

Pseudogap and superconductivity from Mott physics

A.-M. Tremblay

G. Sordi, K. Haule, P. Sémon

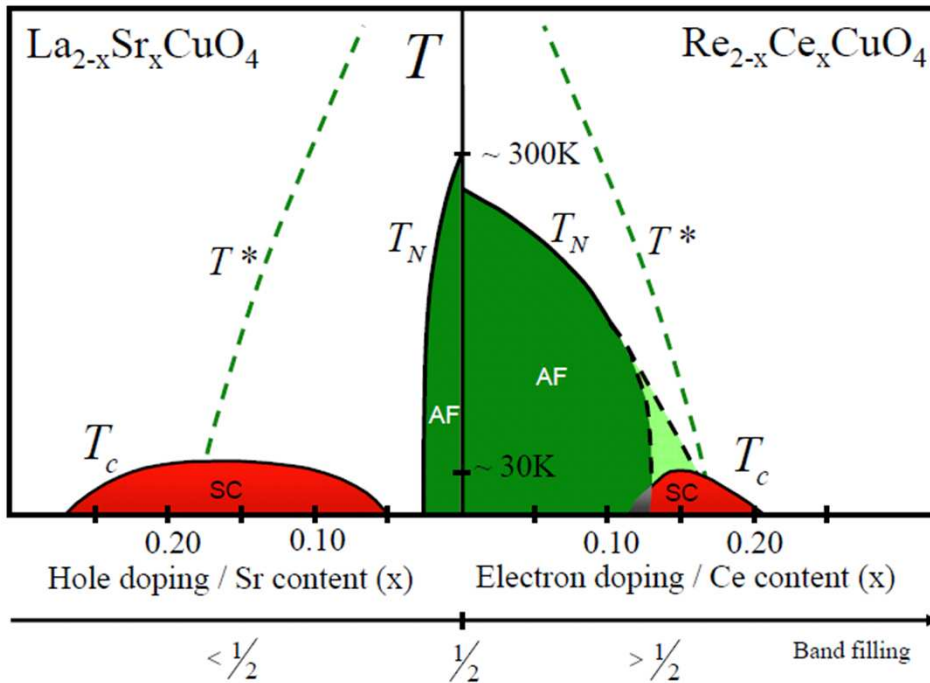


ICSM 2012, 30 avril 2012



High-temperature superconductors

Armitage, Fournier, Greene, RMP (2009)



- 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) ...

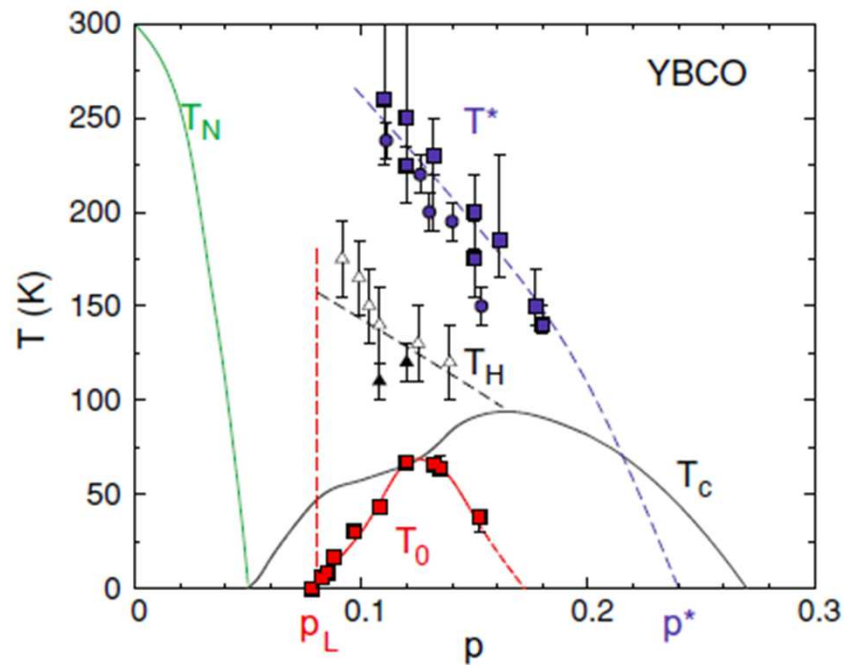
- Or Mott Physics?

- RVB: P.A. Lee Rep. Prog. Phys. **71**, 012501 (2008)

What is under the dome?
Mott Physics away from $n = 1$



Ordered phases

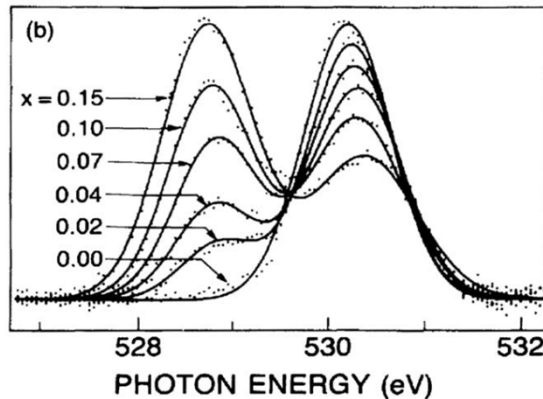


Leboeuf, Doiron-Leyraud et al. PRB **83**, 054506 (2011)

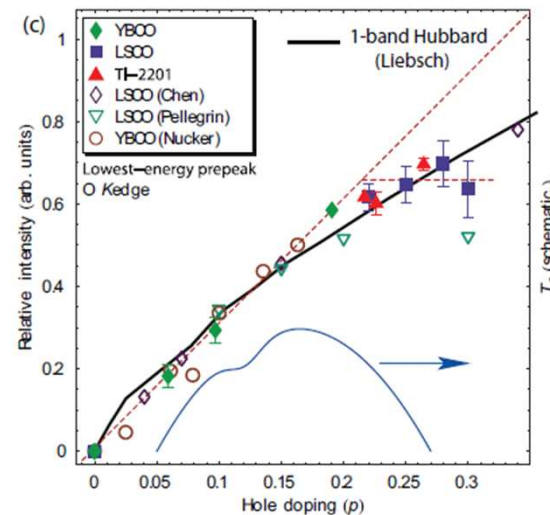
Cuprates as doped Mott insulators



Experiment: X-Ray absorption



Chen et al. PRL **66**, 104 (1991)



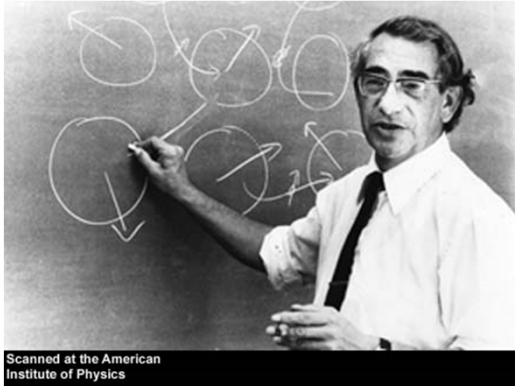
Peets et al. PRL **103**, (2009),

Phillips, Jarrell PRL , vol. **105**, 199701 (2010)

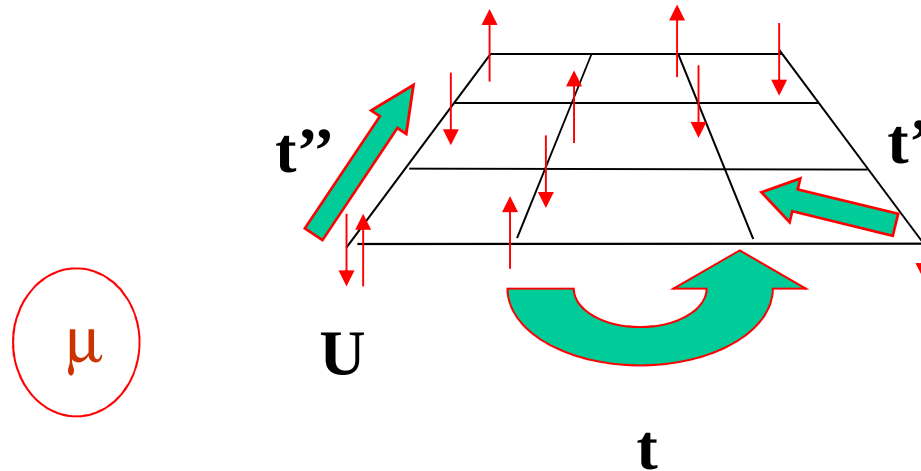
Number of low energy states above $\omega = 0$ scales as $2x +$
Not as $1+x$ as in Fermi liquid

Meinders *et al.* PRB **48**, 3916 (1993)

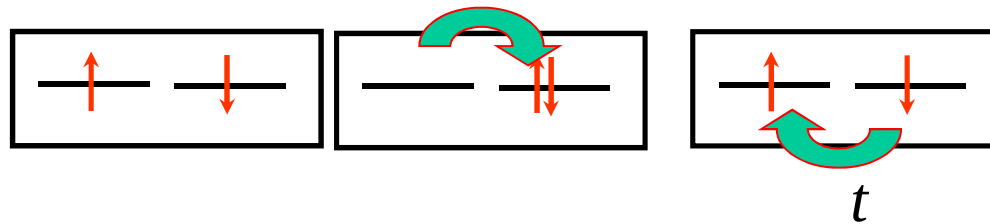
Hubbard model



1931-1980



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



$t = 1$

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



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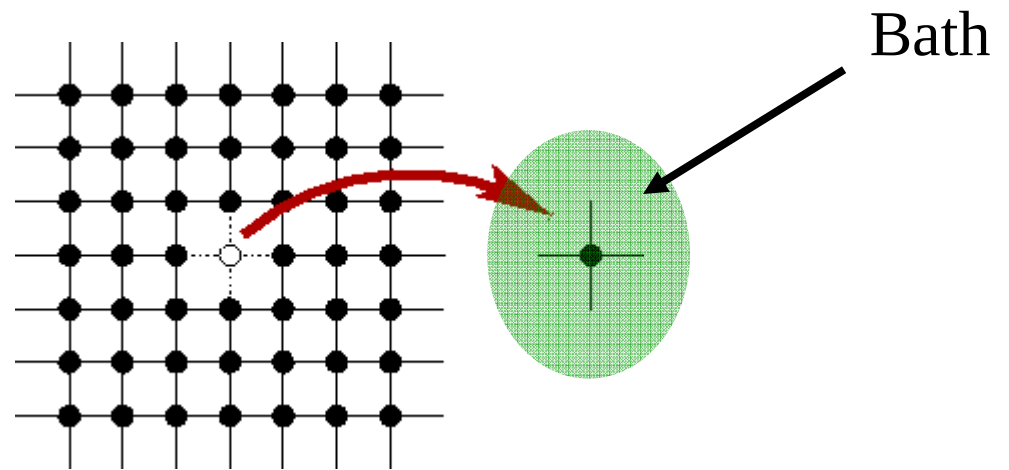
Method



Mott transition and Dynamical Mean-Field Theory.

The beginnings in $d = \text{infinity}$

- 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.



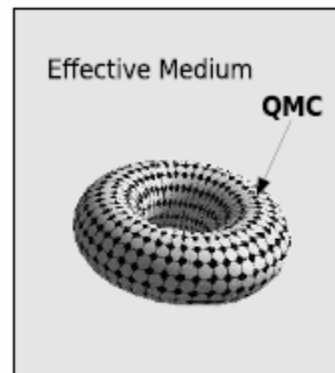
W. Metzner and D. Vollhardt, PRL (1989)

A. Georges and G. Kotliar, PRB (1992)

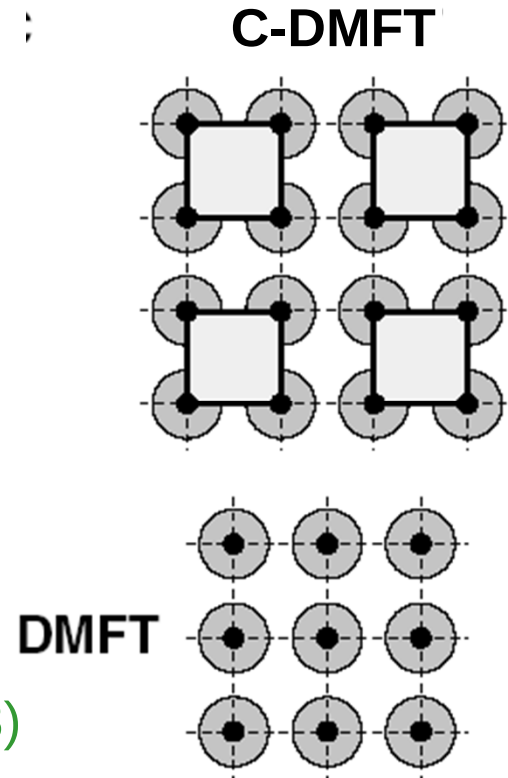
M. Jarrell PRB (1992)

DMFT, ($d = 3$)

2d Hubbard: Quantum cluster method



DCA



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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MDC

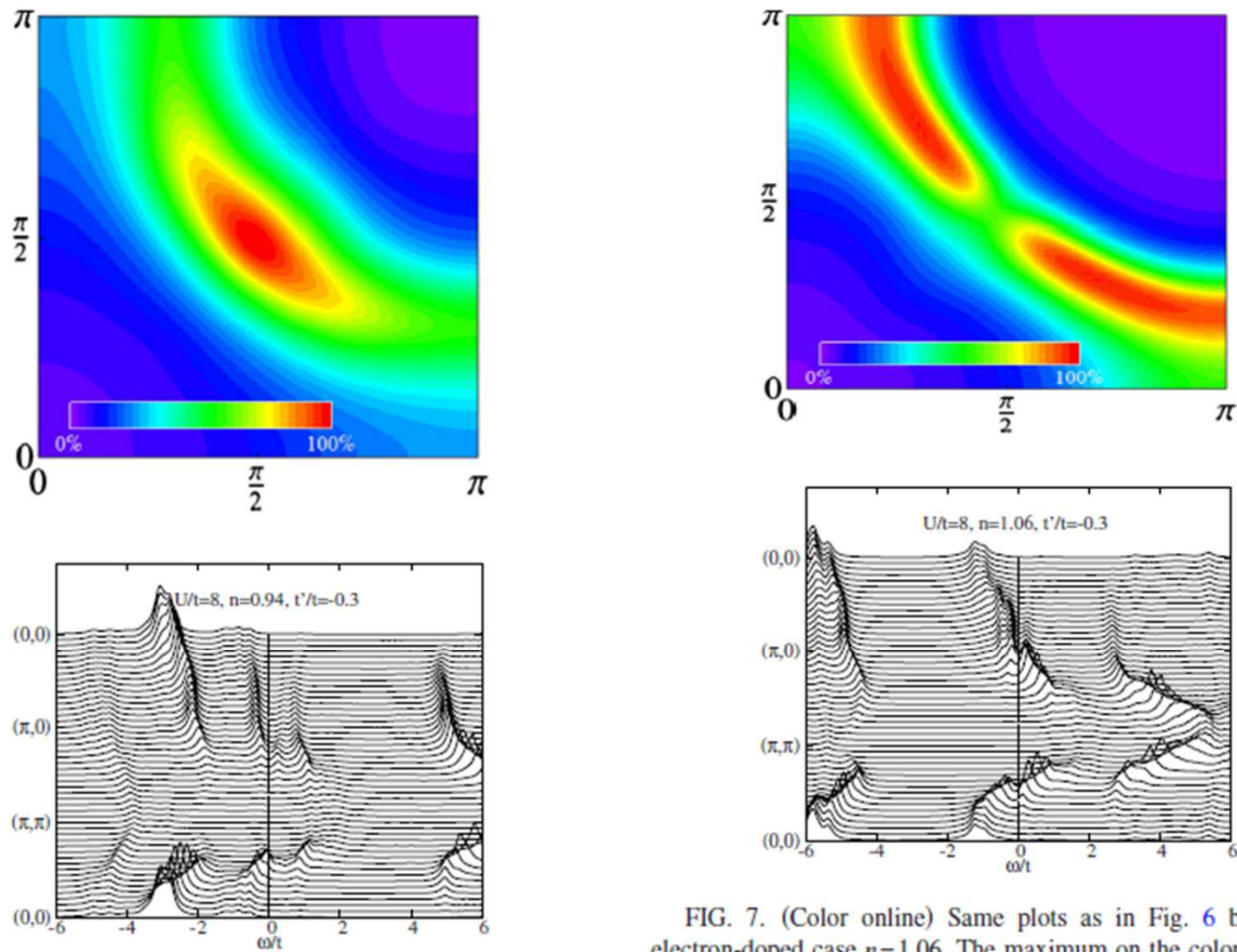
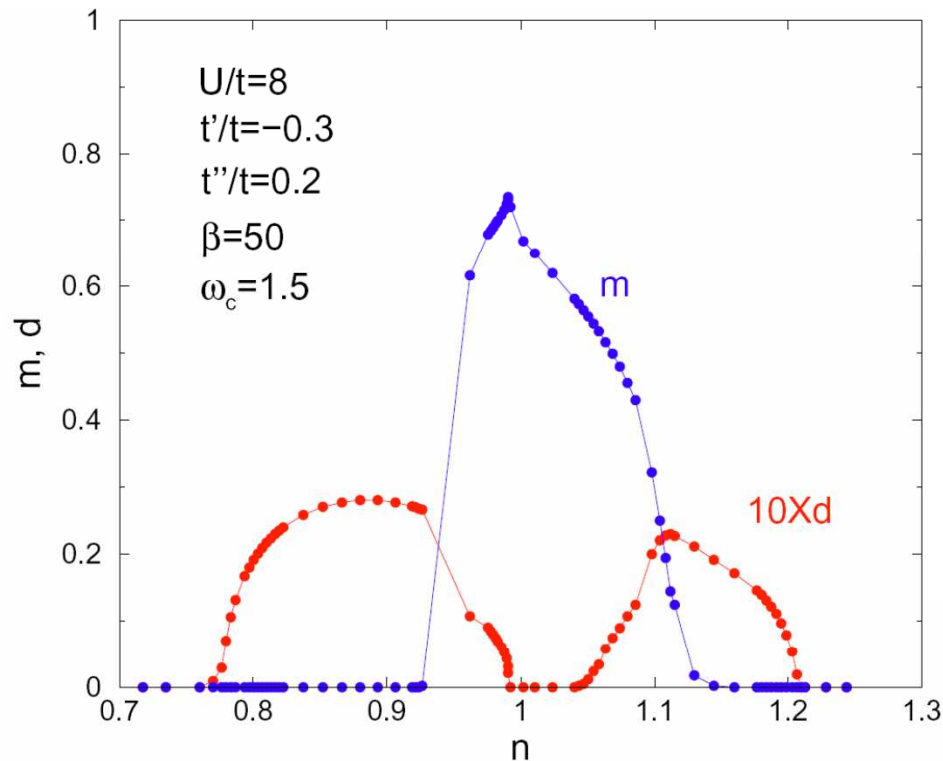
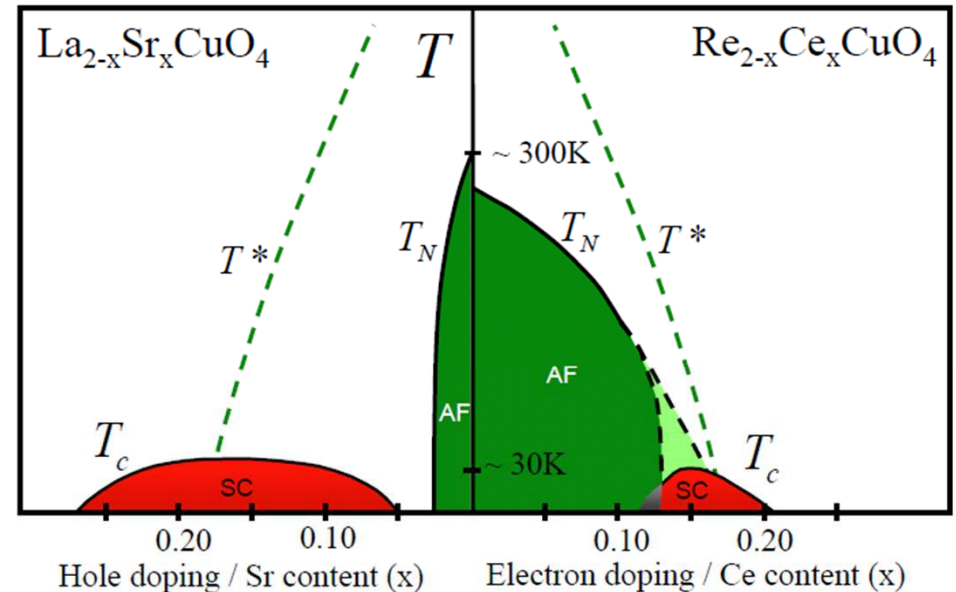


FIG. 7. (Color online) Same plots as in Fig. 6 but for the electron-doped case $n=1.06$. The maximum on the color scale cor-

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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+ and -

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



Outline

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

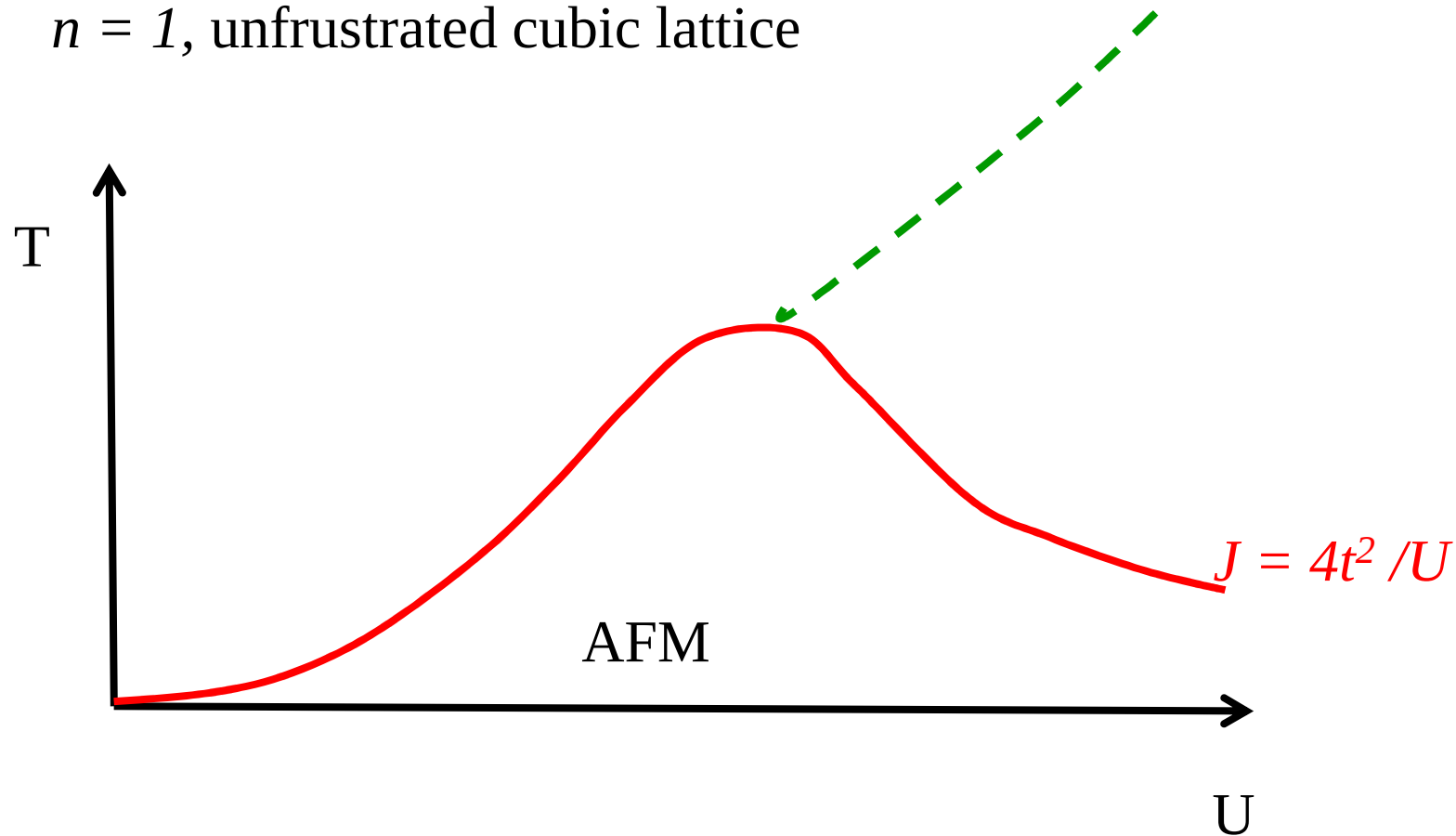


The Mott transition



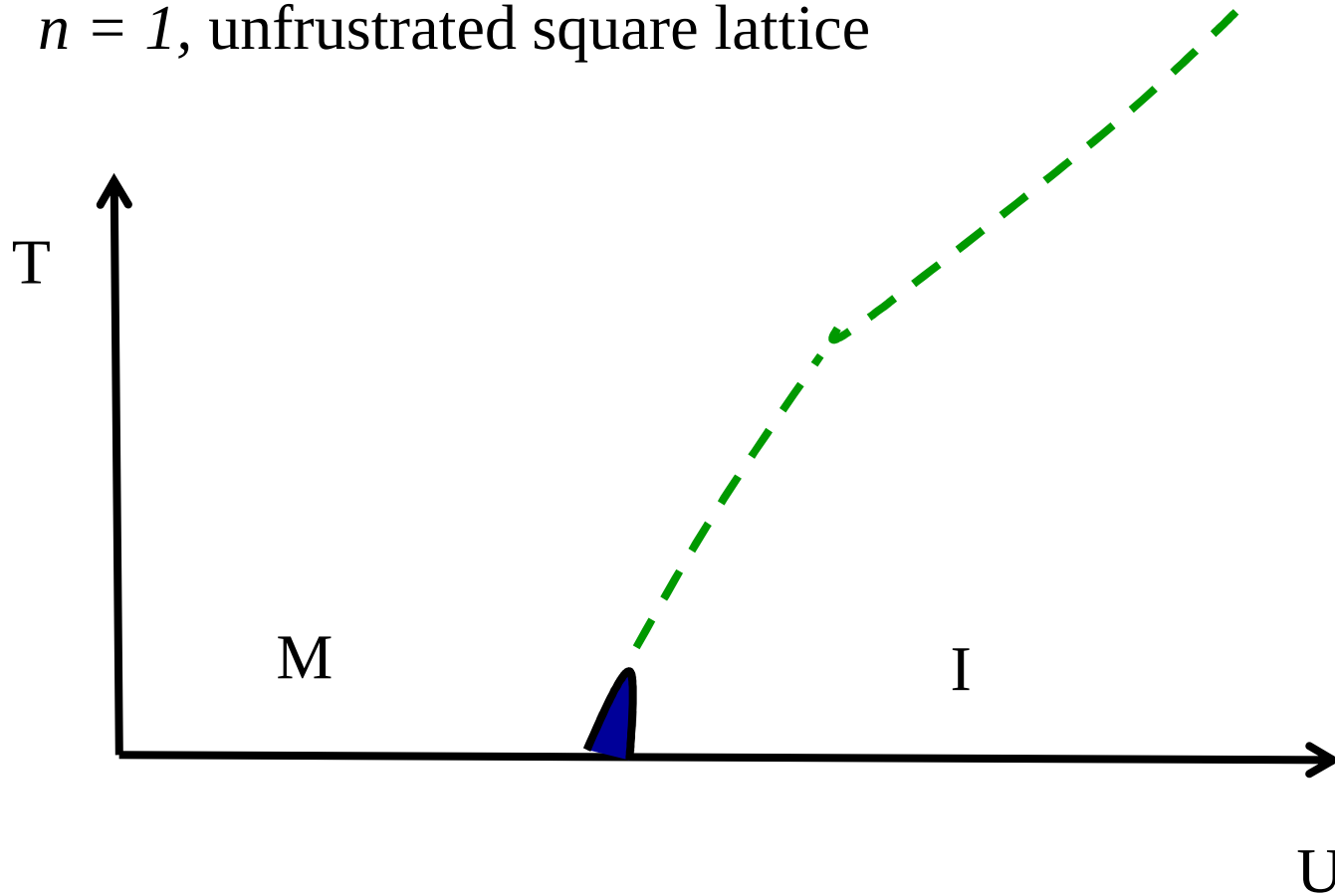
Local moment and Mott transition

$n = 1$, unfrustrated cubic lattice



Local moment and Mott transition

$n = 1$, unfrustrated square lattice





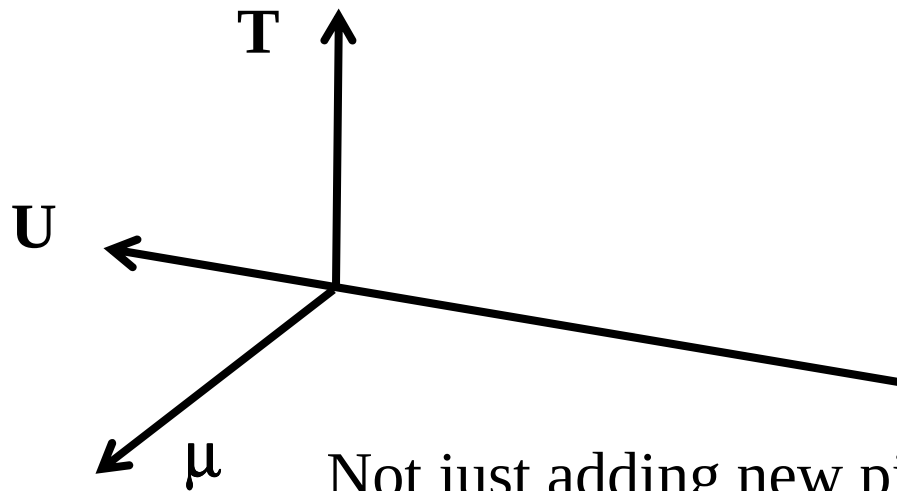
Giovanni Sordi

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

and

Phys. Rev. B. **84**, 075161 (2011)

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



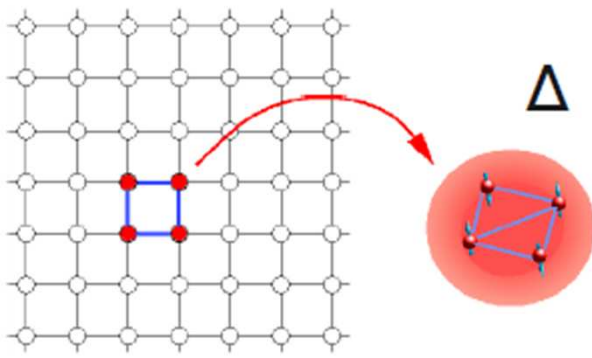
Kristjan Haule

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



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C-DMFT



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

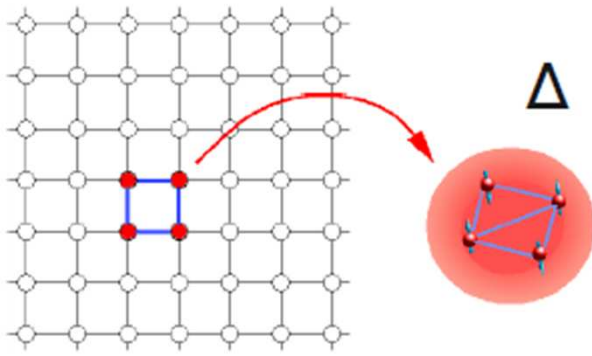
$$Z = \int \mathcal{D}[\psi^\dagger, \psi] e^{-S_c - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\mathbf{k}} \psi_{\mathbf{k}}^\dagger(\tau) \Delta_{\mathbf{k}}(\tau, \tau') \psi_{\mathbf{k}}(\tau')}$$

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).

C-DMFT



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

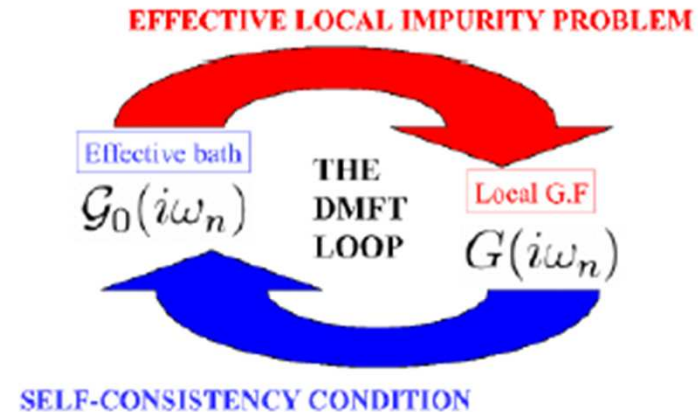
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K. Haule, PRB 2007

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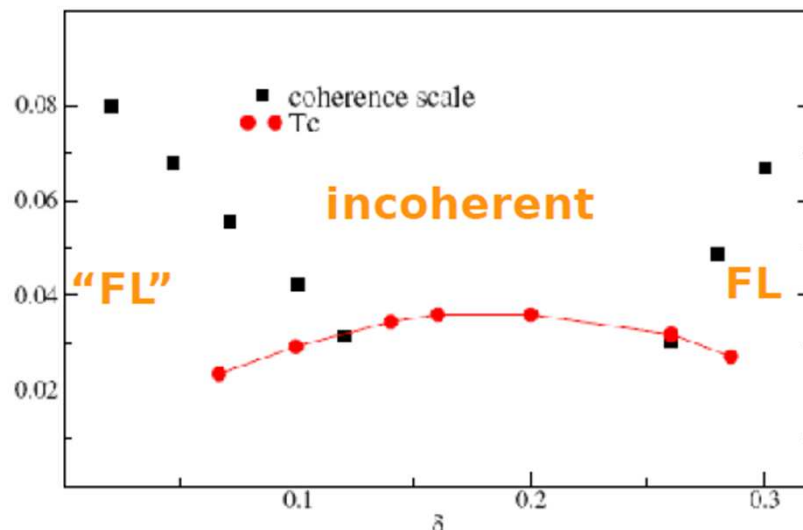


$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n)$$

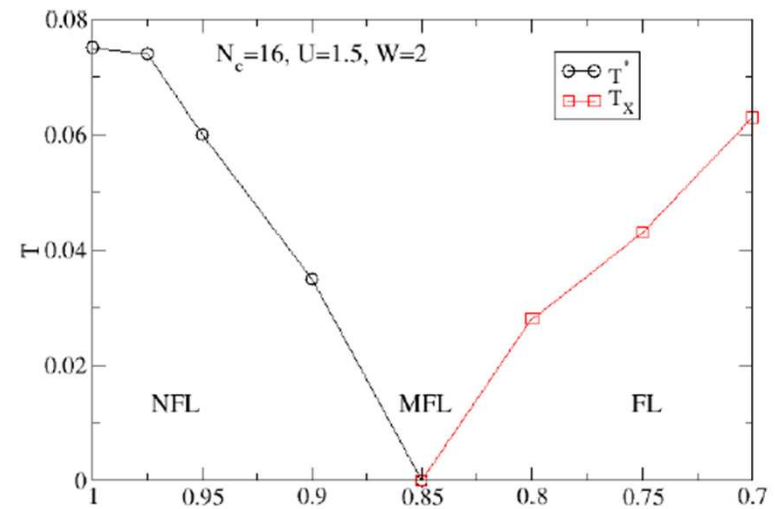
$$- \left[\sum_{\tilde{k}} \frac{1}{i\omega_n + \mu - t_c(\tilde{k}) - \Sigma_c(i\omega_n)} \right]^{-1}$$

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)

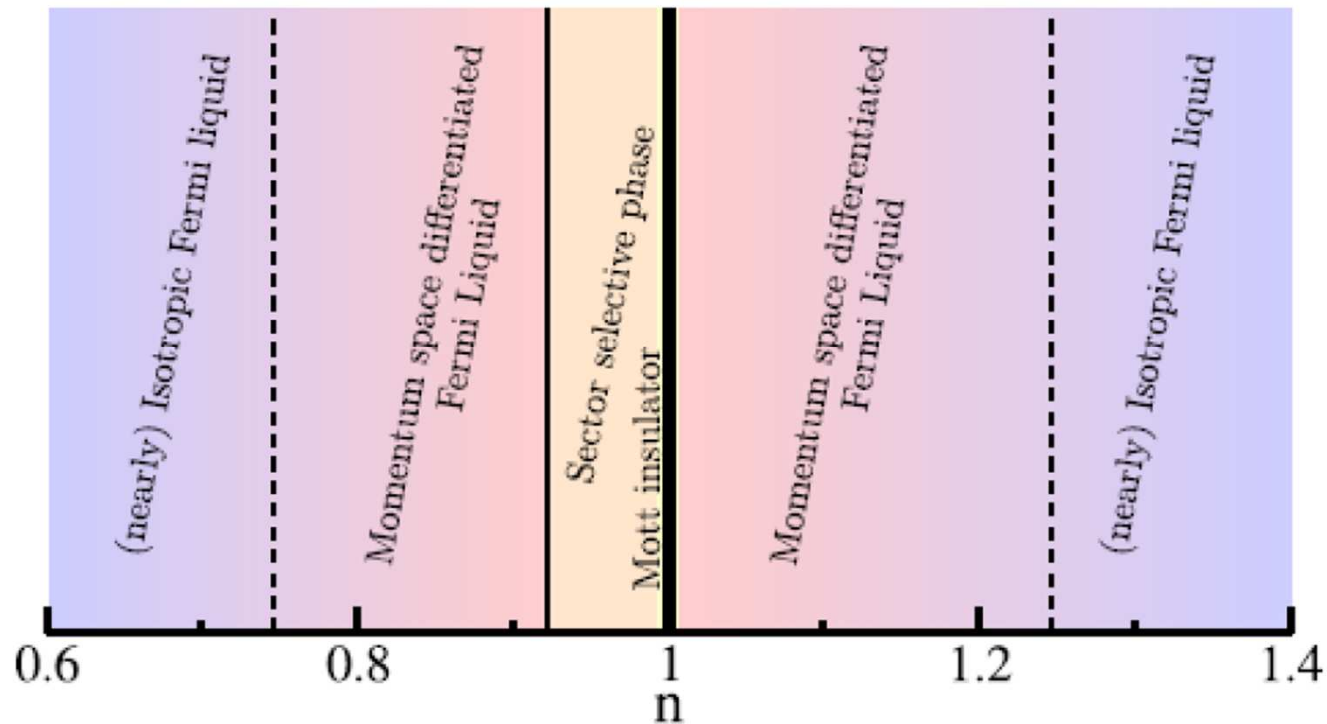


K. Haule, G. Kotliar, PRB (2008)



Vildhyadhiraja, PRL (2009)

Doping driven Mott transition

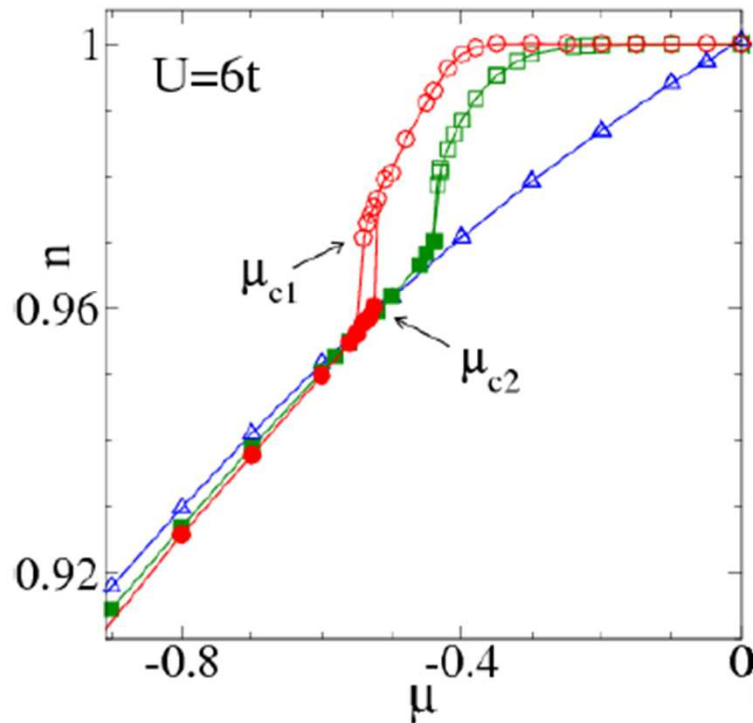


Gull, Werner, Millis, (2009)

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



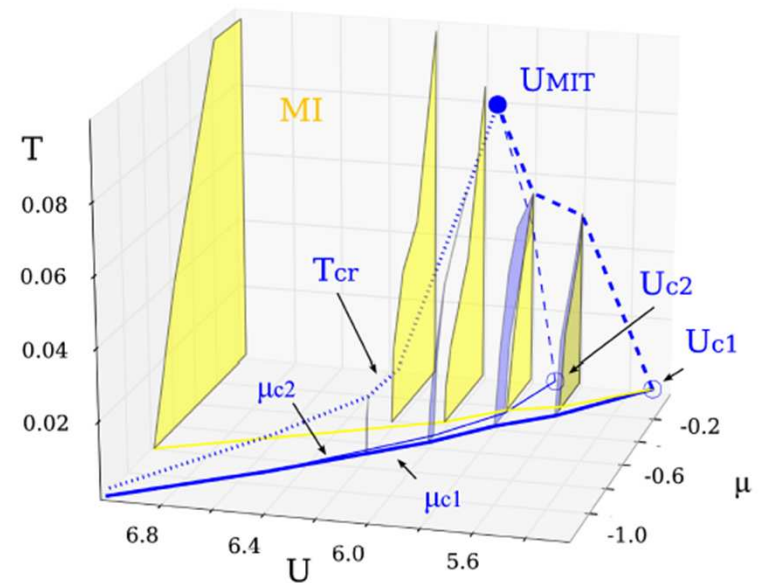
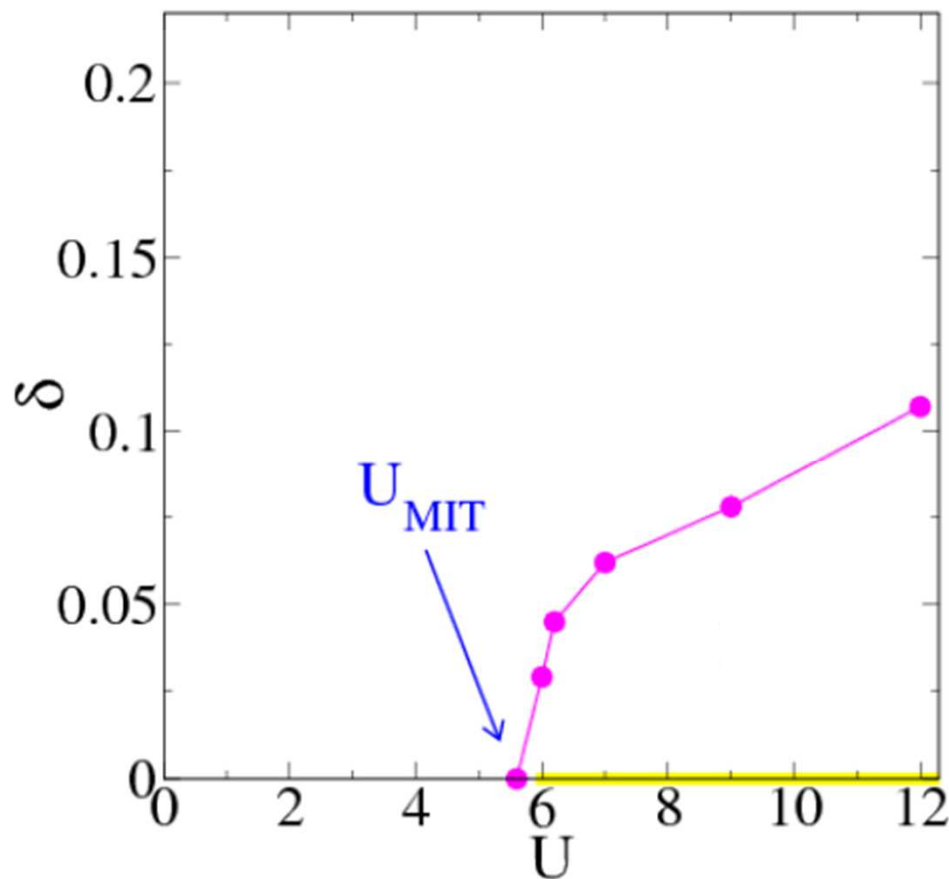
First order transition at finite doping



$n(\mu)$ 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



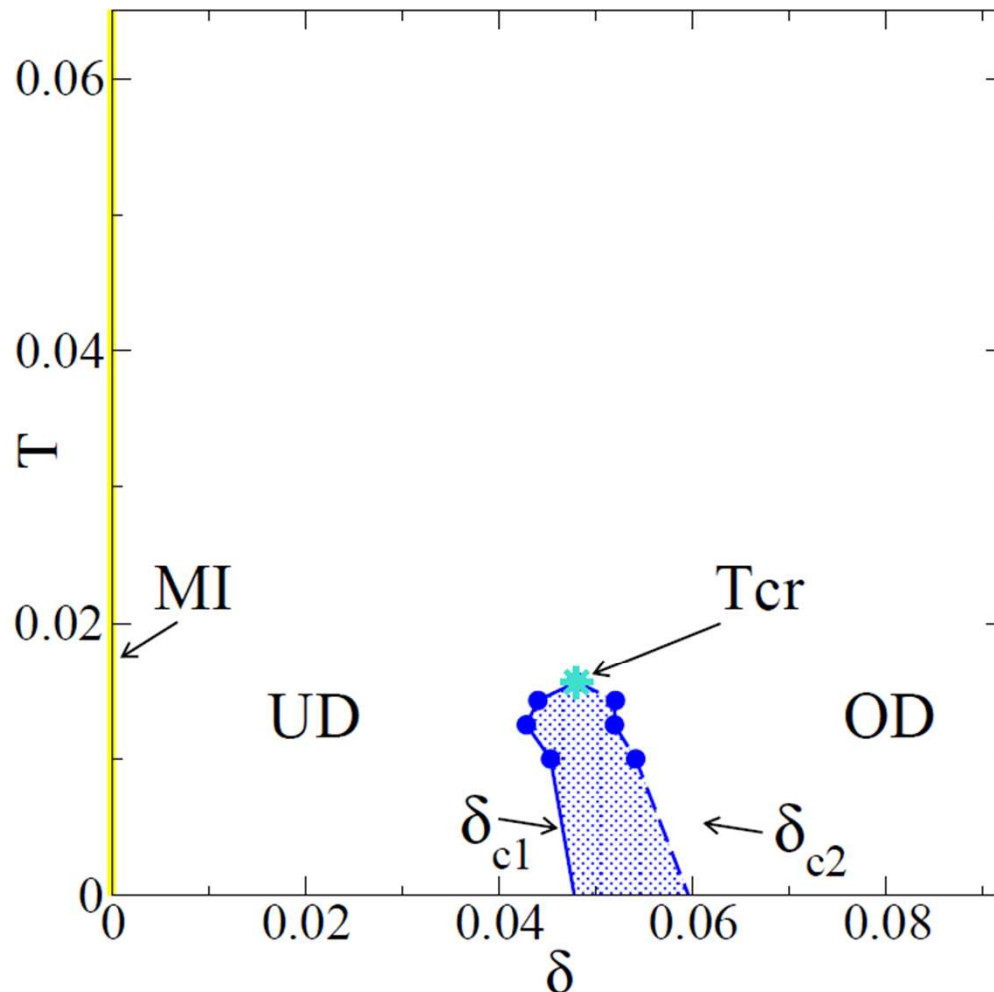
Characterisation of the phases ($U=6.2t$)

$U > U_{\text{MIT}}$:

1. Mott insulator (MI)
2. Underdoped phase (UD):
 $\delta < \delta_c$
3. Overdoped phase (OD):
 $\delta > \delta_c$
4. Coexistence/forbidden region

Here “optimal doping” δ_c =
doping at which the 1st order
transition occurs

How does the UD phase differ
from the OD phase?

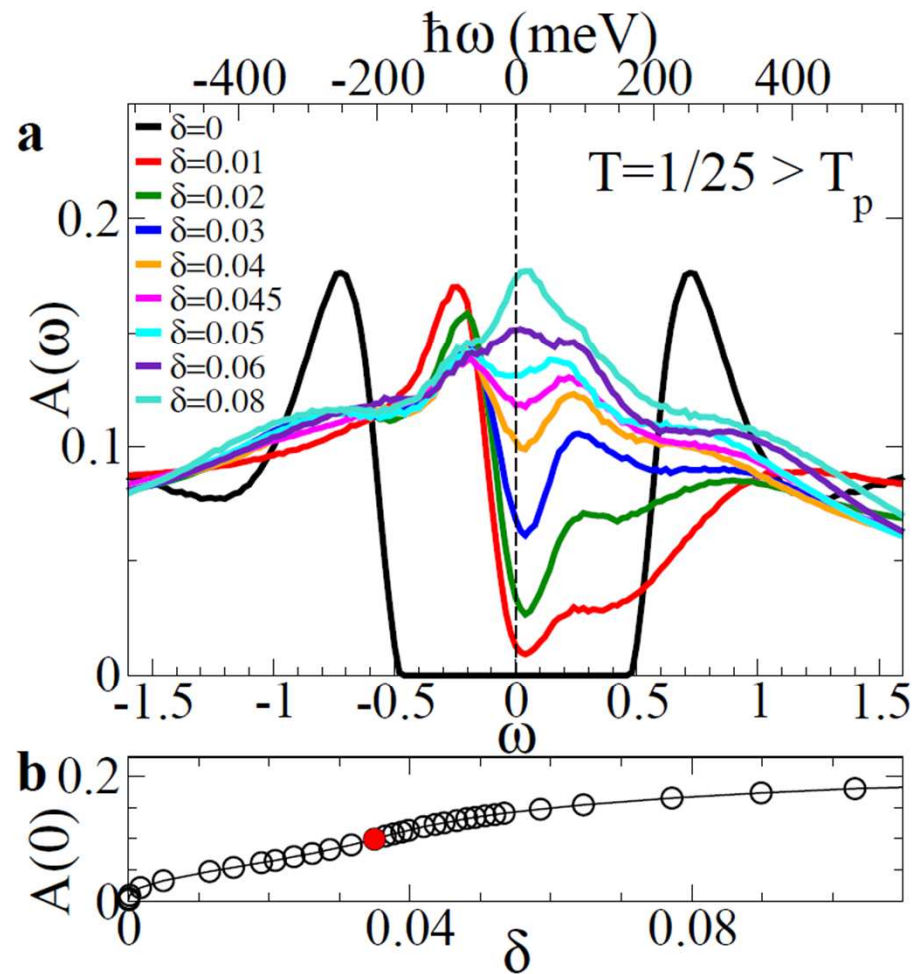
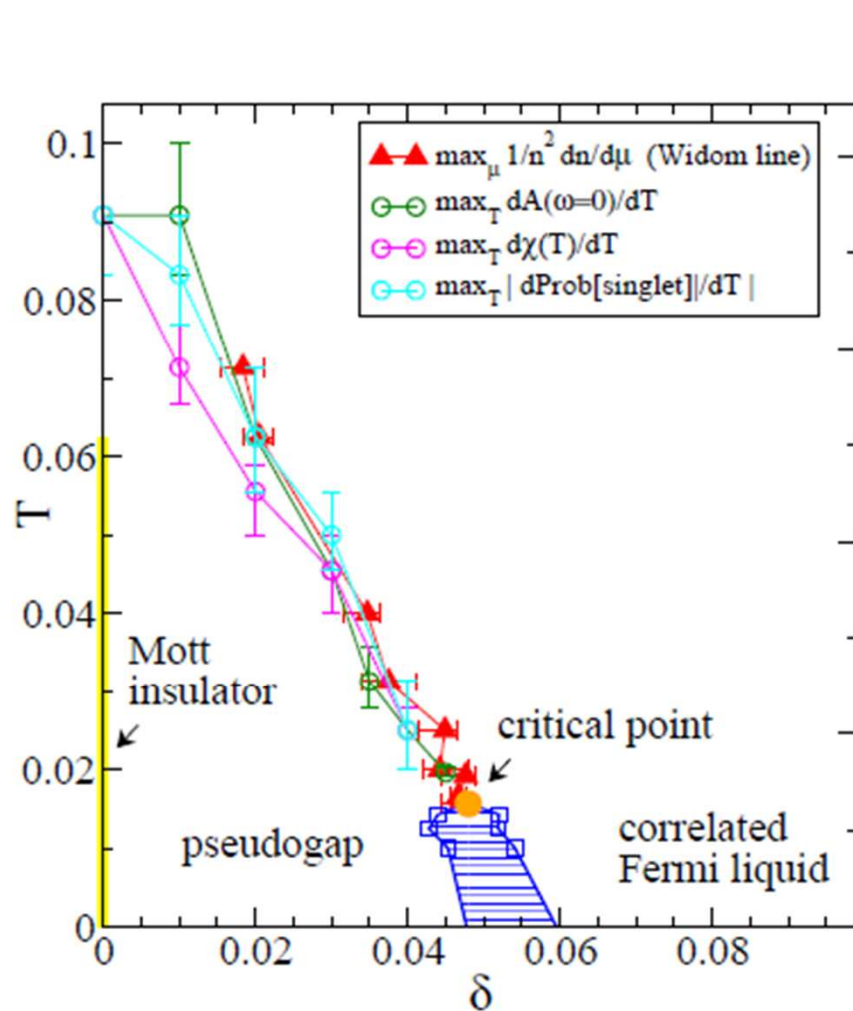


Smaller D and S

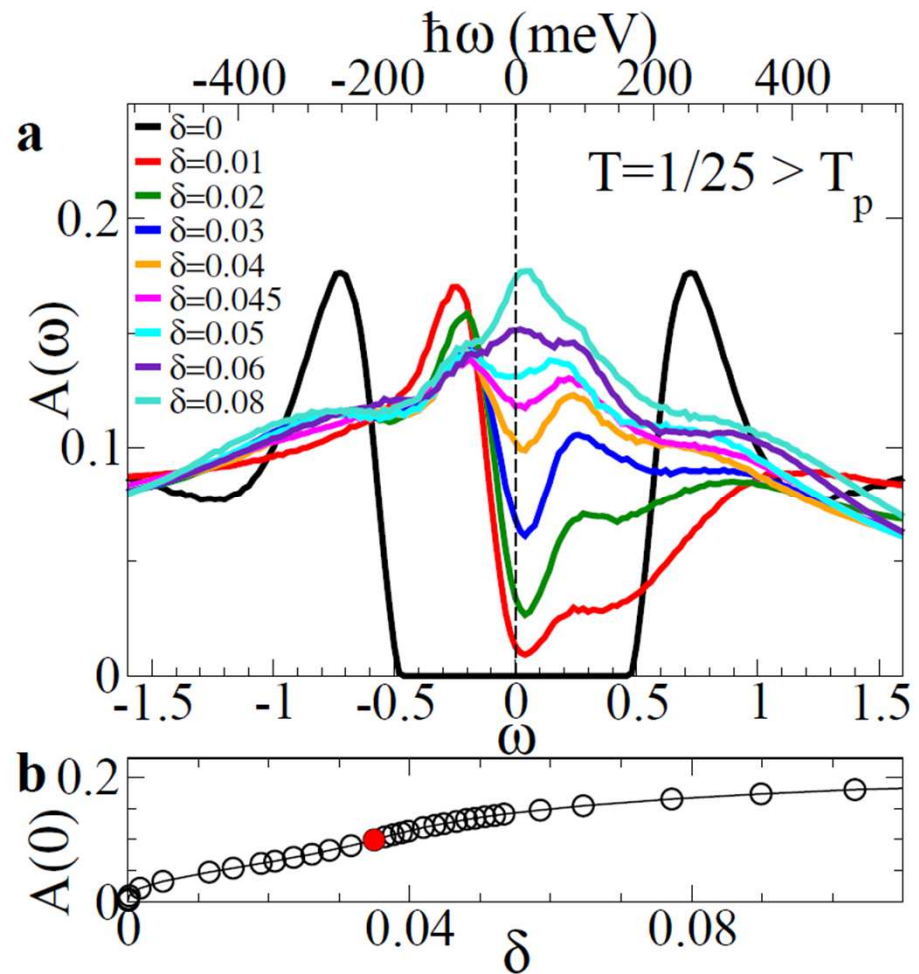
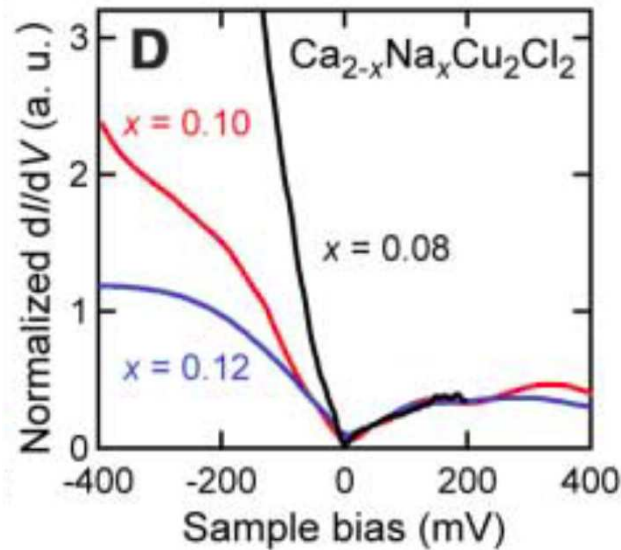


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Density of states

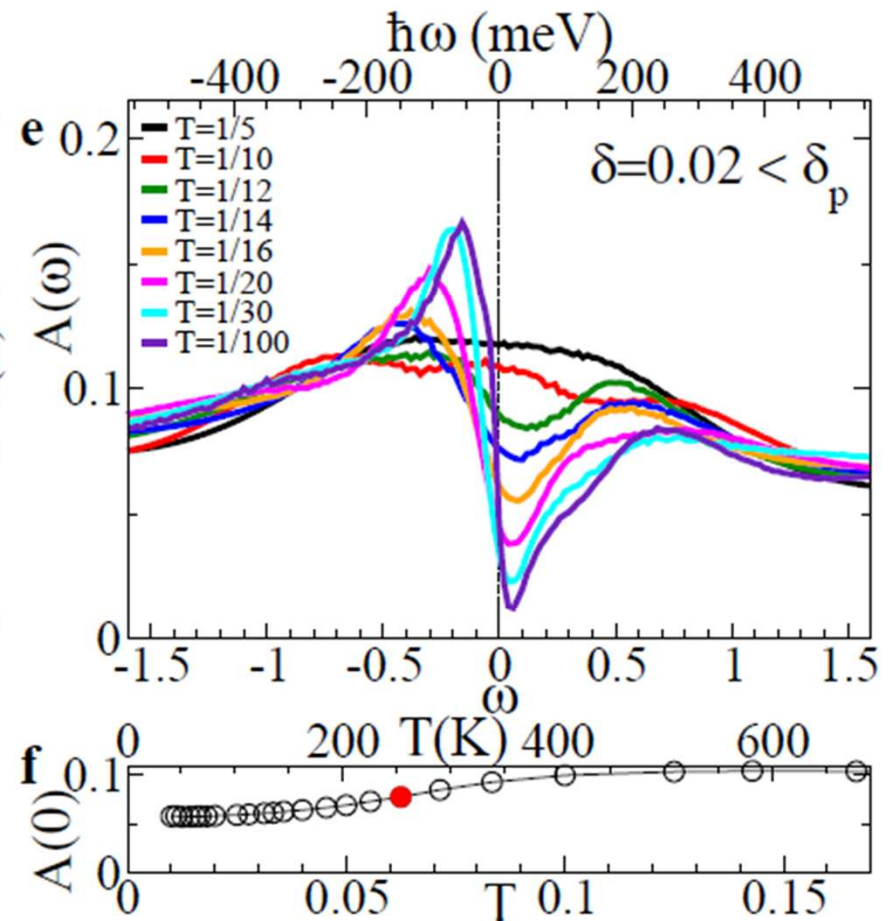
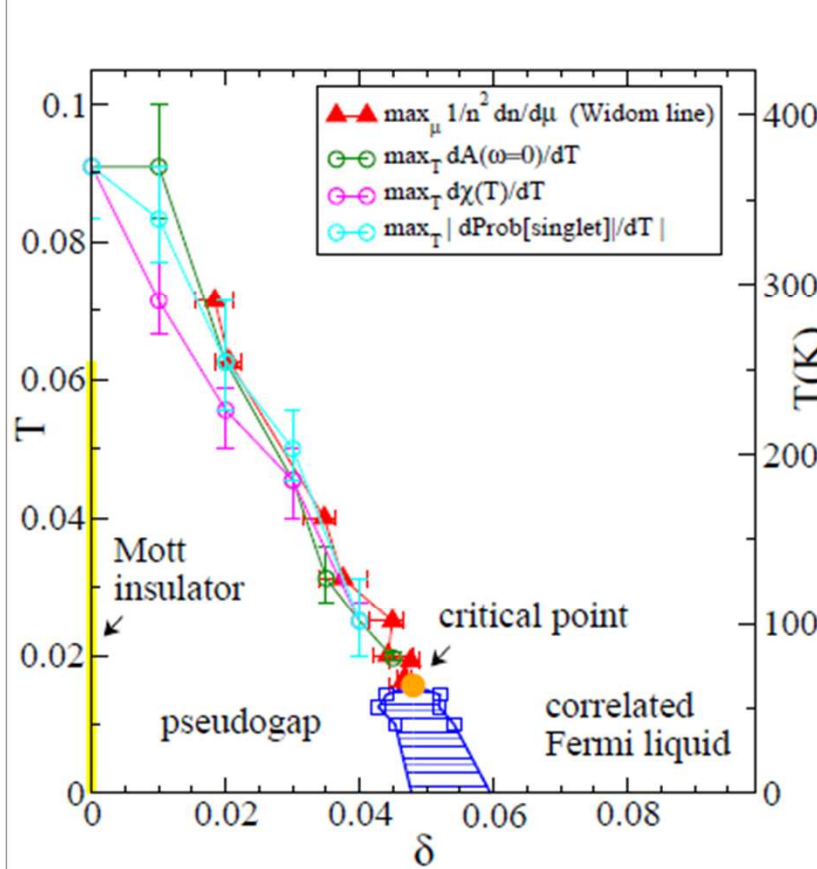


Density of states

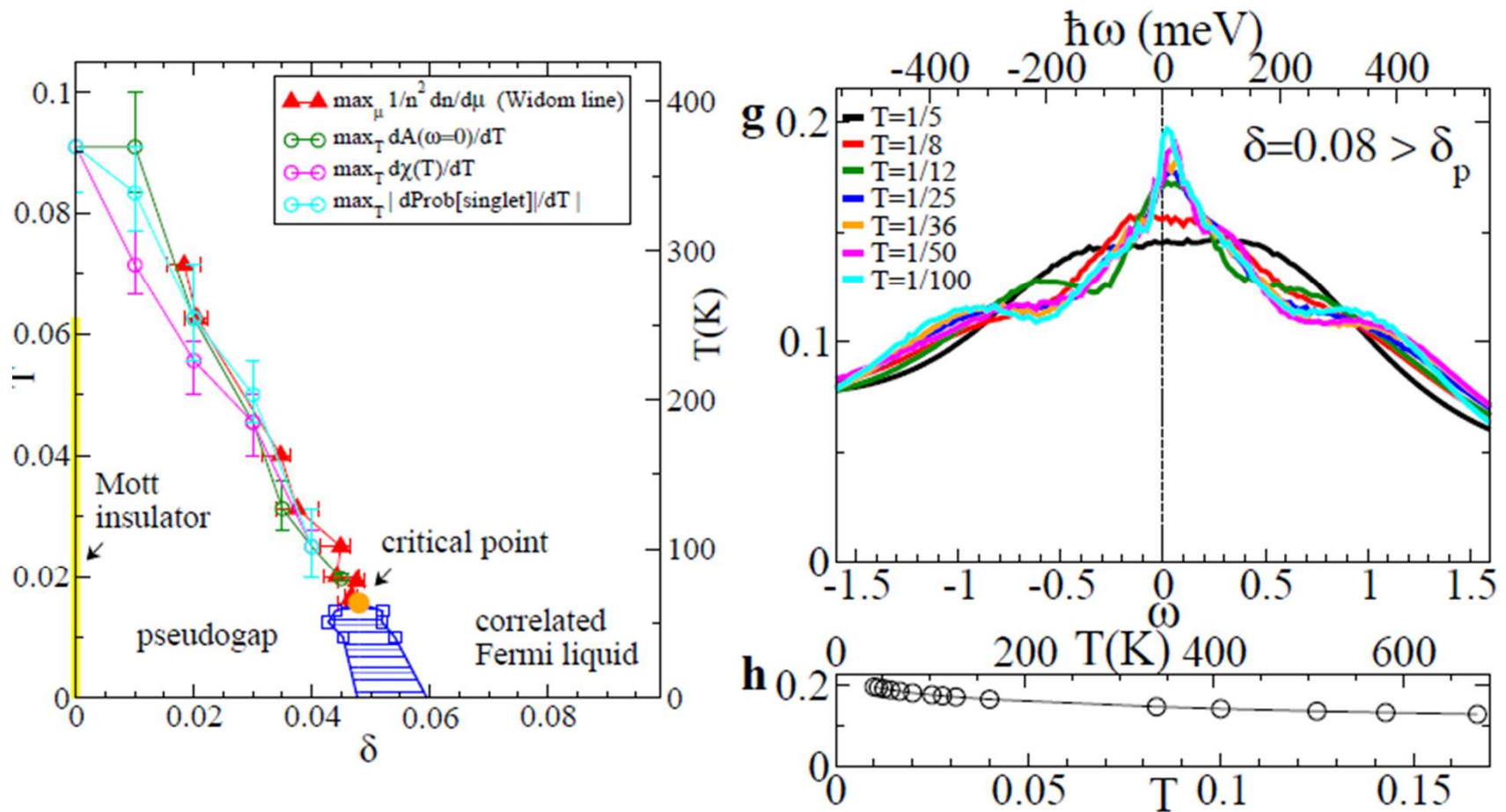


Khosaka et al. *Science* **315**, 1380 (2007);

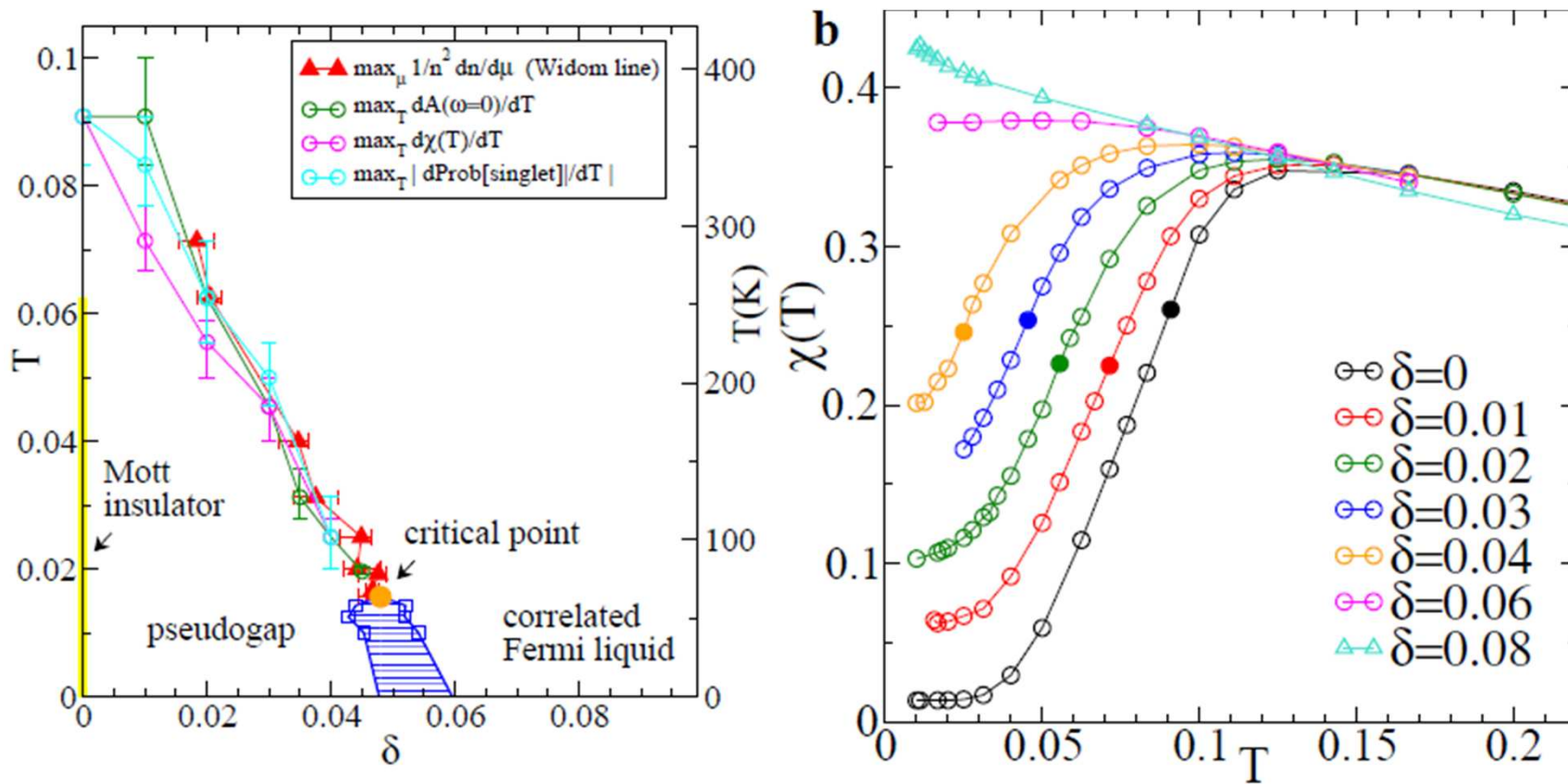
Density of states



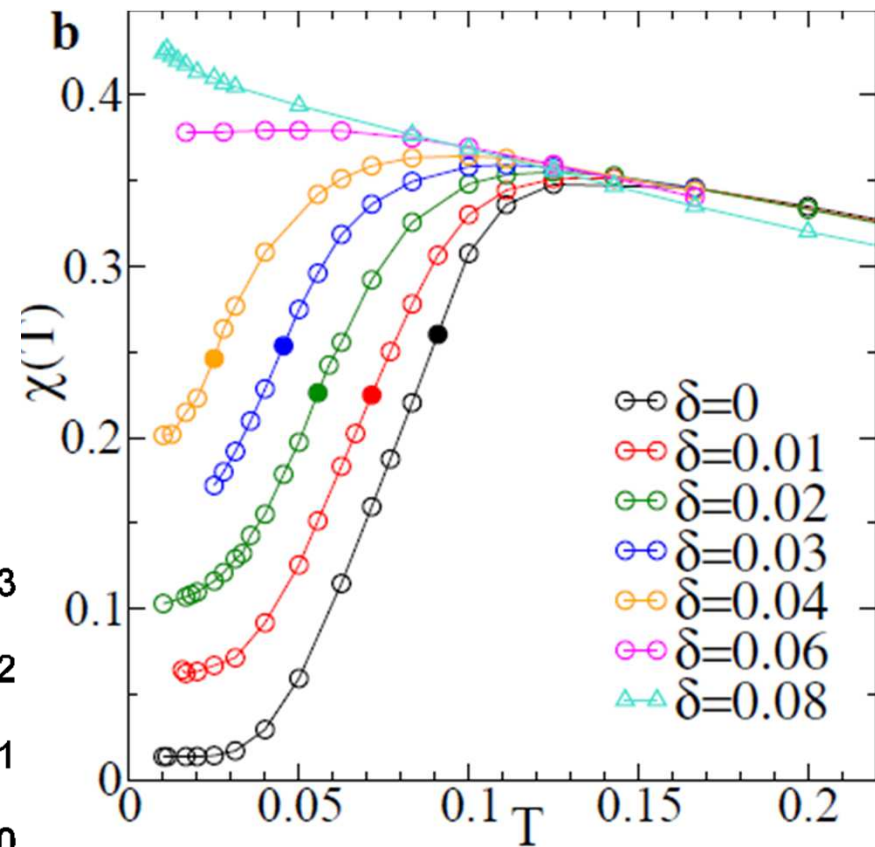
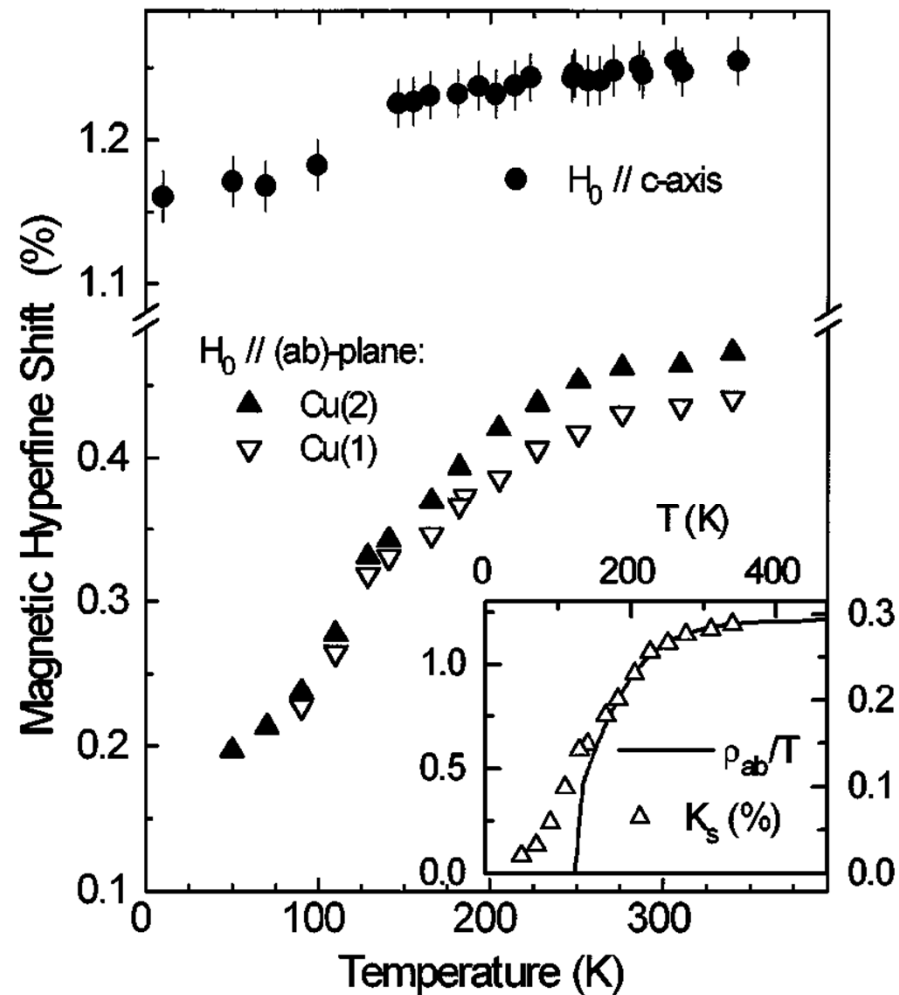
Density of states



Spin susceptibility



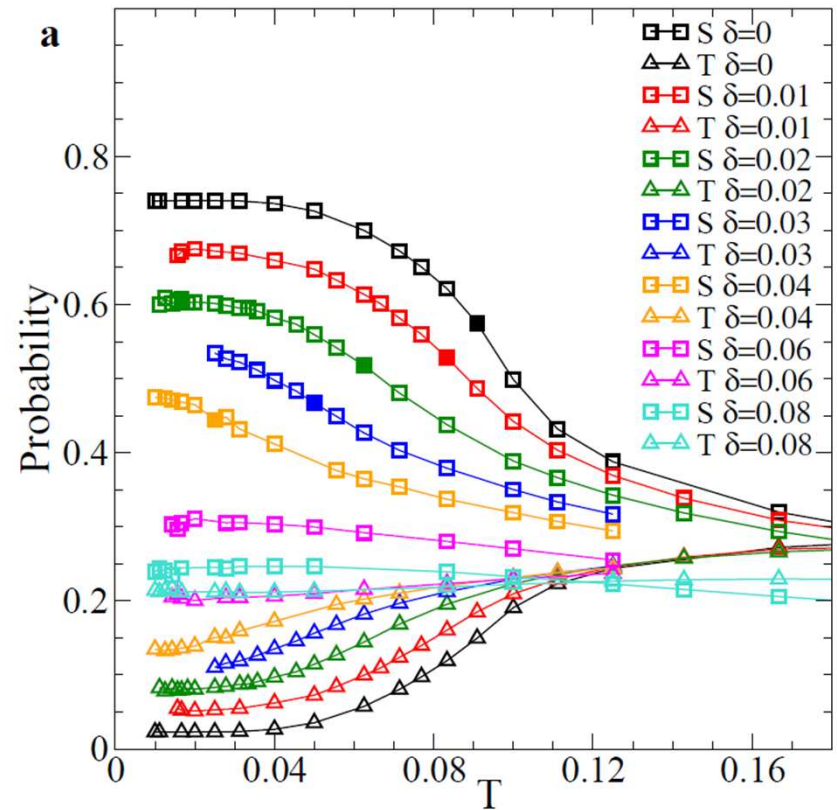
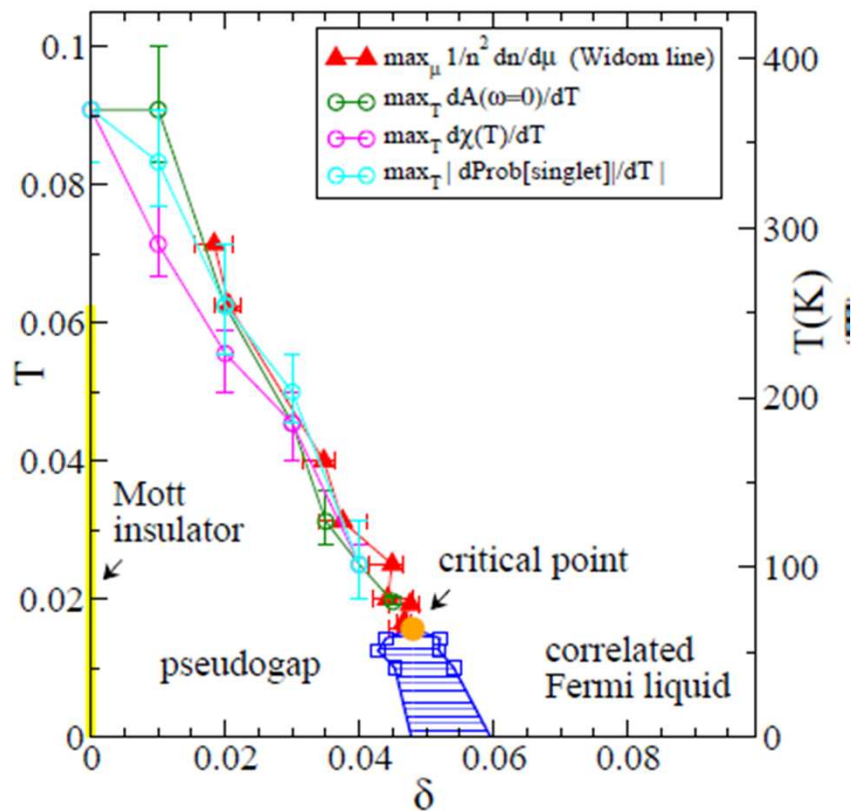
Spin susceptibility



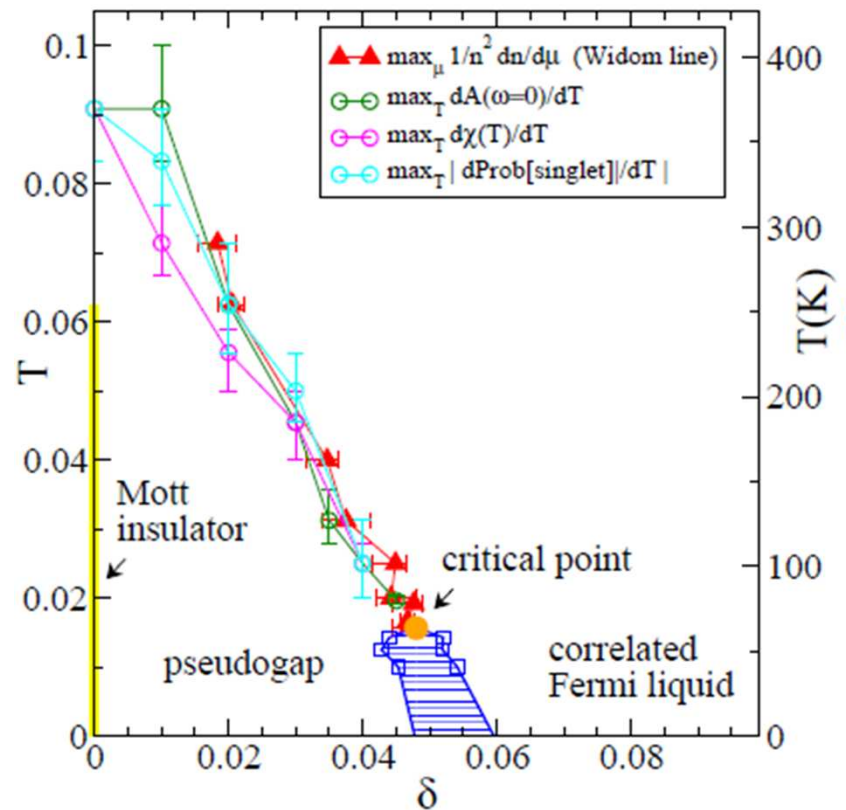
Underdoped Hg1223

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

Plaquette eigenstates



Pseudogap T^* along the Widom line





Giovanni Sordi



Patrick Sémon



Kristjan Haule

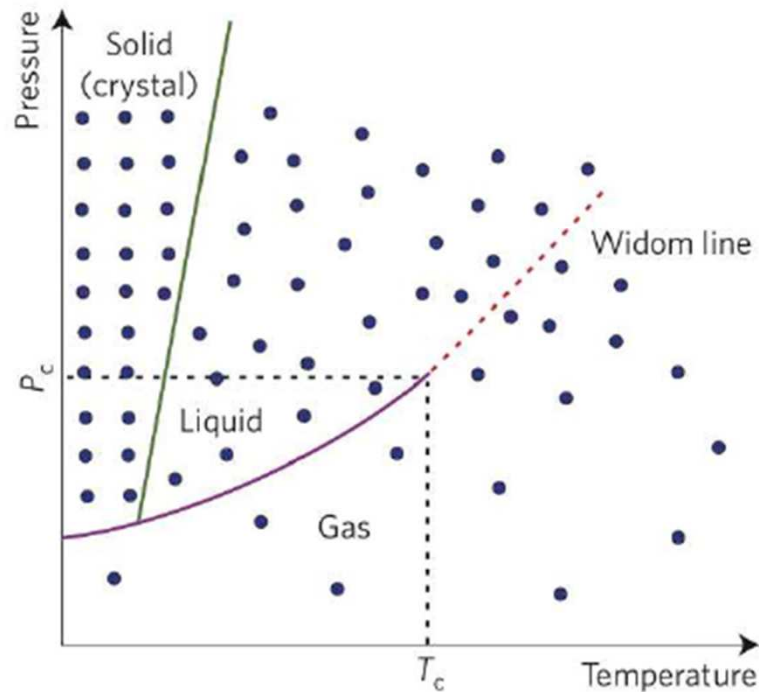
The Wisdom line

arXiv:1110.1392



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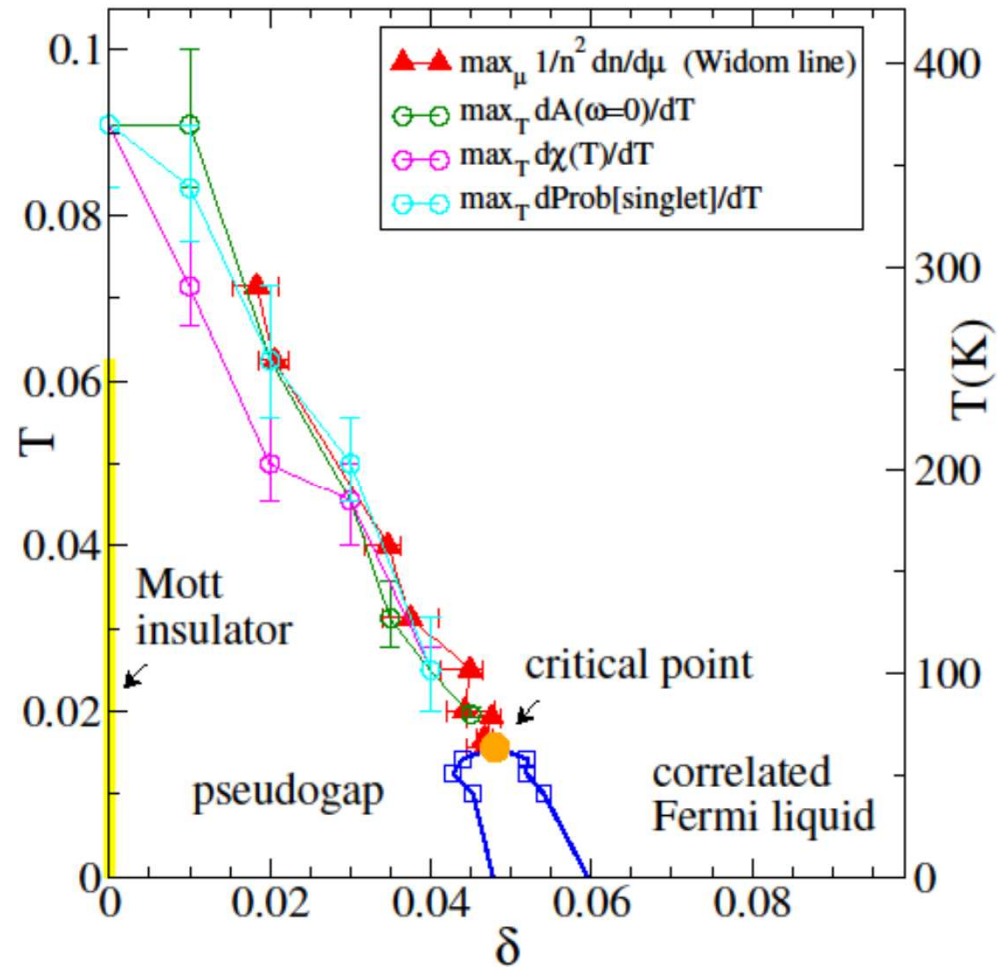
What is the Widom line?



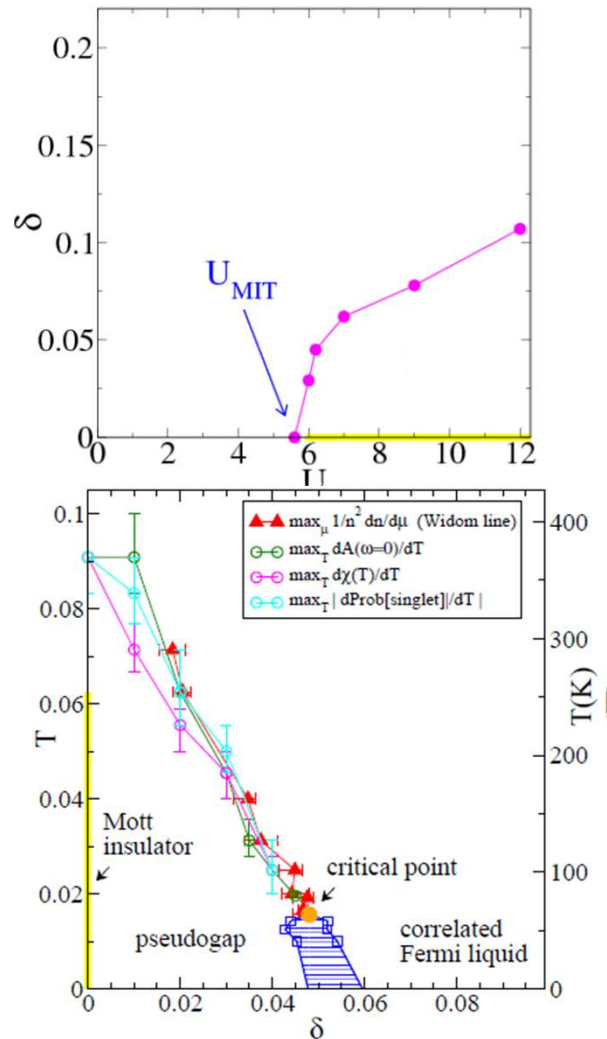
McMillan and Stanley, Nat Phys 2010

- ▶ 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 $T \rightarrow T_p$
- ▶ 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

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?)



Giovanni Sordi



Patrick Sémon



Kristjan Haule

Finite T phase diagram

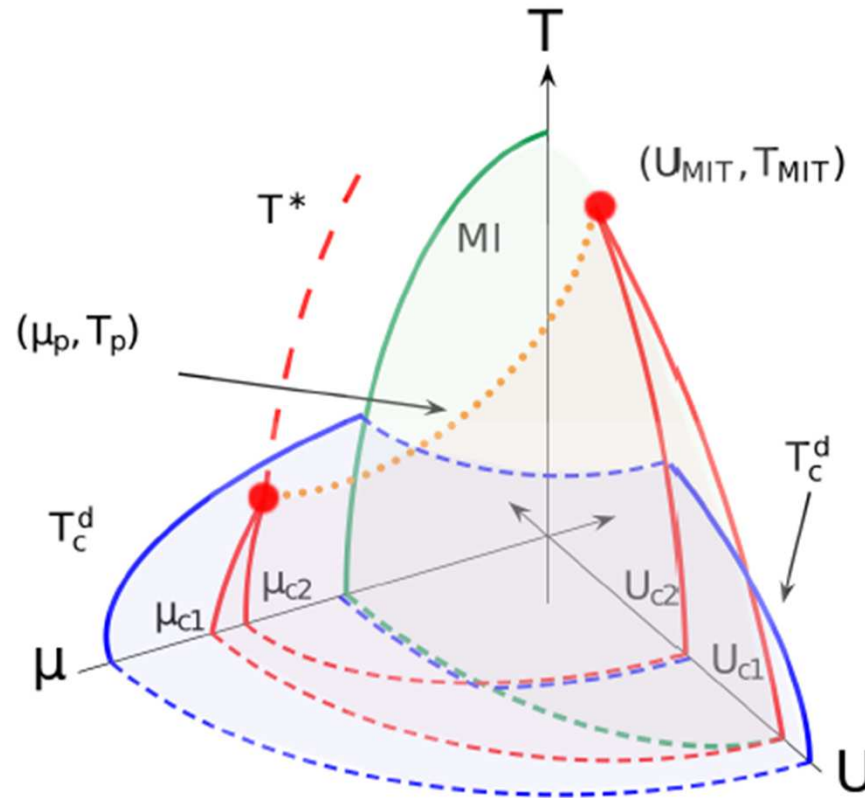
Superconductivity

arXiv:1201.1283v1

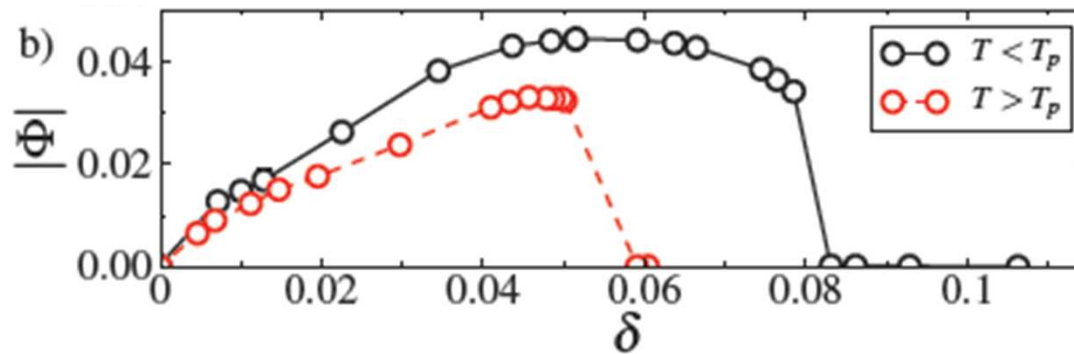


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Unified phase diagram

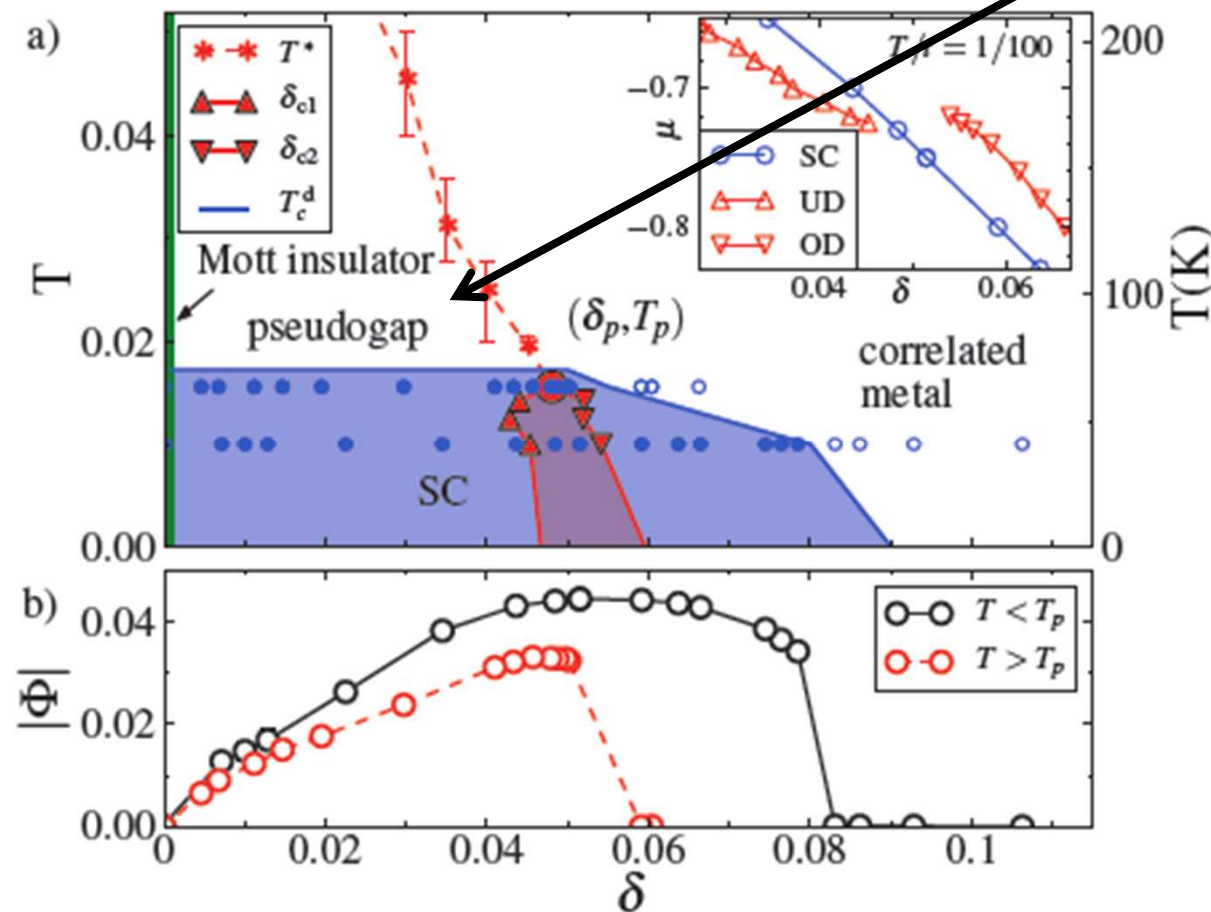


Cuprates (doping driven transition)



Cuprates (doping driven transition)

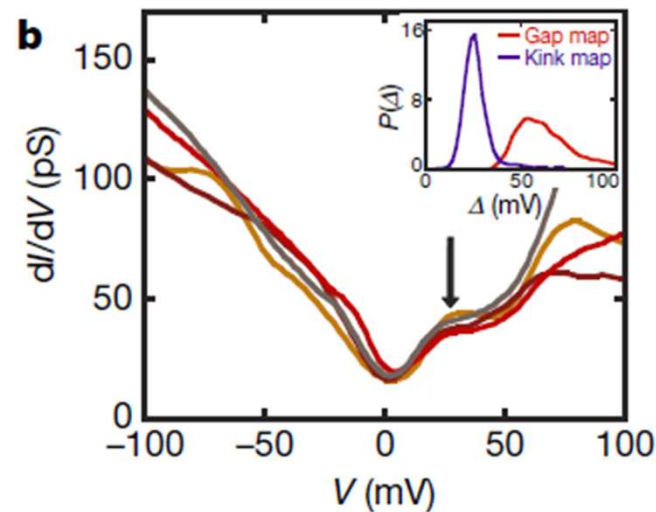
Pseudogap vs pair



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

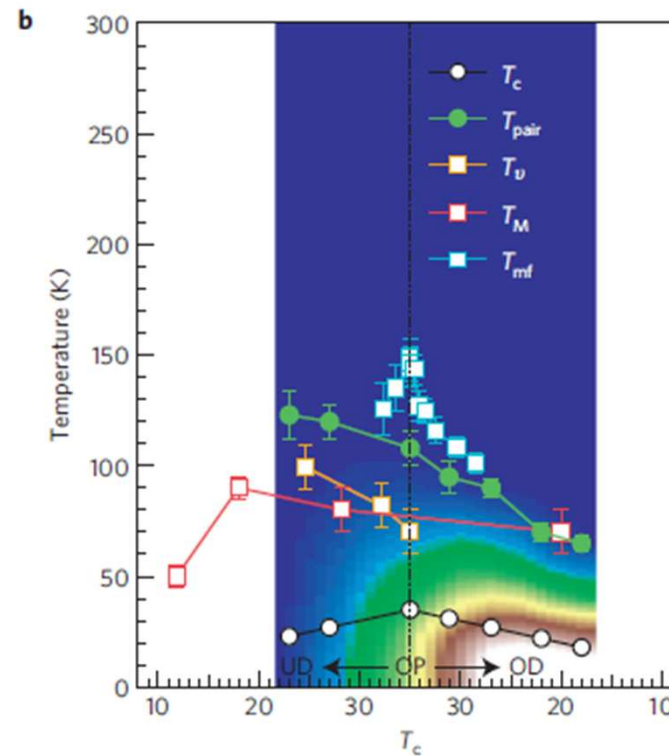
Meaning of T_c^d

- Local pair formation



K. K. Gomes, A. N. Pasupathy, A. Pushp,
S. Ono, Y. Ando, and A. Yazdani,
Nature **447**, 569 (2007)

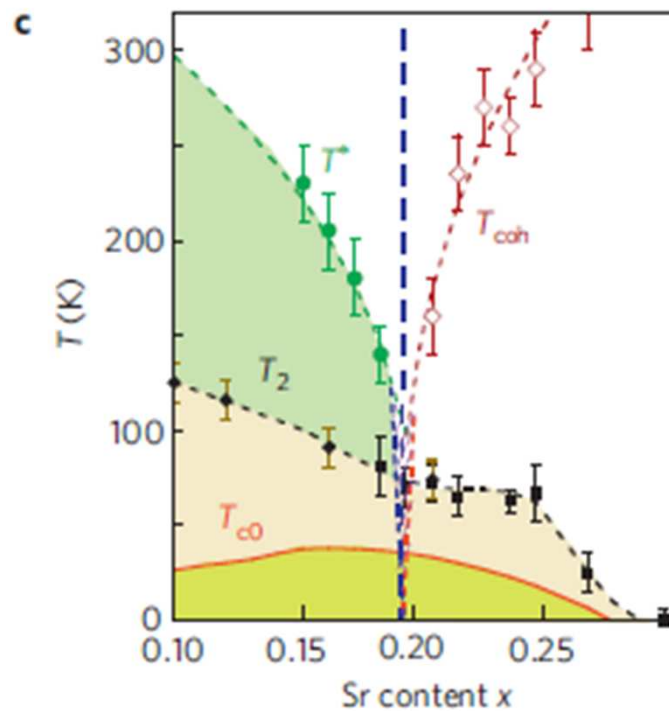
T_{pair}



ARPES
Bi2212

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

$$T_2$$



Magnetoresistance, LSCO
Fluctuating vortices

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



Giant proximity effect

$$T_c = 32 \text{ K}$$
$$T_c < 5 \text{ K}$$

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

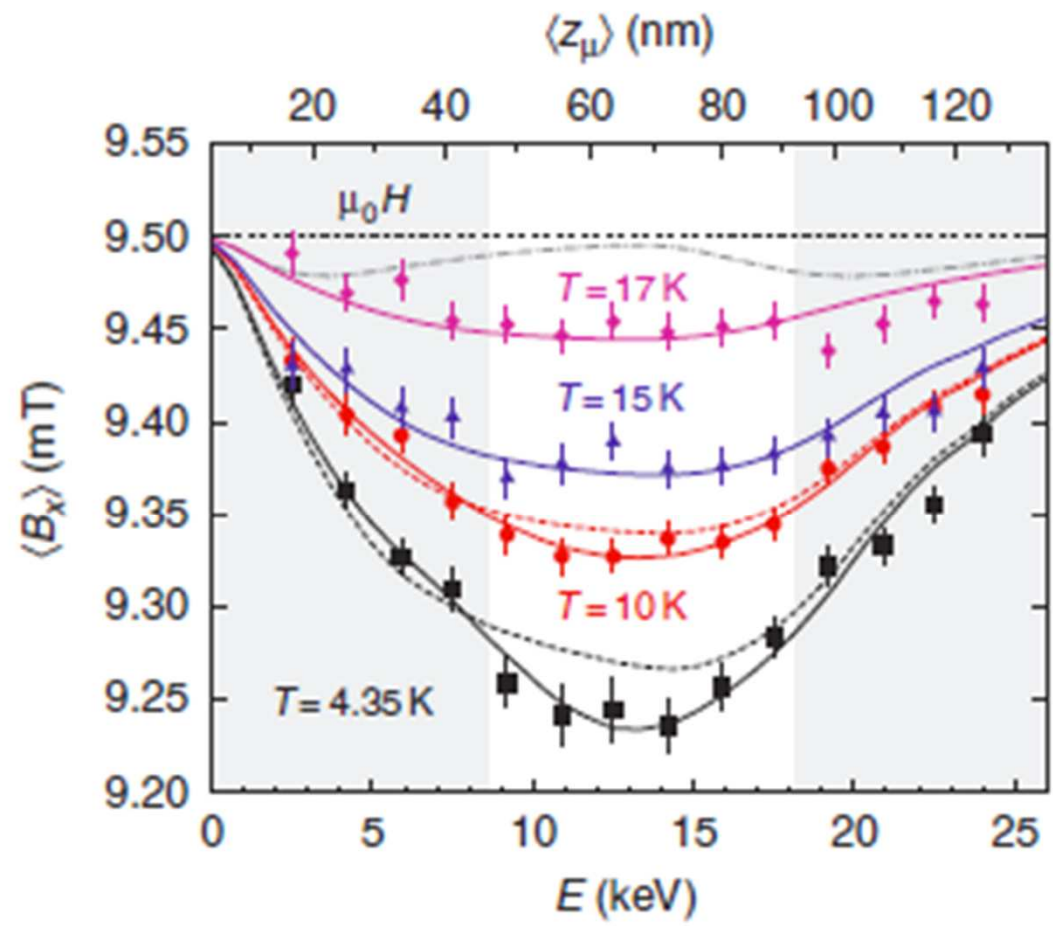


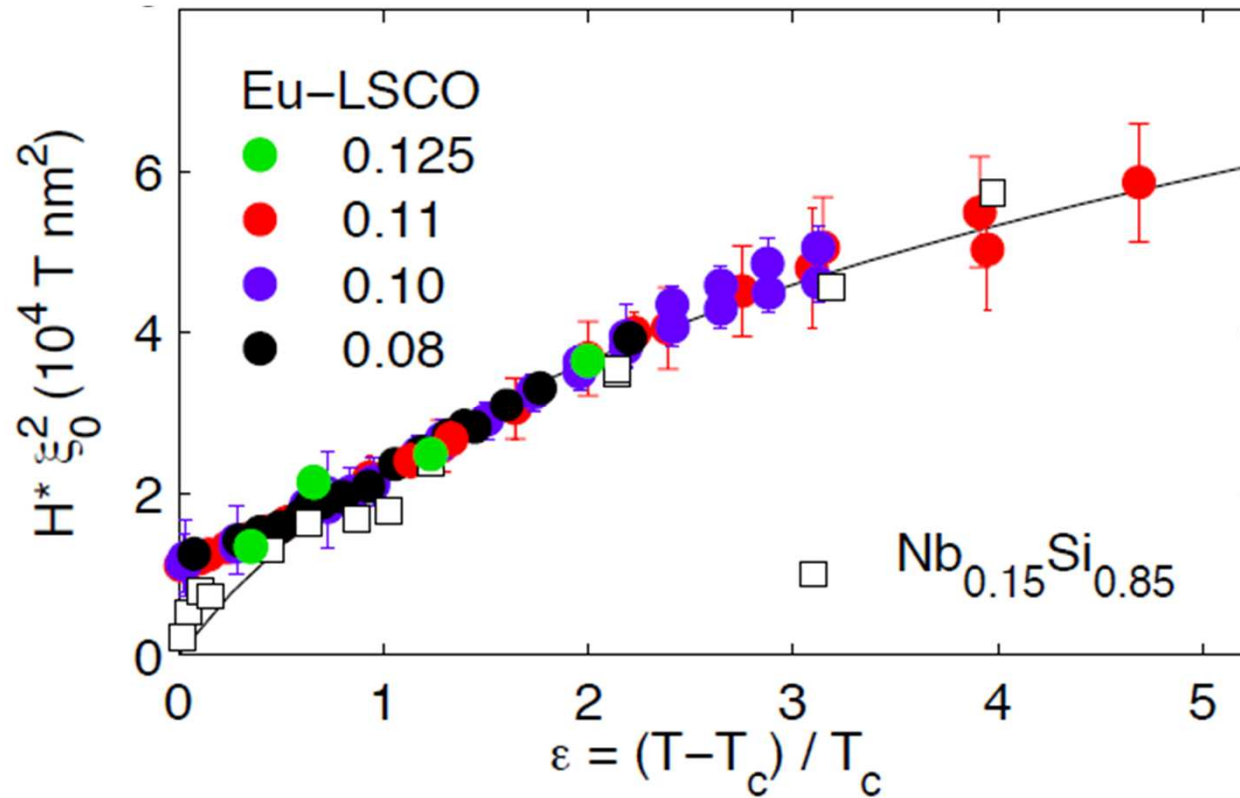
Figure 6 | Depth profile of the local field at different temperatures. The

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

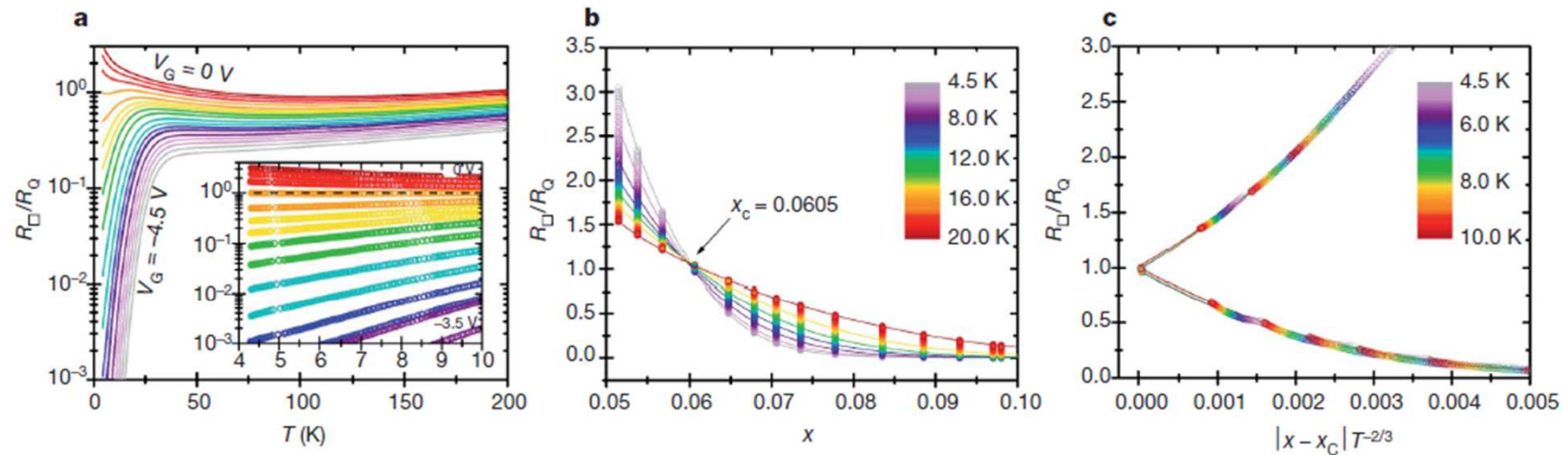
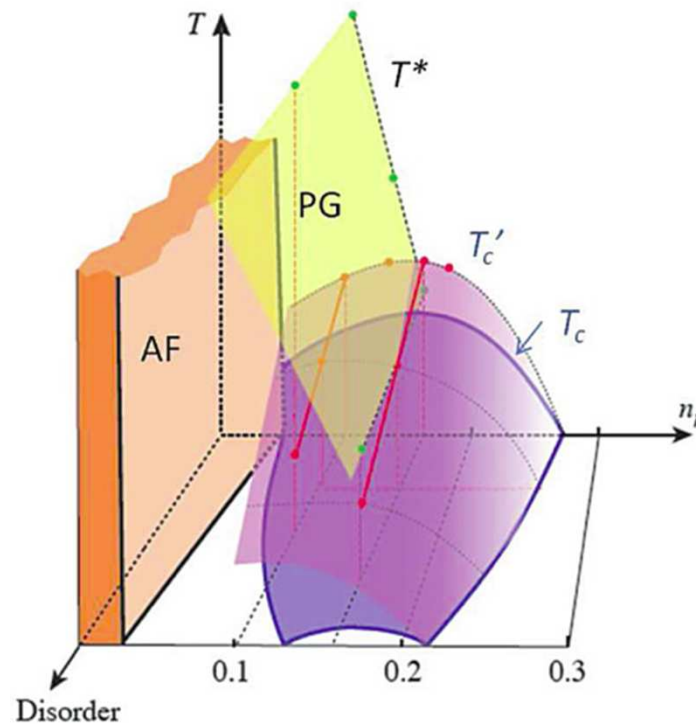


Figure 2 | Superconductor–insulator transition driven by electric field. a, Temperature dependence of normalized resistance $r = R_{\square}(x, T)/R_Q$ of an initially heavily underdoped and insulating film (see Supplementary Fig. 12 for linear scale). The device (Supplementary section B) employs a coplanar 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 $R_{\square}(x_c, T) = R_Q = 6.45$ k Ω . 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 $R_c = 6.45 \pm 0.10$ k Ω . 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 K $< T < 10$ 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

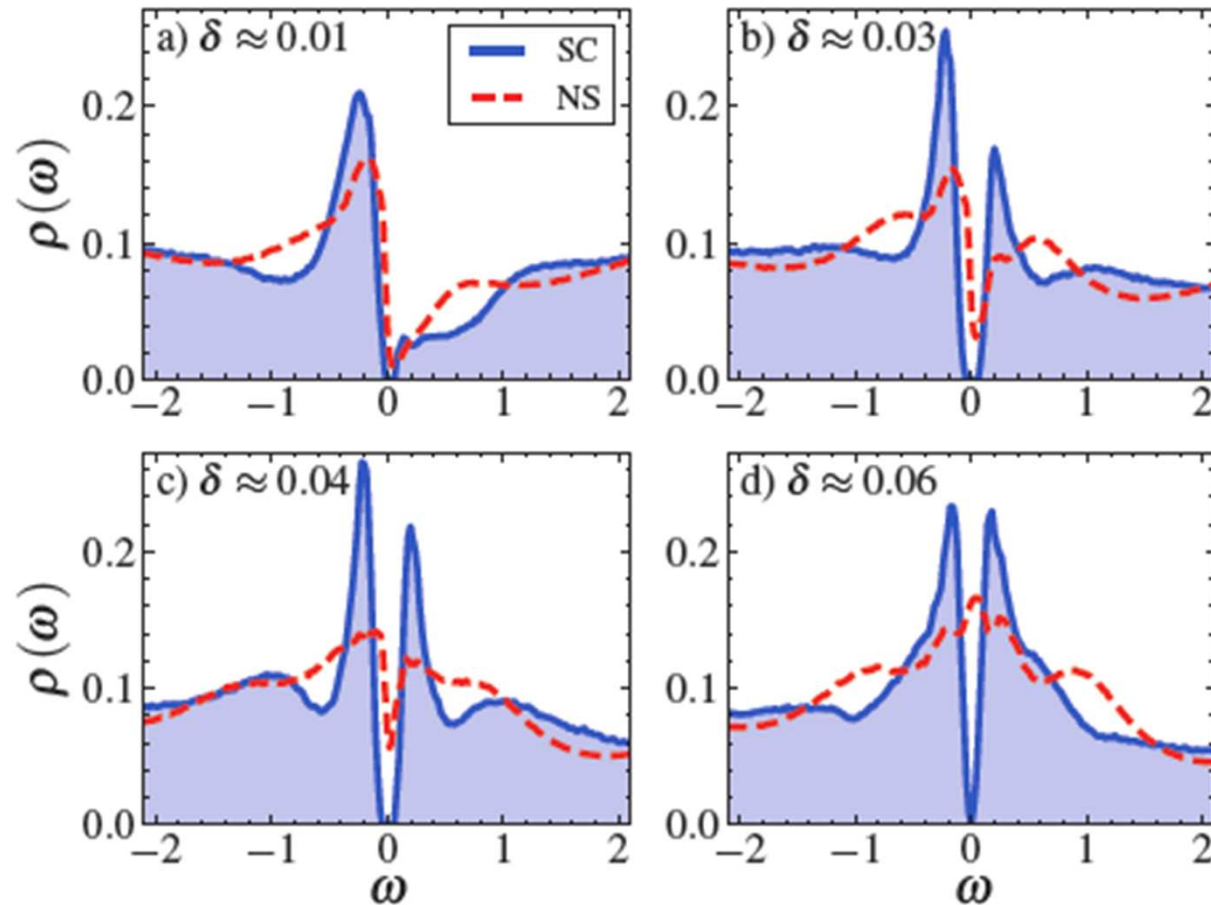


F. Rullier-Albenque, H. Alloul, and G. Rikken,
Phys. Rev. B **84**, 014522 (2011).

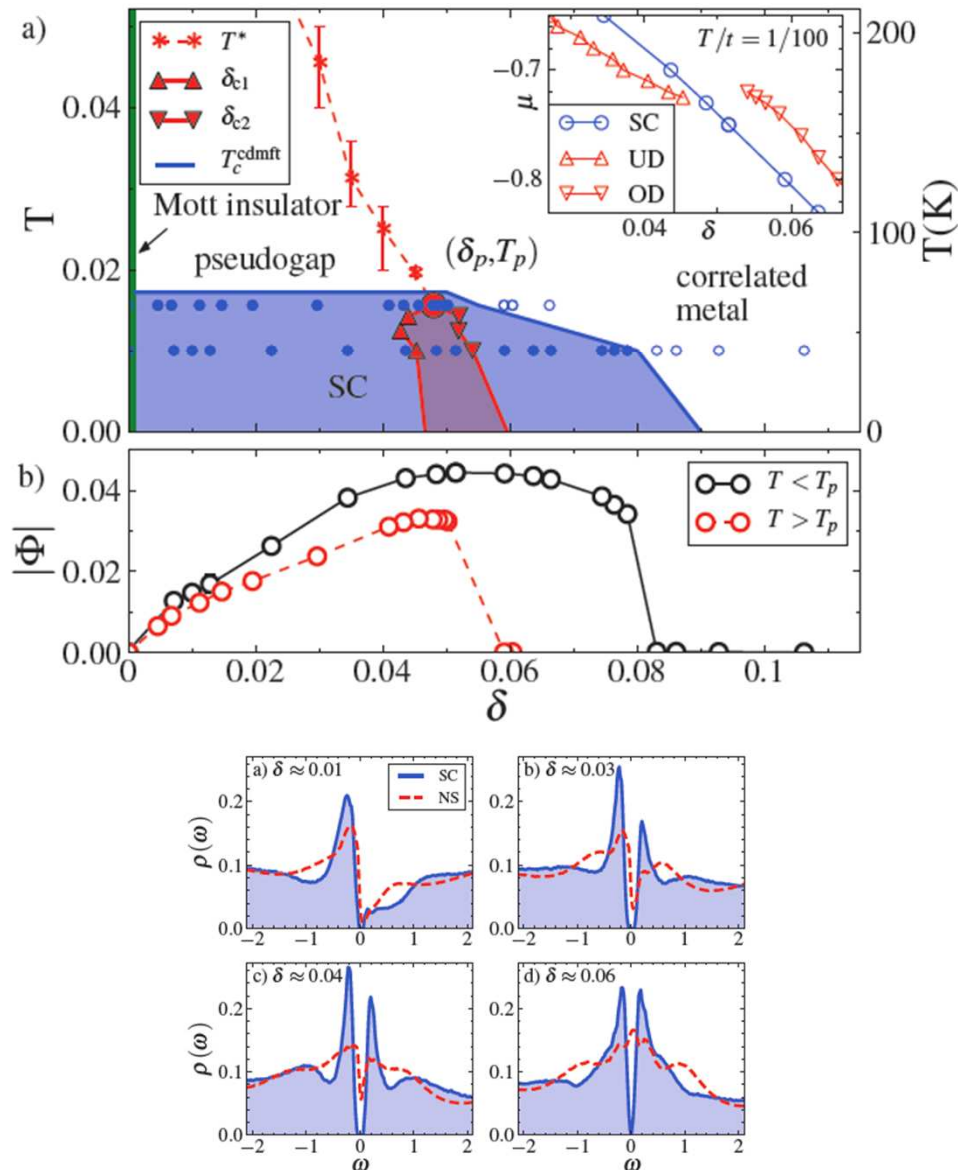
Superconductivity in underdoped vs BCS



First-order transition leaves its mark

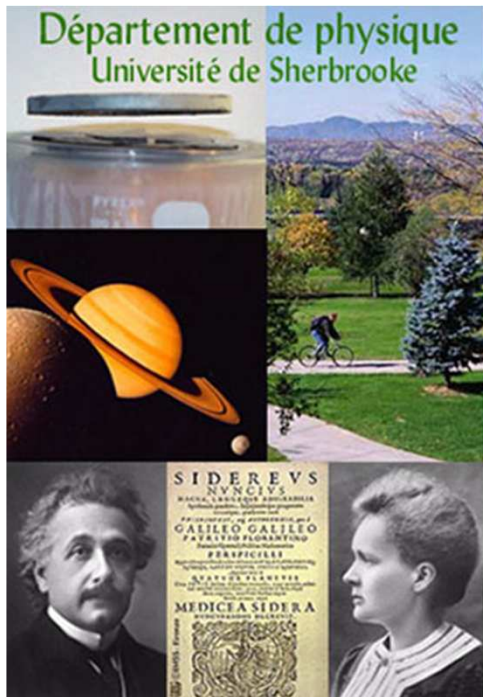


Summary



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

André-Marie Tremblay



Le regroupement québécois sur les matériaux de pointe



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Merci

Thank you

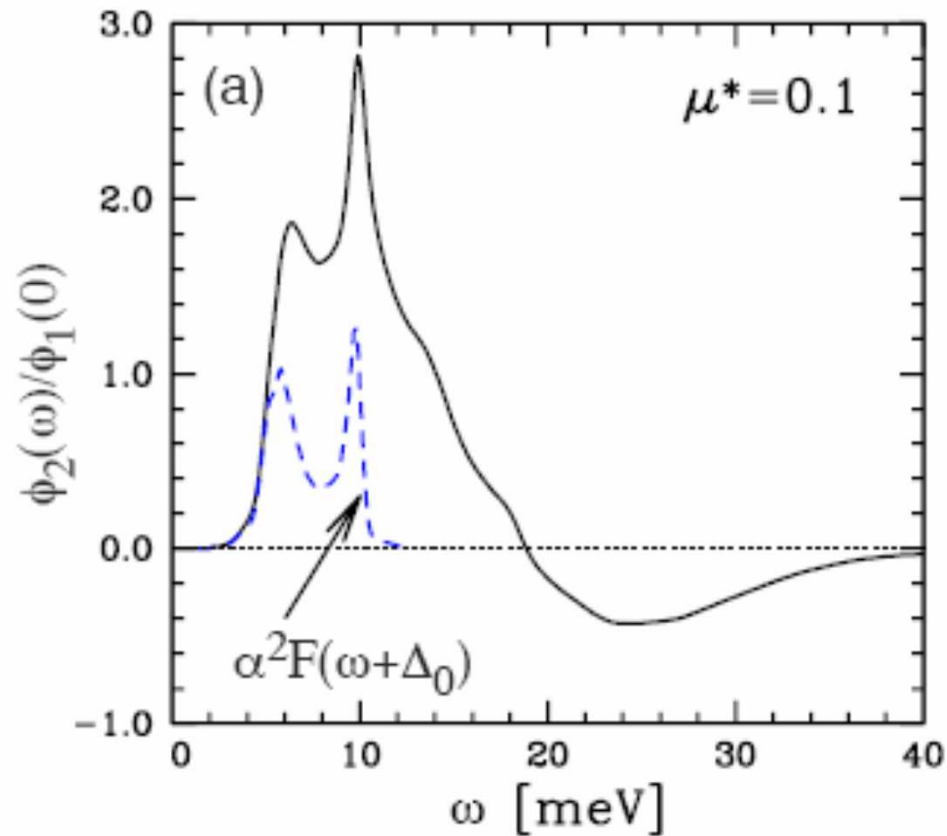
$T = 0$ phase diagram

The glue



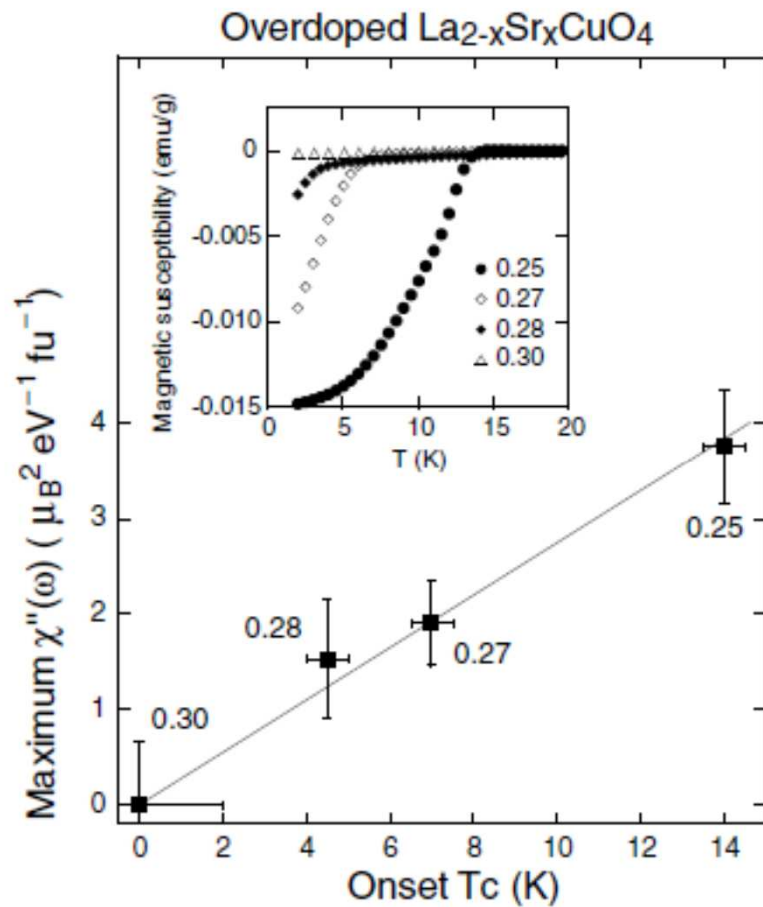
$\text{Im } \Sigma_{\text{an}}$ and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

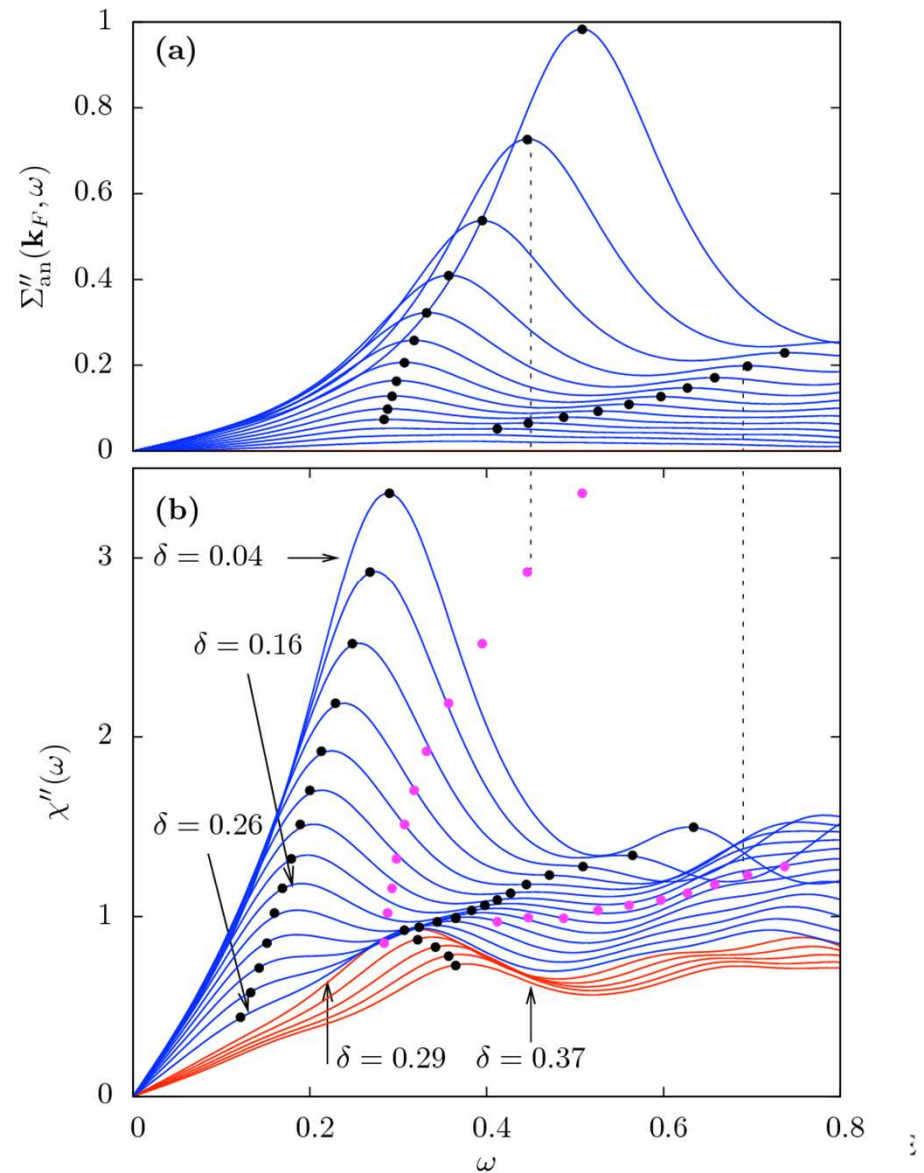


The glue

Kyung, S  n  chal, Tremblay, Phys. Rev. B
80, 205109 (2009)



Wakimoto ... Birgeneau
 PRL (2004)



The glue and neutrons

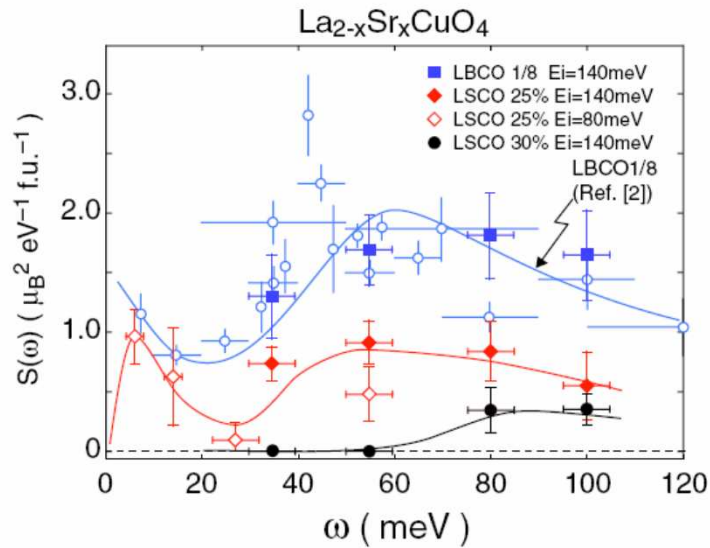


FIG. 3 (color online). $\mathbf{Q}$ -integrated dynamic structure factor $S(\omega)$ which is derived from the wide- H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i = 140$ meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$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

