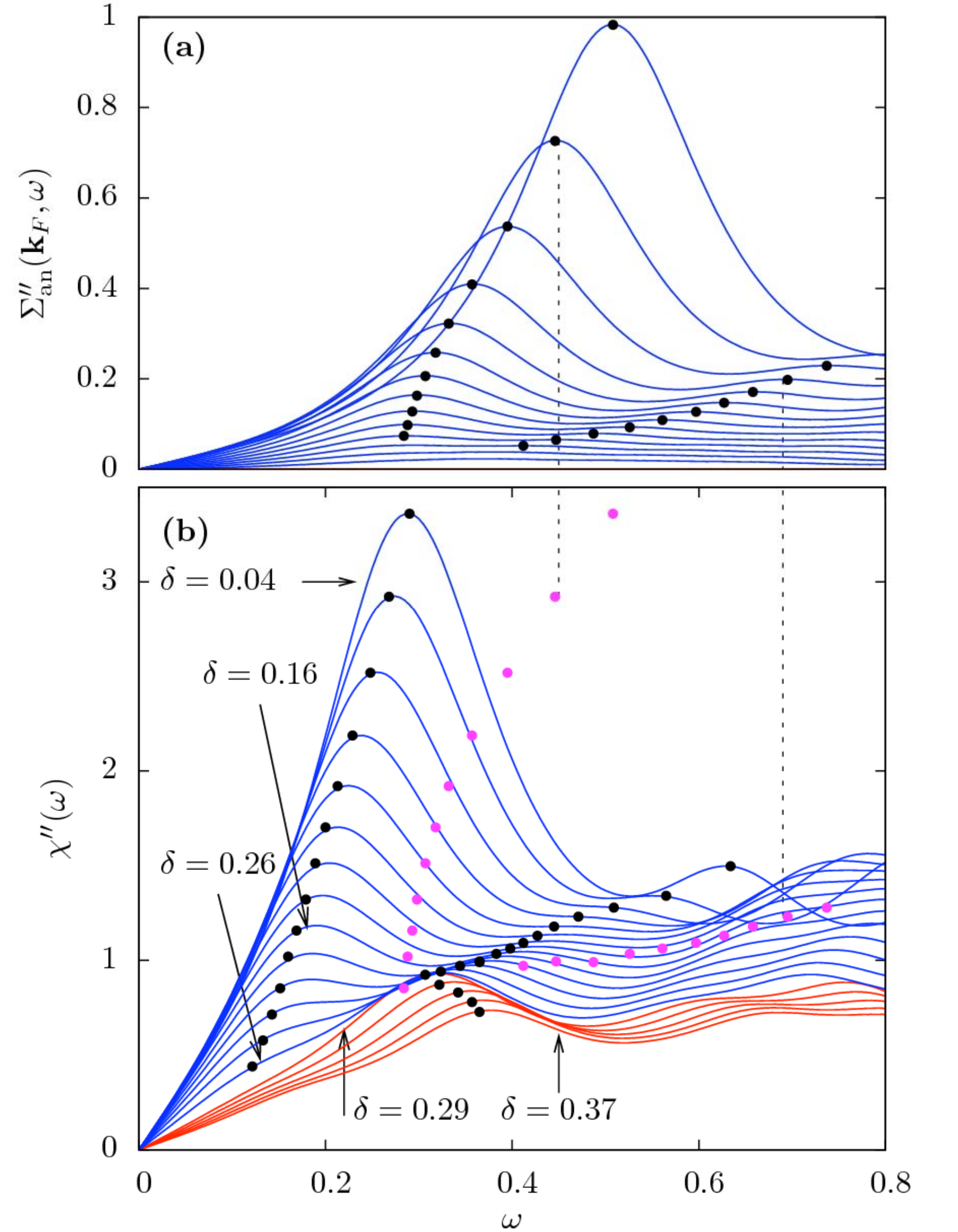
The glue

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



Wakimoto … Birgeneau PRL (2004)



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The glue and neutrons

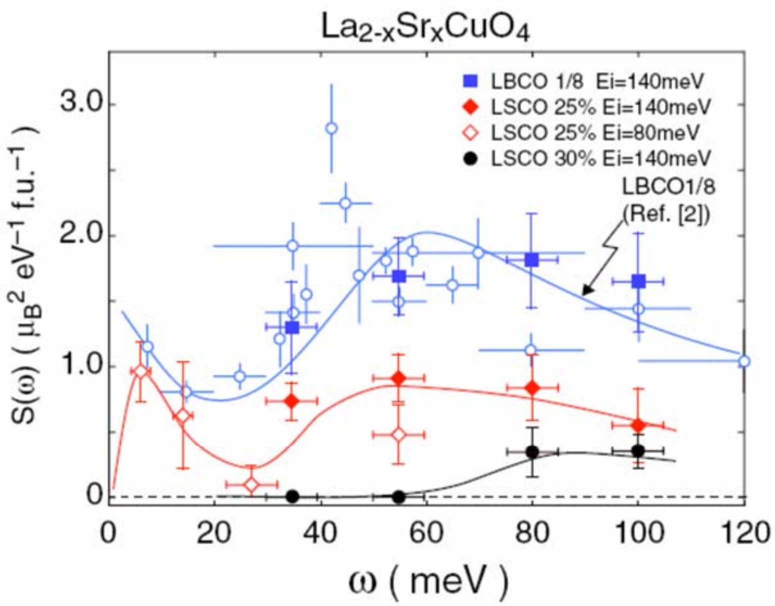
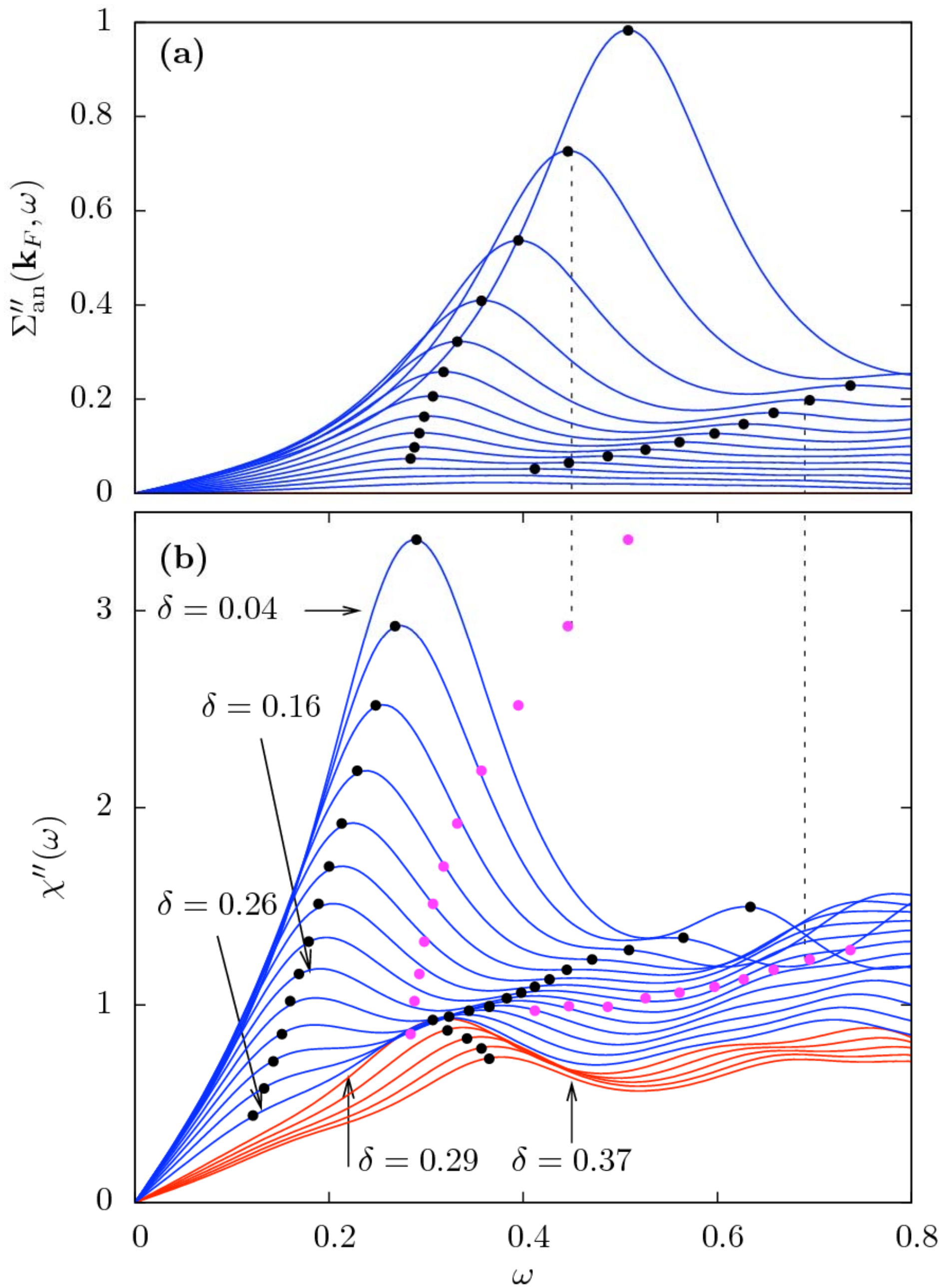


FIG. 3 (color online). **Q**-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for E_i = 140 meV, open for E_i = 80 meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO 1/8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

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