And yet they attract: Superconductivity in the presence of strong repulsion

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Tuesday January 17, 2017

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VERITATEM IN CHARITATE

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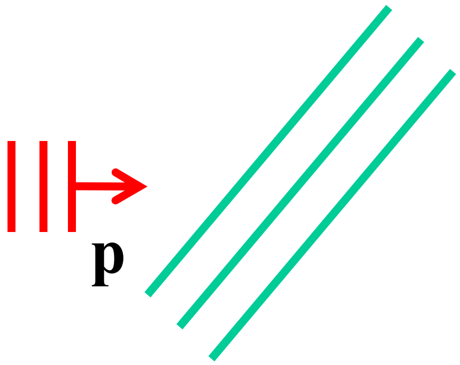
Two pillars of Condensed Matter Physics

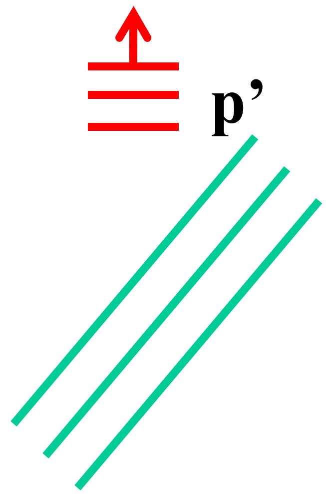
- Band theory
  - DFT
  - Fermi liquid Theory
    - Metals
    - Semiconductors: transistor
- BCS theory of superconductivity
  - Broken symmetry
  - Emergent phenomenon
    - Also in particle physics, astrophysics…

Superconductivity

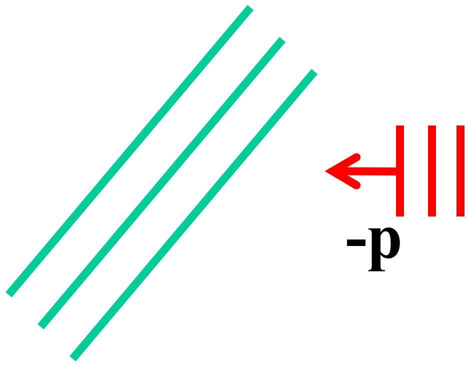
Attraction mechanism in the metallic state



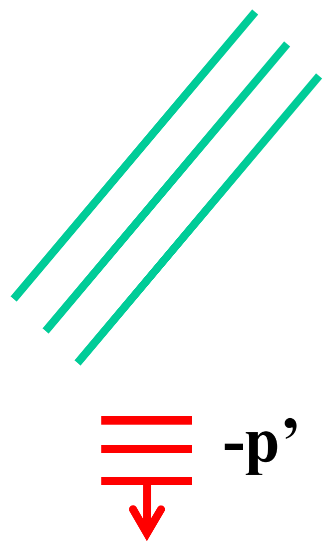
Attraction mechanism in the metallic state



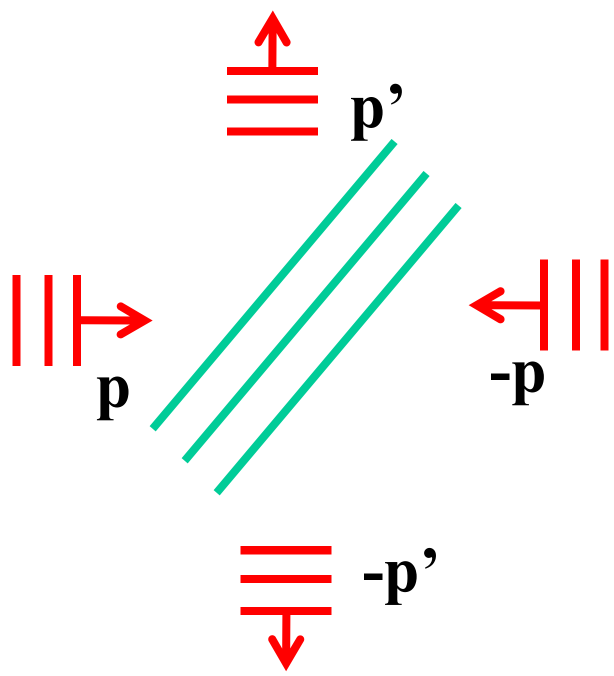
Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



#1 Cooper pair, #2 Phase coherence

$$E_P = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \psi^*_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow} \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow}$$

$$E_P = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \left\langle \psi^*_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow} \right\rangle \left\langle \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow} \right\rangle$$

$$|\mathrm{BCS}(\theta)\rangle = \ldots + e^{iN\theta}|N\rangle + e^{i(N+2)\theta}|N+2\rangle + \ldots .$$

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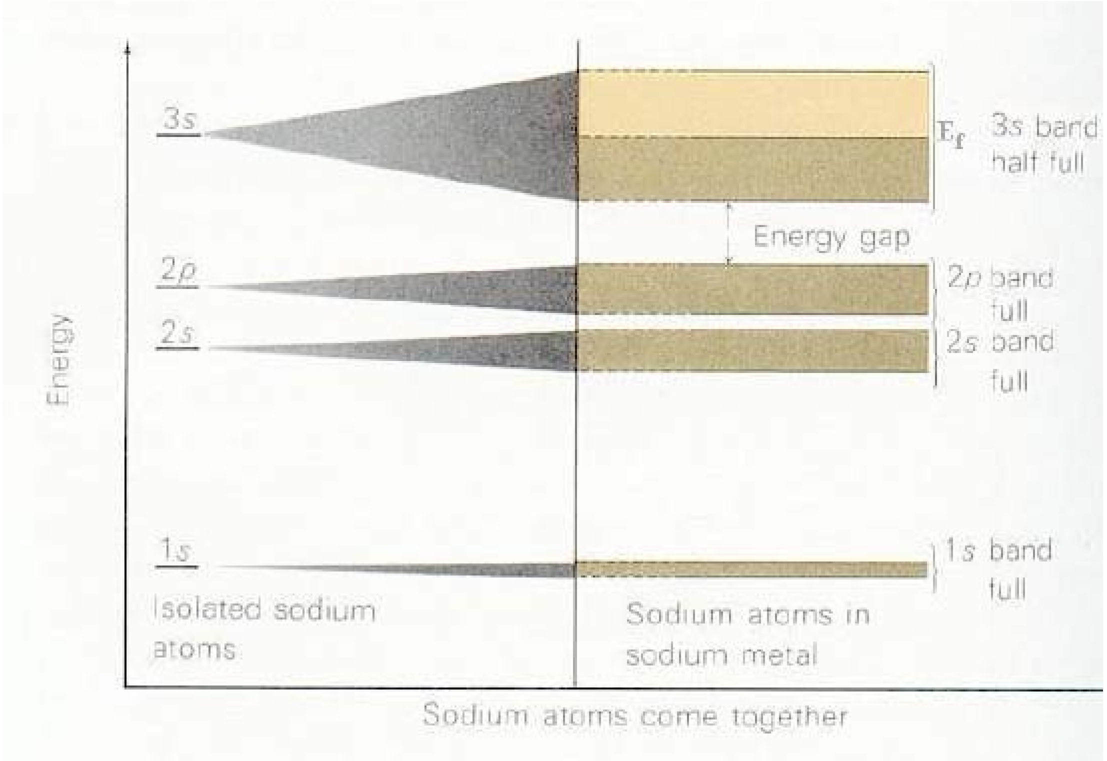
Breakdown of band theory
Half-filled band is metallic?

Metals and insulators: standard theory



http://chem.libretexts.org/Textbook_Maps/

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Half-filled band: Not always a metal

NiO, Boer and Verway

Peierls, 1937

Mott, 1949

« Conventional » Mott transition

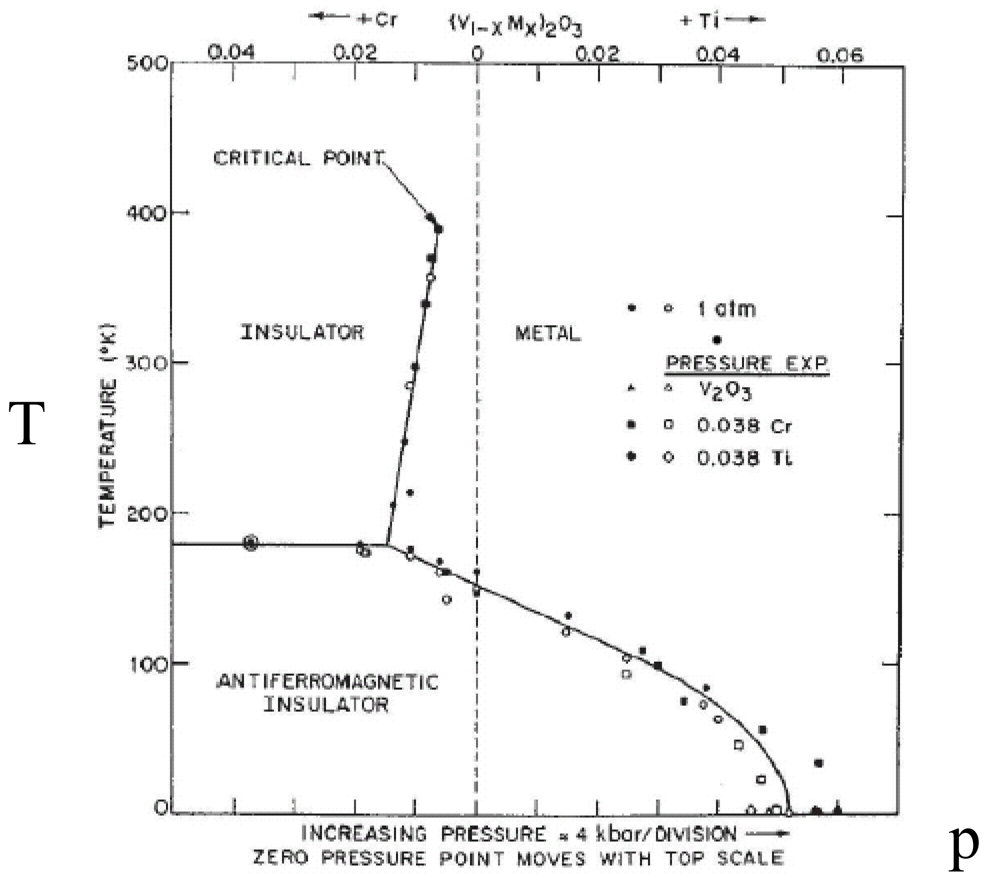
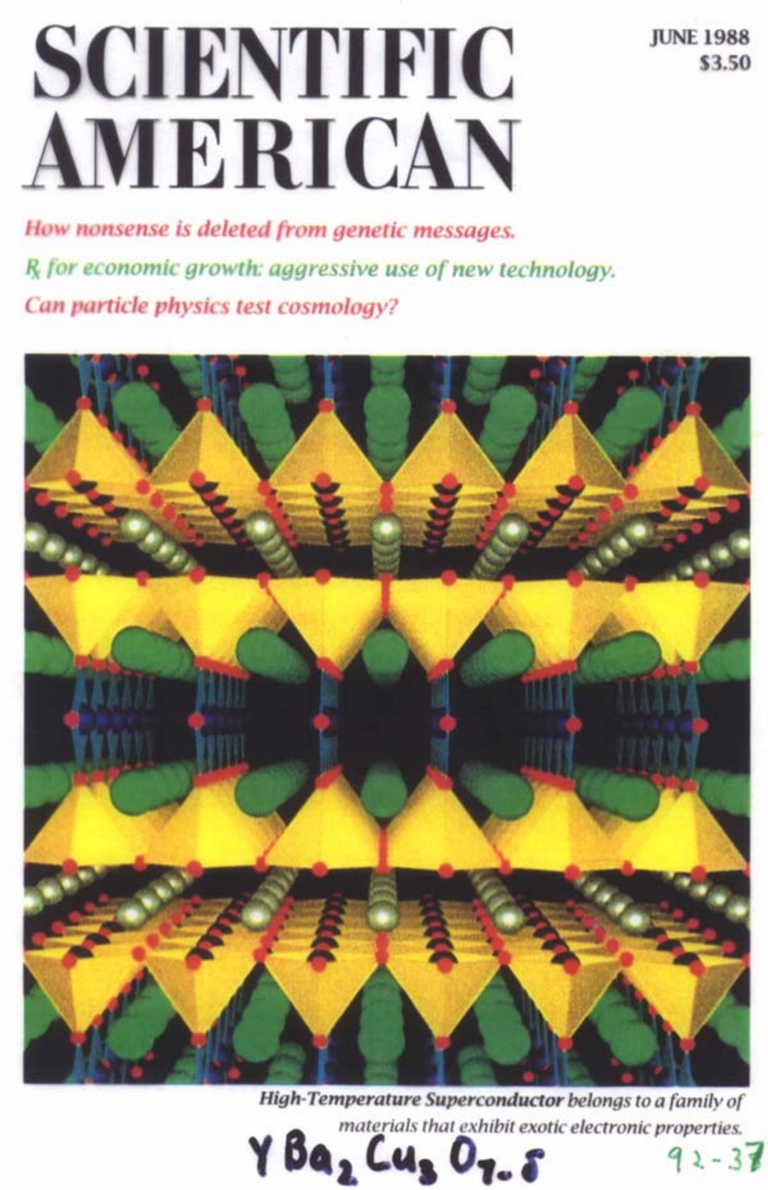
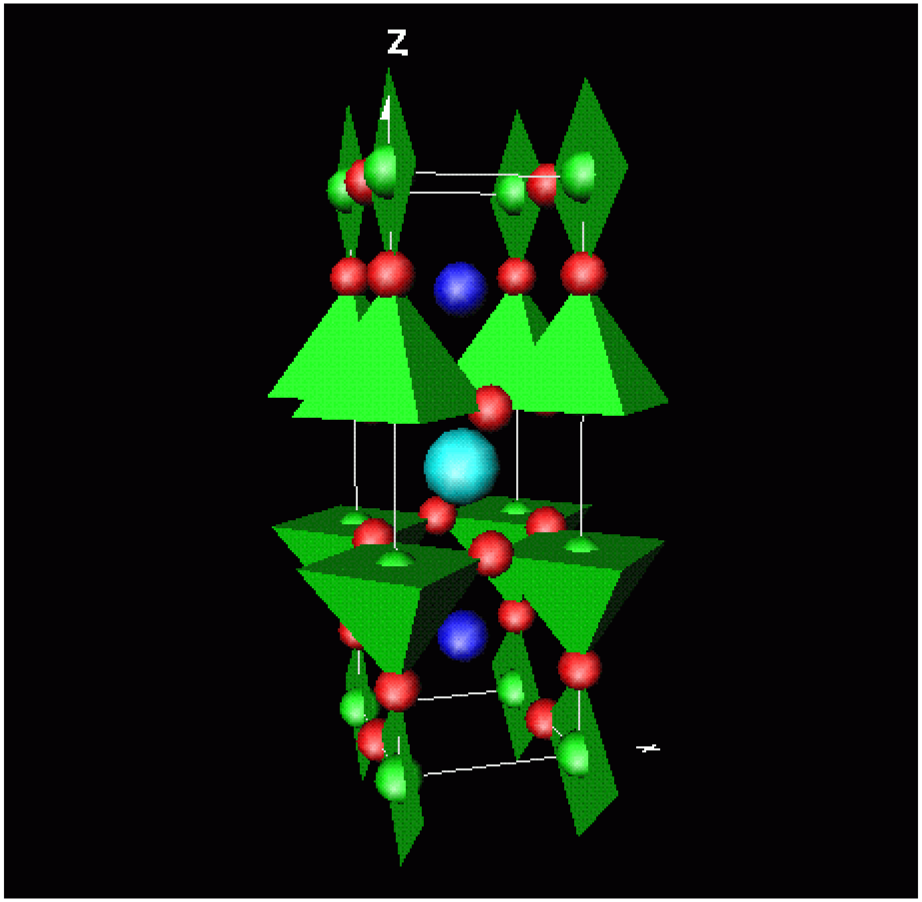


Figure: McWhan, PRB 1970; Limelette, Science 2003

Atomic structure





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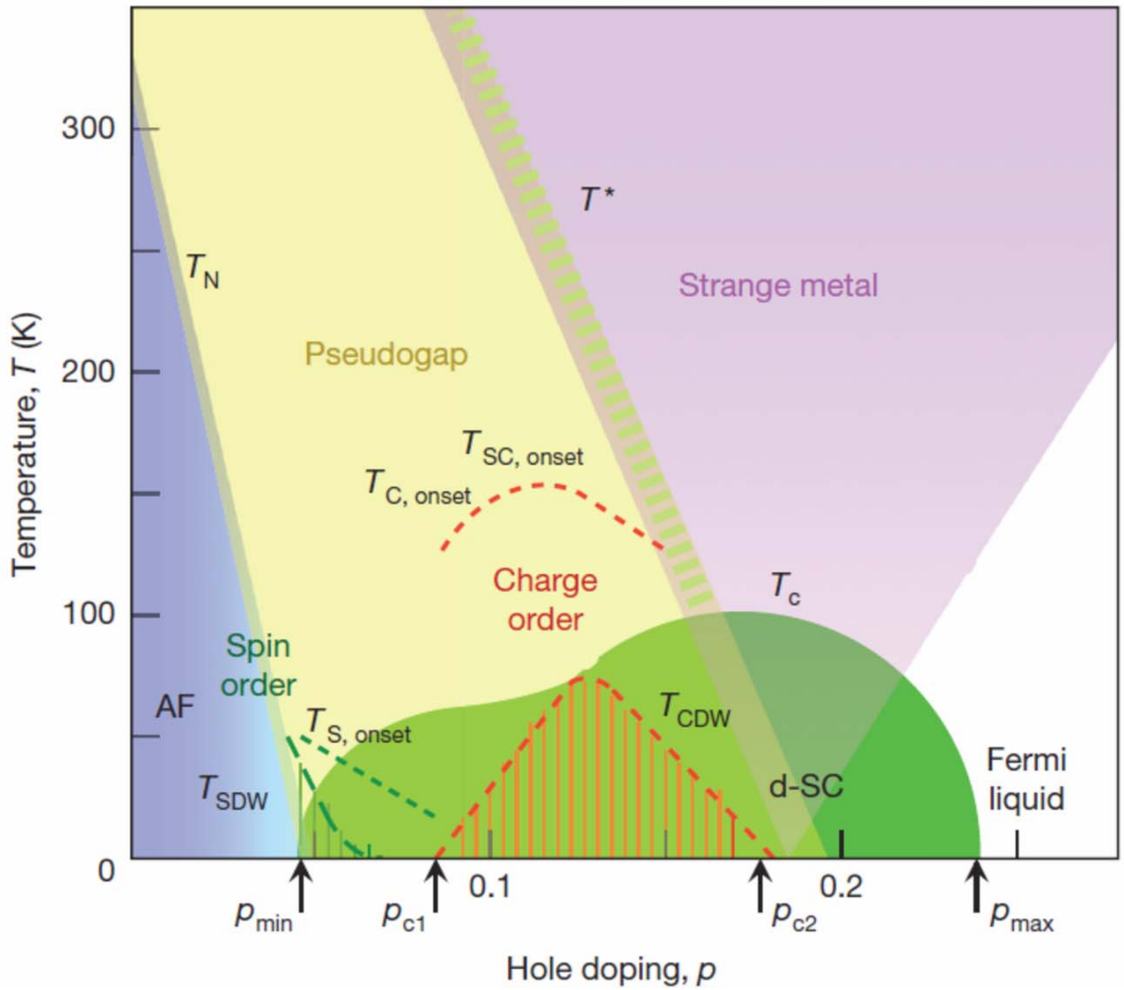
Phase diagram $YBa_2Cu_3O_{7-x}$



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

Outline

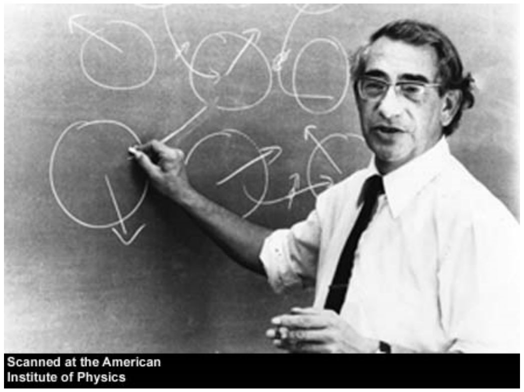
1. The model
2. The method

Part I: Weakly and strongly correlated electrons

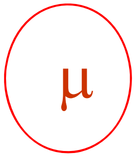
Part II: Strongly correlated superconductivity

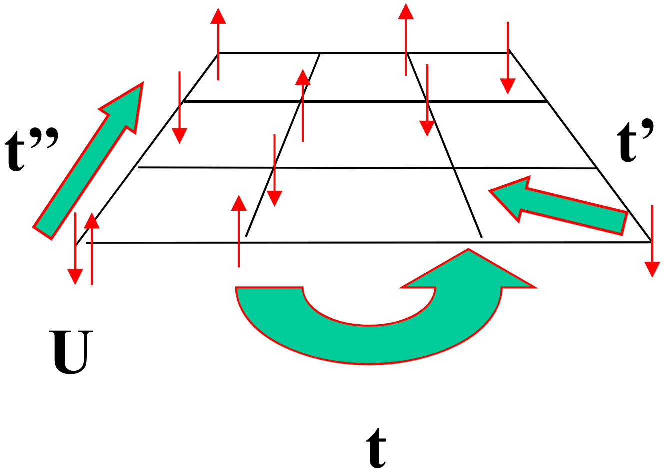
2. The model

Hubbard model



1931-1980





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

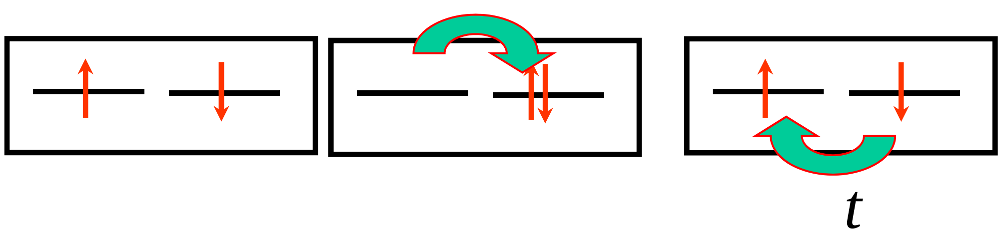
Attn: Charge transfer insulator

Interesting in the general case

No mean-field factorization for d-wave superconductivity

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

Mott transition



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

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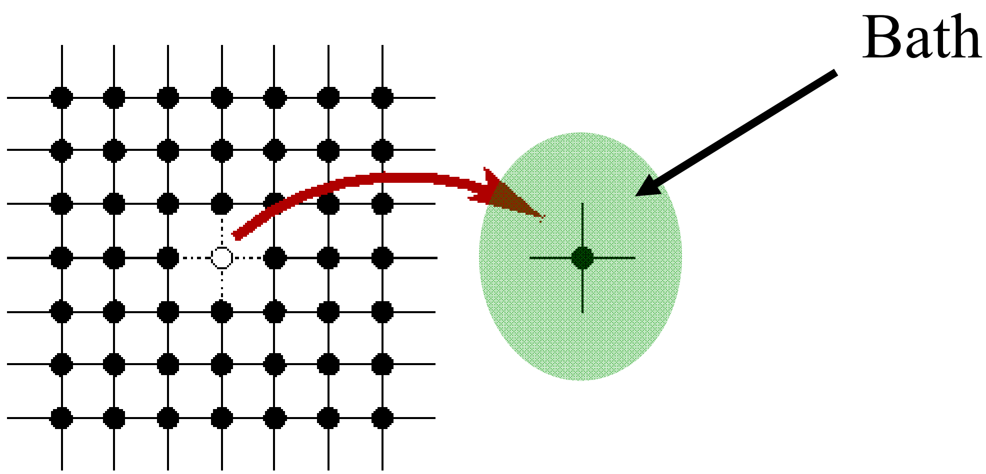
Method for strongly correlated matter

Dynamical Mean Field Theory (+ clusters)

Concept: atomic localized correlations consistent with delocalized aspect

Mott transition and Dynamical Mean-Field Theory. The beginnings in *d = infinity*

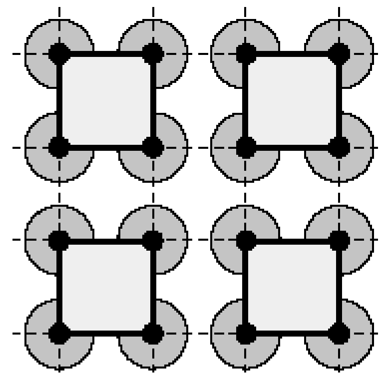


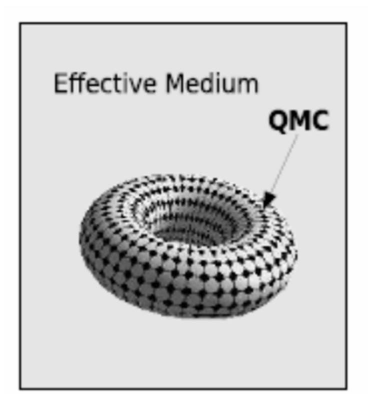
W. Metzner and D. Vollhardt, PRL (1989)
A. Georges and G. Kotliar, PRB (1992)
M. Jarrell PRB (1992)

DMFT, (*d = 3)*

2d Hubbard: Quantum cluster method

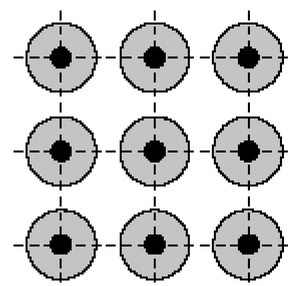
C-DMFT





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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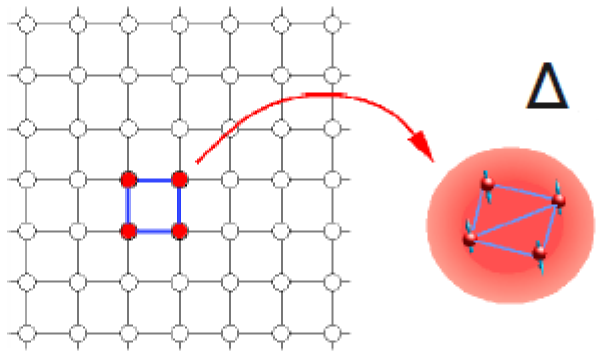
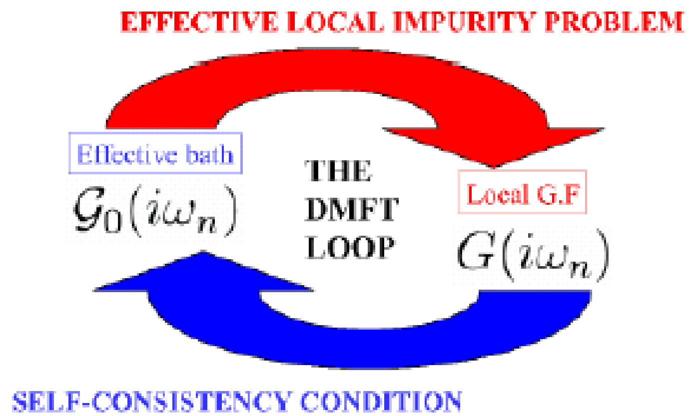
Impurity solver

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





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

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

+ 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

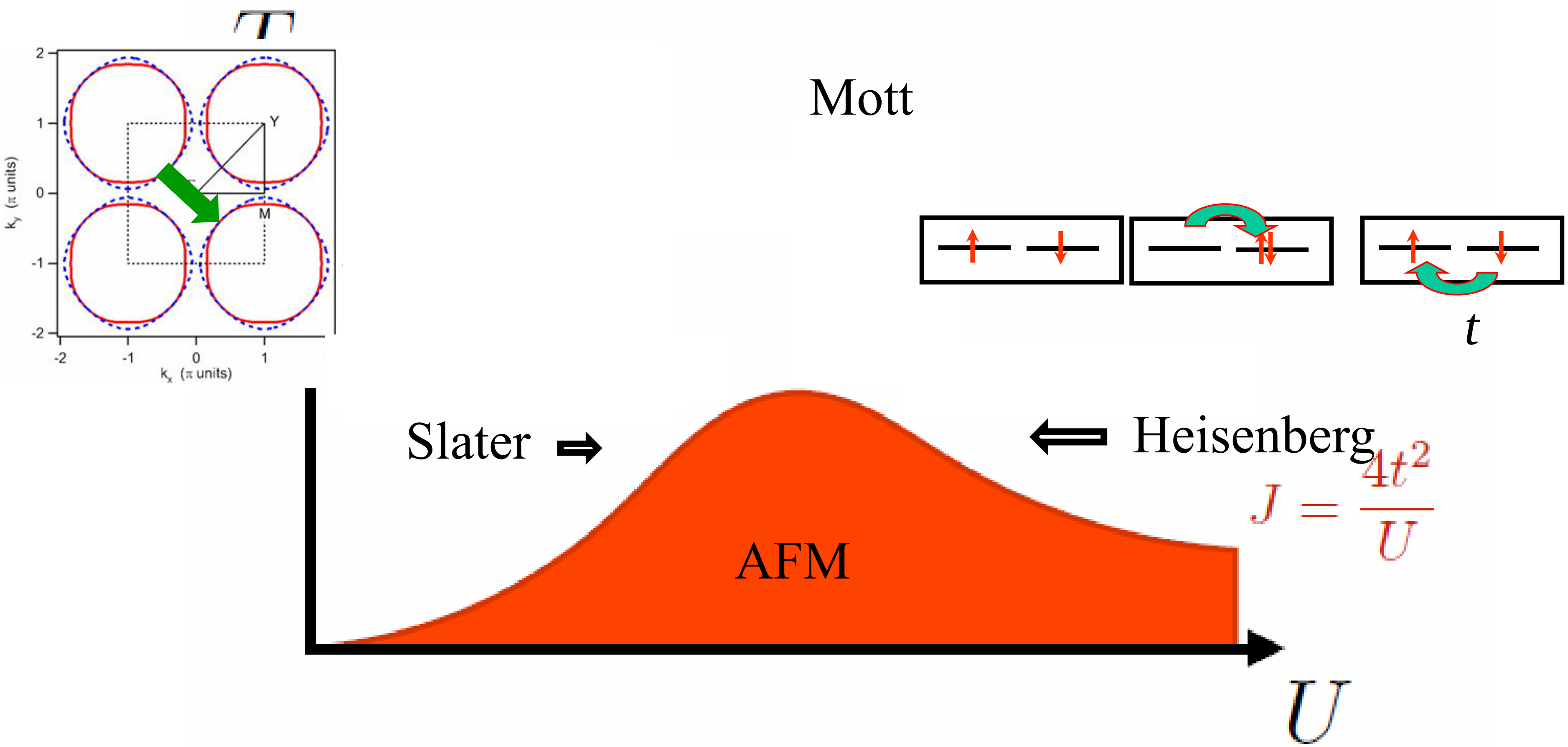
- Europe:
  - Georges, Parcollet, Ferrero, Civelli, (Paris)
  - de Medici (Grenoble) Capone (Italy)
- USA:
  - Gull (Michigan) Millis (Columbia)
  - Kotliar, Haule (Rutgers)
  - Jarrell (Louisiana)
  - Maier, Okamoto (Oakridge)
- Japan
  - Imada (Tokyo) Sakai, Tsunetsugu, Motome

Part I

Weakly vs strongly correlated electrons
Normal and antiferromagnetic state

Weak vs Strong correlations

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



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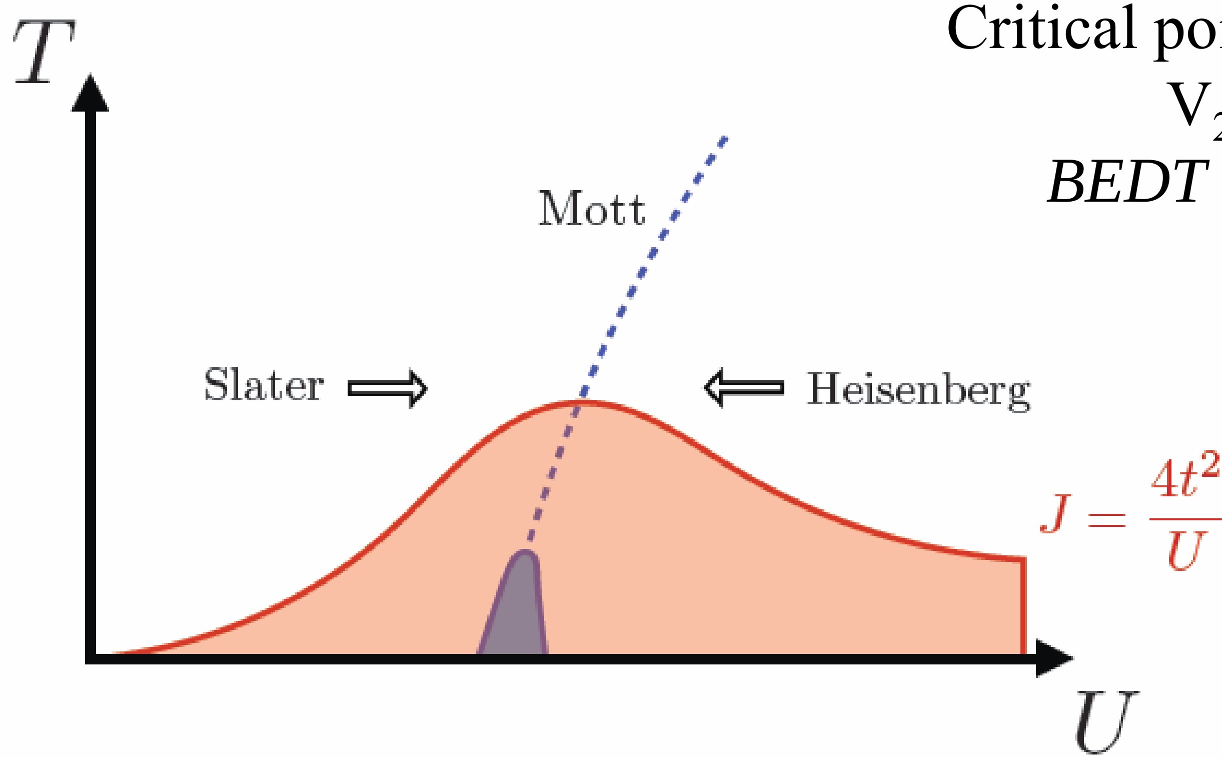
Local moment and Mott transition

n = 1, *d = 2* square lattice

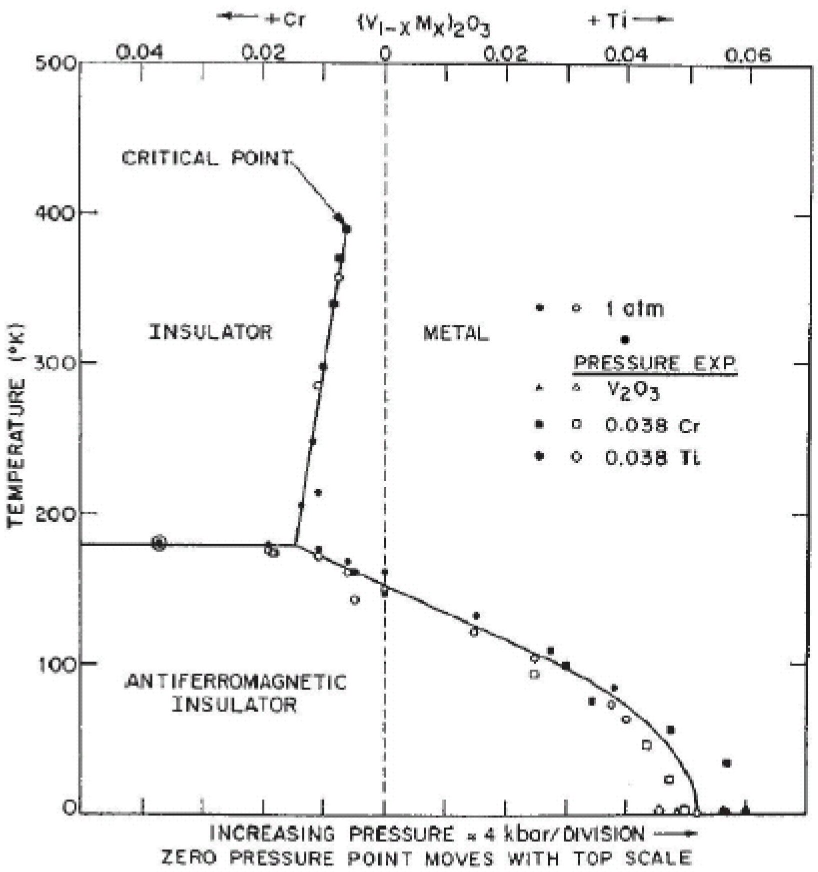


Critical point visible in V_2O_3, *BEDT* organics

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

« Conventional » Mott transition

T

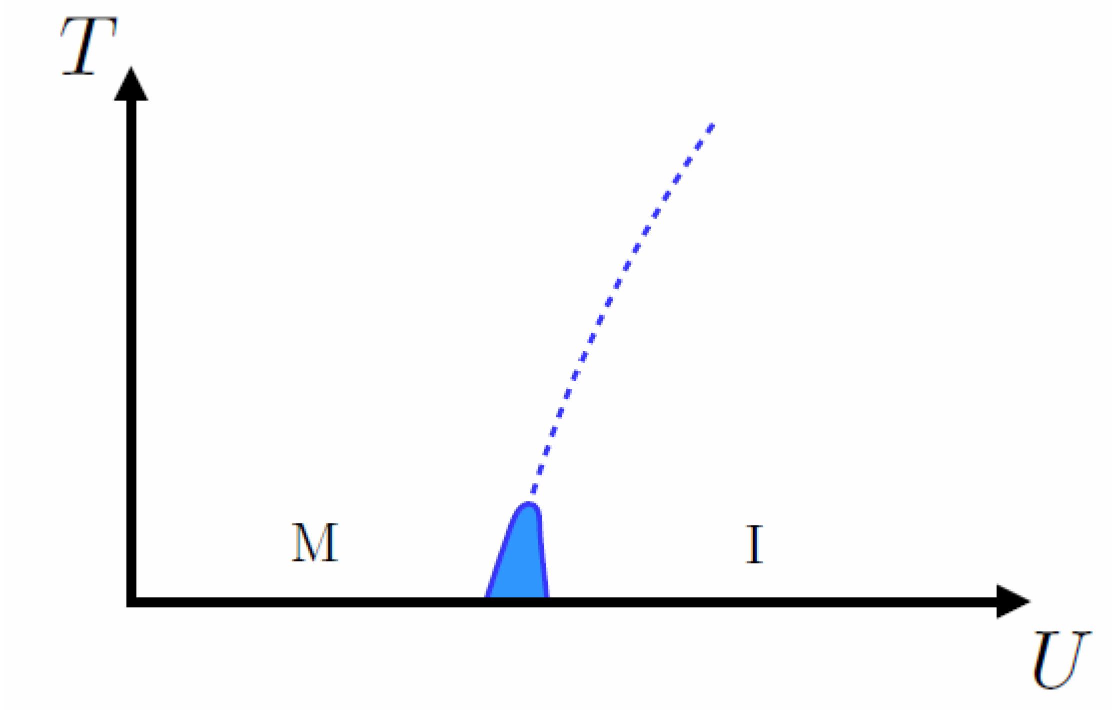


p

Figure: McWhan, PRB 1970; Limelette, Science 2003

Influence of Mott transition away from half-filling

n = 1, d = 2 square lattice



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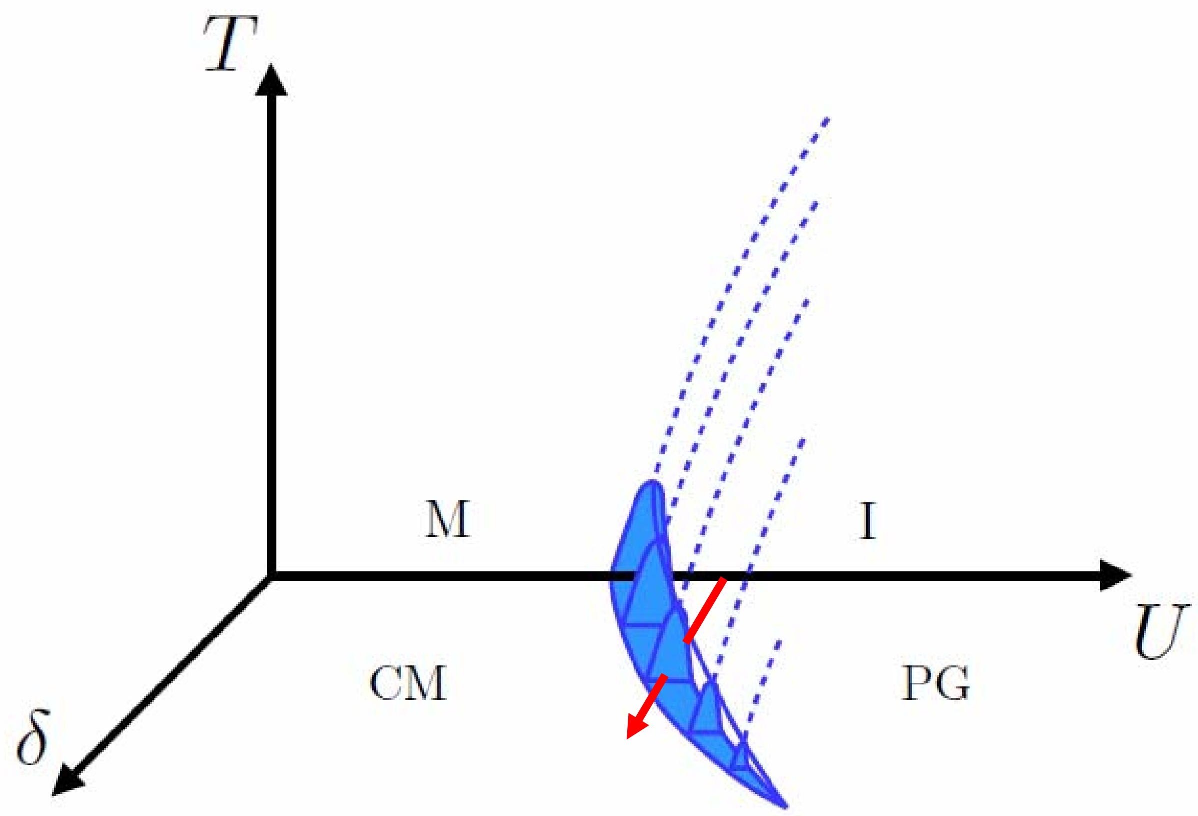
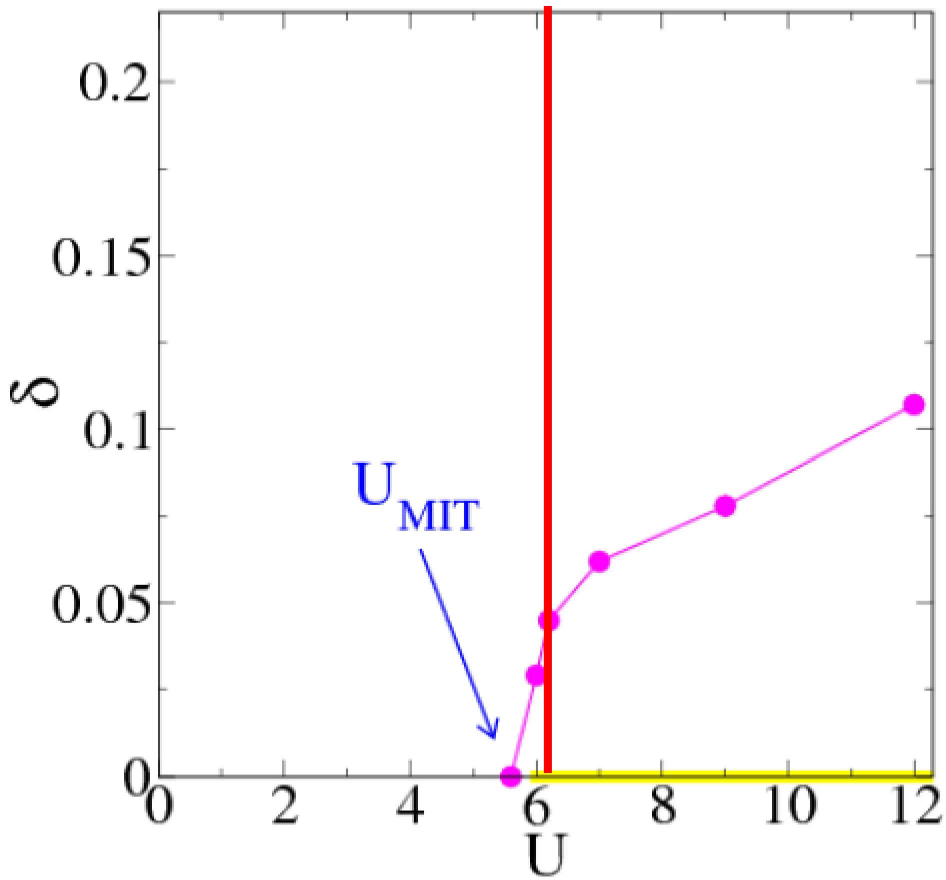
Influence of Mott transition away from half-filling

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

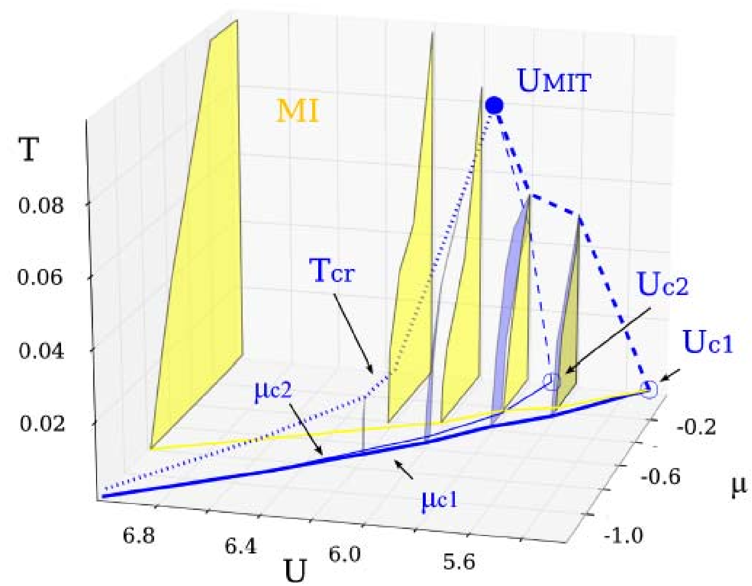


Link to Mott transition up to optimal doping
Another emergent transition

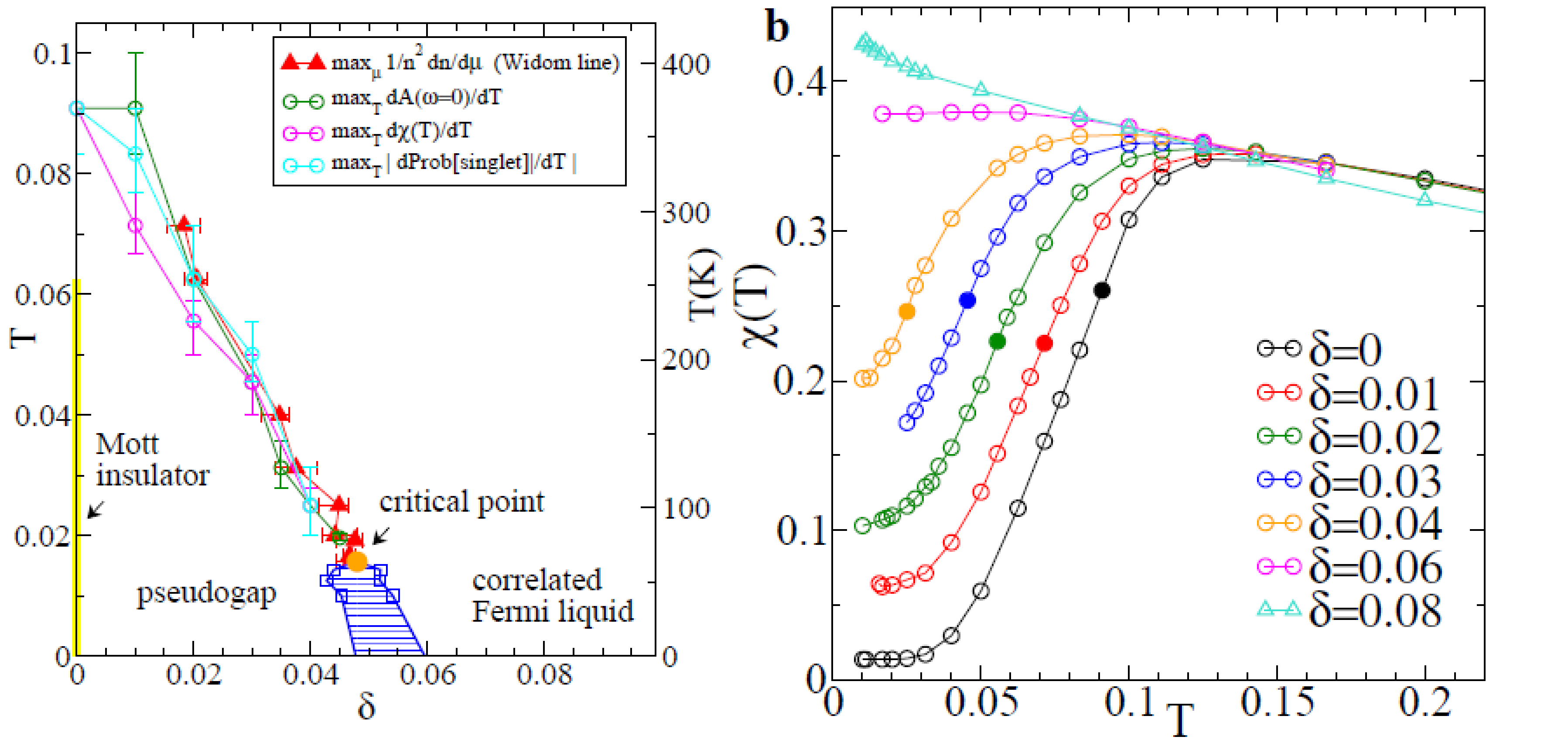
Doping dependence of critical point as a function of *U*



Smaller *D* and *S*

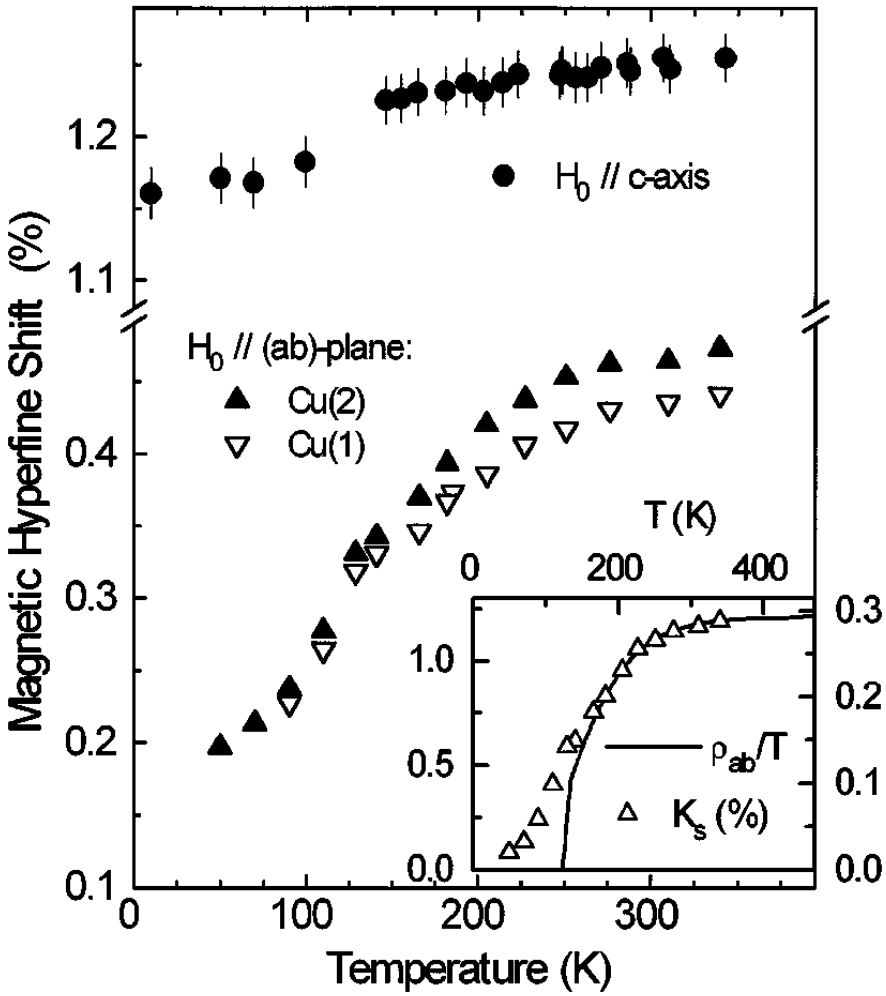


Spin susceptibility



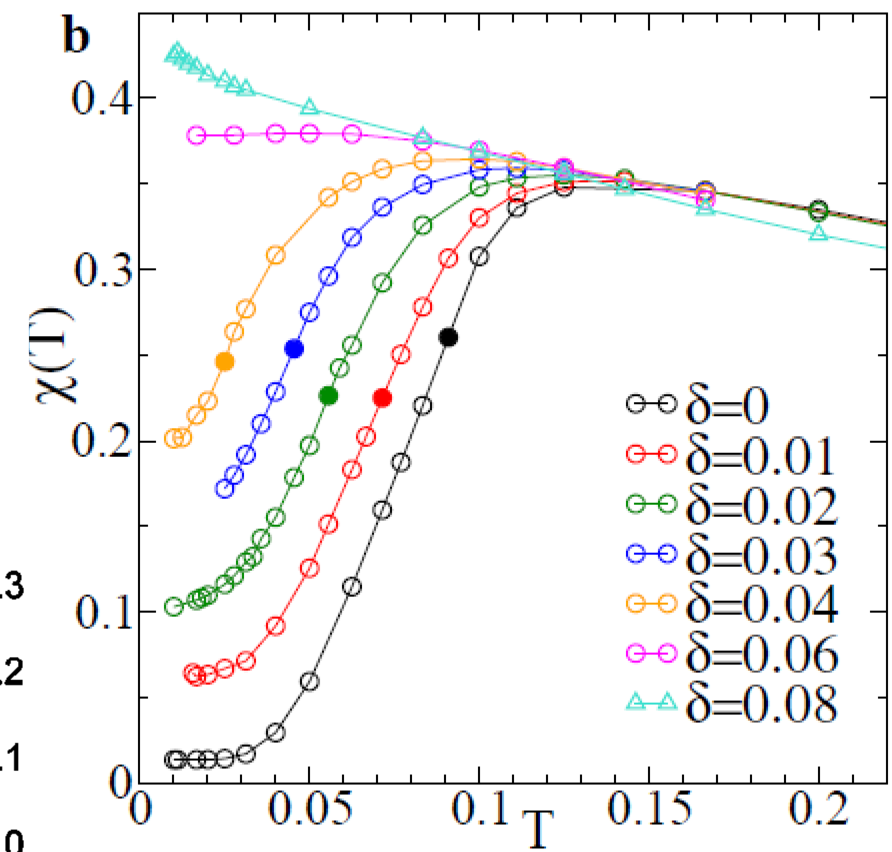
G. Sordi, *et al*. Scientific Reports 2, 547 (2012)

Spin susceptibility



Underdoped Hg1223

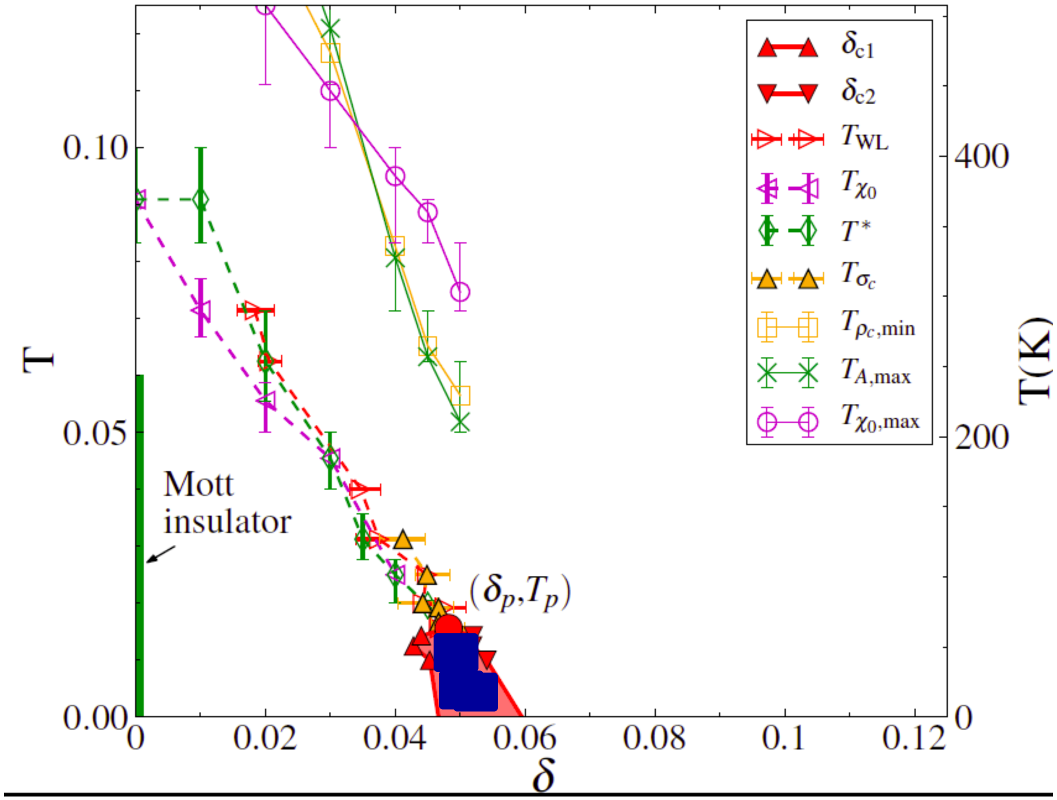
Julien et al. PRL **76,** 4238 (1996)



Two crossover lines

Giovanni Sordi

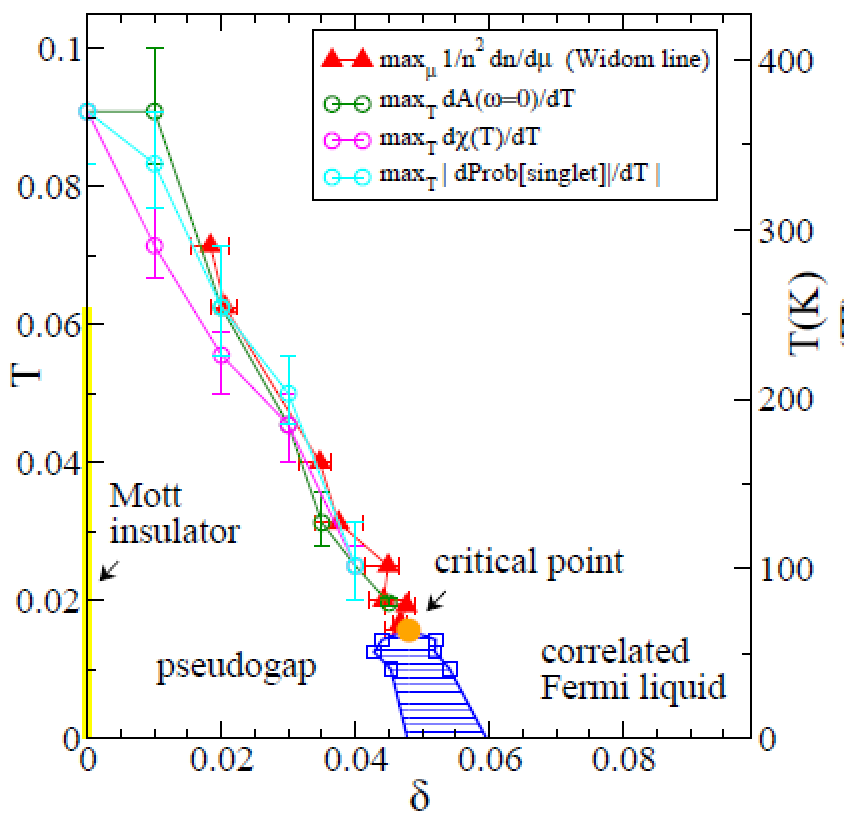
Patrick Sémon

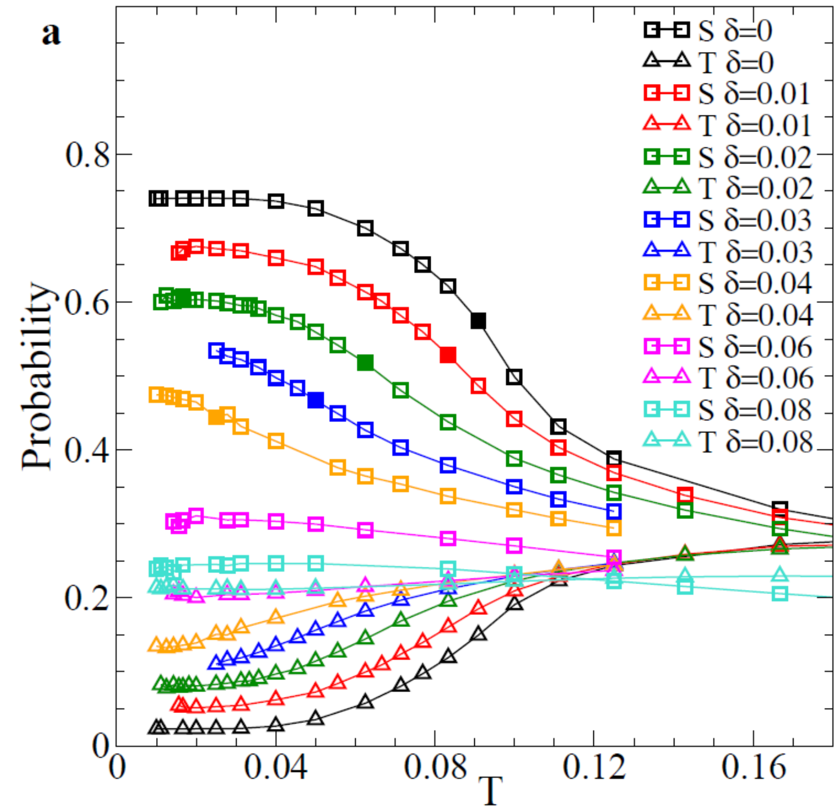


G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)
P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B **89**, 165113/1-6 (2014)

Physics

Plaquette eigenstates





See also:

Michel Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, A. Georges
PRB **80**, 064501 (2009)

Giovanni Sordi

Patrick Sémon

Kristjan Haule

The Widom line

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

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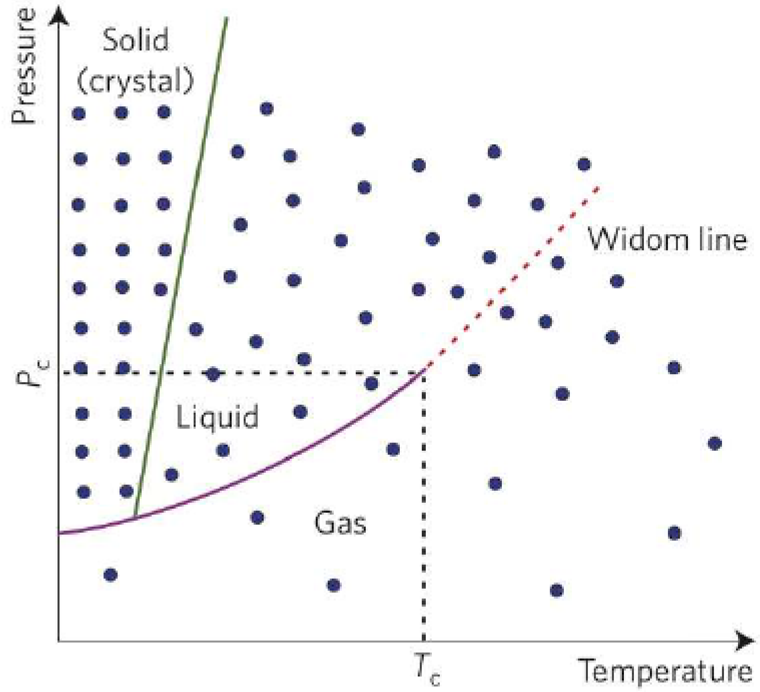
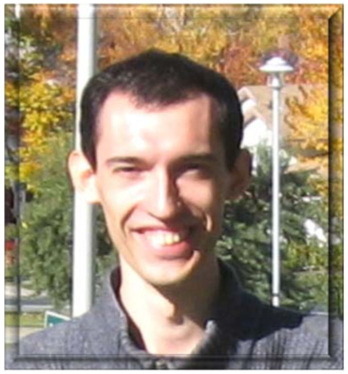
What is the Widom line?



McMillan and Stanley, Nat Phys 2010

- it is the continuation of the coexistence line in the supercritical region
- line where the maxima of different response functions touch each other asymptotically as $T \to T_p$
- liquid-gas transition in water: max in isobaric heat capacity C_p, isothermal compressibility, isobaric heat expansion, etc
- DYNAMIC crossover arises from crossing the Widom line!
  water: Xu et al, PNAS 2005, Simeoni et al Nat Phys 2010


Giovanni Sordi


Maxime Charlebois


Patrick Sémon

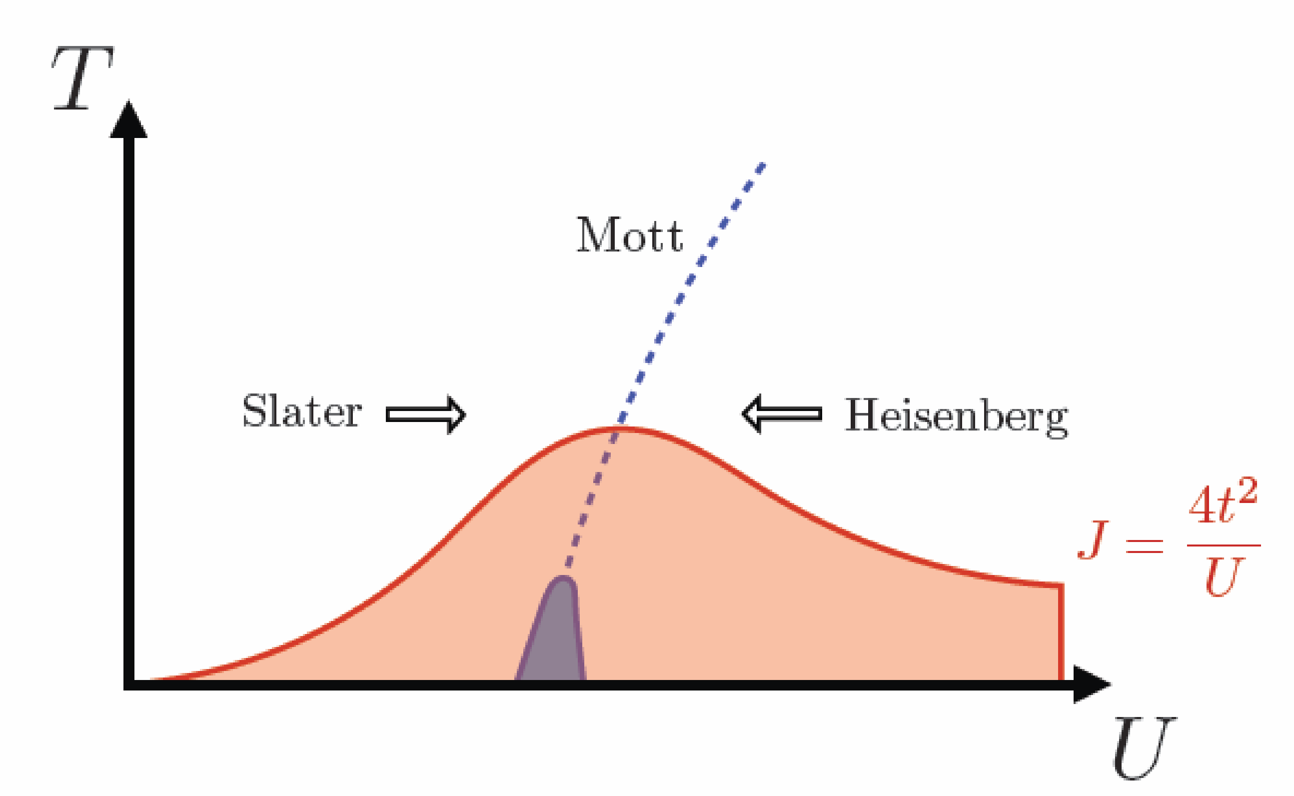

Lorenzo Fratino

Intermezzo

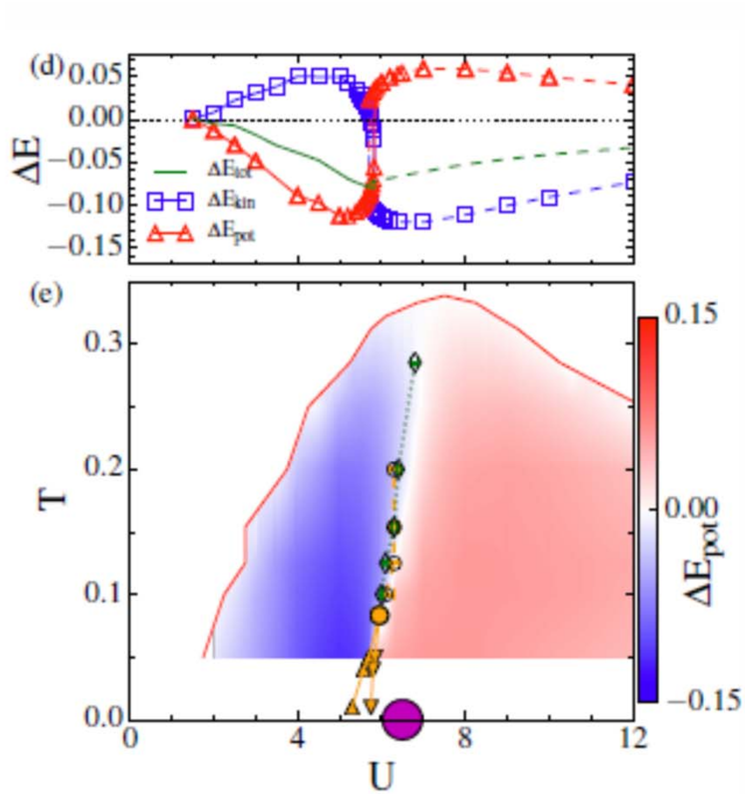
Influence of the underlying normal state on the ordered state

Crossovers inside the AFM phase

n = 1, unfrustrated d = 3 cubic lattice



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]

unpublished

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Patrick Sémon

Lorenzo Fratino

Part II

Strongly correlated Superconductivity

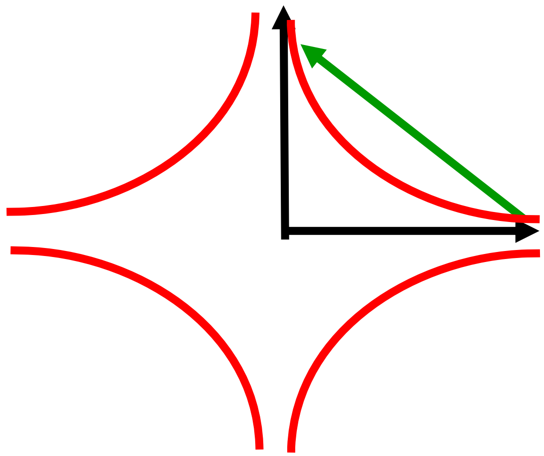
Sordi et al. PRL **108**, 216401 (2012)

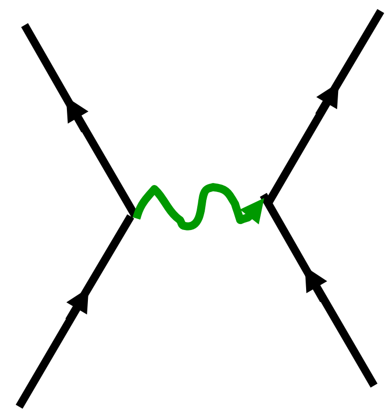
Fratino et al.

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

Cartoon « BCS » weakly-correlated picture

$$E_P = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \left\langle \psi^*_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow} \right\rangle \left\langle \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow} \right\rangle$$





Béal–Monod, Bourbonnais, Emery
P.R. B. **34**, 7716 (1986).

Exchange of spin waves?
Kohn-Luttinger
T_c with pressure

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)

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A cartoon strongly-correlated picture

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

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

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

Pitaevskii Brückner:

Pair state orthogonal to repulsive core of Coulomb interaction

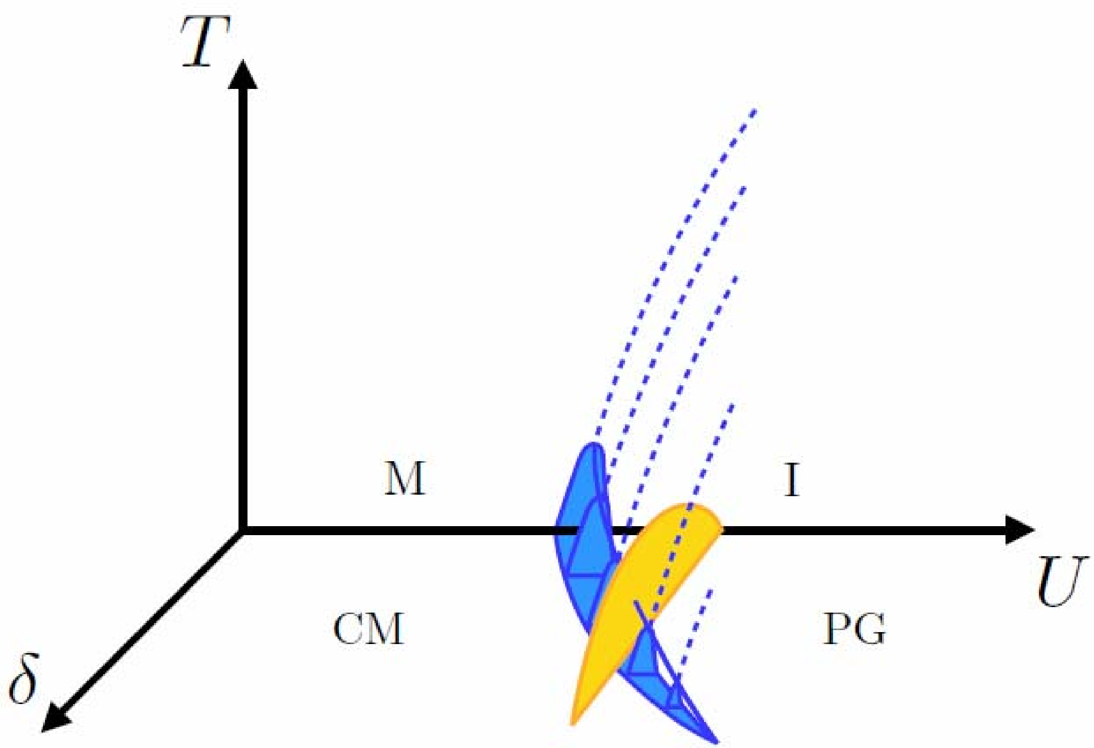
P.W. Anderson Science 317, 1705 (2007)

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

More sophisticated Slave Boson: Kotliar Liu PRB 1988

Superconductiviy in Doped Mott insulator

n = 1, d = 2 square lattice



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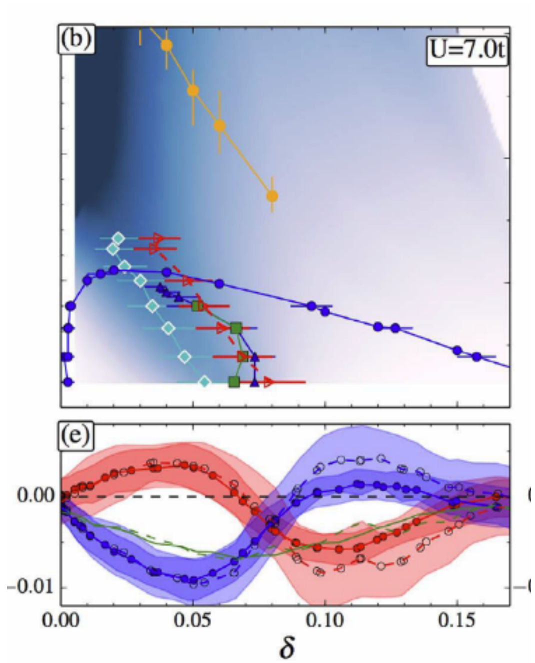
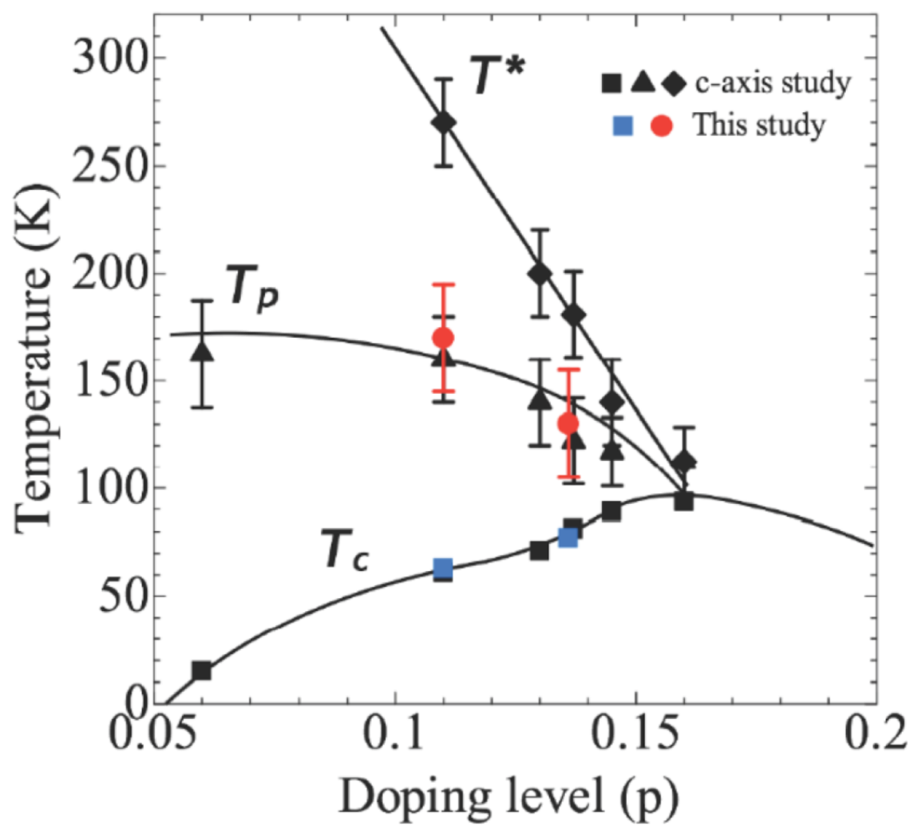
An organizing principle



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

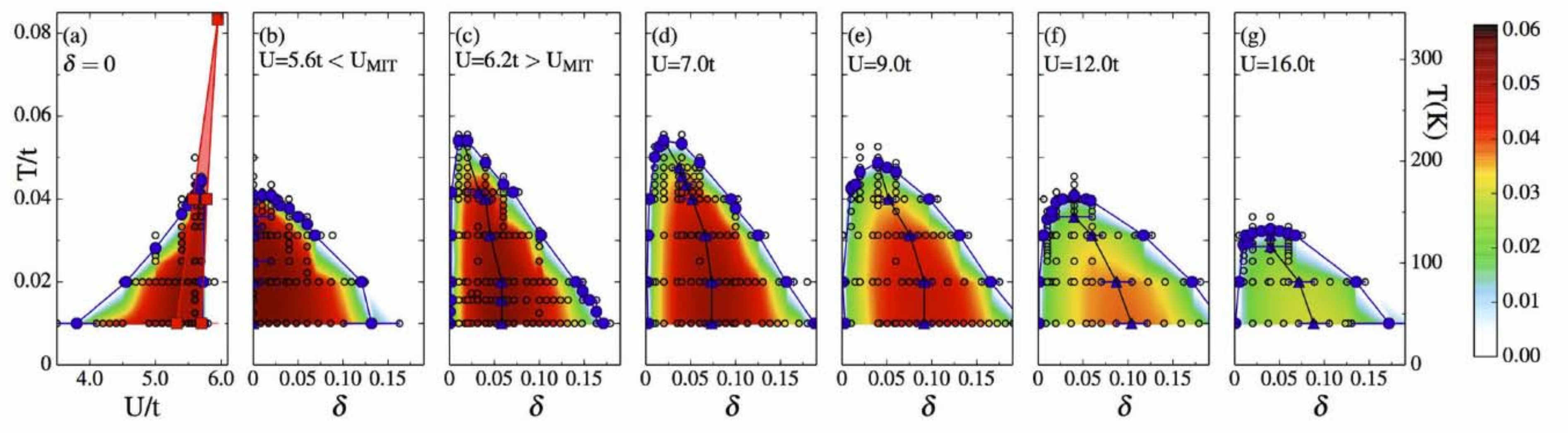
Theory, see also Jarrel PRL (2004), Gull Millis PRB (2014)
Experiments: Bontemps, Van der Marel …

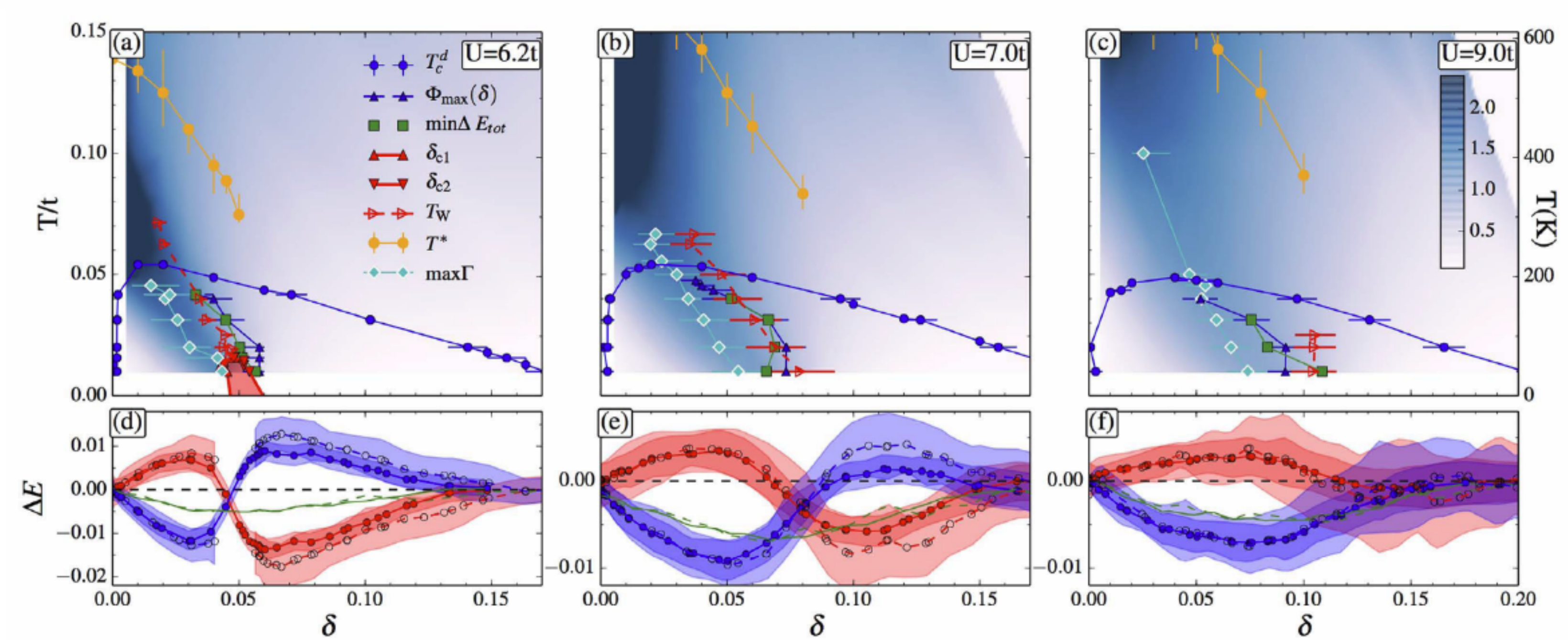
Evidence for local pairs from $\sigma_2(\omega)$



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

An organizing principle





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

3 bands, charge transfer insulator

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

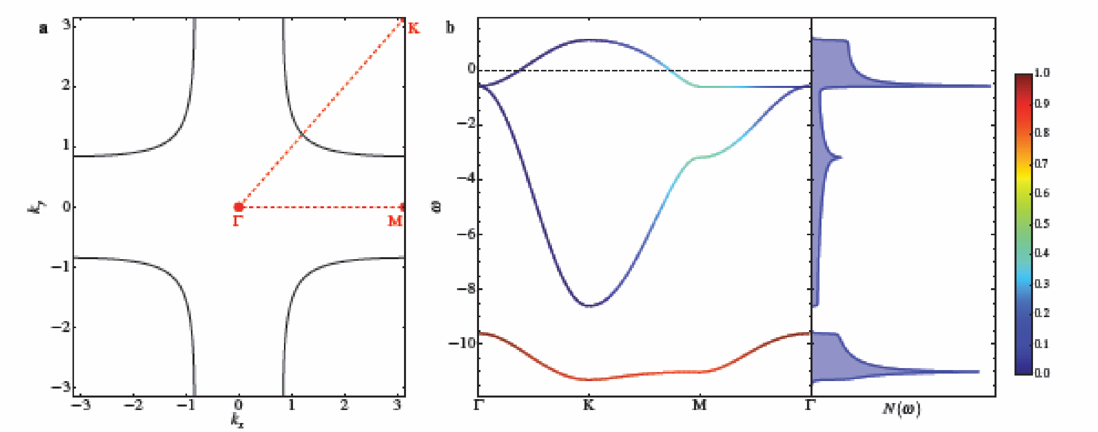
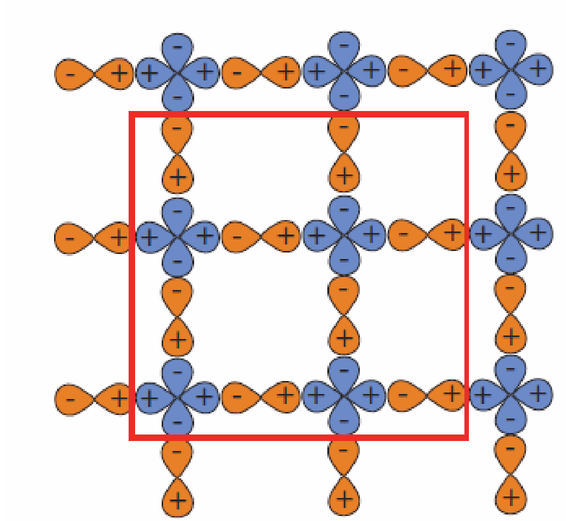


FIG. 2. (a) Noninteracting Fermi surface for the model parameter investigated in Fig. 1a of main text, namely $\epsilon_p = 9$, $t_{pp} = 1$, $t_{pd} = 1.5$, which gives a total occupation n_{tot} equal to five. (b) Non-interacting band structure for the same model parameter along with the resulting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



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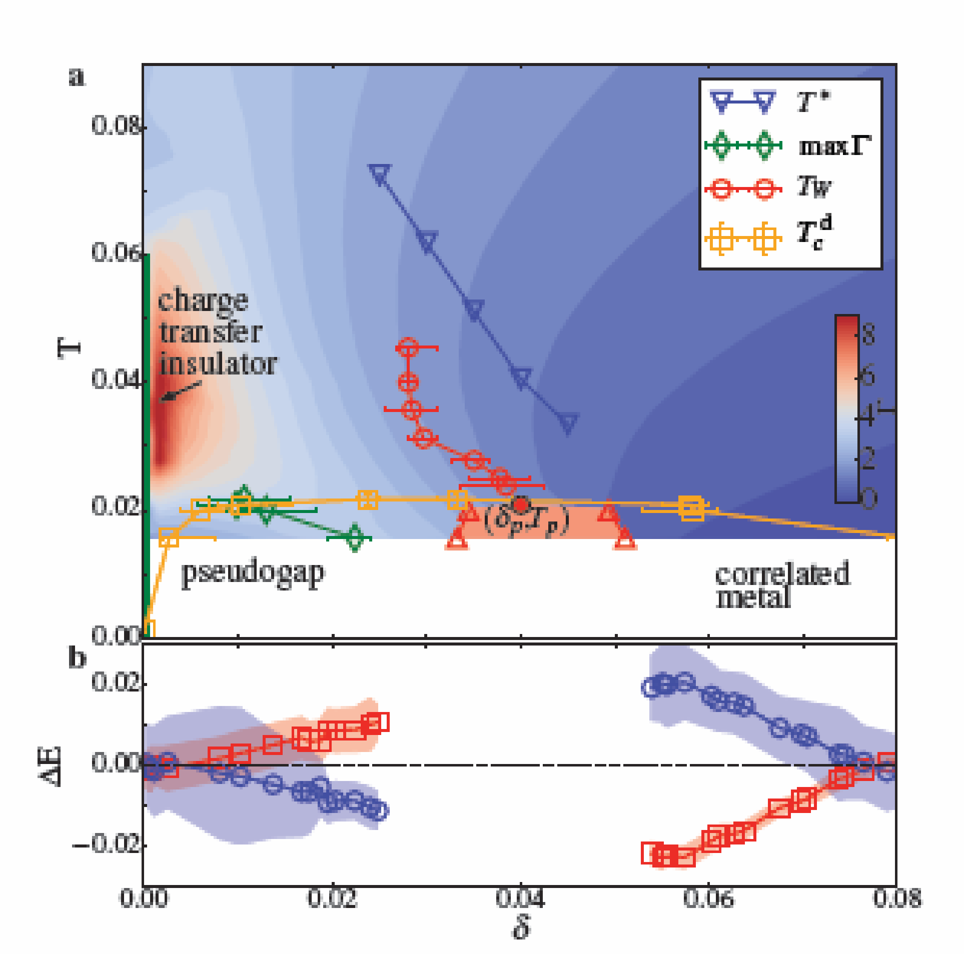
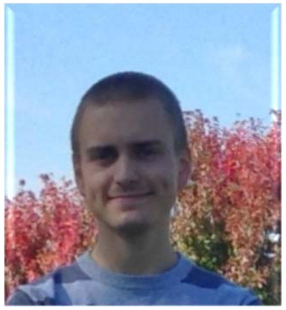
3 bands, charge transfer insulator



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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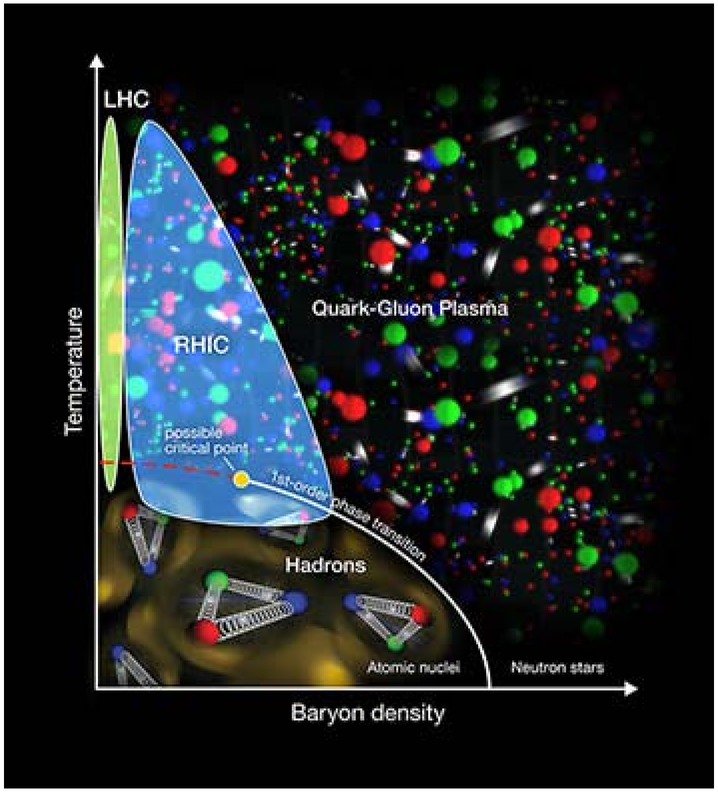
A general principle in strongly correlated matter?



Swagato Mukherjee, Raju Venugopalan, and Yi Yin
Phys. Rev. Lett. **117**, 222301 (2016)

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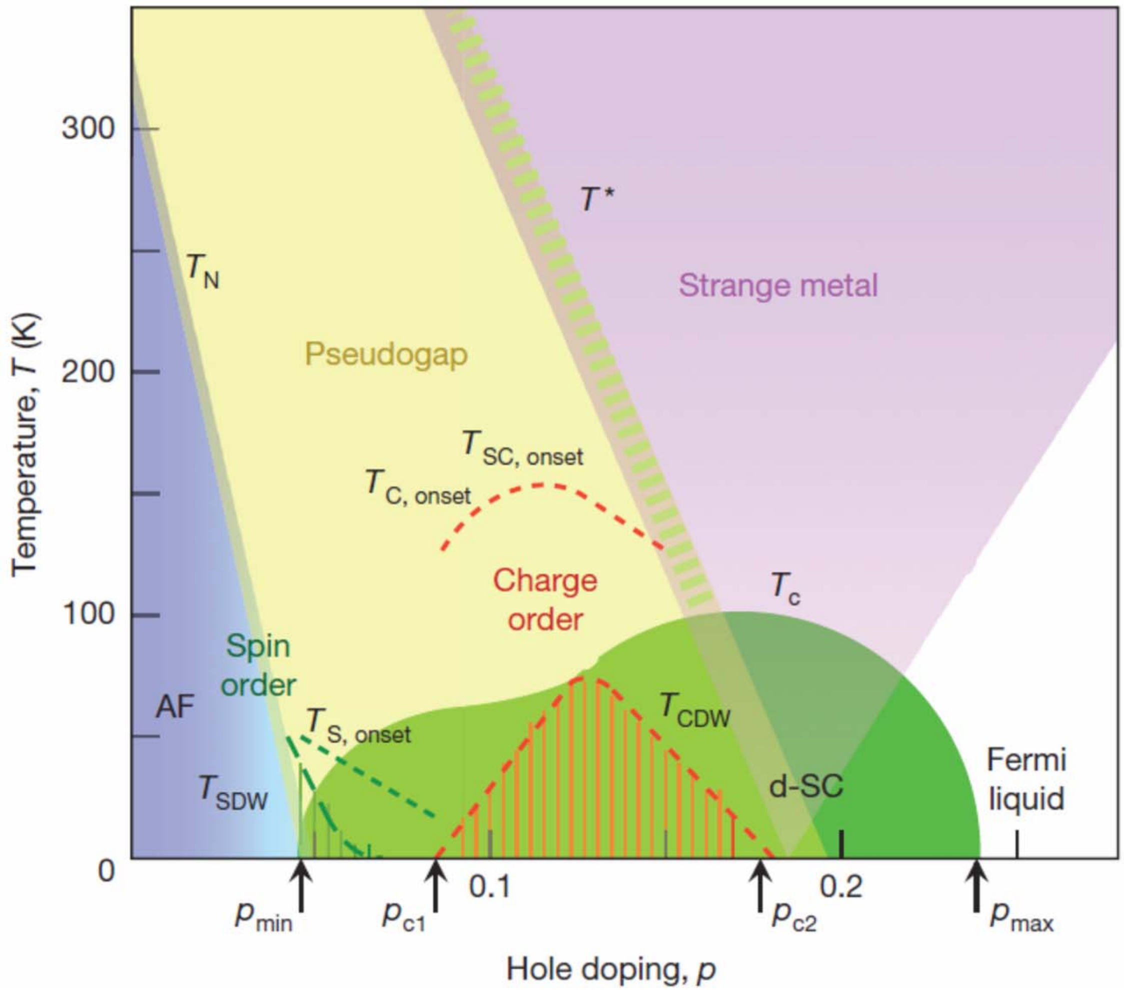
Phase diagram



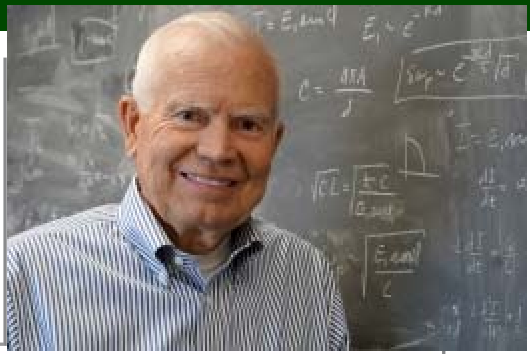
Keimer et al., Nature 518, 179 (2015)

P.W. Anderson

Raising the question

D.J. Scalapino

Is There Glue in Cuprate Superconductors?
Philip W. Anderson
Science **316**, 1705 (2007);
DOI: 10.1126/science.1140970



Is There Glue in Cuprate Superconductors?

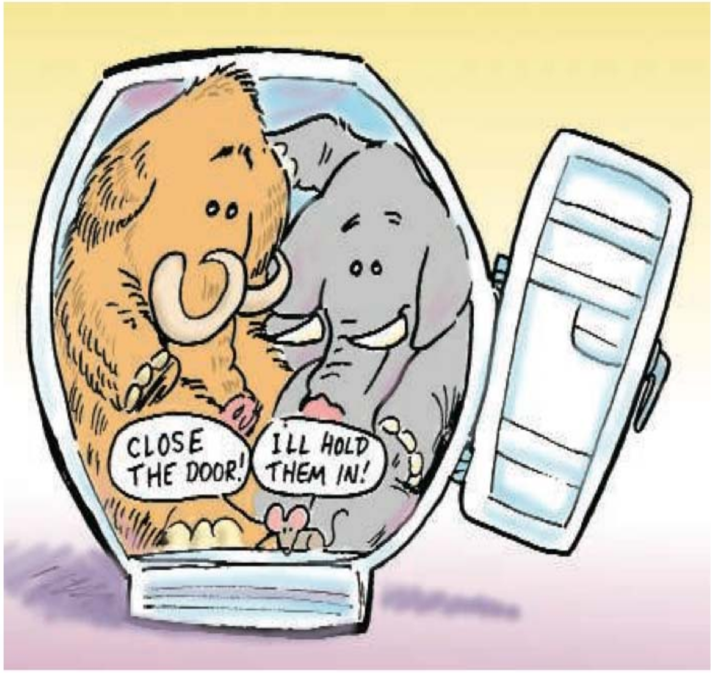
Philip W. Anderson

Many theories about electron pairing in cuprate superconductors may be on the wrong track.

Science e-letter, 5 and 10 Dec. 2007

Retardation

$$V^{eff}_{él-ph}(\vec{q},\omega) = \frac{e^2}{4\pi\varepsilon_0(q^2+k^2_{TF})}\left[1+\frac{\omega^2_{ph}(\vec{q})}{\omega^2-\omega^2_{ph}(\vec{q})}\right]$$



"We have a mammoth and an elephant in our refrigerator—do we care much if there is also a mouse?"

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Conclusion

- Even within a single phase, there can be qualitative differences between the strong and weak correlation limit

- A phase transition in the underlying normal state can act as an organizing principle for the phase diagram.

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