Superconductivity, pseudogap and Mott transition

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Montauk, 6 Sept. 2012

VERITATEM IN CHARITATE

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Three broad classes of mechanisms for pseudogap

- Rounded first order transition
- *d =2* precursor to a lower temperature broken symmetry phase
- Mott physics

- Competing order
  - Current loops: Varma, PRB **81,** 064515 (2010)
  - Stripes or nematic: Kivelson et al. RMP 75 1201(2003); J.C.Davis
  - d-density wave : Chakravarty, Nayak, Phys. Rev. B **63**, 094503 (2001); Affleck et al. flux phase
  - SDW: Sachdev PRB **80**, 155129 (2009) ...
- Or Mott Physics?
  - RVB: P.A. Lee Rep. Prog. Phys. **71,** 012501 (2008)

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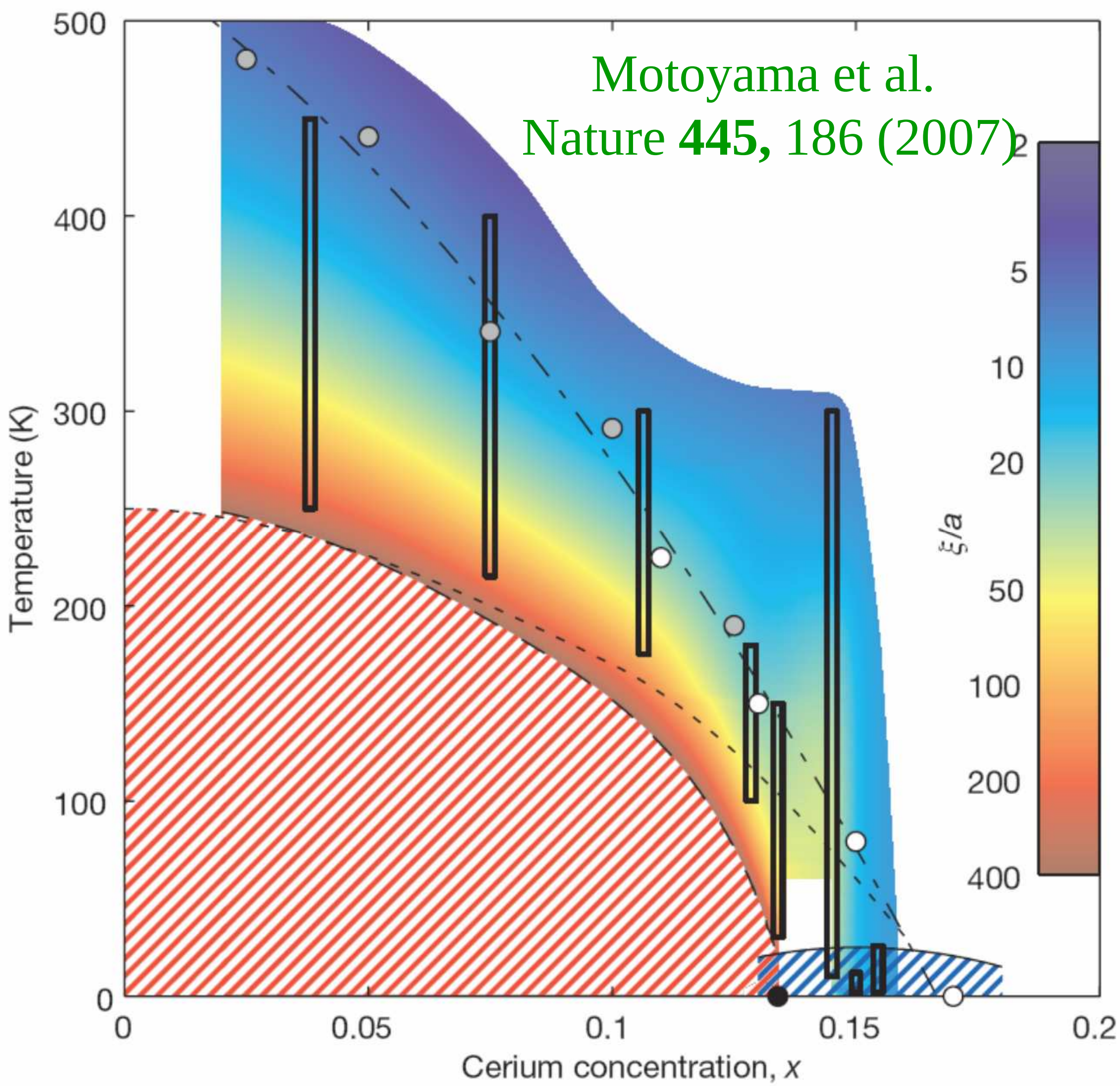
$d = 2$ precursors, e-doped



Motoyama et al.
Nature **445,** 186 (2007)

$$\xi^{\star} = 2.6(2)\xi_{\mathrm{th}}$$

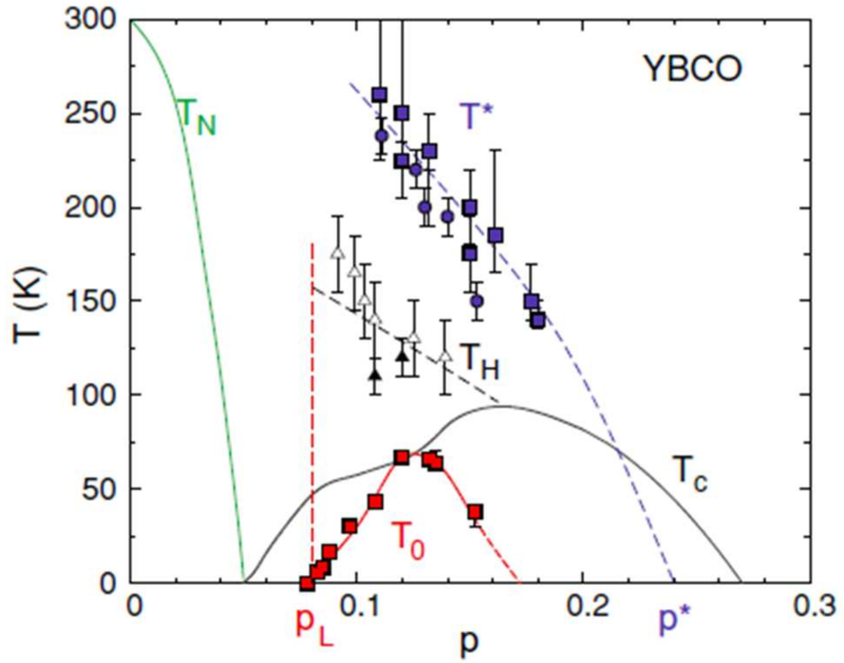
Vilk, A.-M.S.T (1997)

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

Semi-quantitative fits of both ARPES and neutron

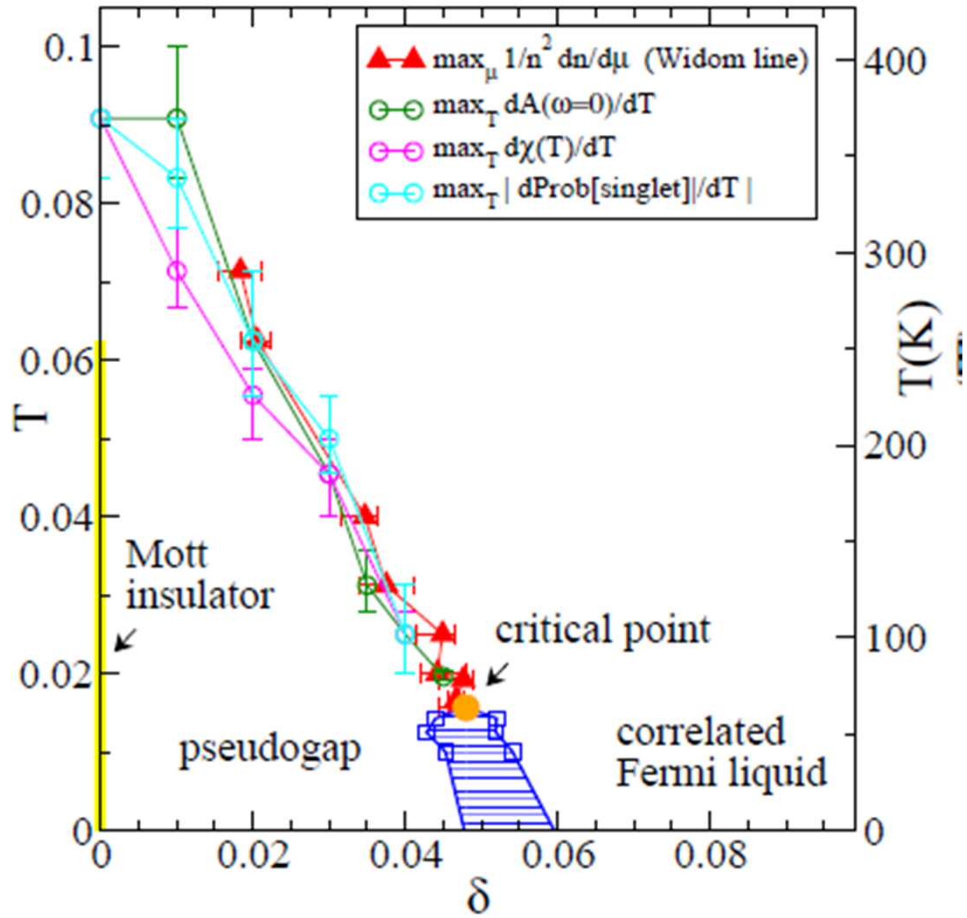
Université de Sherbrooke

Hole-doped case: Competing phases?



Leboeuf, Doiron-Leyraud et al. PRB **83,** 054506 (2011)

Pseudogap from Mott physics



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

Competing order is a consequence of the pseudogap, not its cause:

Parker et al. Nature 468, 677 (2010)

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Model

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

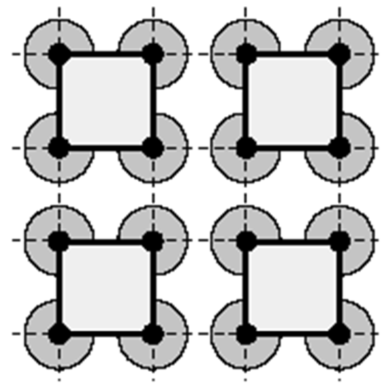
Outline

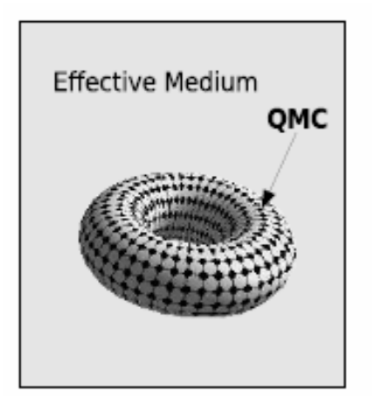
- Method
- *T=0* phase diagram
- Finite *T* phase diagram
  - Normal state (no LRO, what is below the dome)
    - First order transition
    - Widom line and pseudogap
  - Superconductivity

Method

2d Hubbard: Quantum cluster method

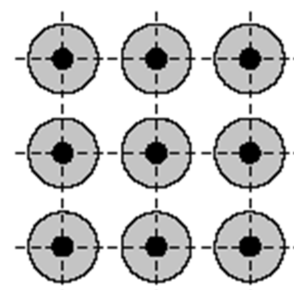
C-DMFT





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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Another way to look at this (Potthoff)

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

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

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

Still stationary (chain rule)

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

M. Potthoff, Eur. Phys. J. B 32, 429 (2003).

SFT : Self-energy Functional Theory

With $F[\Sigma]$ Legendre transform of Luttinger-Ward funct.

$$\Omega_{\mathbf{t}}[\Sigma] = F[\Sigma] + \mathrm{Tr}\ln(-(G_0^{-1} - \Sigma)^{-1})$$

is stationary with respect to Σ and equal to grand potential there.

$$\Omega_{\mathbf{t}}[\Sigma] = \Omega_{\mathbf{t}'}[\Sigma] - \mathrm{Tr}\ln(-(G_0'^{-1} - \Sigma)^{-1}) + \mathrm{Tr}\ln(-(G_0^{-1} - \Sigma)^{-1}).$$

Vary with respect to parameters of the cluster (including Weiss fields)

Variation of the self-energy, through parameters in $H_0(\mathbf{t}')$

M. Potthoff, Eur. Phys. J. B 32, 429 (2003).

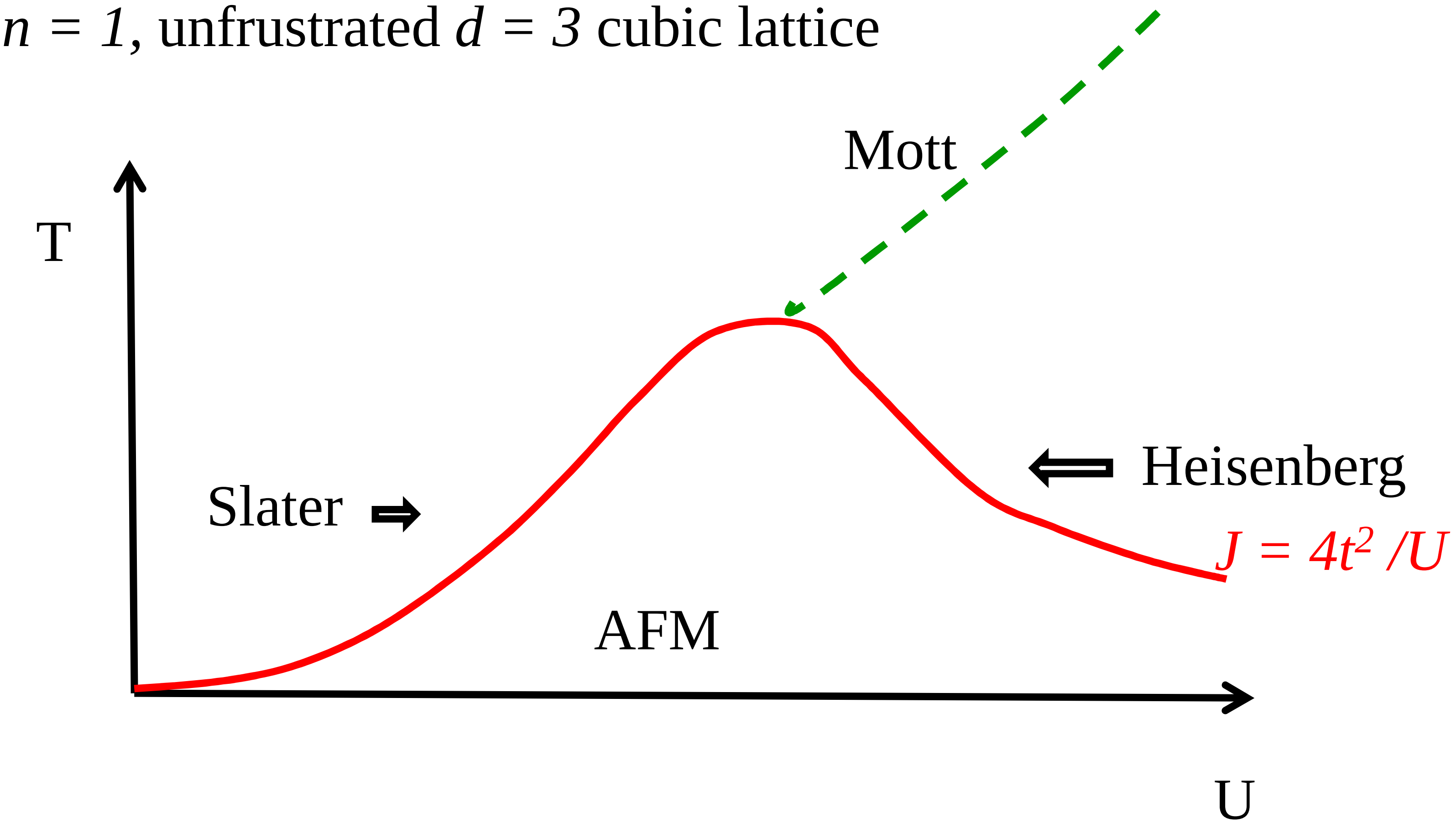
+ and -

- 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

What is it useul for?
Example: The Mott transition

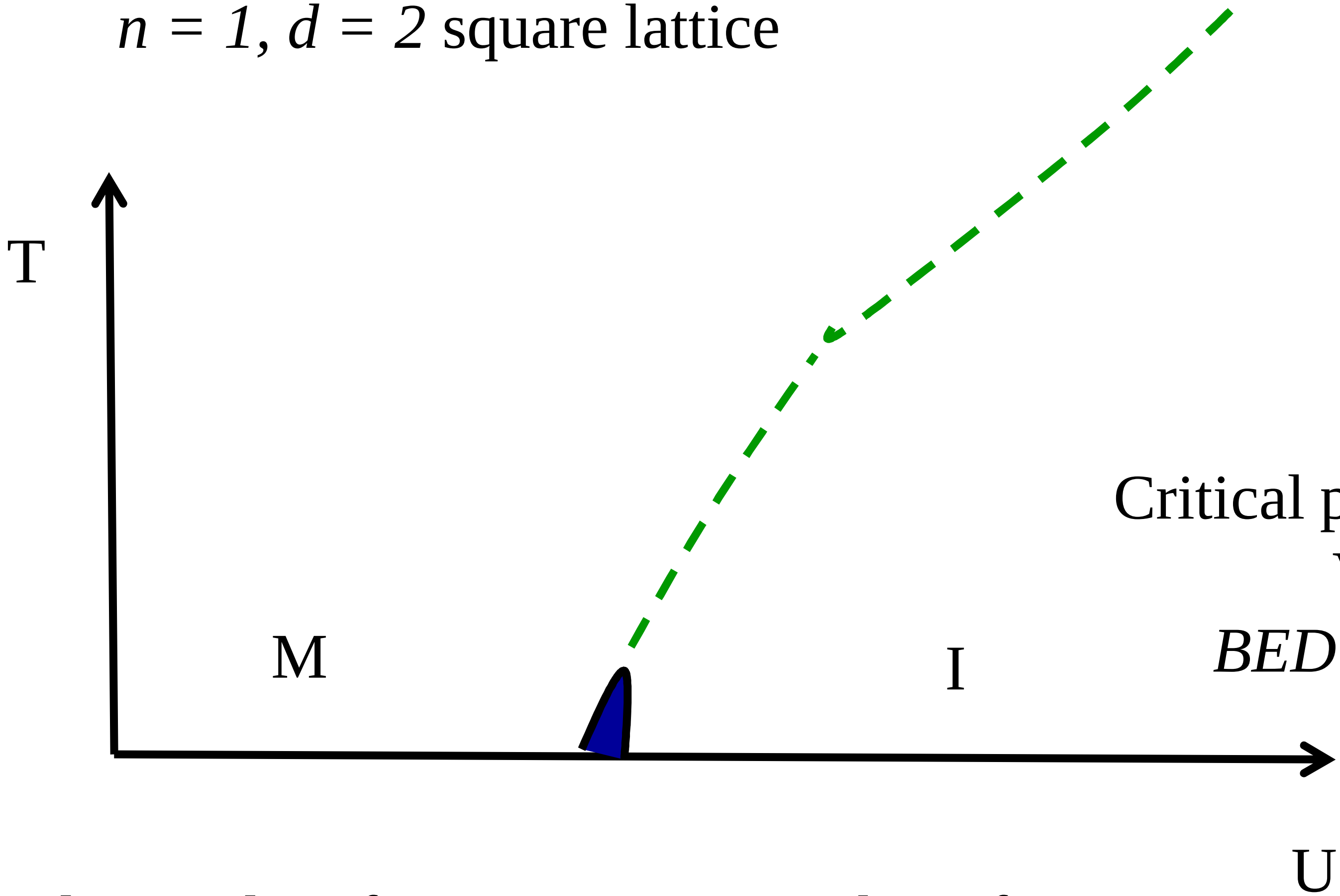
Local moment and Mott transition

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



Local moment and Mott transition

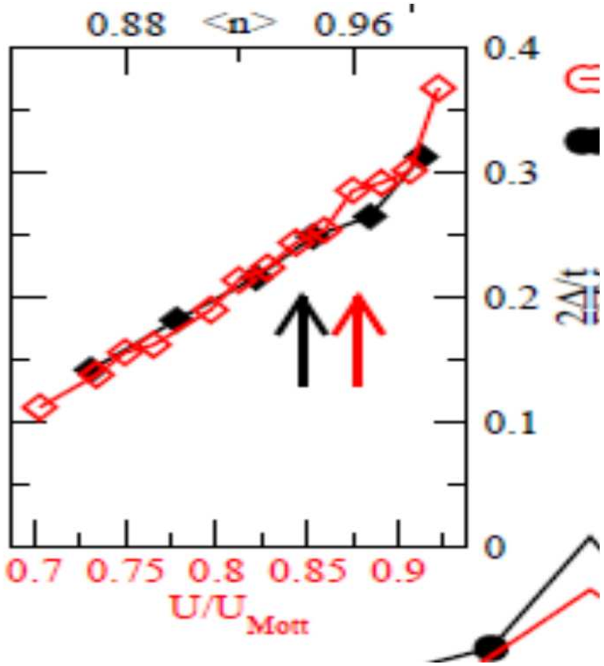
n = 1, *d = 2* square lattice



Critical point visible in
V_2O_3,
BEDT organics

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

Size dependence



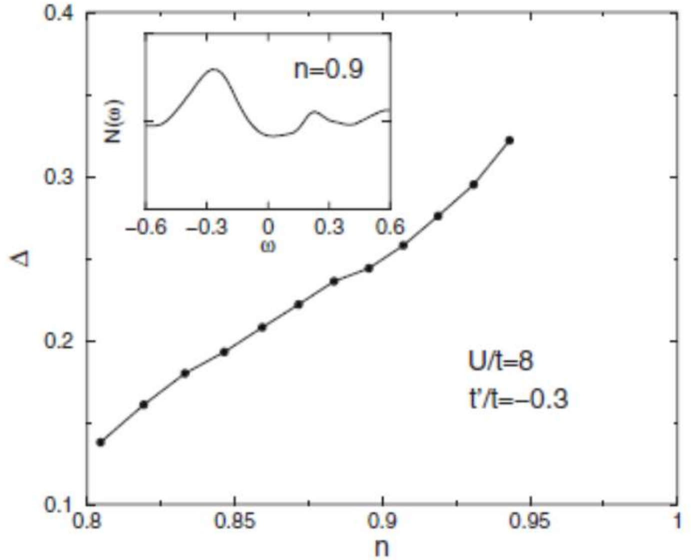


FIG. 5. The gap as a function of filling, for $U=8t$, $t'=-0.3t$. The gap is defined as half the distance between the two peaks on either side of $\omega=0$, as they appear, for example, in the inset.

Gull, Parcollet, Millis
arXiv:1207.2490v1

Kancharla et al. PRB **77**, 184516 (2008)

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$T = 0$ phase diagram: cuprates

Phase diagram

Exact diagonalization as impurity solver ($T=0$).

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T = 0 phase diagram: Pseudogap in the normal state

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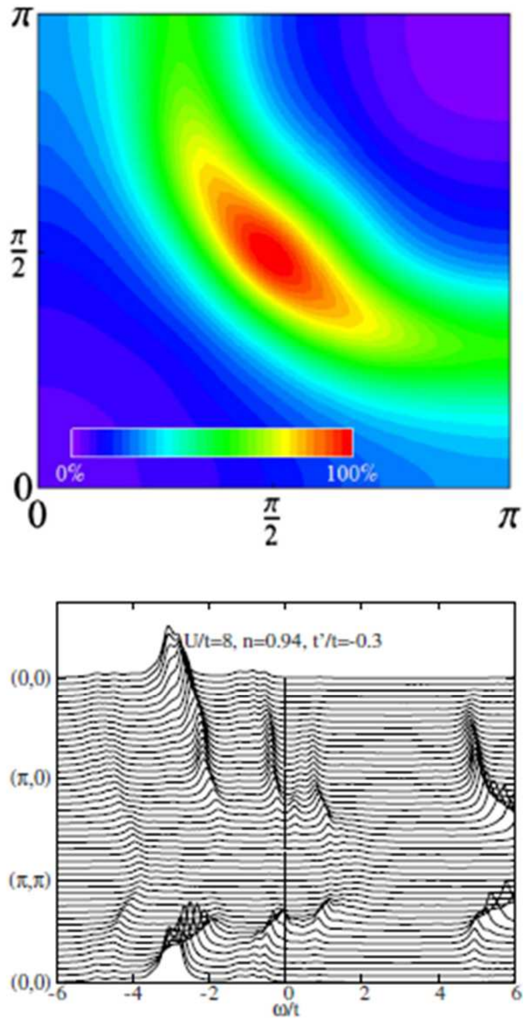
$\omega = 0$ (CDMFT)



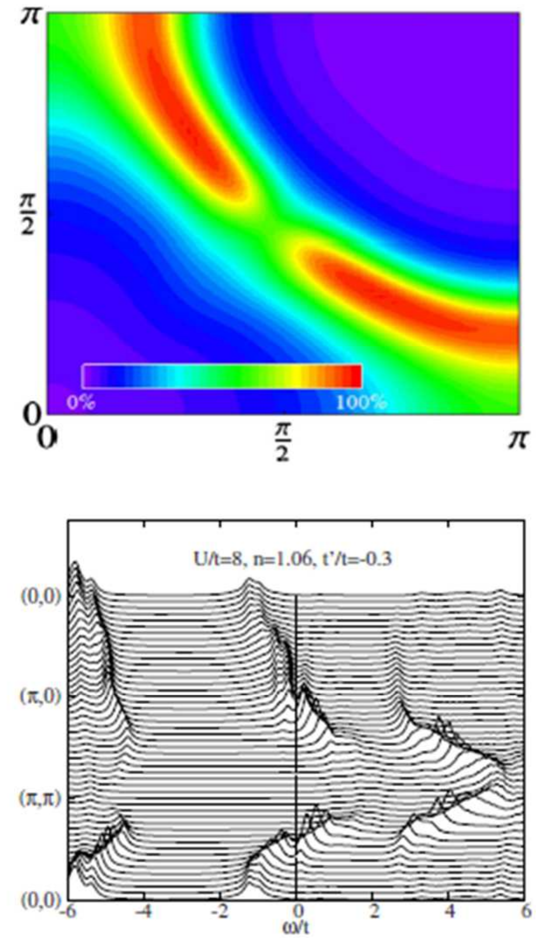
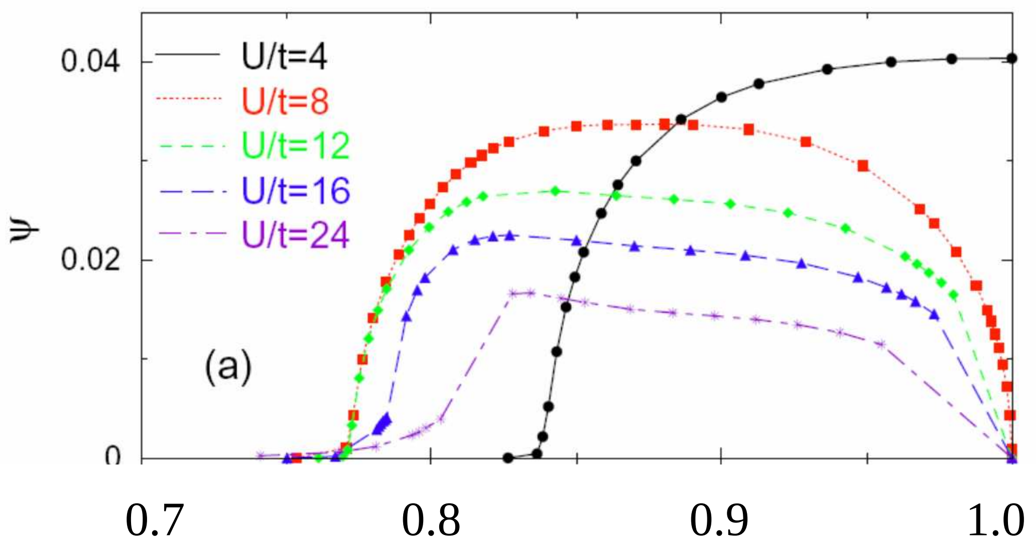


FIG. 7. (Color online) Same plots as in Fig. 6 but for the electron-doped case $n = 1.06$. The maximum on the color scale cor-

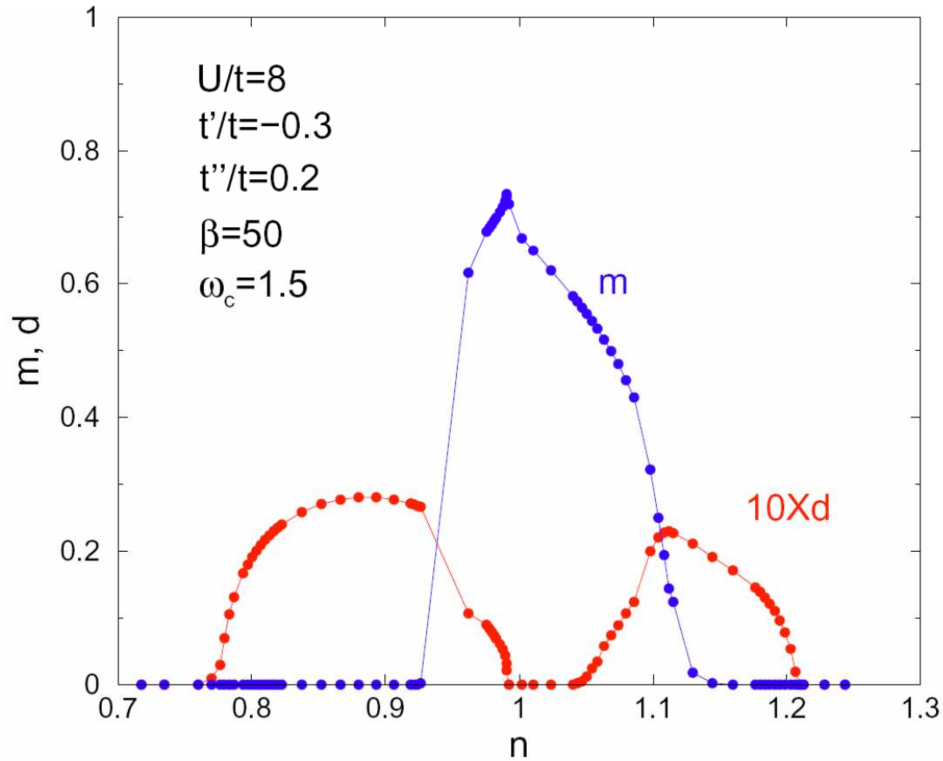
$T = 0$ phase diagram: superconductivity

Dome vs Mott (CDMFT)

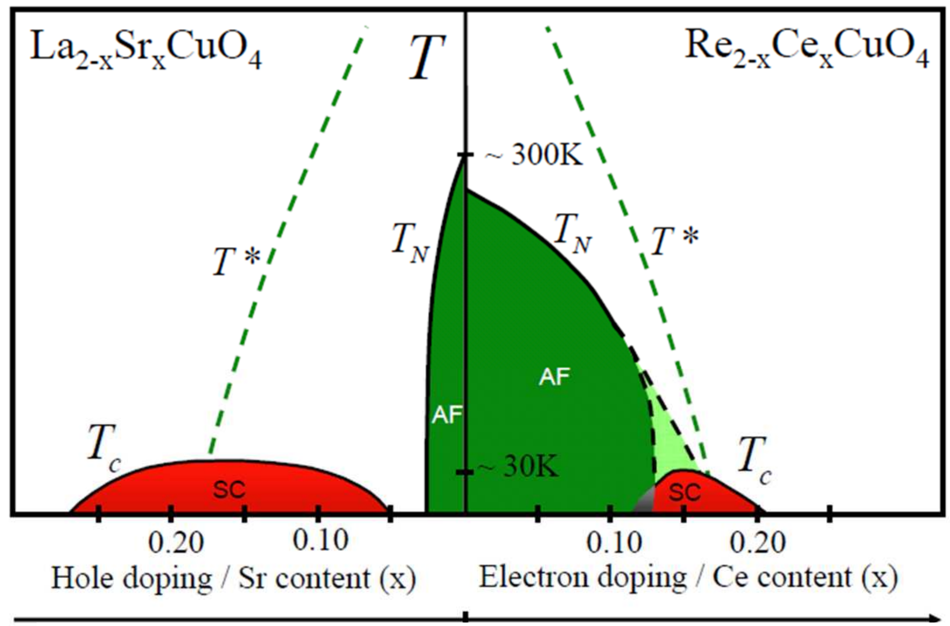


Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008)

CDMFT global phase diagram



Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008) AND Capone, Kotliar PRL (2006)



Armitage, Fournier, Greene, RMP (2009)



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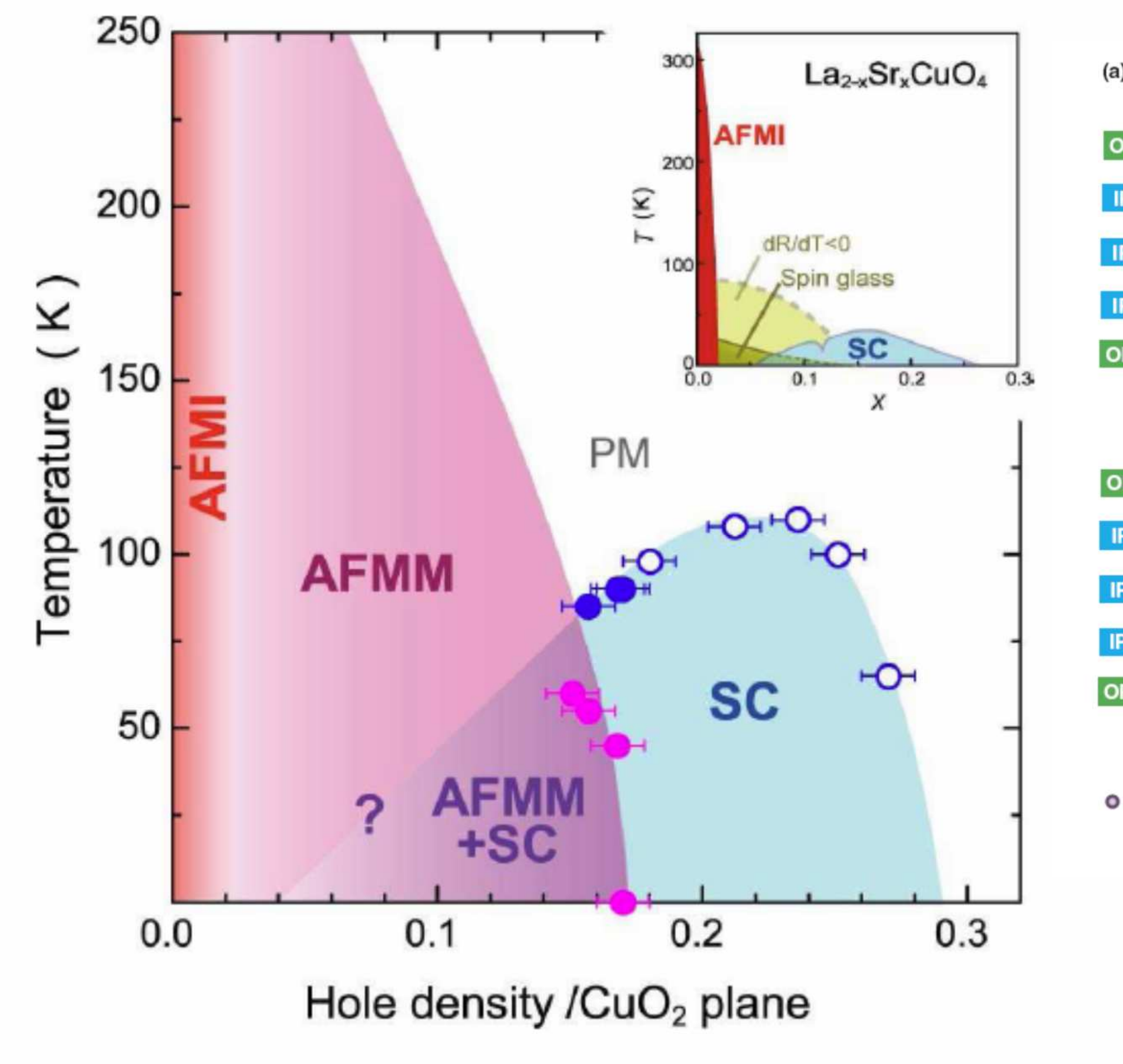
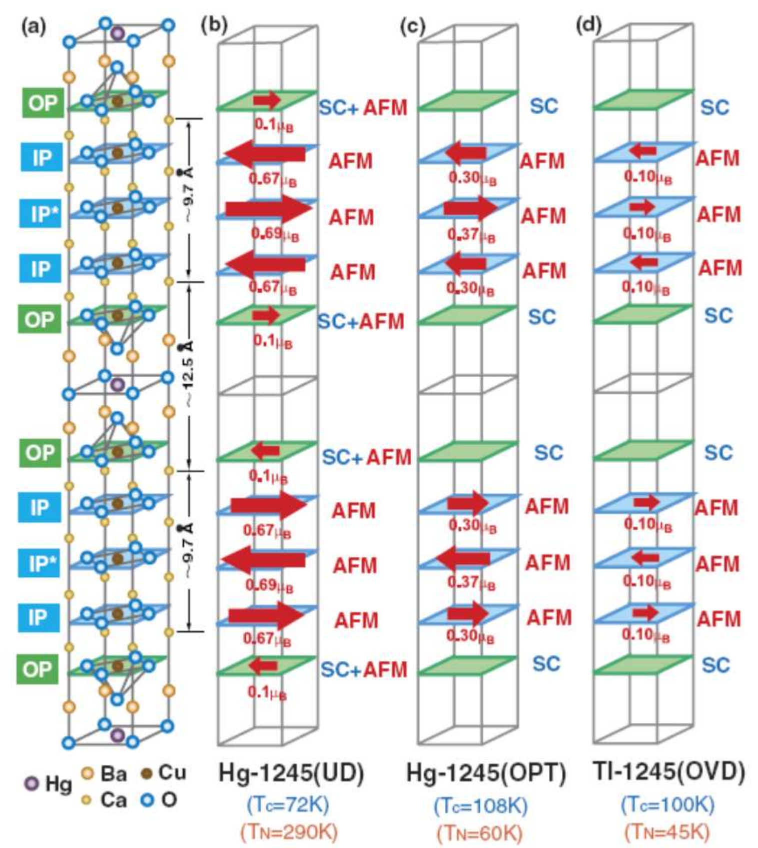
Consistent with following experiments

H. Mukuda, Y. Yamaguchi, S. Shimizu, … A. Iyo JPSJ **77**, 124706 (2008)





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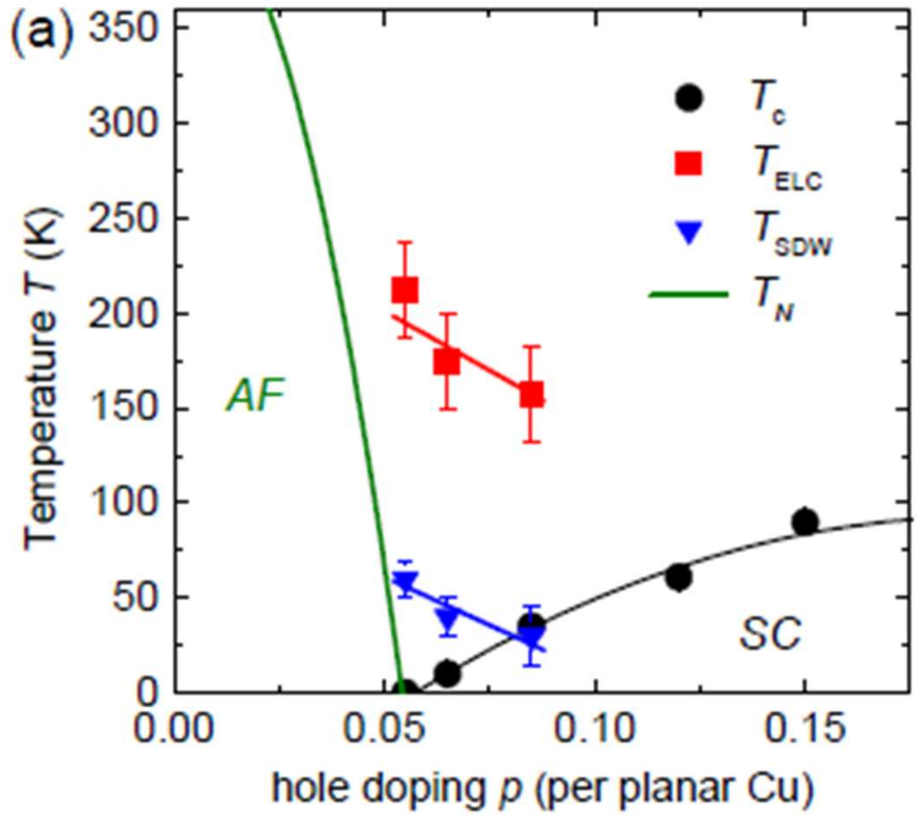
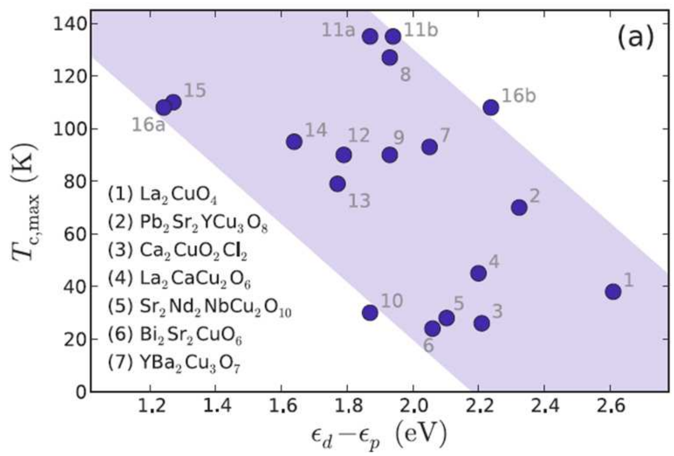
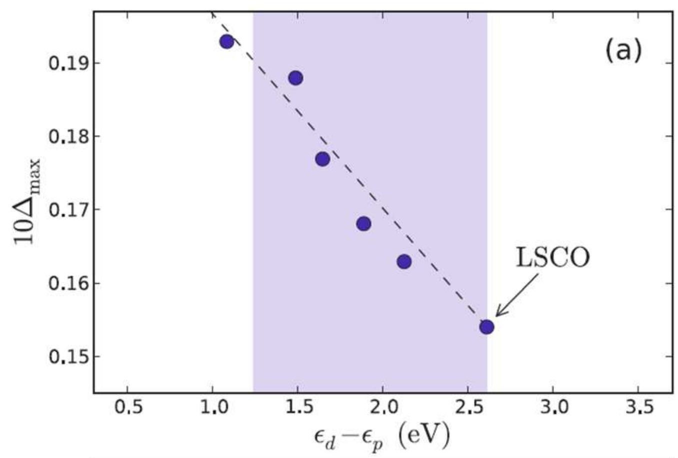
Magnetic phase diagram of YBCO



Haug, … Keimer, New J. Phys. 12, 105006 (2010)

Materials dependent properties





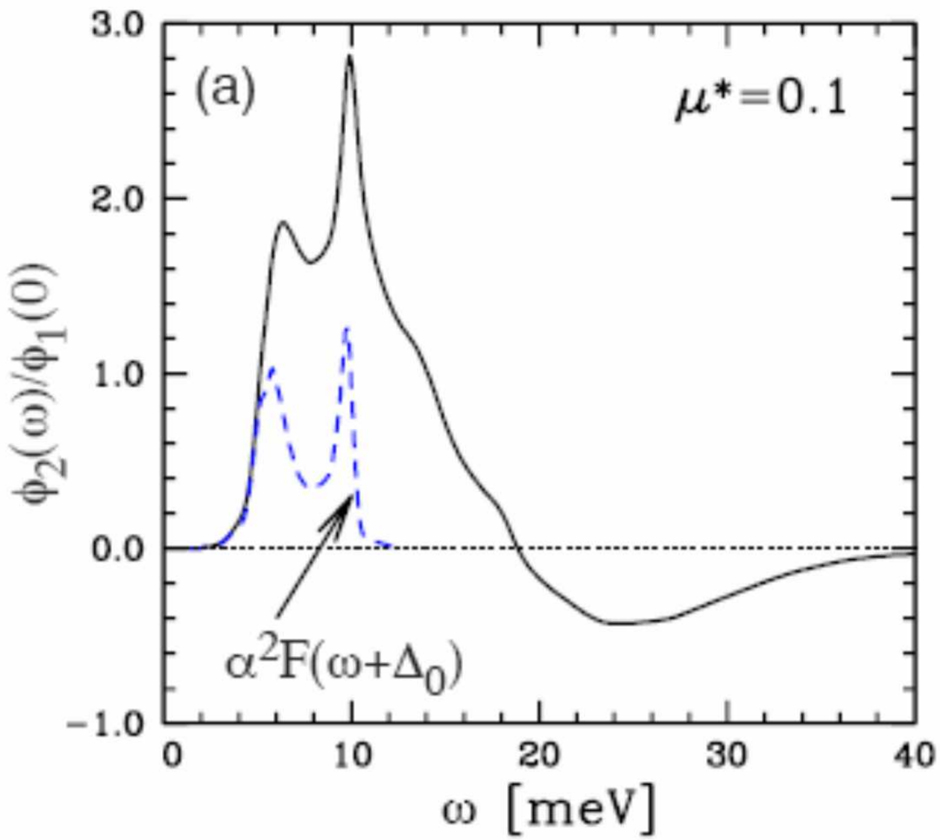
C. Weber, C.-H. Yee, K. Haule, and G. Kotliar, ArXiv e-prints (2011), 1108.3028.

T = 0 phase diagram

The glue

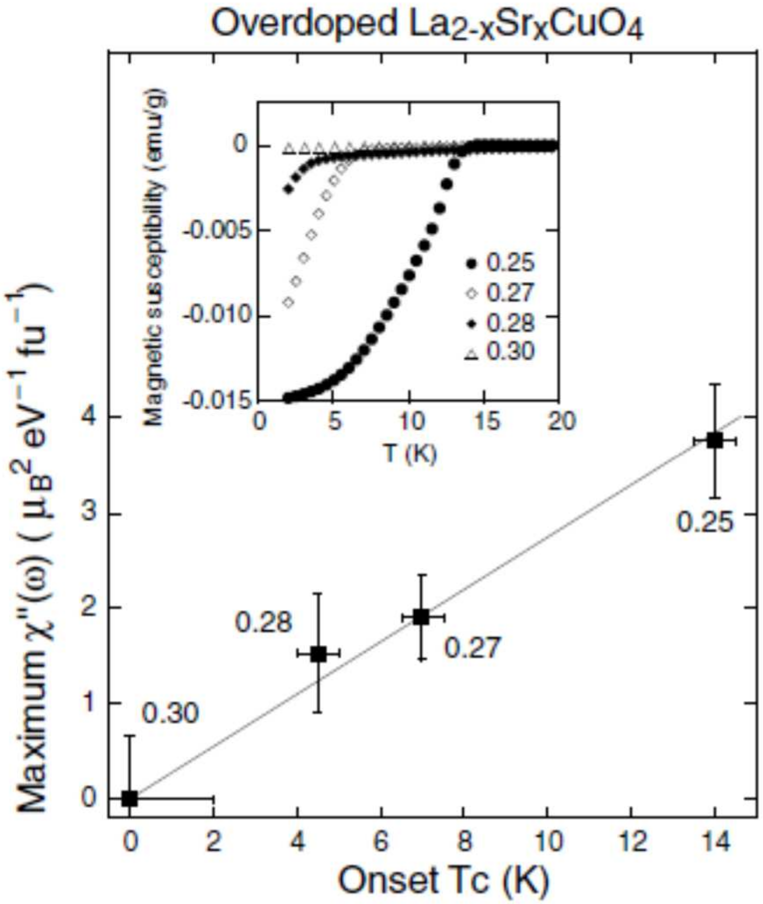
Im Σ_{an} and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

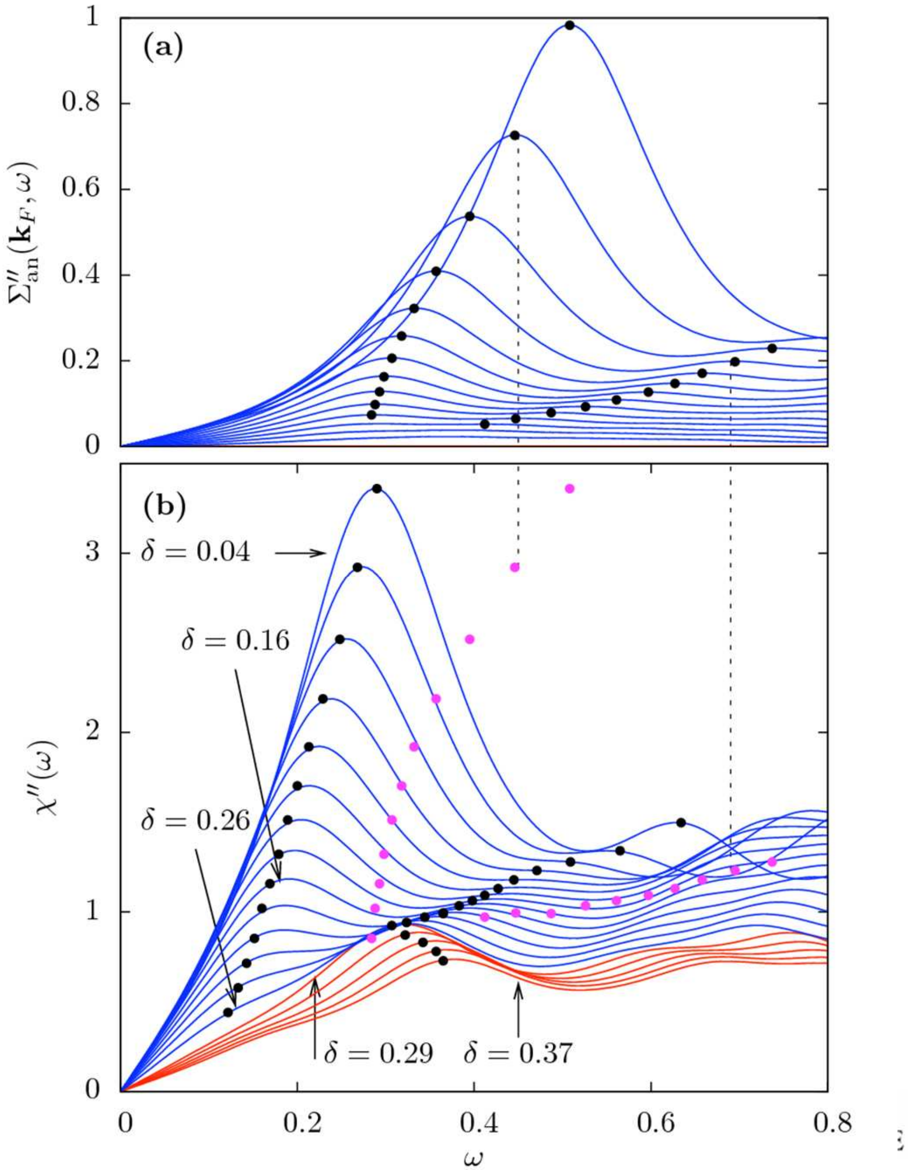


The glue

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



Wakimoto … Birgeneau PRL (2004)



The glue and neutrons

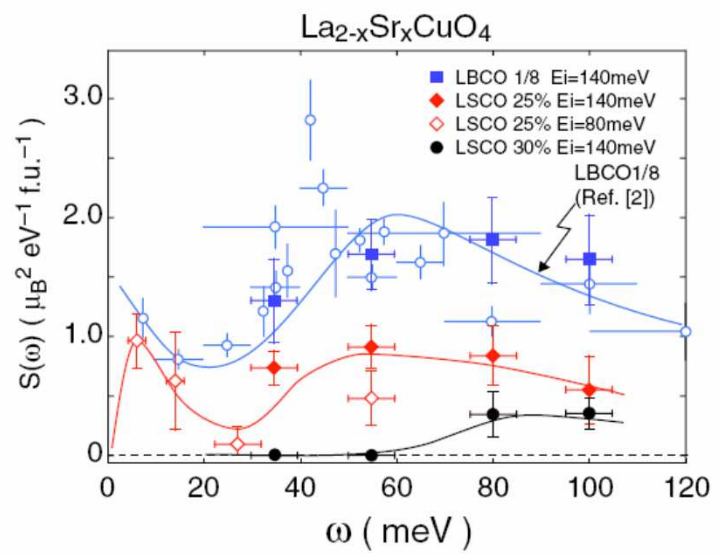
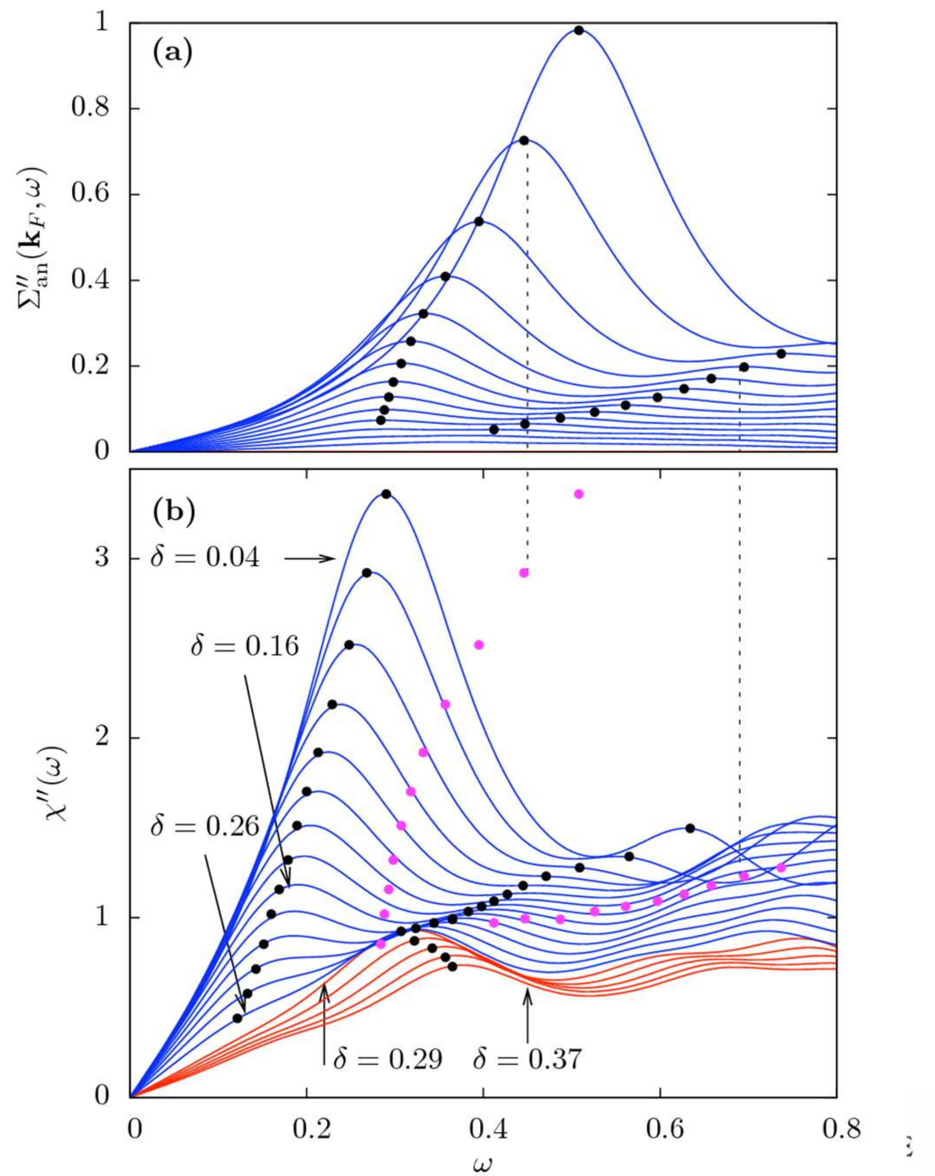


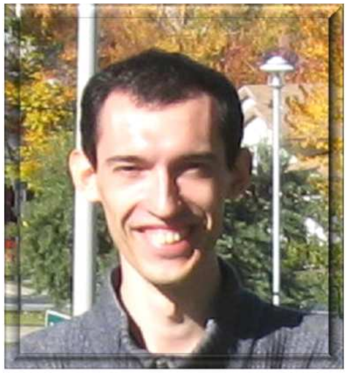
FIG. 3 (color online). **Q**-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i = 140$ meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO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

Finite *T* phase diagram

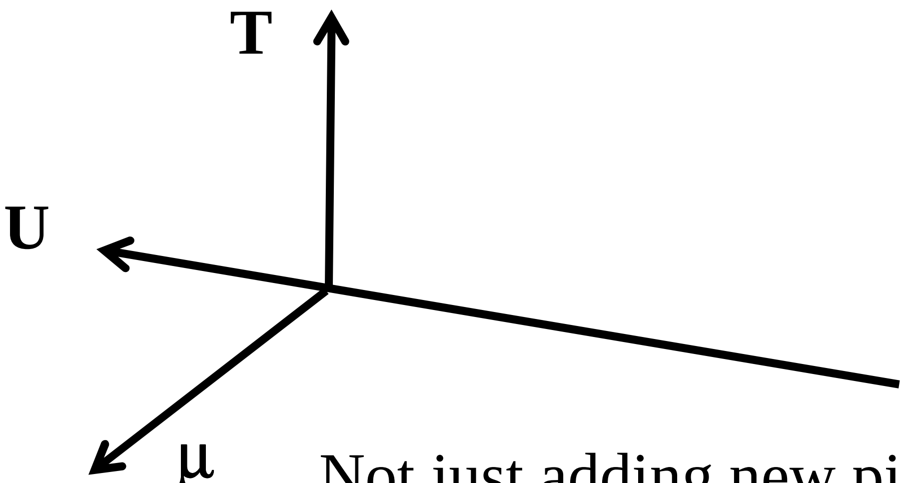
Normal state of the cuprates



Giovanni Sordi

G. Sordi, K. Haule, A.-M.S.T
PRL, **104**, 226402 (2010)
and
Phys. Rev. B. **84**, 075161 (2011)

Doping-induced Mott transition (*t'=0*)

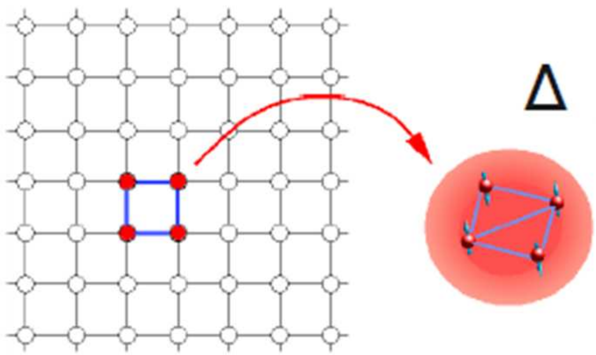


Kristjan Haule

Not just adding new piece:
Lesson from DMFT, first order transition + critical point governs phase diagram

C-DMFT

$$Z = \int \mathcal{D}[\psi^\dagger, \psi]\, \mathrm{e}^{-S_c - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\mathbf{K}} \psi^\dagger_{\mathbf{K}}(\tau) \Delta_{\mathbf{K}}(\tau,\tau') \psi_{\mathbf{K}}(\tau')}$$



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

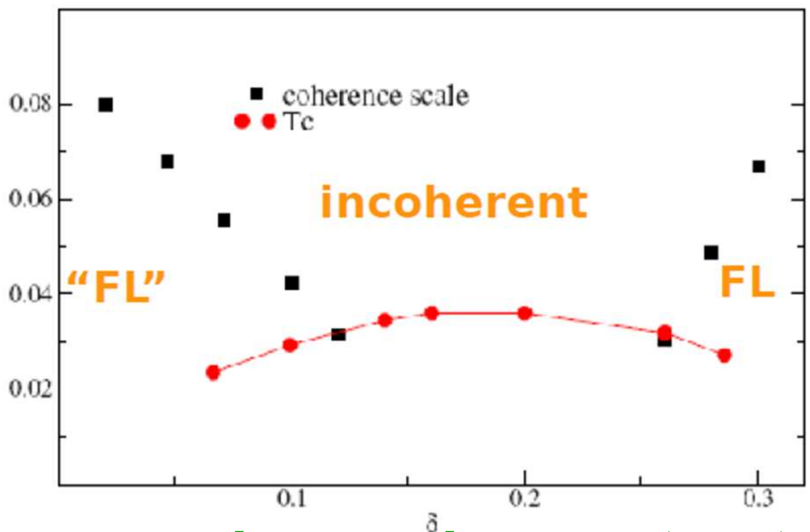
Continuous-time Quantum Monte Carlo calculations to sum all diagrams generated from expansion in powers of hybridization.

P. Werner, A. Comanac, L. de' Medici, M. Troyer, and A. J. Millis, Phys. Rev. Lett. **97**, 076405 (2006).

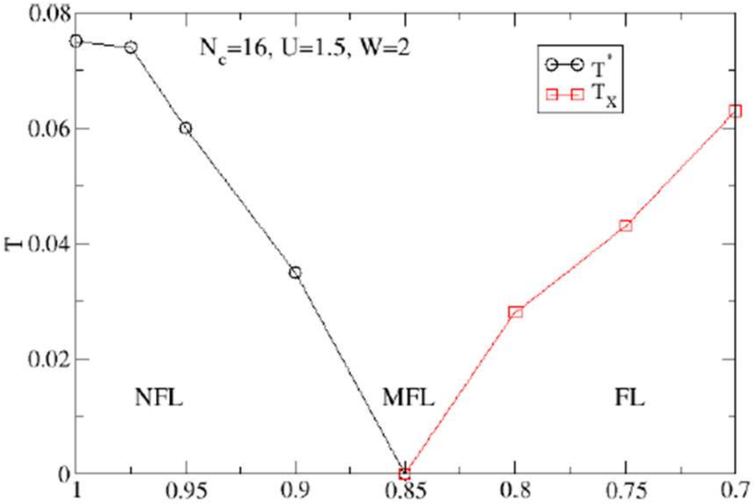
K. Haule, Phys. Rev. B **75**, 155113 (2007).

Doping driven Mott transition, *t' = 0*

Method	t'	Orbital selective	U	Critical point	Ref.
D+C+H 8			7		Werner et al. cond-mat (2009)
D+C+H 4					Gull et al. EPL (2008)
	-0.3		10,6		Liebsch, Merino… (2008)
					Ferrero et al. PRB (2009)
D+C+H 8			7		Gull, et al. PRB (2009)

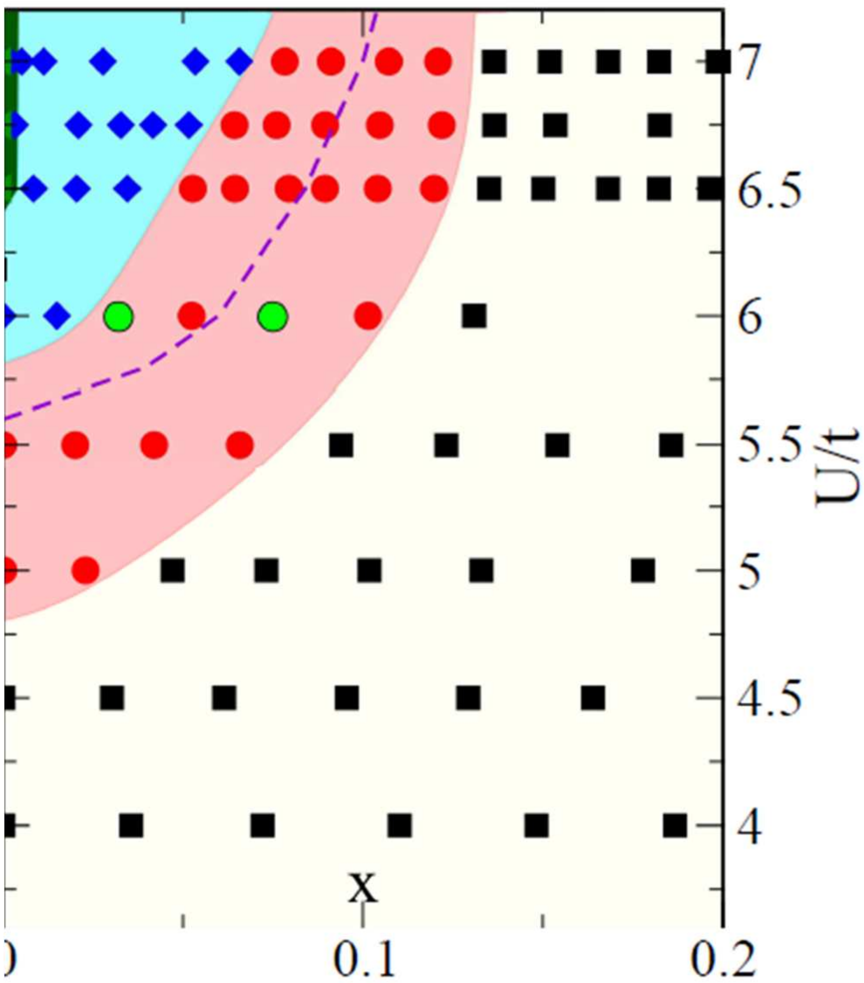


K. Haule, G. Kotliar, PRB (2007)



Vildhyadhiraja, PRL (2009)

Doping driven Mott transition



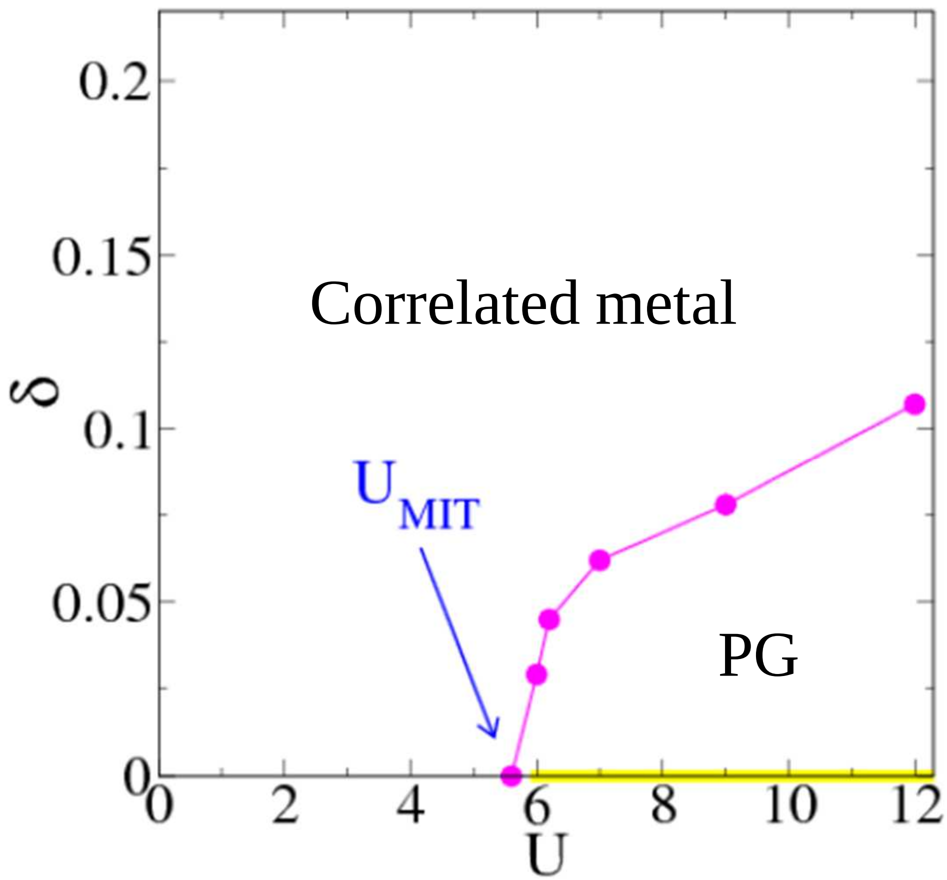
T = 0.25 t

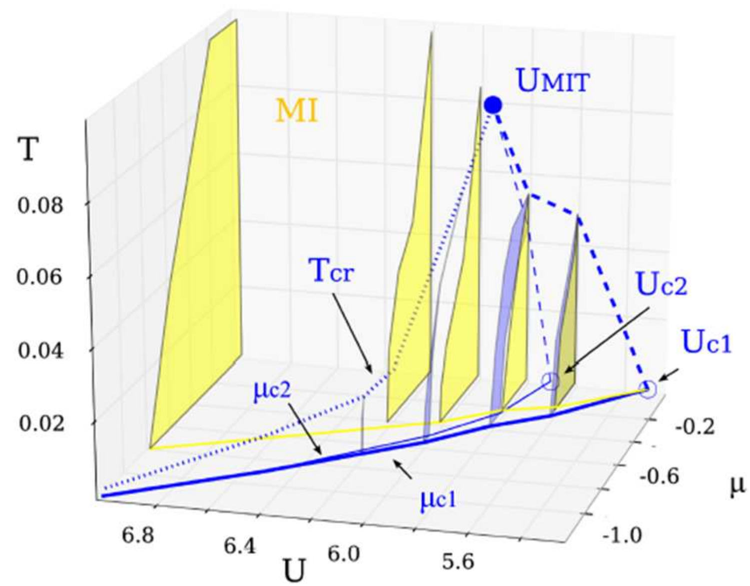
Gull, Parcollet, Millis
arXiv:1207.2490v1

Gull, Werner, Millis, (2009)
E. Gull, M. Ferrero, O. Parcollet, A. Georges, and A. J. Millis (2010)

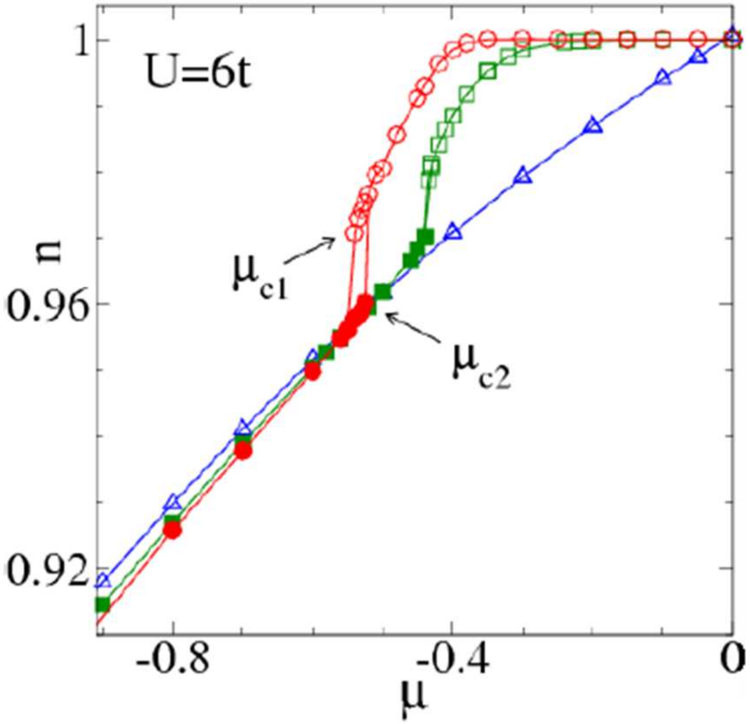
Link to Mott transition up to optimal doping

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





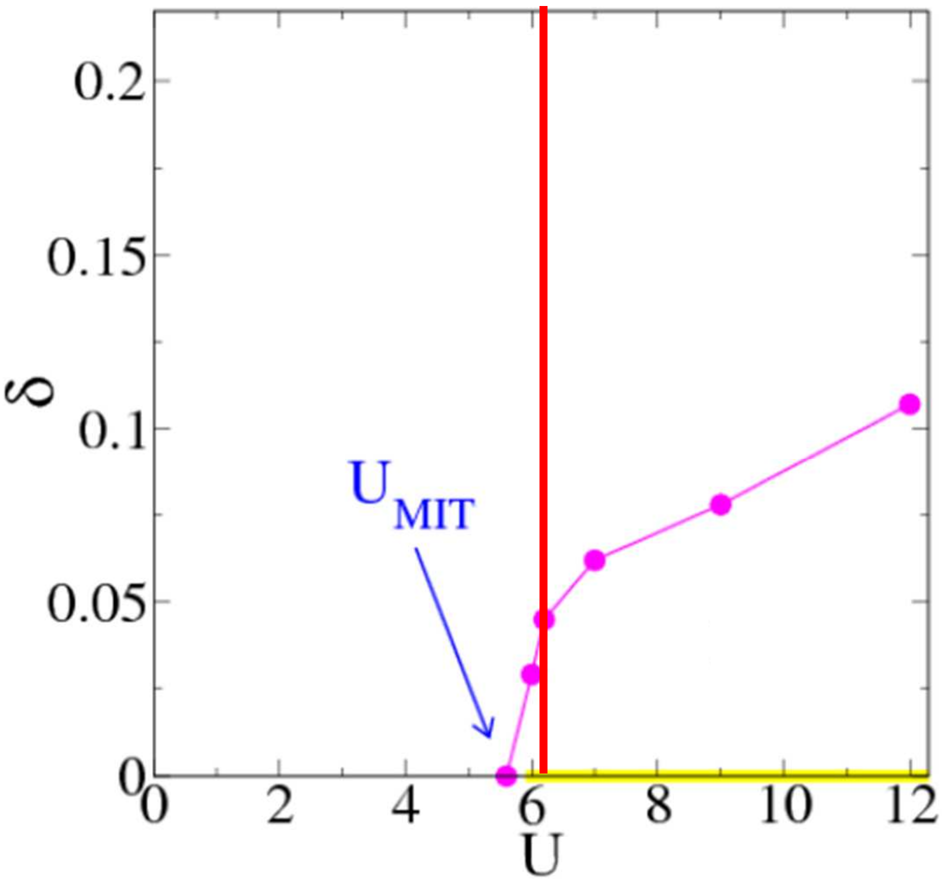
First order transition at finite doping



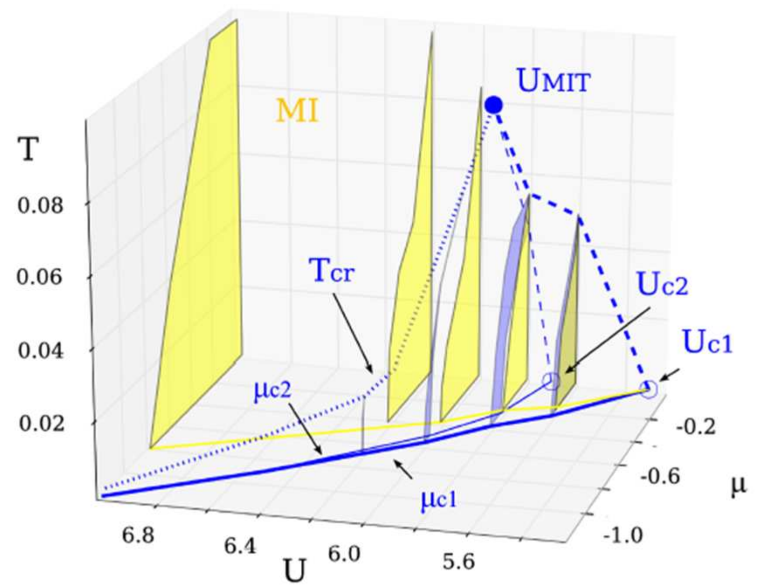
$n(\mu)$ for several temperatures:
$T/t =$1/10, 1/25, 1/50

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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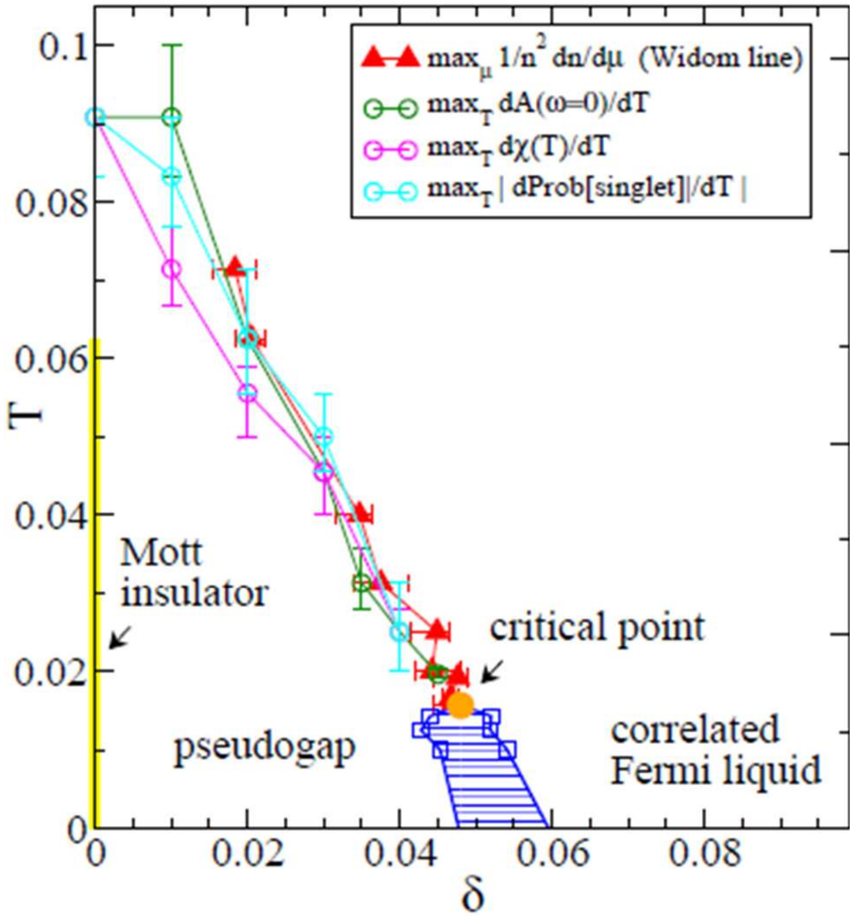
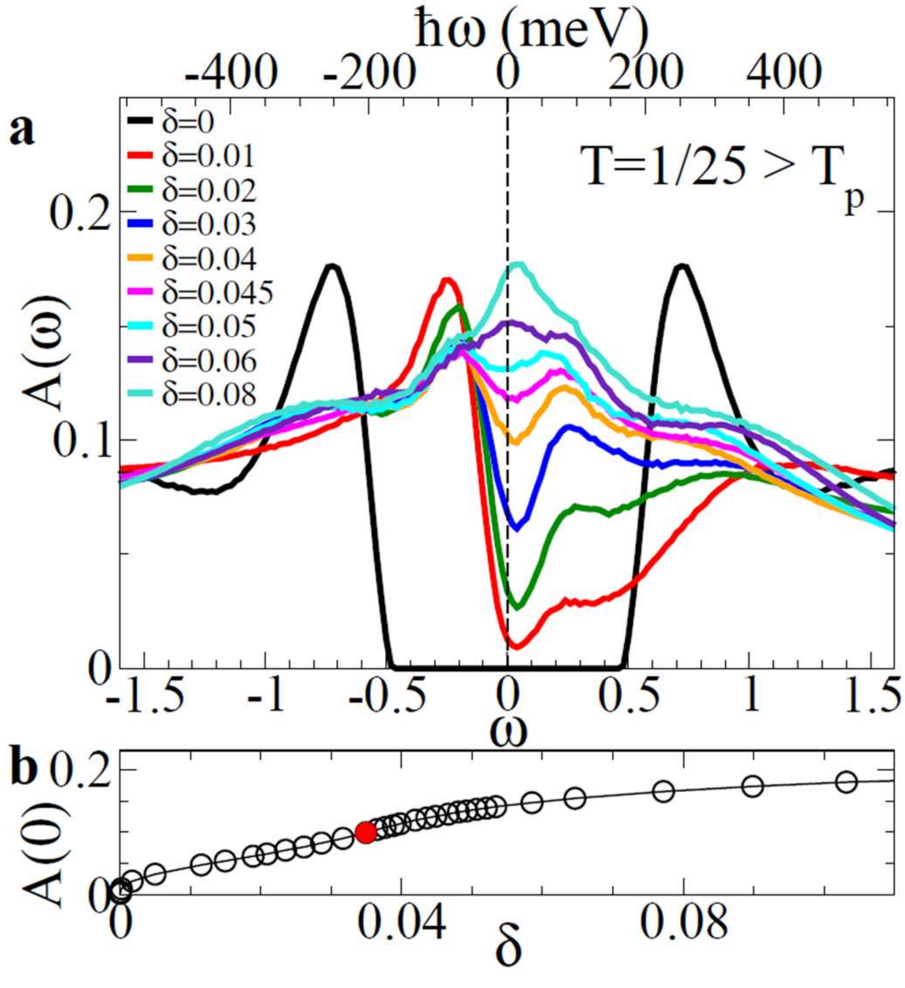
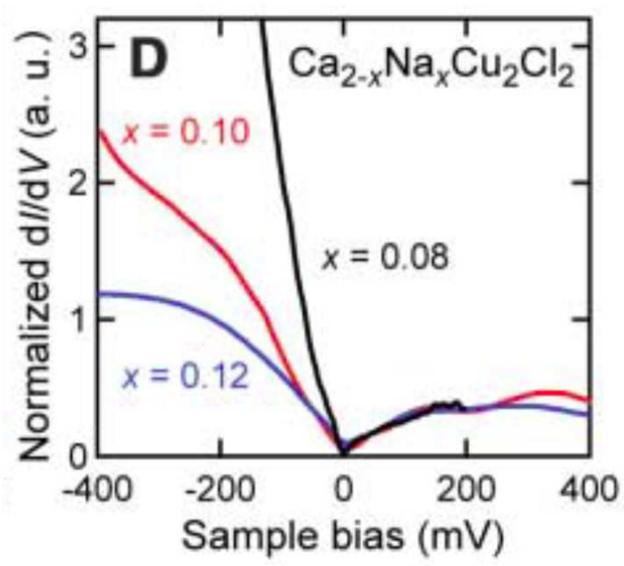
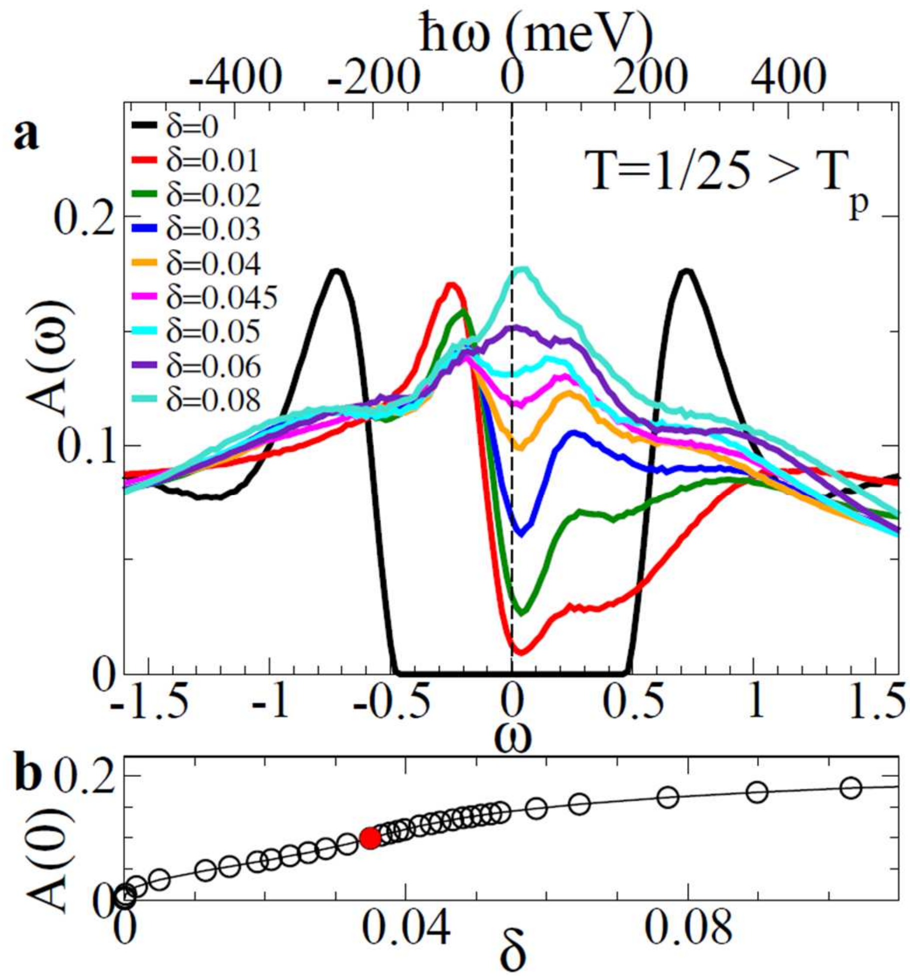
Density of states





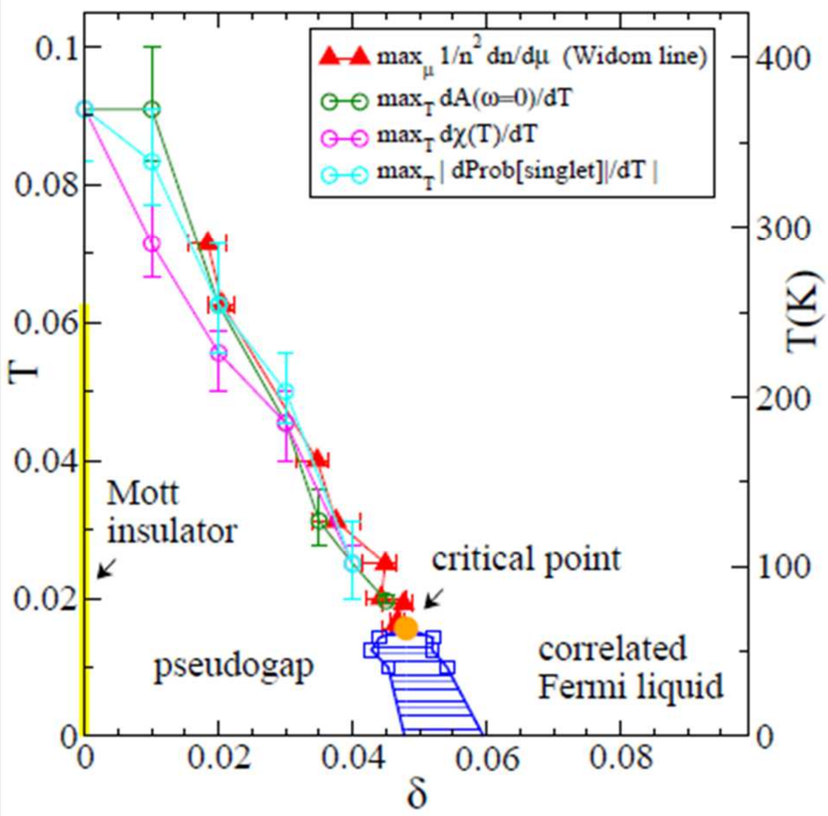
Density of states

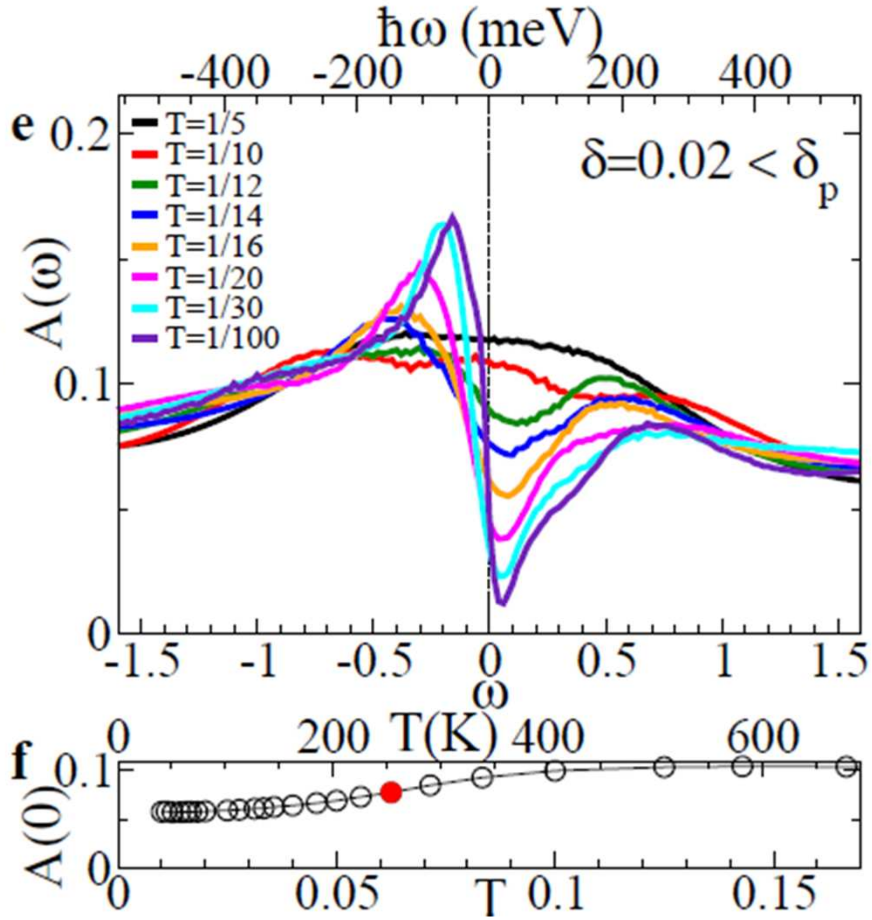




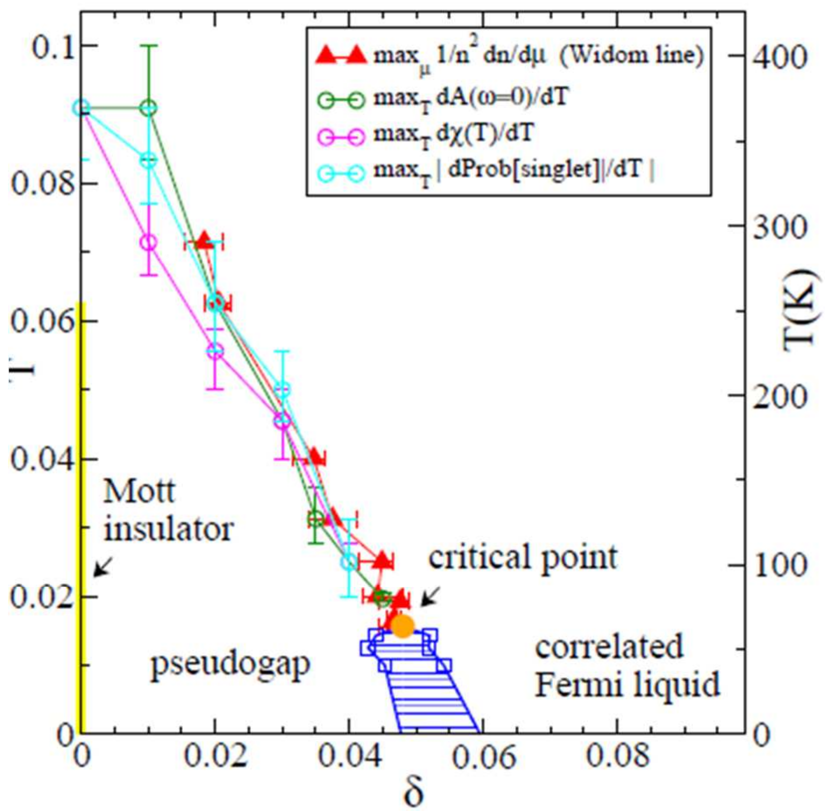
Khosaka et al. *Science* **315**, 1380 (2007);

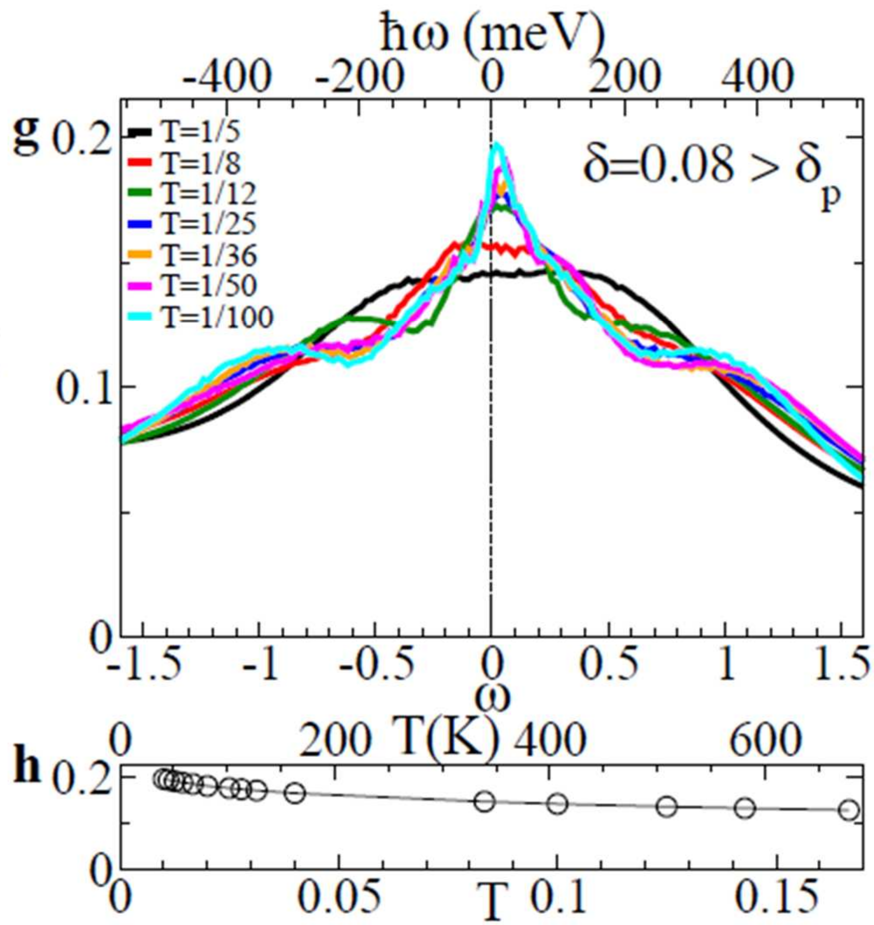
Density of states



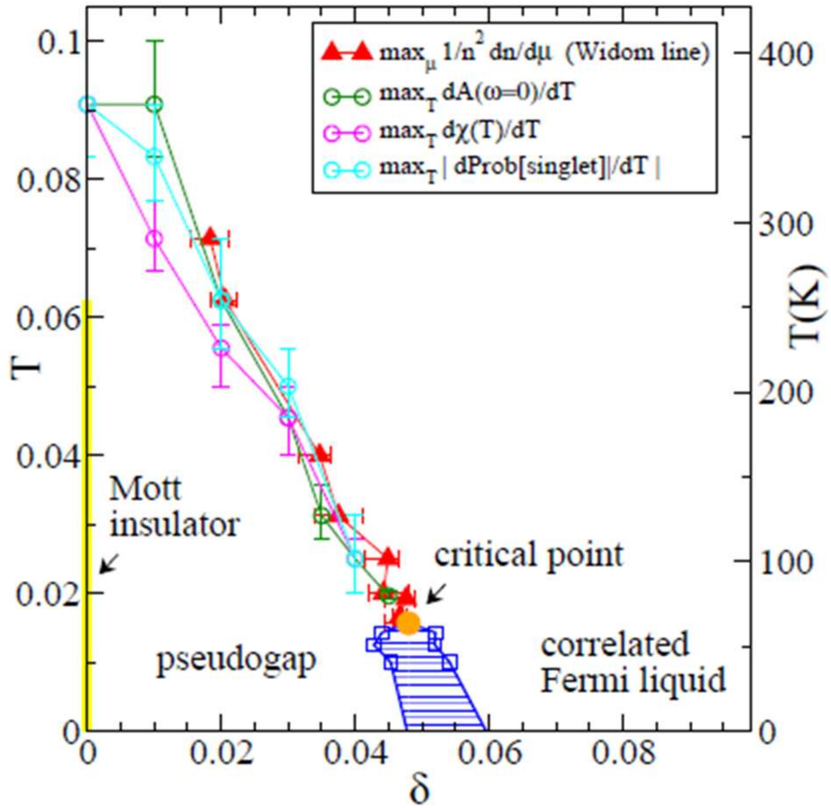


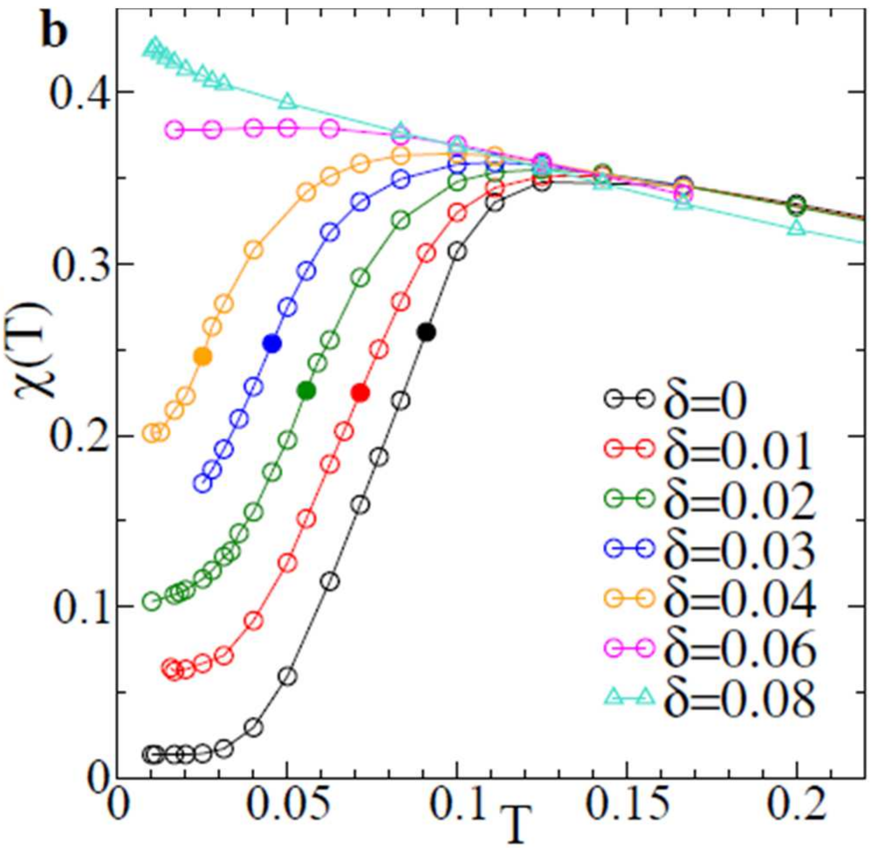
Density of states





Spin susceptibility





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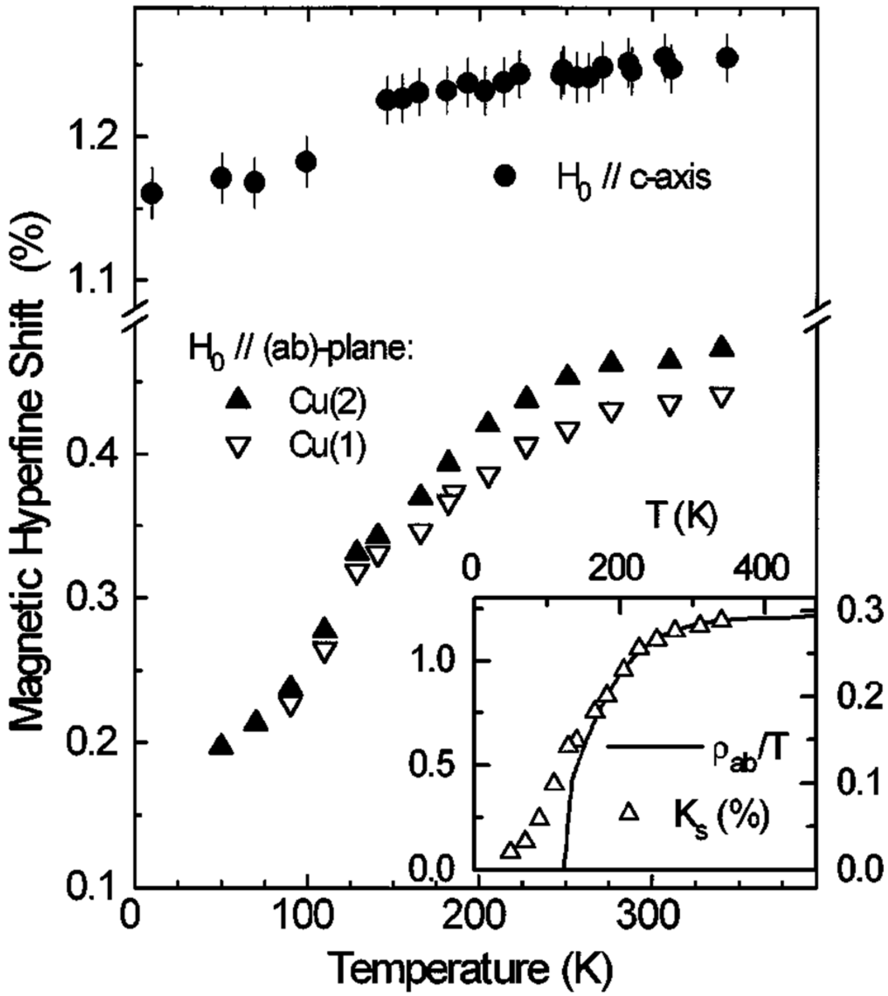
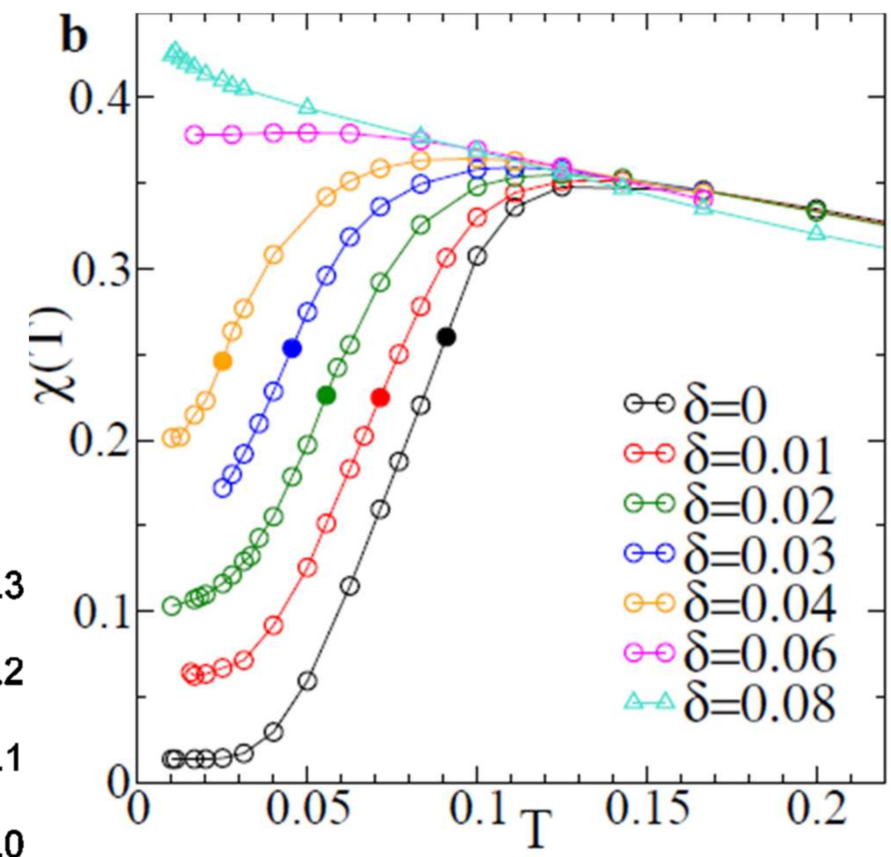
Spin susceptibility

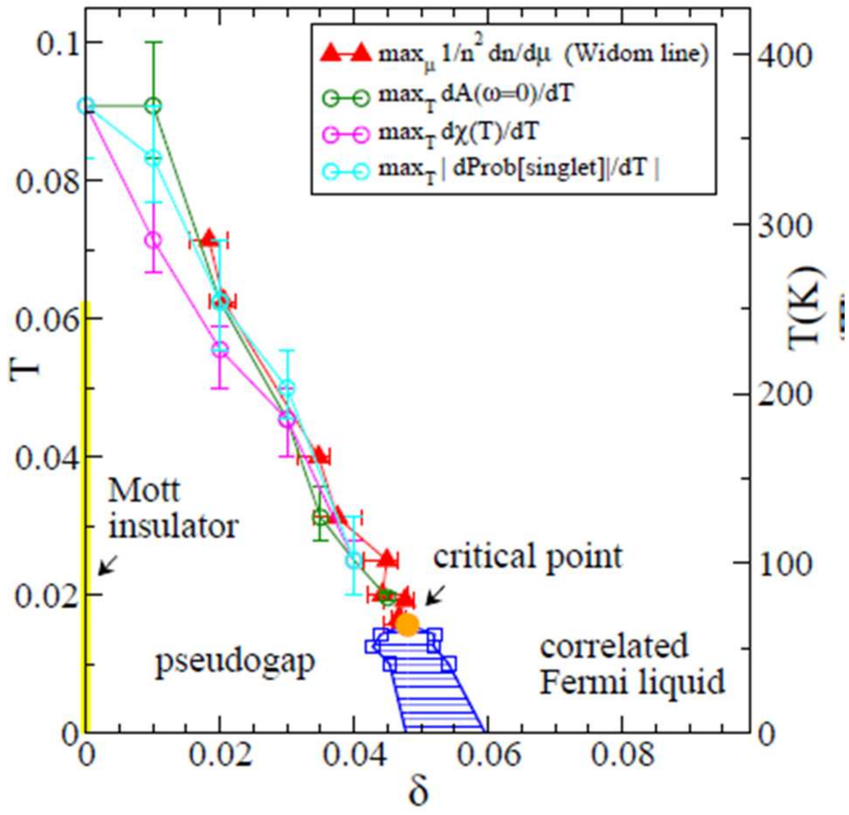


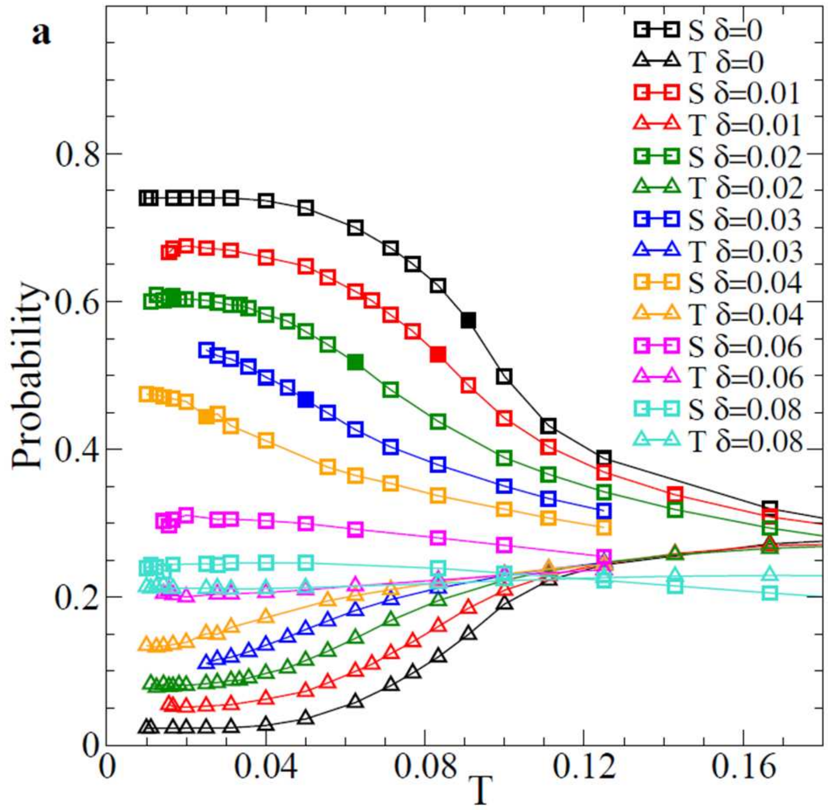
Underdoped Hg1223

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



Plaquette eigenstates





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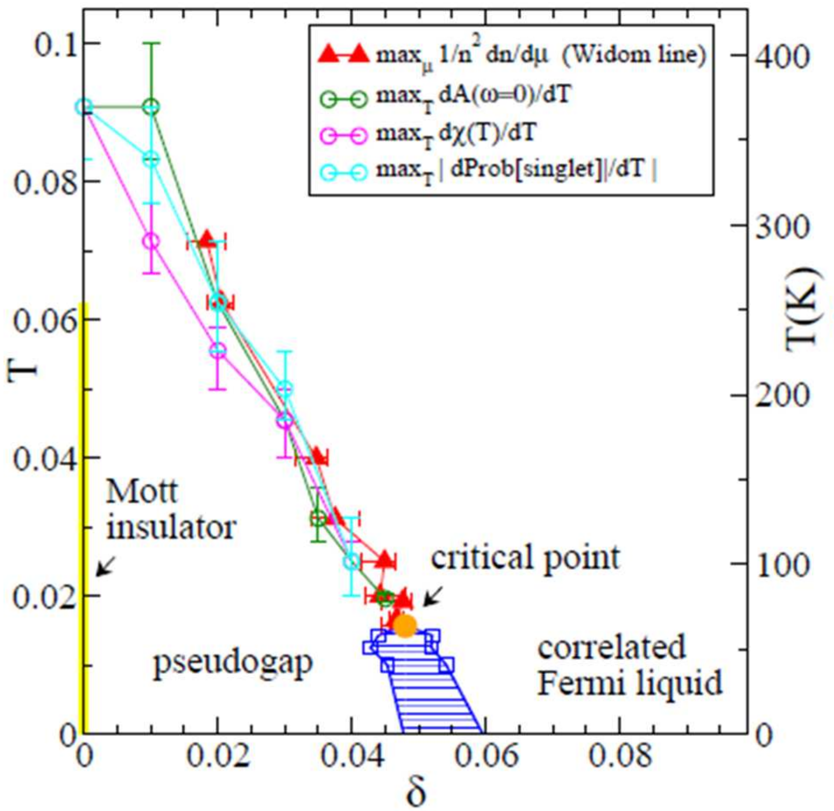
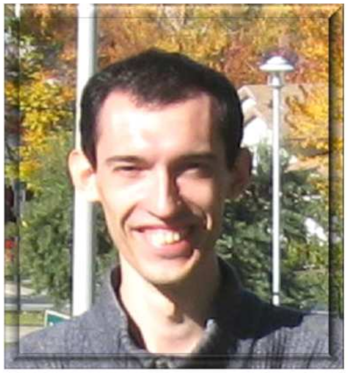
Pseudogap *T** along the Widom line





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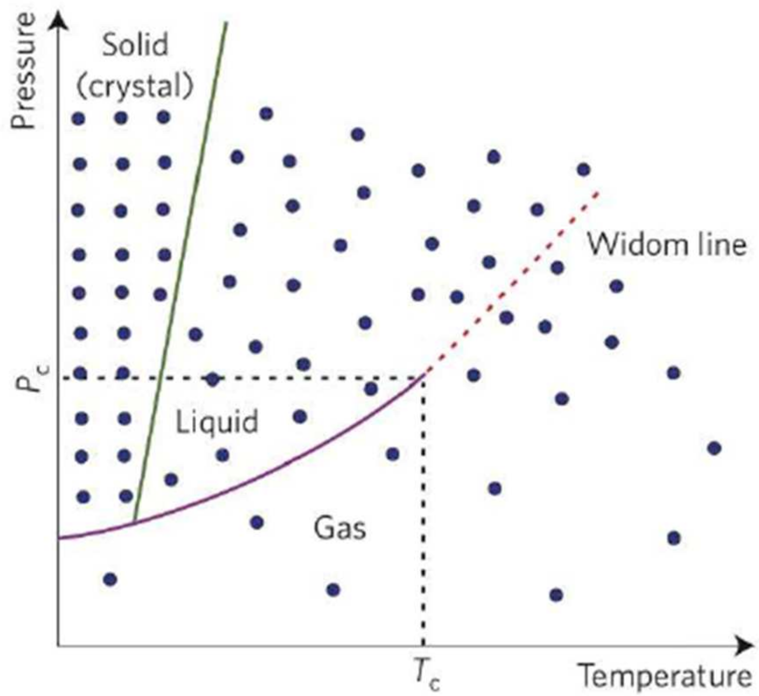
Patrick Sémon

Kristjan Haule

The Widom line

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

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

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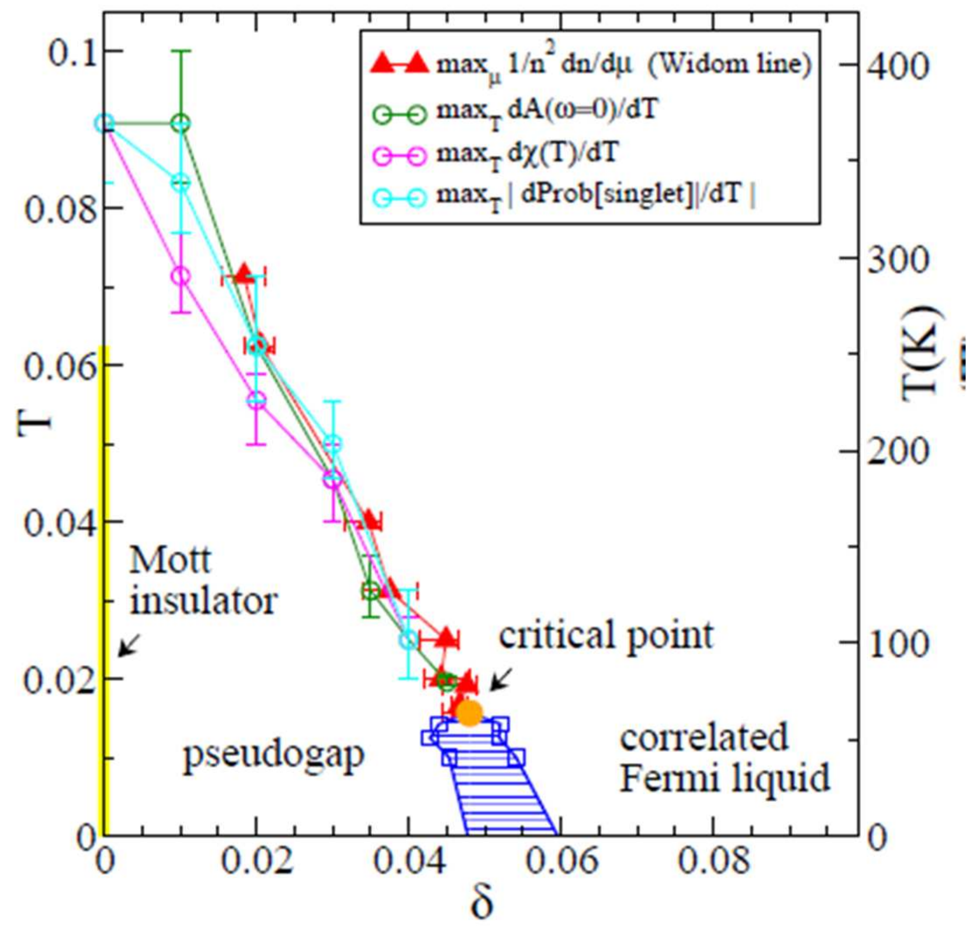
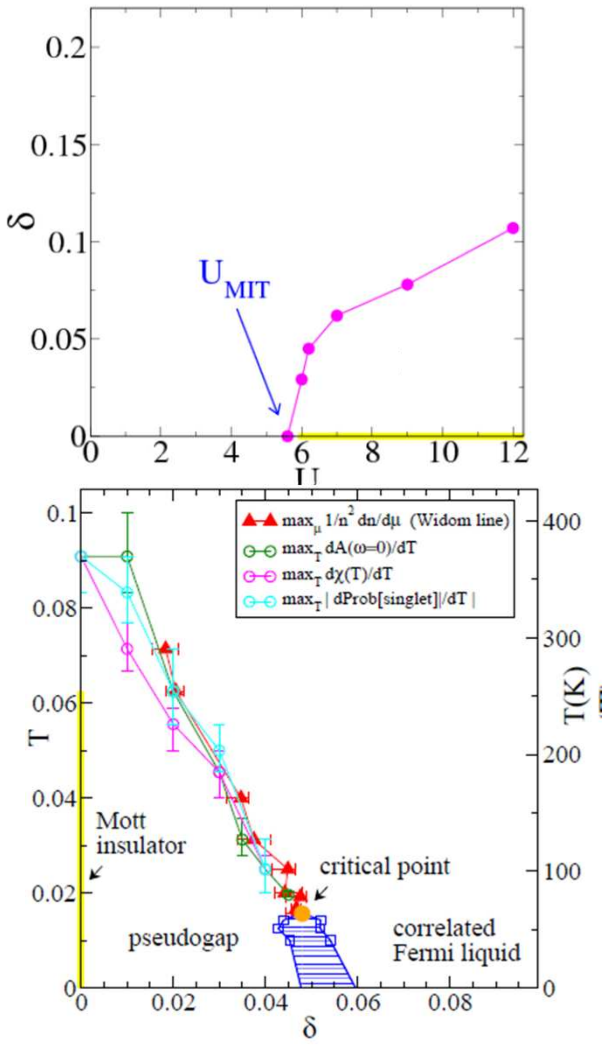
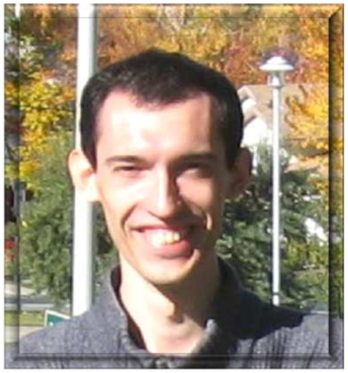
Phase diagram



Summary: normal state



- Mott physics extends way beyond half-filling
- Pseudogap is a phase
- Pseudogap *T** is a Widom line
- High compressibility (stripes?)



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Finite *T* phase diagram

Superconductivity

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

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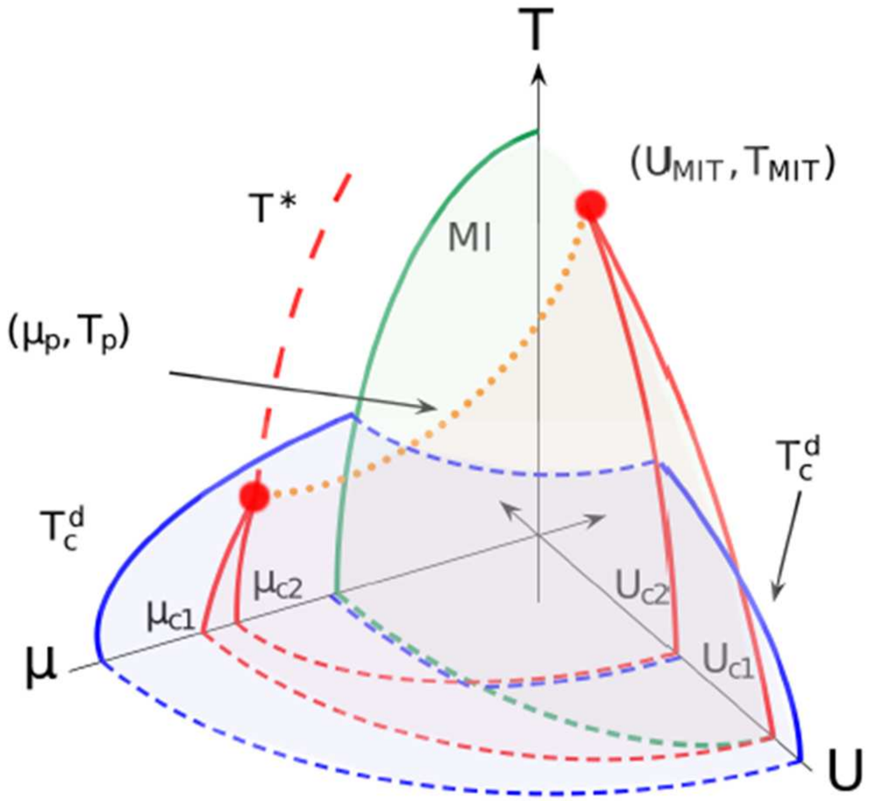
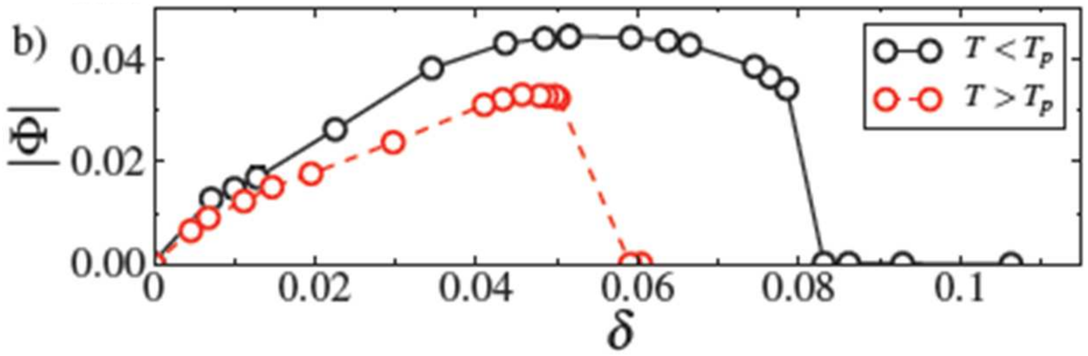
Unified phase diagram

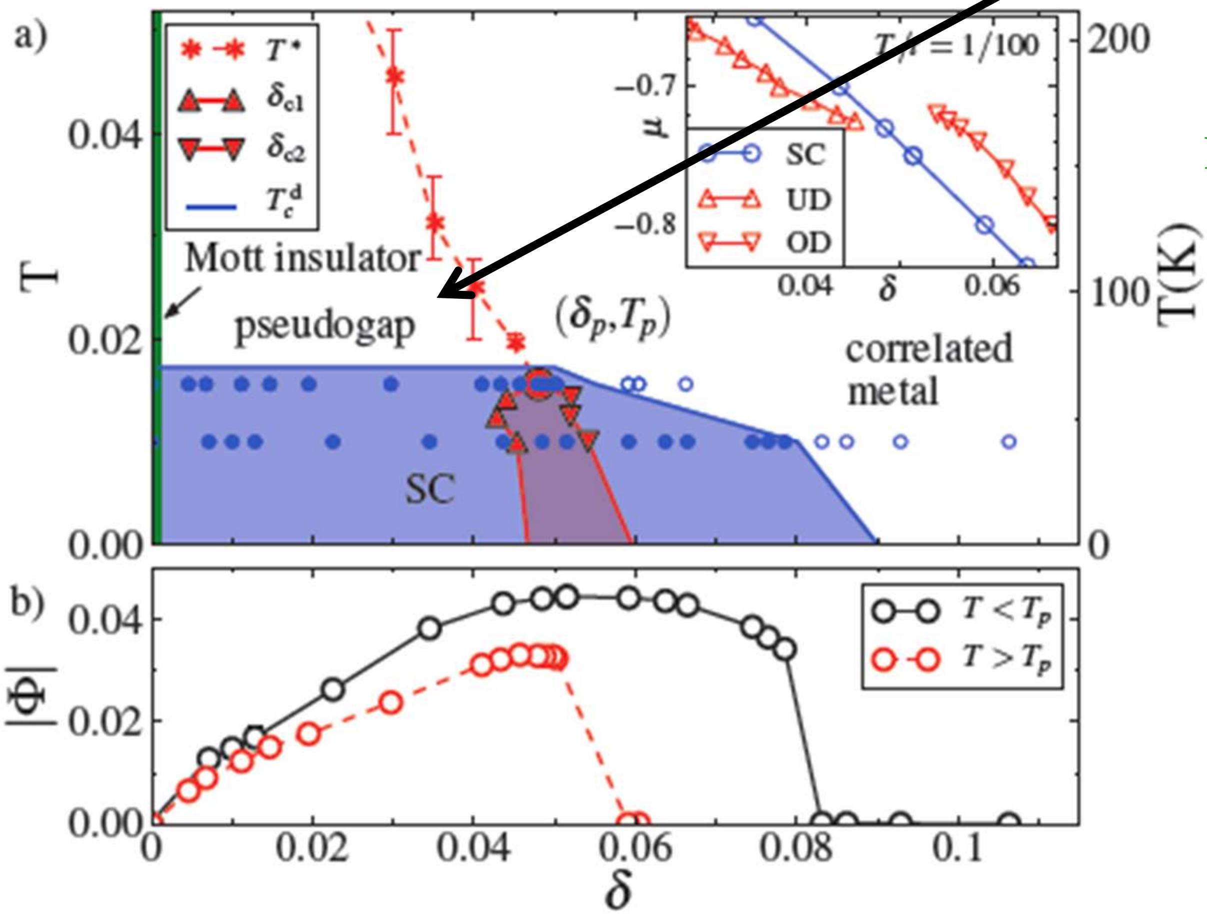


Cuprates (doping driven transition)



Cuprates (doping driven transition)

Pseudogap vs pair

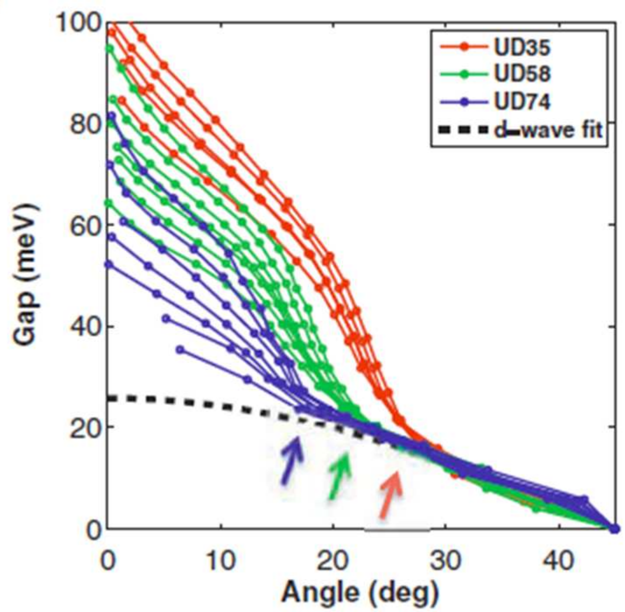


F. Rullier-Albenque, H. Alloul, and G.Rikken, Phys. Rev. B **84**, 014522 (2011).

Larger clusters

- Is there a minimal size cluster where T_c vanishes before half-filling?
- Learn something from small clusters as well
- Local pairs in underdoped

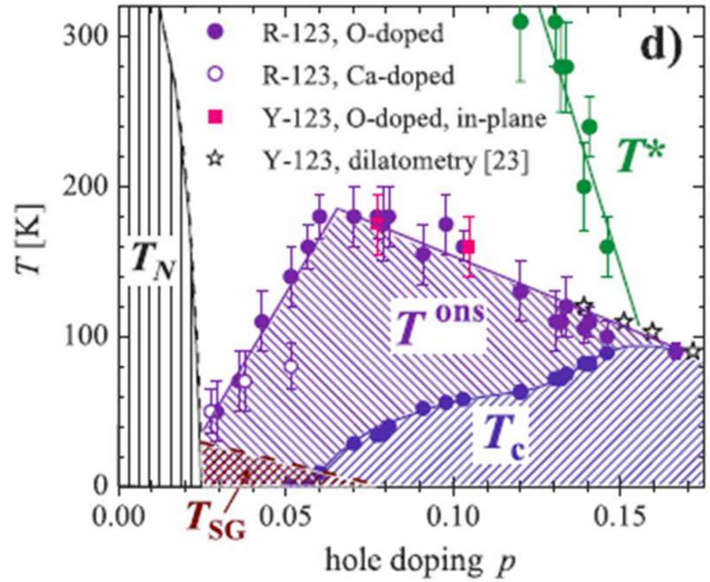
Meaning of T_c^d : Local pair formation



A. Pushp, Parker, … A. Yazdani, Science **364**, 1689 (2007)

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.

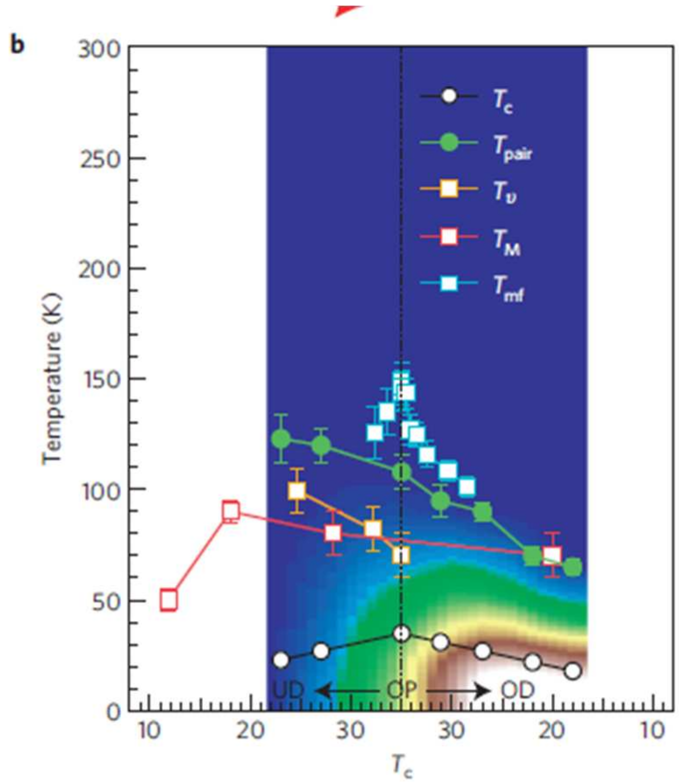
Fluctuating region



Infrared response

Dubroka et al. 106, 047006 (2011)

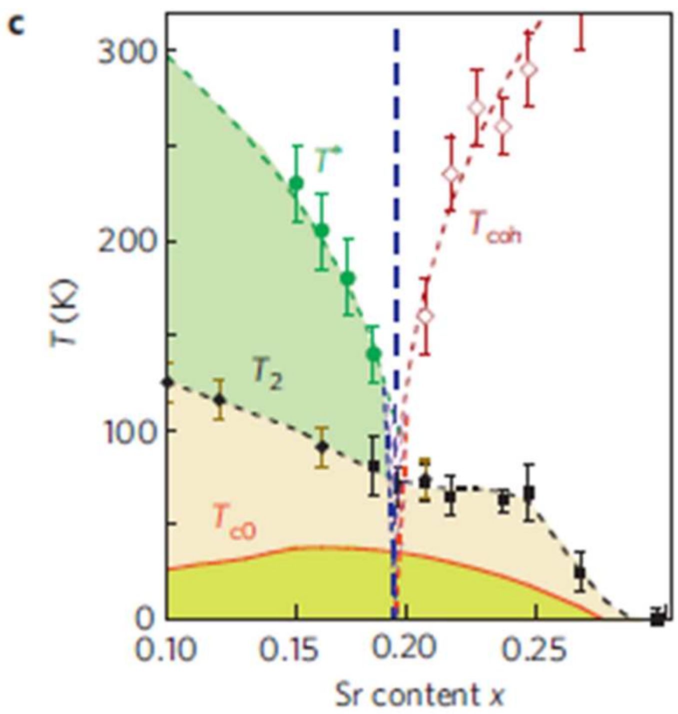
Tpair



ARPES
Bi2212

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

T_2



Magnetoresistance, LSCO
Fluctuating vortices

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

Giant proximity effect

$T_c = 32\ K$
$T_c < 5K$

Morenzoni et al.,
Nature Comms. **2** (2011)

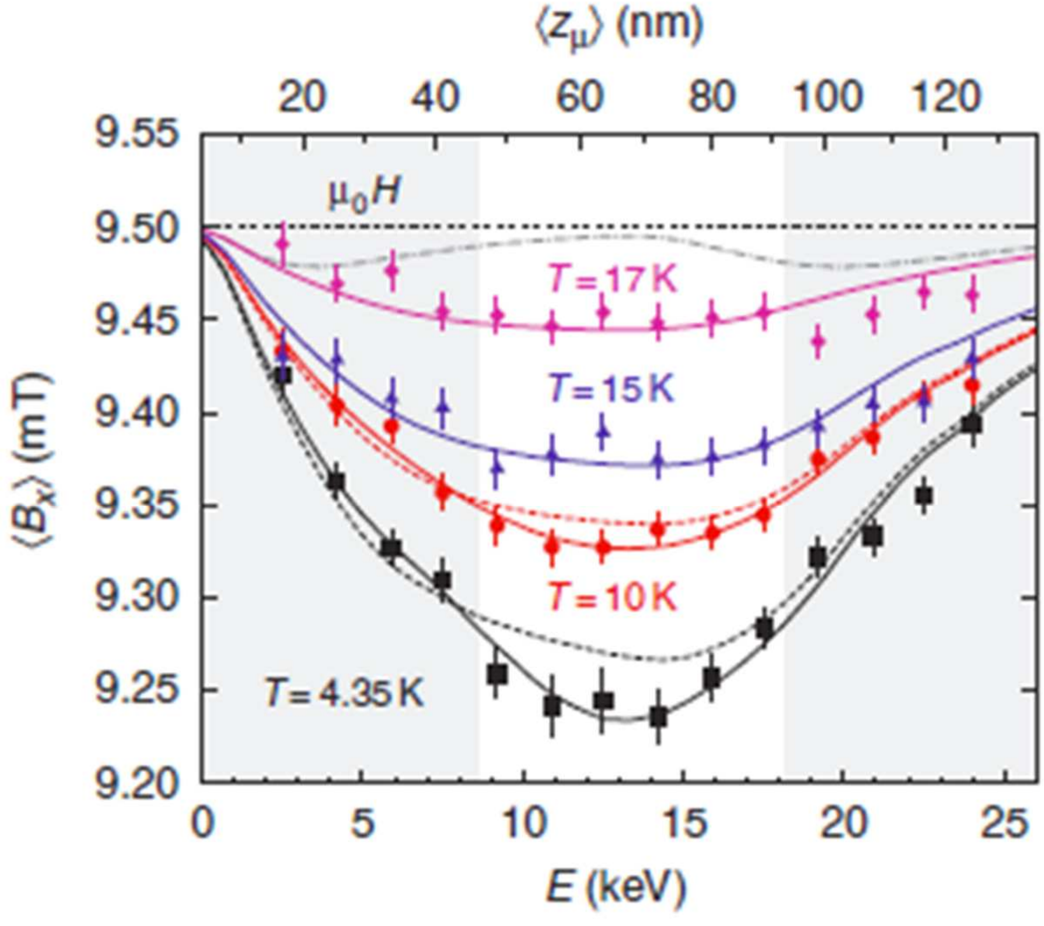
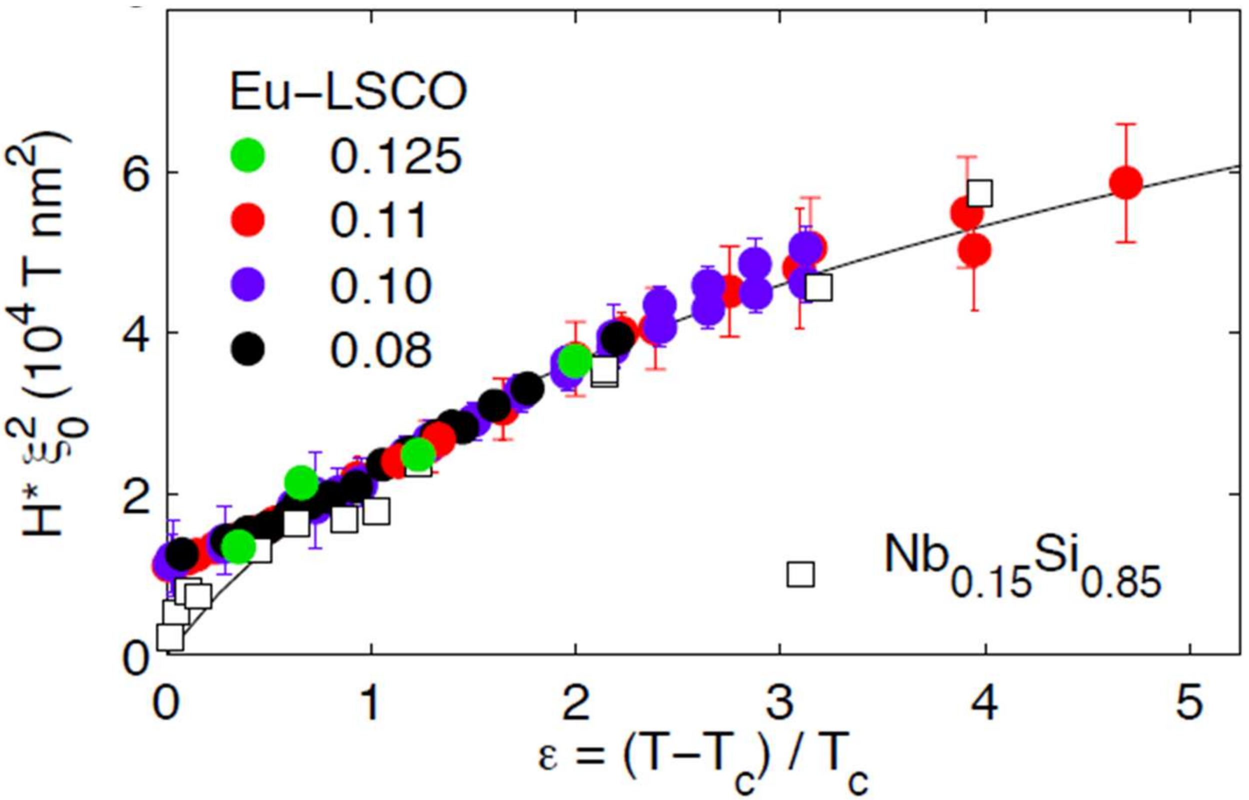


Figure 6 | Depth profile of the local field at different temperatures. The

Actual T_c in underdoped

- Quantum and classical phase fluctuations
  - V. J. Emery and S. A. Kivelson, Phys. Rev. Lett. **74**, 3253 (1995).
  - V. J. Emery and S. A. Kivelson, Nature **374**, 474 (1995).
  - D. Podolsky, S. Raghu, and A. Vishwanath, Phys. Rev. Lett. **99**, 117004 (2007).
  - Z. Tesanovic, Nat Phys **4**, 408 (2008).
- Magnitude fluctuations
  - I. Ussishkin, S. L. Sondhi, and D. A. Huse, Phys. Rev. Lett. **89**, 287001 (2002).
- Competing order
  - E. Fradkin, S. A. Kivelson, M. J. Lawler, J. P. Eisenstein, and A. P. Mackenzie, Annual Review of Condensed Matter Physics **1**, 153 (2010).
- Disorder
  - F. Rullier-Albenque, H. Alloul, F. Balakirev, and C. Proust, EPL (Europhysics Letters) **81**, 37008 (2008).
  - H. Alloul, J. Bobro, M. Gabay, and P. J. Hirschfeld, Rev. Mod. Phys. **81**, 45 (2009).

Gaussian amplitude fluctuations in Eu-LSCO



Chang, Doiron-Leyraud et al.

Phase fluctuations and disorder?

Monolayer LSCO, field doped

A. T. Bollinger et al. & I. Božović, Nature **472**, 458–460

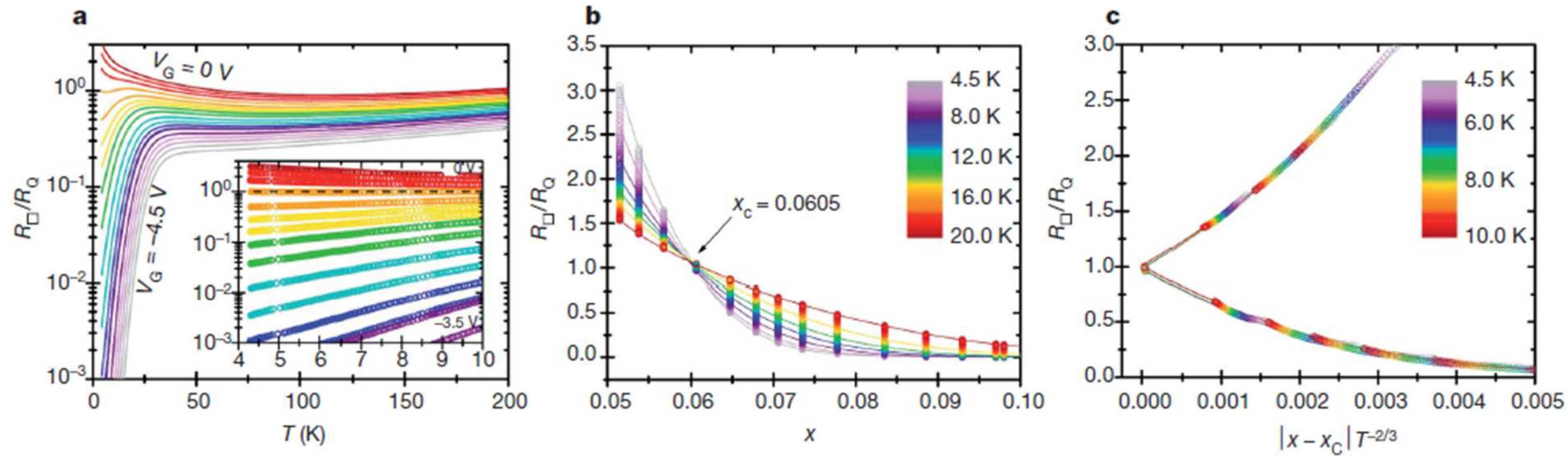
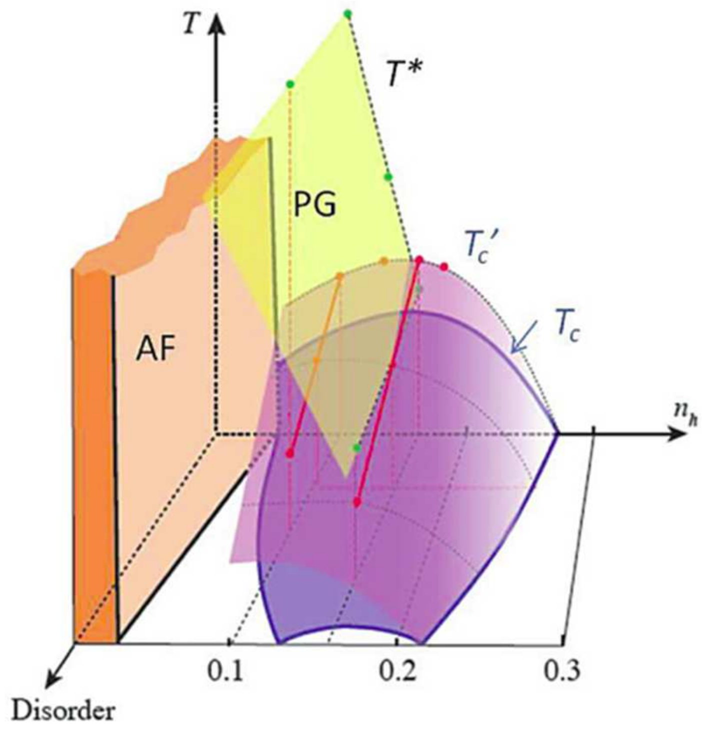


Figure 2 | Superconductor–insulator transition driven by electric field. **a**, Temperature dependence of normalized resistance $r = R_\square(x,T)/R_Q$ of an initially heavily underdoped and insulating film (see Supplementary Fig. 12 for linear scale). The device (Supplementary section B) employs a coplanar Au gate and DEME-TFSI ionic liquid. The carrier density, fixed for each curve, is tuned by varying the gate voltage from 0 V to −4.5 V in 0.25 V steps; an insulating film becomes superconducting via a QPT. The inset highlights a separatrix independent of temperature below 10 K. The open circles are the actual raw data points; the black dashed line is $R_\square(x_c,T) = R_Q = 6.45$ kΩ. **b**, The inverse representation of the same data, that is, the $r_T(x)$ dependence at fixed temperatures below 20 K. Each vertical array of (about 100) data points corresponds to one fixed carrier density, that is, to one $r_x(T)$ curve in Fig. 2a. The colours refer to the temperature, and the continuous lines are interpolated for selected temperatures (4.5, 6.0, 8.0, 10.0, 12.0, 15.0 and 20.0 K). The crossing point defines the critical carrier concentration $x_c = 0.06 \pm 0.01$, and the critical resistance $R_c = 6.45 \pm 0.10$ kΩ. **c**, Scaling of the same data with respect to a single variable $u = |x - x_c| T^{-1/z\nu}$, with $z\nu = 1.5$. This figure is derived by folding panel **b** at x_c and scaling the abscissa of each $r_T(|x - x_c|)$ curve by $T^{-2/3}$. For $4.3\,\mathrm{K} < T < 10\,\mathrm{K}$, the discrete groups of points of Fig. 2b collapse accurately onto a two-valued function, with one branch corresponding to x larger and the other to x smaller than x_c. The critical exponents are identical on both sides of the superconductor–insulator transition. The raw data points cover the interpolation lines almost completely, except close to the origin.

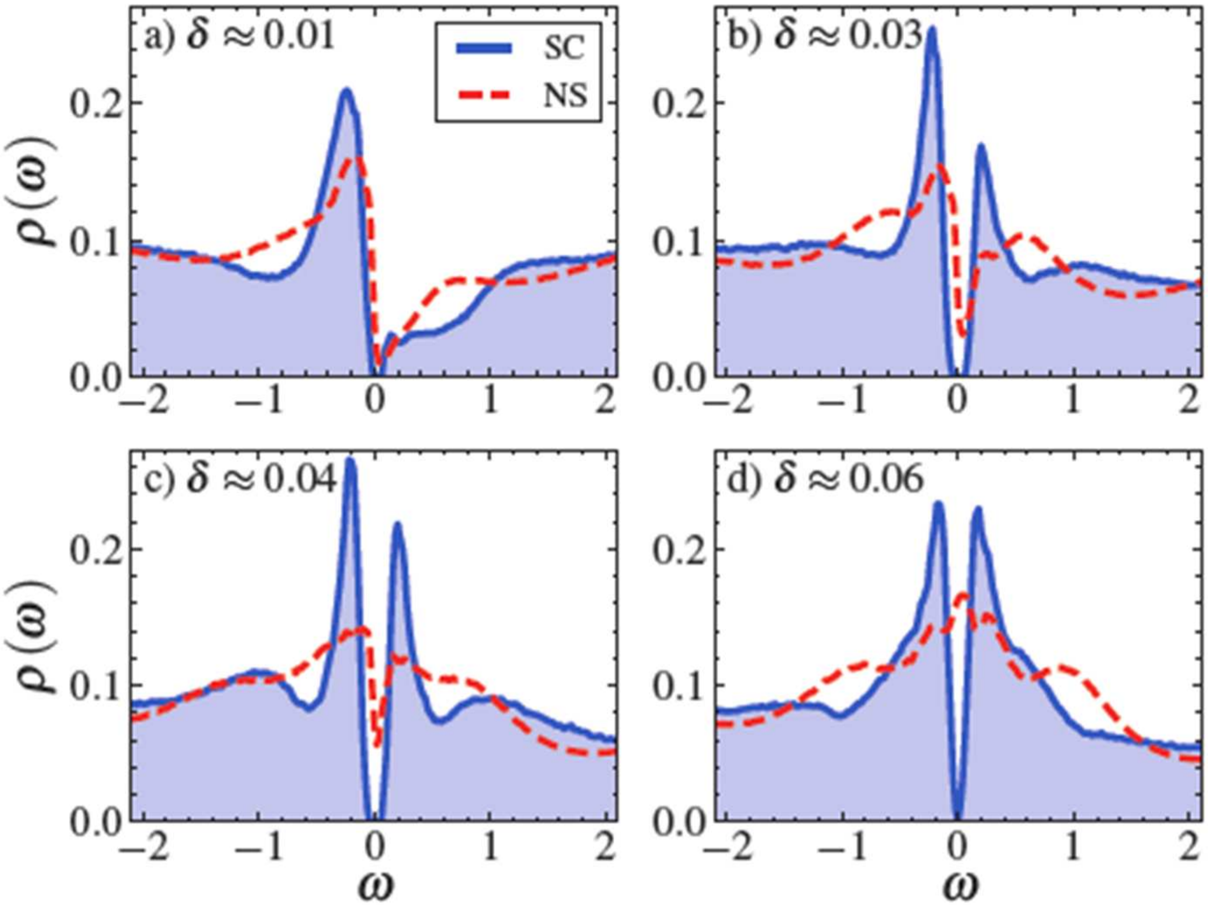
Effect of disorder



F. Rullier-Albenque, H. Alloul, and G.Rikken,
Phys. Rev. B **84**, 014522 (2011).

Superconductivity in underdoped vs BCS

First-order transition leaves its mark



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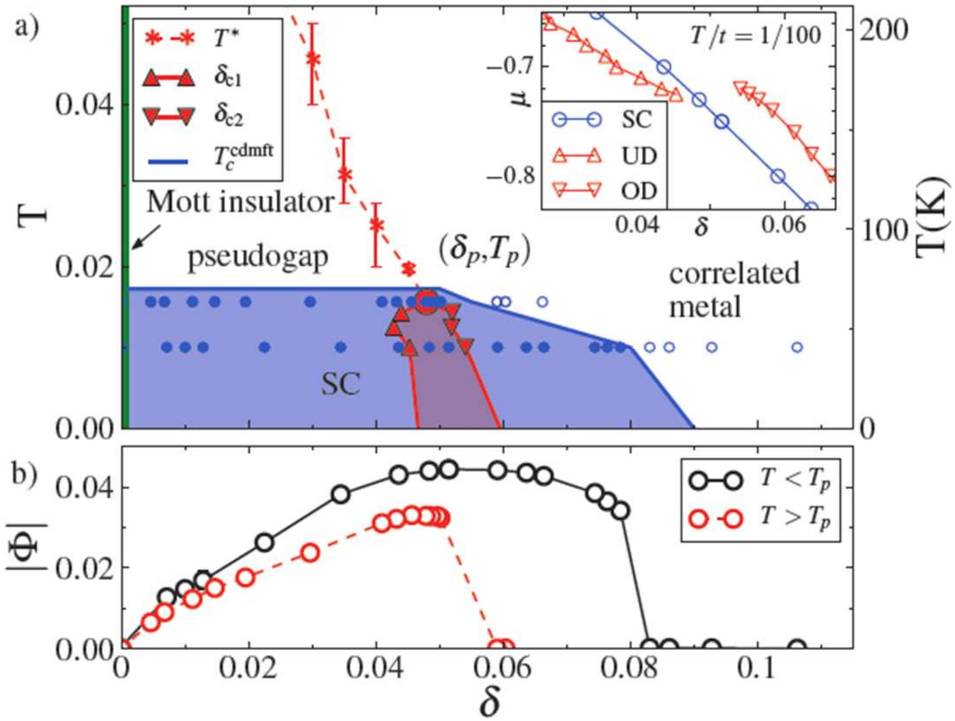
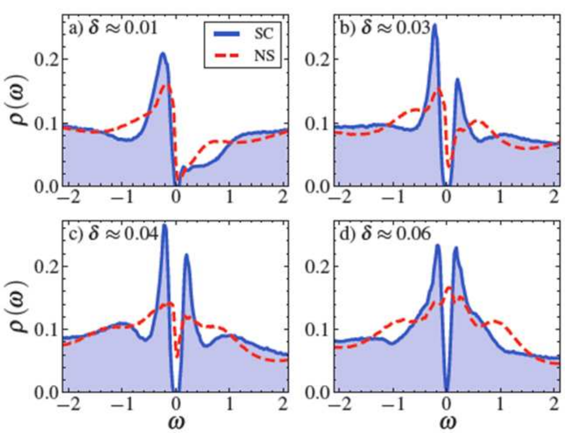
Summary





- Below the dome finite T critical point (not QCP) controls normal state
- First-order transition destroyed but traces in the dynamics
- Pseudogap different from pairing.
- Actual T_c in underdoped
  - Competing order
  - Long wavelength fluctuations (see O.P.)
  - Disorder

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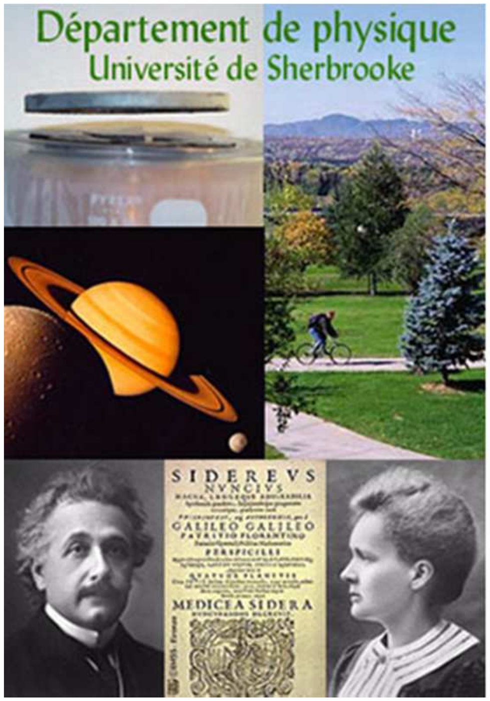

André-Marie Tremblay

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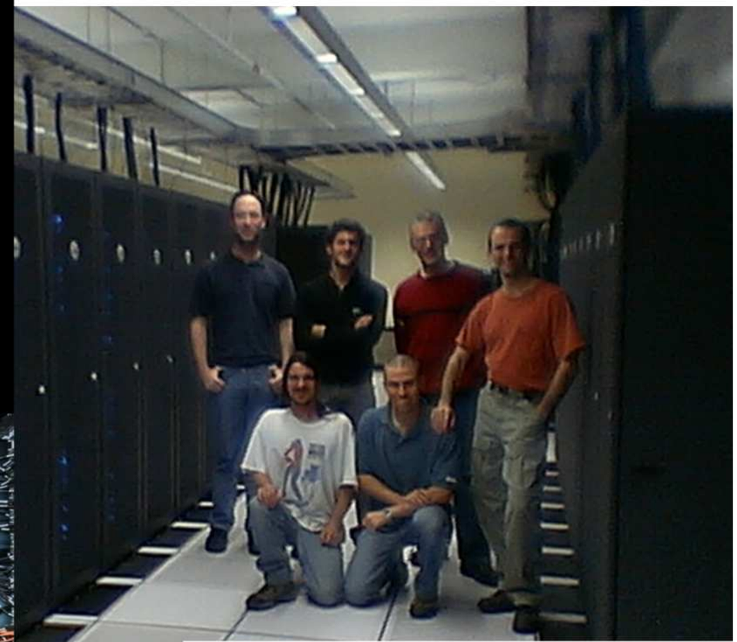

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Merci

Thank you