Strongly correlated superconductivity and quantum criticality

A.-M. Tremblay

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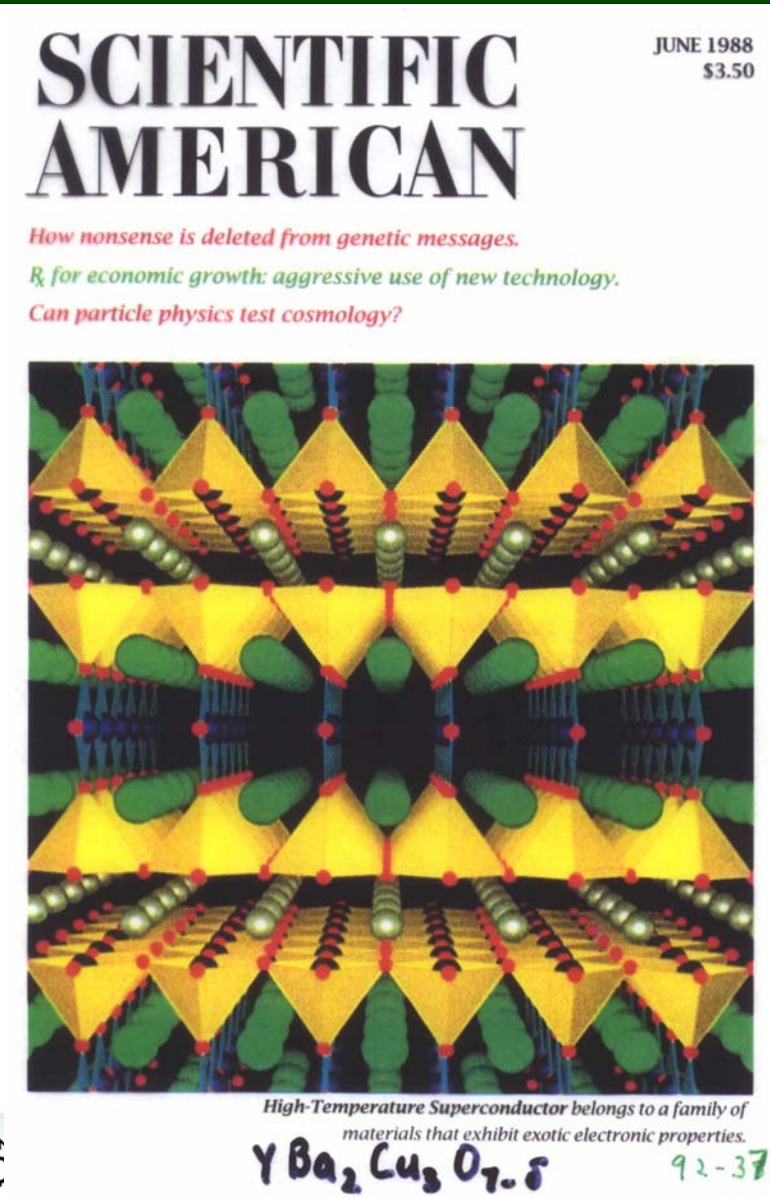
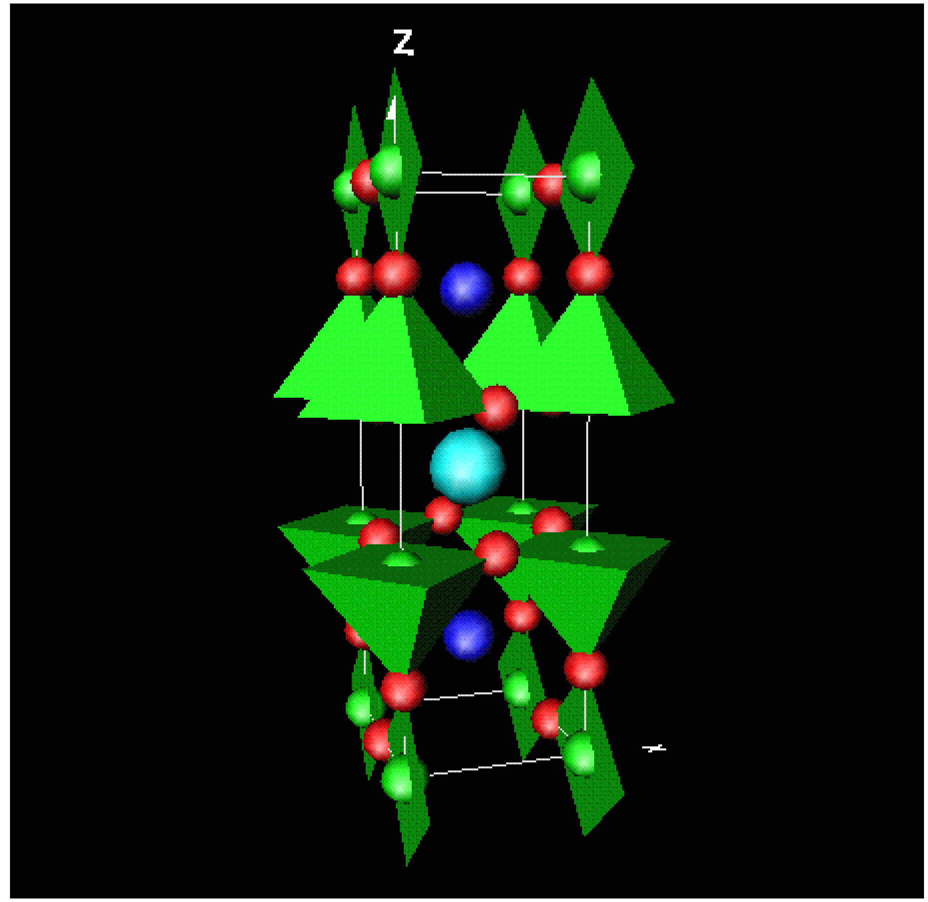
March Meeting of the American Physical Society
New Orleans - C23.00003

CIFAR
CANADIAN INSTITUTE for ADVANCED RESEARCH

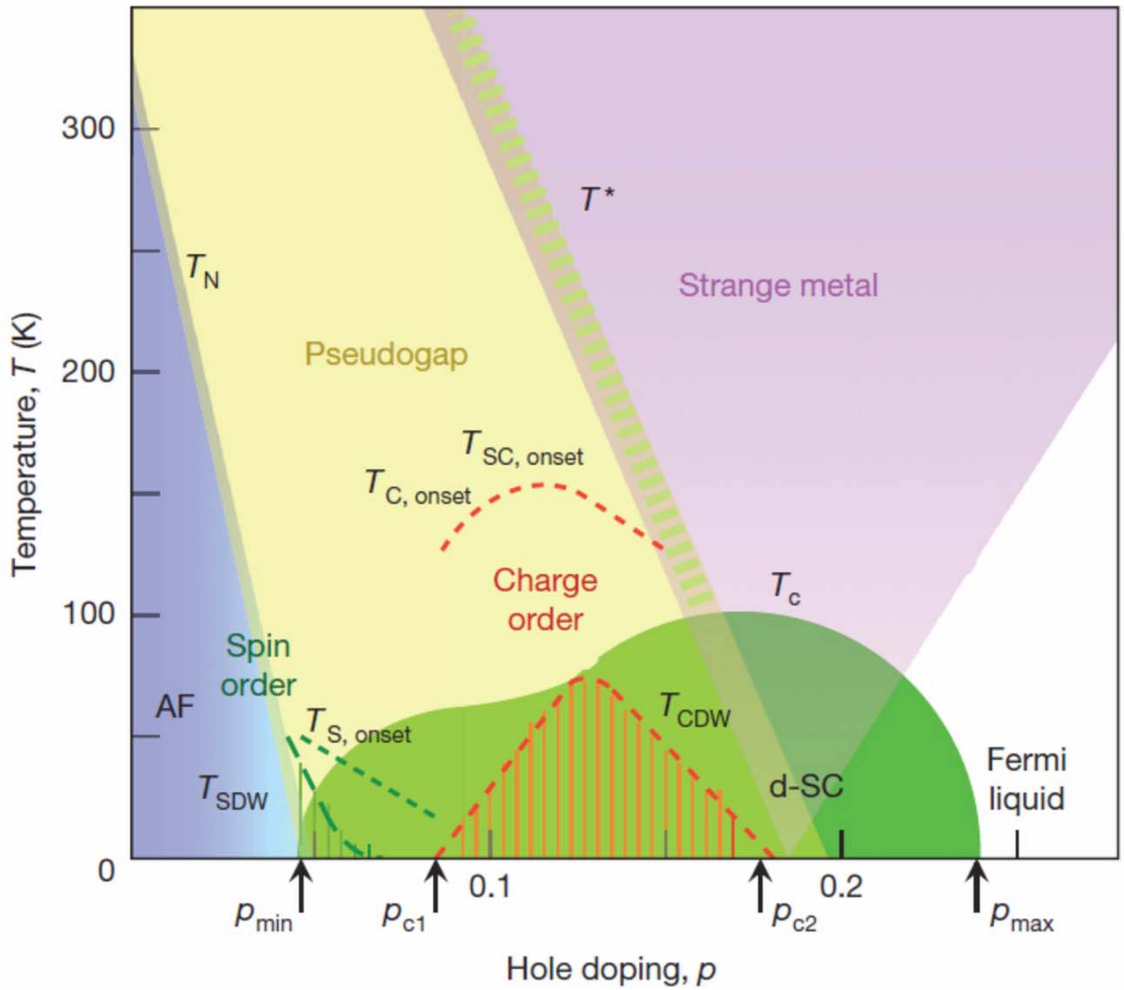
VERITATEM IN CHARITATE

Atomic structure





Phase diagram $YBa_2Cu_3O_{7-x}$



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

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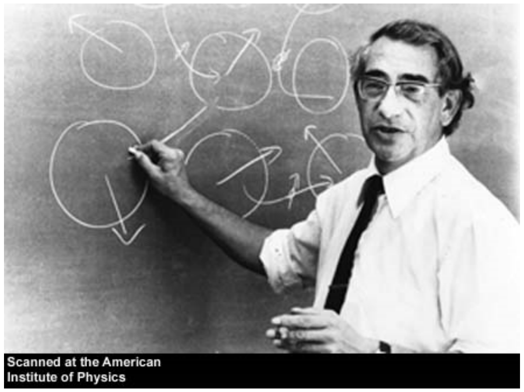
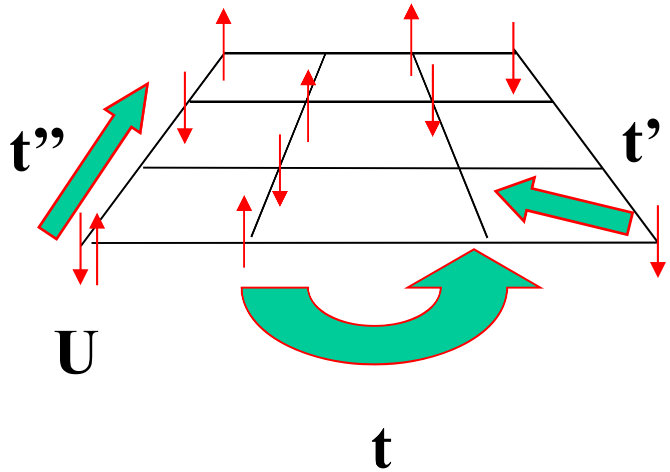
Hubbard model



1931-1980

μ



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

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

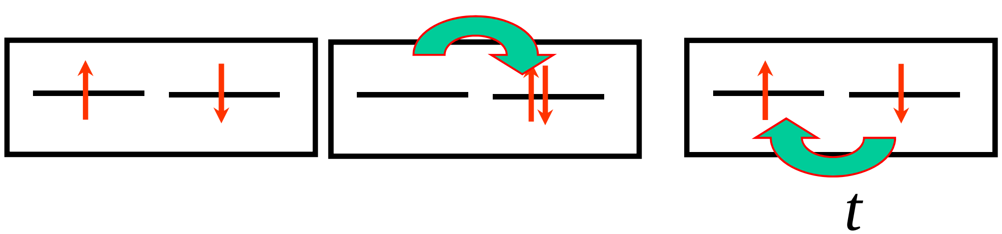
Attn: Charge transfer insulator

Interesting in the general case

No mean-field factorization for d-wave superconductivity

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

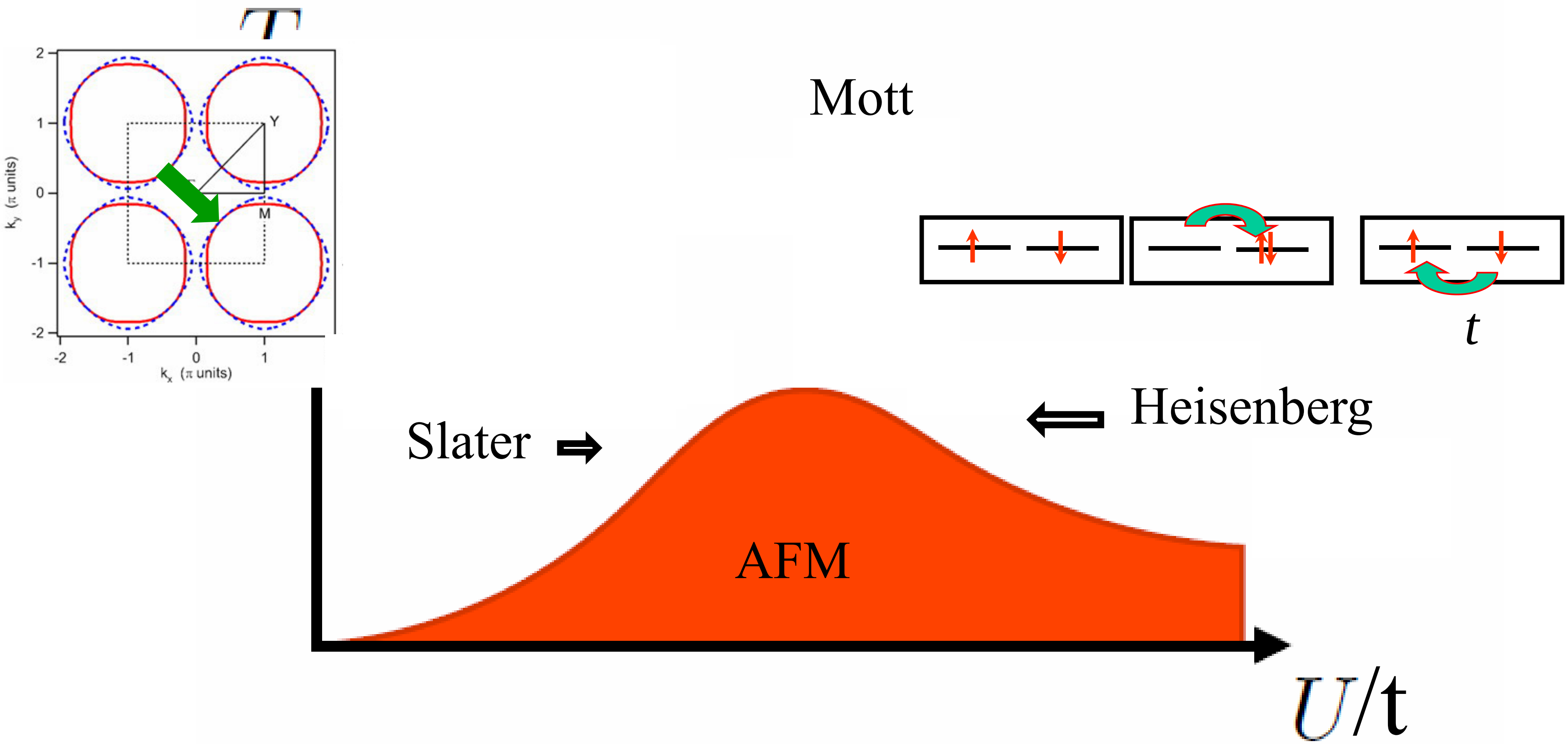
Interaction-induced metal-insulator (Mott) transition



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

Weak vs Strong correlations

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



2. Method for strongly correlated matter

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)

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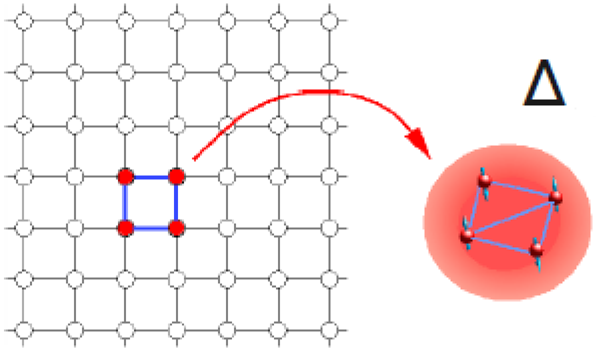
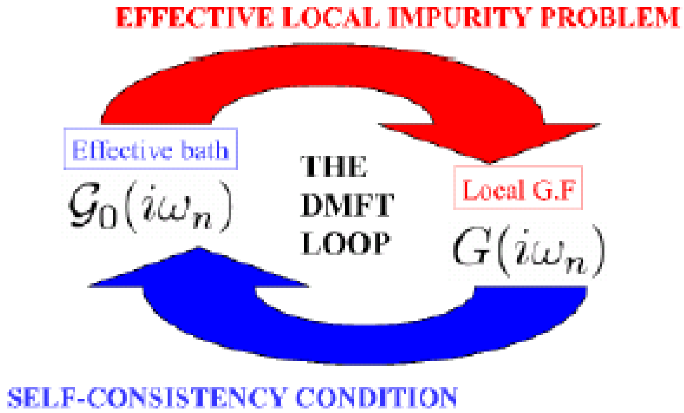
Method





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

+ 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

Some groups using these methods for cuprates

- Europe:
  - Georges, Parcollet, Ferrero, Civelli, (Paris)
  - 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

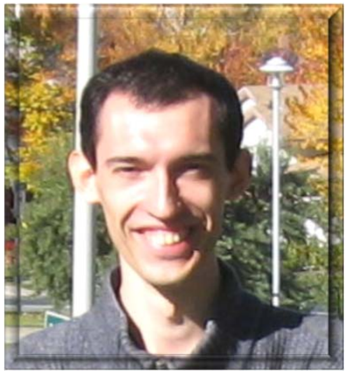
- The model
- The method

- Part I: Weakly and strongly correlated electrons

- Part II: Strongly correlated superconductivity
  - Cuprates
  - Organics

Part I

Weakly vs strongly correlated electrons
Normal and antiferromagnetic state



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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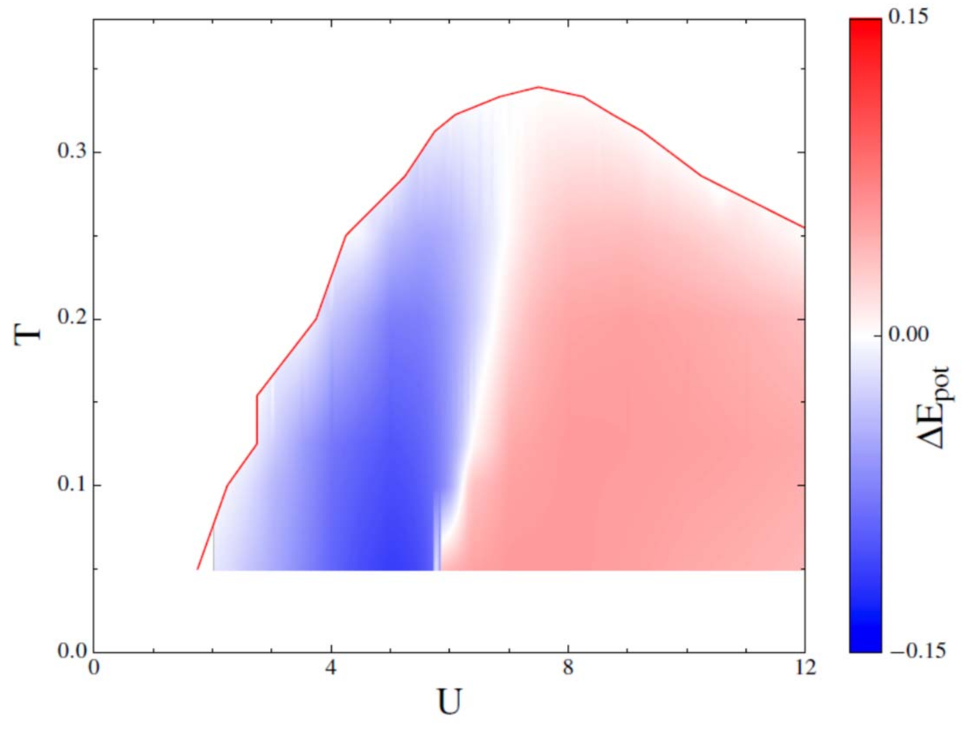
Change in potential energy due to large ξ



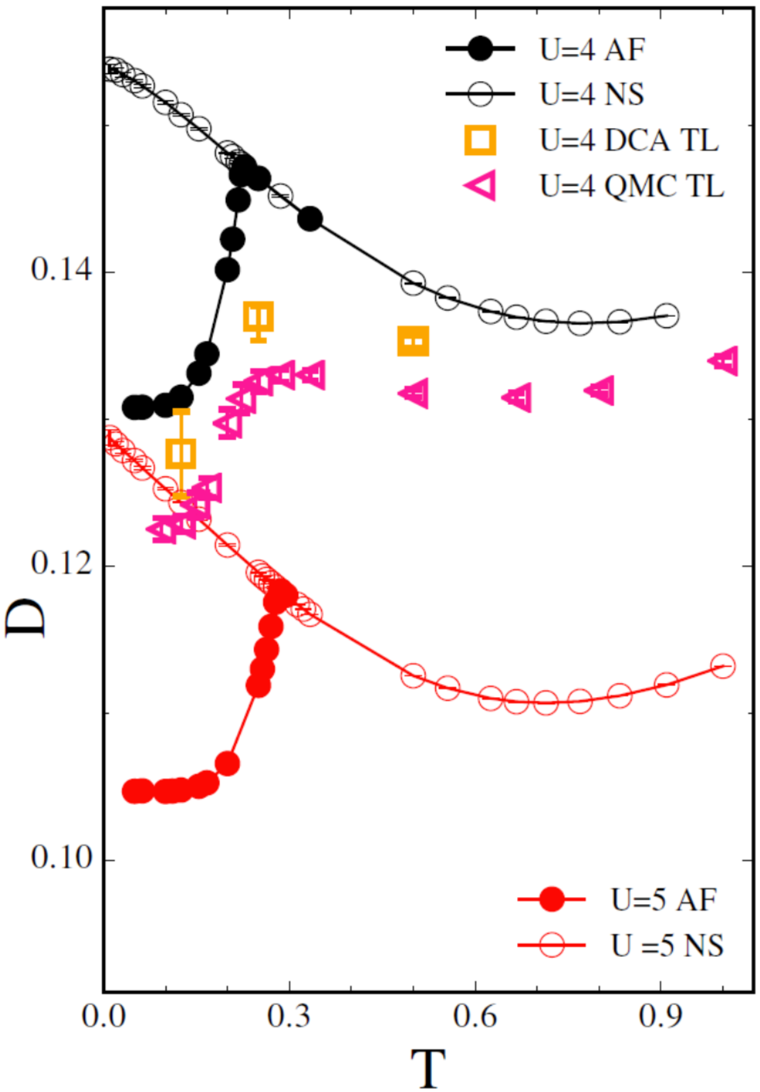
L. Fratino,[1] P. Sémon,[2] M. Charlebois,[2] G. Sordi,[1] and A.-M. S. Tremblay[2,3]

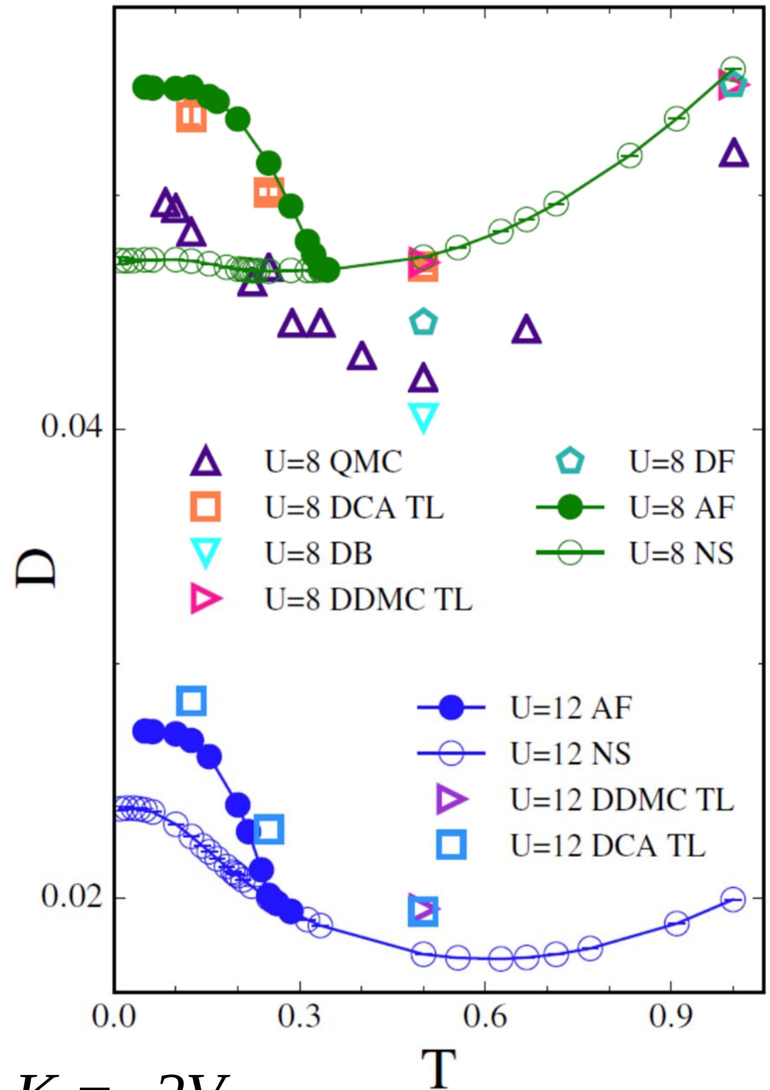
arXiv:1702.01821

L. Fratino: **Competing order in correlated electrons**

B37b.00007

Double occupancy at weak and strong interactions: benchmarks

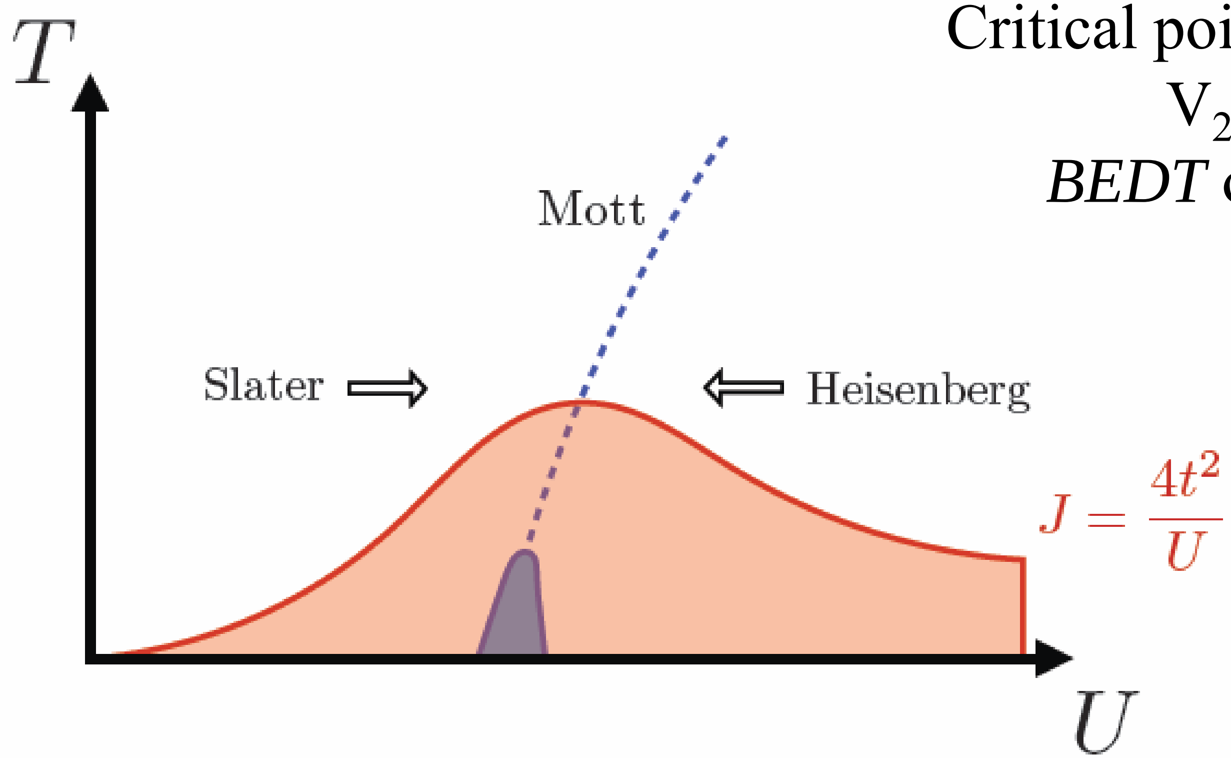




K = -2V

Underlying Mott transition

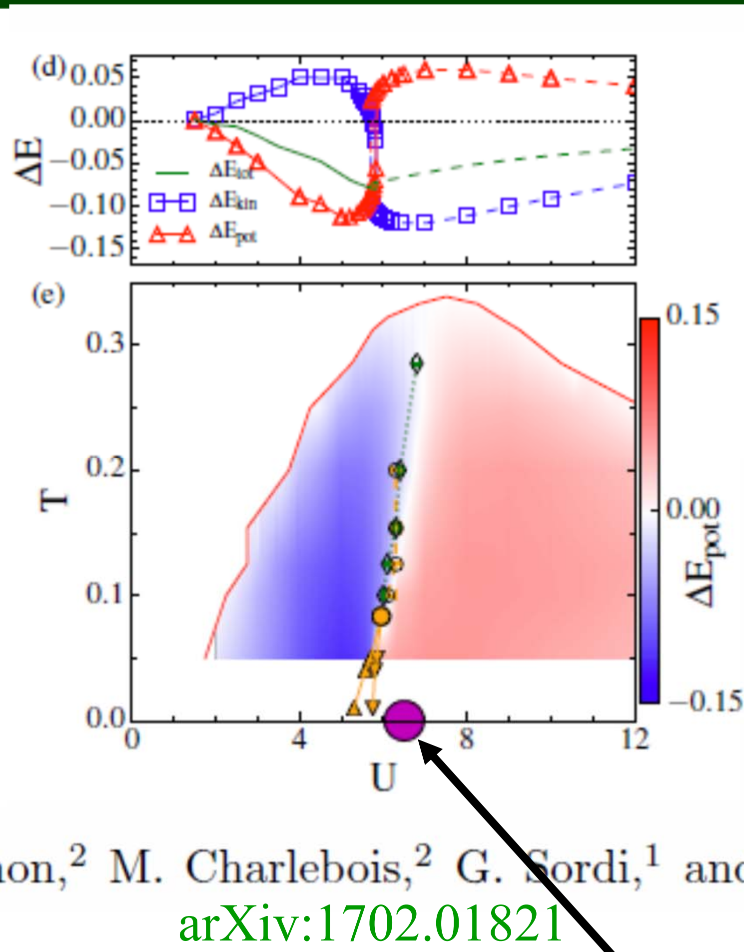
n = *1*, *d* = *2* square lattice



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

arXiv:1702.01821

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

Giovanni Sordi

Kristjan Haule

Influence of the Mott transition away from half-filling

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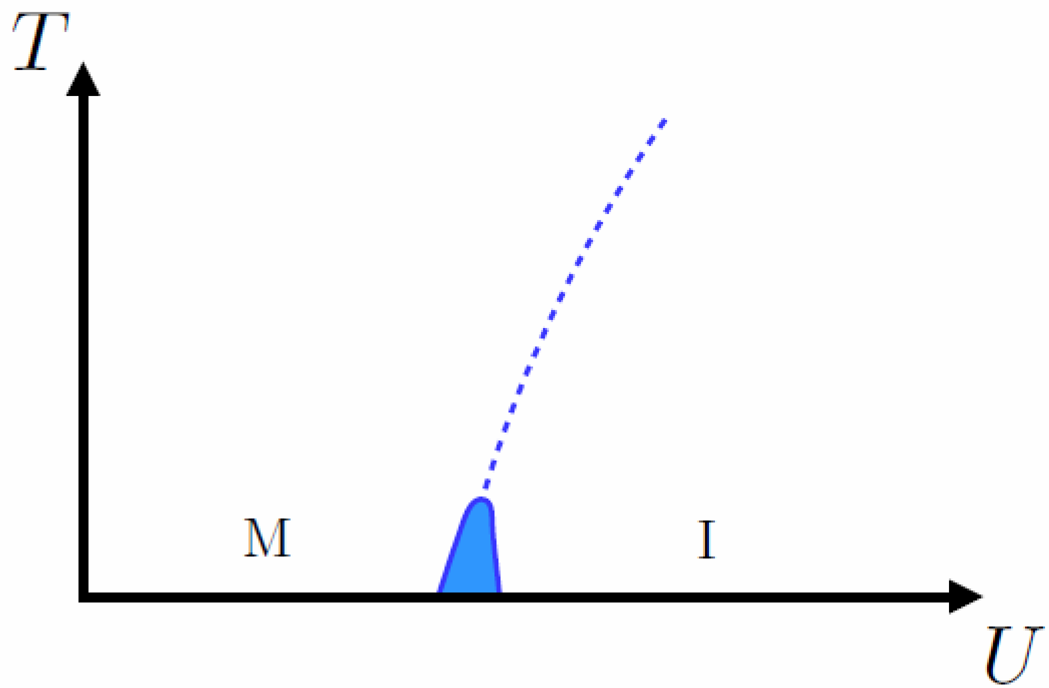
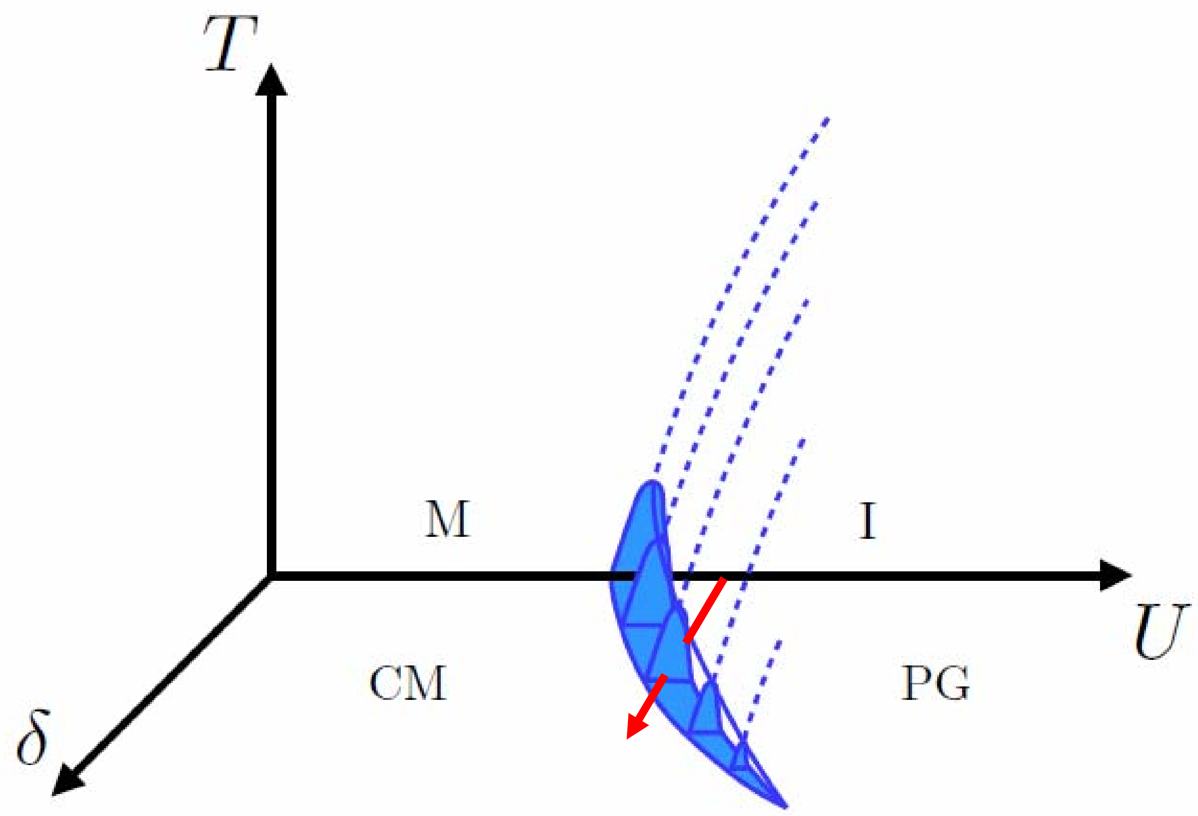
Influence of Mott transition away from half-filling

n = 1, d = 2 square lattice

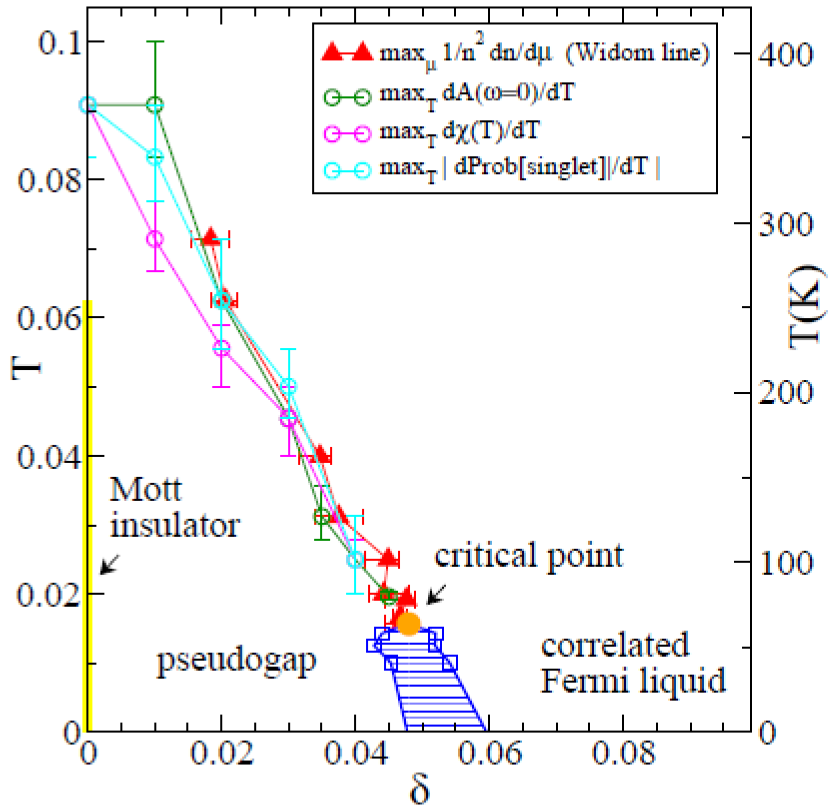


Influence of Mott transition away from half-filling

$n = 1, d = 2$ square lattice

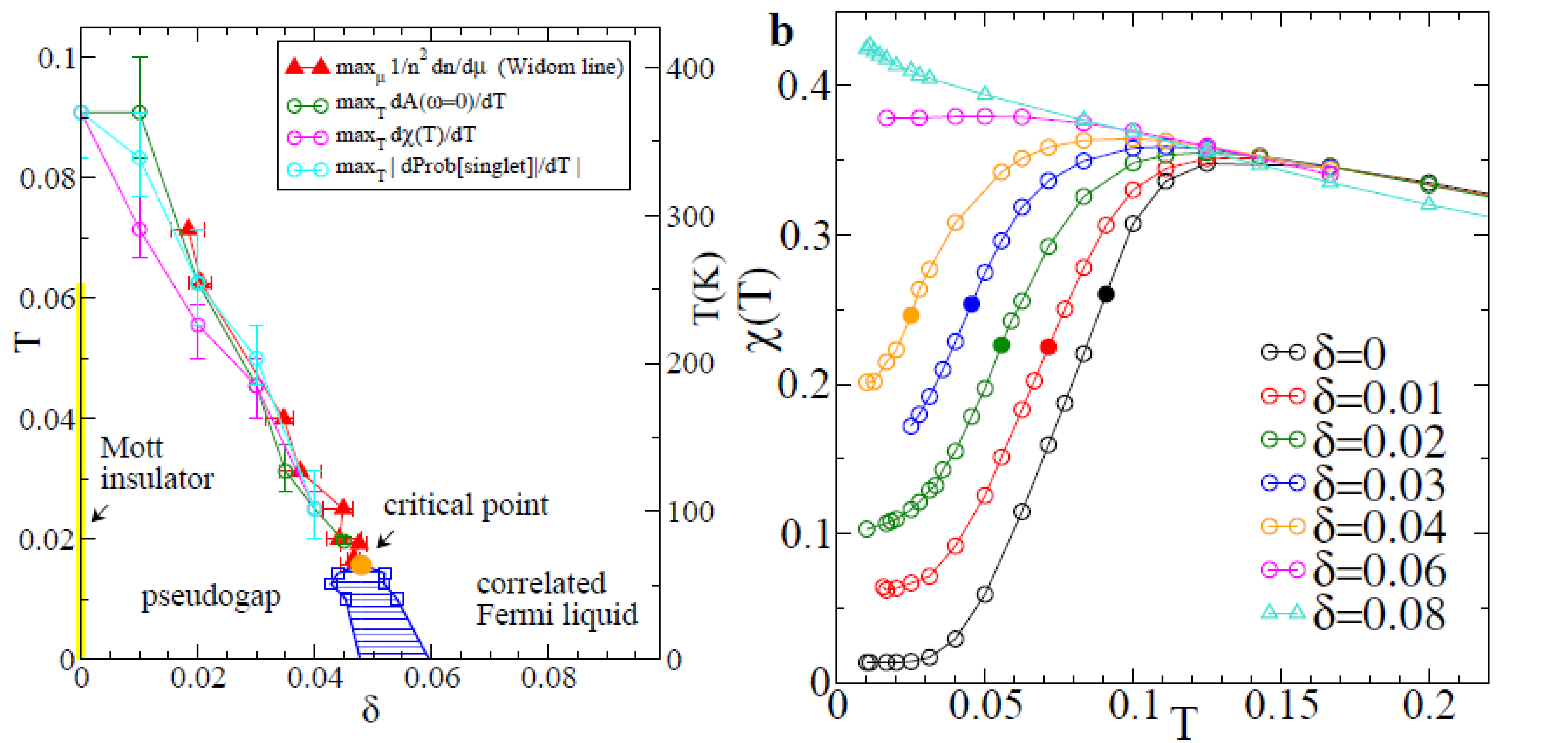


Spin susceptibility



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

Spin susceptibility



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

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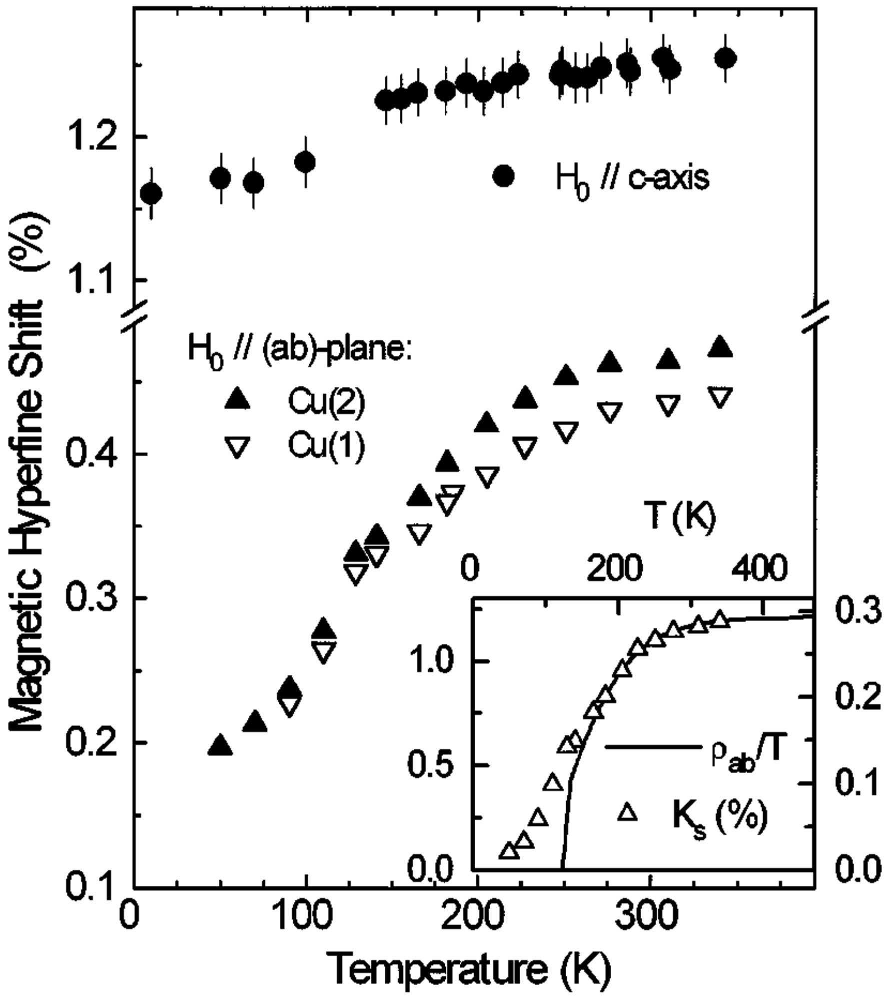
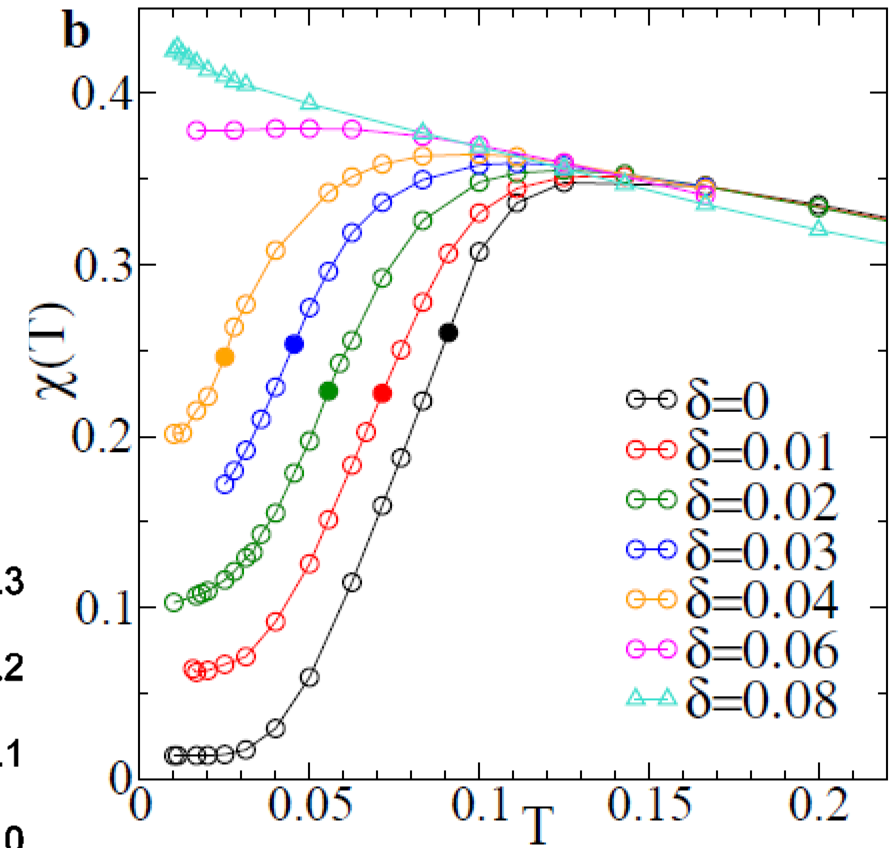
Spin susceptibility



Underdoped Hg1223

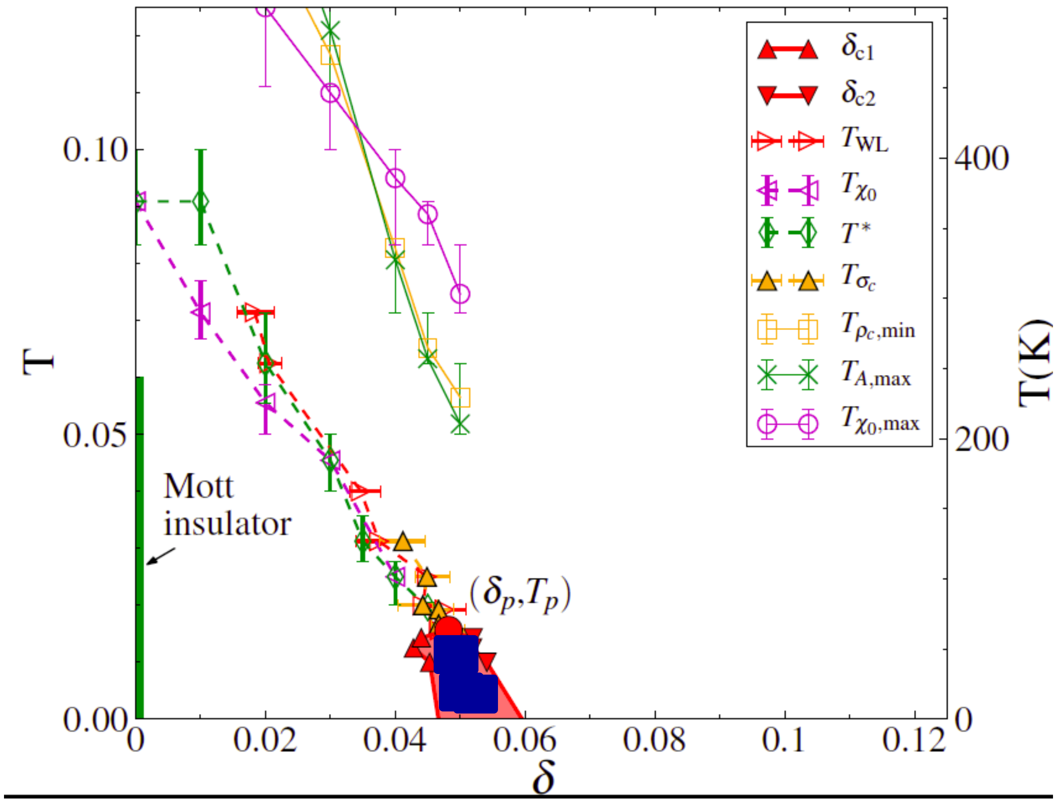
Julien et al. PRL **76,** 4238 (1996)



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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Physics

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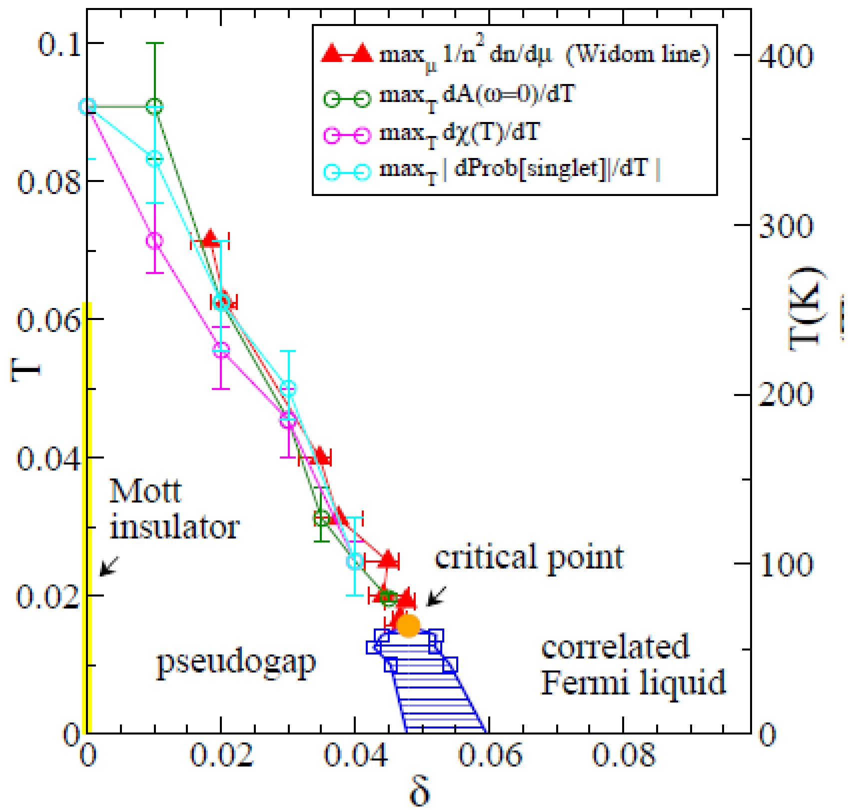
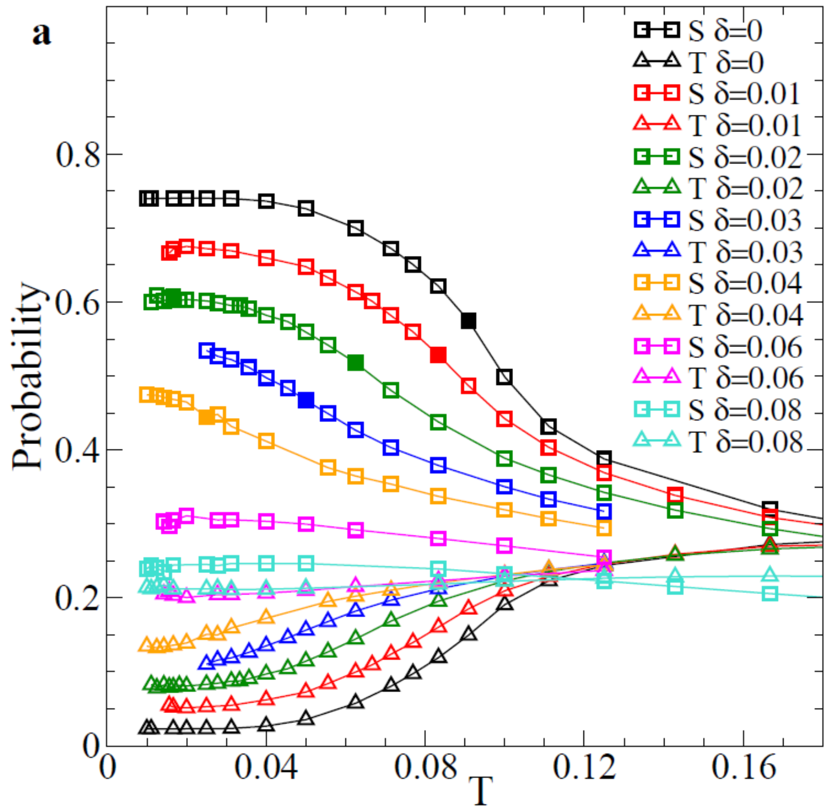
Plaquette eigenstates





See also:

Michel Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, A. Georges

PRB **80**, 064501 (2009)

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Patrick Sémon

Lorenzo Fratino

Part II

Strongly correlated Superconductivity

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

Fratino et al.

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

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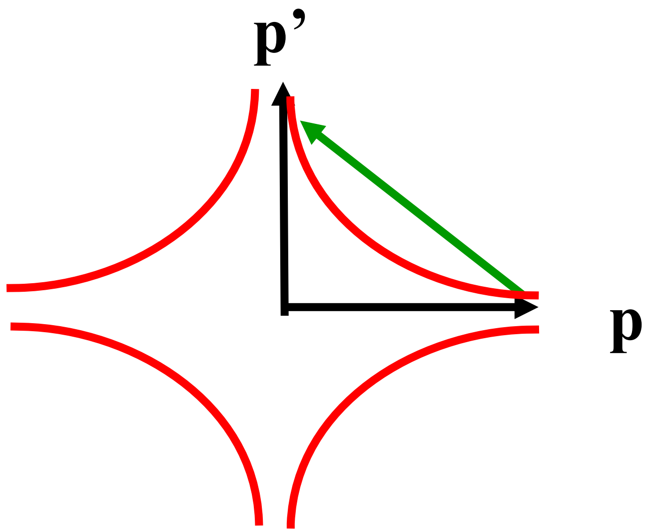
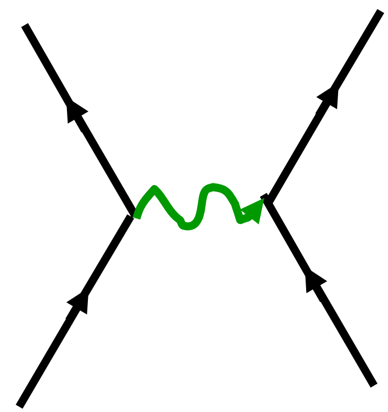
Cartoon « BCS » weak-correlation picture

$$\Delta_{\mathbf{p}} = -\frac{1}{2V}\sum_{\mathbf{p}'} U(\mathbf{p}-\mathbf{p}')\frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}}\left(1-2n\left(E_{\mathbf{p}'}\right)\right)$$





Exchange of spin waves?
Kohn-Luttinger
T_c with pressure

Béal–Monod, Bourbonnais, Emery
P.R. B. **34**, 7716 (1986).
D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch
P.R. B **34**, 8190-8192 (1986).
Kohn, Luttinger, P.R.L. **15**, 524 (1965).

P.W. Anderson Science 317, 1705 (2007)

A cartoon strong correlation picture

$$J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j = J\sum_{\langle i,j\rangle}\left(\frac{1}{2}c_i^\dagger\vec{\sigma}c_i\right)\cdot\left(\frac{1}{2}c_j^\dagger\vec{\sigma}c_j\right)$$

$$d = \langle\hat{d}\rangle = 1/N\sum_{\vec{k}}(\cos k_x - \cos k_y)\langle c_{\vec{k},\uparrow}c_{-\vec{k},\downarrow}\rangle$$

$$H_{MF} = \sum_{\vec{k},\sigma}\varepsilon(\vec{k})c^\dagger_{\vec{k},\sigma}c_{\vec{k},\sigma} - 4Jm\hat{m} - Jd(\hat{d}+\hat{d}^\dagger) + F_0$$

Pitaevskii Brückner:

Pair state orthogonal to repulsive core of Coulomb interaction

P.W. Anderson Science 317, 1705 (2007)

Miyake, Schmitt–Rink, and Varma P.R. B **34**, 6554-6556 (1986)

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More sophisticated Slave Boson: Kotliar Liu PRB 1988

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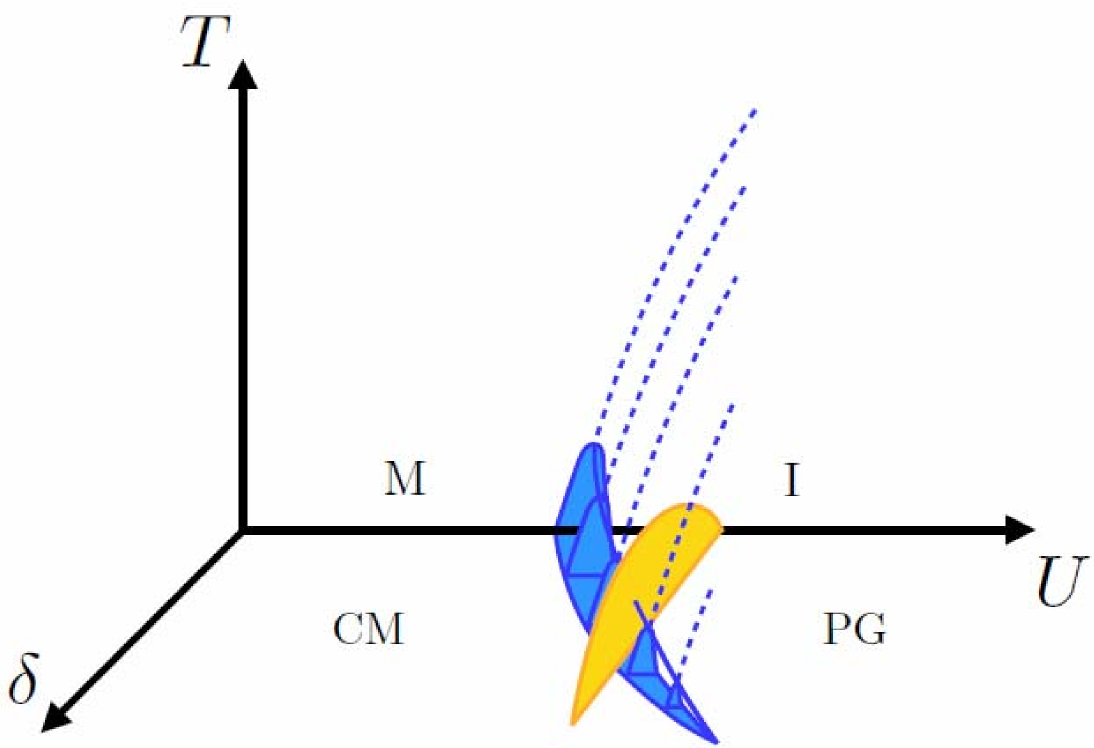
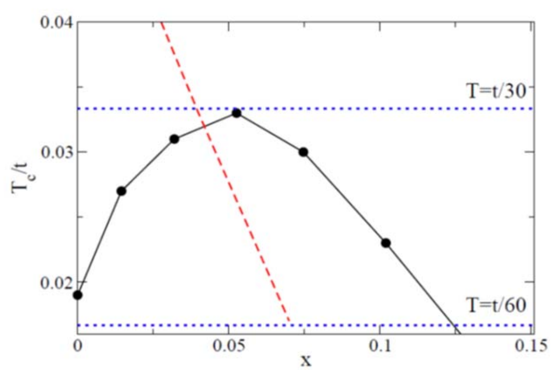
Superconductiviy in Doped Mott insulator

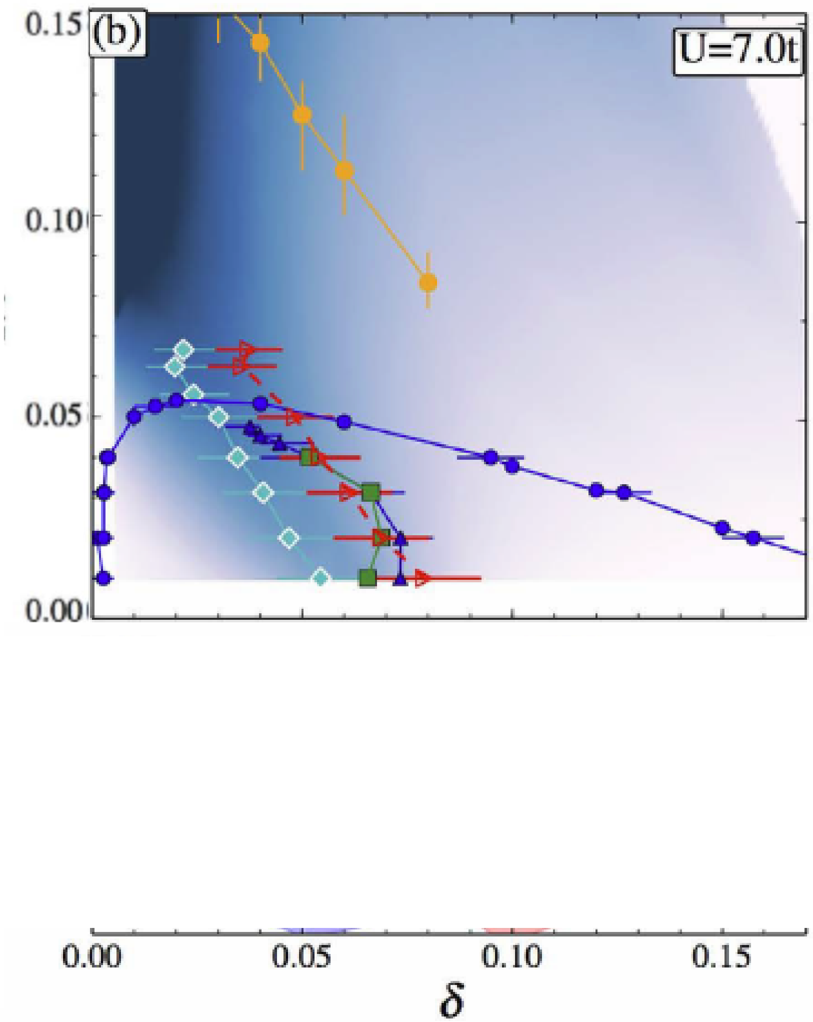
$n = 1, d = 2$ square lattice



An organizing principle



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



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

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

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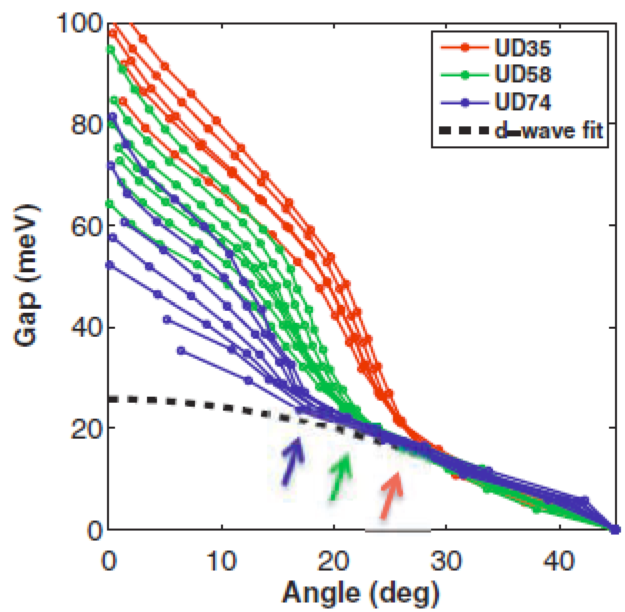
Meaning of T_c^d : Local pair formation



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

However, our measurements demonstrate that the nodal gap does not change with reduced doping. The pairing strength does not get weaker or stronger as the Mott insulator is approached; rather, it saturates.

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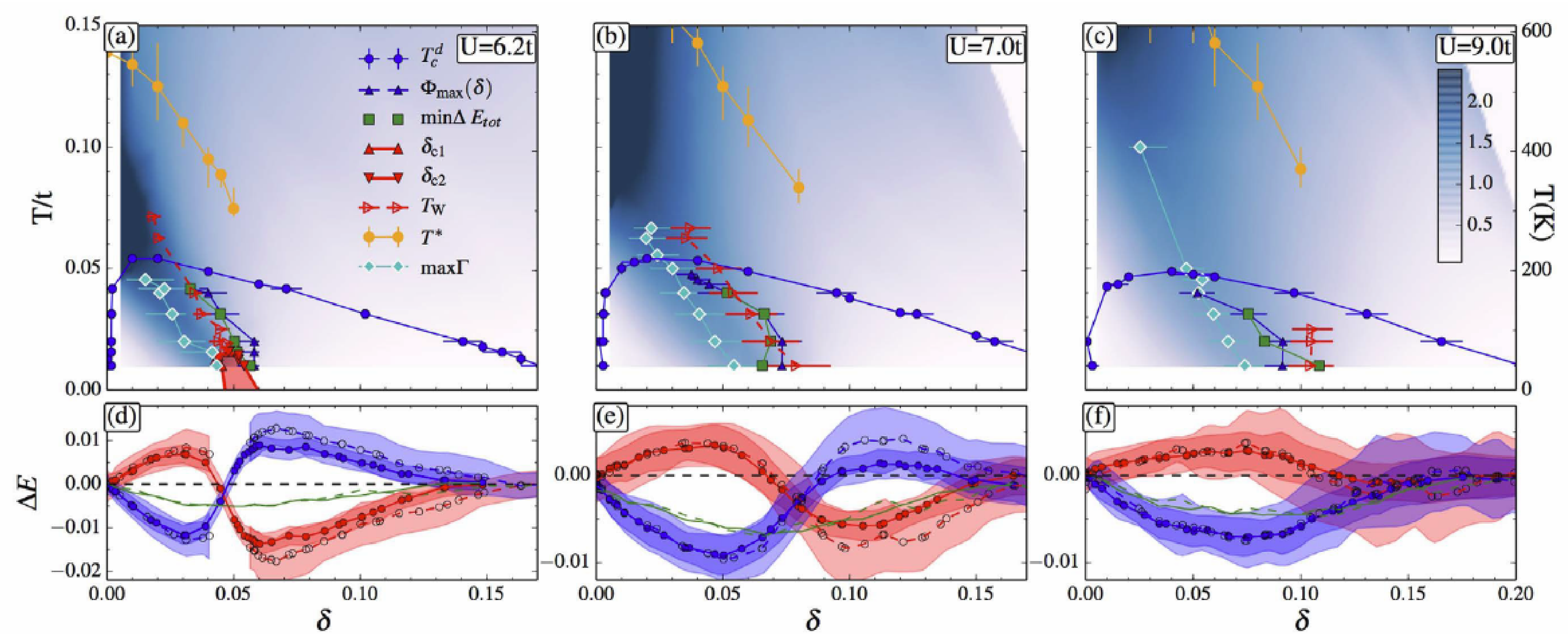
An organizing principle



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

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h-doped as charge-transfer insulator

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3 bands, charge transfer insulator

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

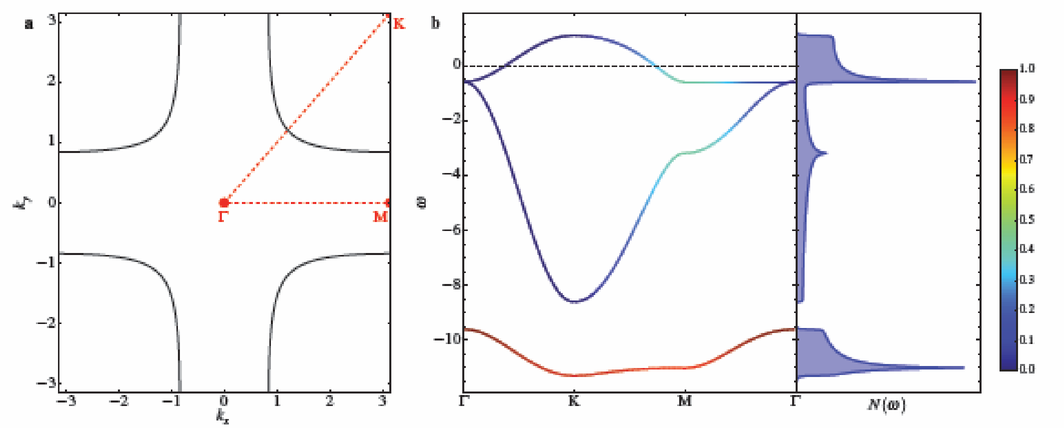
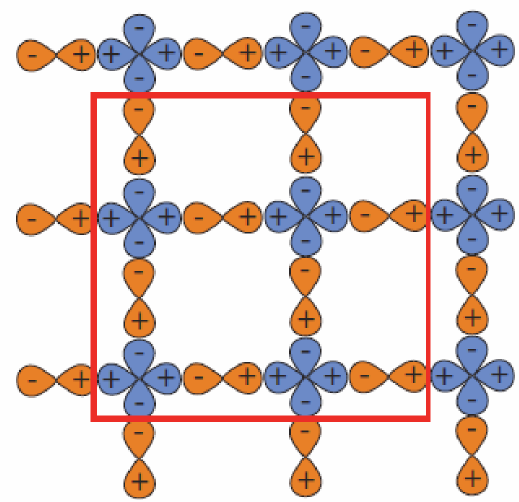
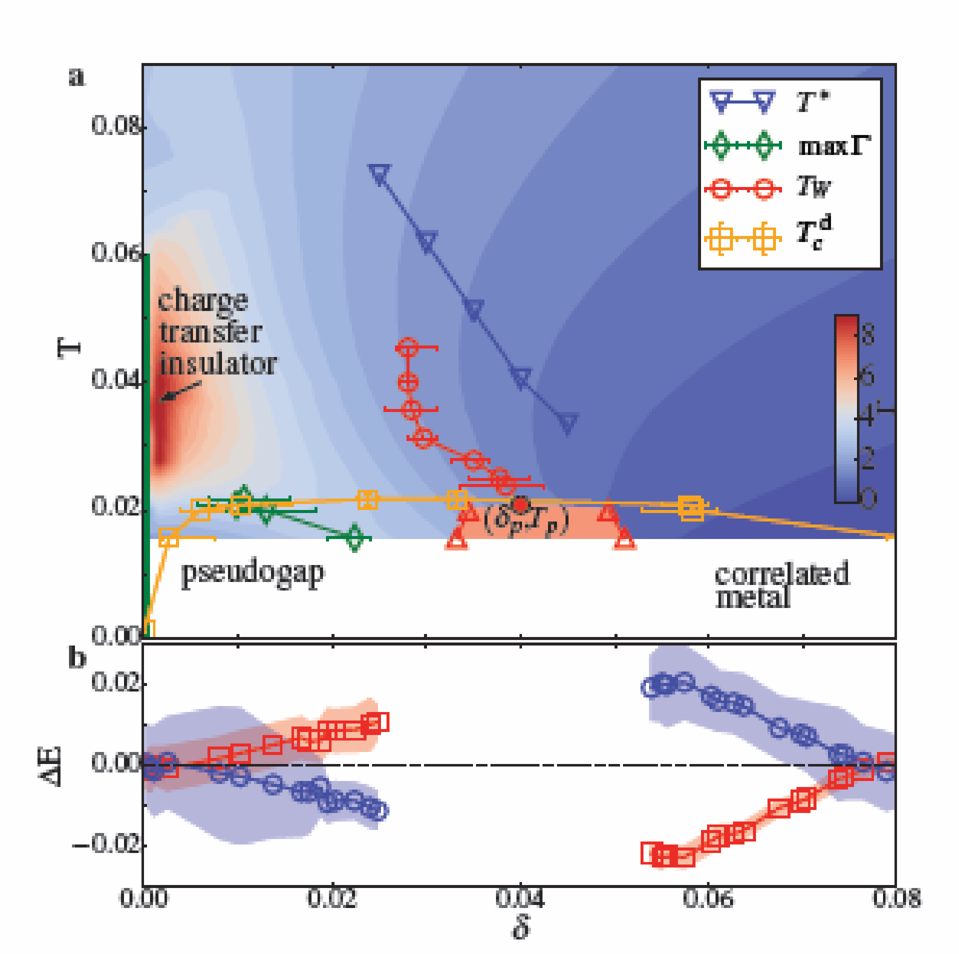


FIG. 2. (a) Noninteracting Fermi surface for the model parameter investigated in Fig. 1a of main text, namely $\epsilon_p = 9$, $t_{pp} = 1$, $t_{pd} = 1.5$, which gives a total occupation n_{tot} equal to five. (b) Non-interacting band structure for the same model parameter along with the resulting total density of states. Color corresponds to the d-character of the hybridised bands. The band crossing the Fermi level has mostly oxygen character.



No interaction on oxygen

3 bands, charge transfer insulator



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

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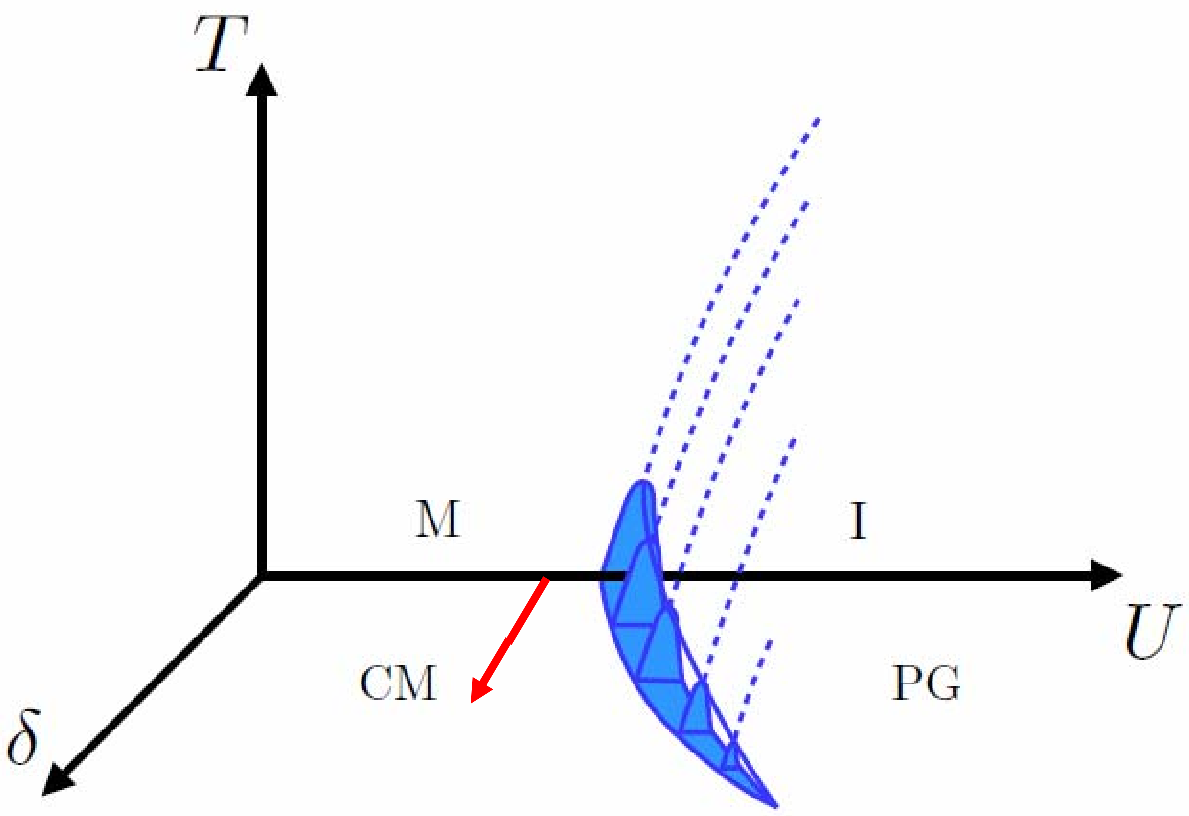
Other materials

e-doped cuprates

Influence of Mott transition away from half-filling

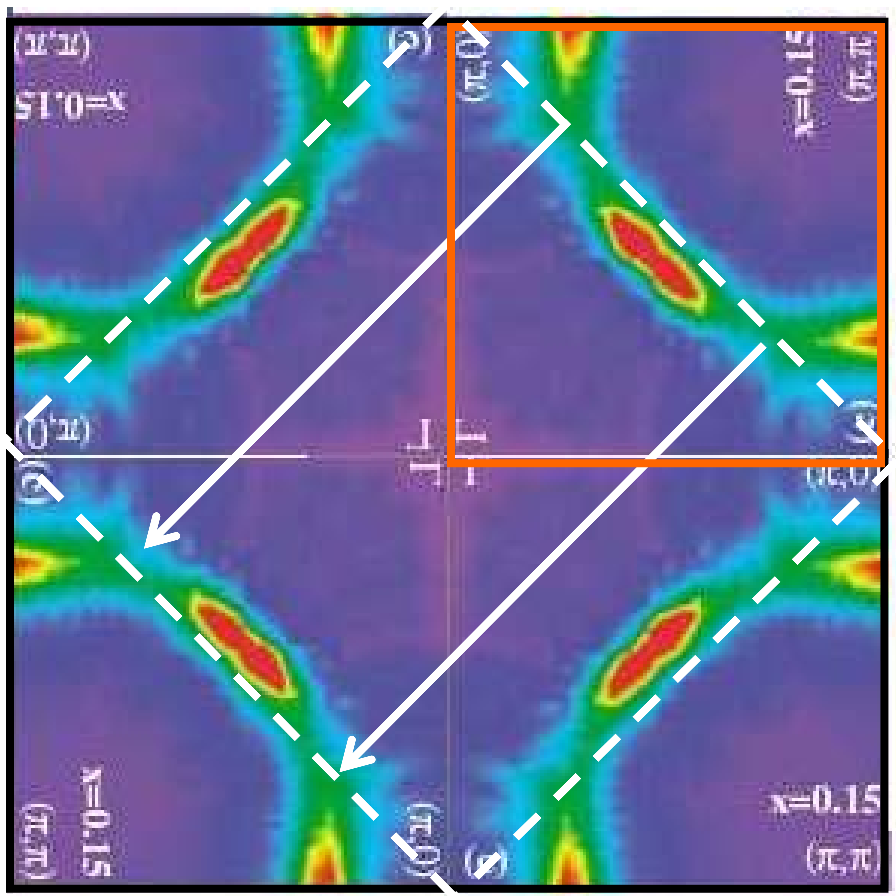
$n = 1, d = 2$ square lattice



Hot spots from AFM quasi-static scattering

Mermin-Wagner

$d = 2$



Vilk, A.-M.S.T (1997)
Kyung, Hankevych, A.-M.S.T., PRL, 2004

Armitage et al. PRL 2001

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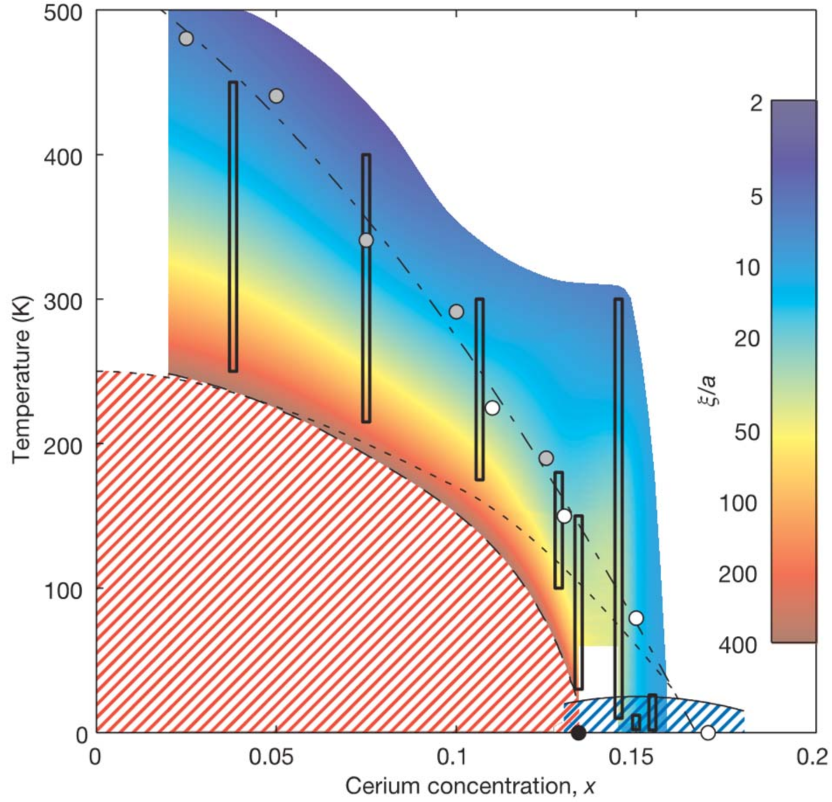
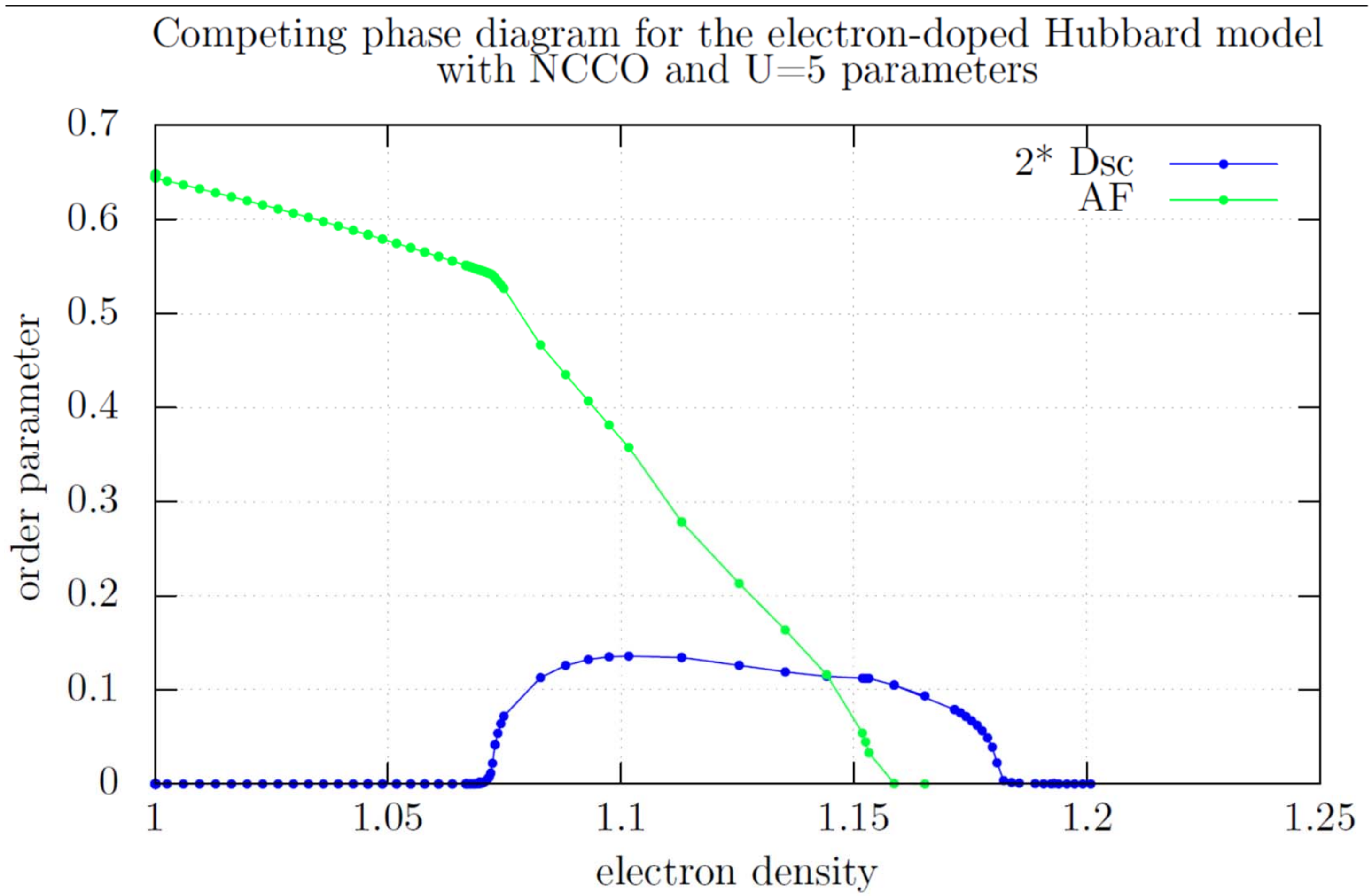
e-doped pseudogap

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



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

e-doped: Ground State AFM-QCP and dSC



A. Foley and D. Sénéchal, unpublished

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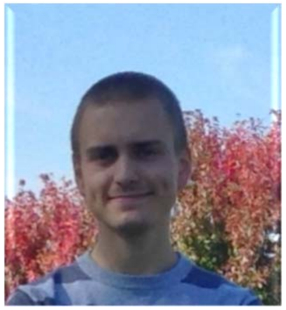

Charles-David Hébert

Patrick Sémon

Organics : Phase diagram, finite T

Made possible by algorithmic improvements

P. Sémon *et al.*
PRB **85**, 201101(R) (2012)
PRB **90** 075149 (2014);
and PRB **89**, 165113 (2014)

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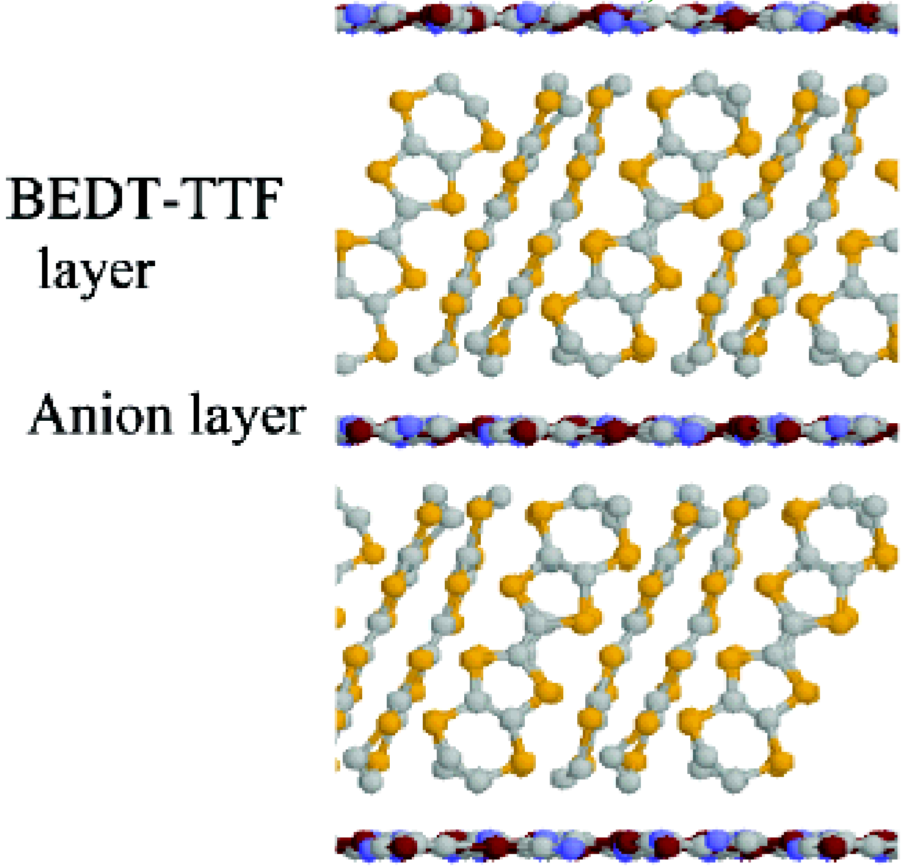
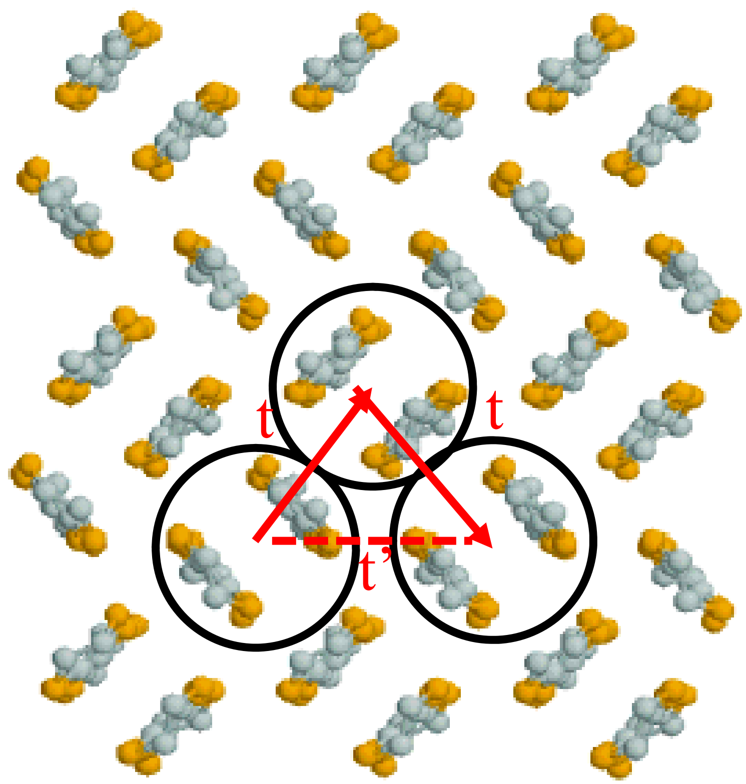
Layered organics (κ–BEDT-X family)

H. Kino + H. Fukuyama, J. Phys. Soc. Jpn **65** 2158 (1996),
R.H. McKenzie, Comments Condens Mat Phys. **18**, 309 (1998)





$t \approx 50\,\mathrm{meV}$

$\Rightarrow U \approx 400\,\mathrm{meV}$

$t'/t \sim 0.6 - 1.1$

Y. Shimizu, et al. Phys. Rev. Lett. **91**, 107001(2003)

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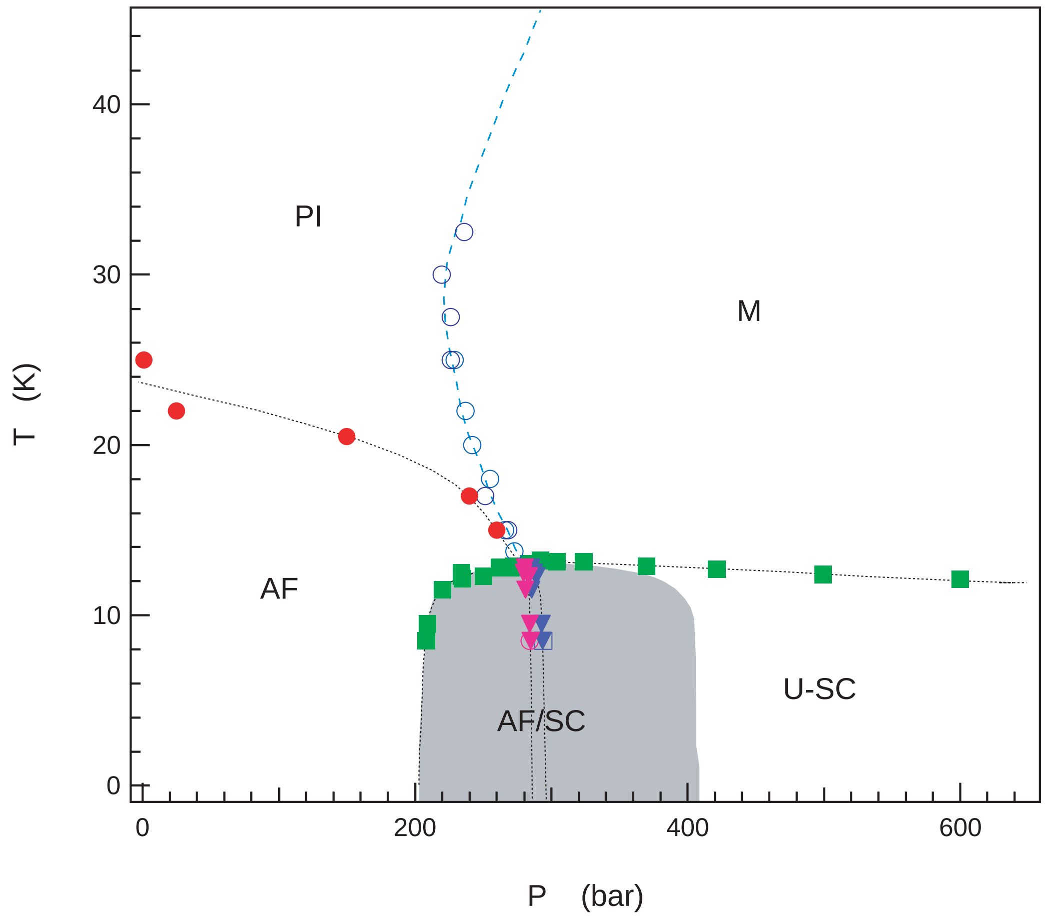
Phase diagram for organics

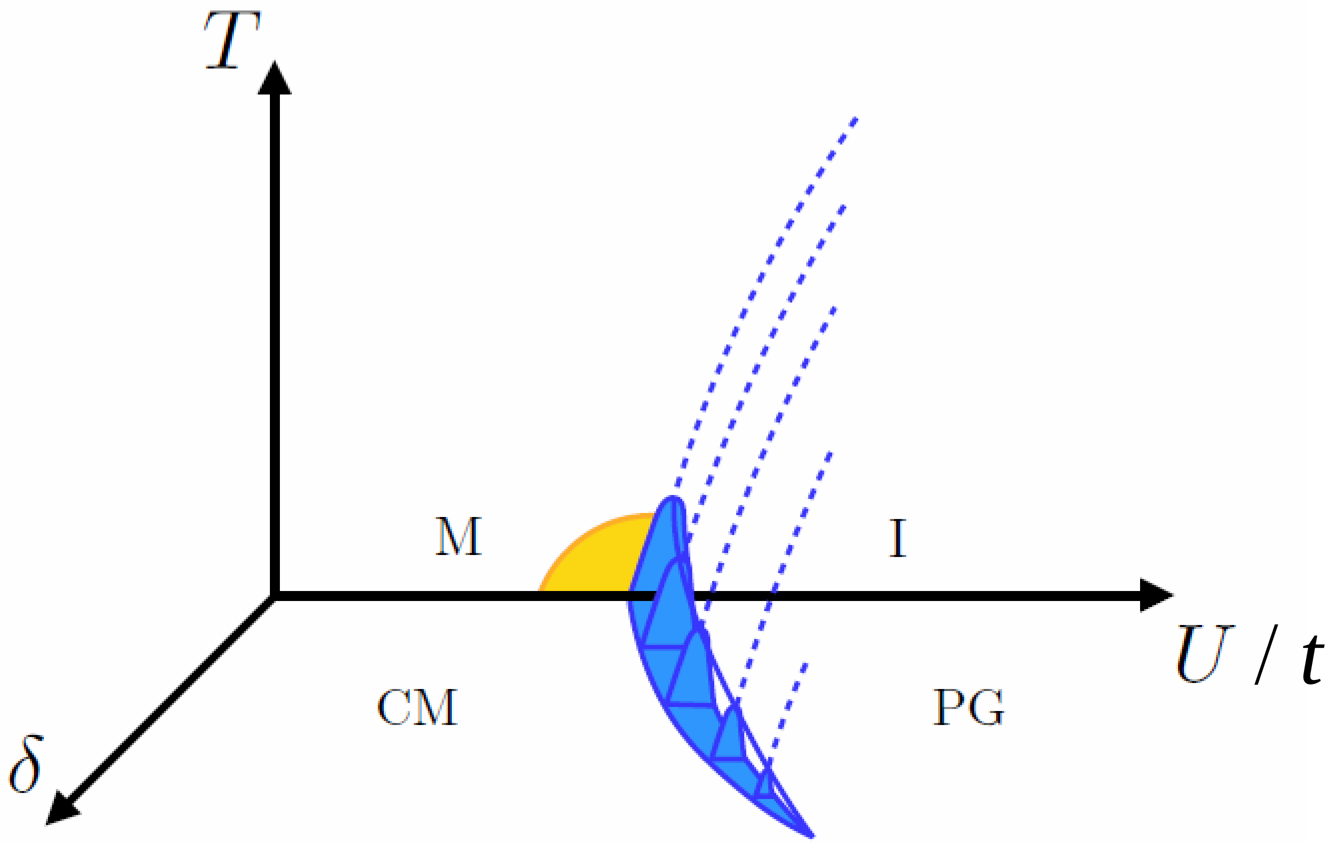


Phase diagram (X=Cu[N(CN)$_2$]Cl)

S. Lefebvre et al. PRL **85**, 5420 (2000), P. Limelette, et al. PRL 91 (2003)

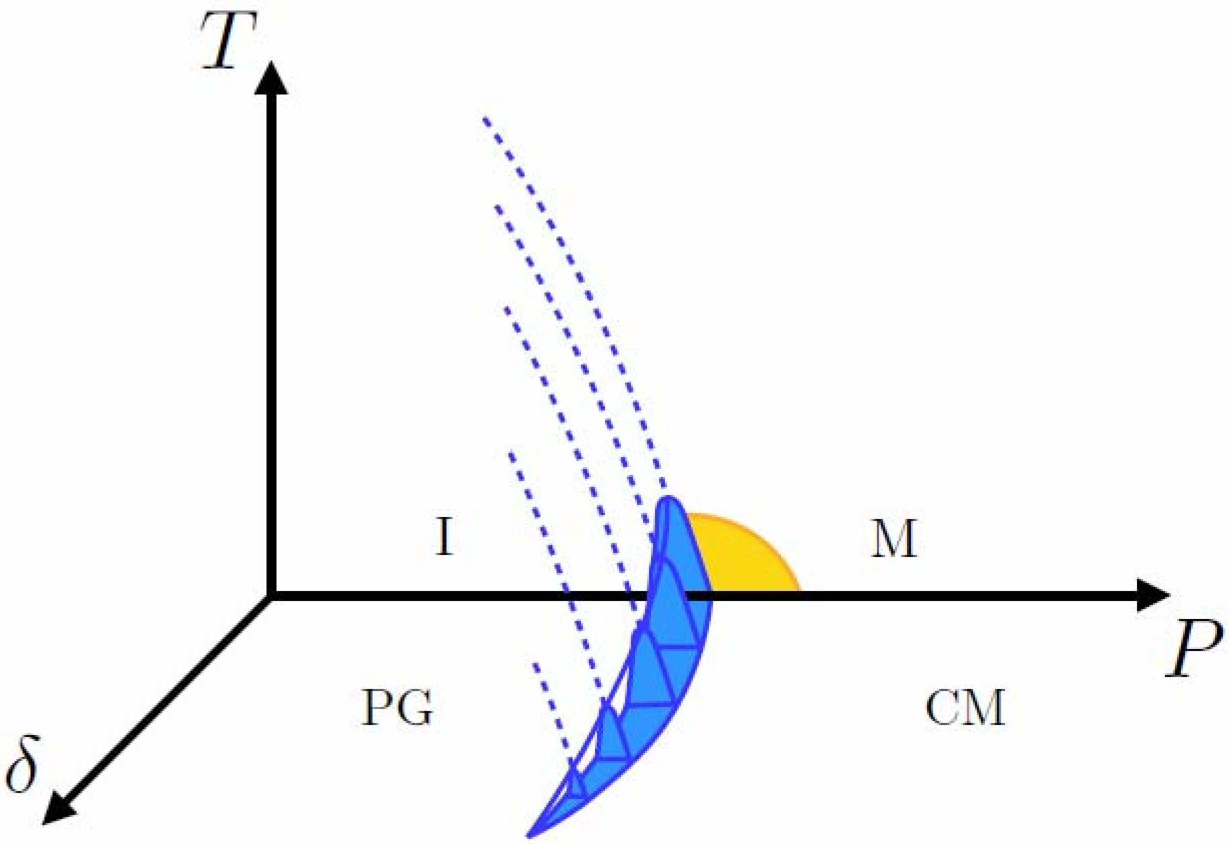
Superconductivity near the Mott transition

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



Superconductivity near the Mott transition

$n = 1, d = 2$ square lattice



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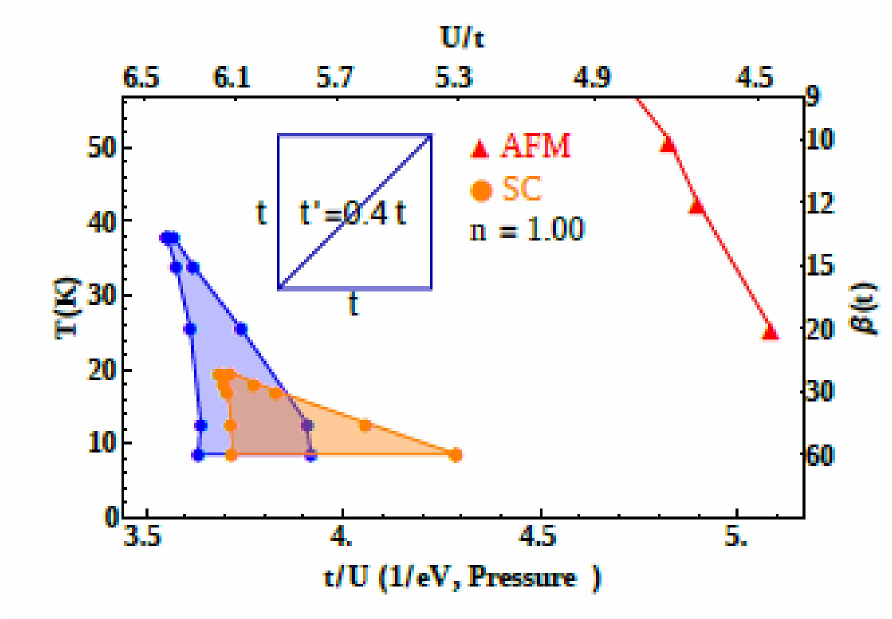
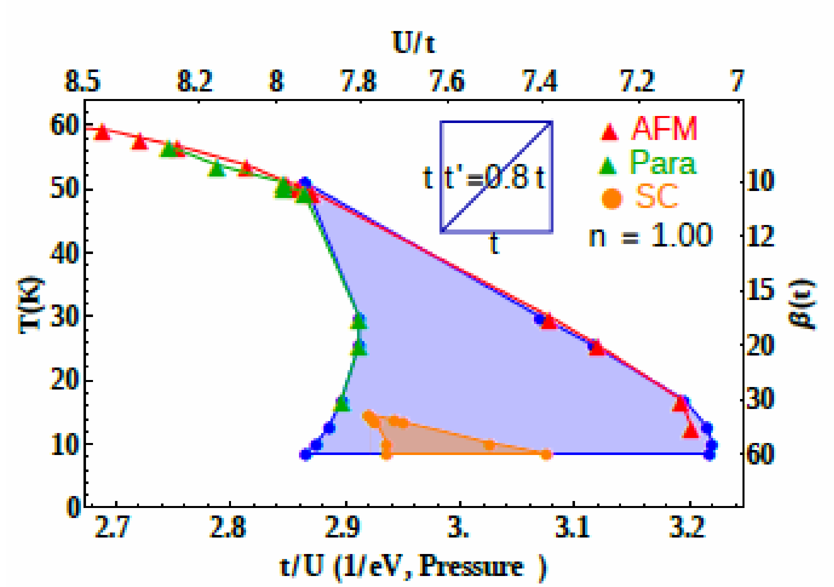
Superconductivity near Mott transition (*n* = *1*)



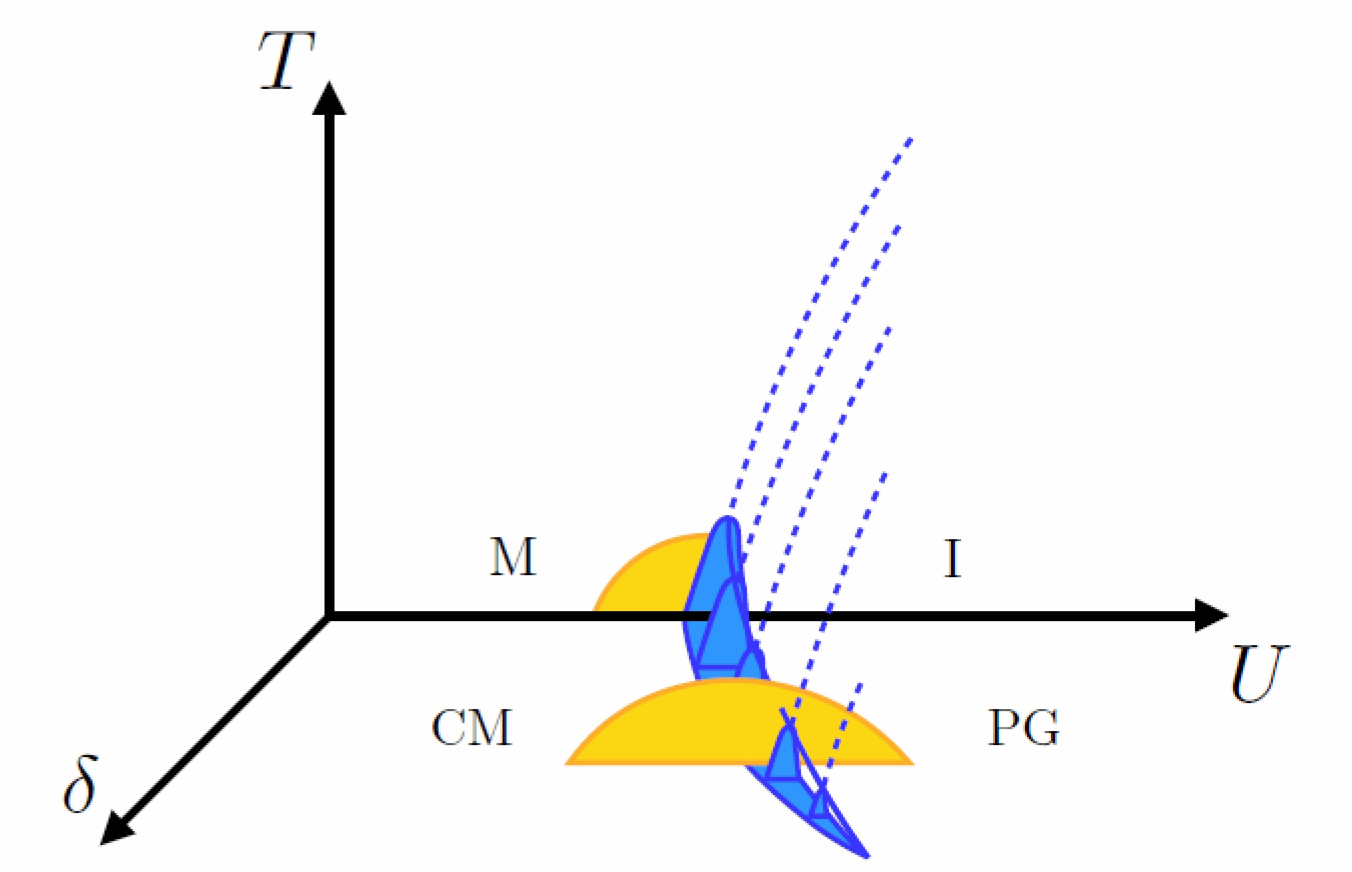


C.-D. Hébert, P. Sémon, A.-M.S. T PRB **92**, 195112 (2015)

Doped Organics

Doped organics

n = 1, d = 2 square lattice



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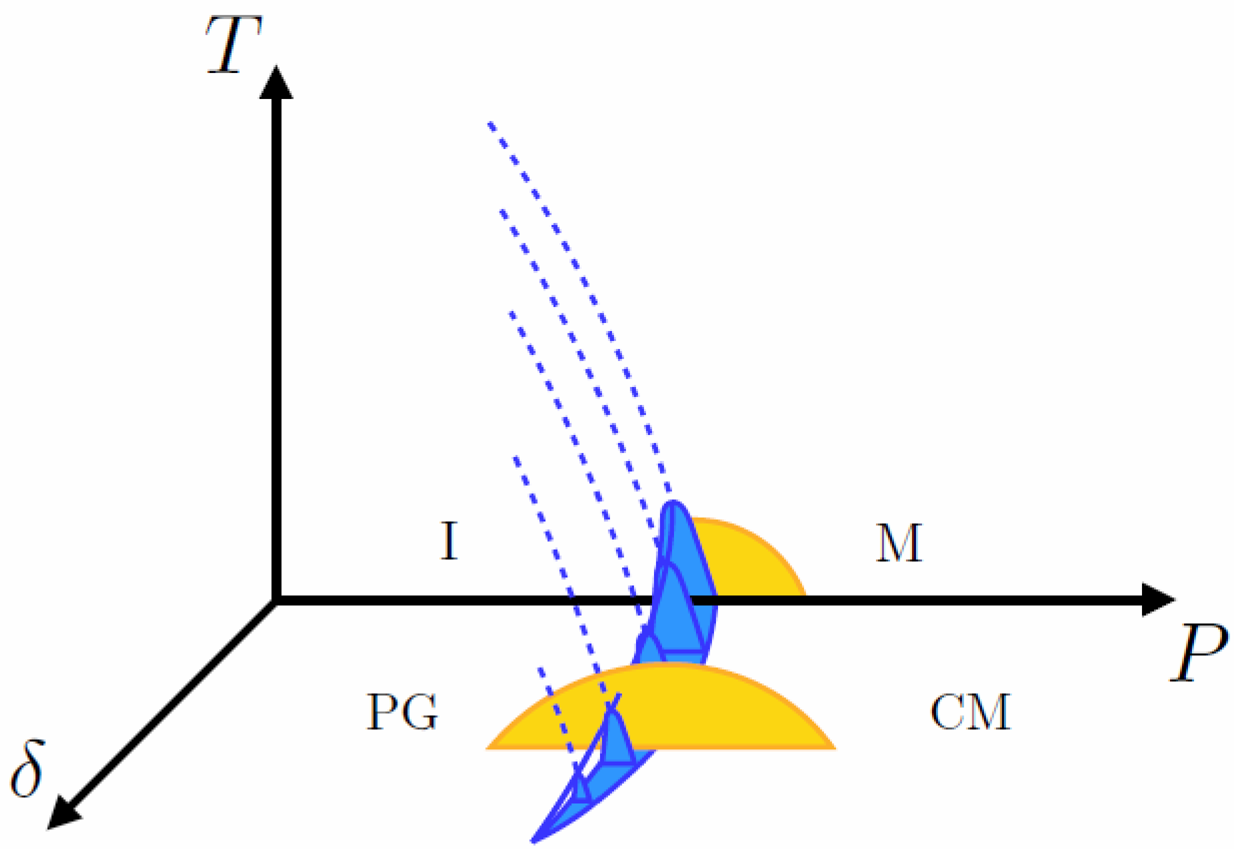
Doped organics

n = 1, d = 2 square lattice



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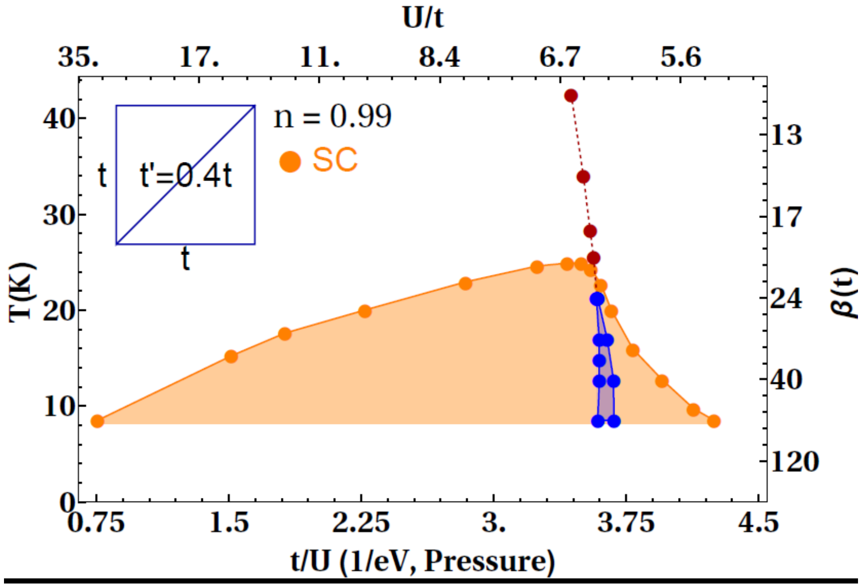
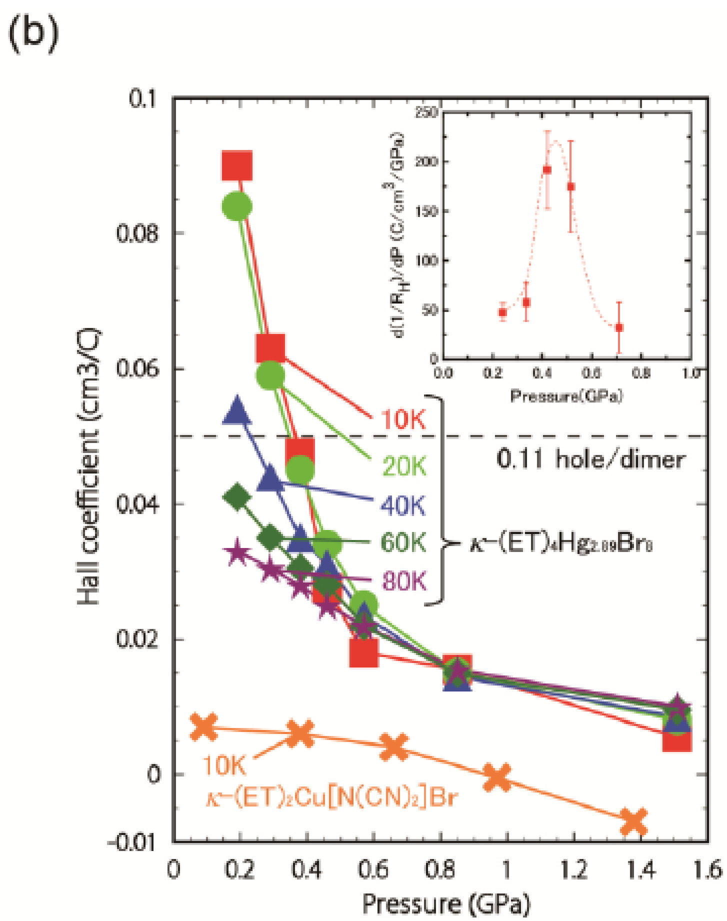
First order and Widom line in organics

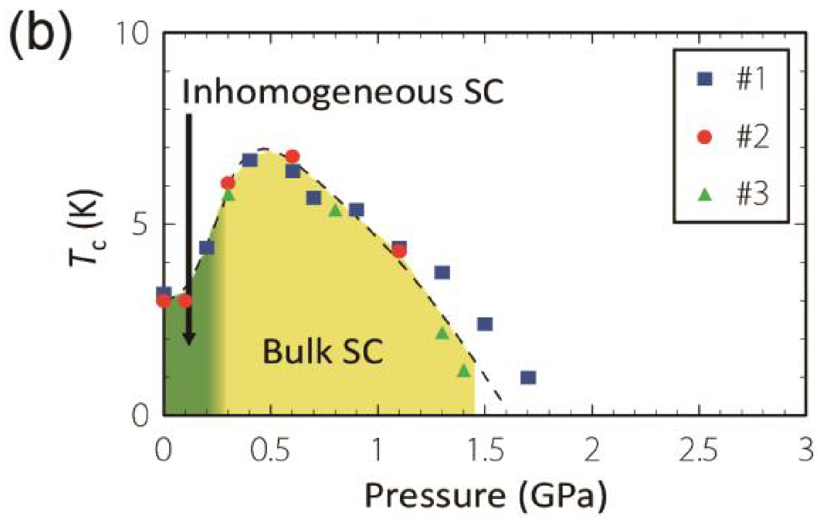


Compare: T. Watanabe, H. Yokoyama and M. Ogata JPS Conf. Proc. **3**, 013004 (2014)

C.-D. Hébert, P. Sémon, A.-M.S. T PRB **92**, 195112 (2015)

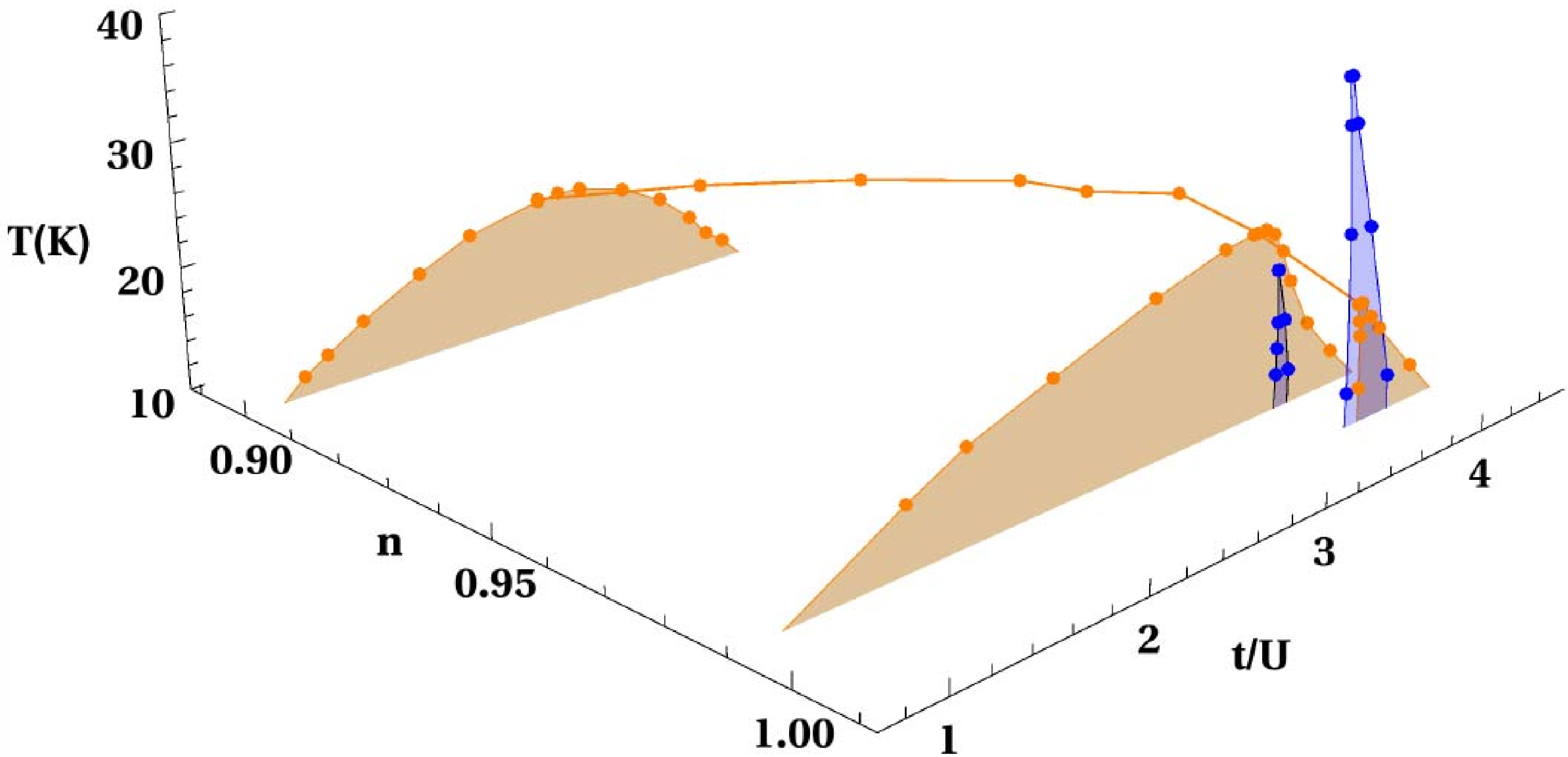
Doped BEDT





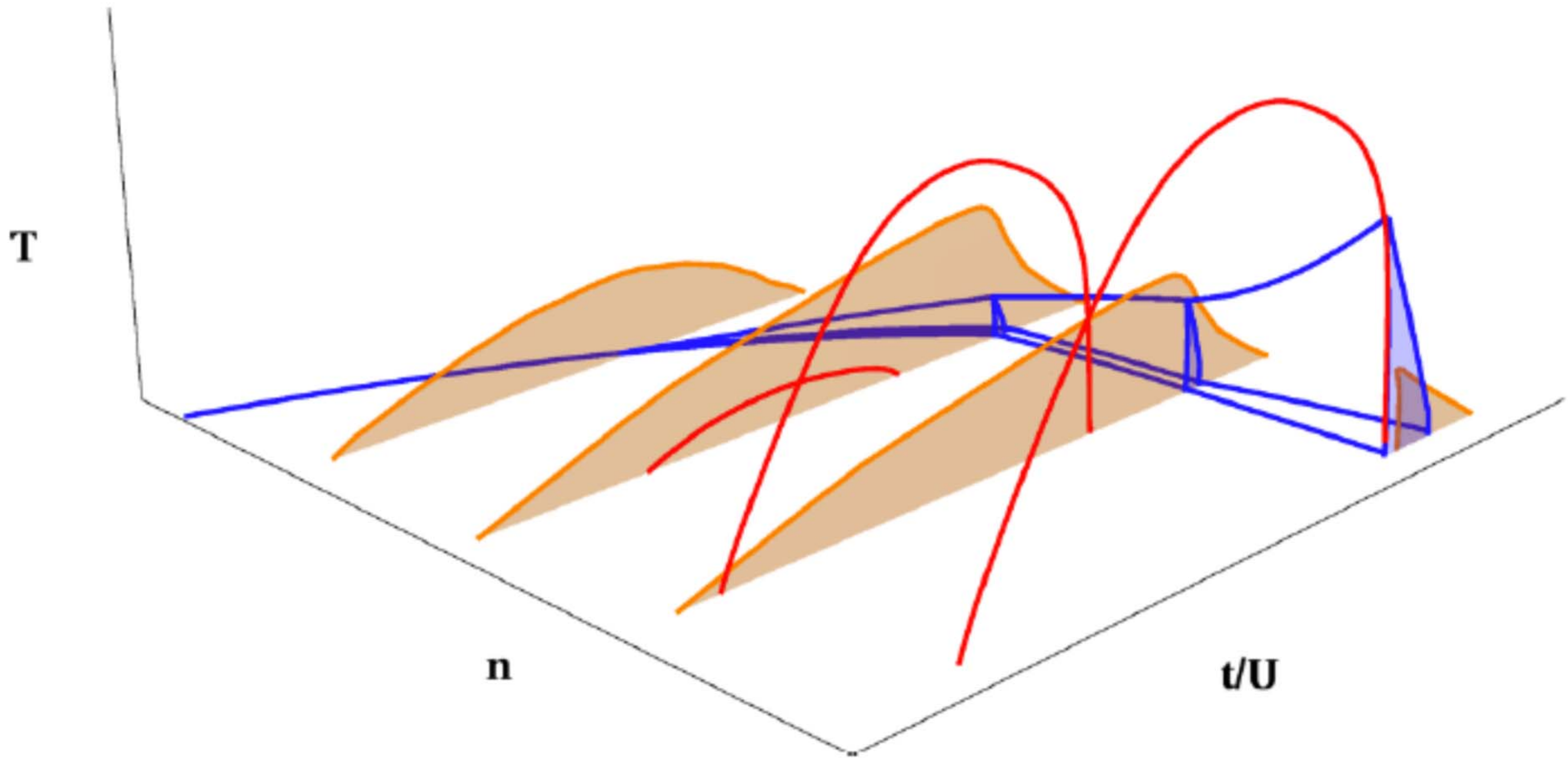
H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

$t' = 0.4t$ overview



Compare: T. Watanabe, H. Yokoyama and M. Ogata
JPS Conf. Proc. **3**, 013004 (2014)

Generic case highly frustrated case



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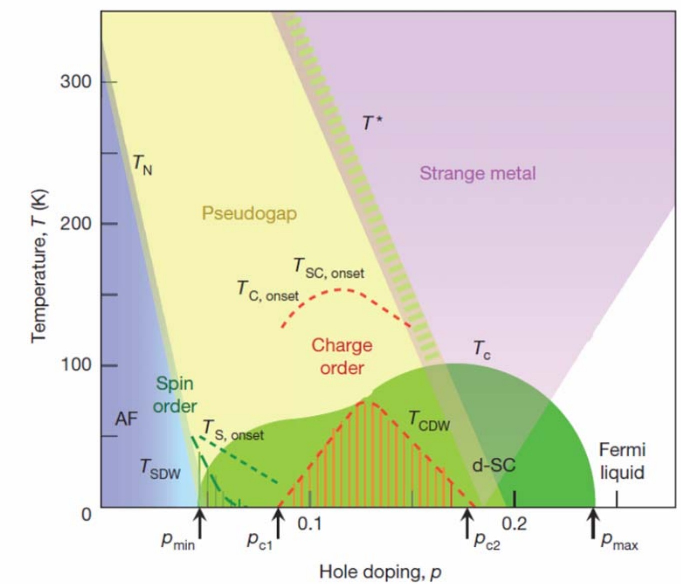
Conclusion

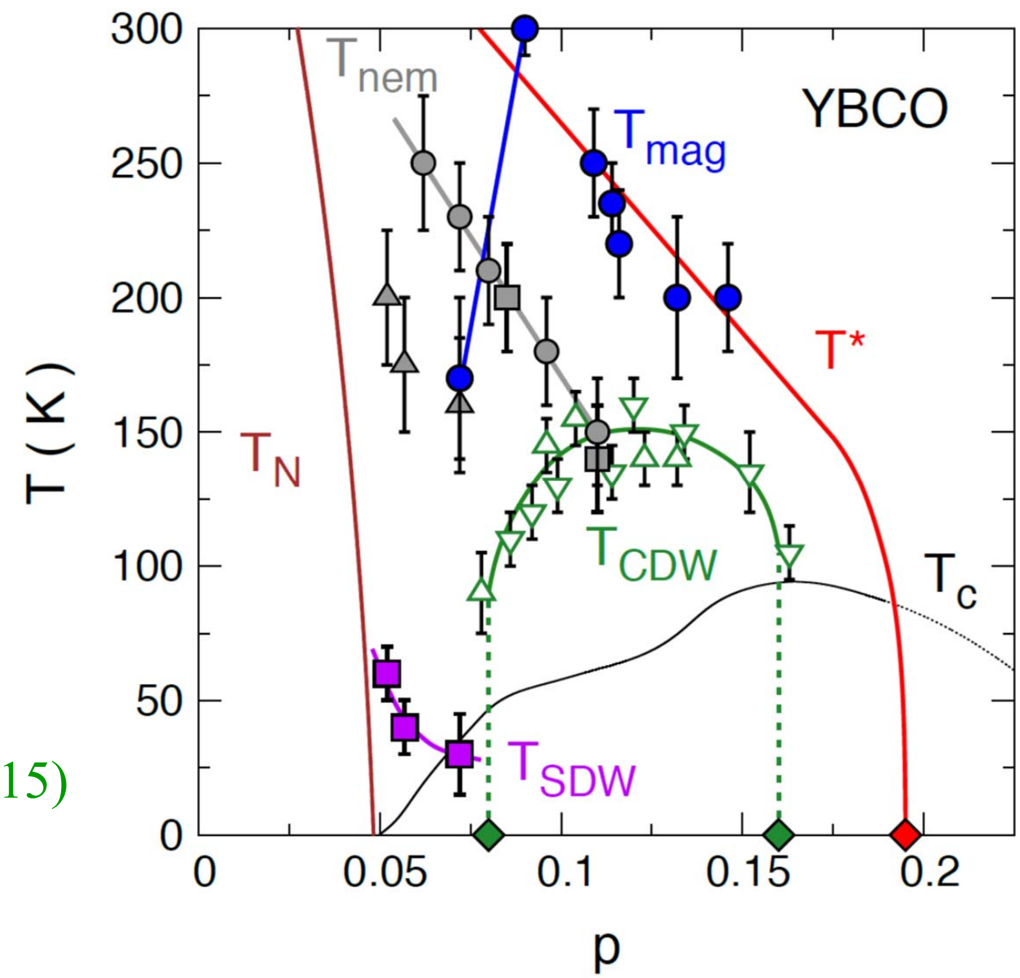
- Even within a single phase, there can be qualitative differences between the strong and weak correlation limits
- The underlying normal state organizes the ordered state
- Mott + J suffices for many qualitative properties of both pseudogap and d-SC
- A quantum critical point is not a necessary condition to have a dome shape

Prologue

Phase diagram $YBa_2Cu_3O_{7-x}$



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



Cyr-Choinières… Taillefer (unpublished)

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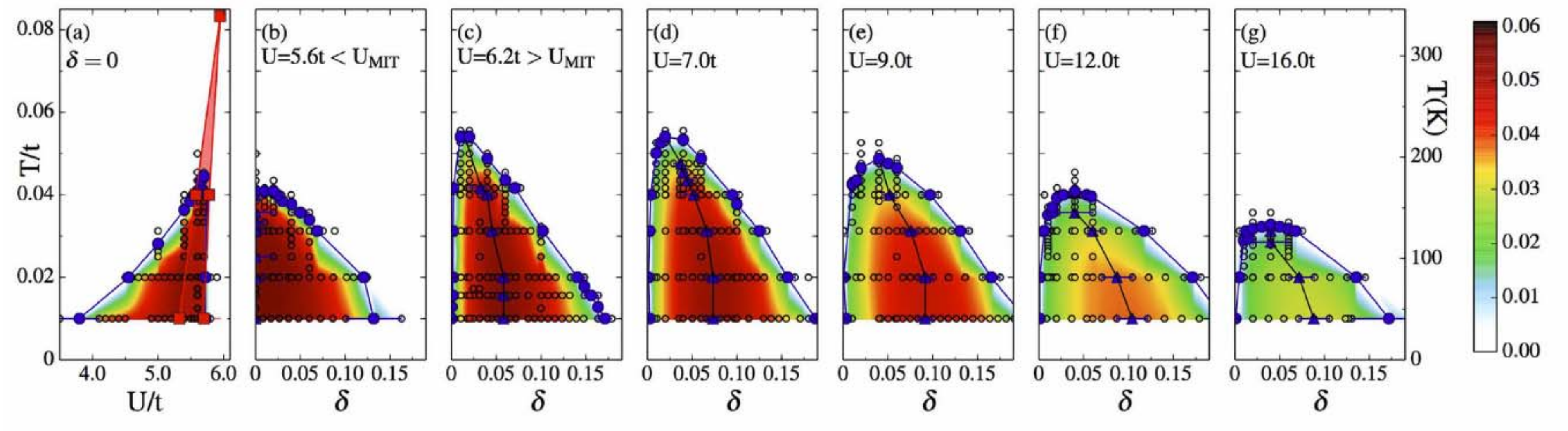
Pairing mechanism



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

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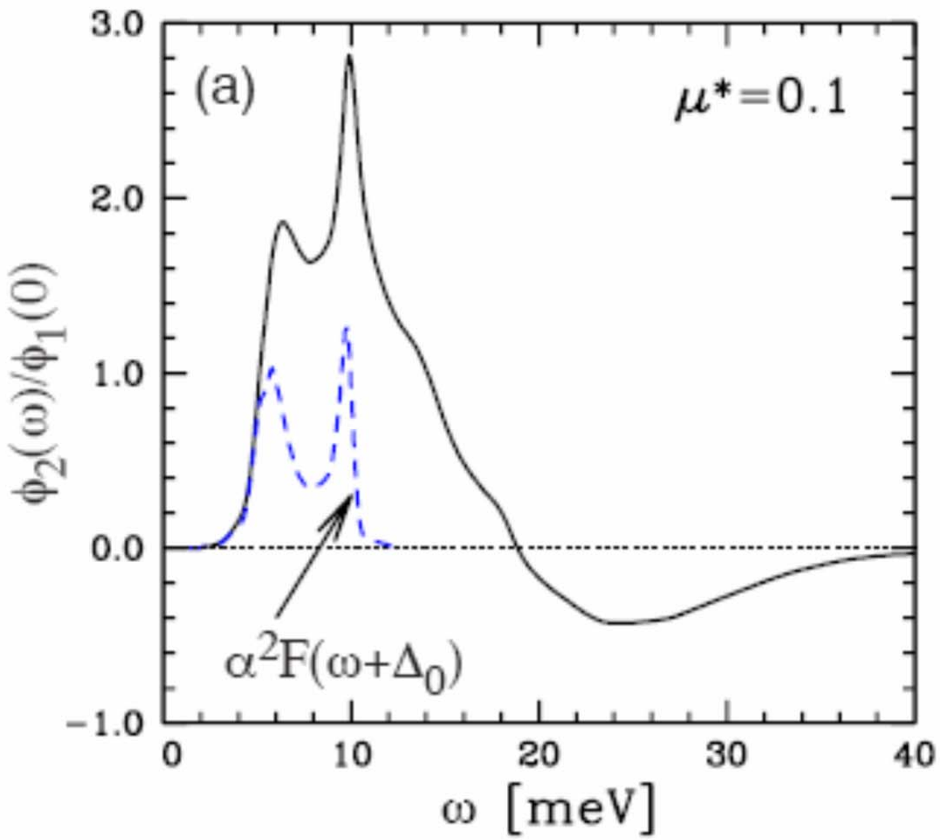
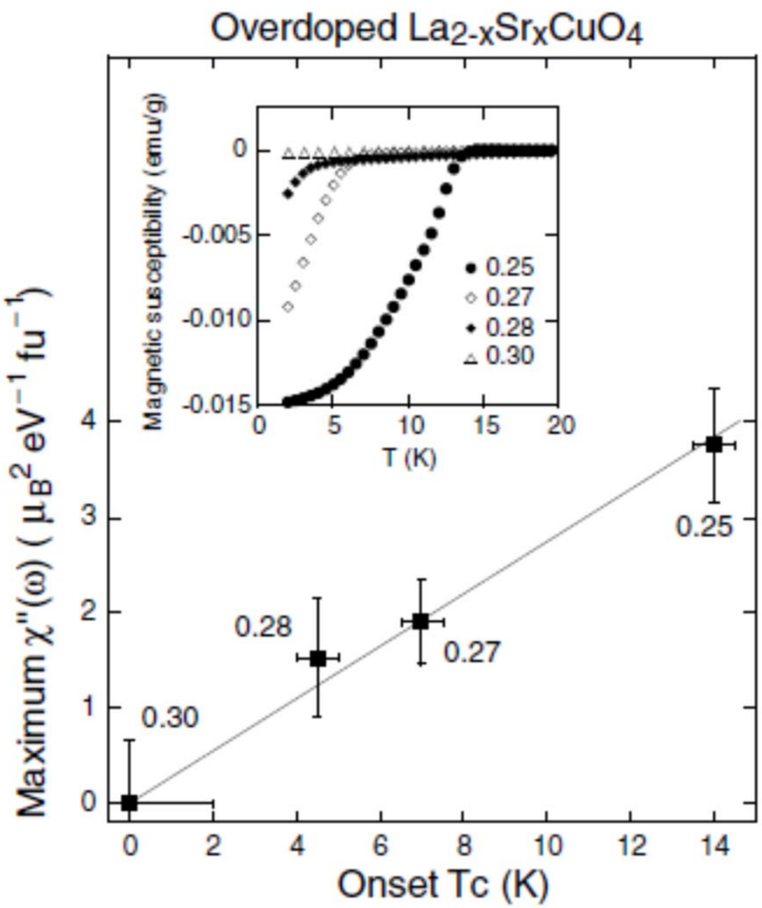
Im Σ_{an} and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

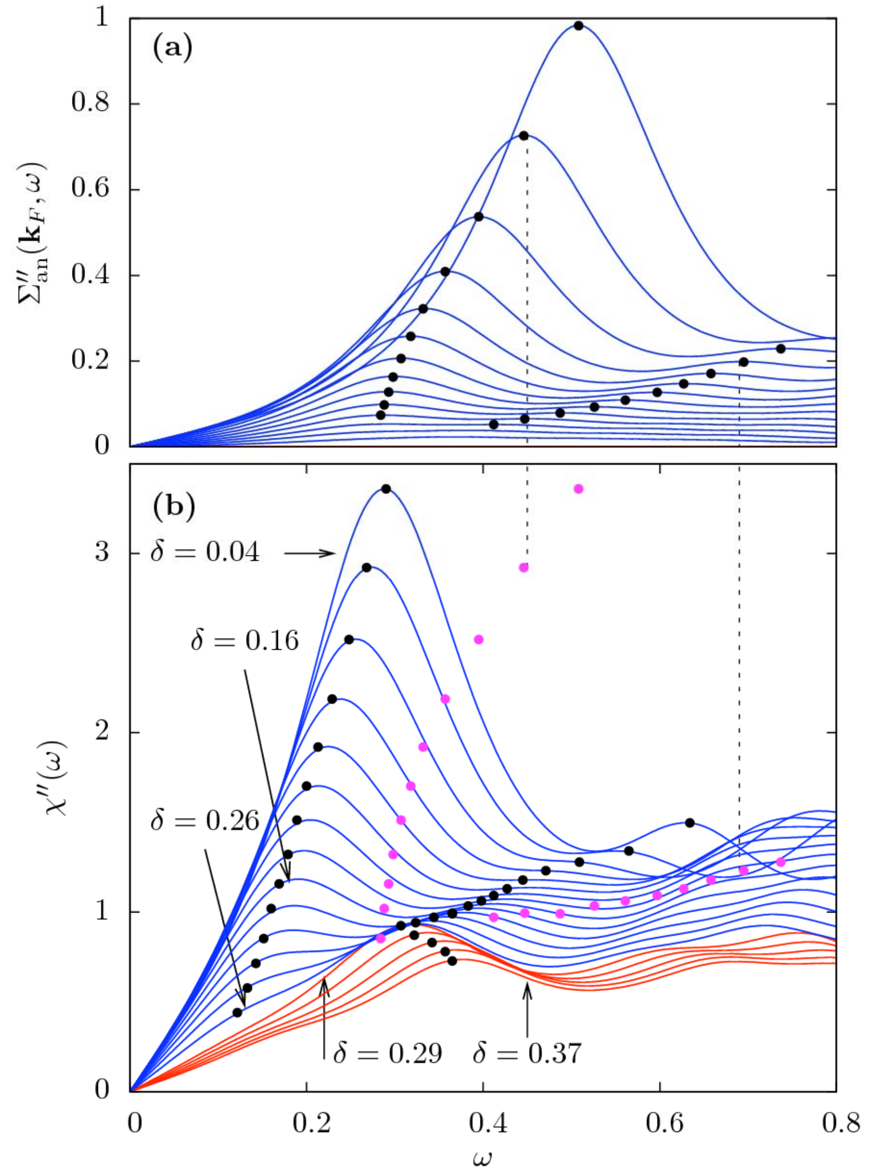


The glue

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



Wakimoto … Birgeneau PRL (2004)



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The glue and neutrons

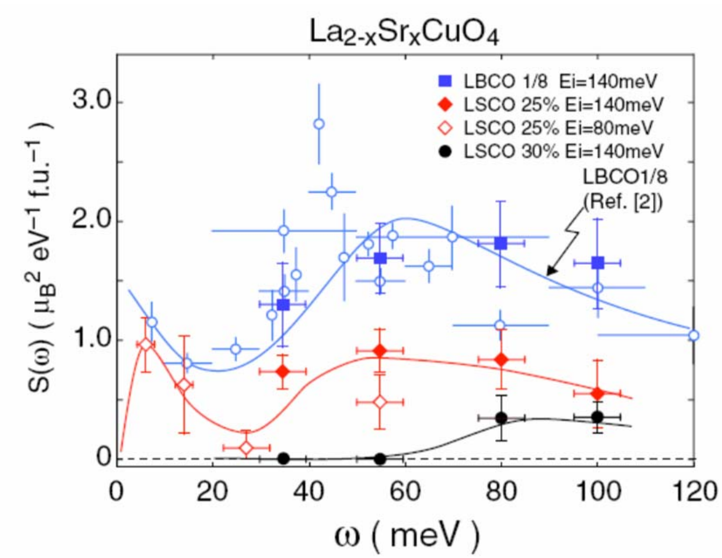
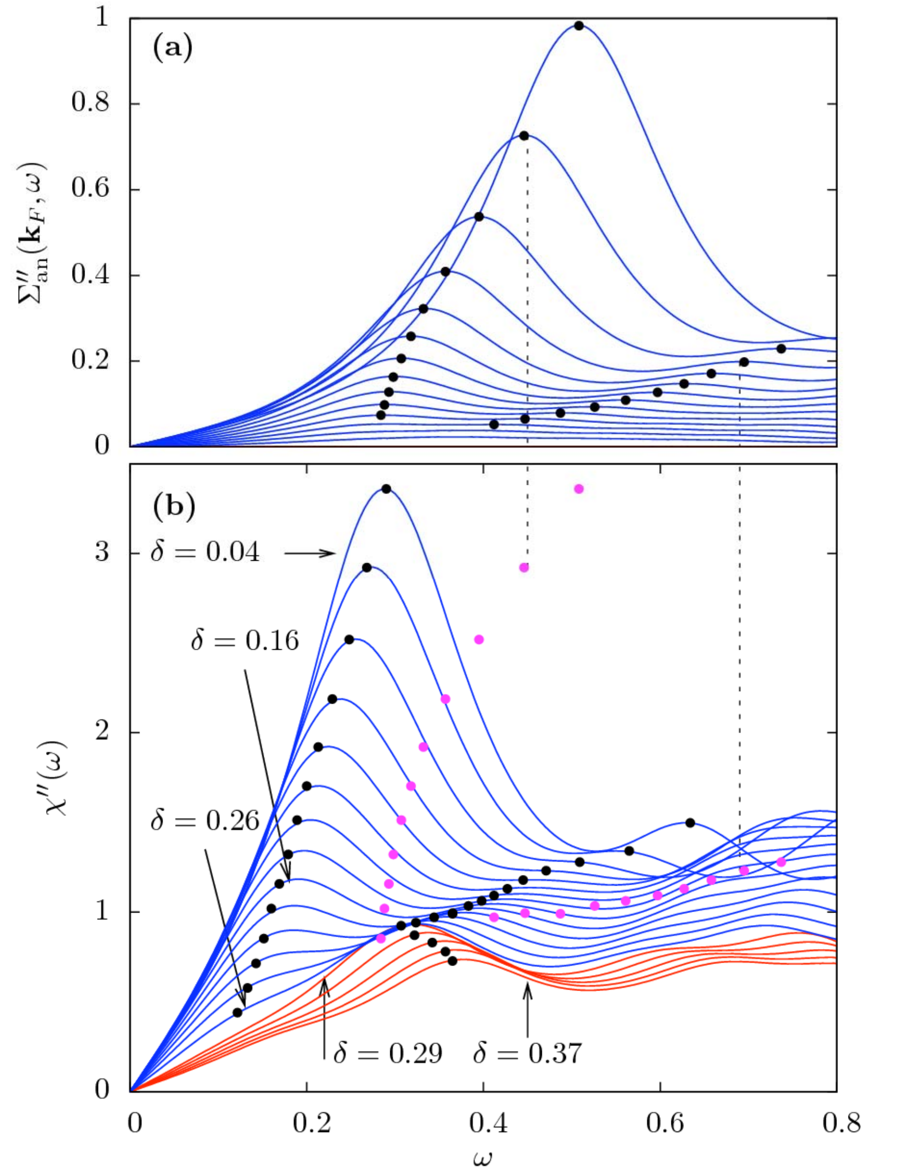


FIG. 3 (color online). **Q**-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i = 140$ meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO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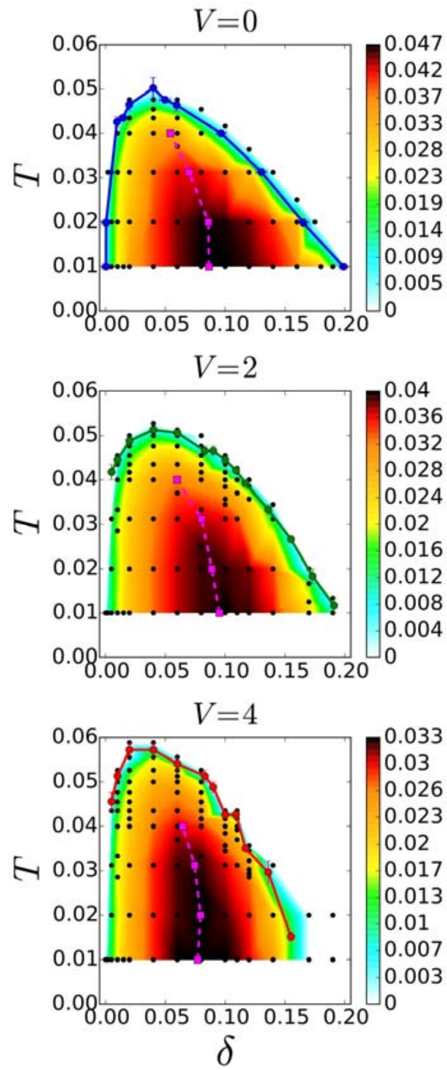
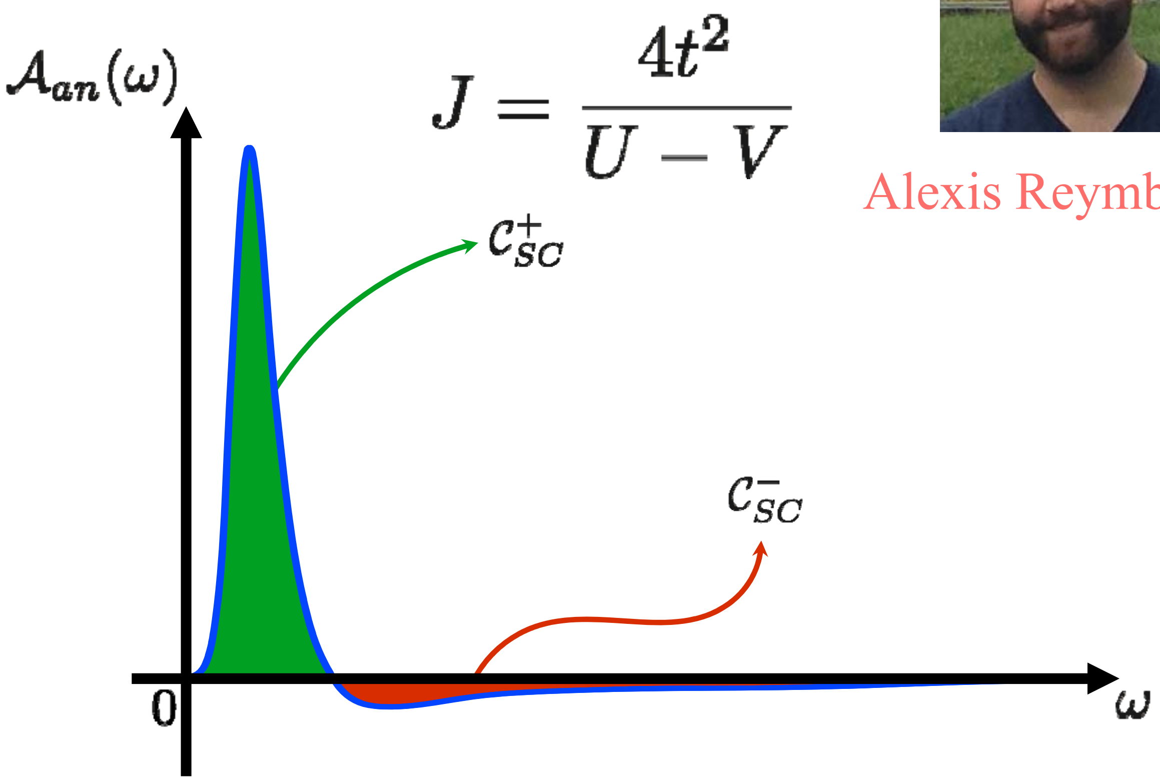
Antagonistic effects of *V* at finite T





Alexis Reymbaut

A. Reymbaut *et al*. PRB **94** 155146 (2016)

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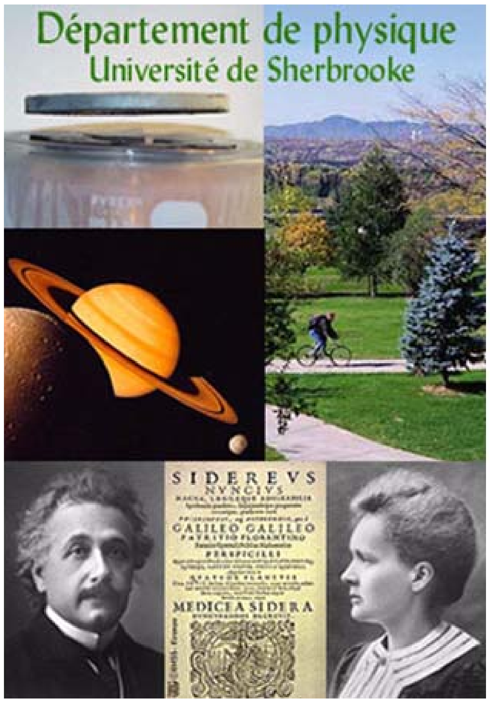
André-Marie Tremblay



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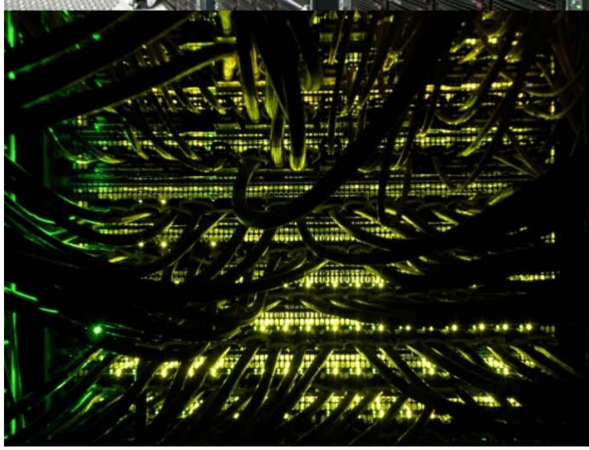
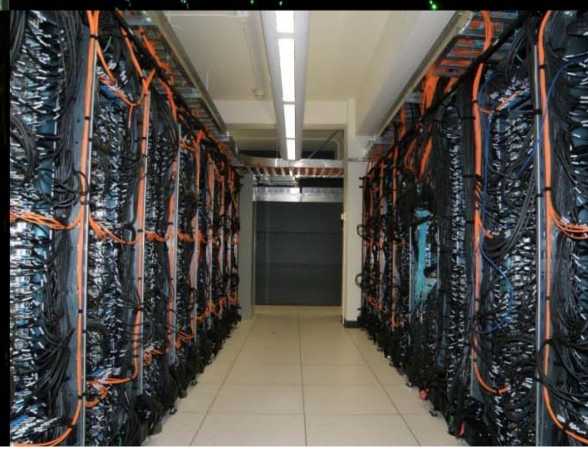


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Review: A.-M.S.T. arXiv: 1310.1481

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