CIFAR
CANADIAN INSTITUTE
for ADVANCED RESEARCH

The pseudogap

André-Marie Tremblay

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26 April 2016

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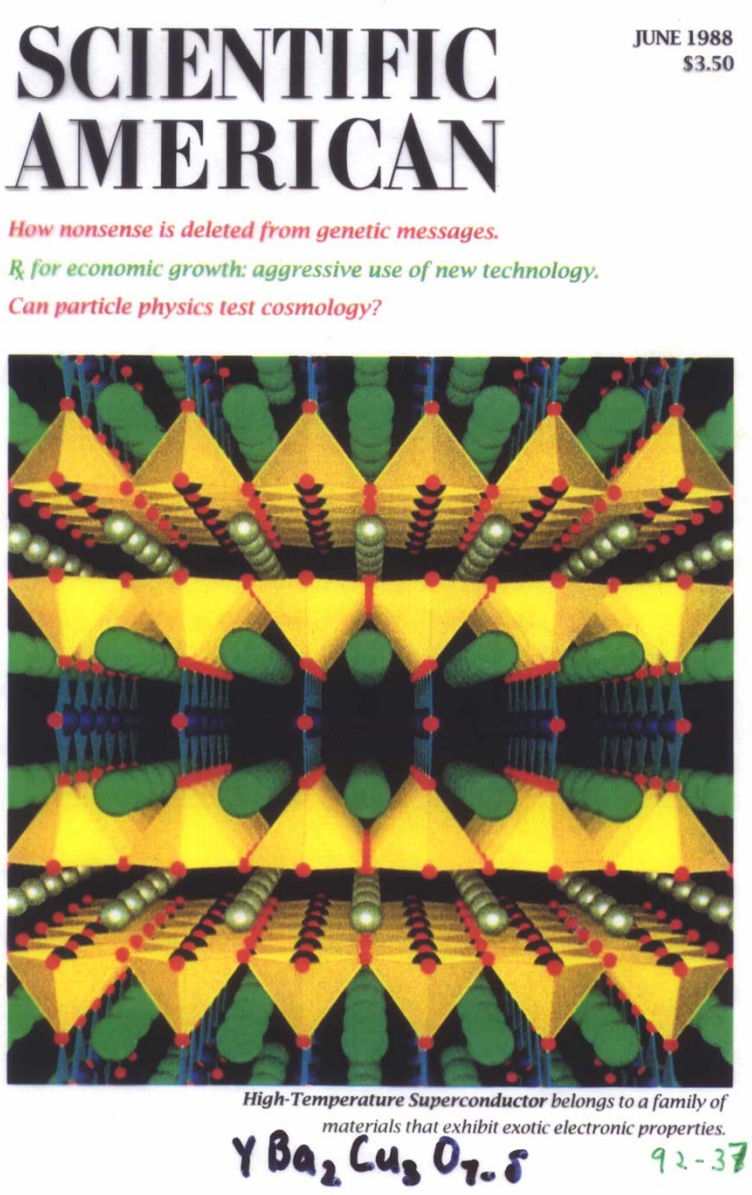
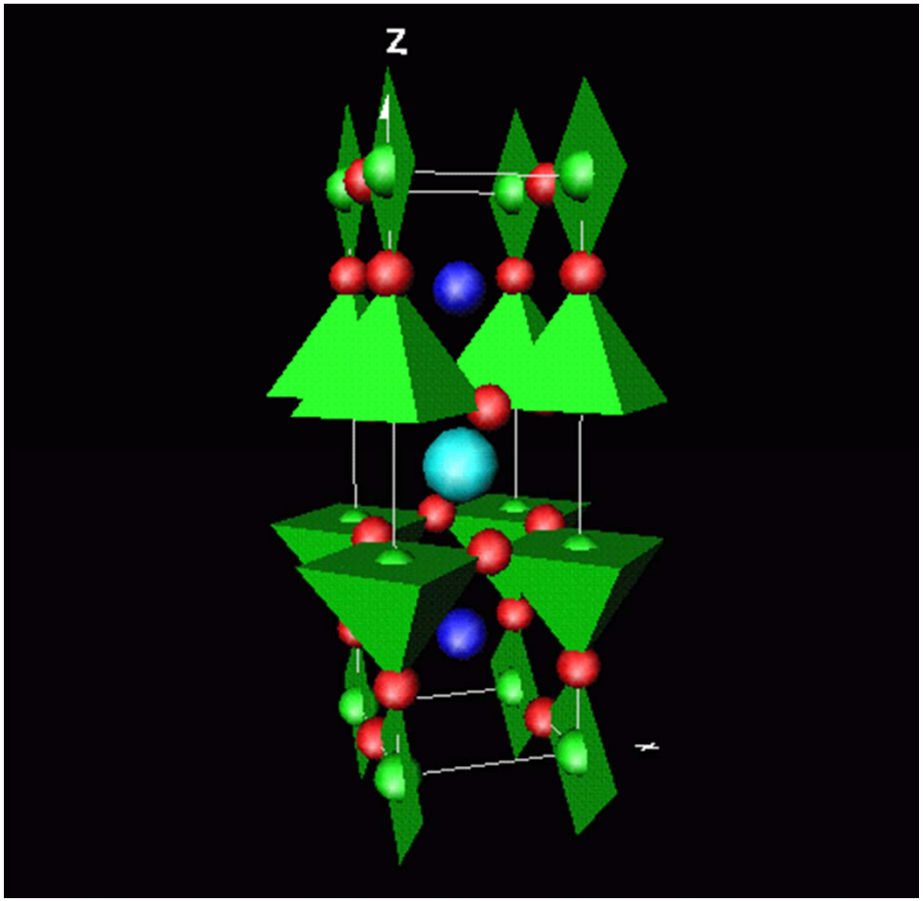
Atomic structure





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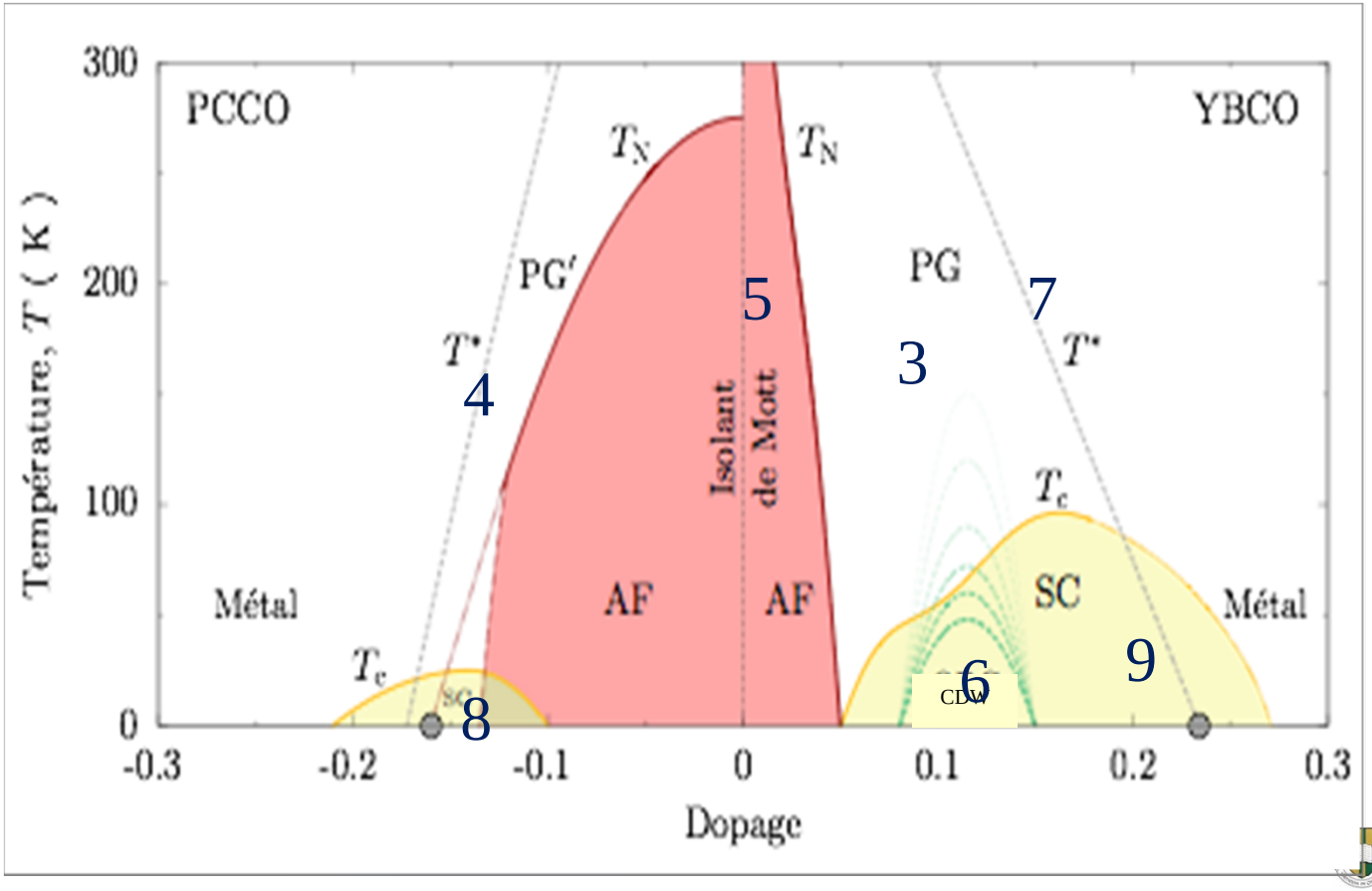
Outline

For references, September 2013 Julich summer school
Strongly Correlated Superconductivity
http://www.cond-mat.de/events/correl13/manuscripts/tremblay.pdf



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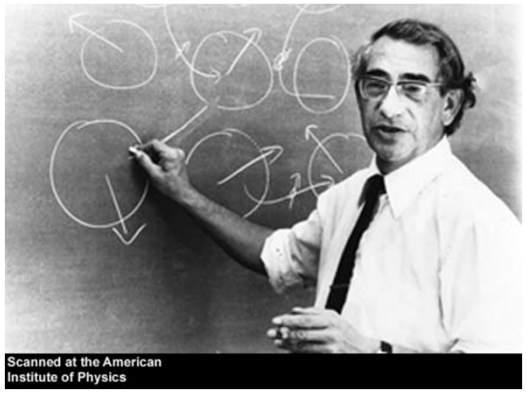
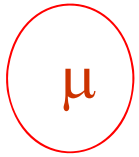
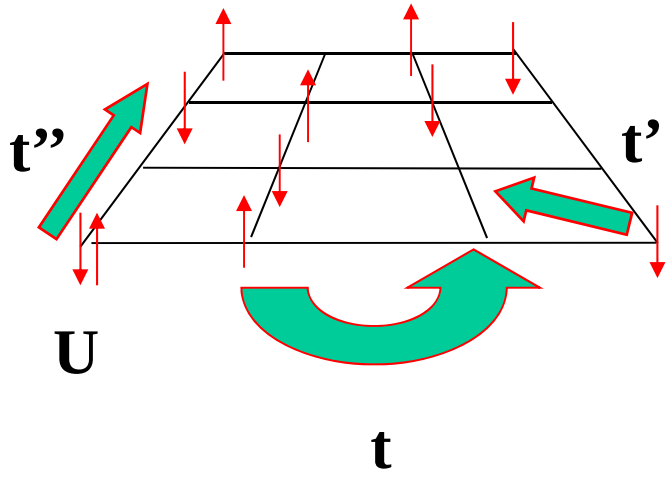
Hubbard model



1931-1980

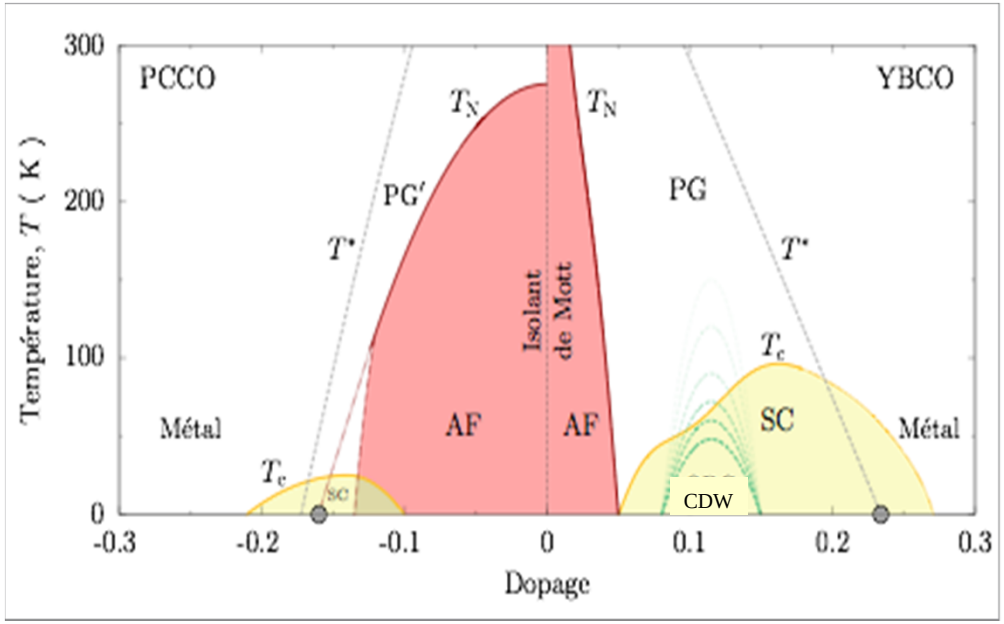


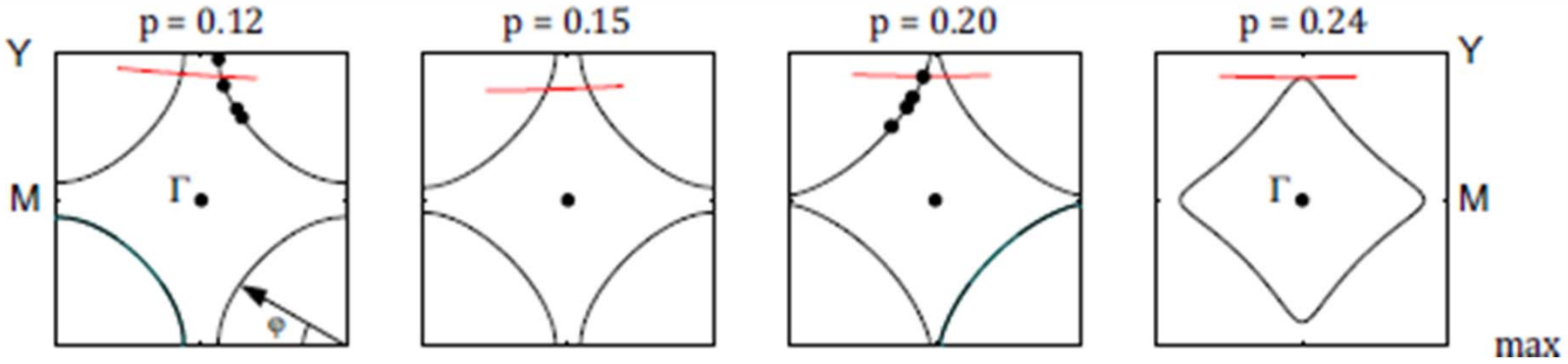


$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

Attn: Charge transfer insulator

Non-interacting Fermi surface





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Speakers

Friday 29 April, Forest Hill Ballroom

07:00-08:45 **Breakfast, High Park Ballroom**

09:00-09:45 Jeff TALLON (Wellington) – *Pseudogap in cuprate superconductors – what, when, why, where, how?*

09:45-10:30 Dan DESSAU (Colorado) – *Direct connection of ARPES with optics, transport, and thermodynamics experiments in cuprate cuperconductors: the key role of electron self-energies*

11:30-12:15 Louis TAILLEFER (Sherbrooke) – *Normal-state signatures of the pseudogap quantum critical point*

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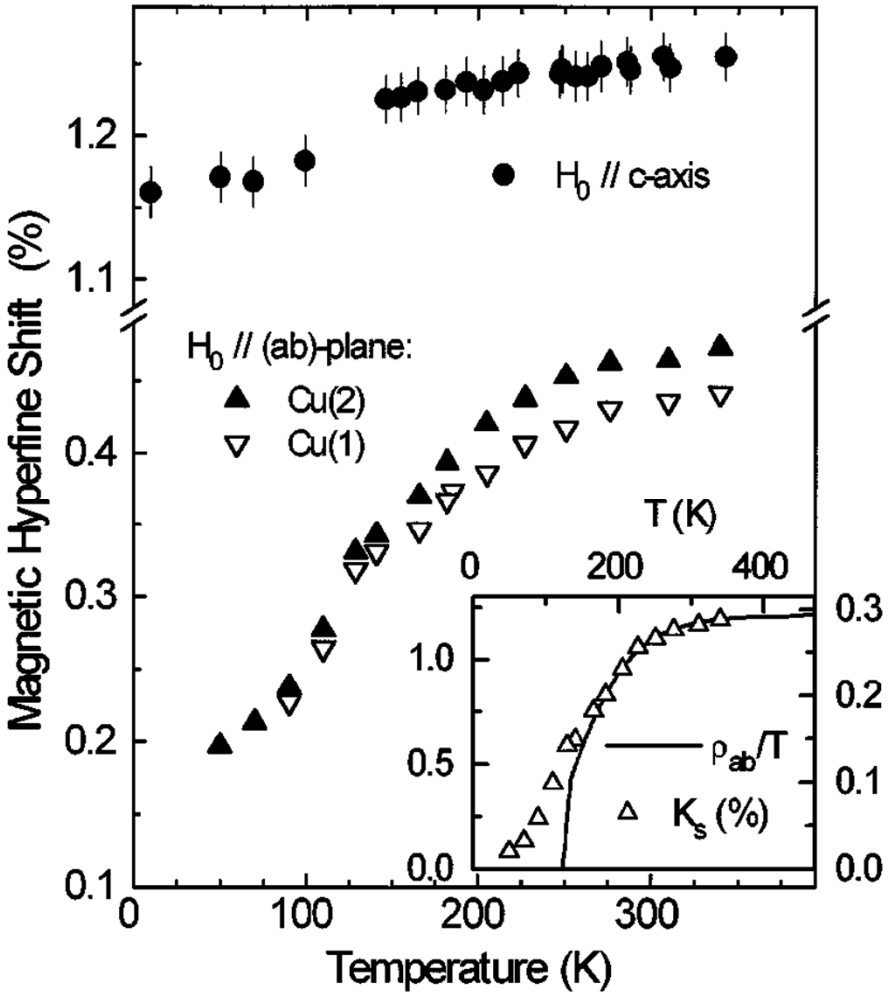
- Pseudogap: not an ordinary metal
  - Experimental evidence (Tallon)
- Link between various experiments
  - Self-energy etc (Dessau)
- Theories of the pseudogap
  - Broadened first-order transition
  - Precursor of LRO
  - Strong correlations: Mott physics

Pseudogap: not an ordinary metal

Spin susceptibility (Knight shift): Pseudogap



Underdoped Hg1223

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

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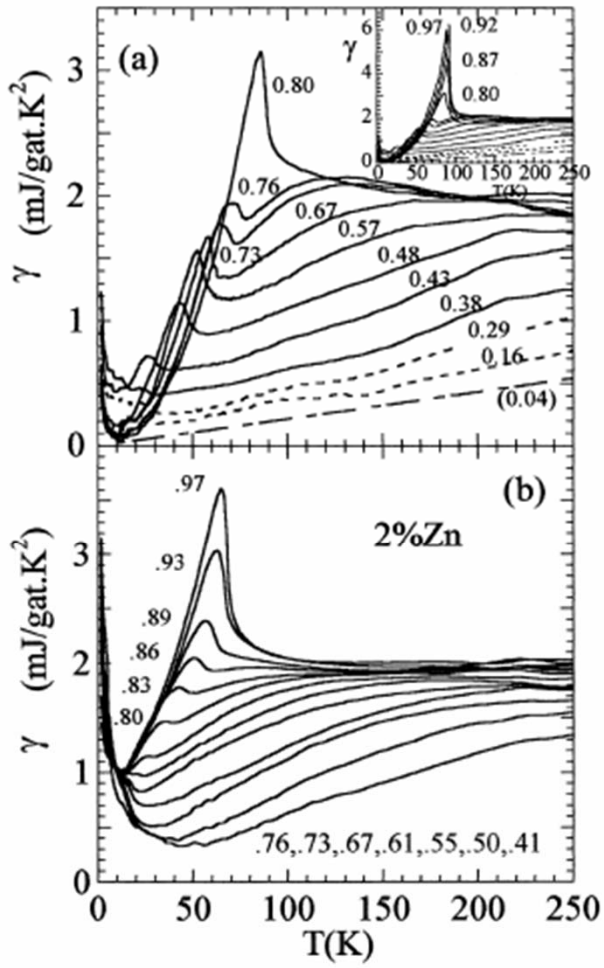
Specific Heat



Loram et al. J. Phys. Chem. Solids, **62**, 59 (2001)

Fig. 5. γ vs T for: (a) $YBa_2Cu_3O_{6+x}$; and (b) $YBa_2(Cu_{0.98}Zn_{0.02})_3O_{6+x}$. Labels show x [7].

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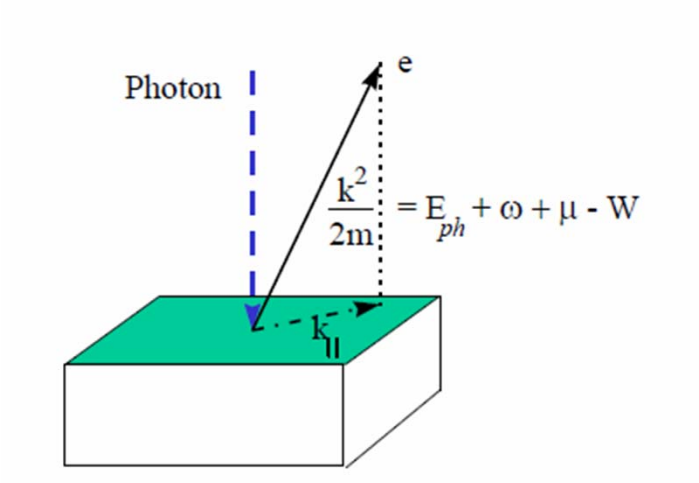
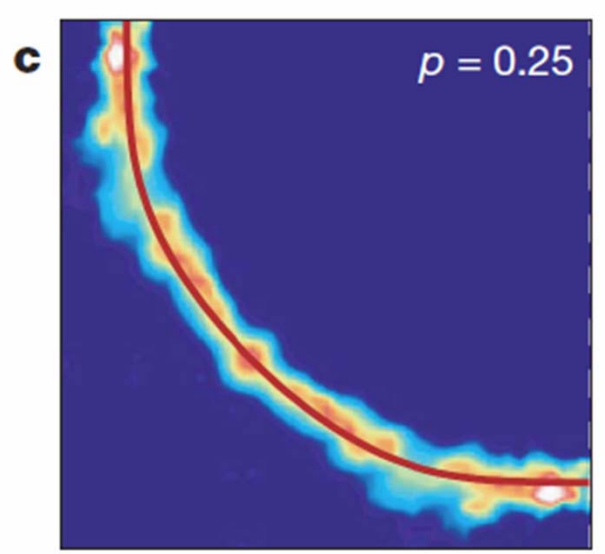
Fermi surface (ARPES)





Tl 2201

Platé *et al.* PRL **95**, 077001 (2005)

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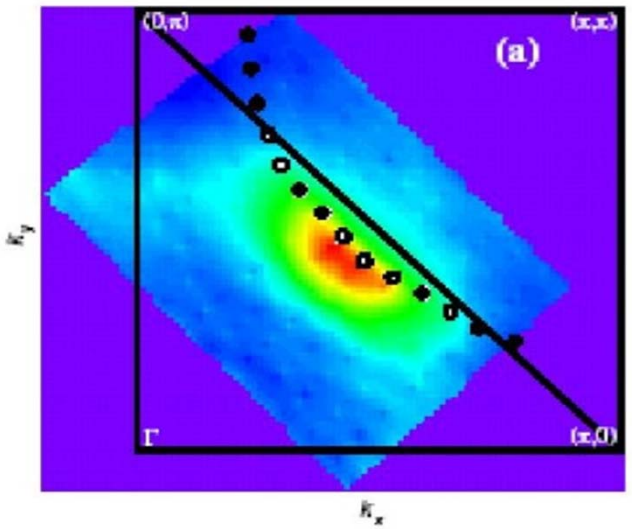
Fermi surface?? ARPES: (Pseudogap)

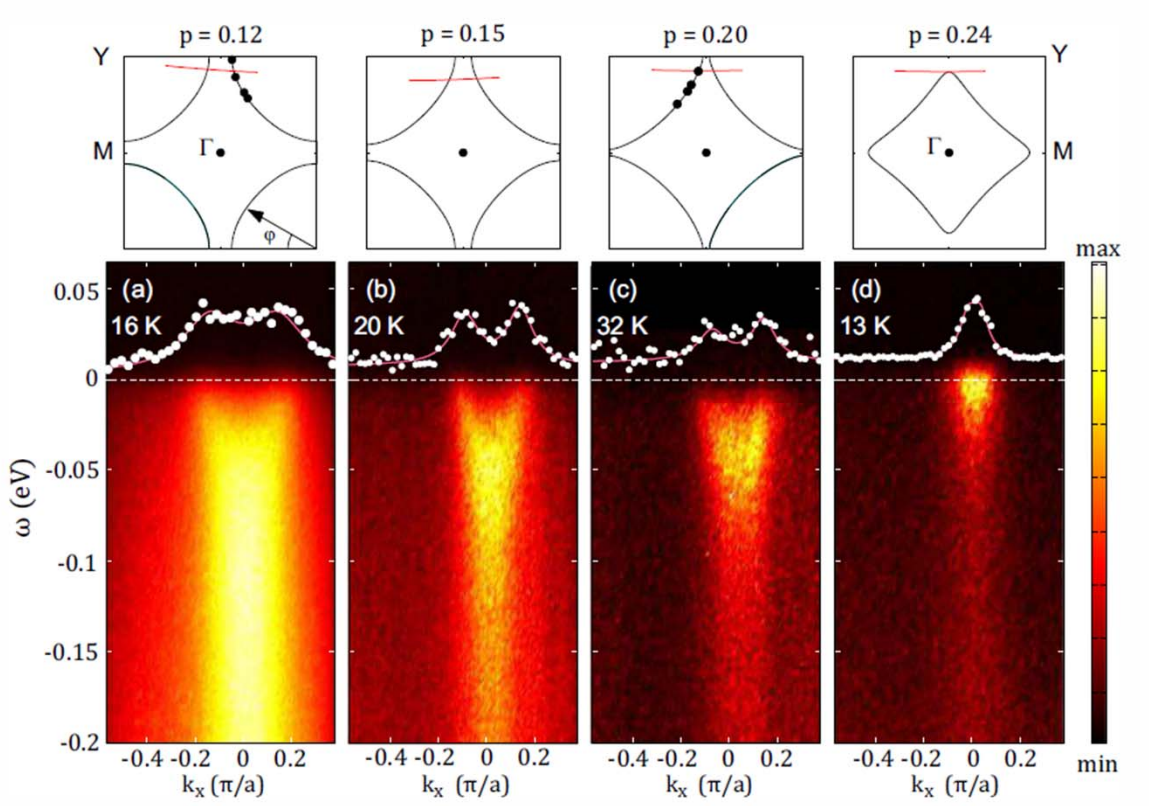
Hole-doped, 10%

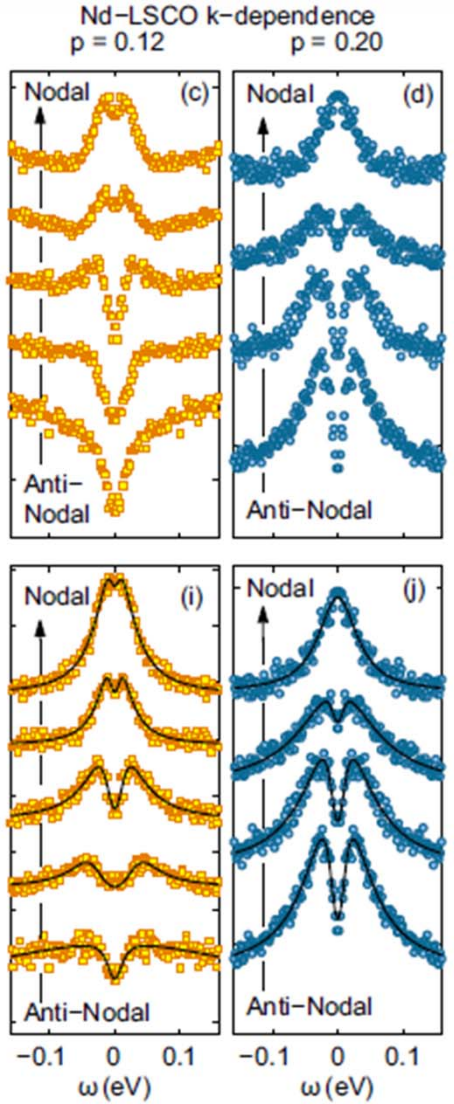


F. Ronning et al. Jan. 2002, $Ca_{2-x}Na_xCuO_2Cl_2$

Ronning *et al.* (PRB 2003)

ARPES pseudogap Nd-LSCO





Matt *et al.* PRB **92**, 134524 (2015)

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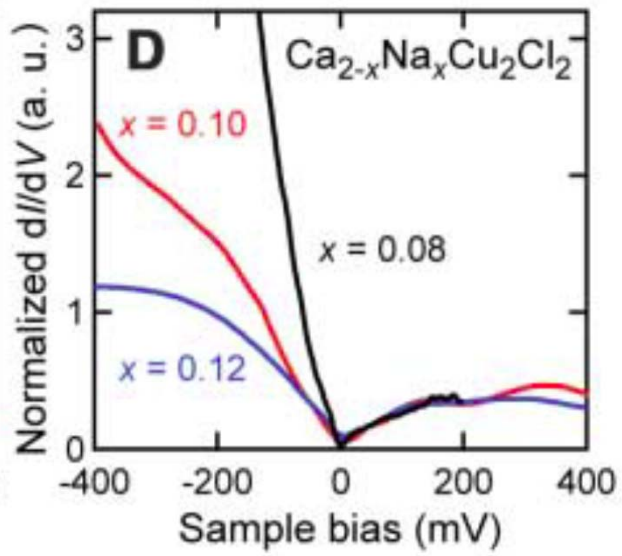
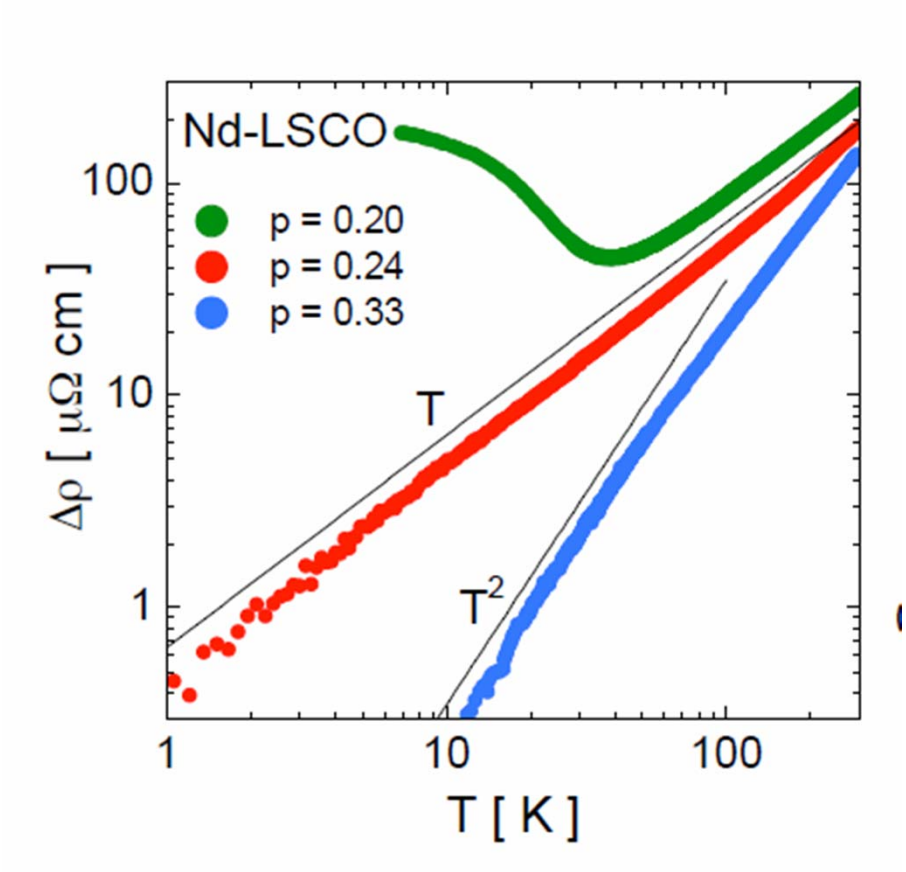
Local density of states (STM)



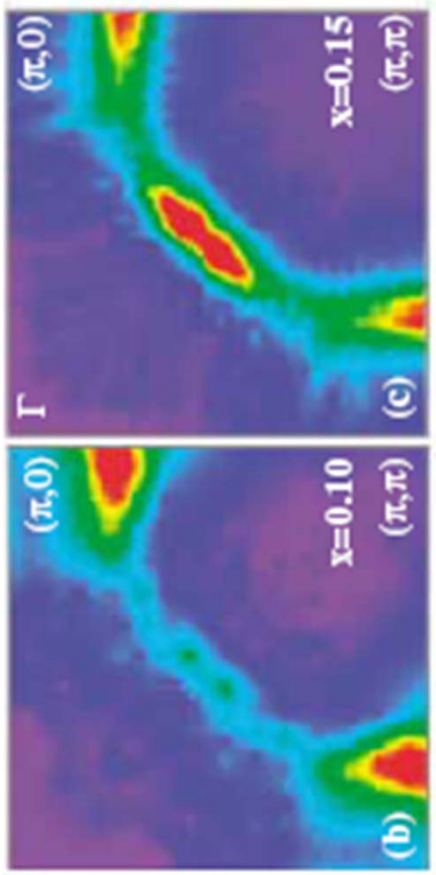
Khosaka et al. *Science* **315**, 1380 (2007);

Strange metal vs pseudogap



Daou R *et al*. Phys. Rev. B **79**,180505 (2009)

Electron-doped cuprates: Fermi surface



Armitage et al. PRL 2001

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Outline

- Pseudogap: not an ordinary metal
  - Experimental evidence (Tallon)
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  - Self-energy etc (Dessau)
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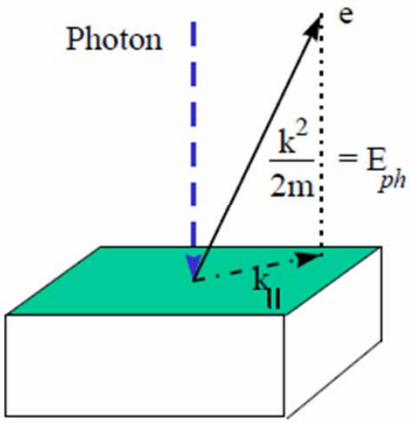
  - Precursor of LRO
  - Strong correlations: Mott physics

What does ARPES measure?



$$-\sum_{\mathbf{k}'} \langle n| \otimes \langle \mathbf{k}| \otimes \langle 0|_{em} \mathbf{j}_{\mathbf{k}'} \cdot \mathbf{A}_{-\mathbf{k}'} |m\rangle \otimes |0\rangle \otimes |1_{\mathbf{q}}\rangle_{em} \cdot$$

$$= -\sum_{\mathbf{k}'} \langle n| \otimes \langle \mathbf{k}| \mathbf{j}_{\mathbf{k}'} |m\rangle \otimes |0\rangle \cdot \langle 0|_{em} \mathbf{A}_{-\mathbf{k}'} |1_{\mathbf{q}}\rangle_{em}$$

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} \propto \sum_{mn} e^{-\beta K_m} \left|\langle n| c_{\mathbf{k}_{||}} |m\rangle\right|^2 \delta\left(\omega + \mu - (E_m - E_n)\right)$$

$$\propto \sum_{mn} e^{-\beta K_m} \left|\langle n| c_{\mathbf{k}_{||}} |m\rangle\right|^2 \delta\left(\omega - (K_m - K_n)\right)$$

$$\propto \int dt e^{i\omega t} \left\langle c^{\dagger}_{\mathbf{k}_{||}} c_{\mathbf{k}_{||}}(t) \right\rangle .$$

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} \propto f(\omega) A\left(\mathbf{k}_{||}, \omega\right)$$

$$c_{\mathbf{k}}(t) = e^{i\hat{H}t} c_{\mathbf{k}} e^{-i\hat{H}t} \quad ; \quad c^{\dagger}_{\mathbf{k}}(t) = e^{i\hat{H}t} c^{\dagger}_{\mathbf{k}} e^{-i\hat{H}t}.$$

Self-energy

$$G^R(\mathbf{k};t) = -i\left\langle\left\{c_{\mathbf{k}}(t), c_{\mathbf{k}}^{\dagger}\right\}\right\rangle\theta(t)$$

Relation to DOS
to kinetic energy…

Non-interacting case

$$\boxed{c_{\mathbf{k}}(t) = e^{-i\epsilon_{\mathbf{k}}t}c_{\mathbf{k}}}$$

$$G^R(\mathbf{k};\omega) = \frac{1}{\omega + i\eta - \varepsilon_{\mathbf{k}}} \qquad A(\omega) = -2\,\mathrm{Im}\,G^R(\omega)$$

Effect of interactions

$$G^R(\mathbf{k},\omega) = \frac{1}{\omega + i\eta - \zeta_{\mathbf{k}} - \sum^R(\mathbf{k},\omega)}$$

$$\begin{aligned} A(\mathbf{k},\omega) &= -2\,\mathrm{Im}\,G^R(\mathbf{k},\omega) \\ &= \frac{-2\,\mathrm{Im}\sum^R(\mathbf{k},\omega)}{\left(\omega - \zeta_{\mathbf{k}} - \mathrm{Re}\sum^R(\mathbf{k},\omega)\right)^2 + \left(\mathrm{Im}\sum^R(\mathbf{k},\omega)\right)^2} \end{aligned}$$

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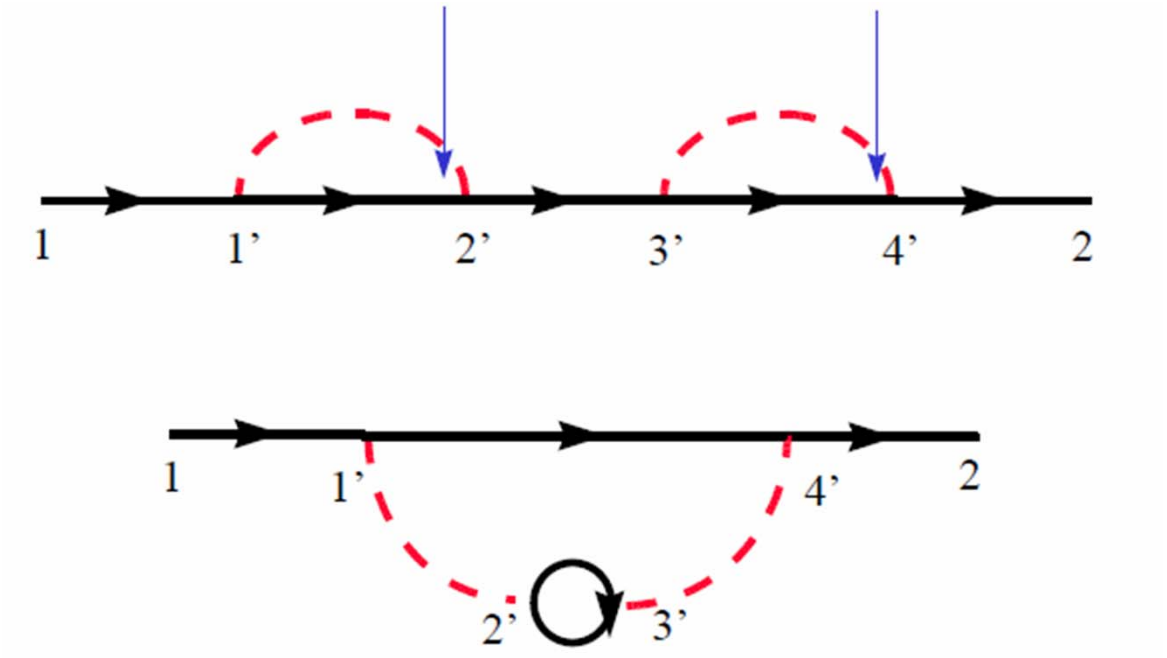
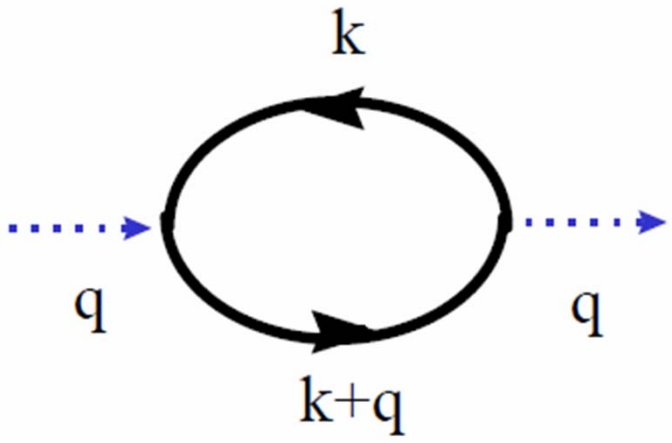
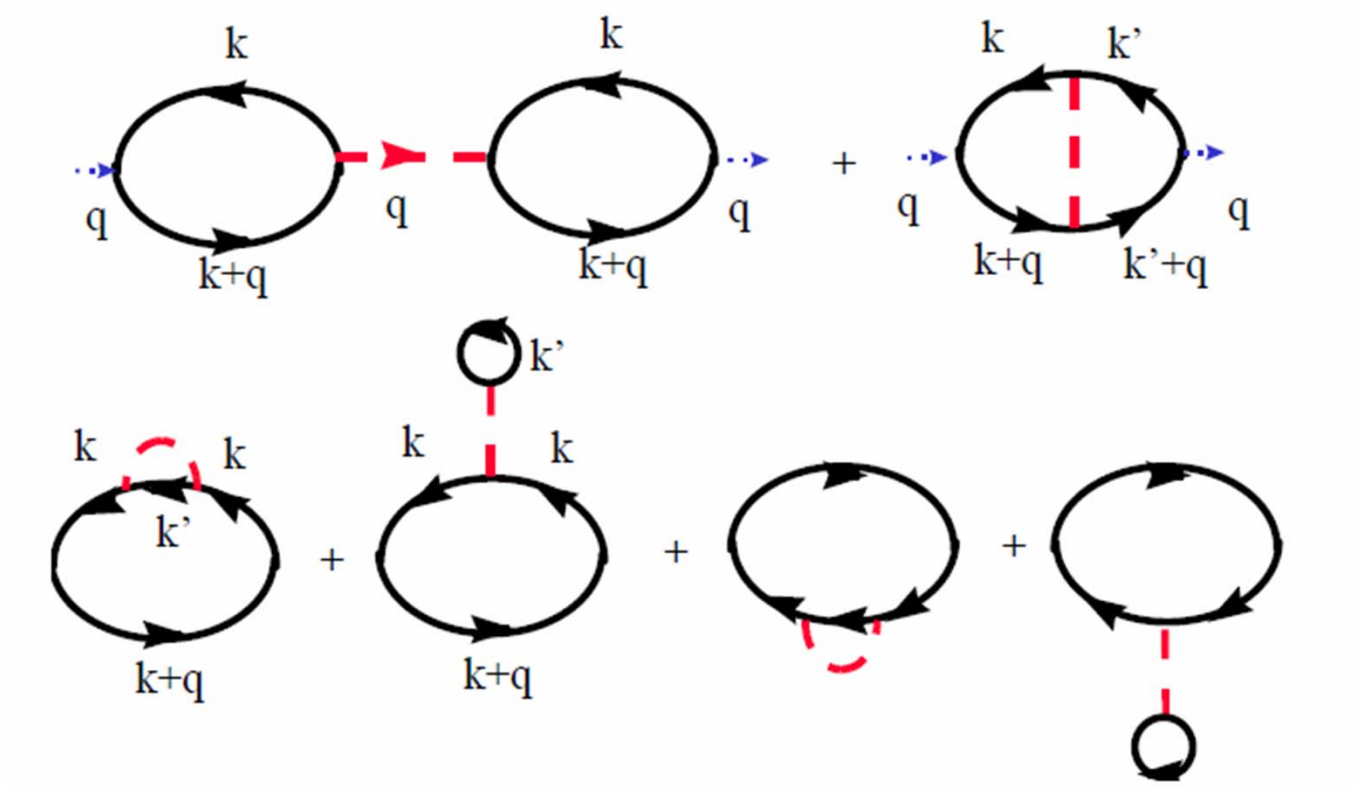
Relation to other observables



Conductivity



Vertex corrections



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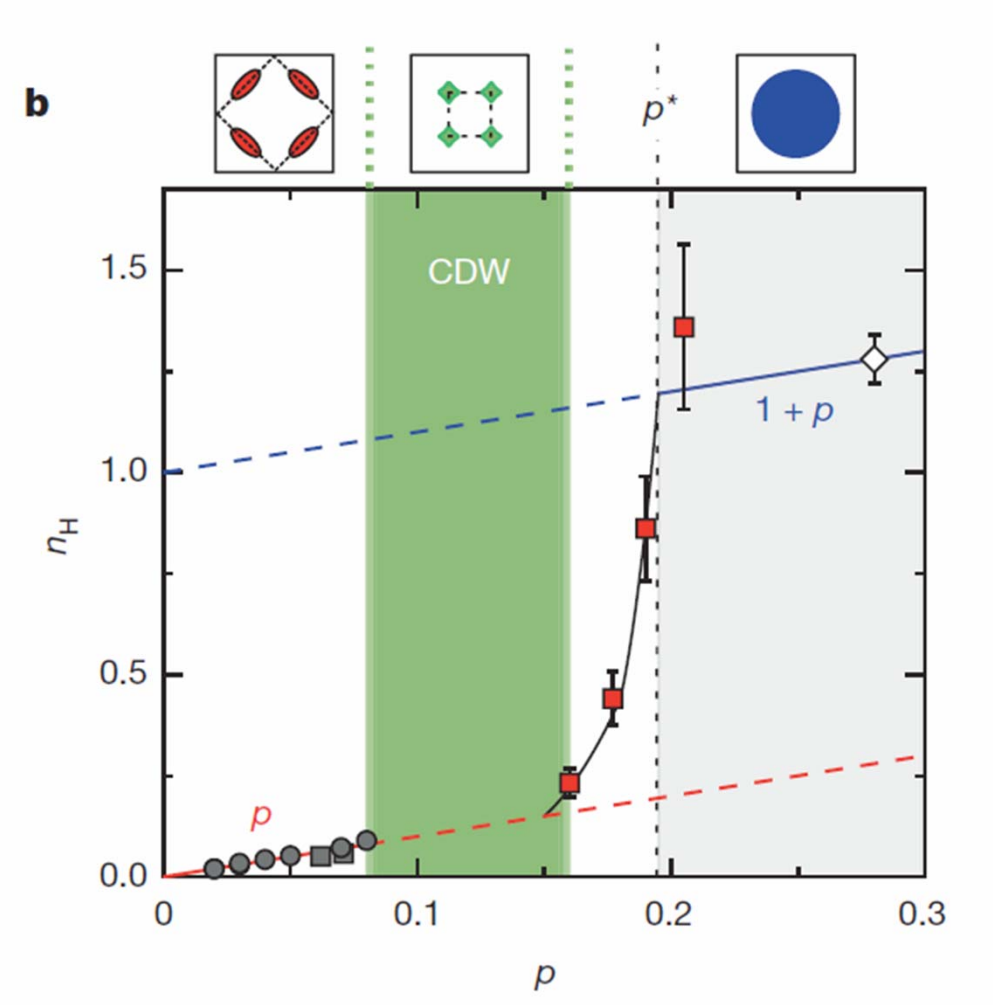
1. First-order transition broadened by disorder

- Loop current order (**q = 0**) (Varma)
- Nematic order (**q = 0**) (Kivelson)
- Charge order ?

- (See Simon Verret and Maxime Charlebois)

Not charge order



Badoux *et al.* Nature, March 2016

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More generally

PHYSICAL REVIEW B 89, 201104(R) (2014)

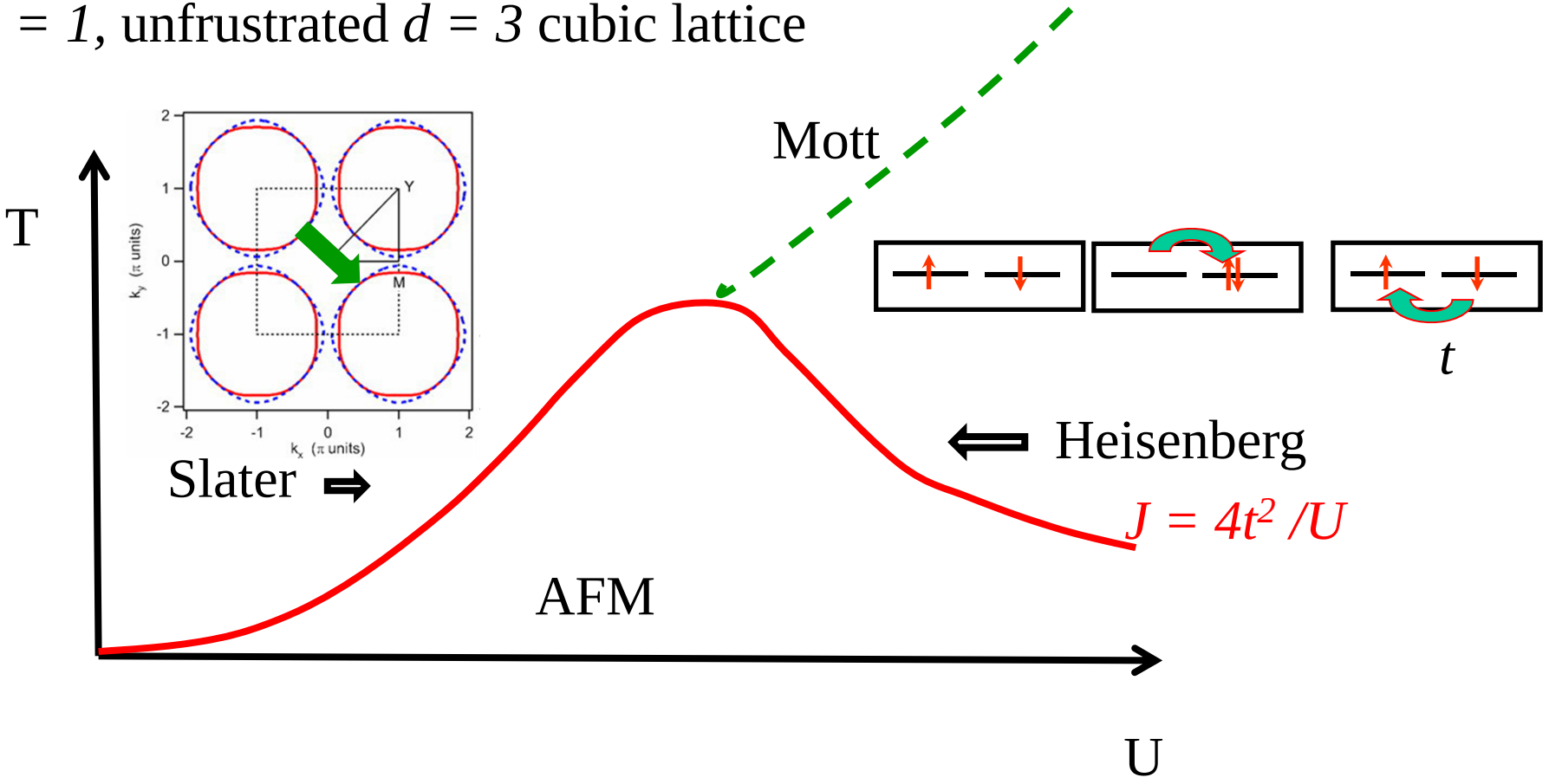
Pseudogap in $YBa_2Cu_3O_{6+\delta}$ is not bounded by a line of phase transitions: Thermodynamic evidence

J. R. Cooper,[1] J. W. Loram,[1] I. Kokanović,[1,2] J. G. Storey,[3] and J. L. Tallon[3]

2. Precursor of $d=2$ long-range order

Weak vs Strong correlations

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



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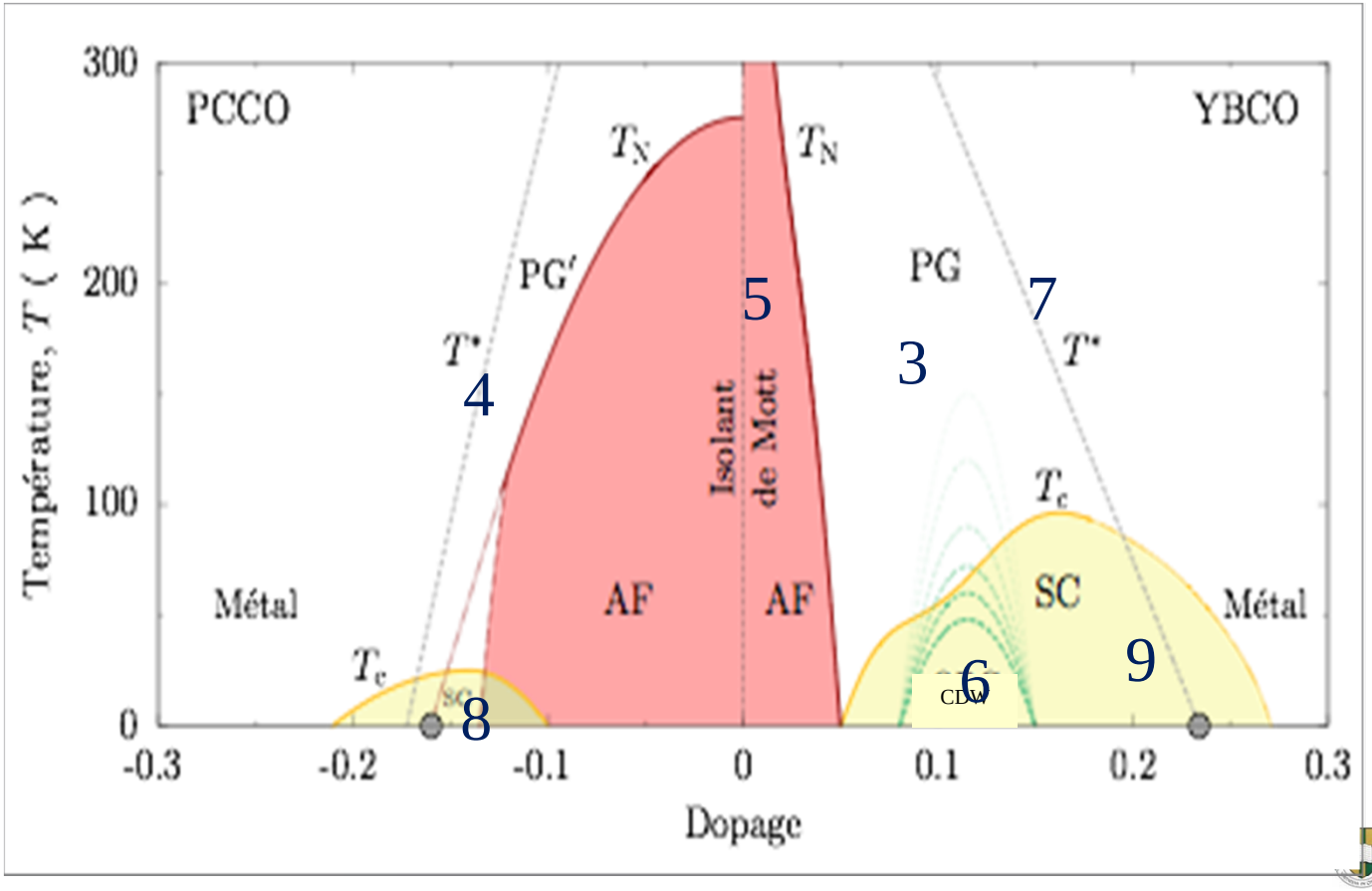

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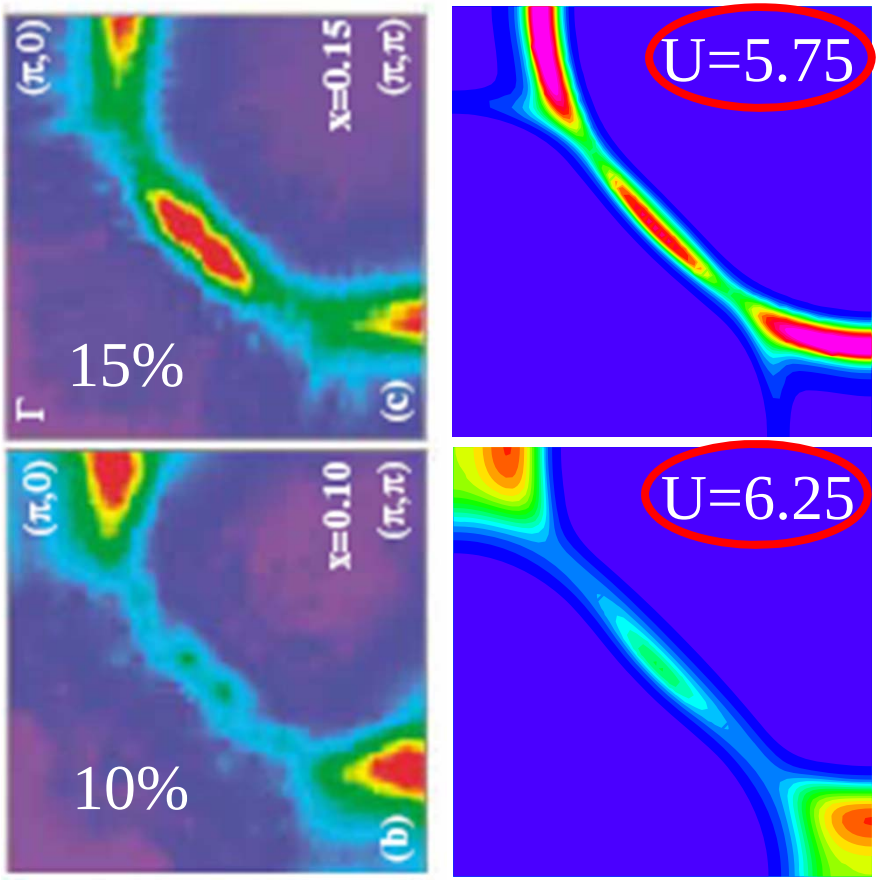
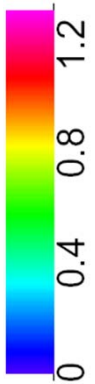
2. Doping an itinerant antiferromagnet Quantum critical point

Electron-doped cuprates

Fermi surface plots

Hubbard repulsion U has to…





be not too large

increase for smaller doping

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

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

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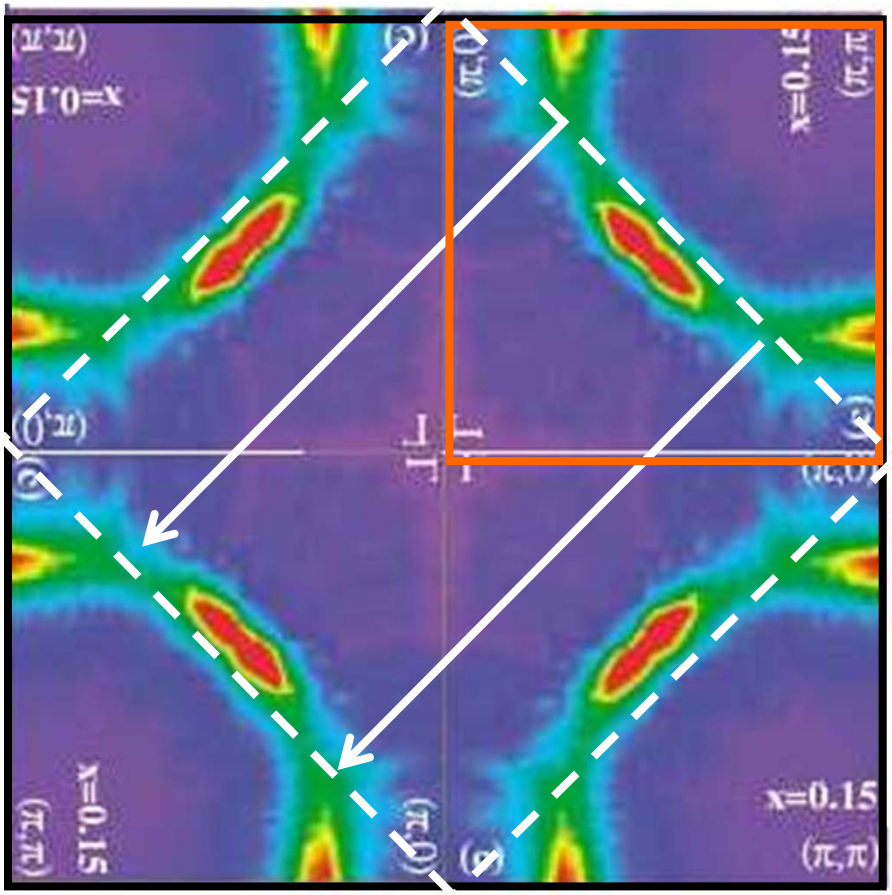
Hot spots from AFM quasi-static scattering

Mermin-Wagner

$d = 2$



Armitage et al. PRL 2001

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

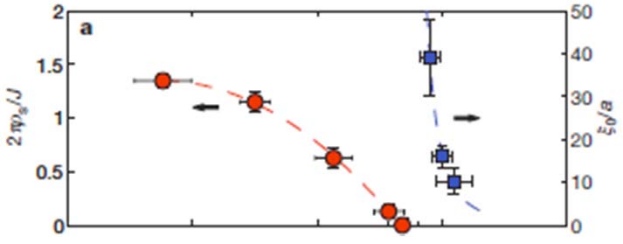
$$\xi^* = 2.6(2)\xi_{th}.$$

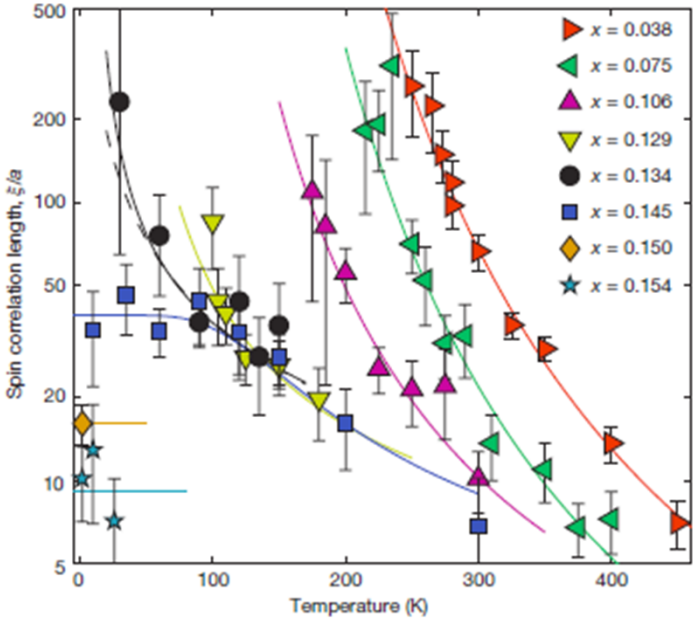
Motoyama, E. M. et al..
445, 186–189 (2007).

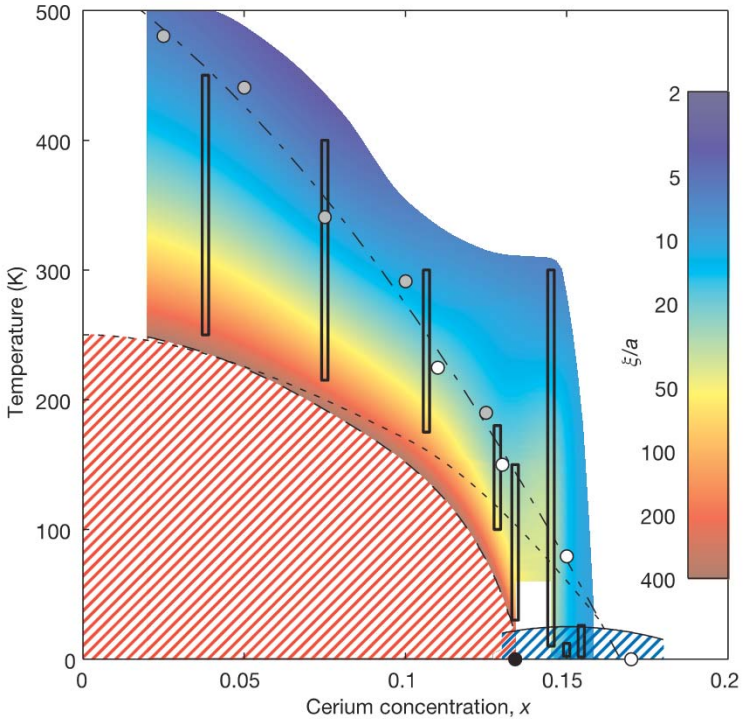
E-doped quantum critical

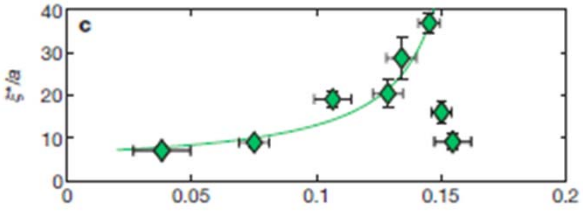
NCCO

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









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

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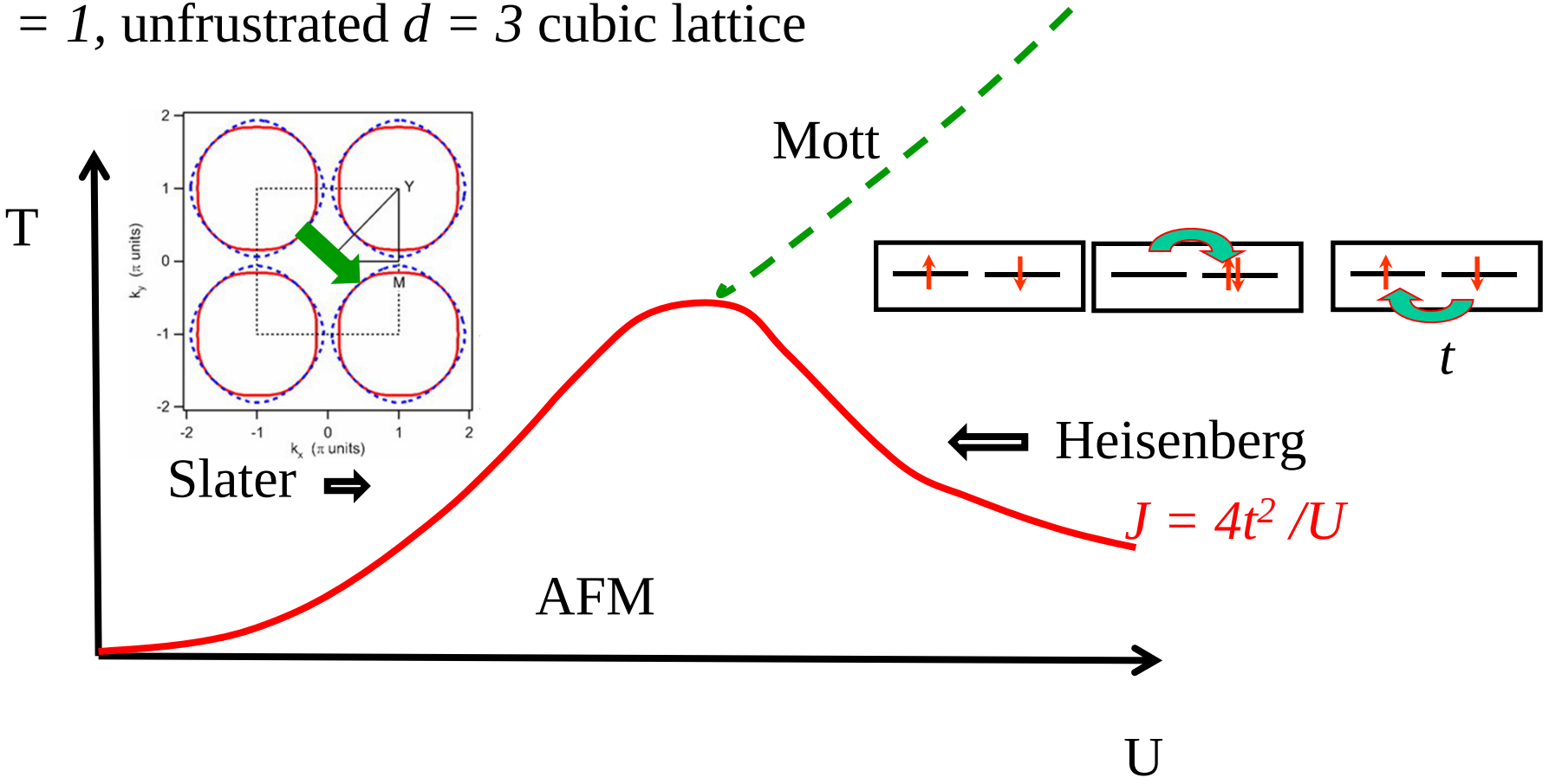
Precursor of d-wave superconducting fluctuations

- In a 15 K interval above T_c

3. Strong correlation physics (Mott insulator)

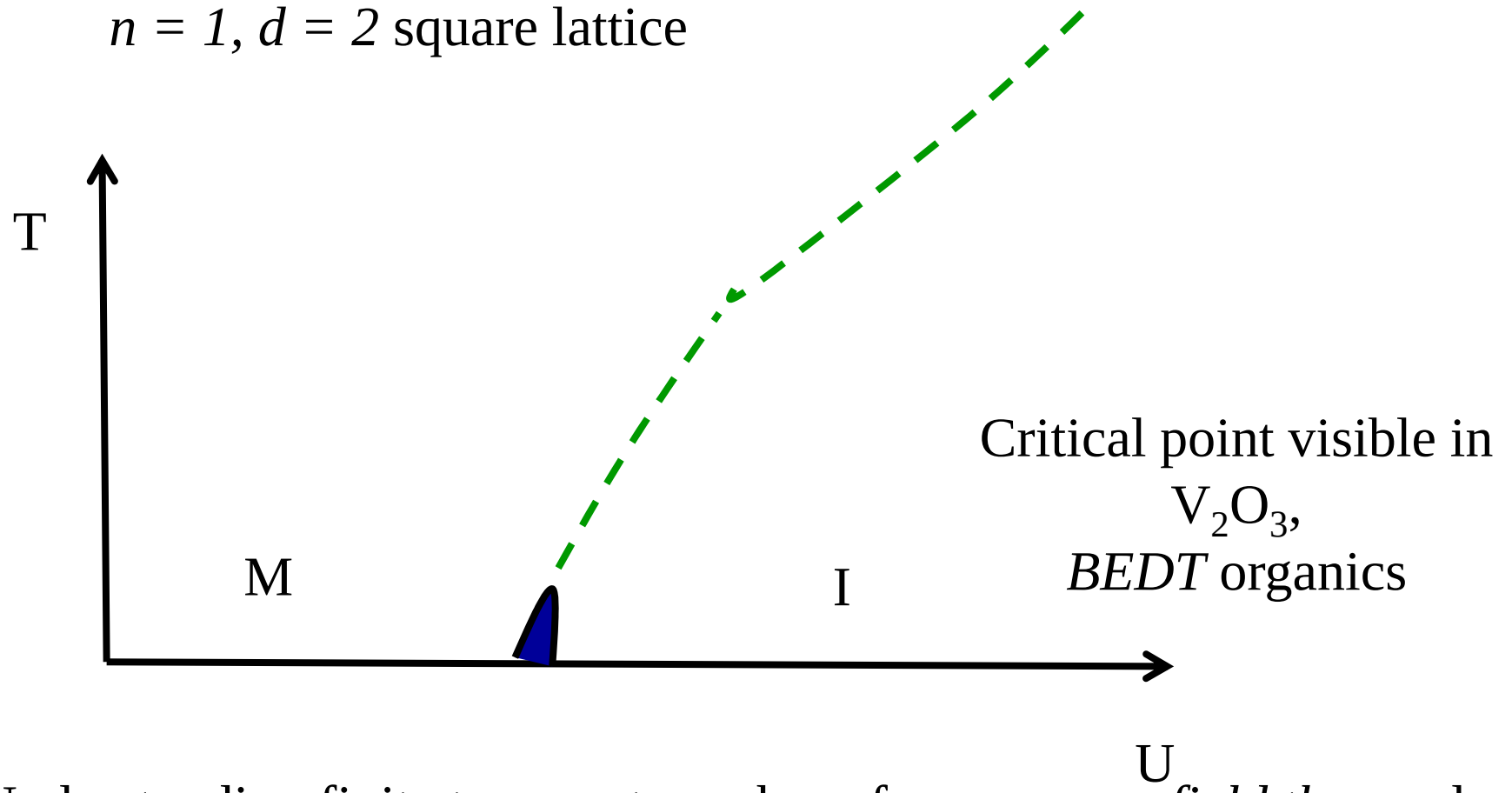
Weak vs Strong correlations

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



Local moment and Mott transition

n = 1, d = 2 square lattice



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

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YRZ

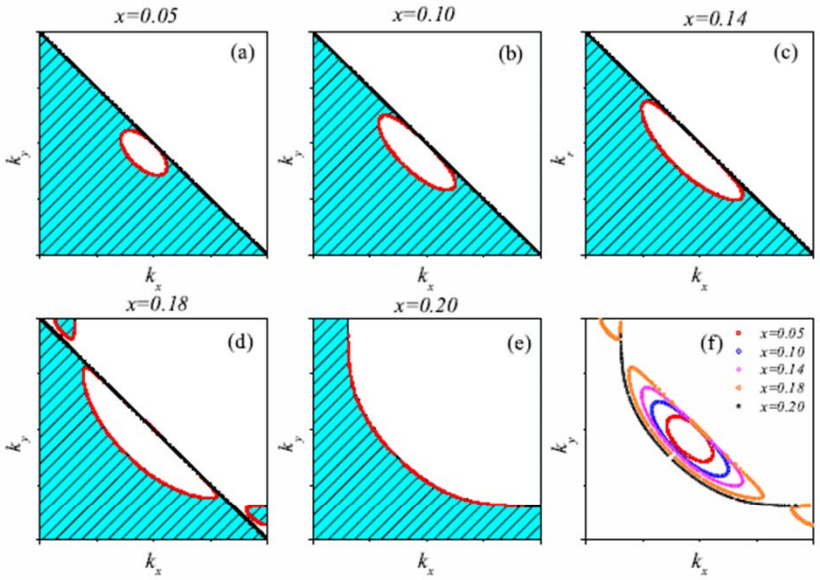

FIG. 1: Contours on which $G(\boldsymbol{k}, 0)$ changes sign at various hole concentrations x are shown in (a)-(e). In the shaded area $G(\boldsymbol{k}, 0) > 0$ satisfying the Luttinger Sum Rule. In the normal pseu[c] See also FL* Sachdev [)] $- (0, \pi)$ is the Luttinge[r] [in] the thick line represent the infinities of $G(\boldsymbol{k}, 0)$. The values of the parameters used here are given in Fig.2. The evolution of the contours of infinities in $G(\boldsymbol{k}, 0)$ is illustrated in (f).

Yang, Rice, Zhang PRB **73**, 174501 (2006)

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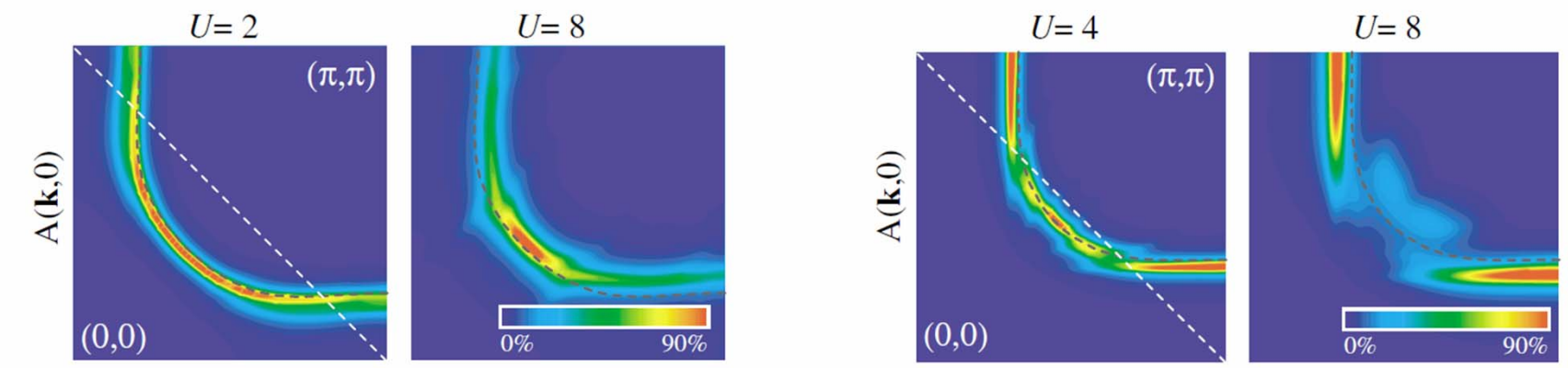
Quantum cluster approaches



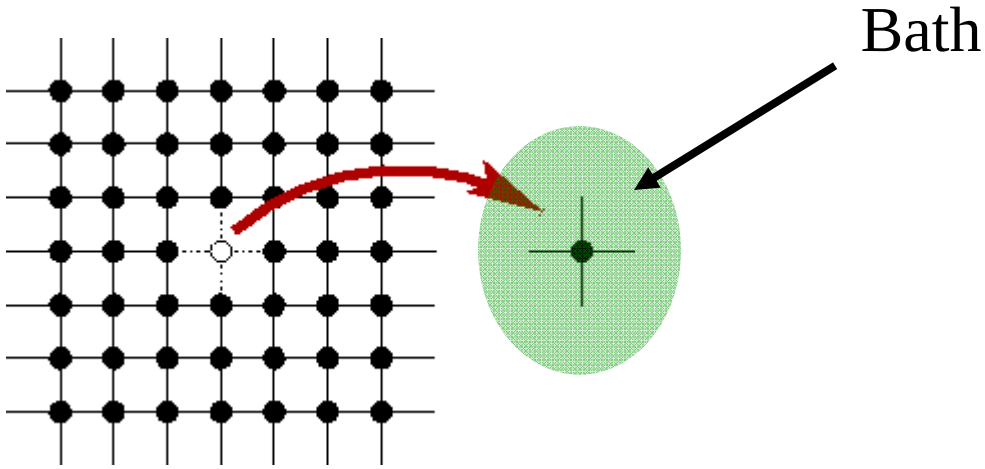
17 % hole doped

17 % electron doped

Sénéchal Tremblay, PRL 92, 126401 (2004)

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

- Compute scattering rate (self-energy) of impurity problem.
- Use that self-energy (ω dependent) for lattice.
- Project lattice on single-site and adjust bath so that single-site DOS obtained both ways be equal.



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

DMFT, (*d = 3*)

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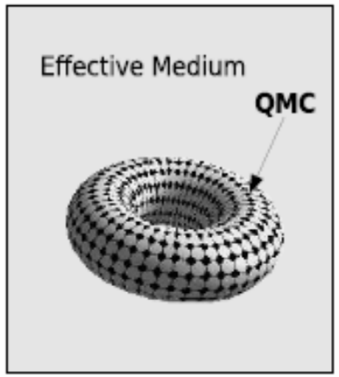
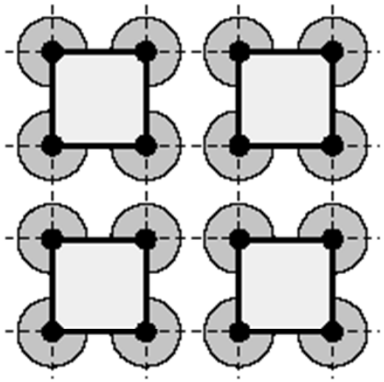
2d Hubbard: Quantum cluster method

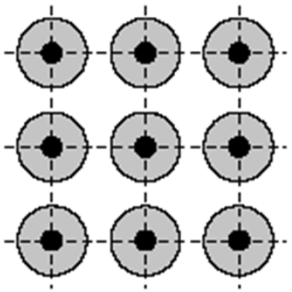


DCA

C-DMFT



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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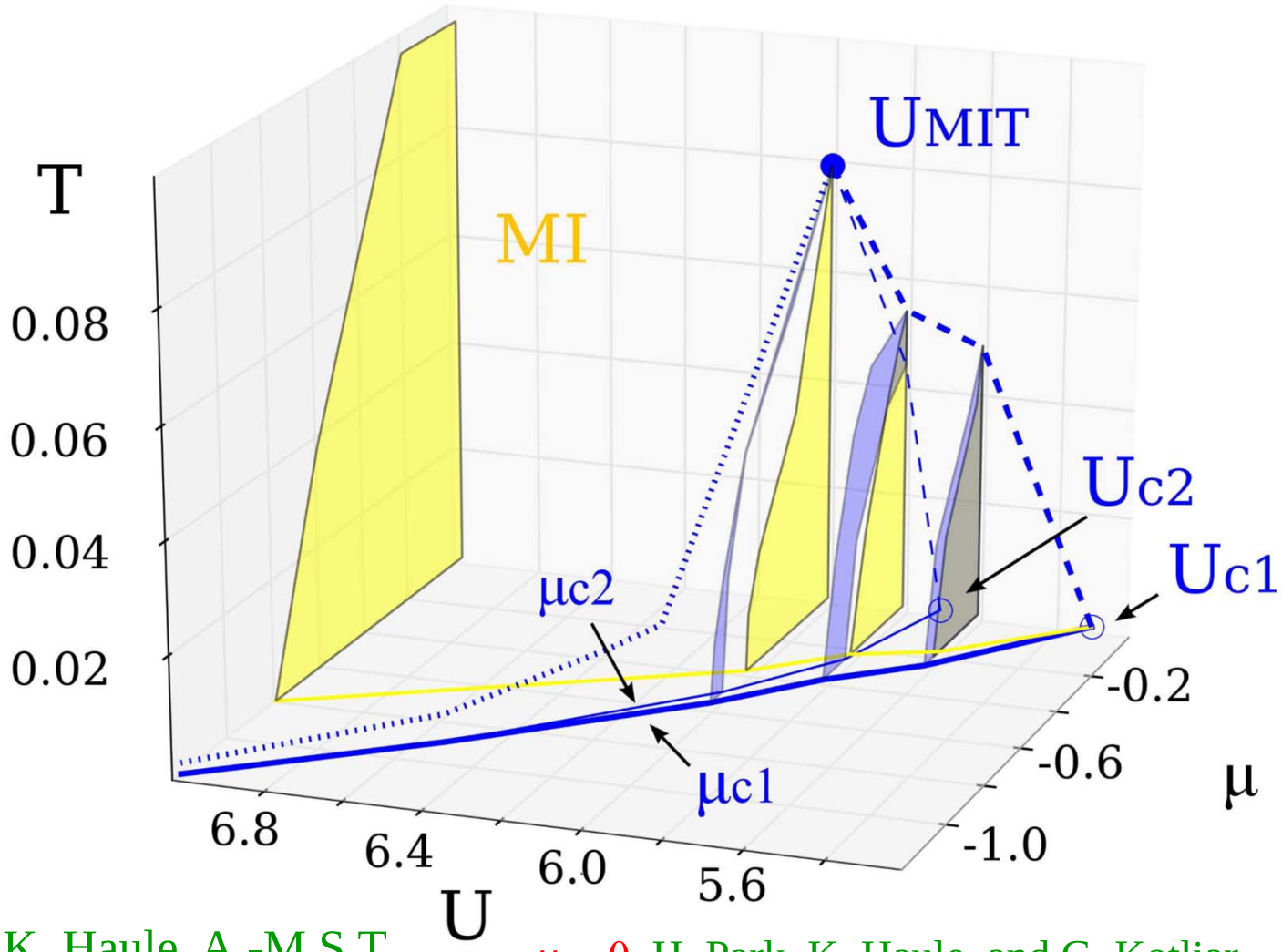
Normal state phase diagram



G. Sordi, K. Haule, A.-M.S.T
PRL, **104**, 226402 (2010)

μ = 0, H. Park, K. Haule, and G. Kotliar,
Phys. Rev. Lett. 101, 186403 (2008).

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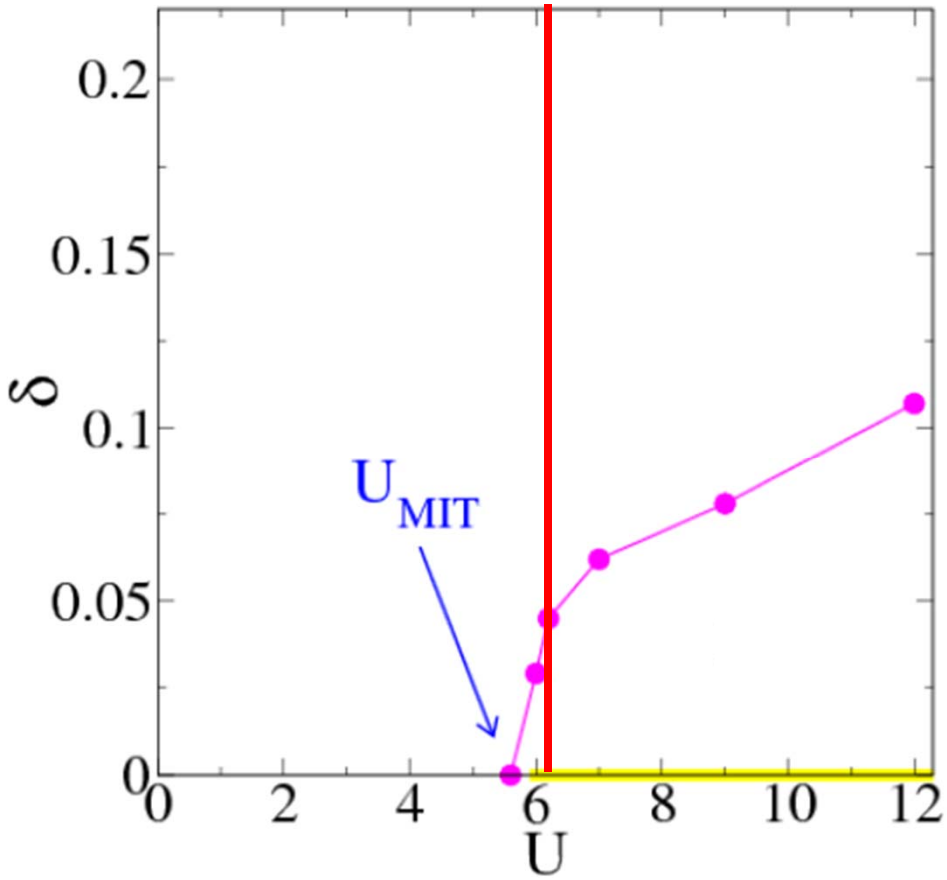
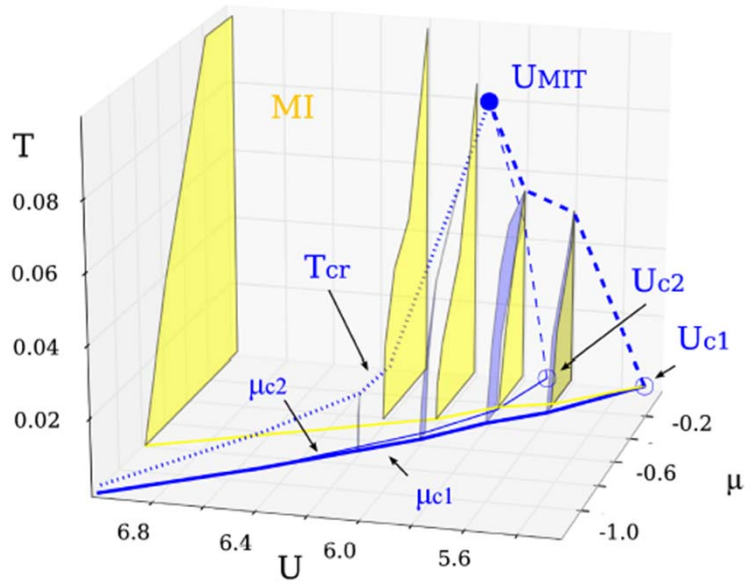
Link to Mott transition up to optimal doping

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





Smaller *D* and *S*

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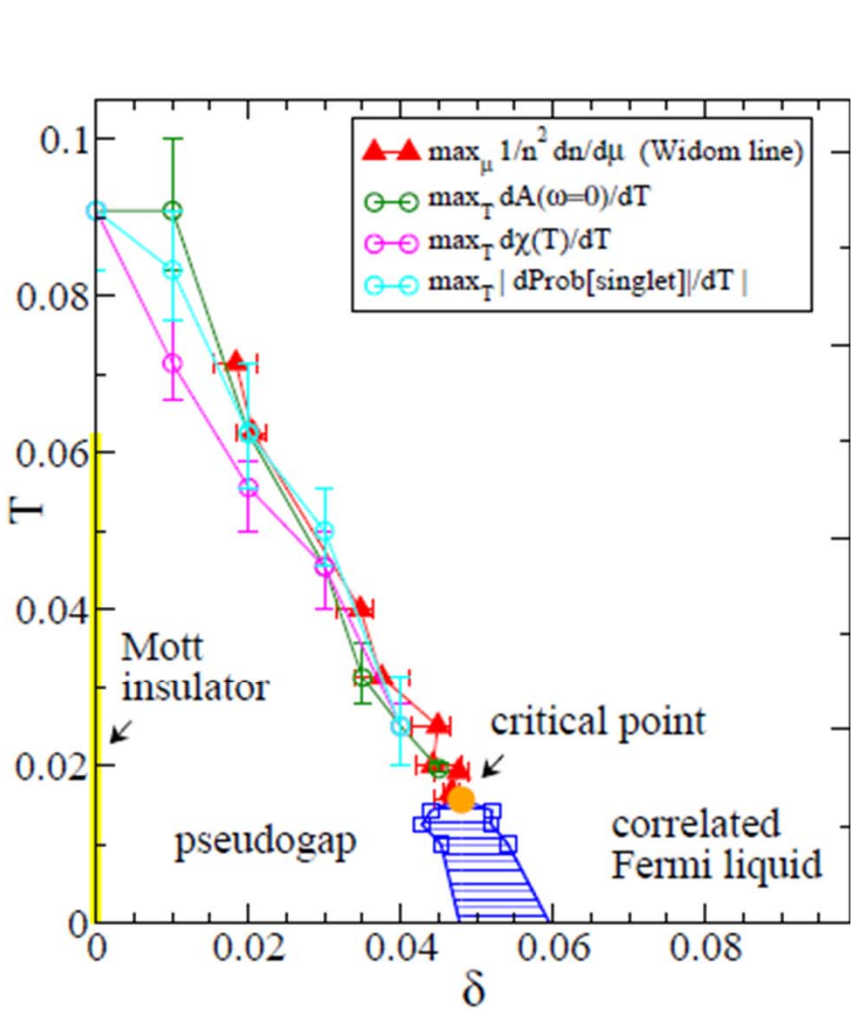
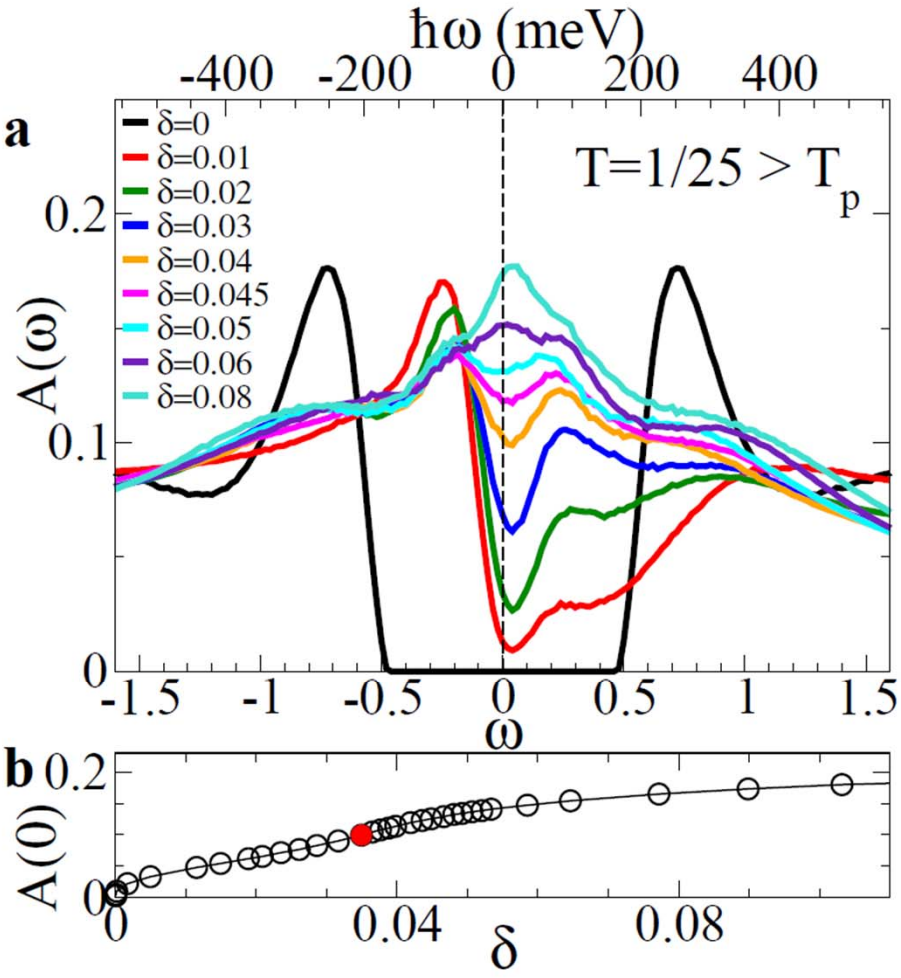
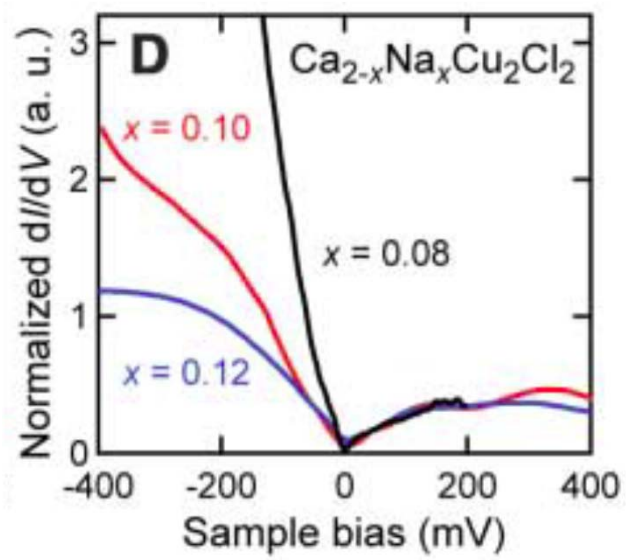
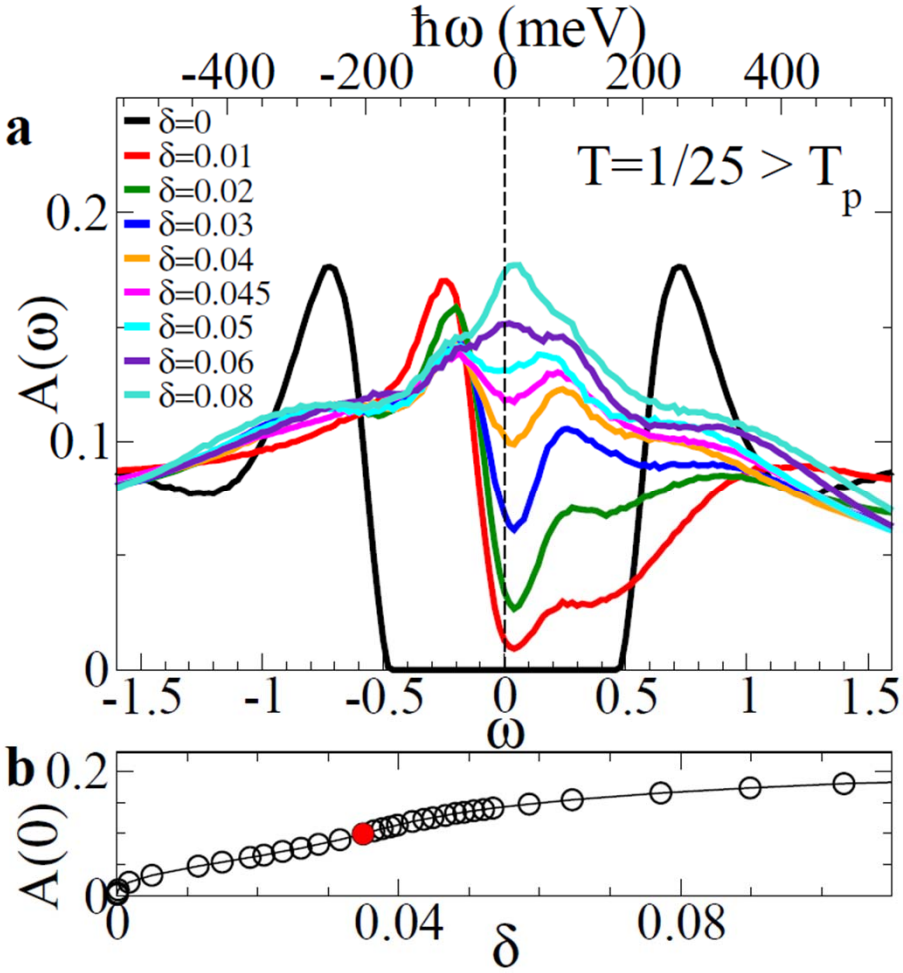
Density of states





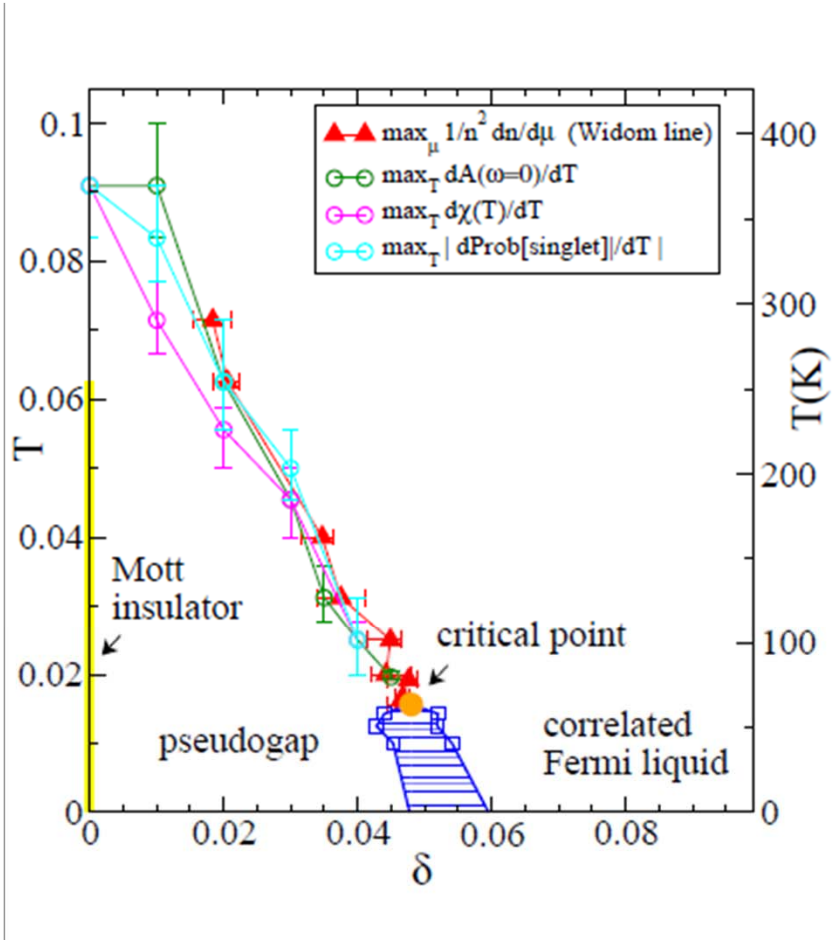
Density of states

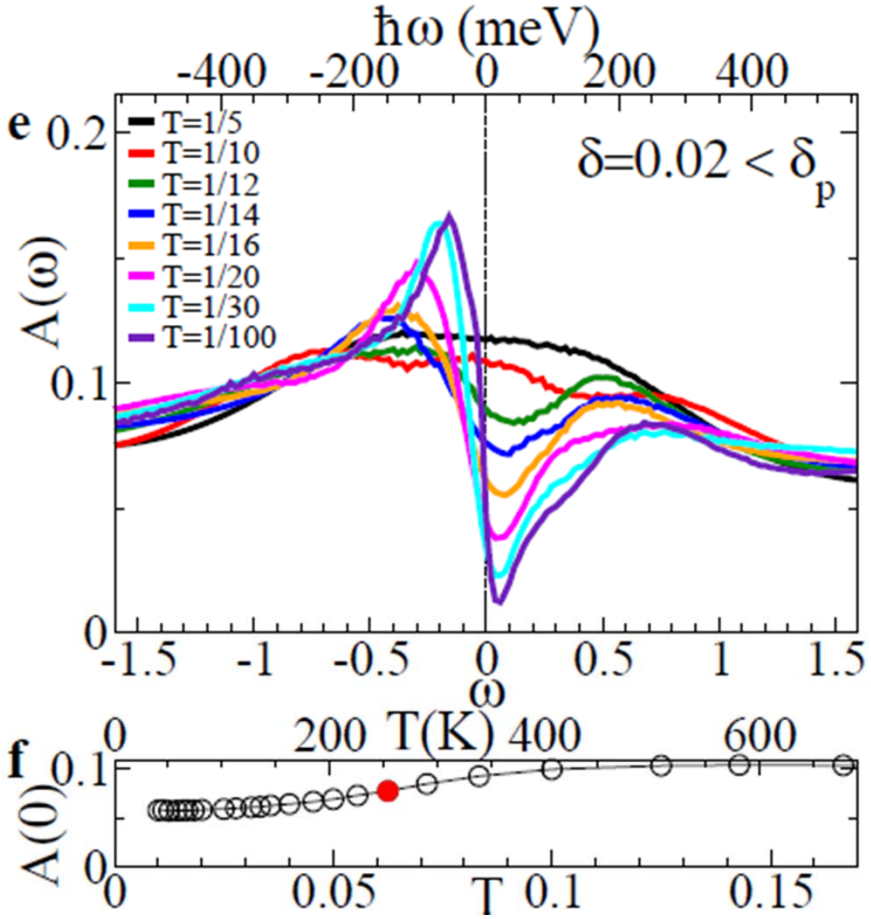




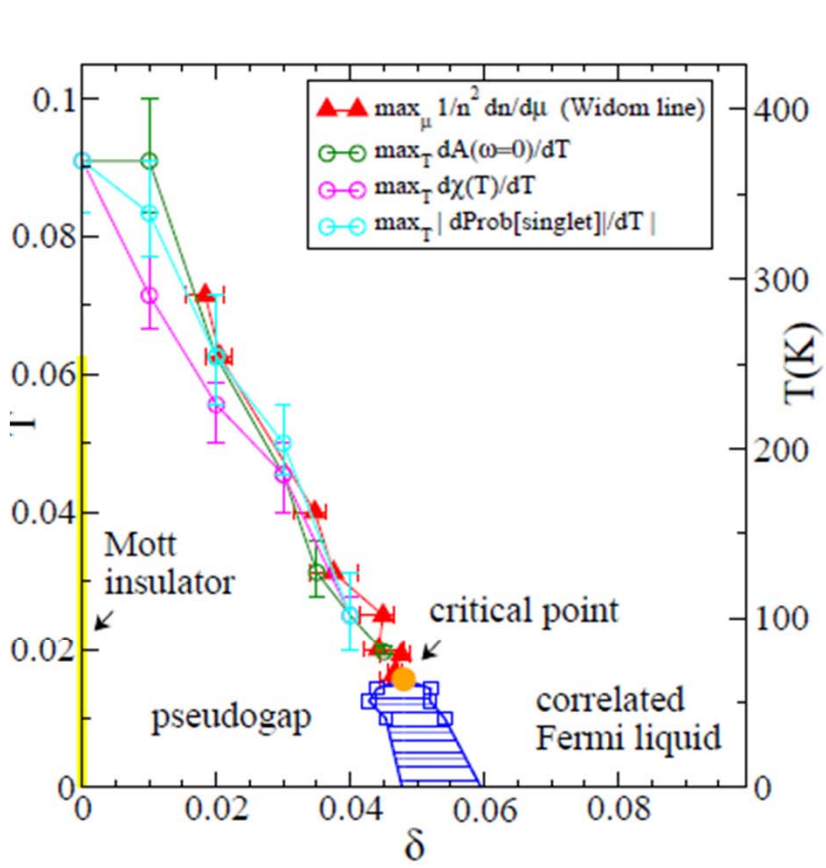
Khosaka et al. *Science* **315**, 1380 (2007);

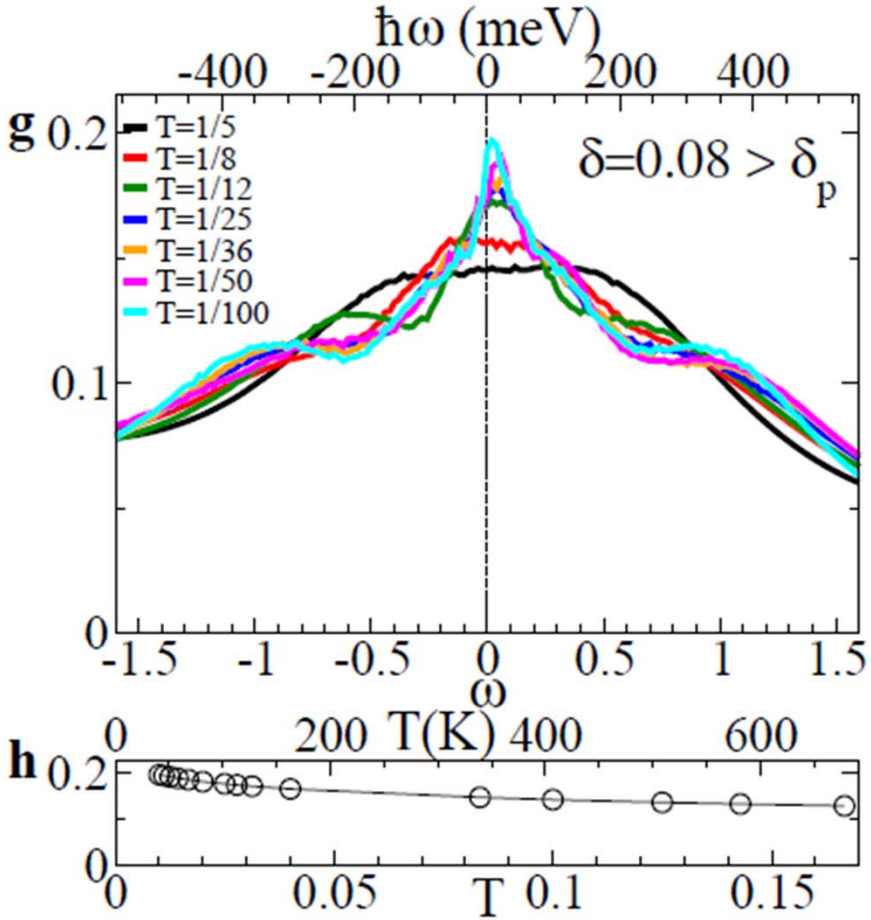
Density of states



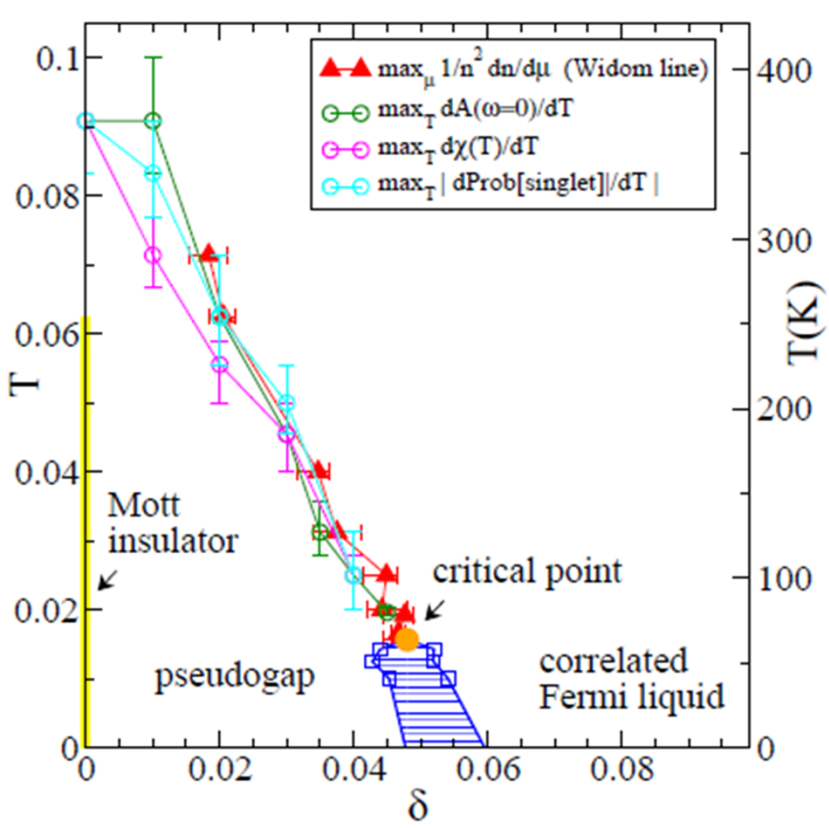


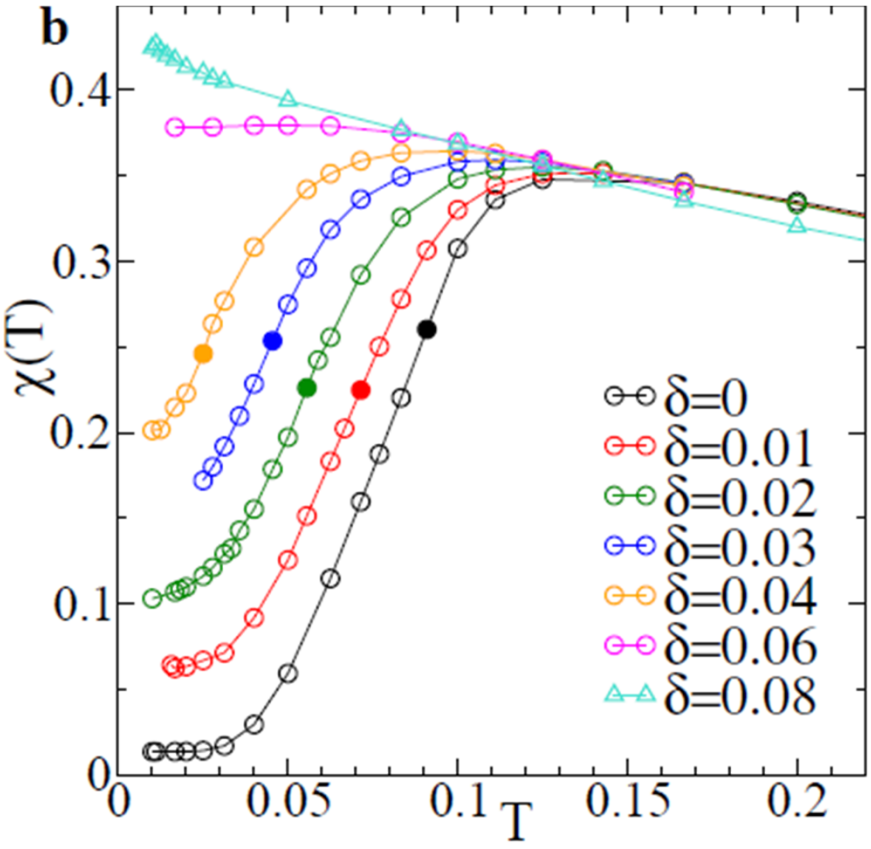
Density of states





Spin susceptibility





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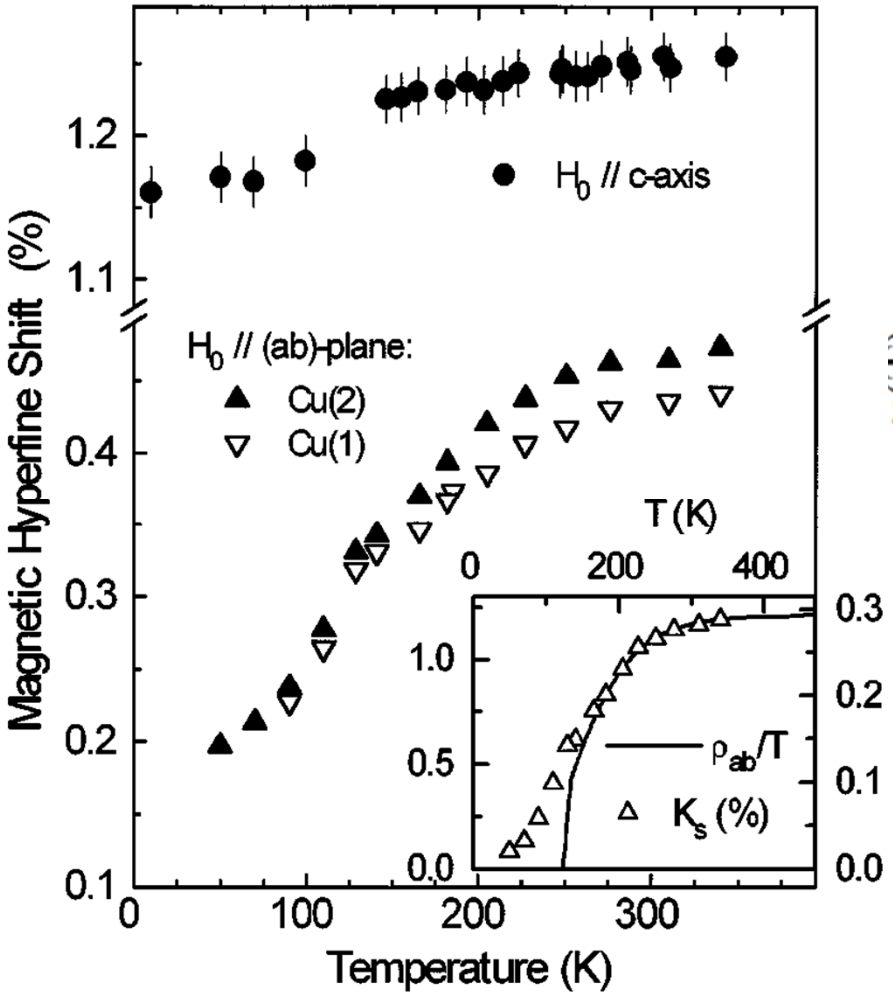
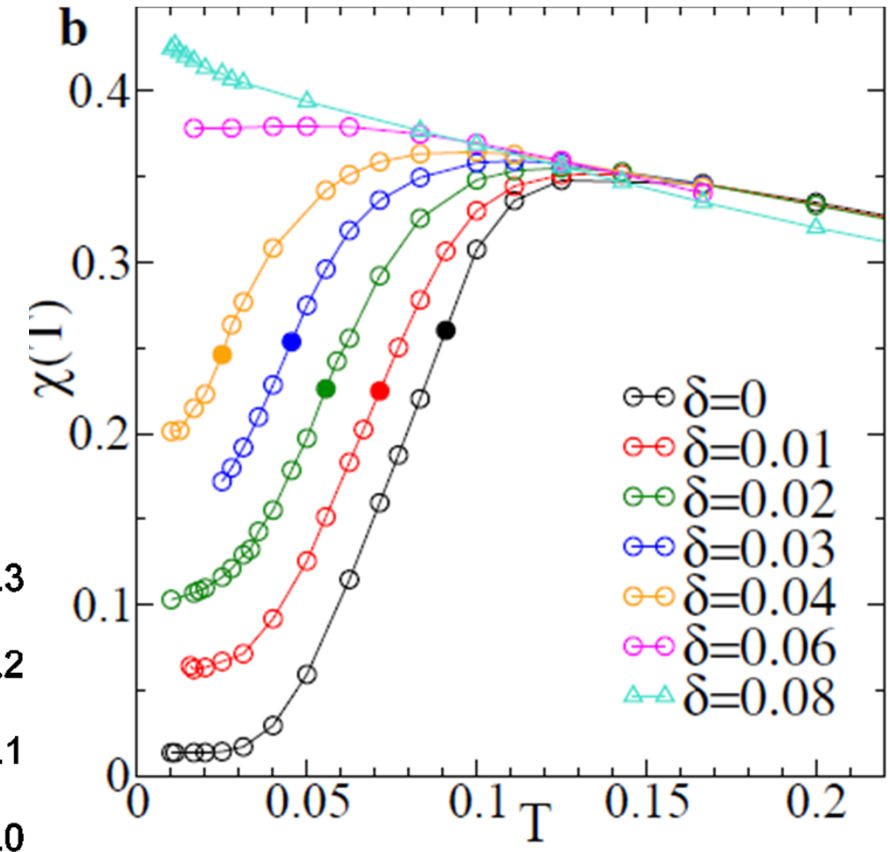
Spin susceptibility





Underdoped Hg1223

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

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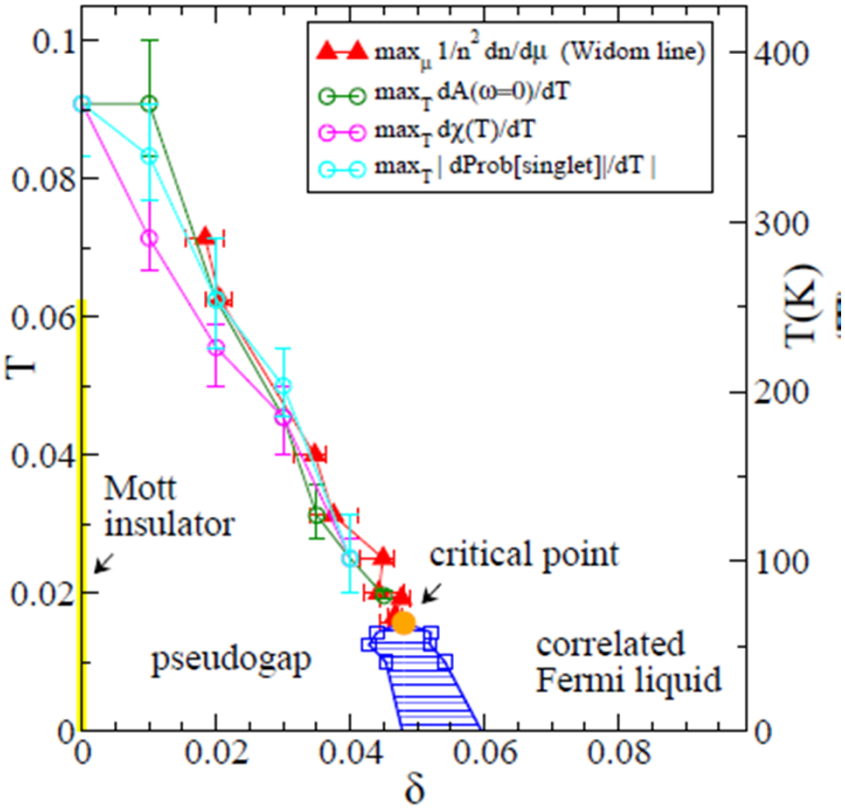
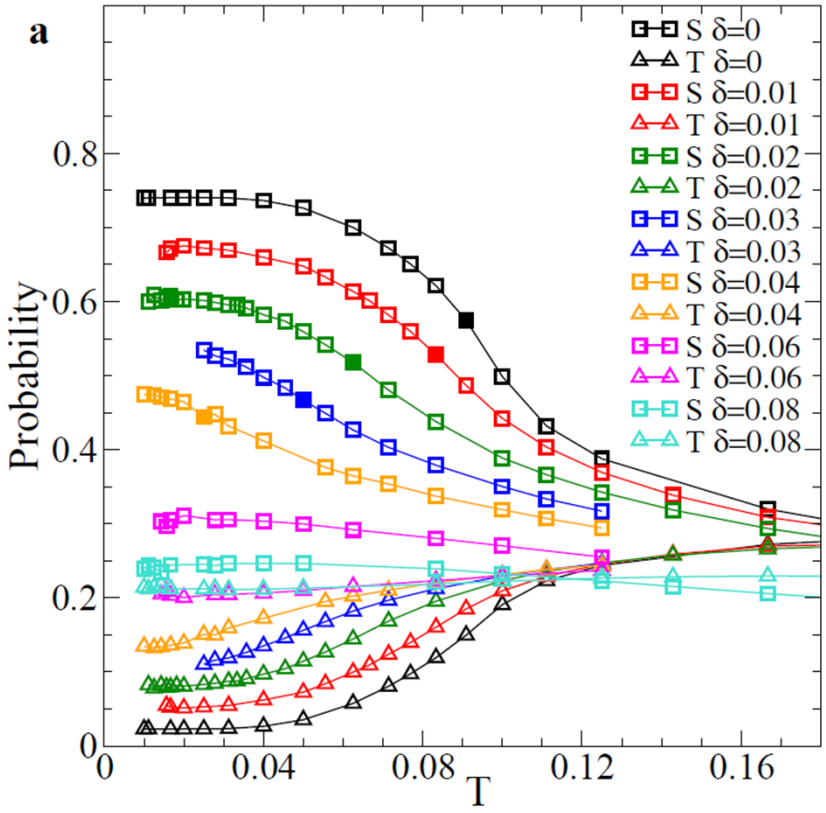
Plaquette eigenstates





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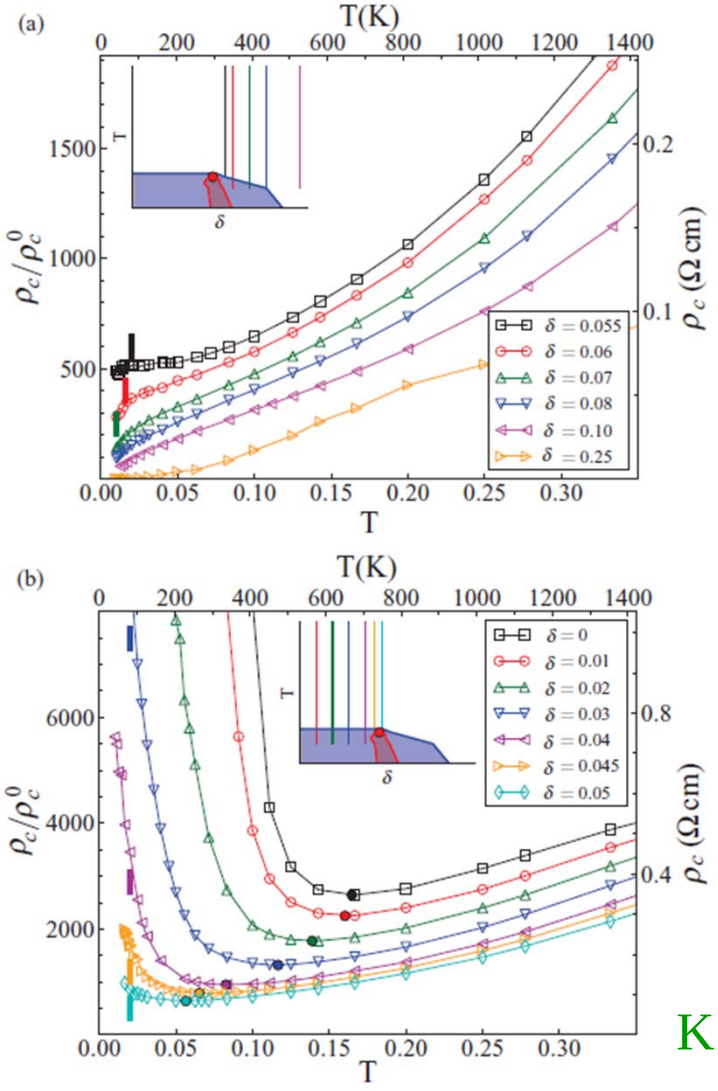
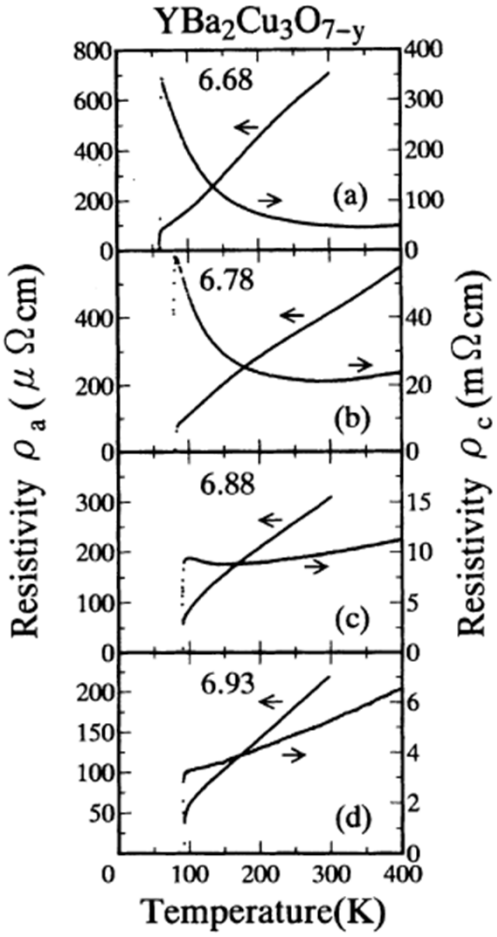
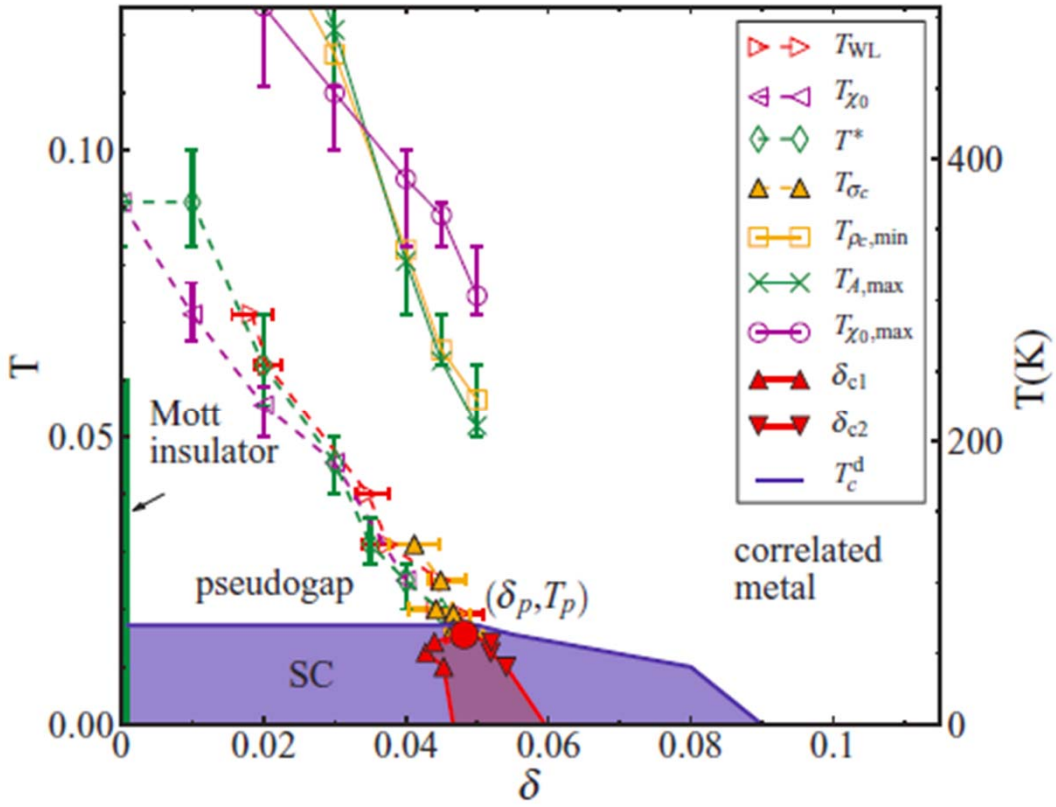
C-axis resistivity





K. Takenaka, K. Mizuhashi, H. Takagi, and S. Uchida, Phys. Rev.B 50, 6534 (1994).

Two crossover lines



Sordi et al. PRL 108, 216401 (2012)
PRB **87**, 041101(R) (2013)

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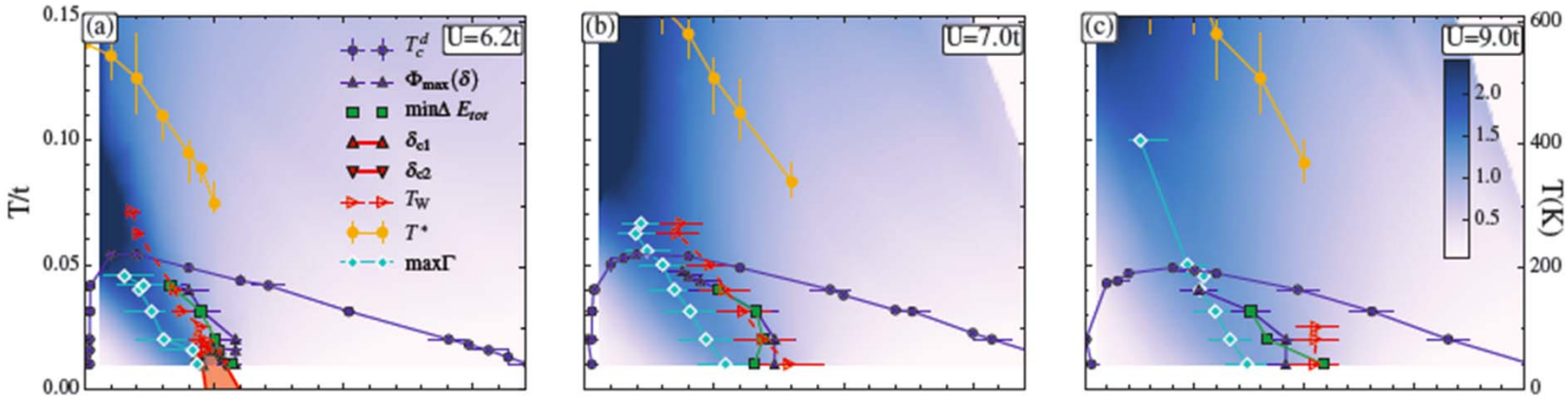
Two crossover lines



Fratino, Sémon, Sordi, A-MS T Sci. Rep. **6**, 22715 (2016)

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What is the minimal model?

H. Alloul arXiv:1302.3473

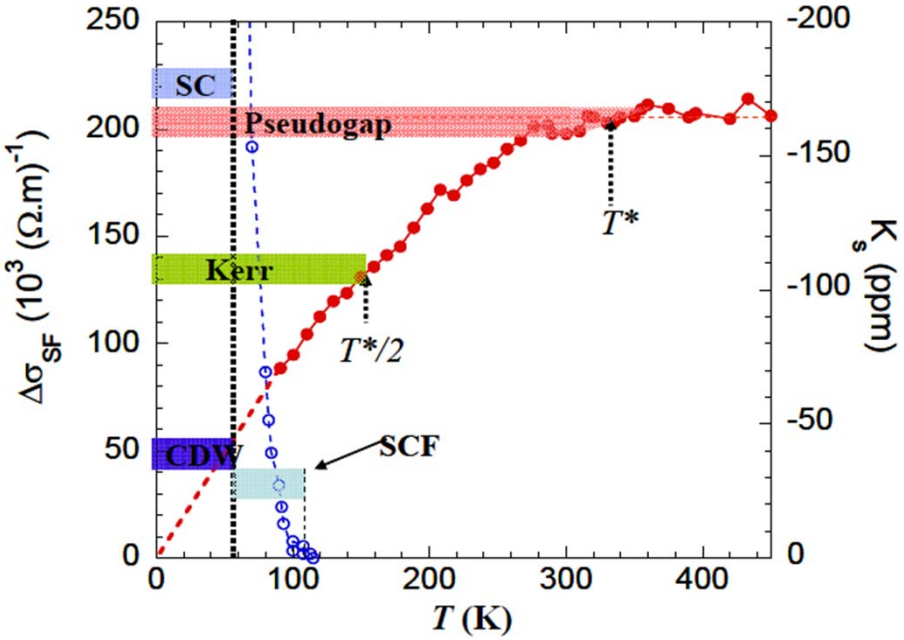
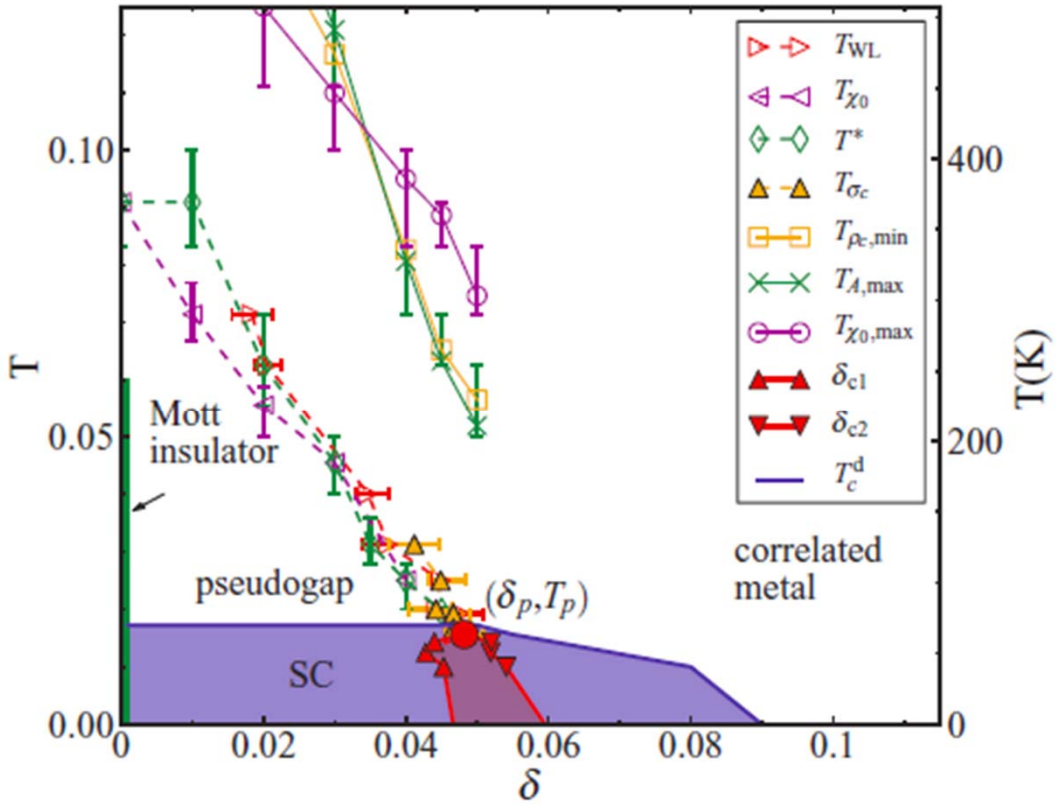


Fig 1 Spin contribution K_s to the ^{89}Y NMR Knight shift [11] for $YBCO_{6.6}$ permit to define the PG onset T^*. Here K_s is reduced by a factor two at $T \sim T^*/2$. The sharp drop of the SC fluctuation conductivity (SCF) is illustrated (left scale) [23]. We report as well the range over which a Kerr signal is detected [28], and that for which a CDW is evidenced in high fields from NMR quadrupole effects [33] and ultrasound velocity data [30]. (See text).

Crossover along the Widom line



Sordi et al. PRL 108, 216401 (2012)
PRB **87**, 041101(R) (2013)

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Giovanni Sordi

Patrick Sémon

Kristjan Haule

The Widom line

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

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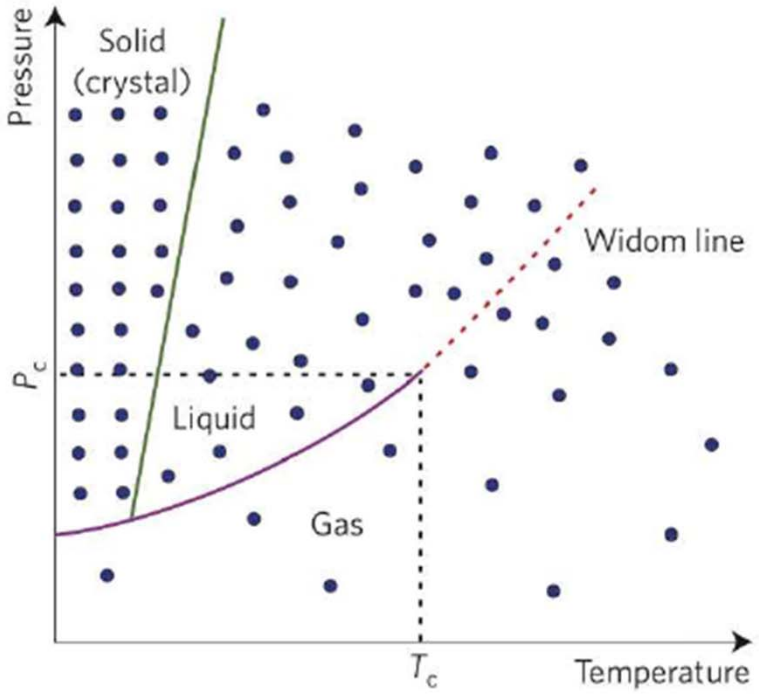
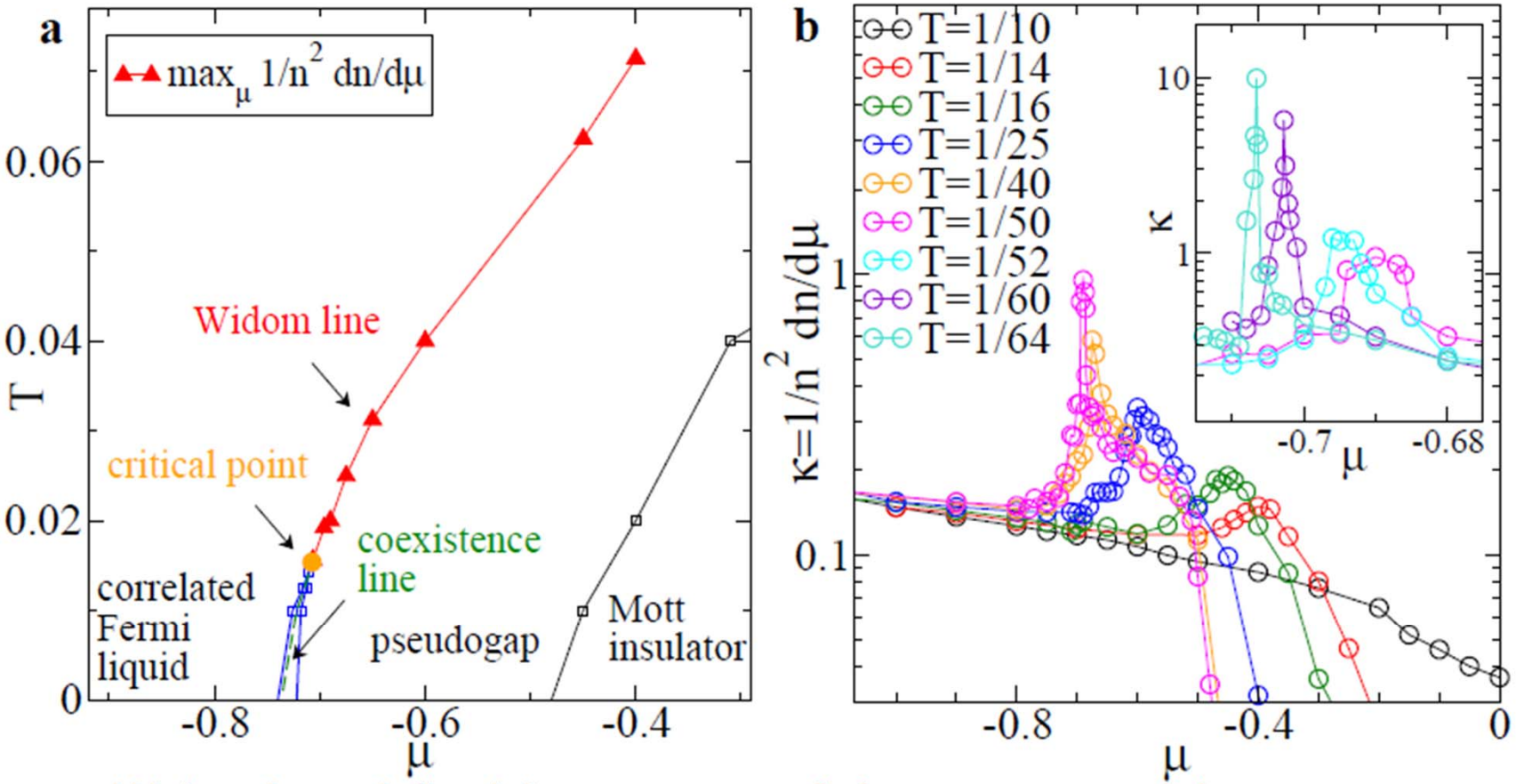
What is the Widom line?



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

Pseudogap T^* along the Widom line



Widom line: defined from maxima of charge compressibility

$\kappa = 1/n^2 (dn/d\mu)_T$

divergence of κ at the (classical) critical point!

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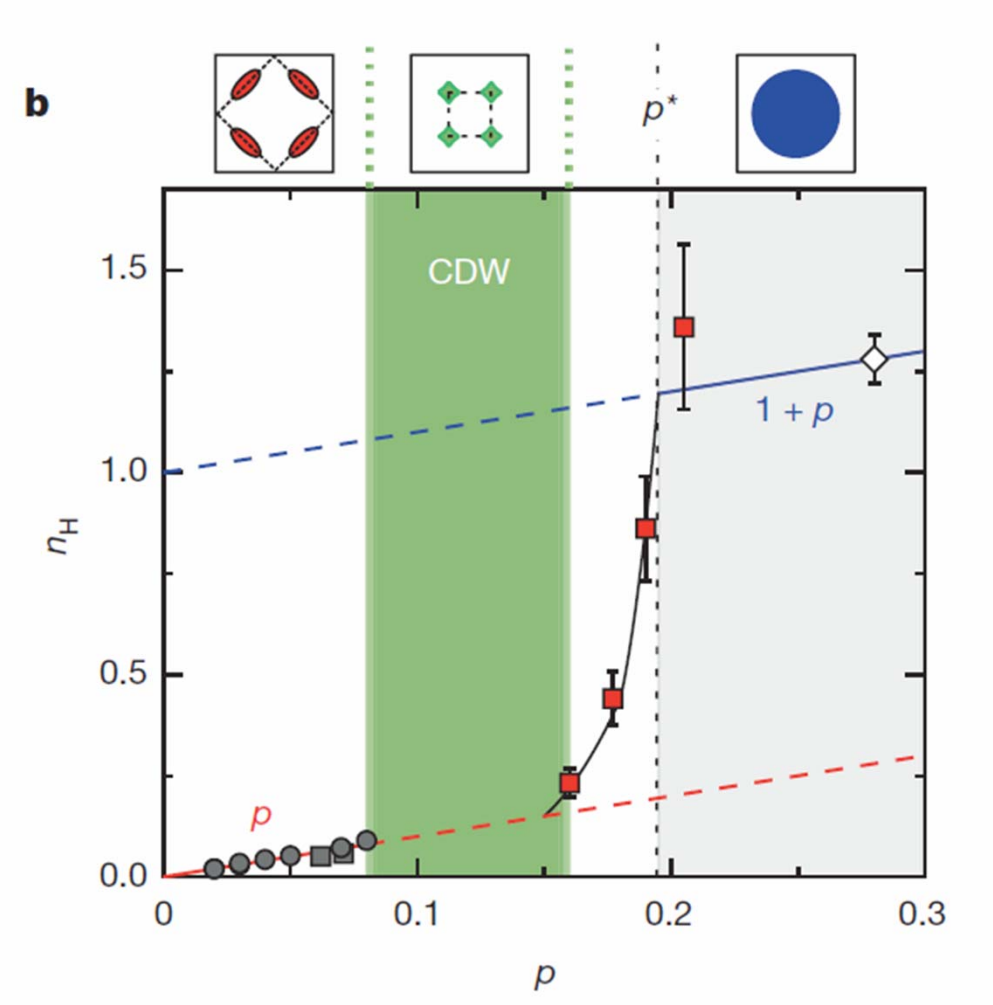
Coming back to: Not charge order



Badoux *et al.* Nature, March 2016

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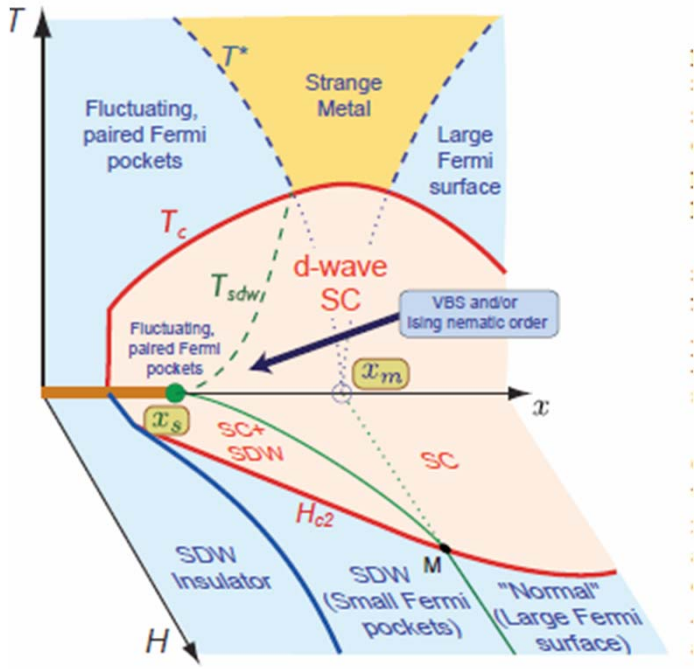
Applying a B field to remove superconductivity



S. Sachdev, Physica C **470**, S4 (2010)

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Antiferromagnetic phase diagram (TPSC)

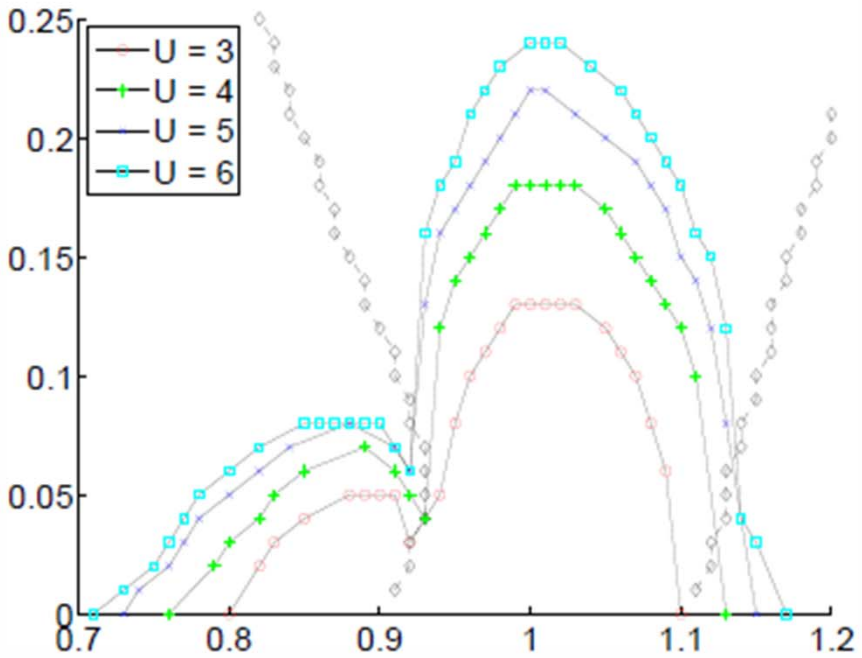


FIGURE 5.5 – Diagramme de phase température-dopage pour $t' = -0.1t$ pour quelques valeurs de U en fonction de n et T. Les diamants ($\Diamond$) indique la frontière commensurable-incommensurable.

Sébastien Roy, PhD thesis 2007

2 possible scenarios

epl A Letters Journal Exploring the Frontiers of Physics

January 2016

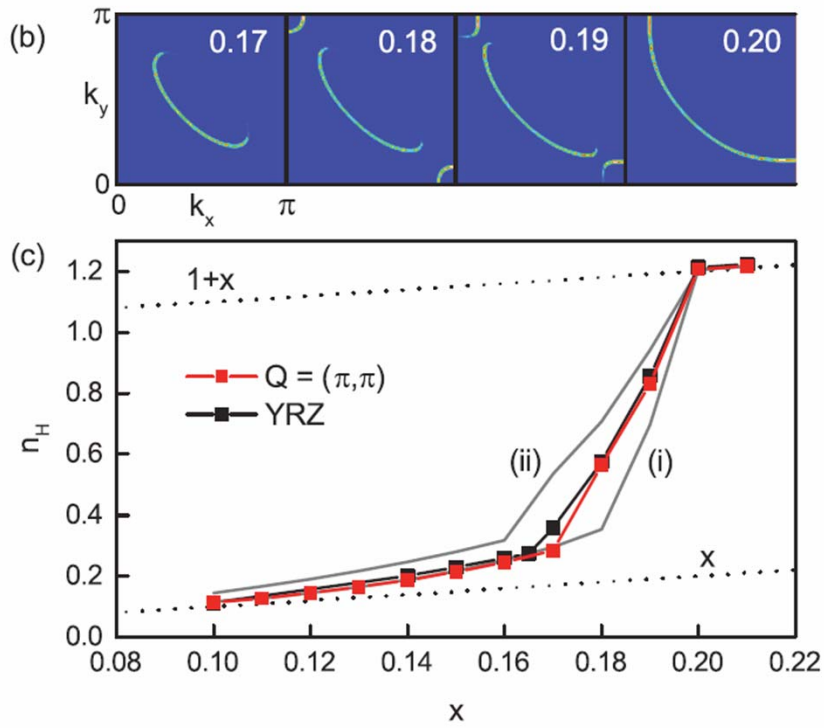
EPL, **113** (2016) 27003
doi: 10.1209/0295-5075/113/27003

www.epljournal.org

Hall effect and Fermi surface reconstruction via electron pockets in the high-T_c cuprates

J. G. Storey

Robinson Research Institute, Victoria University - P.O. Box 600, Wellington, New Zealand



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