Unconventional superconductivity with and without an antiferromagnetic quantum critical point

A.-M. Tremblay

Quantum criticality and topology in itinerant electron systems
15 to 19 August 2016

CIFAR
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VERITATEM IN CHARITATE

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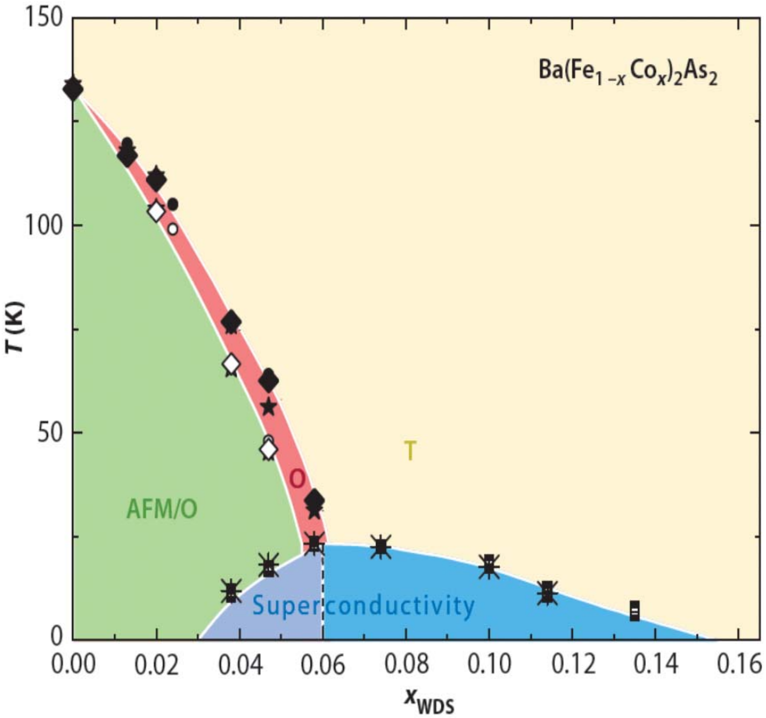
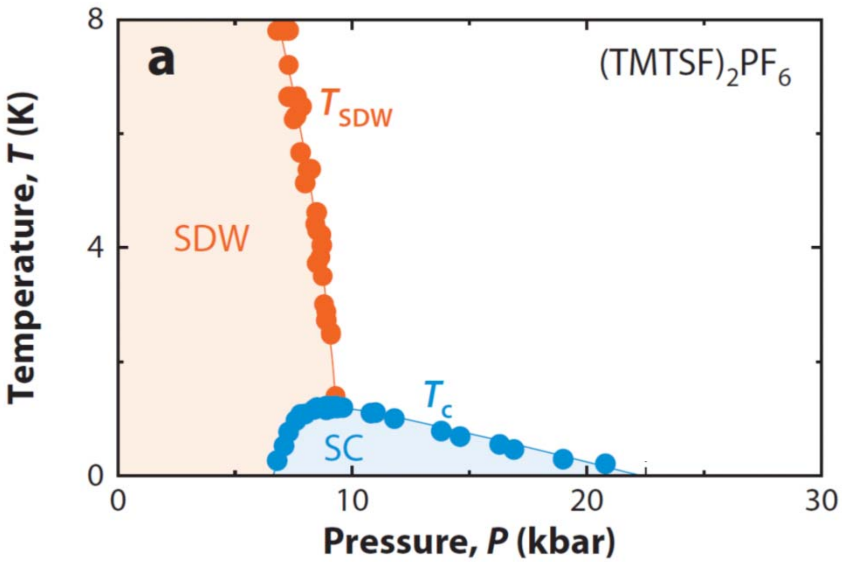
Pnictides and organics

Pnictides



Bechgaard salts



The Archetype

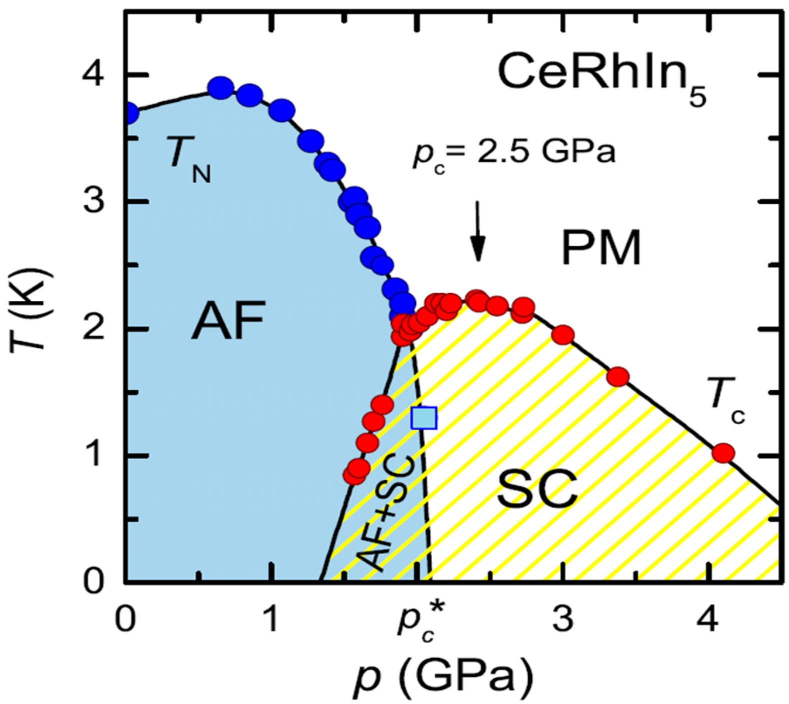
Magnetic superconductivity

Nicolas Doiron-Leyraud, Bourbonnais, Taillefer 2010

Canfield et al. (2010)

Heavy fermions

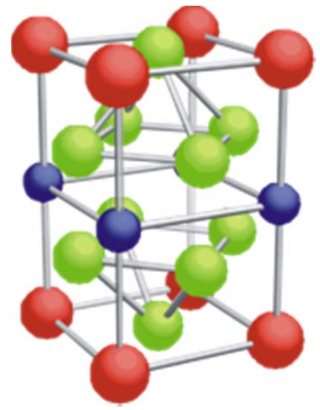
Heavy fermions **3D metals tuned by pressure, field or concentration**



Knebel et al. (2009)

Quantum criticality

$\color{red}{Ce}\color{blue}{RhIn_5}$



Magnetic superconductivity

Mathur et al., Nature 1998

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Method for strongly correlated matter

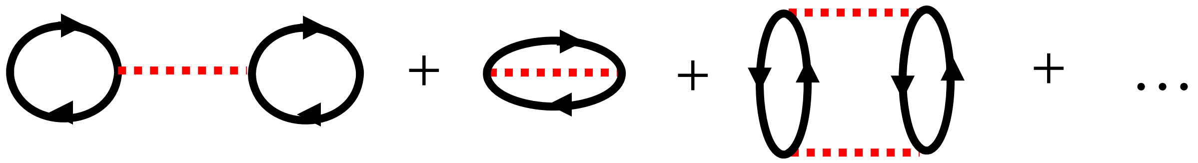
Dynamical Mean Field Theory (+ clusters)

Concept: atomic localized correlations consistent with delocalized aspect

Dynamical "variational" principle

$$\Omega_{\mathbf{t}}[G] = \Phi[G] - Tr[(G_{0\mathbf{t}}^{-1} - G^{-1})G] + Tr\ln(-G)$$

$$\Phi[G] =$$



$$\frac{\delta\Phi[G]}{\delta G} = \Sigma[G]$$

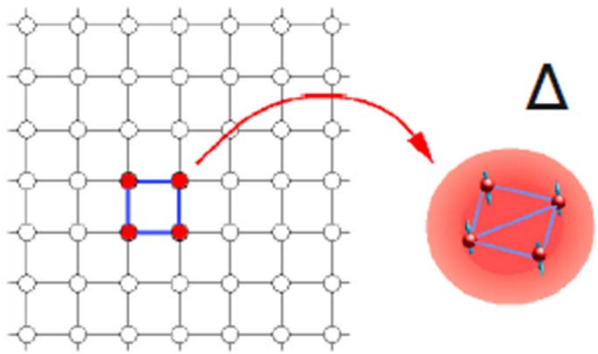
$$\frac{\delta\Omega_t[G]}{\delta G} = \Sigma[G] - G_{0\mathbf{t}}^{-1} + G^{-1} = 0$$

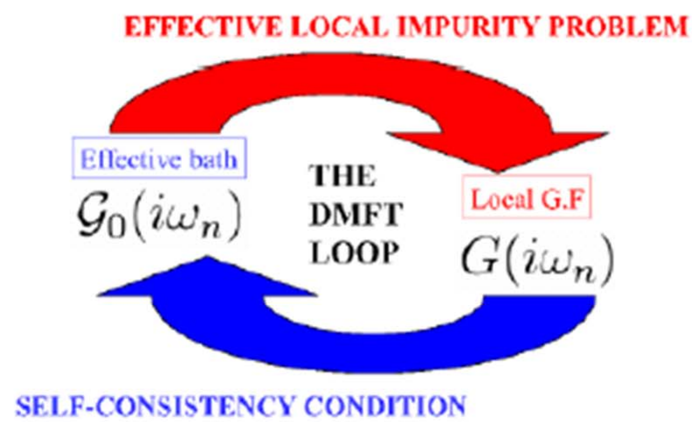
DMFT $$\Phi[G] = \sum_i \Phi[G_{ii}(i\omega_n)]$$

Luttinger and Ward 1960, Baym and Kadanoff (1961)

Impurity solver

$$Z = \int D[d^\dagger, d] \exp\left[-S_c - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_i [d_i^\dagger(\tau) \Delta_{i'i}(\tau,\tau') d_{i'}(\tau')] \right]$$





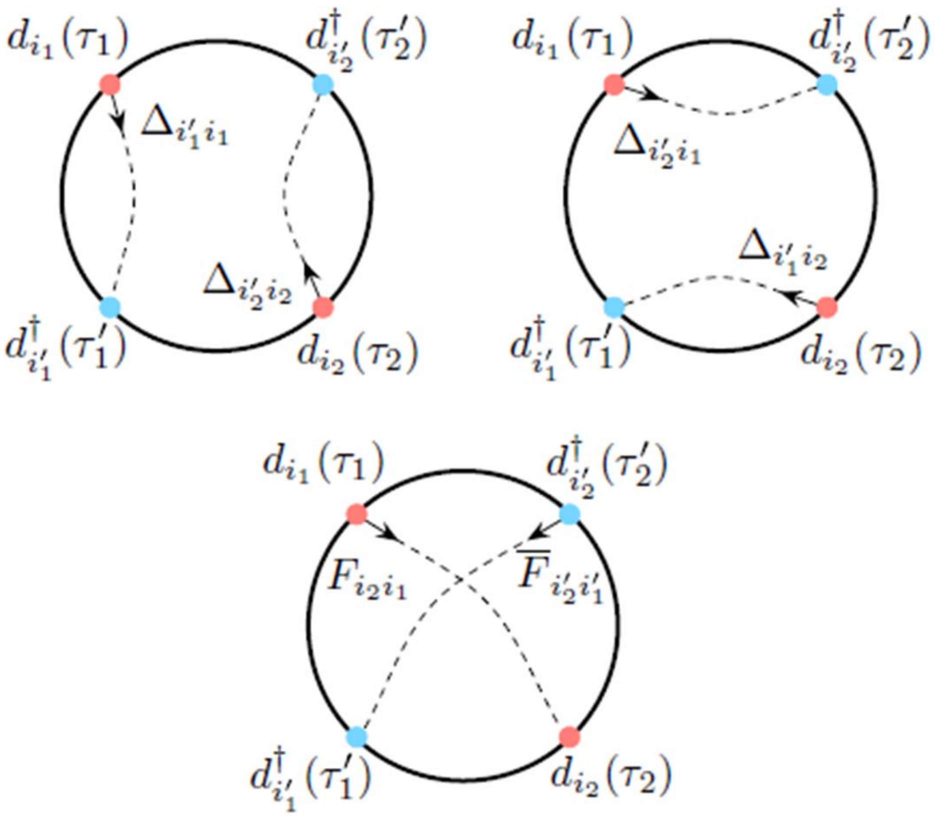
Mean-field is not a trivial problem! Many impurity solvers.

Here: continuous time QMC

P. Werner, PRL 2006
P. Werner, PRB 2007
K. Haule, PRB 2007

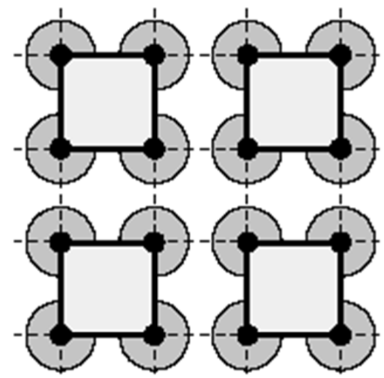
$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n) - \left[\sum_{\tilde{k}} \frac{1}{i\omega_n + \mu - t_c(\tilde{k}) - \Sigma_c(i\omega_n)} \right]^{-1}$$

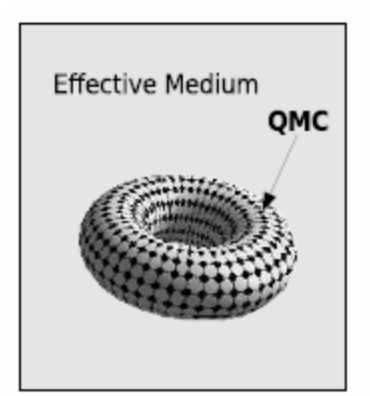
Some not Feynman diagrams



2d Hubbard: Quantum cluster method

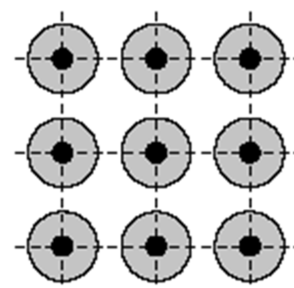
C-DMFT





DCA

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)

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+ and -

- Long range order:
  - Allow symmetry breaking in the bath (mean-field)
- Included:
  - Short-range dynamical and spatial correlations

- Missing:
  - Long wavelength p-h and p-p fluctuations

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

Wei Wu

Superconductivity around an AFM quantum critical point

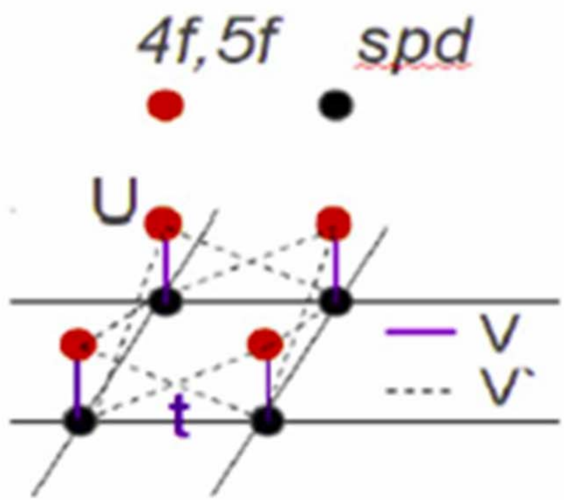
A heavy fermion example

W. Wu A.-M.S.T. Phys. Rev. X, 2015

Heavy fermions

$$H = \sum_{k,\sigma} \epsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{k,\sigma} \epsilon^f f^\dagger_{k,\sigma} f_{k,\sigma}$$

$$+ \sum_{k,\sigma} V_k (f^\dagger_{k,\sigma} c_{k,\sigma} + \text{H.c.}) + \sum_i U \left(n_f^\uparrow - \frac{1}{2}\right)\left(n_f^\downarrow - \frac{1}{2}\right)$$



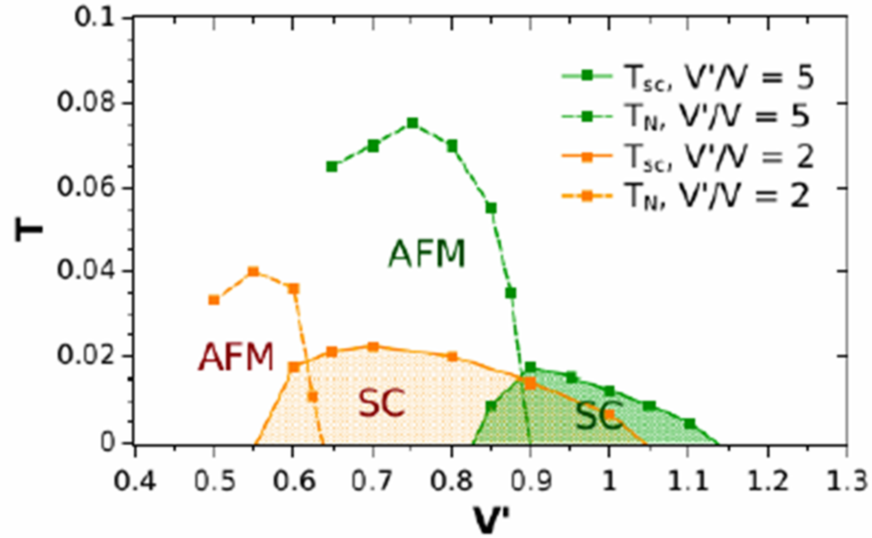
W. Wu A.-M.S.T. Phys. Rev. X, 2015

Phase diagram

U=4

AFM: antiferro-magnetism
SC: superconducting

V'/V = 2 : more frustrated case
V'/V = 5 : less frustrated case

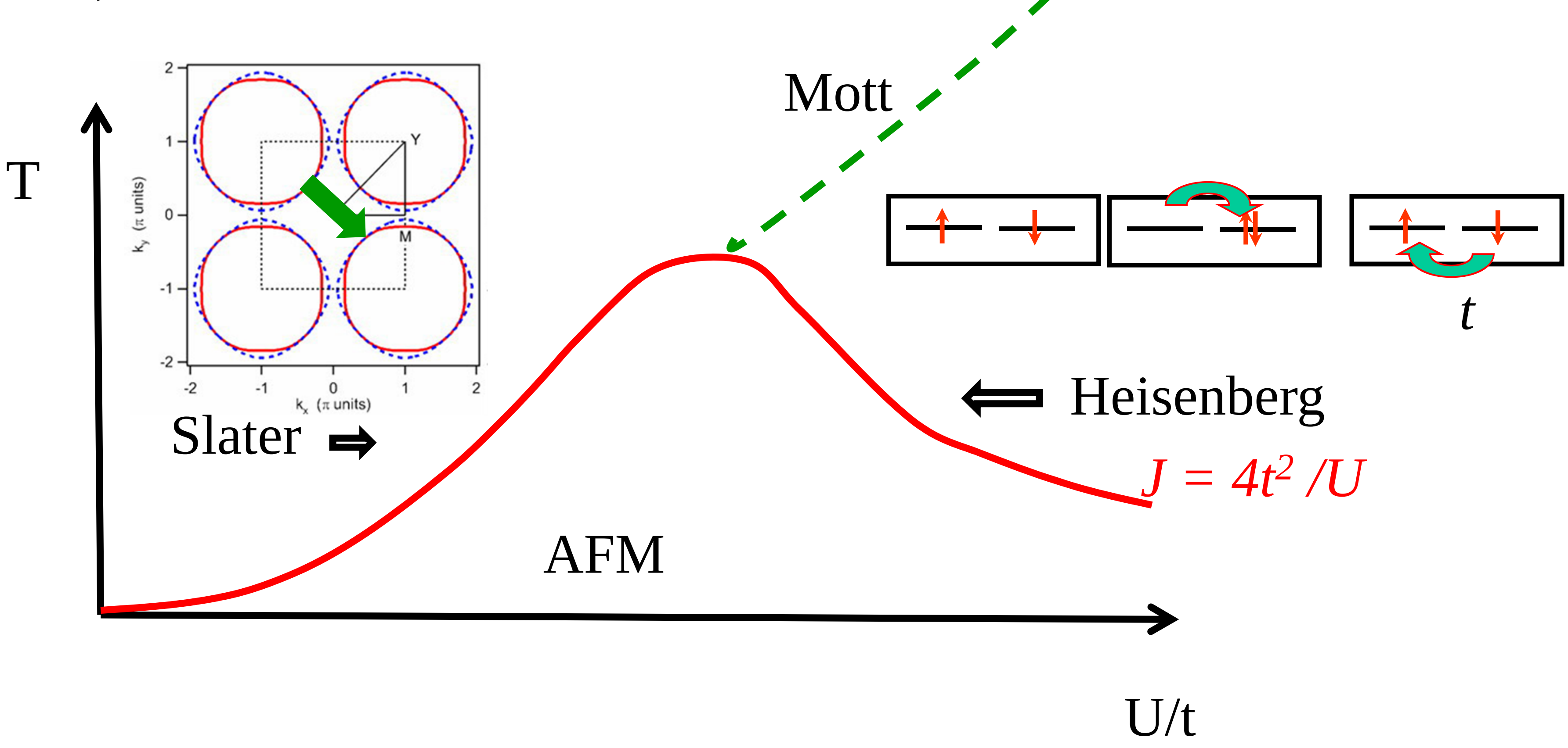


Weakly vs strongly correlated superconductivity

Analog to weakly and strongly correlated antiferromagnets

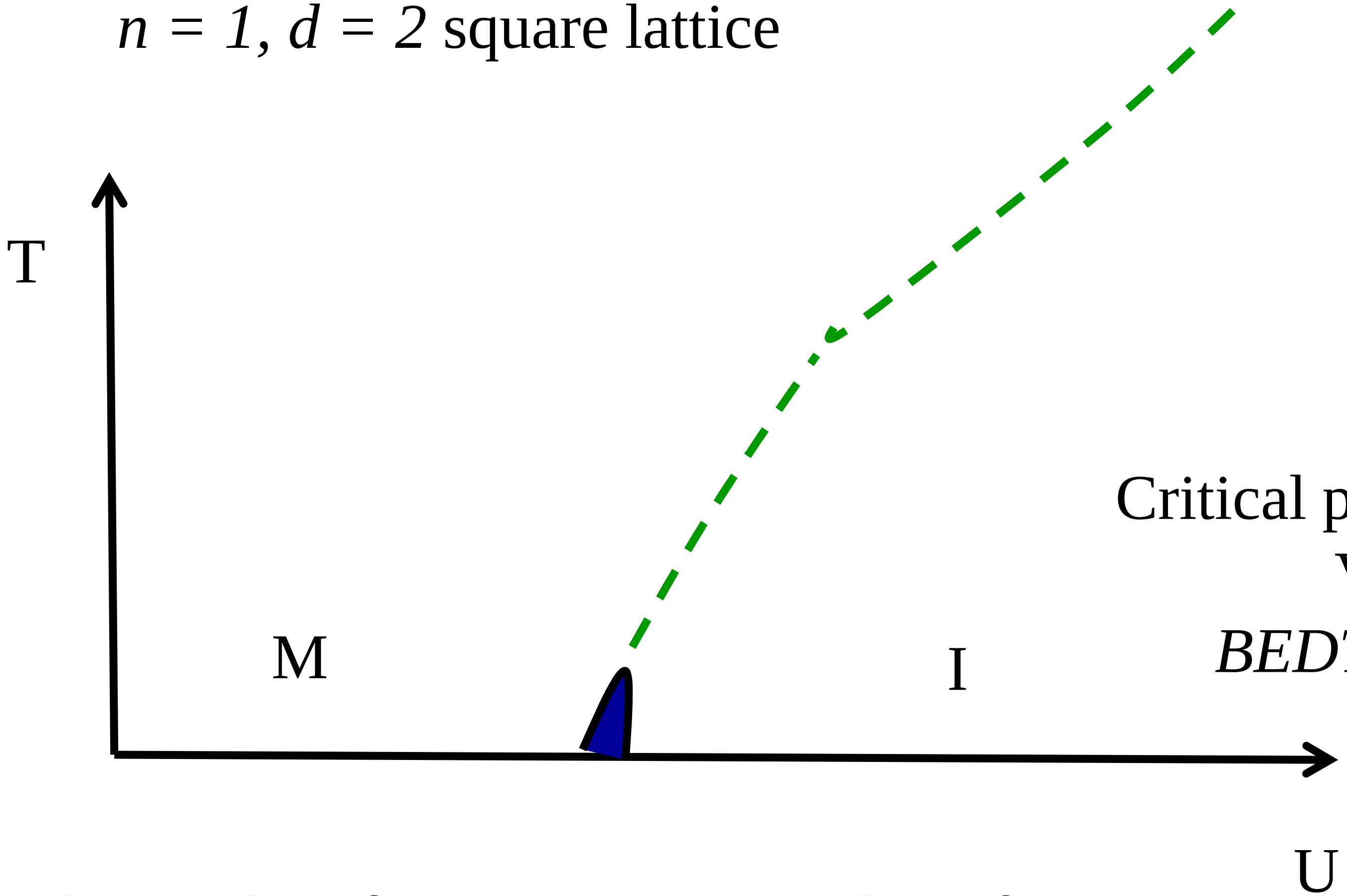
Weak vs Strong correlations

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



Local moment and Mott transition

n = 1, d = 2 square lattice

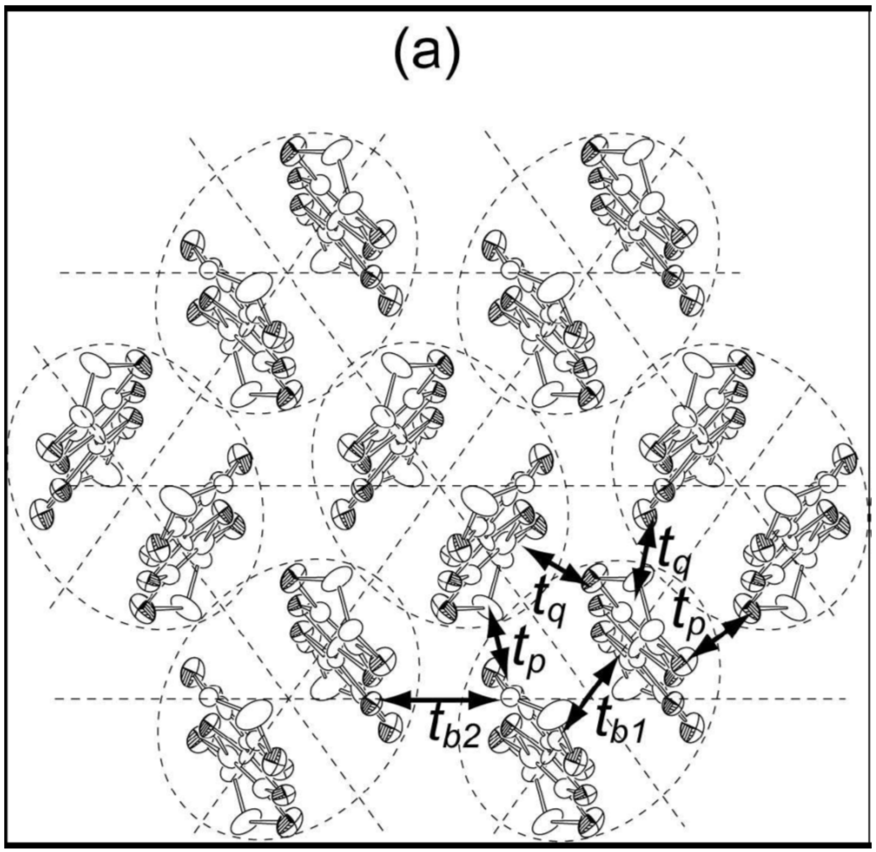


Critical point visible in
V_2O_3,
BEDT organics

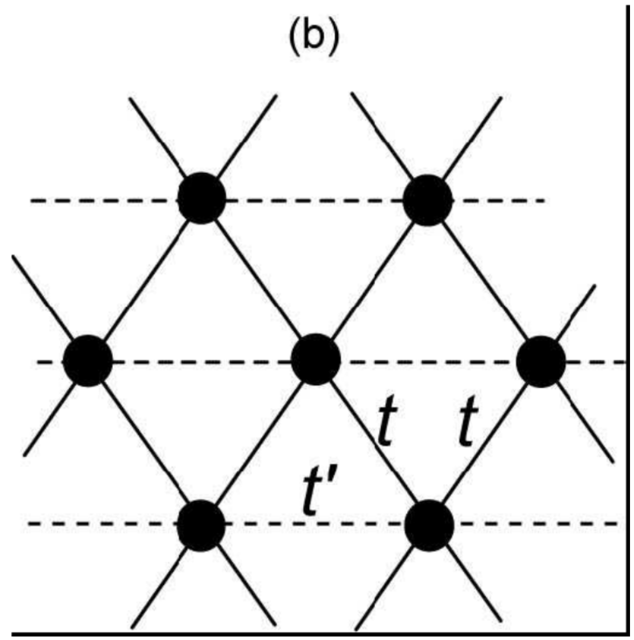
Understanding finite temperature phase from a *mean-field theory* down to *T = 0*

One-band Hubbard model of BEDT organics

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



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



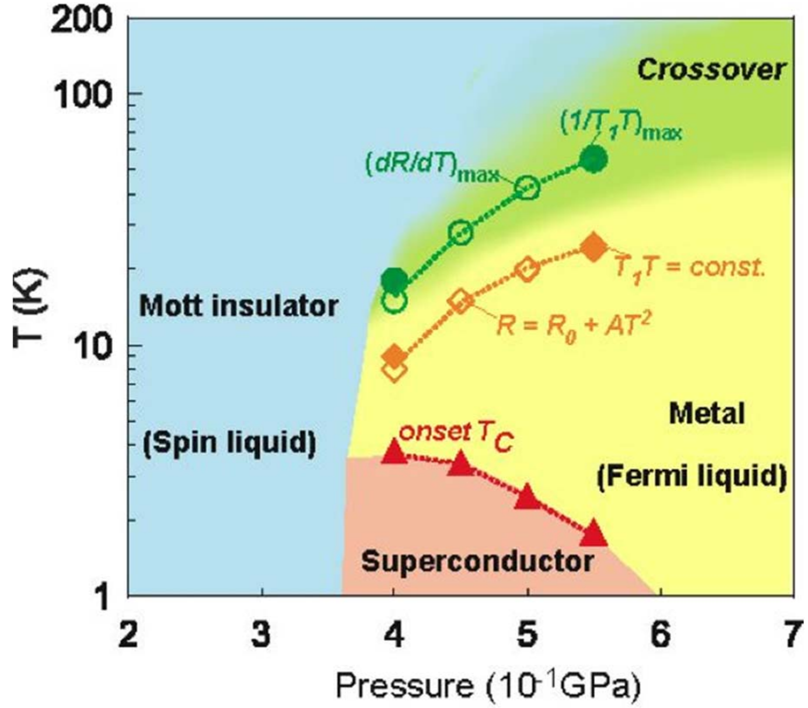
$t \approx 50\,\mathrm{meV}$

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

$t'/t \sim 0.6 - 1.1$

Phase diagram at *n = 1*

X= $Cu_2(CN)_3$ (t'~ t)

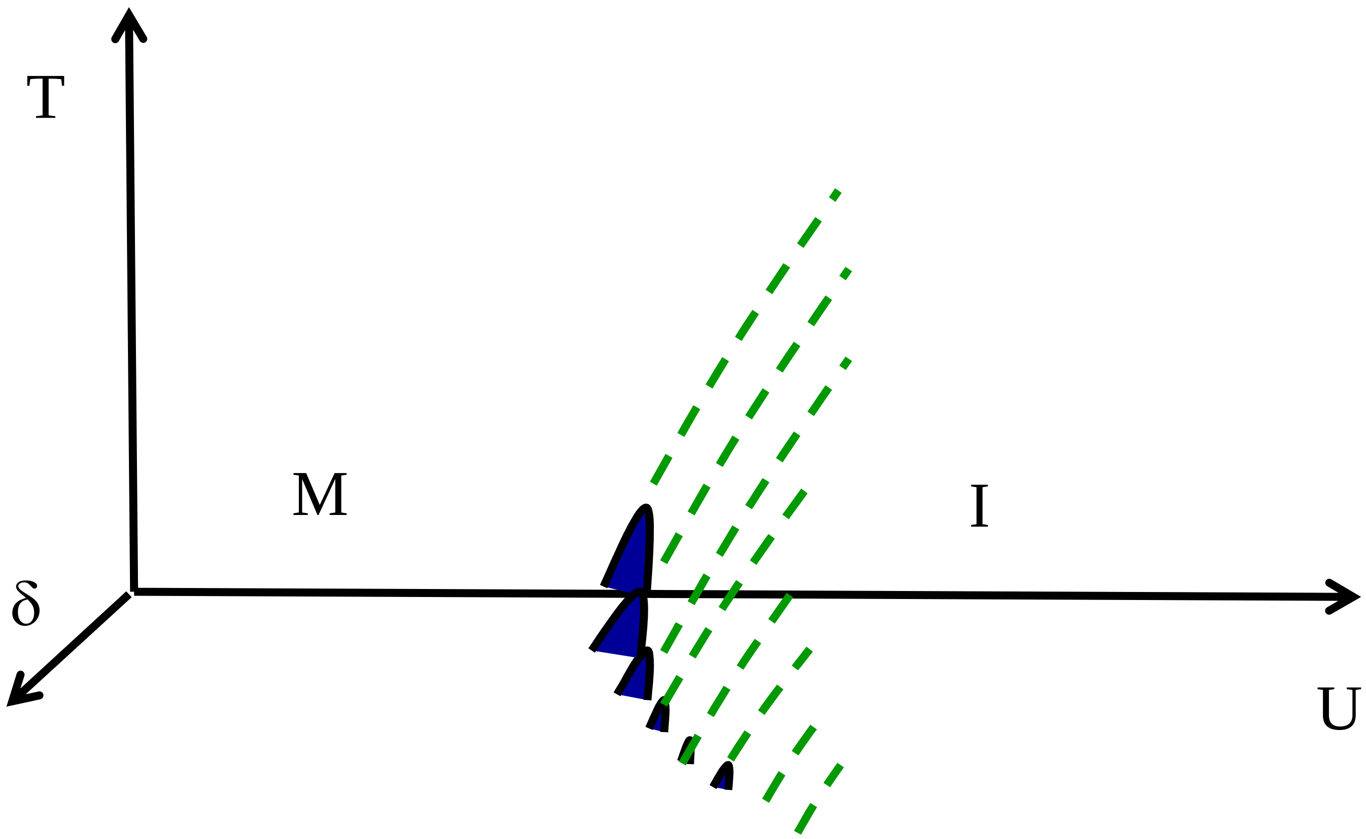


Y. Kurisaki, et al.
Phys. Rev. Lett. **95**, 177001(2005)

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

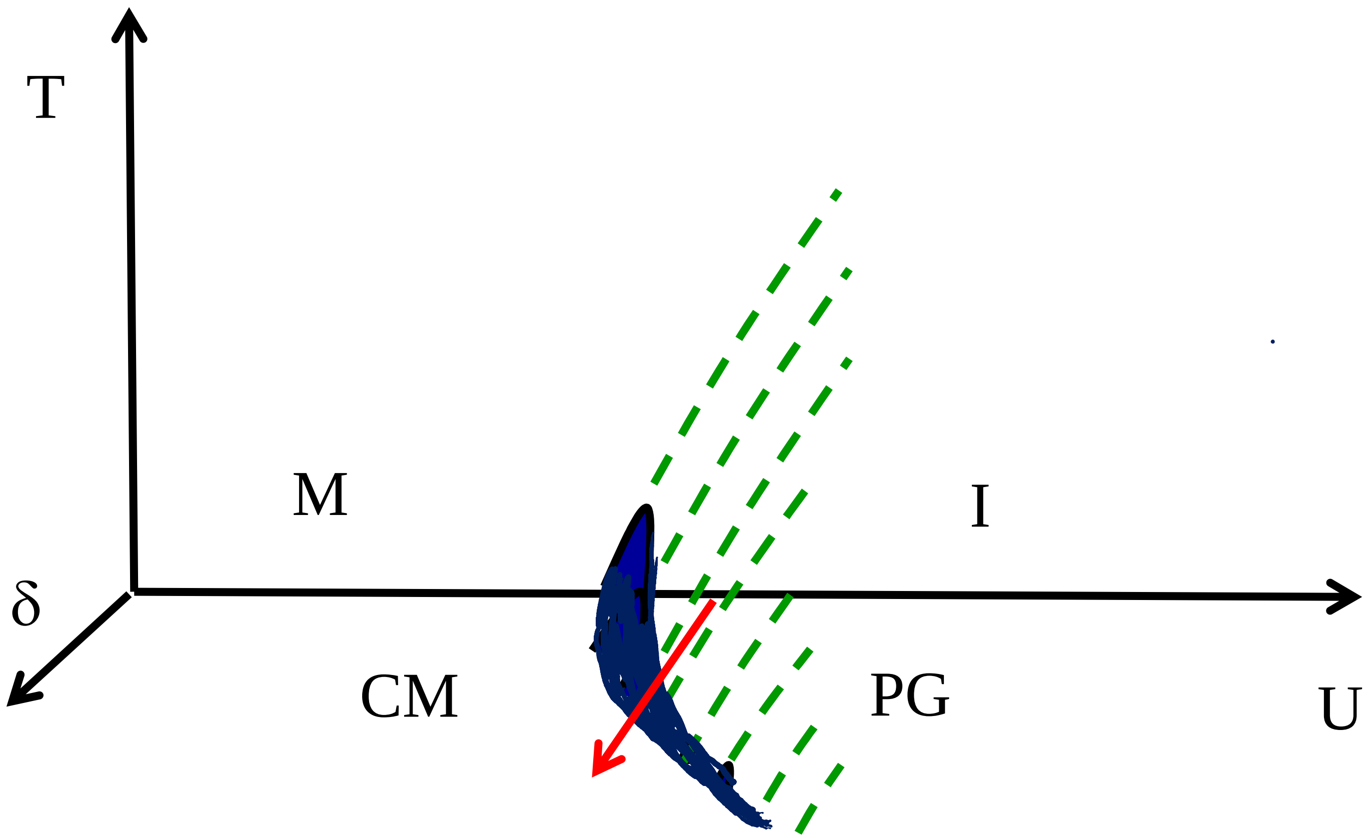
Influence of Mott transition away from half-filling

n = 1, d = 2 square lattice



Influence of Mott transition away from half-filling

$n = 1, d = 2$ square lattice



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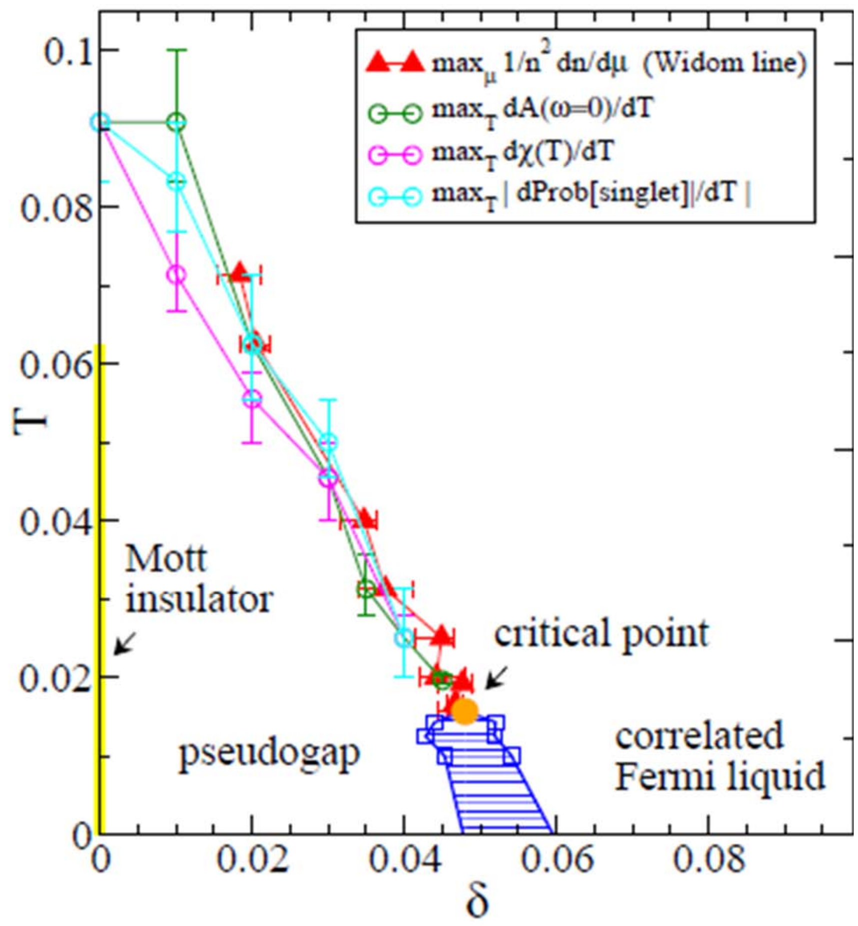
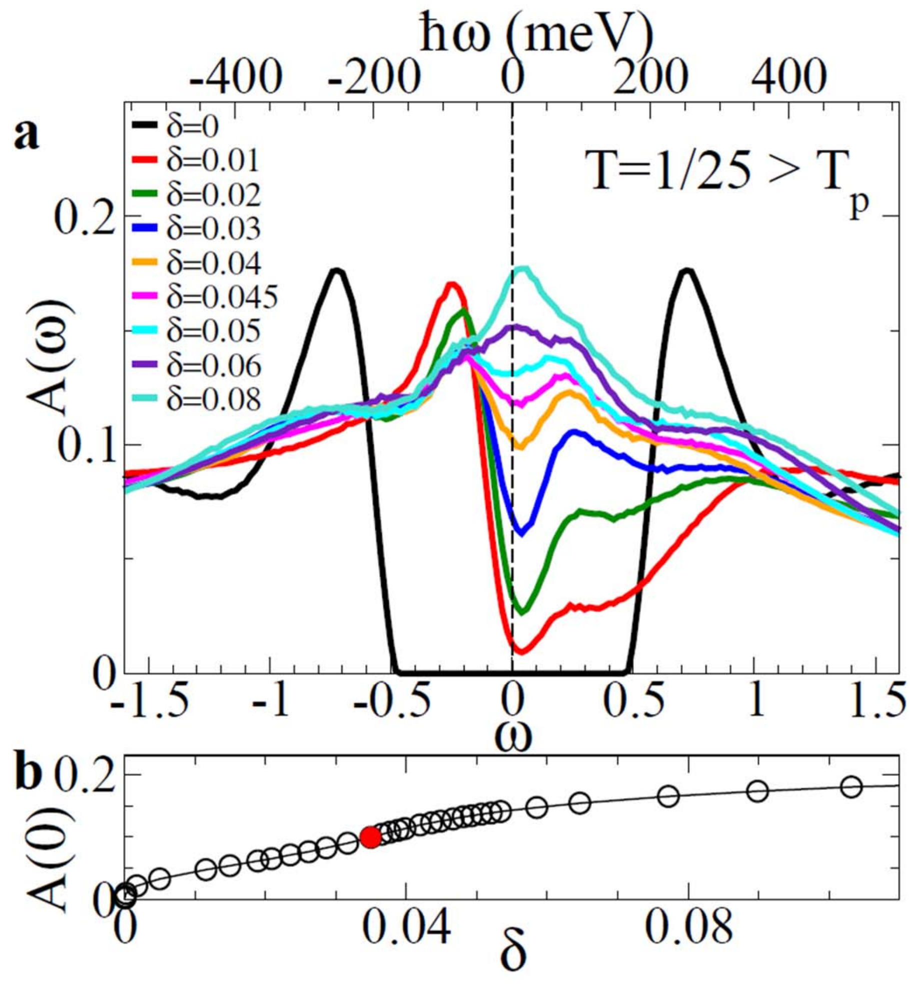
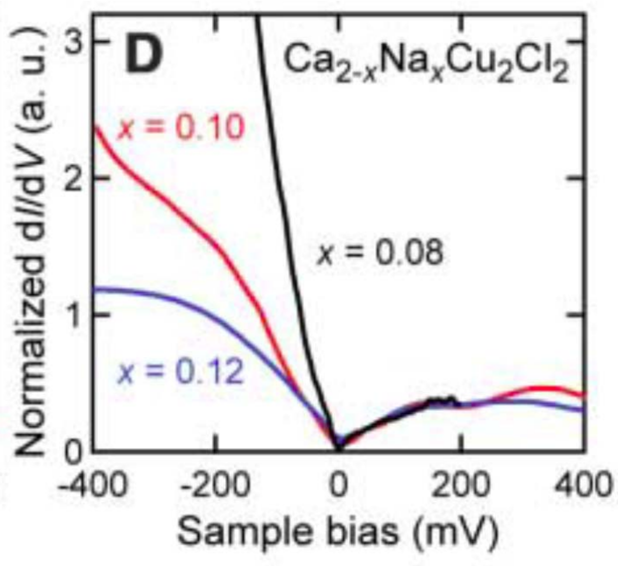
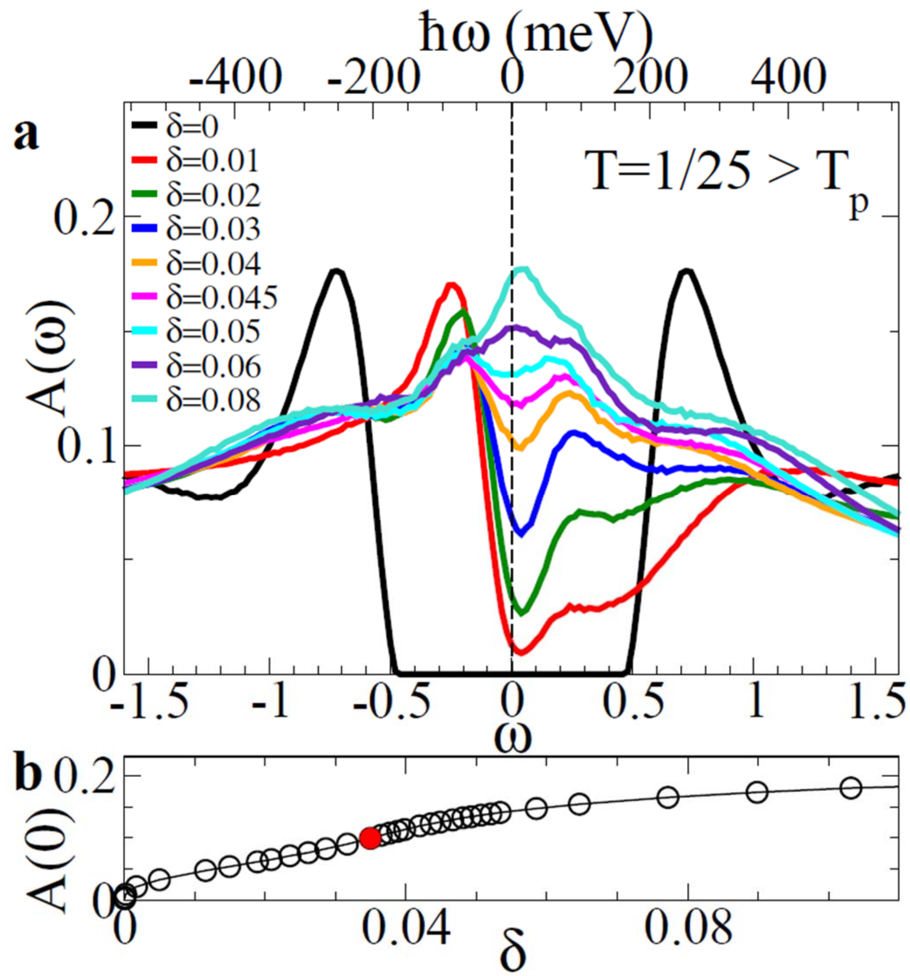
$U = 6.2\,t$ Normal state. Density of states





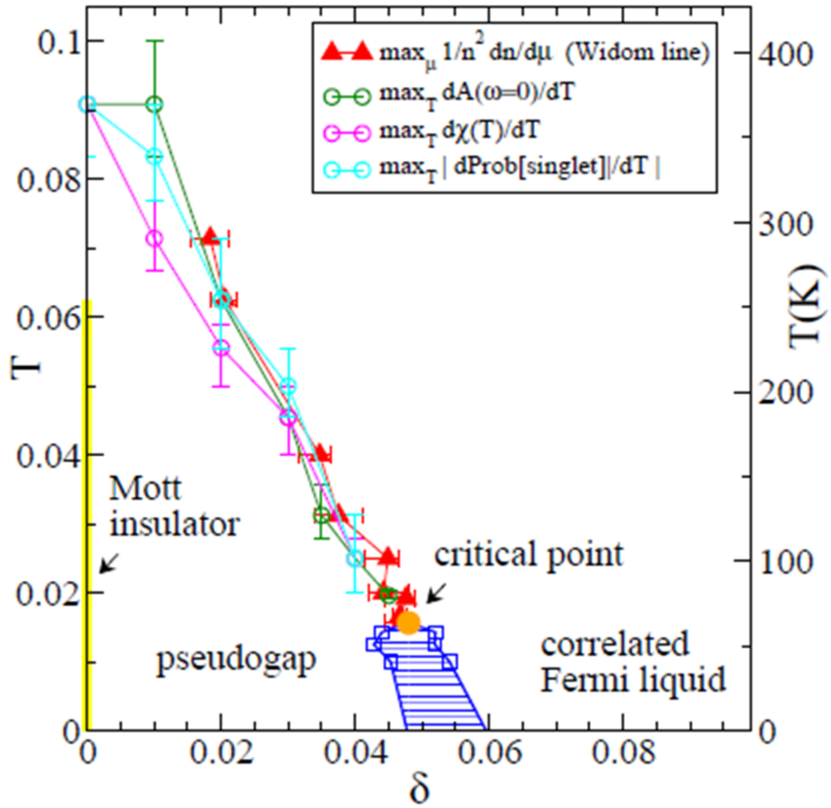
Density of states

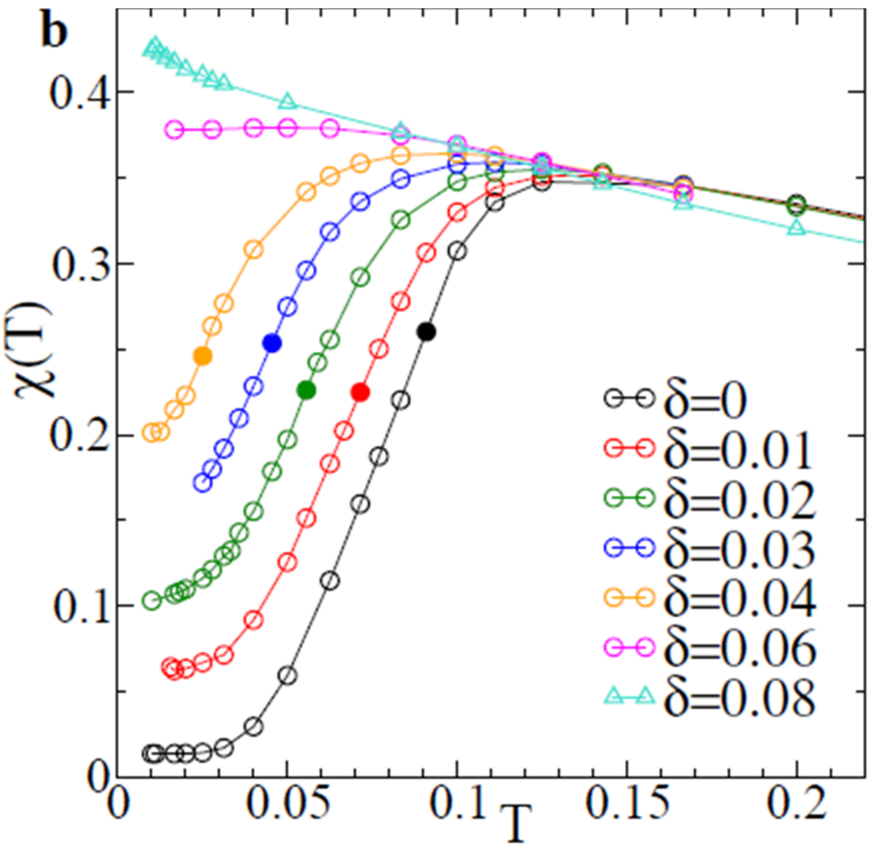




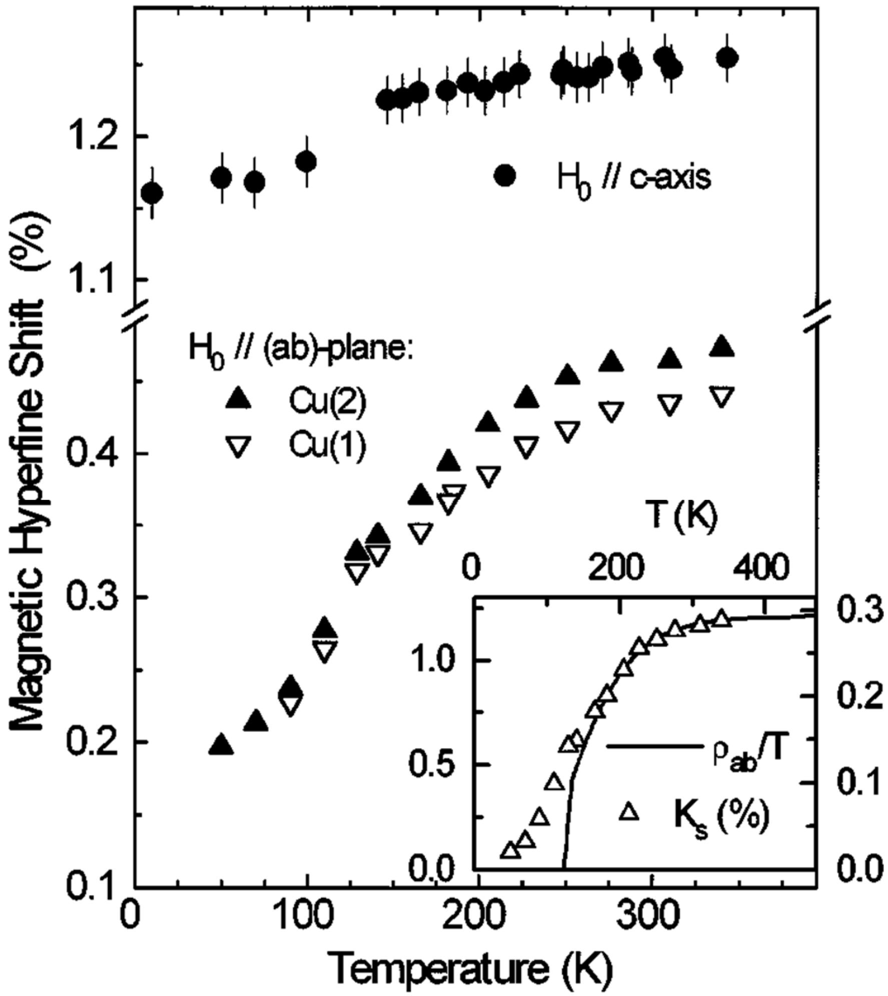
Khosaka et al. *Science* **315**, 1380 (2007);

Spin susceptibility



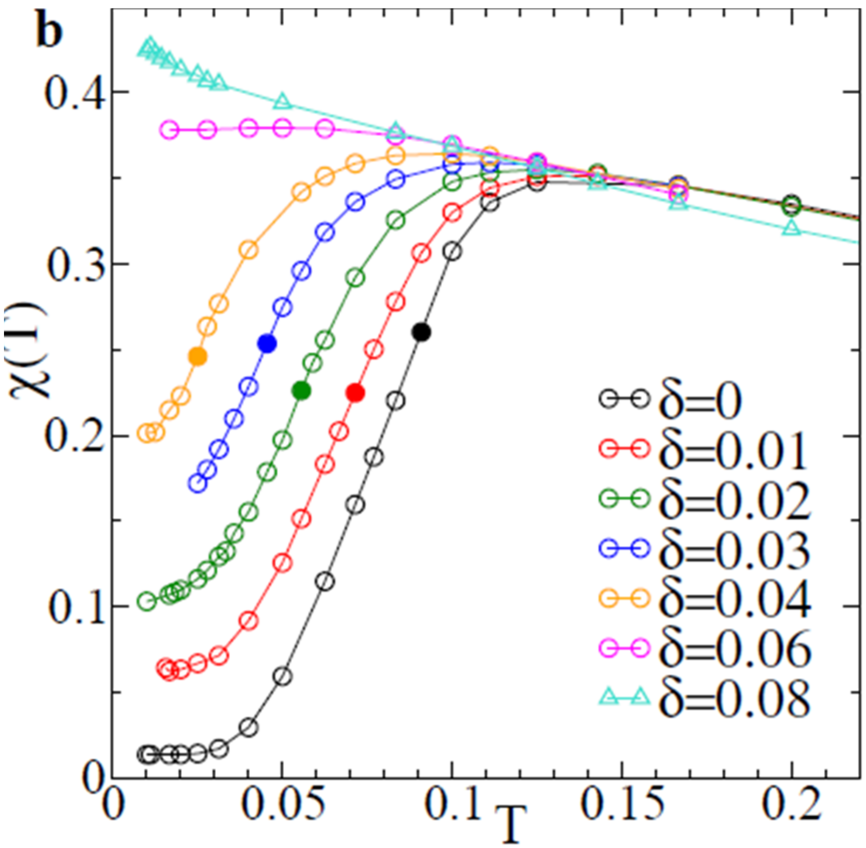


Spin susceptibility



Underdoped Hg1223

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



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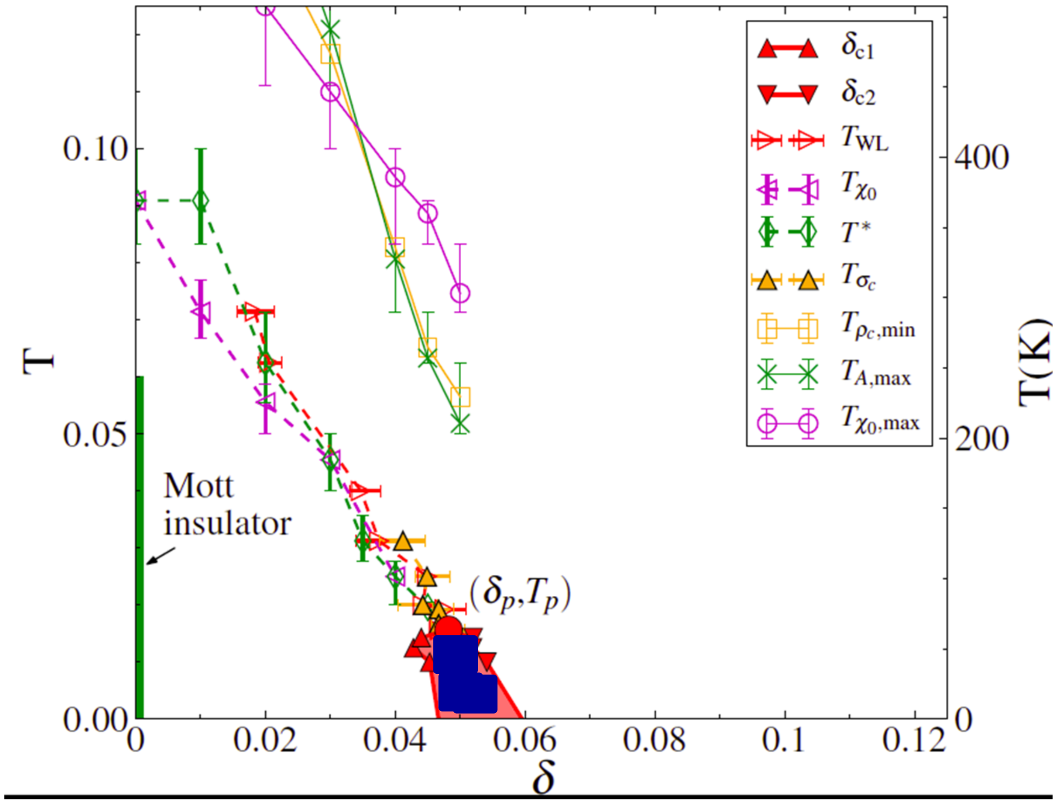
Two crossover lines

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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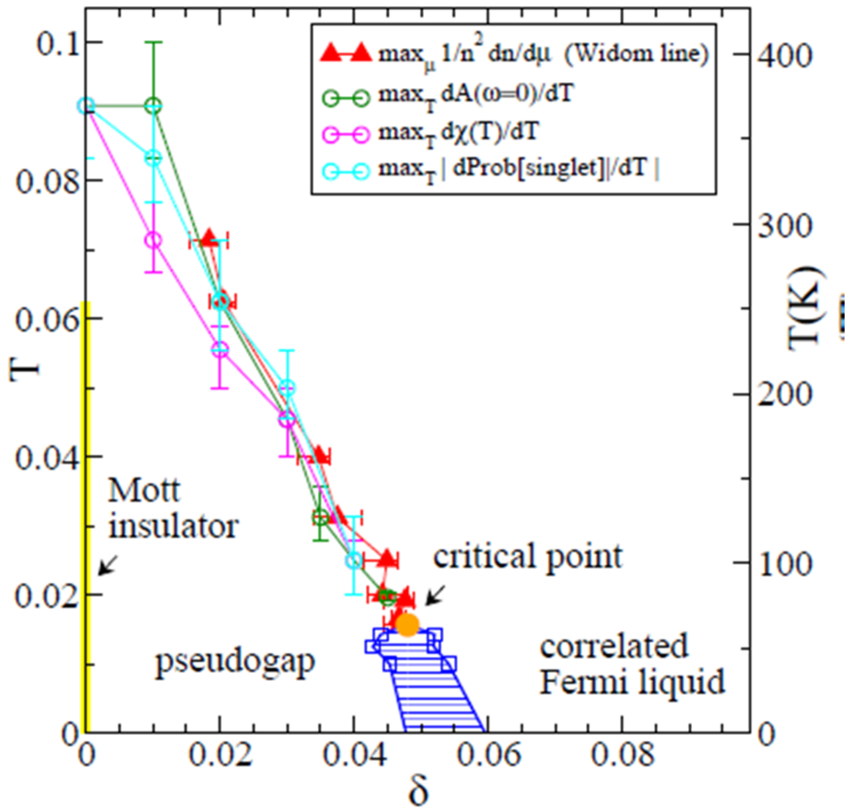
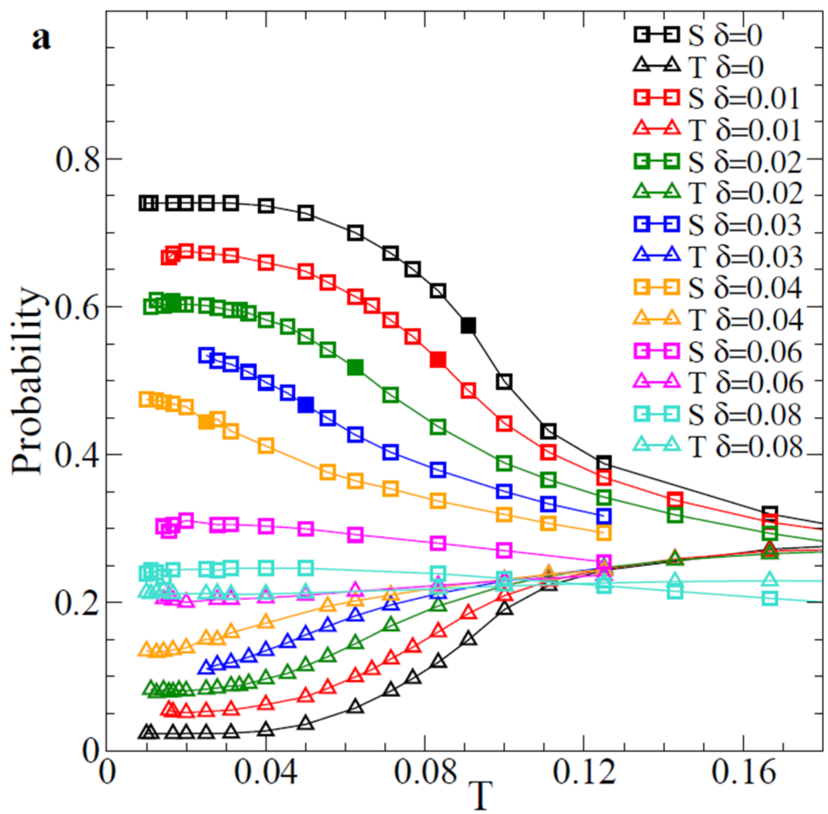
Physics

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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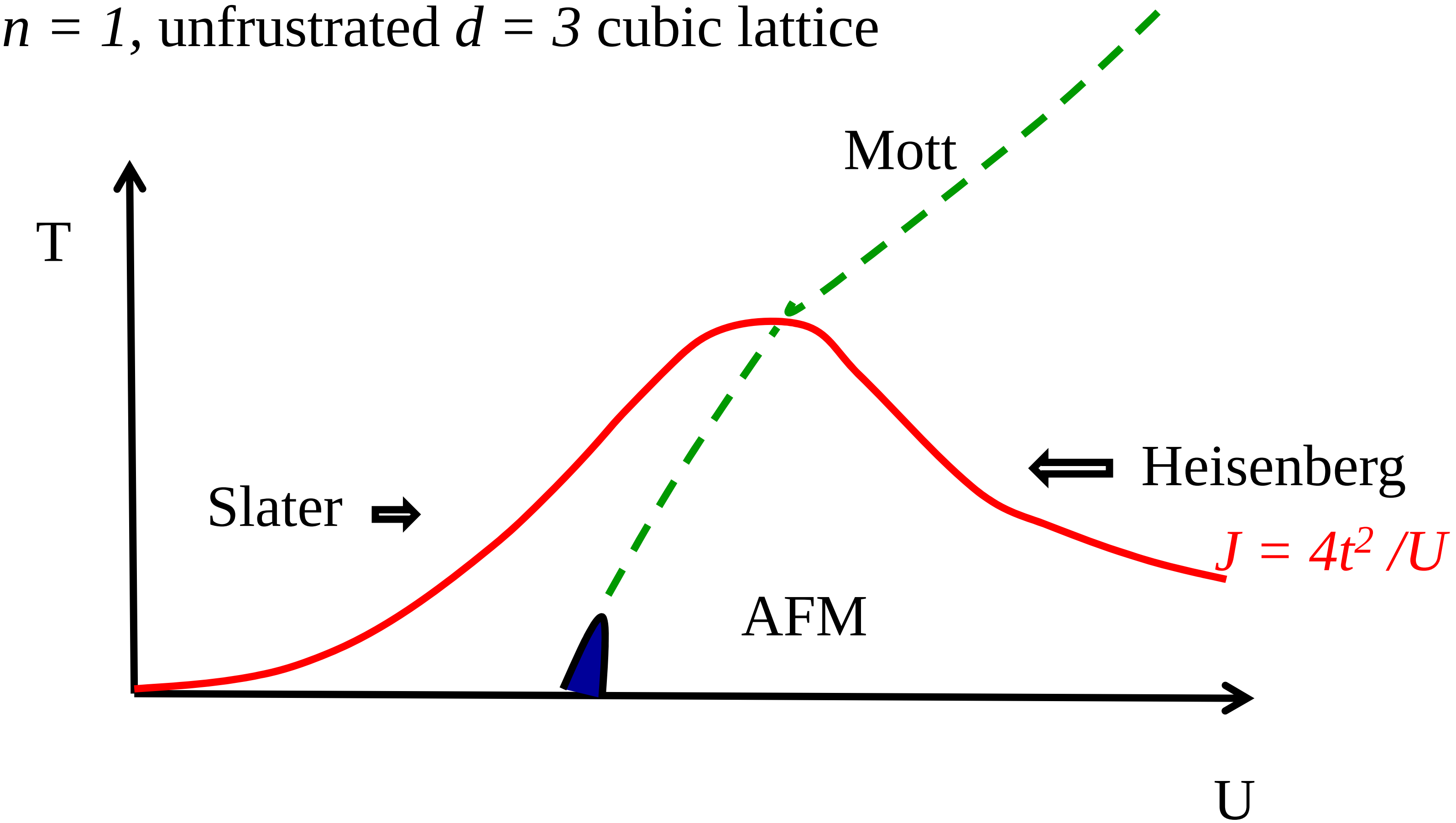
Crossovers inside the AFM phase

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



Giovanni Sordi

Patrick Sémon

Lorenzo Fratino

Finite *T* phase diagram Superconductivity

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

Fratino et al.

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

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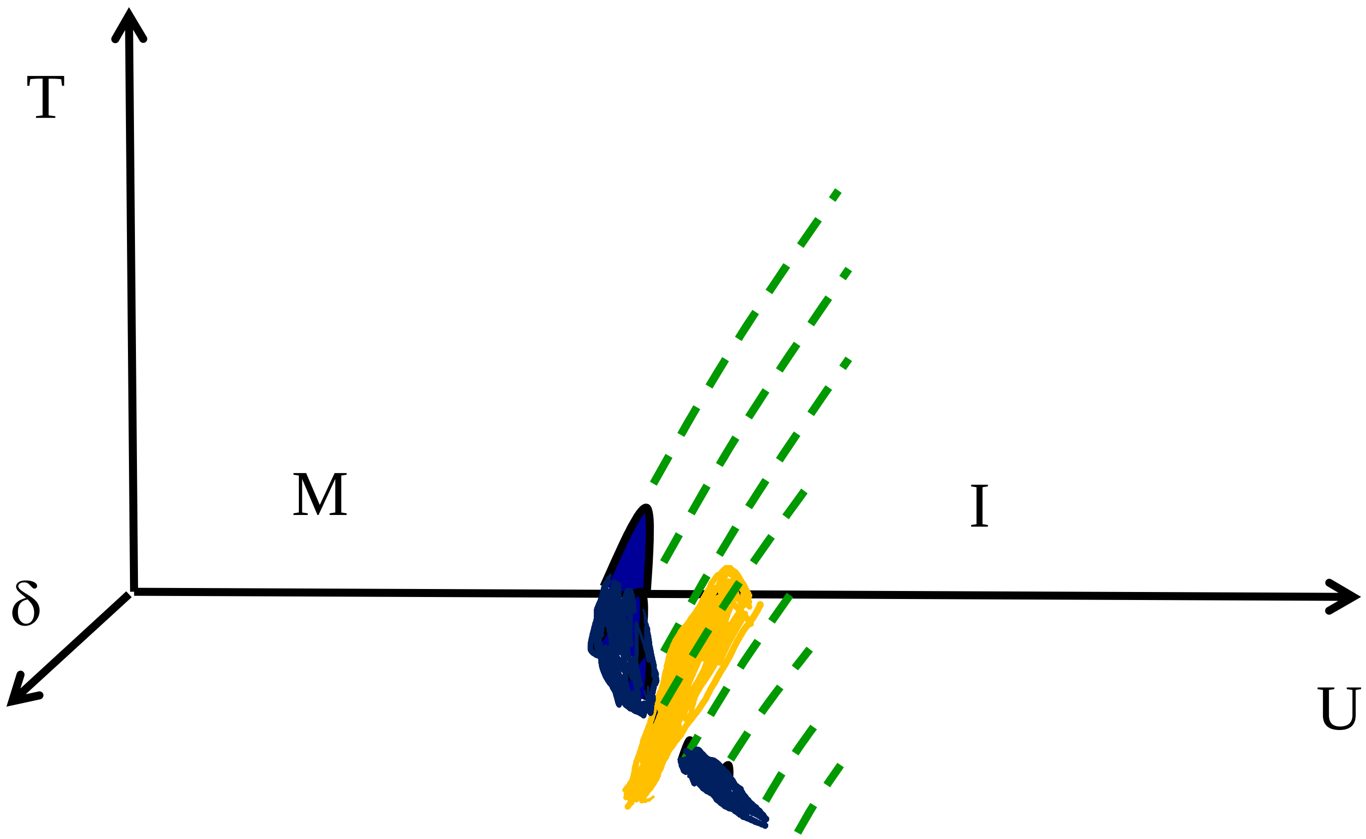
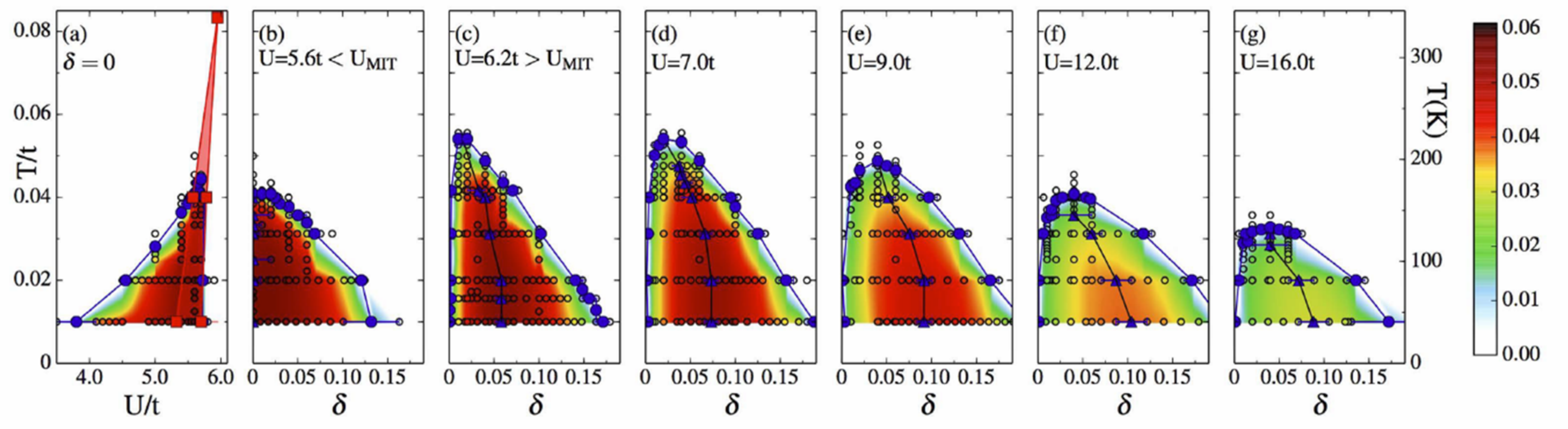
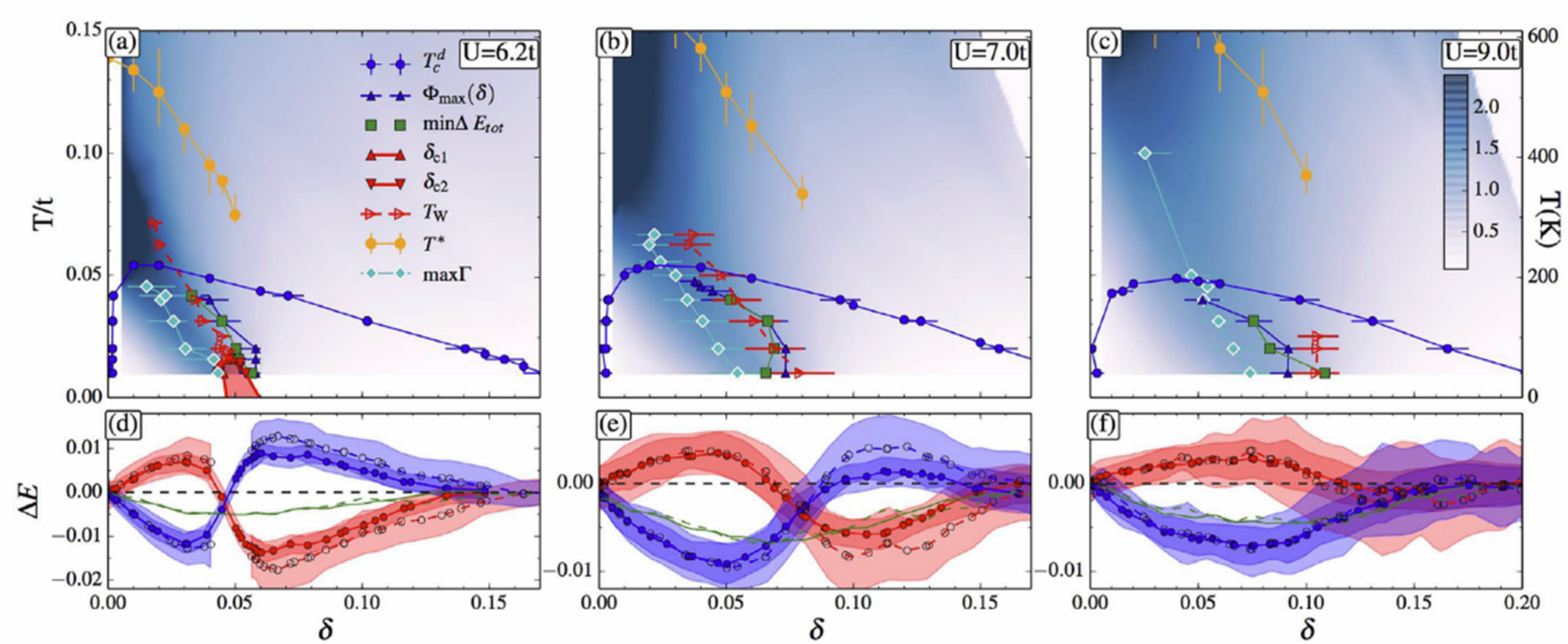
Superconductiviy in Doped Mott insulator

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



An organizing principle





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

3 bands, charge transfer insulator

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

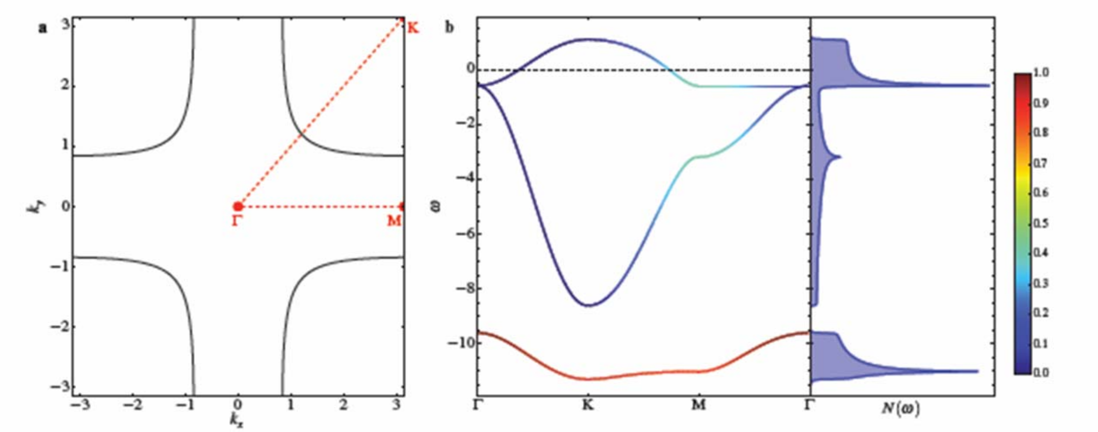
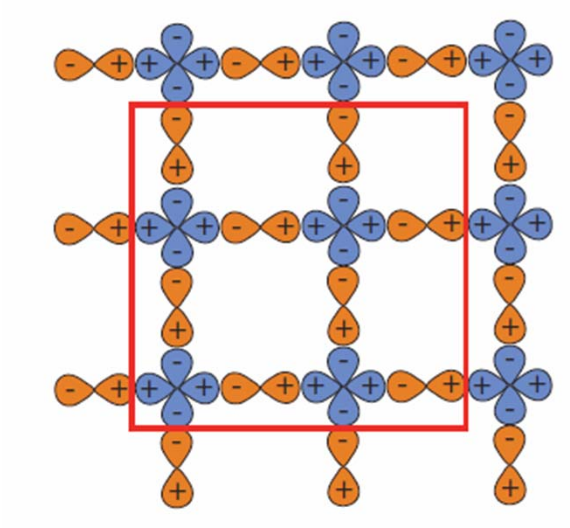


FIG. 2. (a) Noninteracting Fermi surface for the model parameter investigated in Fig. 1a of main text, namely $\epsilon_p = 9$, $t_{pp} = 1$, $t_{pd} = 1.5$, which gives a total occupation n_{tot} equal to five. (b) Non-interacting band structure for the same model parameter along with the resulting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



Giovanni Sordi

Lorenzo Fratino

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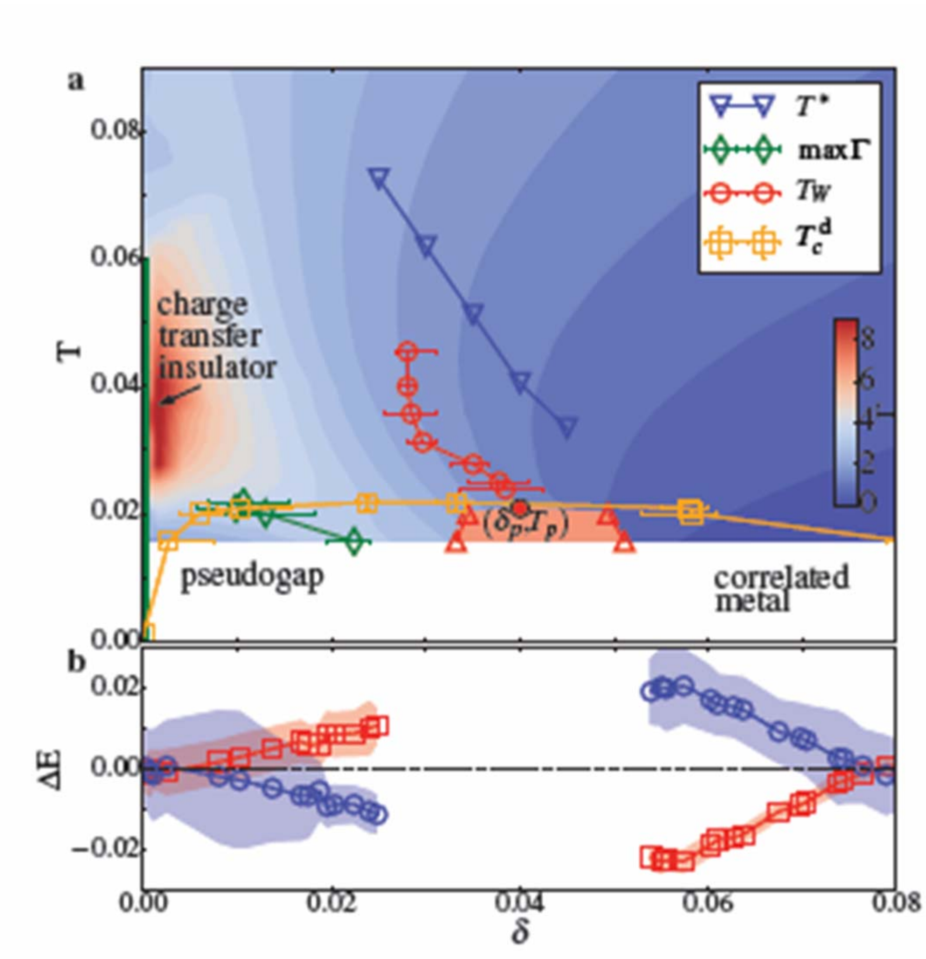
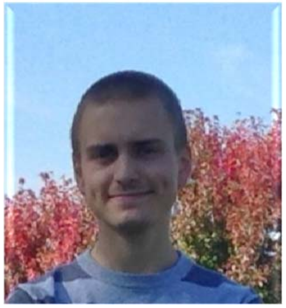
3 bands, charge transfer insulator



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



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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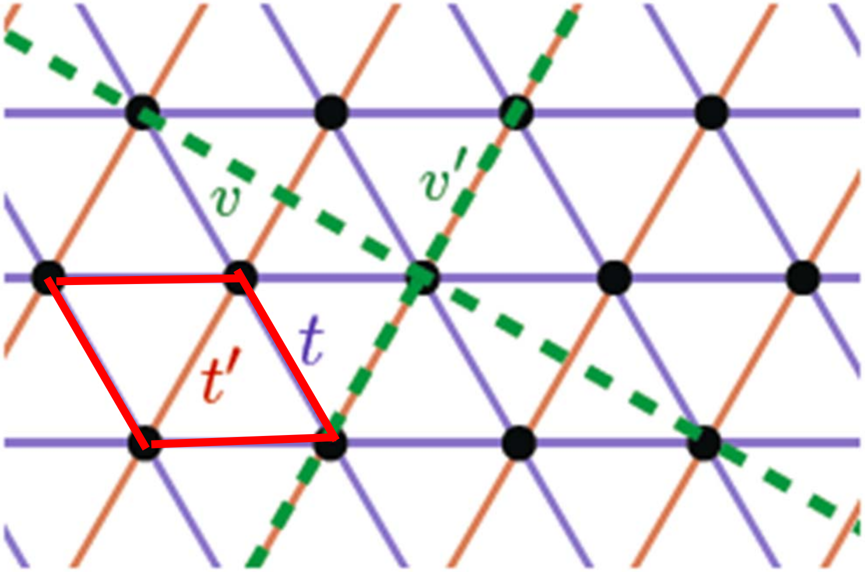
Anisotropic triangular lattice



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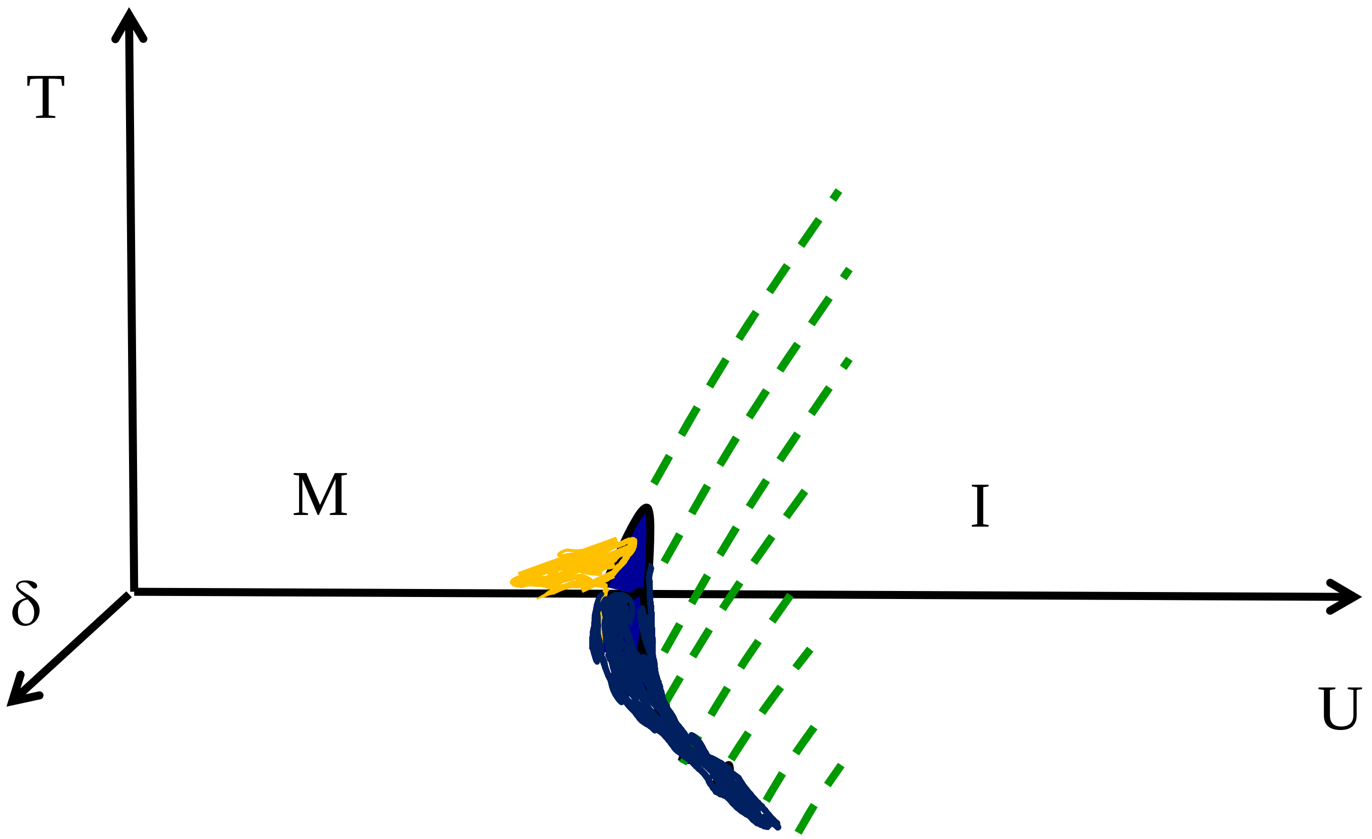
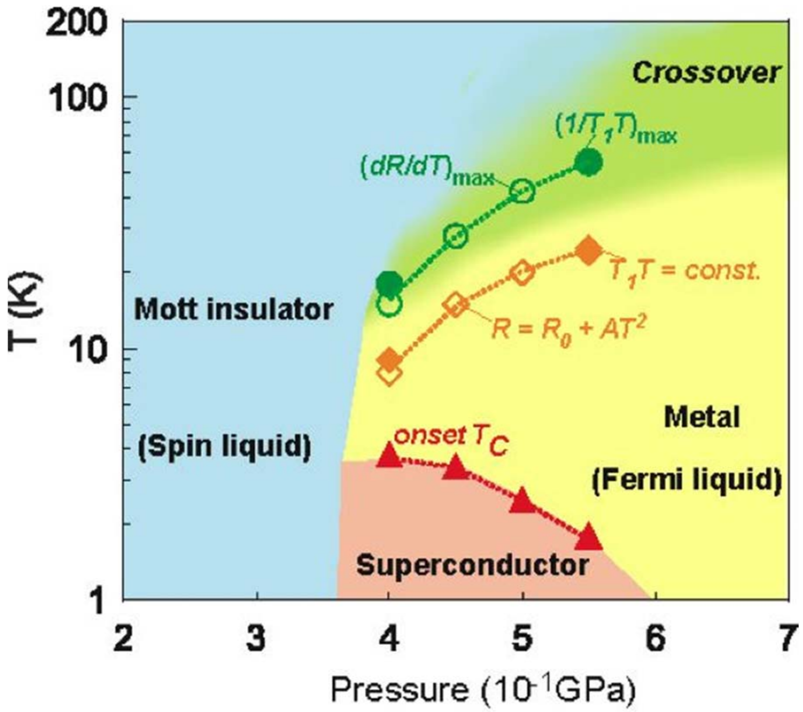
Superconductivity near the Mott transition

n = 1, d = 2 square lattice



Phase diagram at *n = 1*

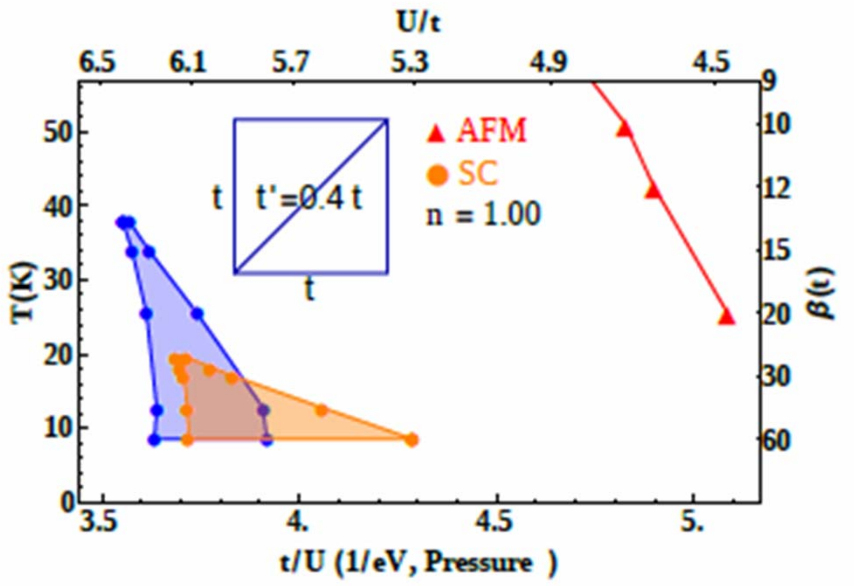
$X = Cu_2(CN)_3$ ($t' \sim t$)

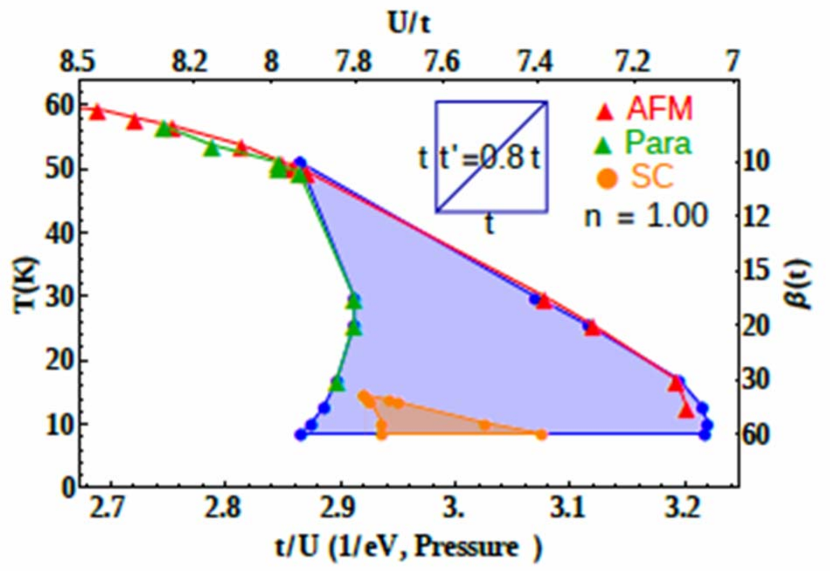


Y. Kurisaki, et al.
Phys. Rev. Lett. **95**, 177001(2005)

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

Effect of frustration on Mott transition ($n = 1$)

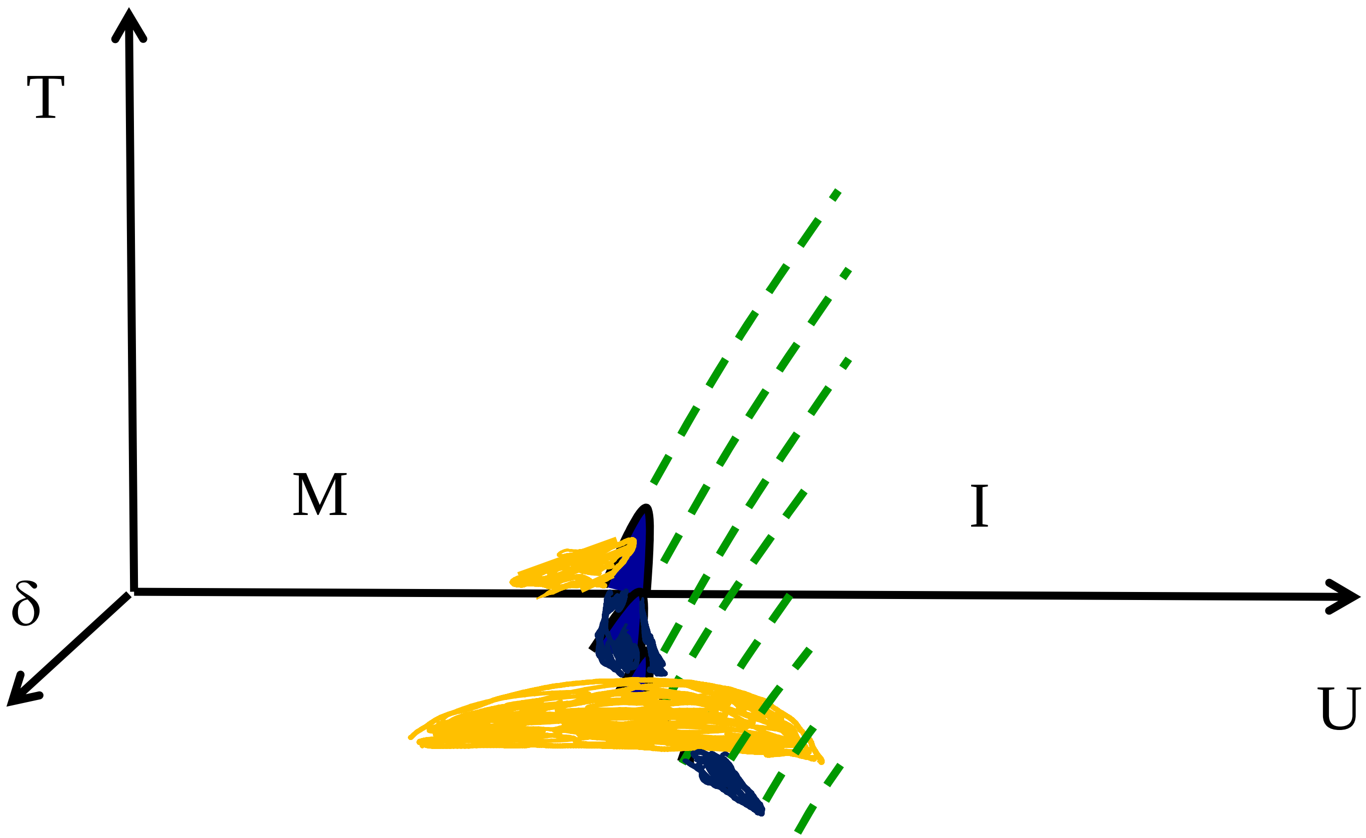




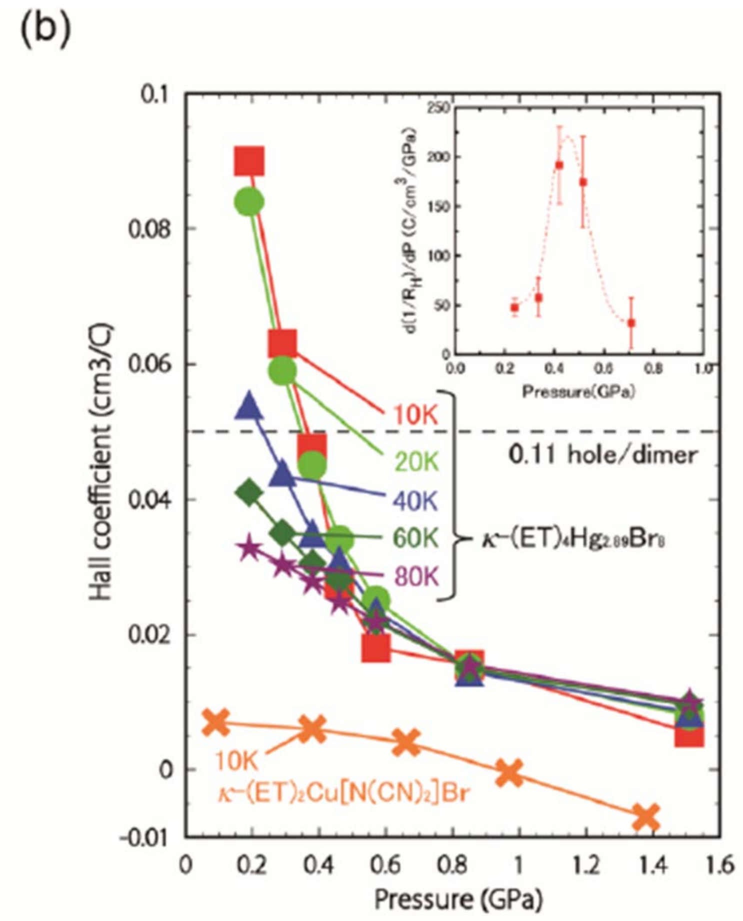
Doped Organics

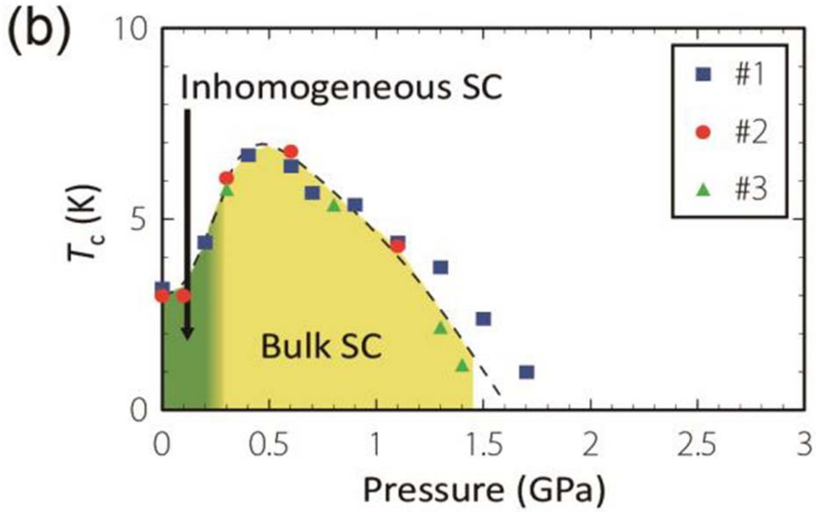
Doped organics

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



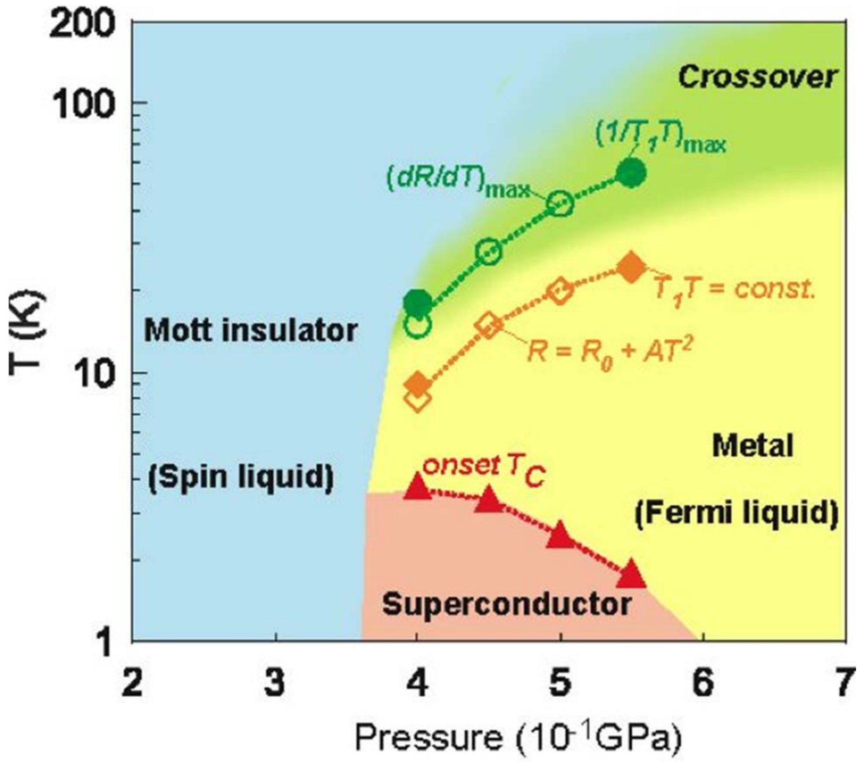
Doped BEDT

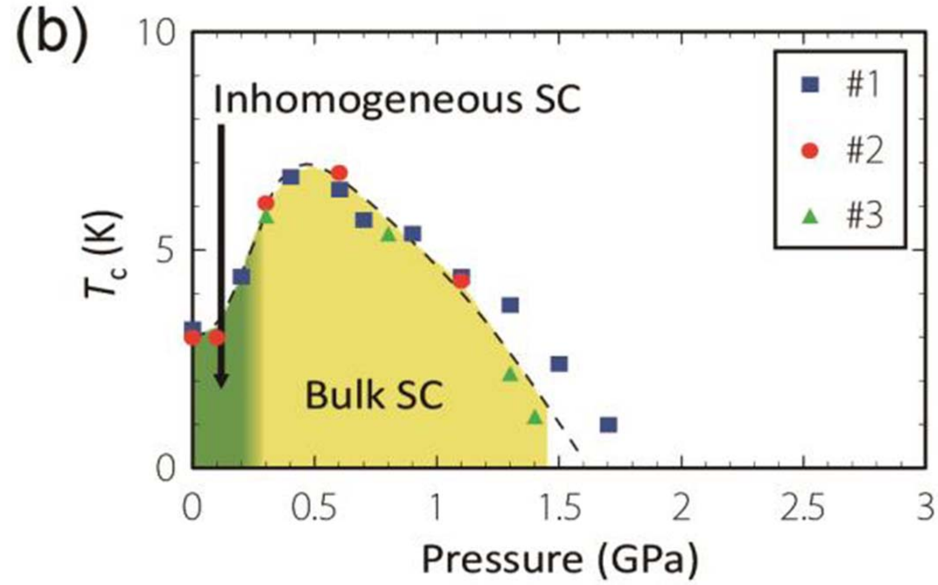




H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

Doped BEDT





$n = 1$

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

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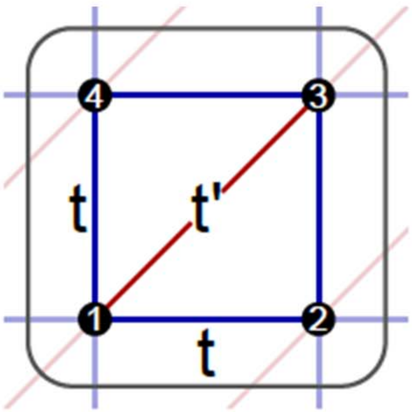
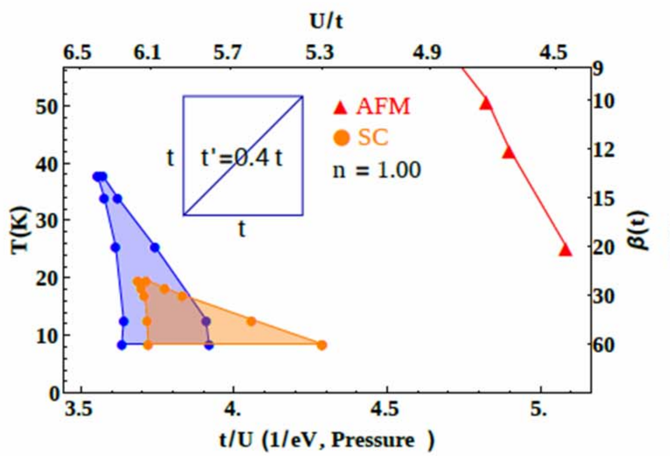
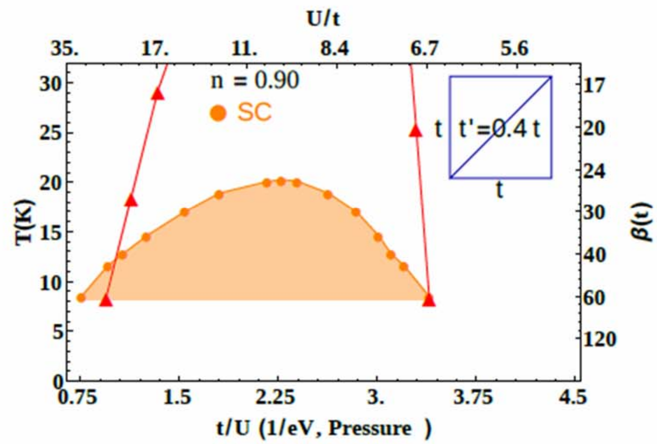
t’=0.4t





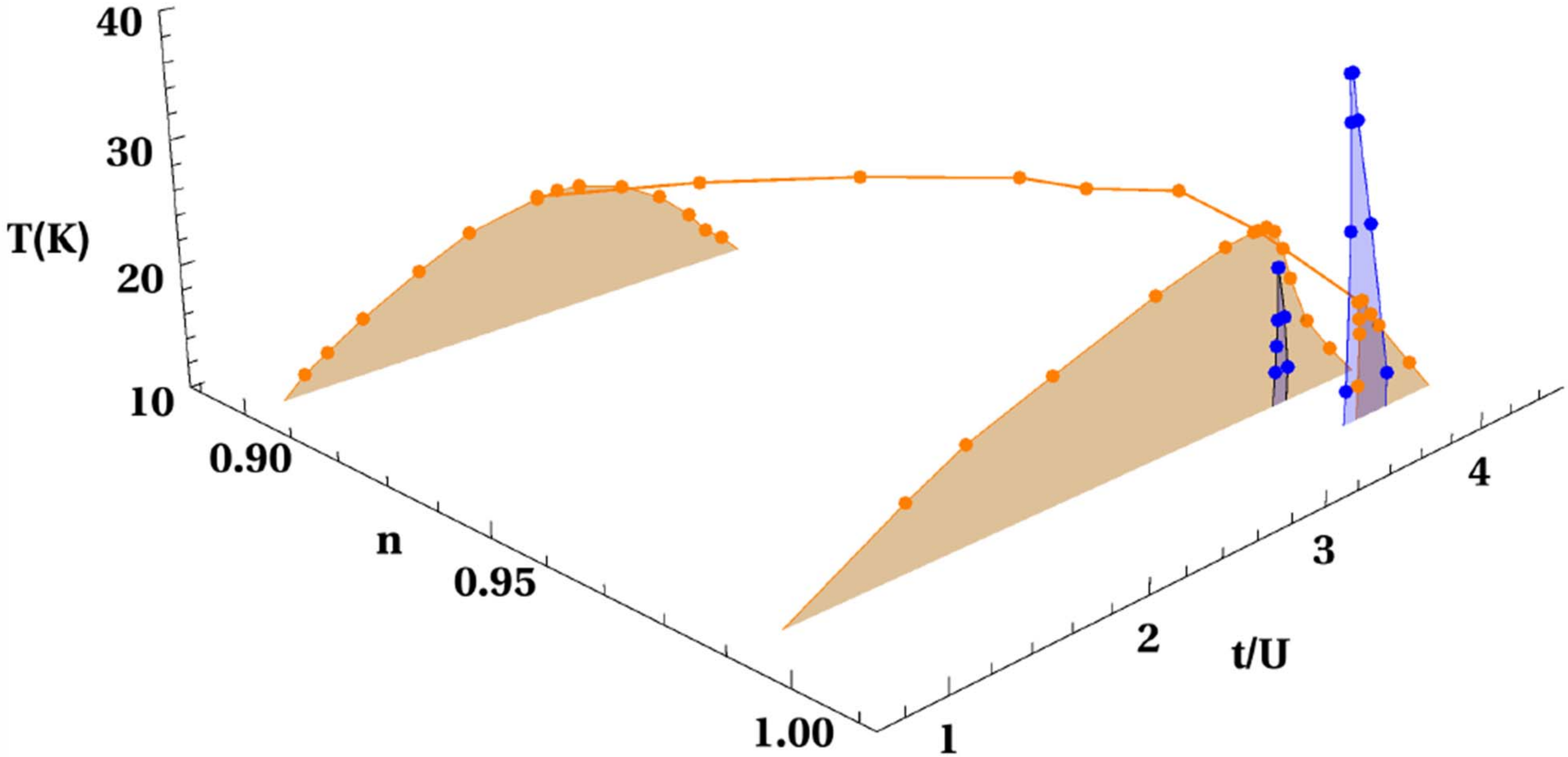
(a)



(c)

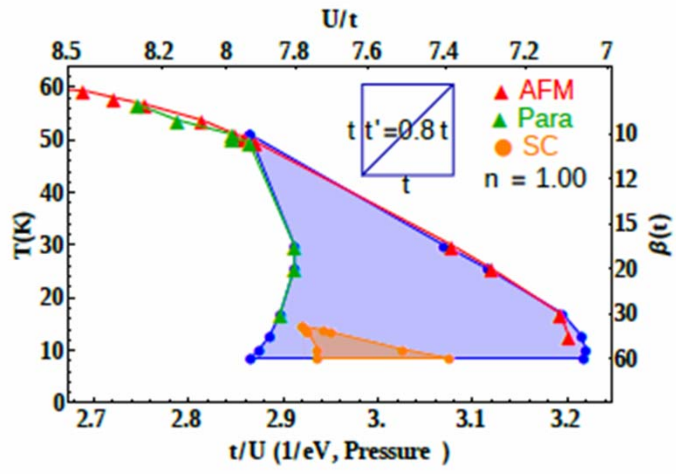
Compare: T. Watanabe, H. Yokoyama and M. Ogata JPS Conf. Proc. **3**, 013004 (2014)

$t' = 0.4t$ overview

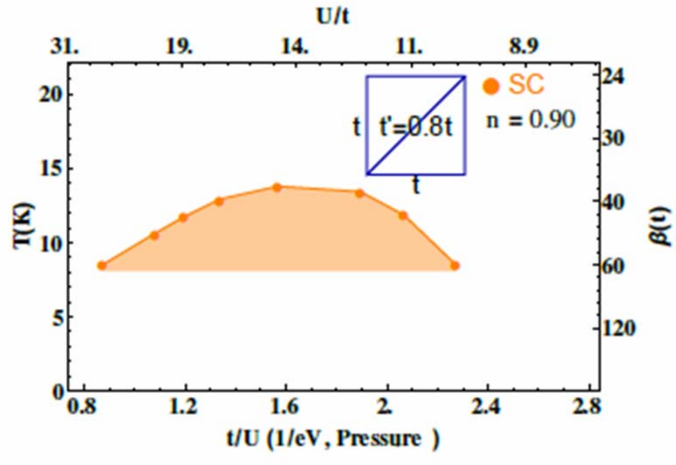


Compare: T. Watanabe, H. Yokoyama and M. Ogata
JPS Conf. Proc. **3**, 013004 (2014)

t’ = 0.8 t



(a)



(b)

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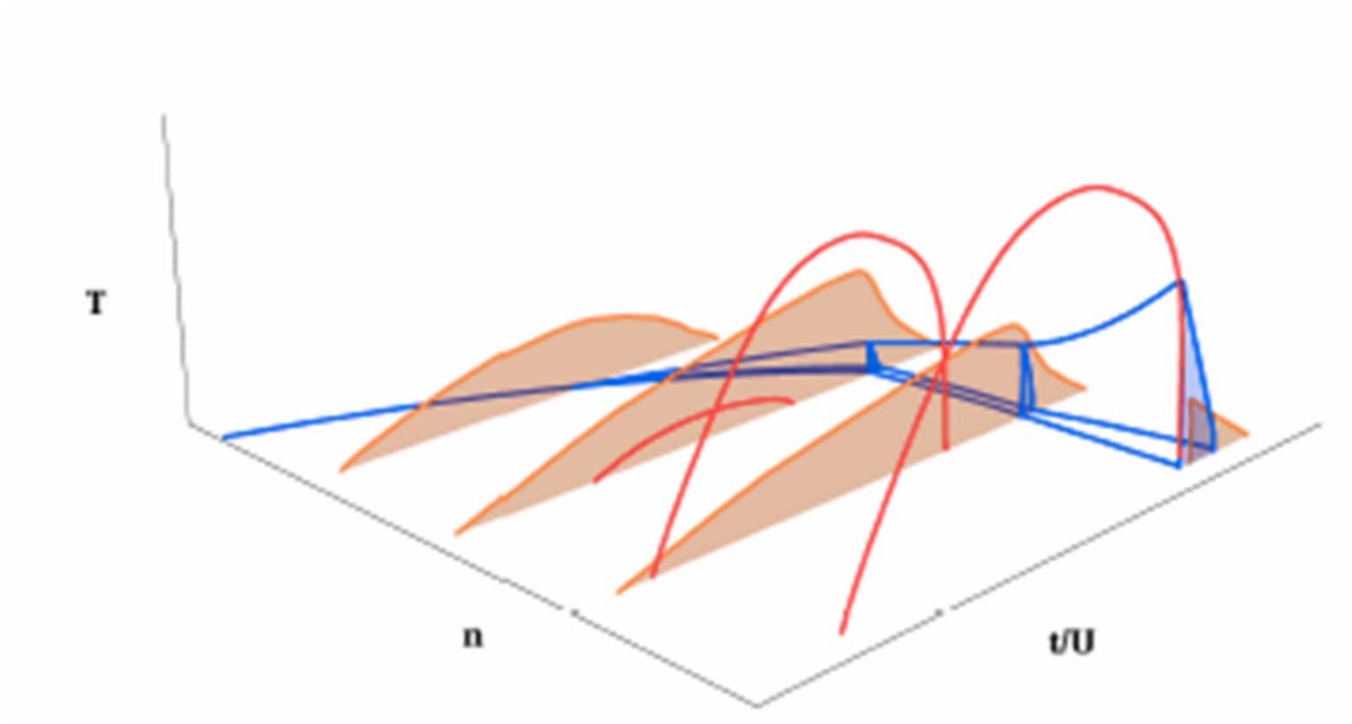
Generic case highly frustrated case



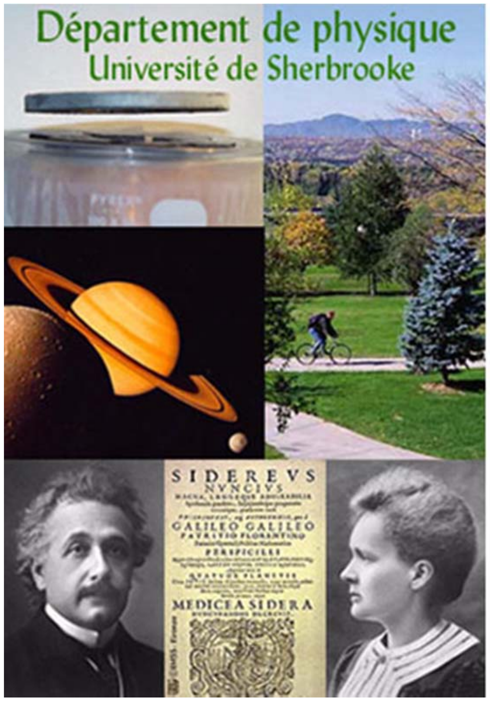
Summary : organics

- Agreement with experiment
  - SC: larger T_c and broader P range if doped
  - Larger frustration: Decrease T_N *much more* than T_c
  - Normal state metal to pseudogap crossover
- Predictions
  - First order transition at low T in normal state (B induced)
  - Crossovers in SC state associated with normal state.
- Physics
  - SC dome without an AFM QCP. Extension of Mott
  - SC from short range J.
  - T_c dome maximum near normal state 1st order

Summary

- AFM QCP for a heavy-fermion model
- No QCP: First order transition that extends Mott physics away from half-filling
- Is an organizing principle for
  - The normal and superconducting states
  - Cuprates and organics are examples
  - Predictions for organics
- Mechanism: *J* short-range (not shown)

André-Marie Tremblay



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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.)

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