CIFAR five year Review, May 2012

A.-M. Tremblay

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CANADIAN INSTITUTE
for ADVANCED RESEARCH

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VERITATEM IN CHARITATE

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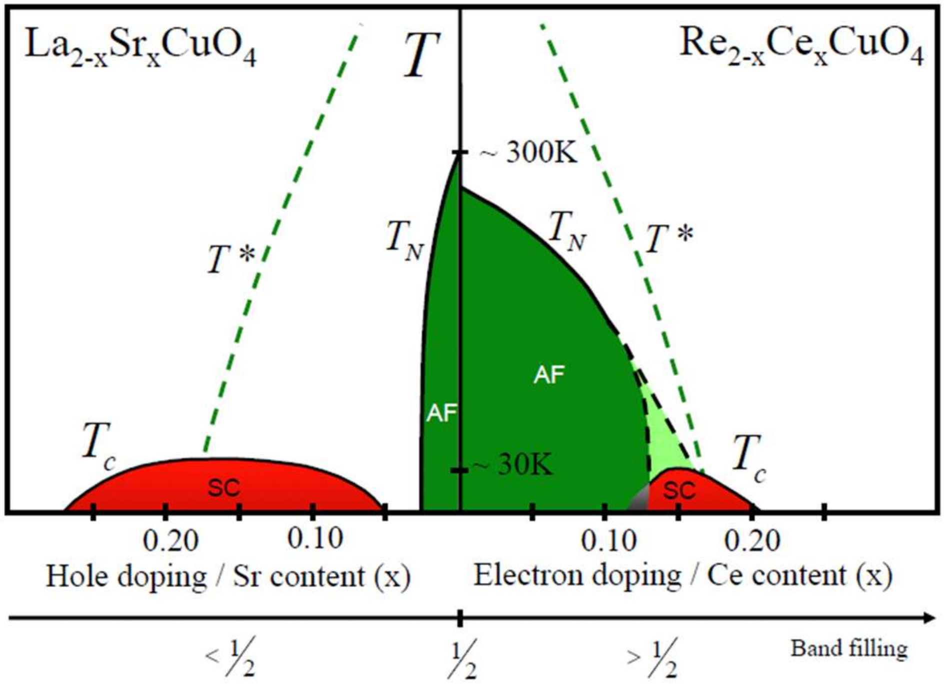
High-temperature superconductors

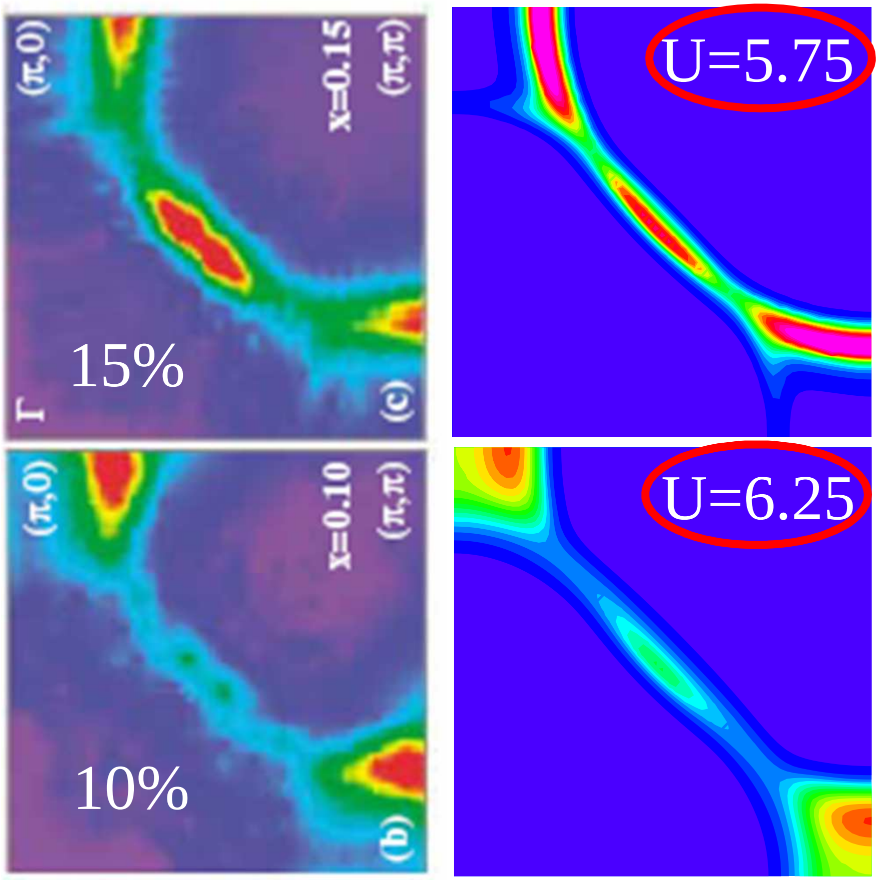
Armitage, Fournier, Greene, RMP (2009)



- 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) ...

Fermi surface plots

Hubbard repulsion *U* has to…



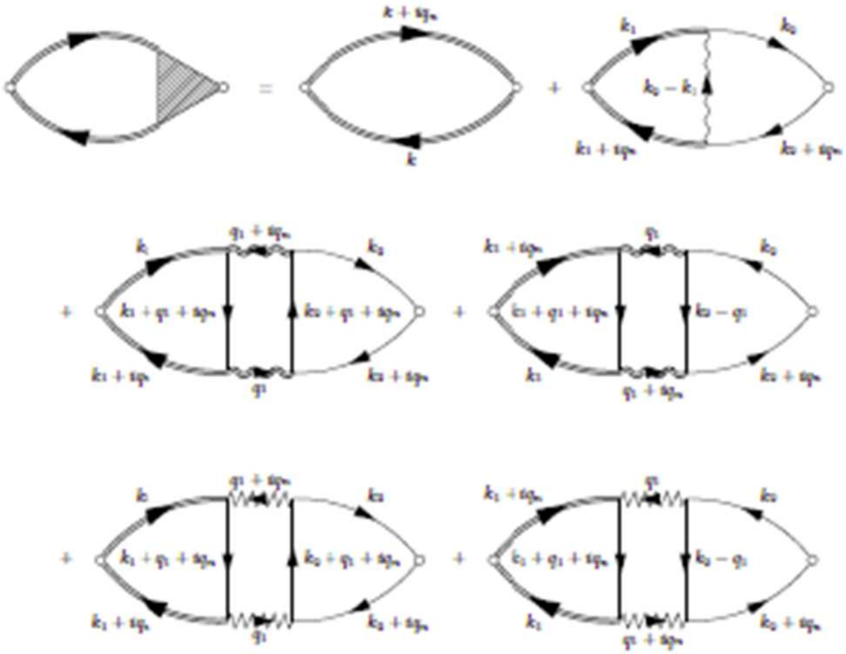
be not too large

increase for
smaller doping

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

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

Resistivity (TPSC)

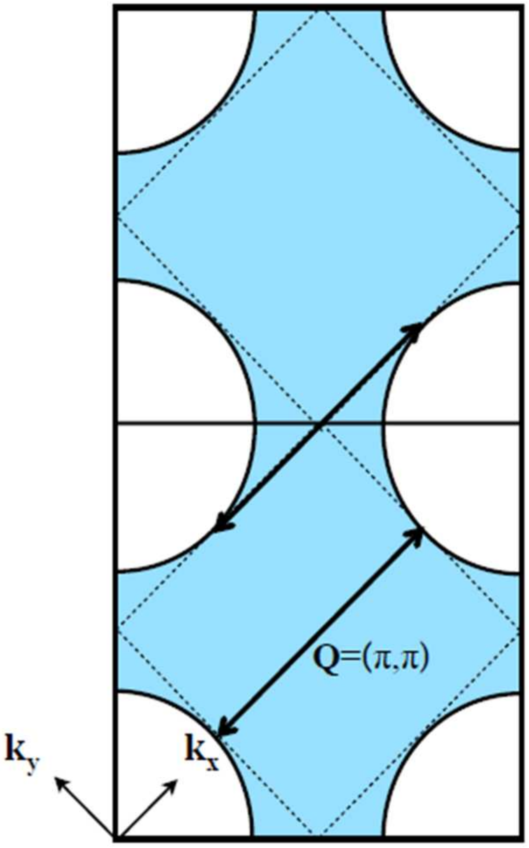


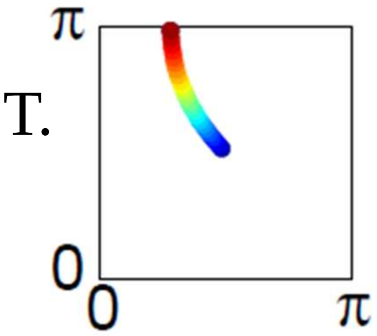
Dominic Bergeron

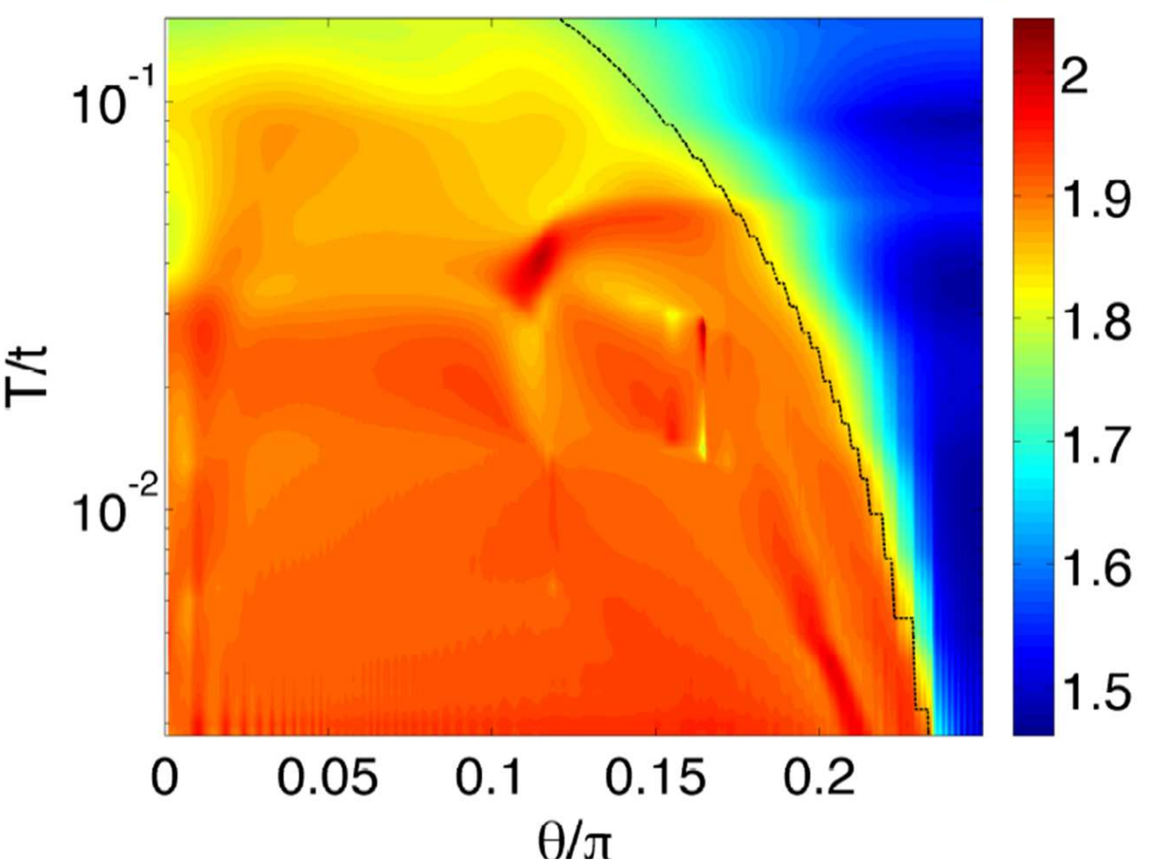
D. Bergeron, V. Hankevych, B. Kyung, and A.-M.S.T.
Phys. Rev. B **84**, 085128/1-35 (2011) (35 pages).

Im Σ for e-doped QCP (TPSC)

D. Bergeron, D. Chowdury, M. Punk, S. Sachdev, A.-M.S.T.

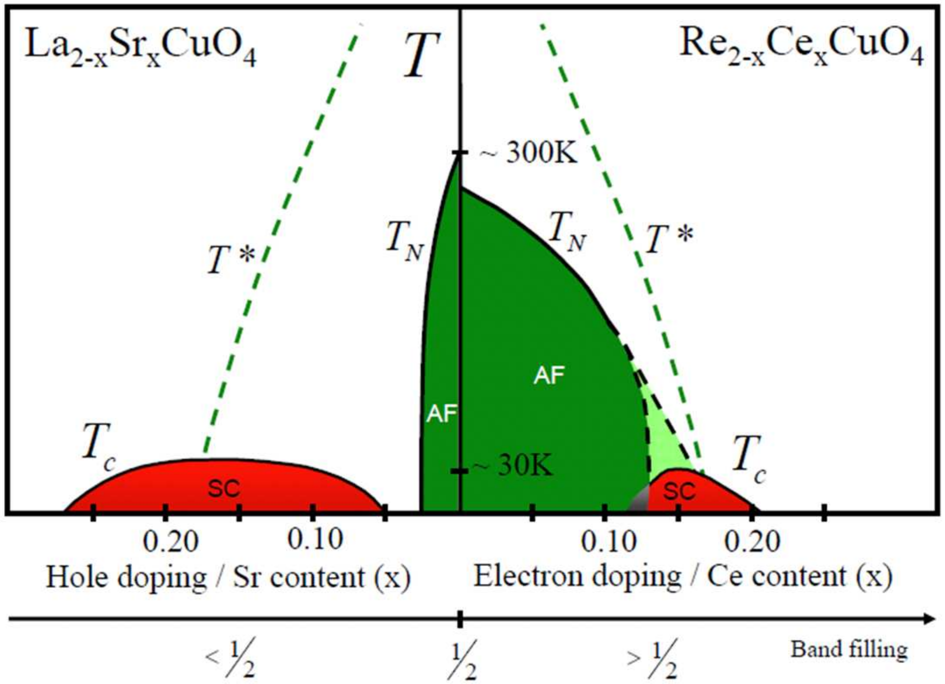






High-temperature superconductors

Armitage, Fournier, Greene, RMP (2009)



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

- 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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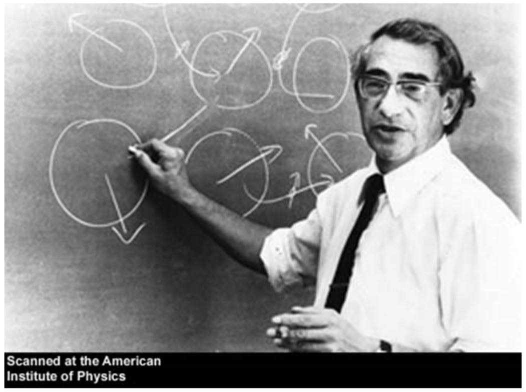
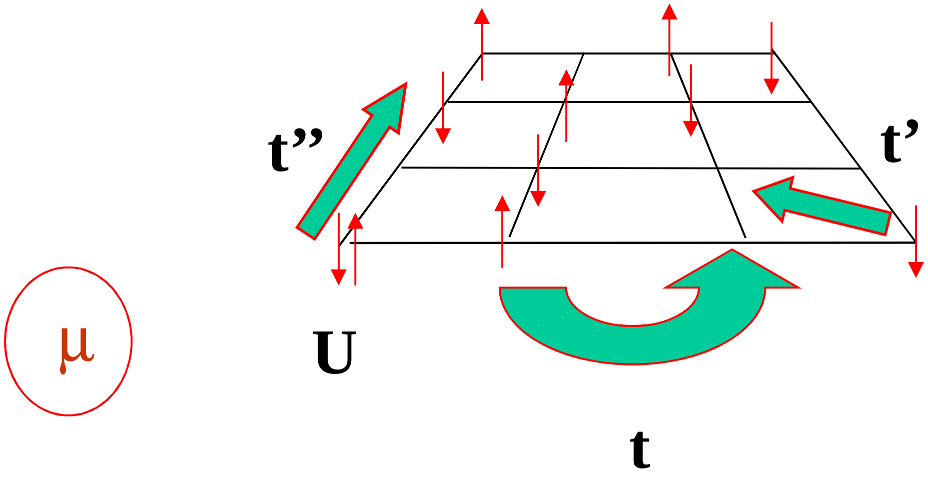
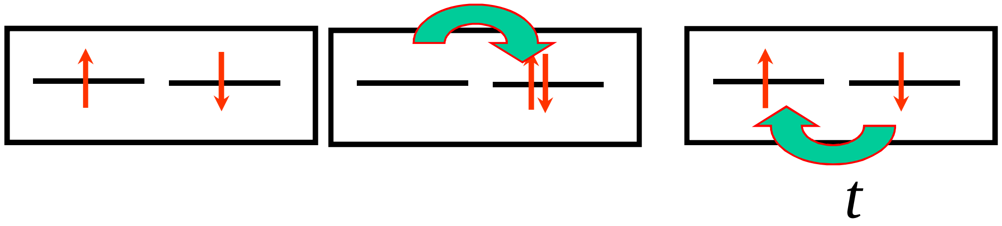
Hubbard model


Scanned at the American Institute of Physics

1931-1980



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



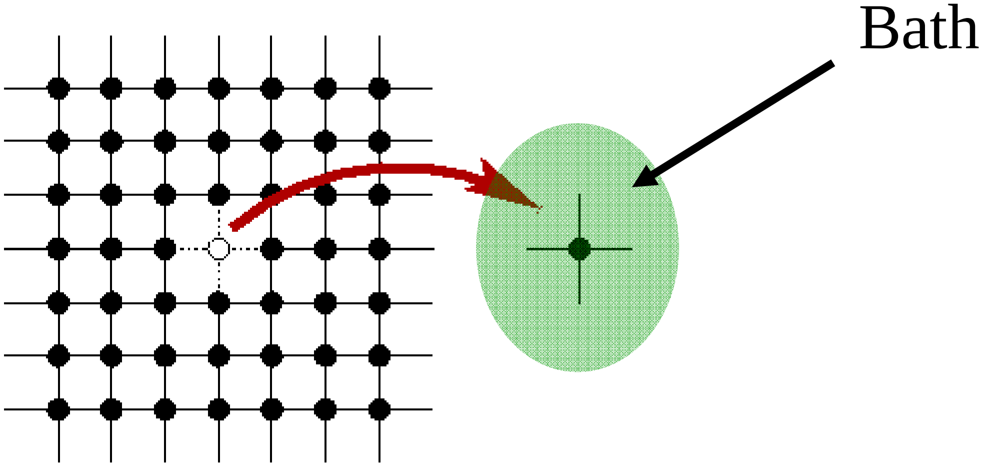
$t = 1$

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

Method

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

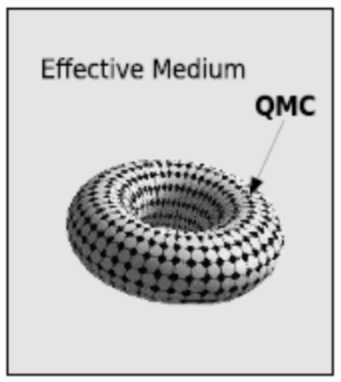
- Compute scattering rate (self-energy) of impurity problem.
- Use that self-energy (ω dependent) for lattice.
- Project lattice on single-site and adjust bath so that single-site DOS obtained both ways be equal.



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

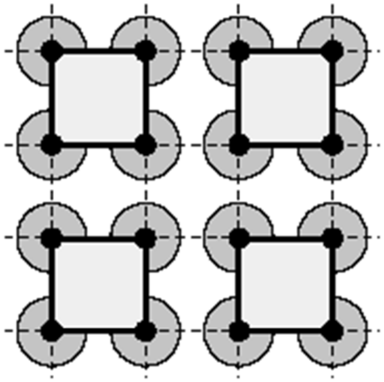
DMFT, (*d = 3*)

2d Hubbard: Quantum cluster method

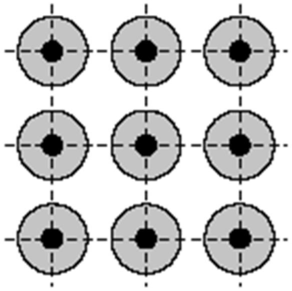


DCA

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)

Not perfect!

- Missing:
  - Long wavelength fluctuations
- Included:
  - Short-range dynamical and spatial correlations

- Long range order:
  - Allow symmetry breaking in the bath (mean-field)

Outline

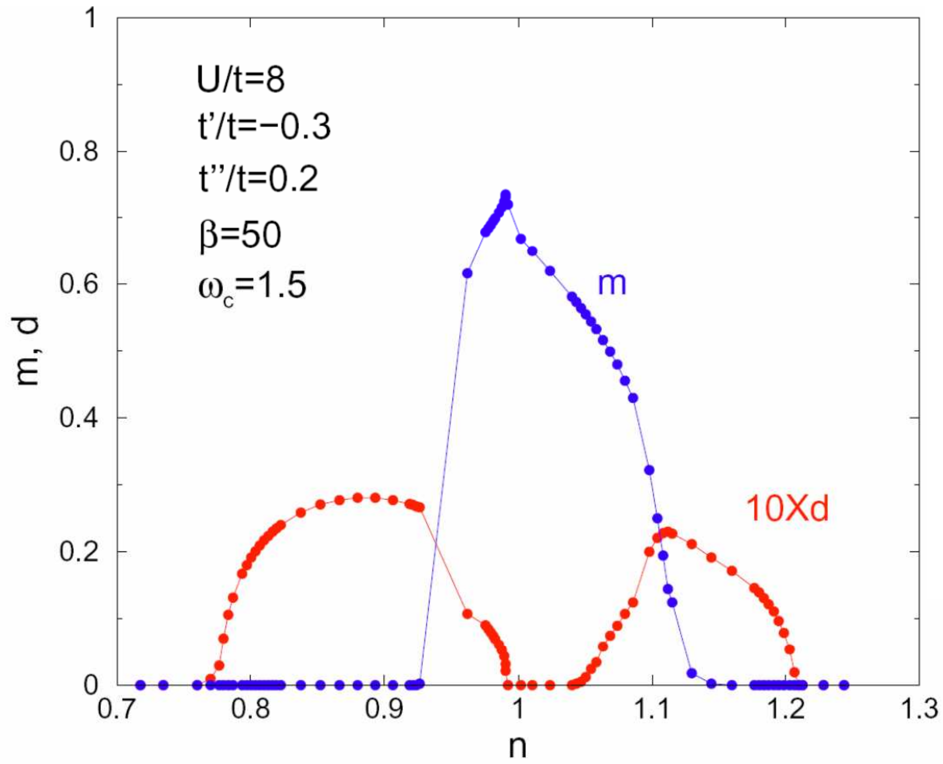
- Method
- *T=0* phase diagram with competing order
- Finite *T* phase diagram
  - – Normal state (no LRO, what is below the dome)
    - First order transition
    - Widom line and pseudogap
  - – Superconductivity

T = 0 phase diagram: cuprates

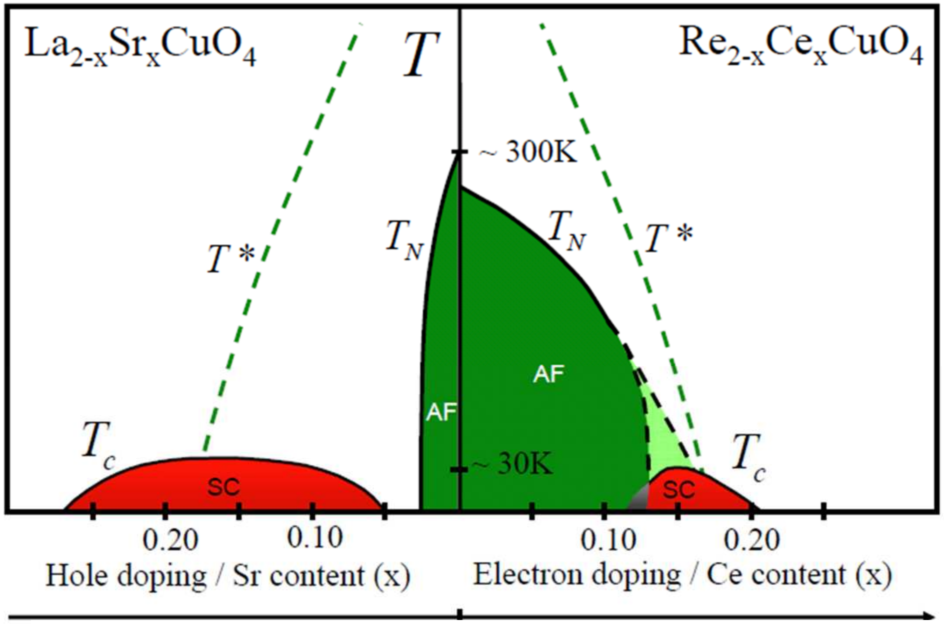
Phase diagram

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

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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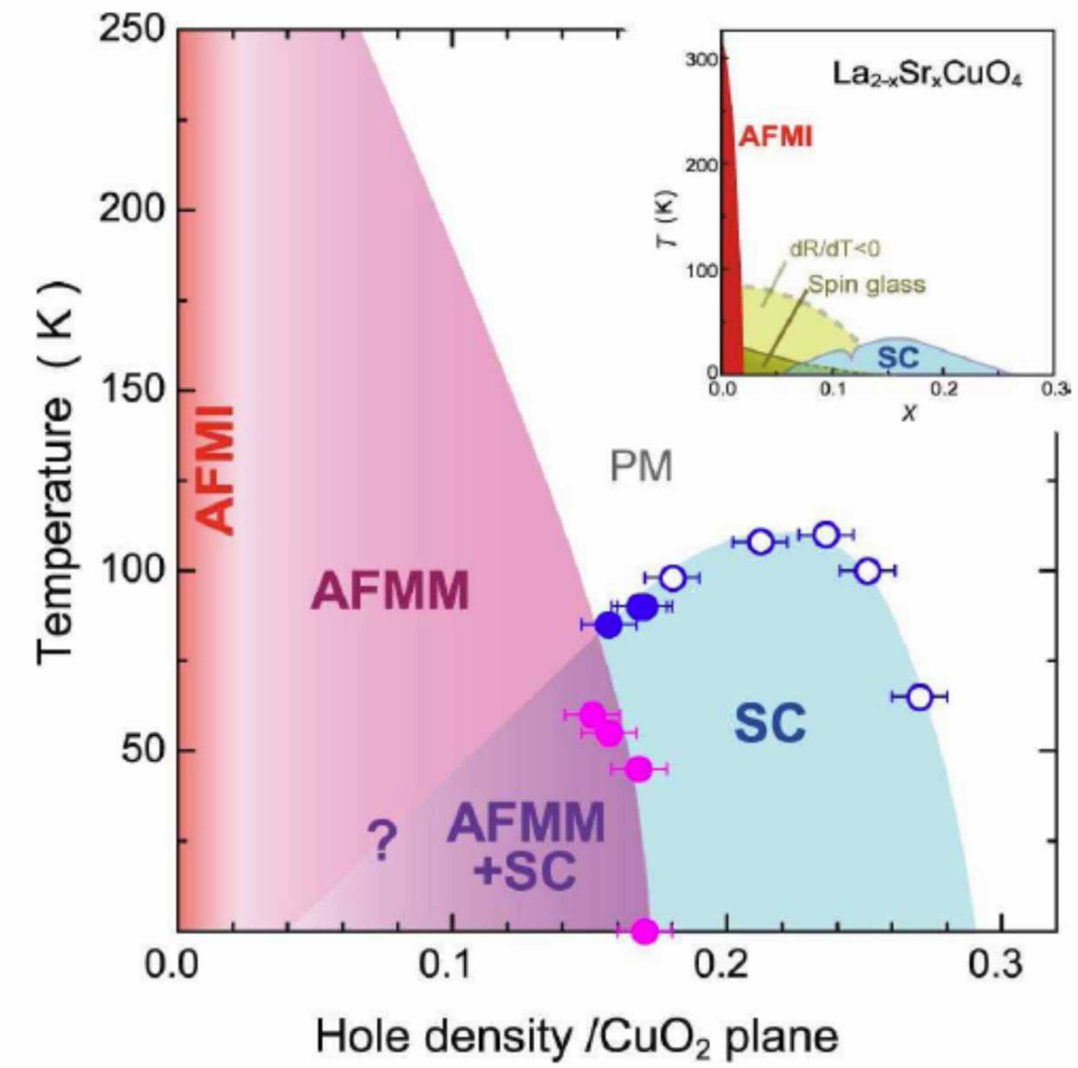
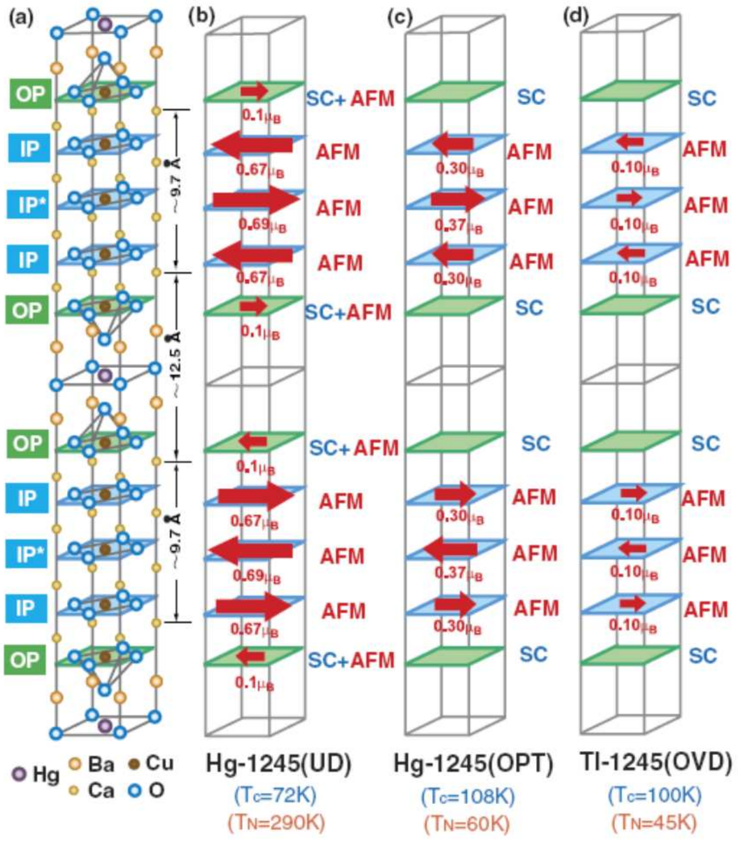
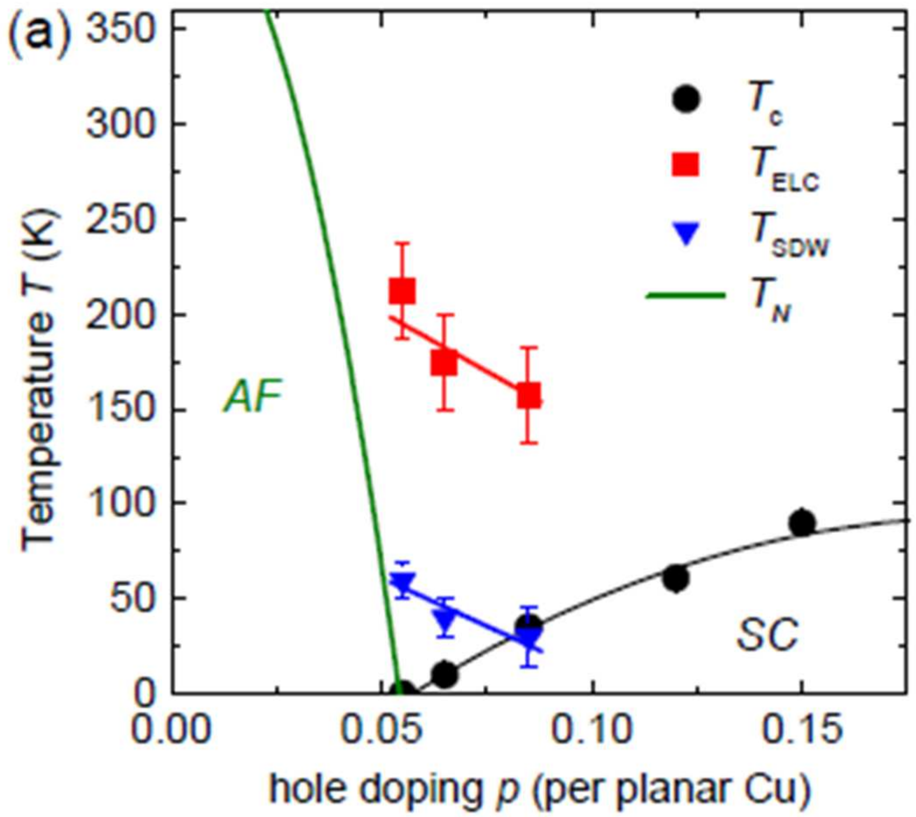
Consistent with following experiments

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





Magnetic phase diagram of YBCO



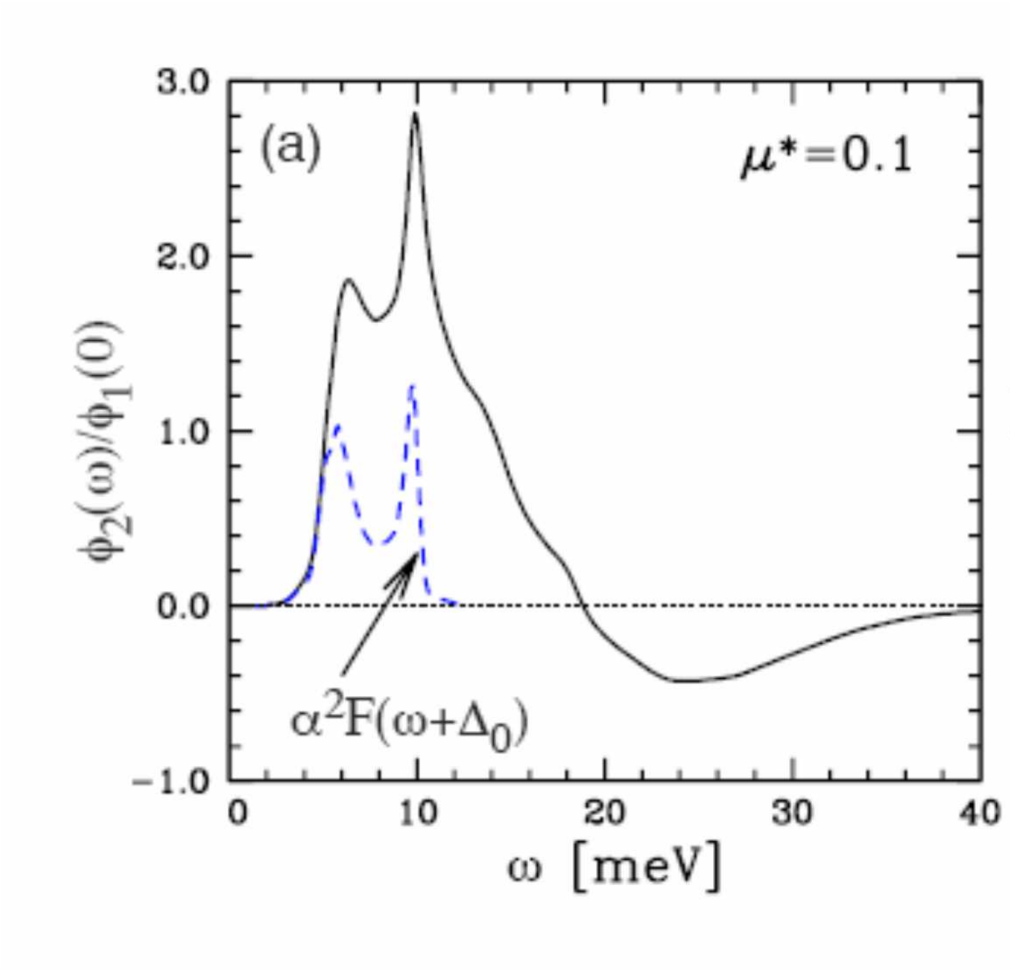
Haug, … Keimer, New J. Phys. 12, 105006 (2010)

$T = 0$ phase diagram

The glue

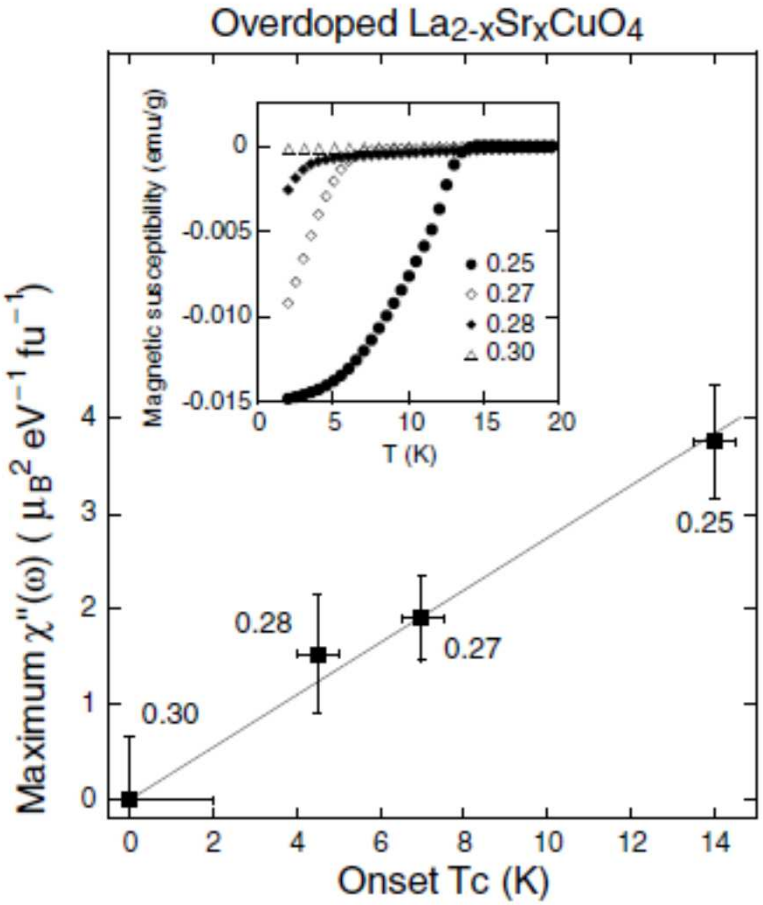
Im Σ_{an} and electron-phonon in Pb

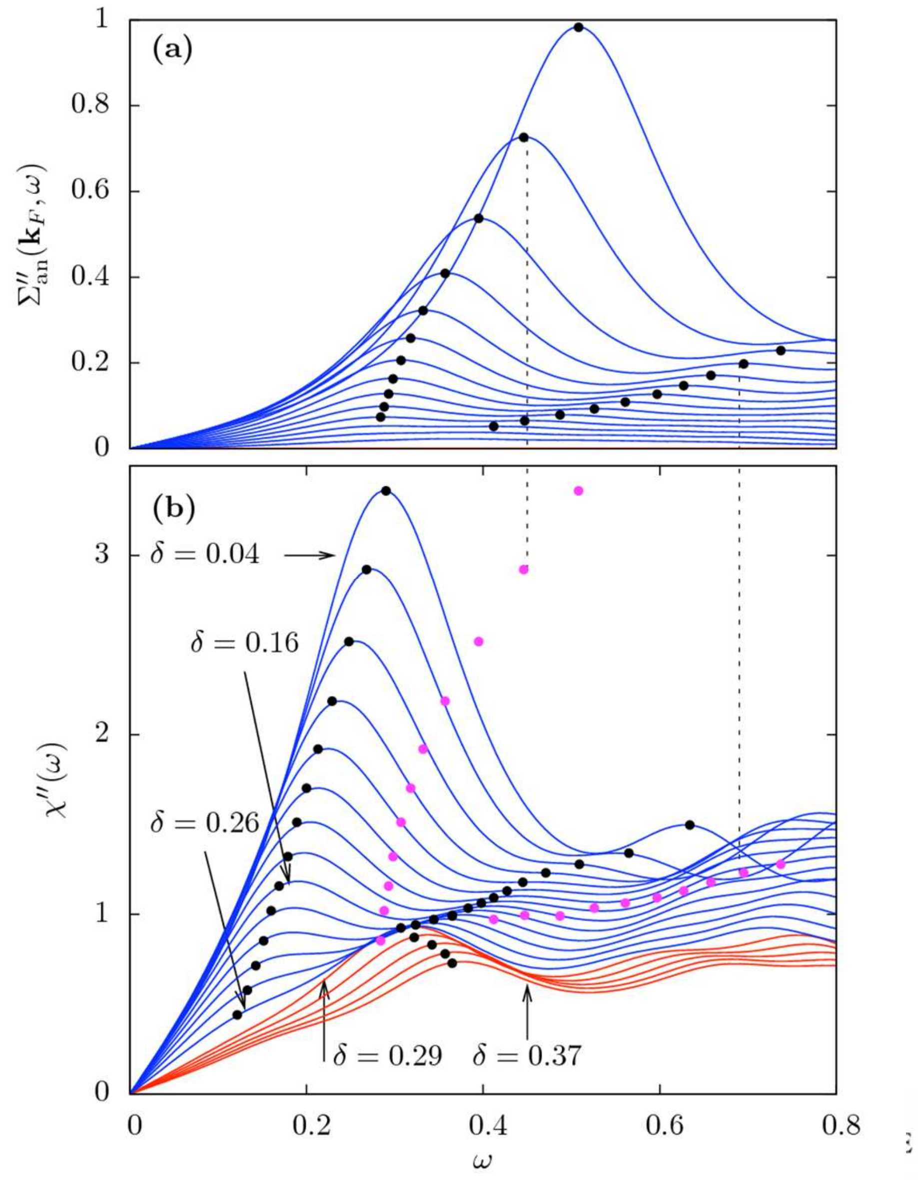
Maier, Poilblanc, Scalapino, PRL (2008)



The glue

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





Wakimoto … Birgeneau PRL (2004)

The glue and neutrons

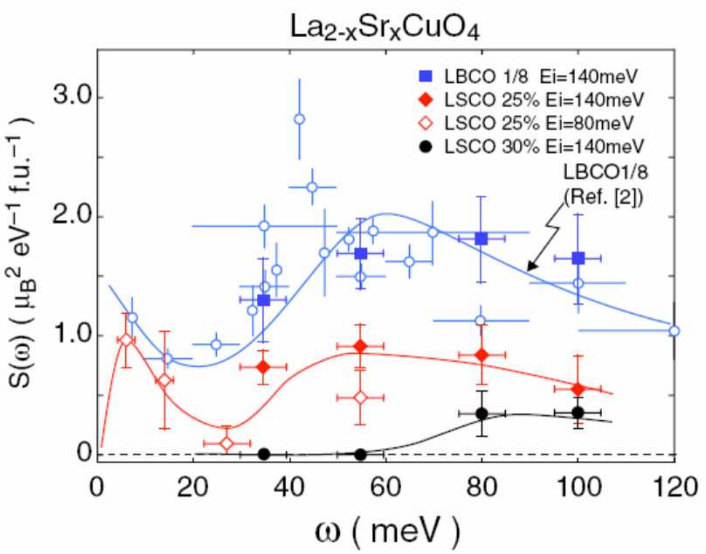
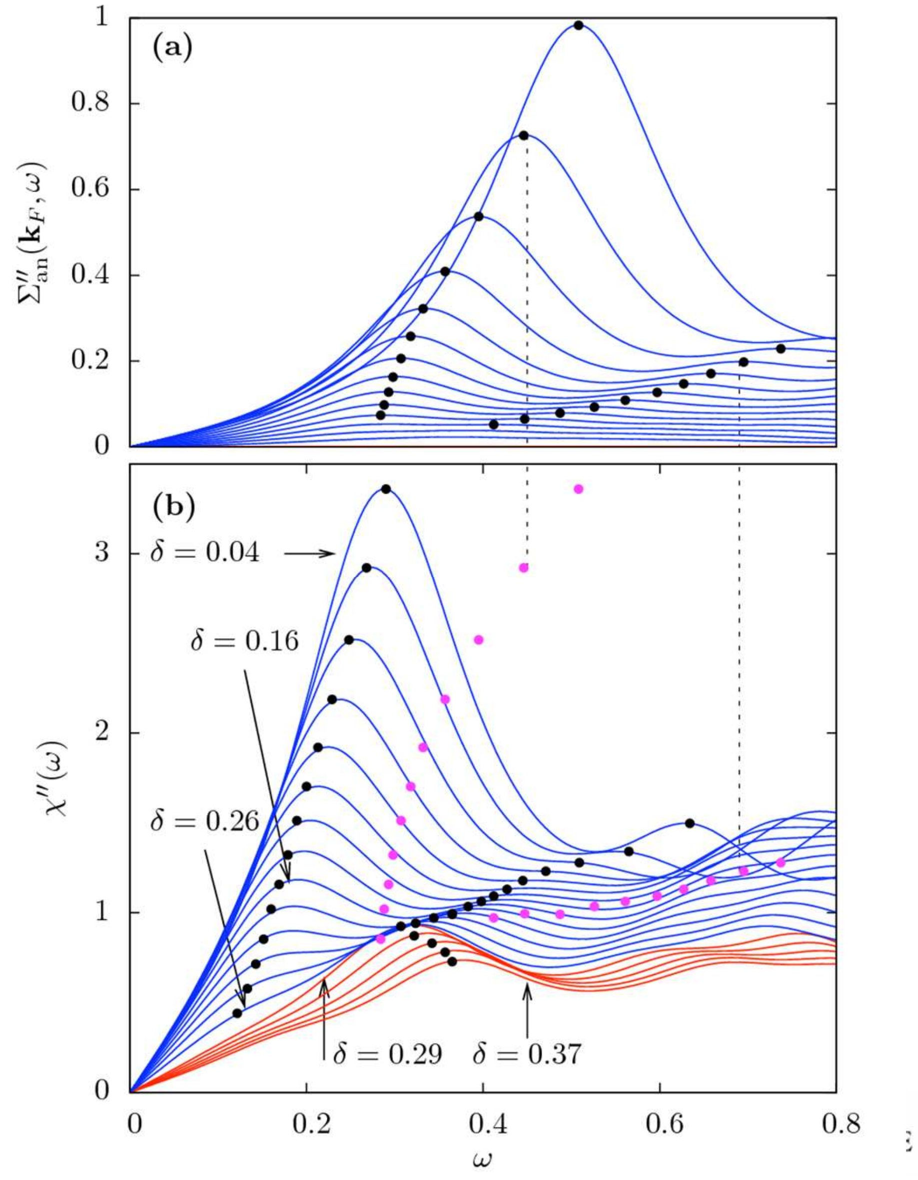


FIG. 3 (color online). **Q**-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for E_i = 140 meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO 1/8 (open circles) from [2]. The solid lines following data of LSCO $x = 0.25$ and 0.30 are guides to the eyes.



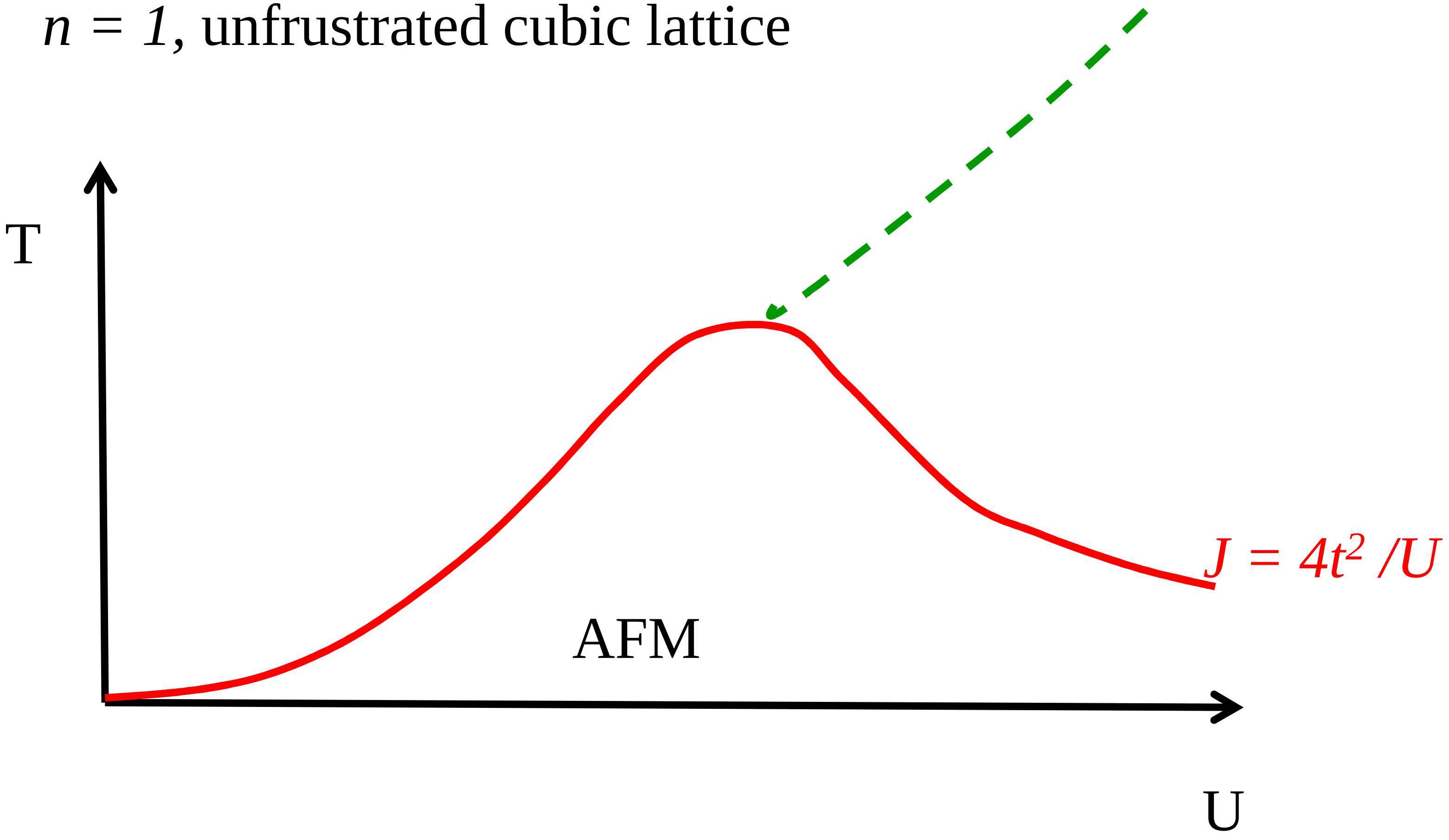
Wakimoto … Birgeneau PRL (2007);
PRL (2004)

Finite temperature

The Mott transition

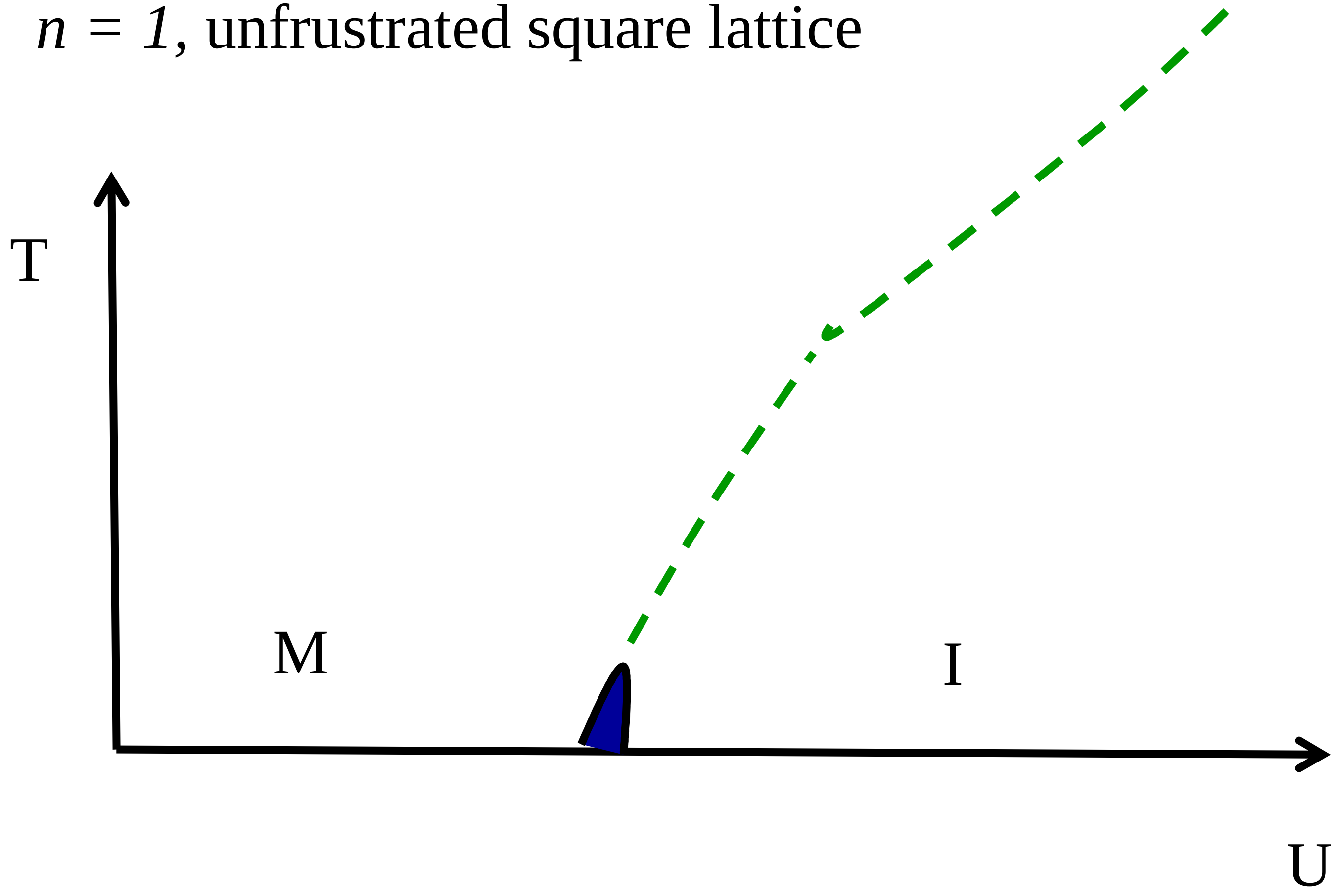
Local moment and Mott transition

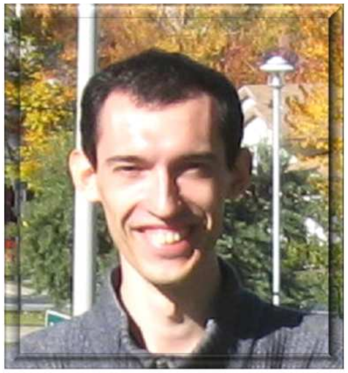
n = *1*, unfrustrated cubic lattice



Local moment and Mott transition

n = *1*, unfrustrated square lattice

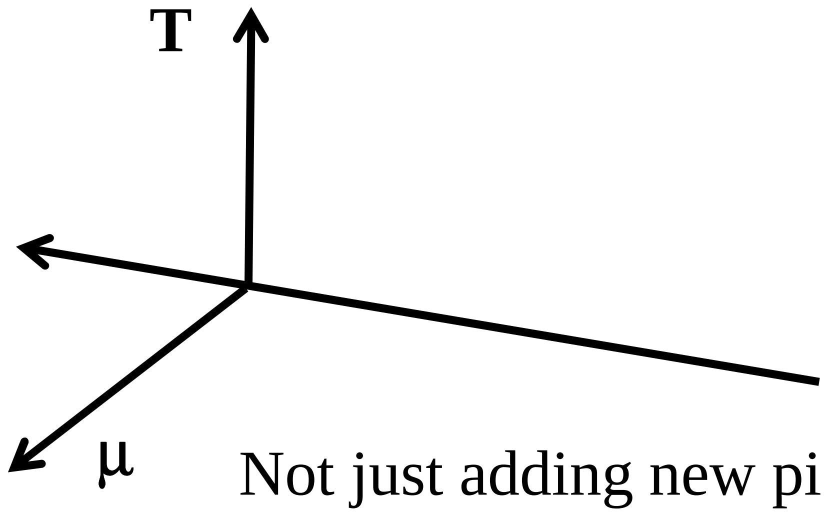




Giovanni Sordi

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

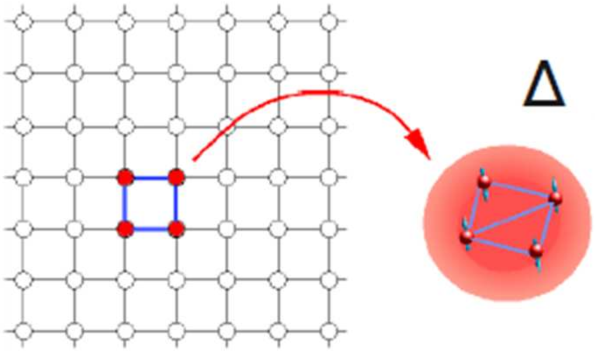
Doping-induced Mott transition ($t'=0$)



Kristjan Haule

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

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

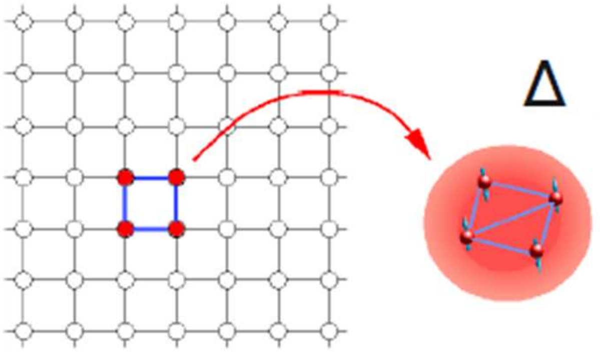
P. Werner, PRL 2006
P. Werner, PRB 2007
K. Haule, PRB 2007

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

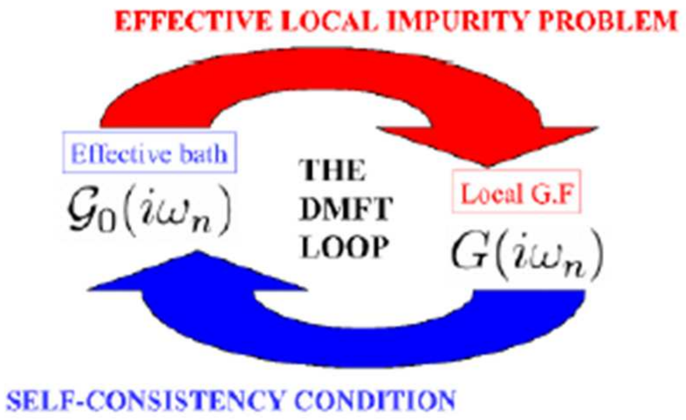
P. Werner, A. Comanac, L. de' Medici, M. Troyer, and A. J. Millis, Phys. Rev. Lett. **97**, 076405 (2006).

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

C-DMFT



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



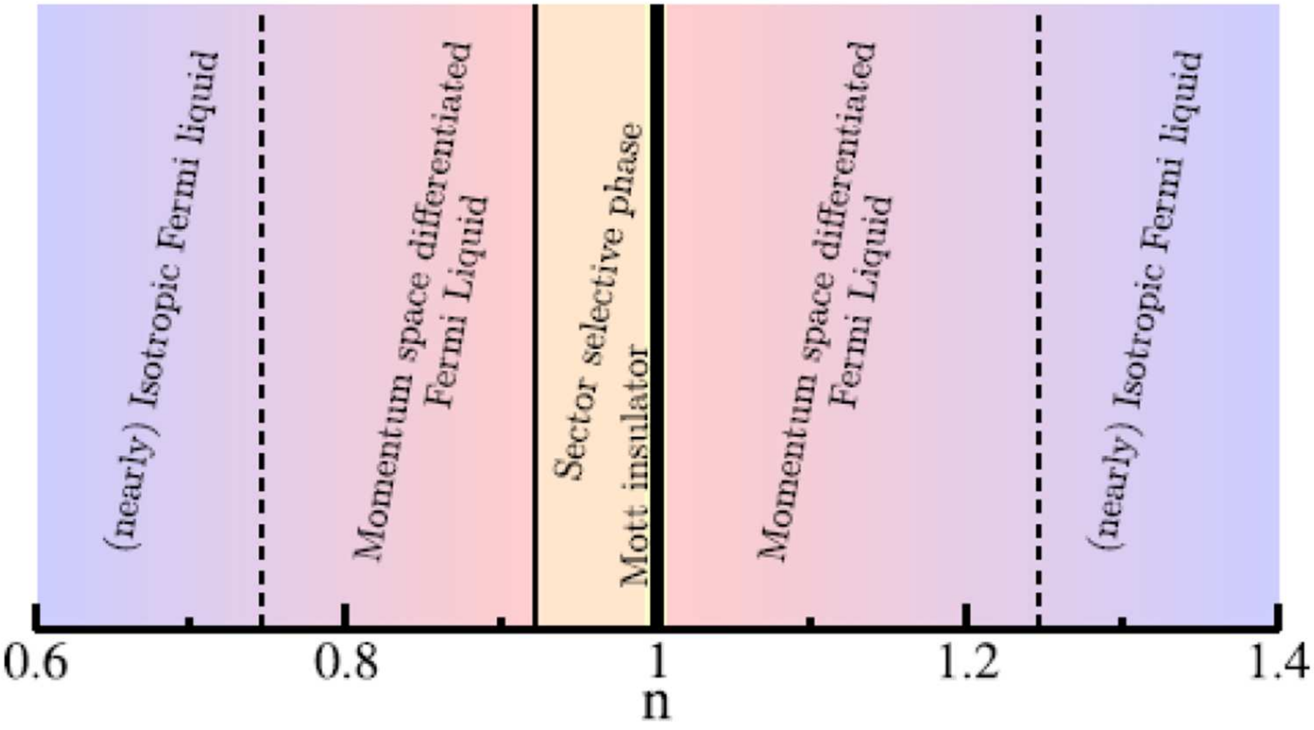
Mean-field is not a trivial problem! Many impurity solvers.

Here: continuous time QMC

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

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

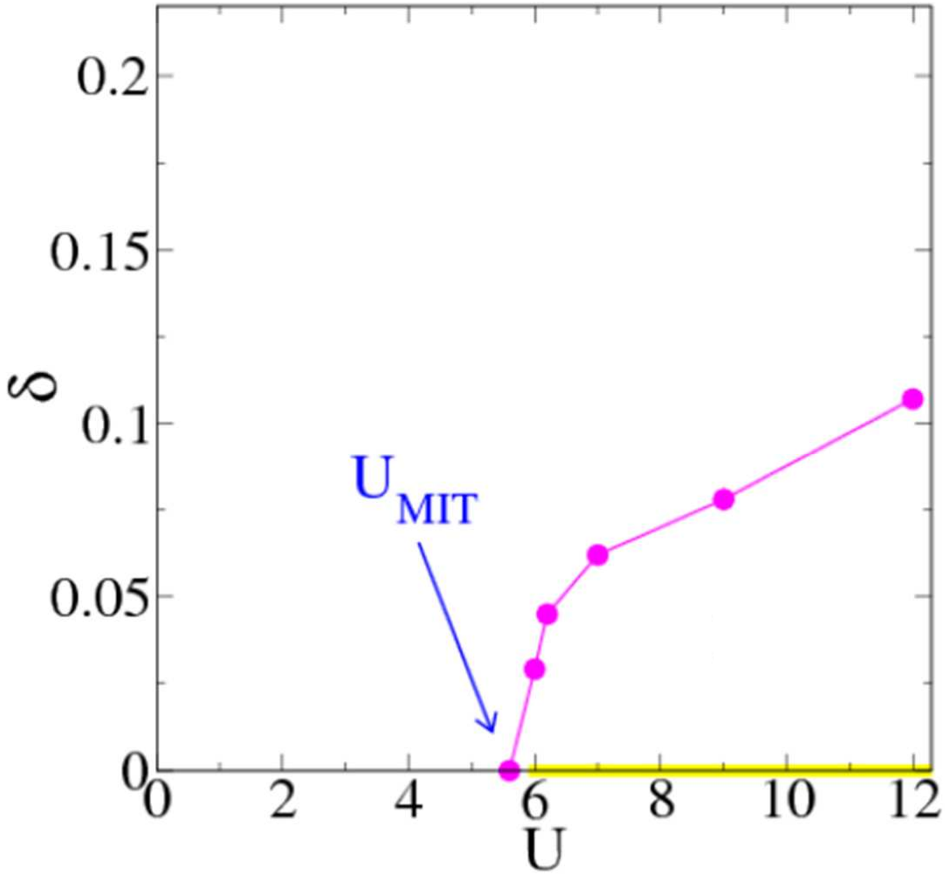
Doping driven Mott transition

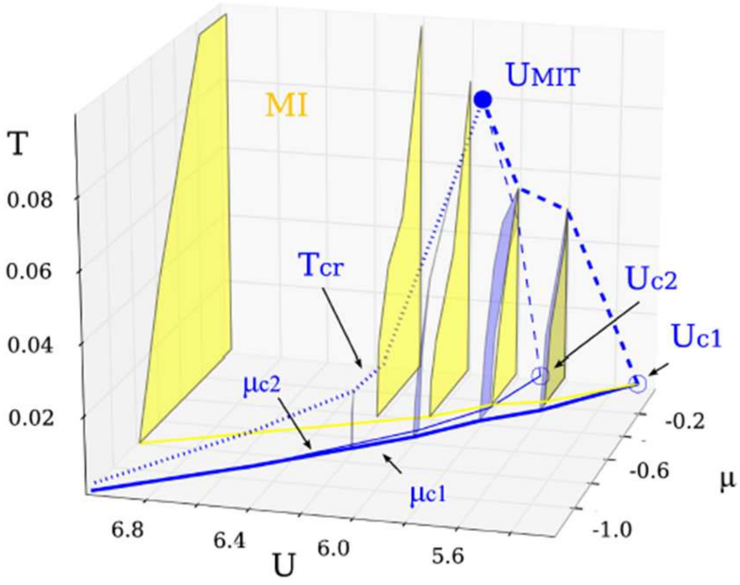


Gull, Werner, Millis, (2009)
E. Gull, M. Ferrero, O. Parcollet, A. Georges, and A. J. Millis (2010)

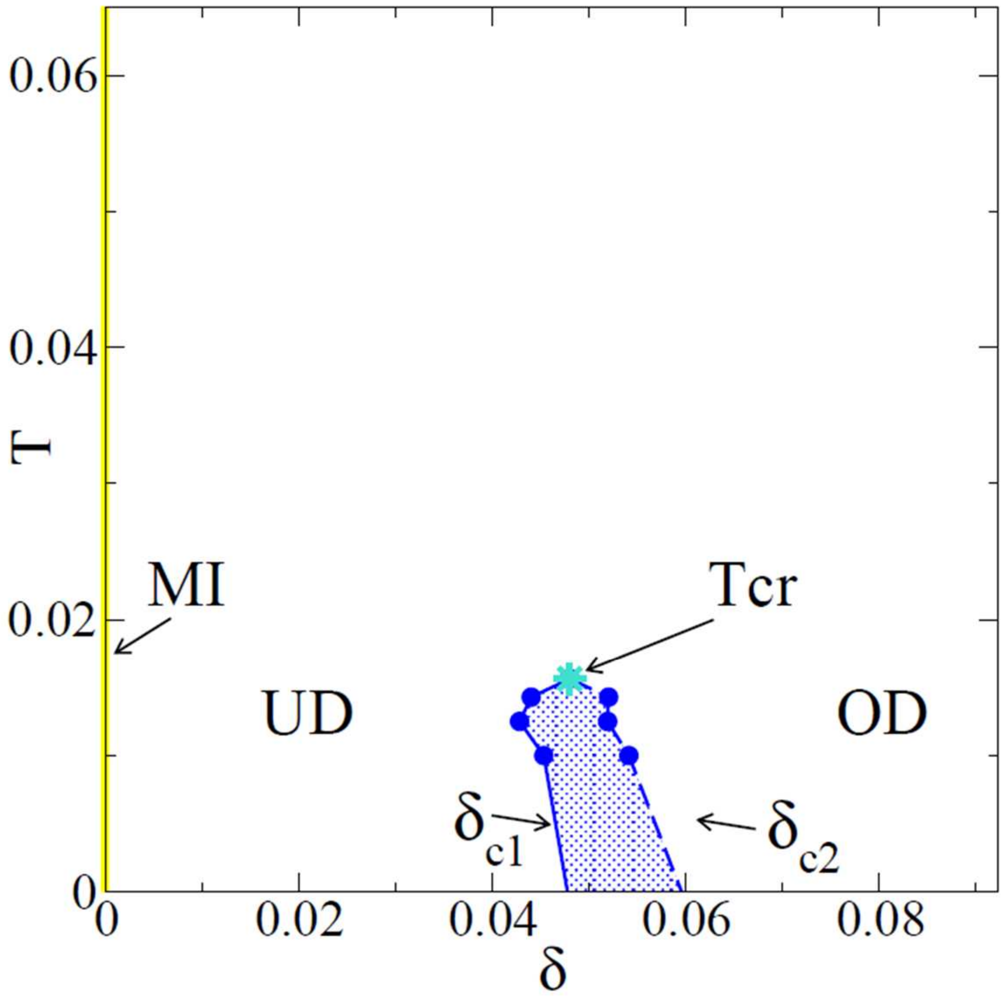
Link to Mott transition up to optimal doping

Doping dependence of critical point as a function of U





Characterisation of the phases (U=6.2t)



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

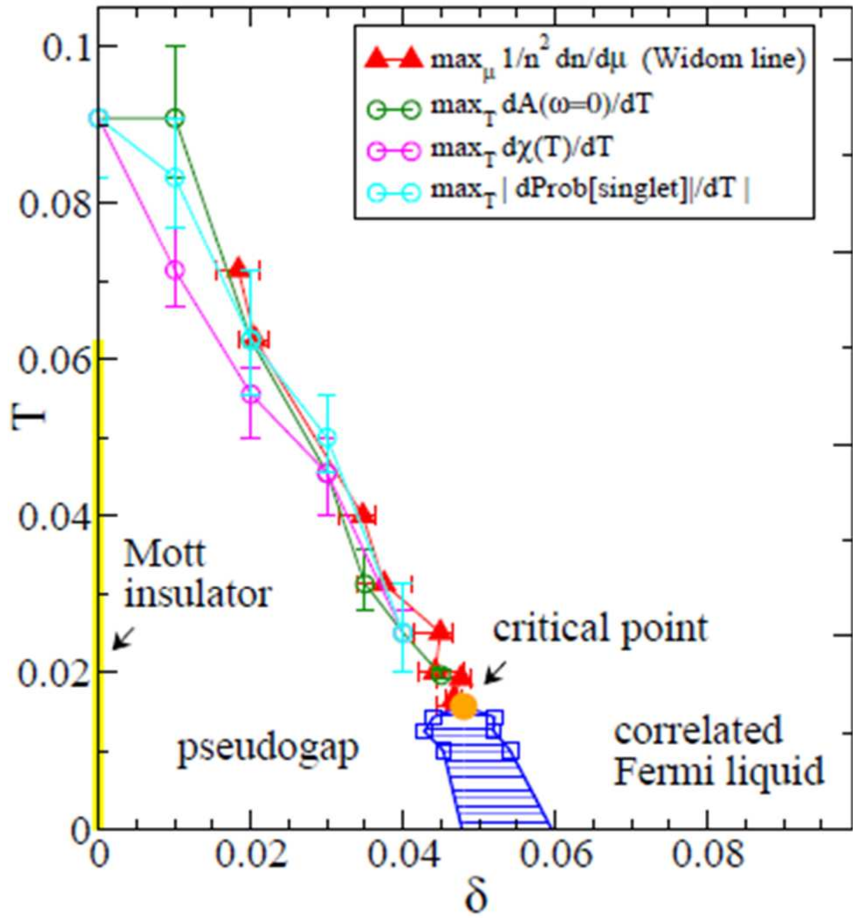
1. Mott insulator (MI)
2. Underdoped phase (UD): $\delta < \delta_c$
3. Overdoped phase (OD): $\delta > \delta_c$
4. Coexistence/forbidden region

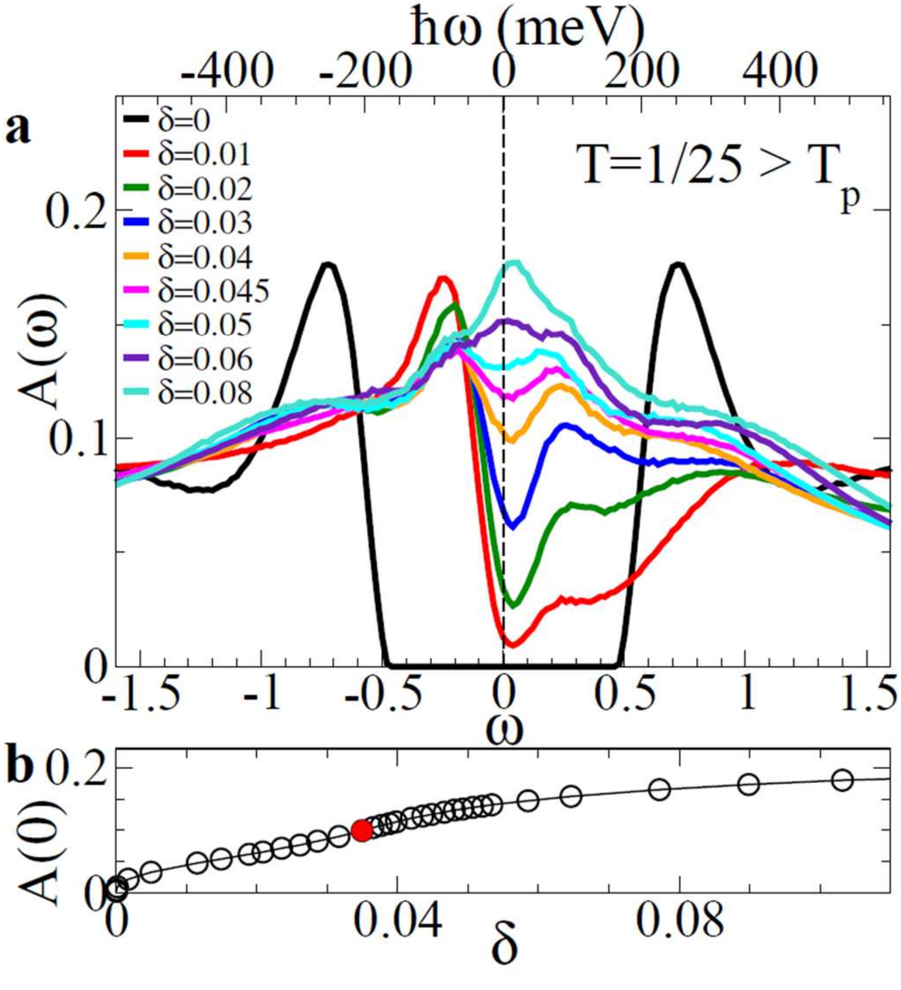
Here "optimal doping" δ_c = doping at which the 1st order transition occurs

How does the UD phase differ from the OD phase?

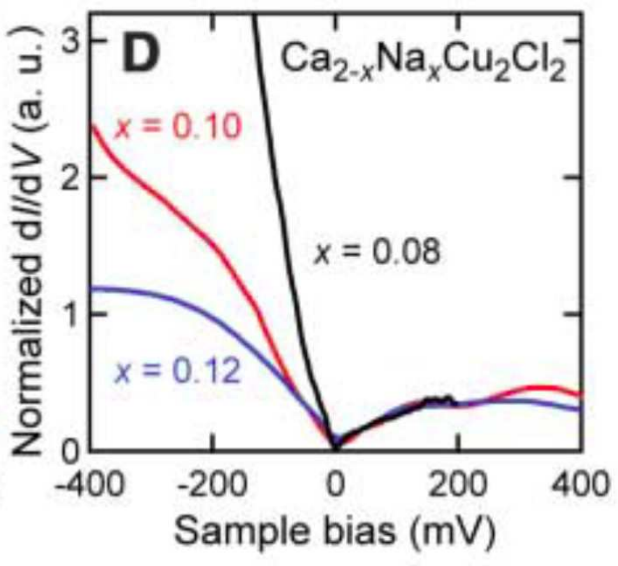
Smaller *D* and *S*

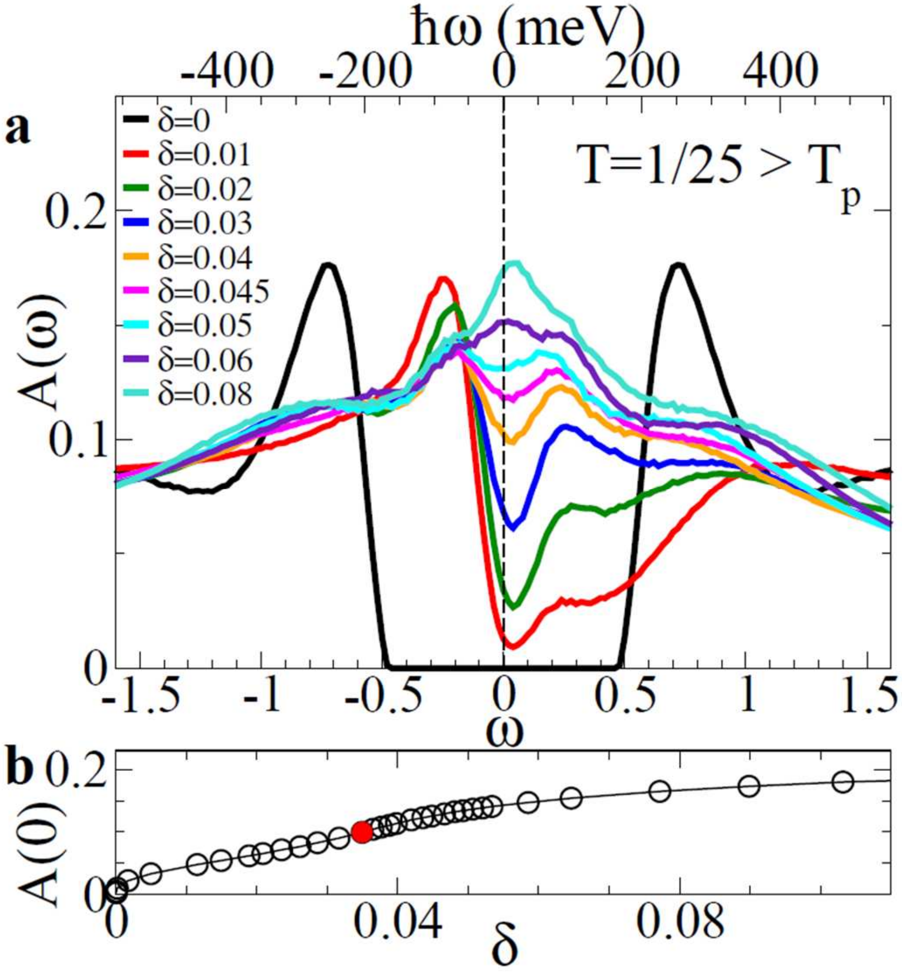
Density of states





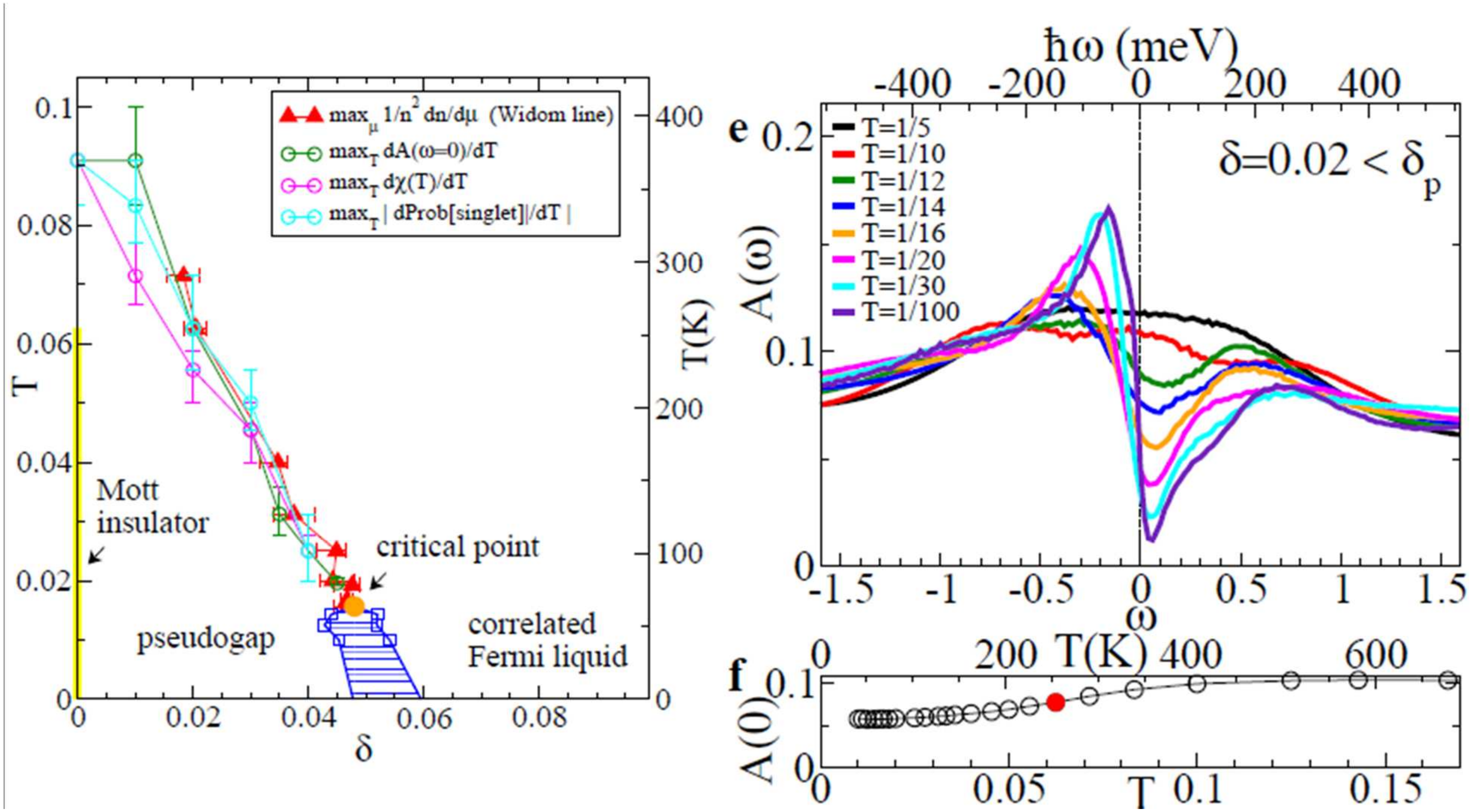
Density of states



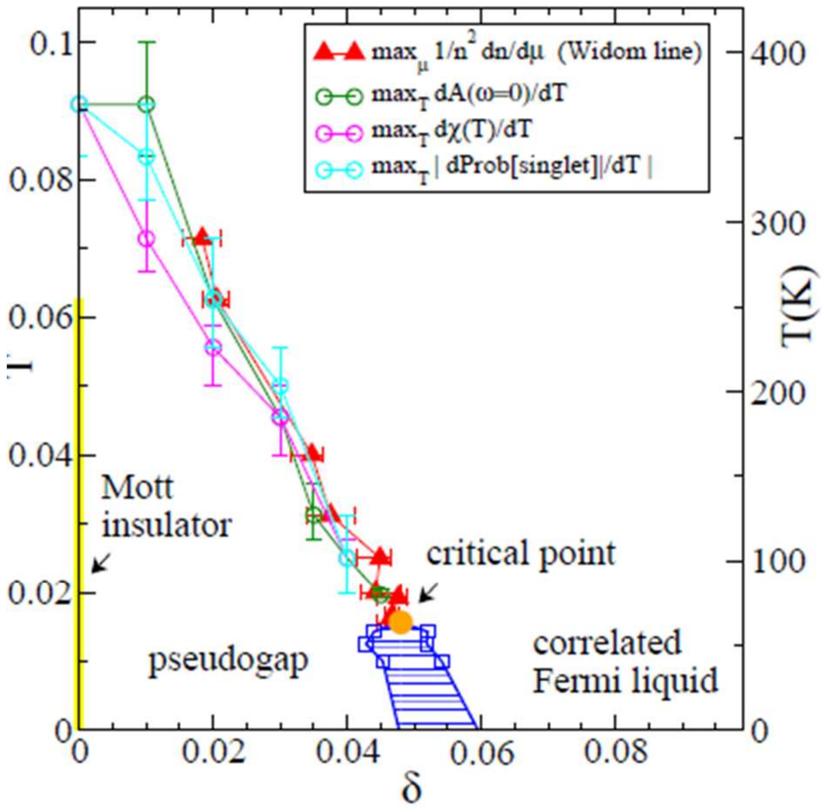


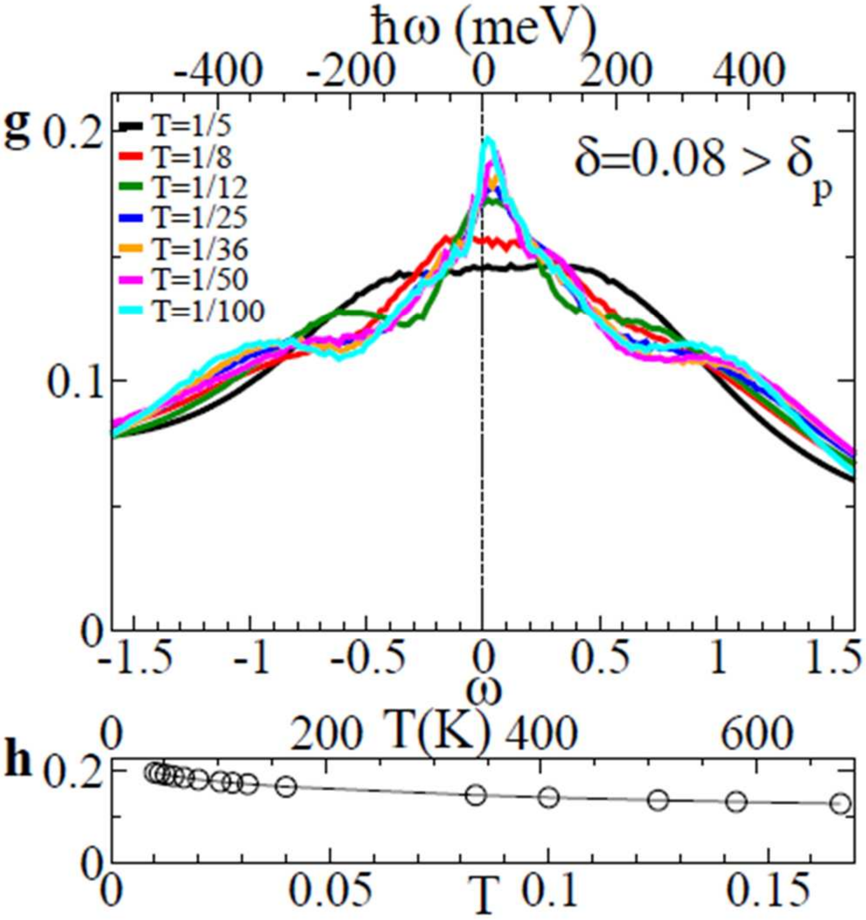
Khosaka et al. *Science* **315**, 1380 (2007);

Density of states

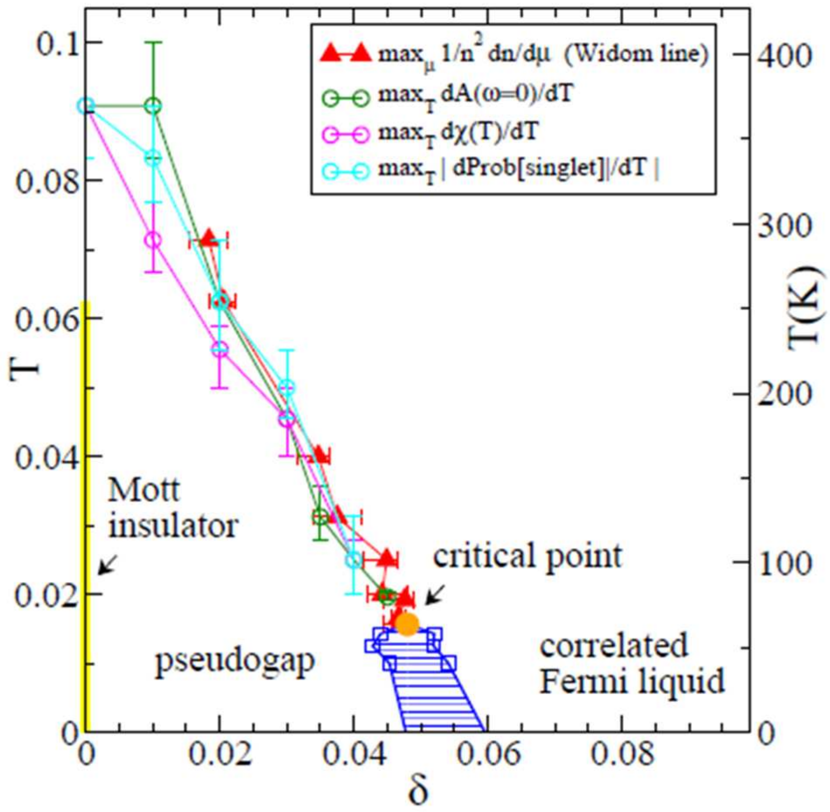


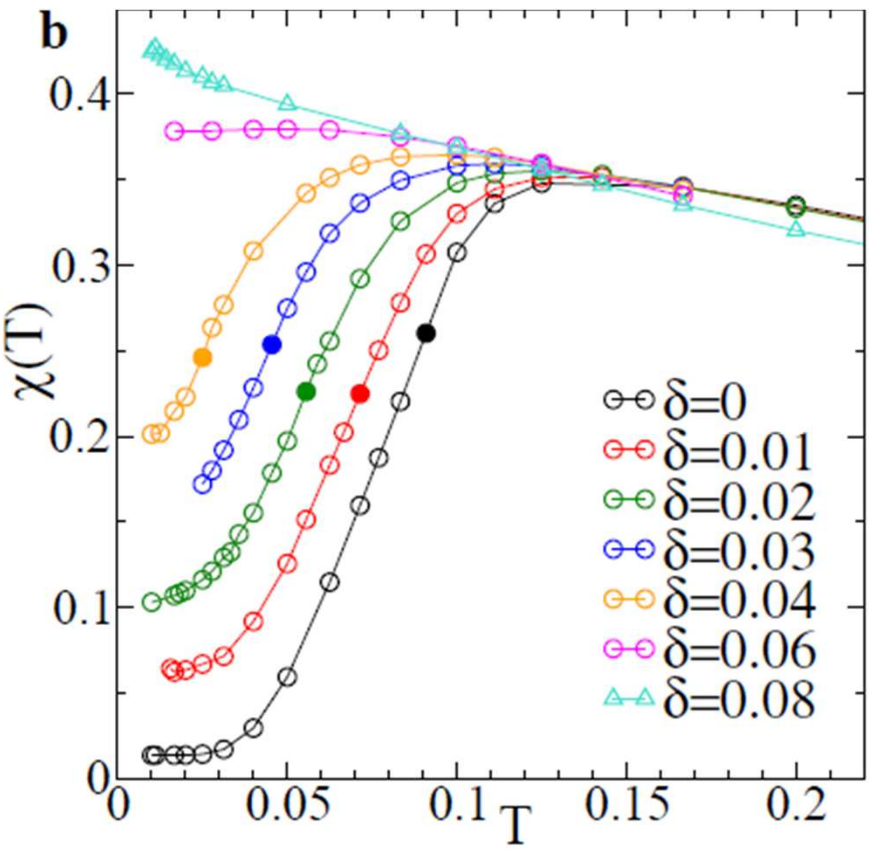
Density of states



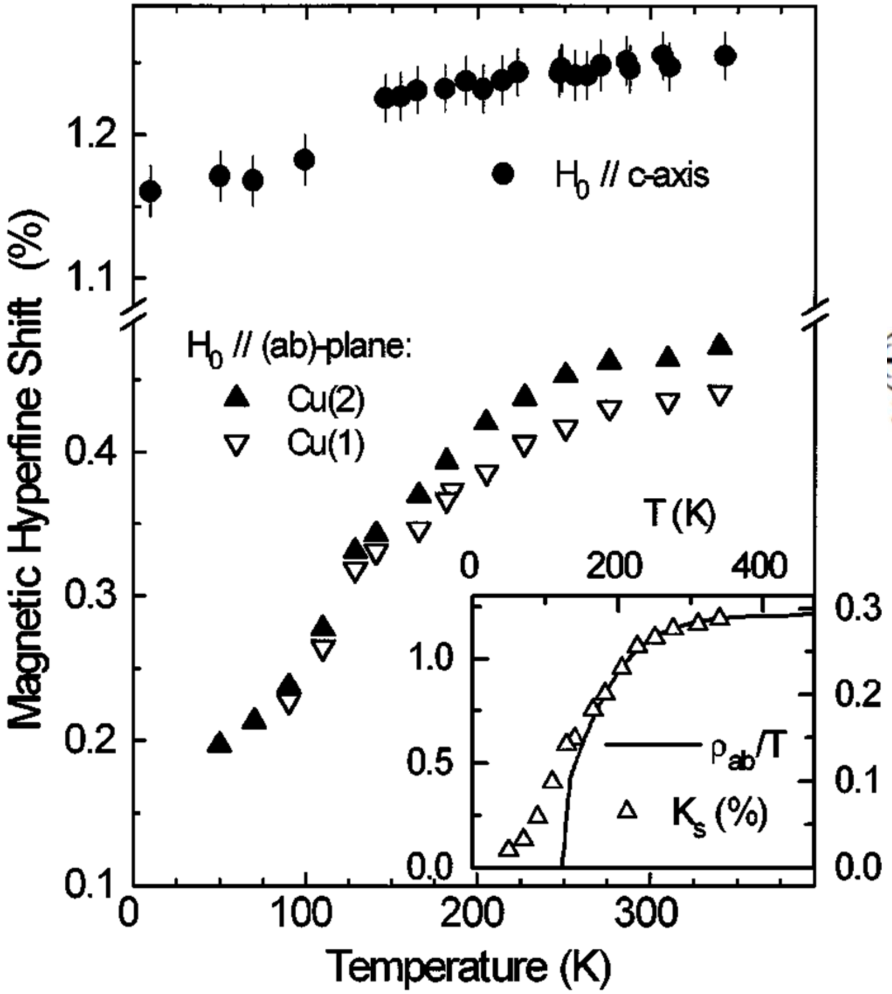


Spin susceptibility



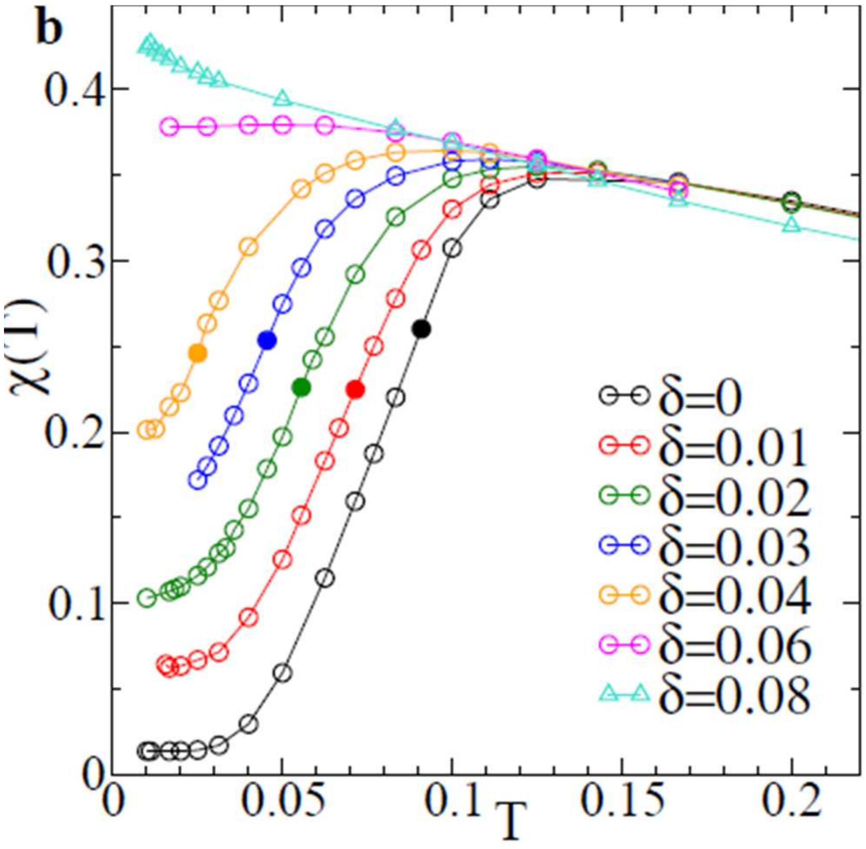


Spin susceptibility

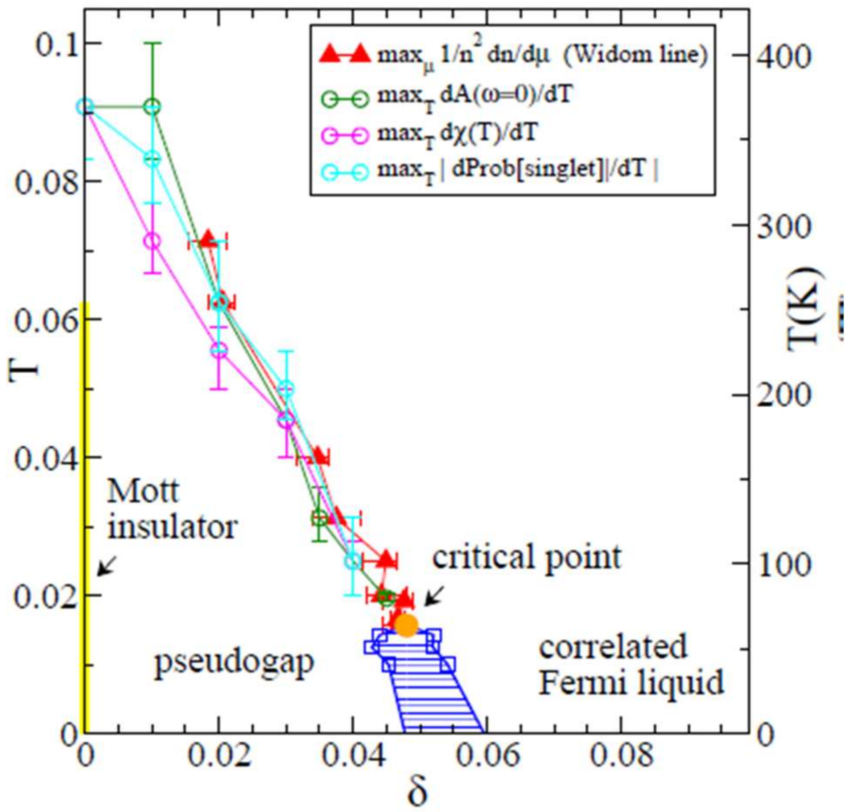


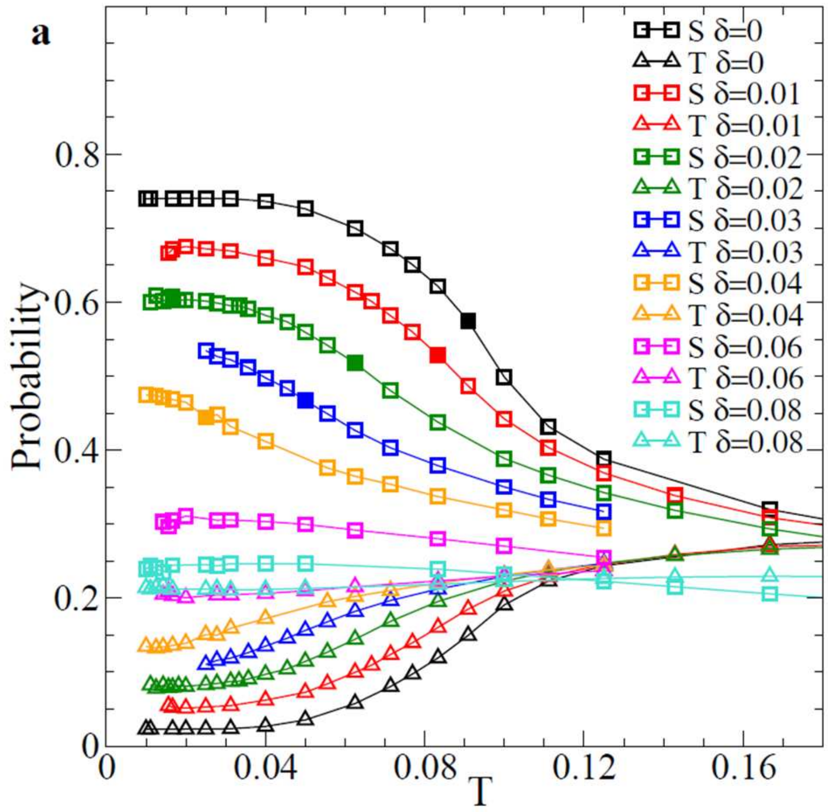
Underdoped Hg1223

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

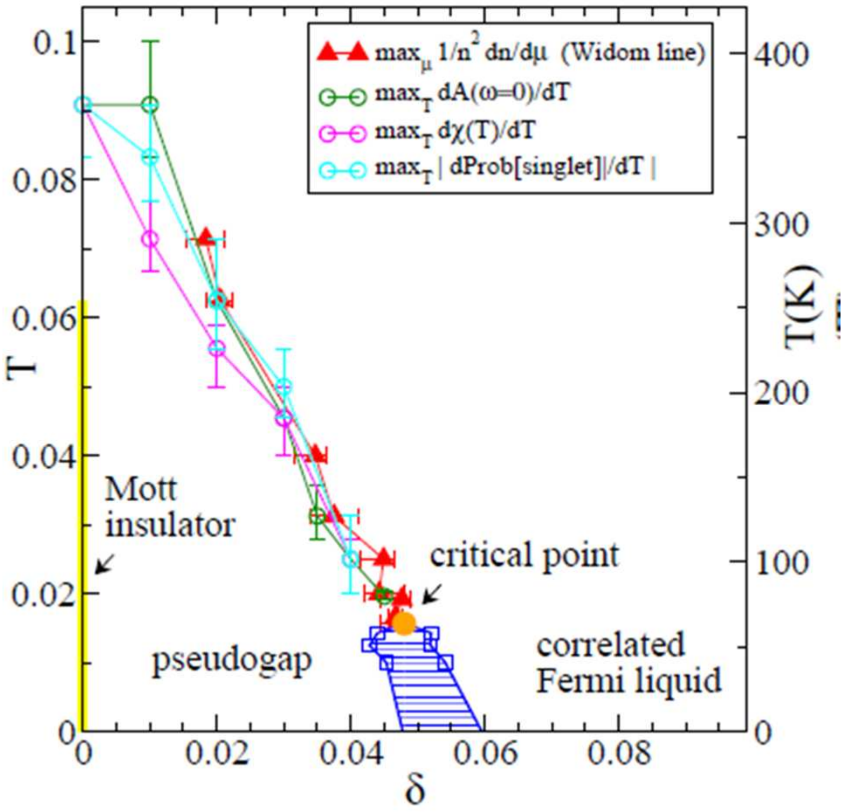


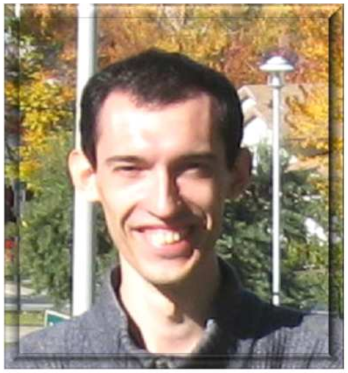
Plaquette eigenstates





Pseudogap *T** along the Widom line





Giovanni Sordi

Patrick Sémon

Kristjan Haule

The Widom line

arXiv:1110.1392

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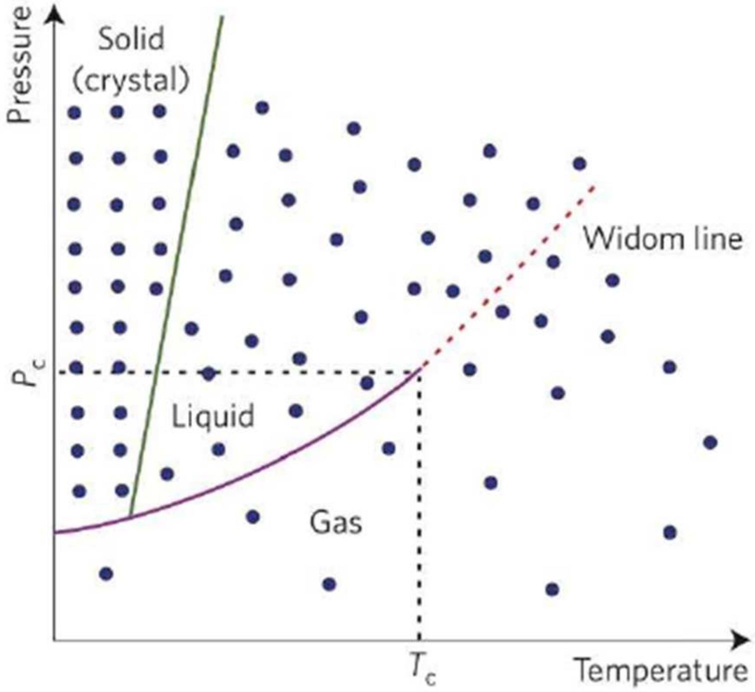
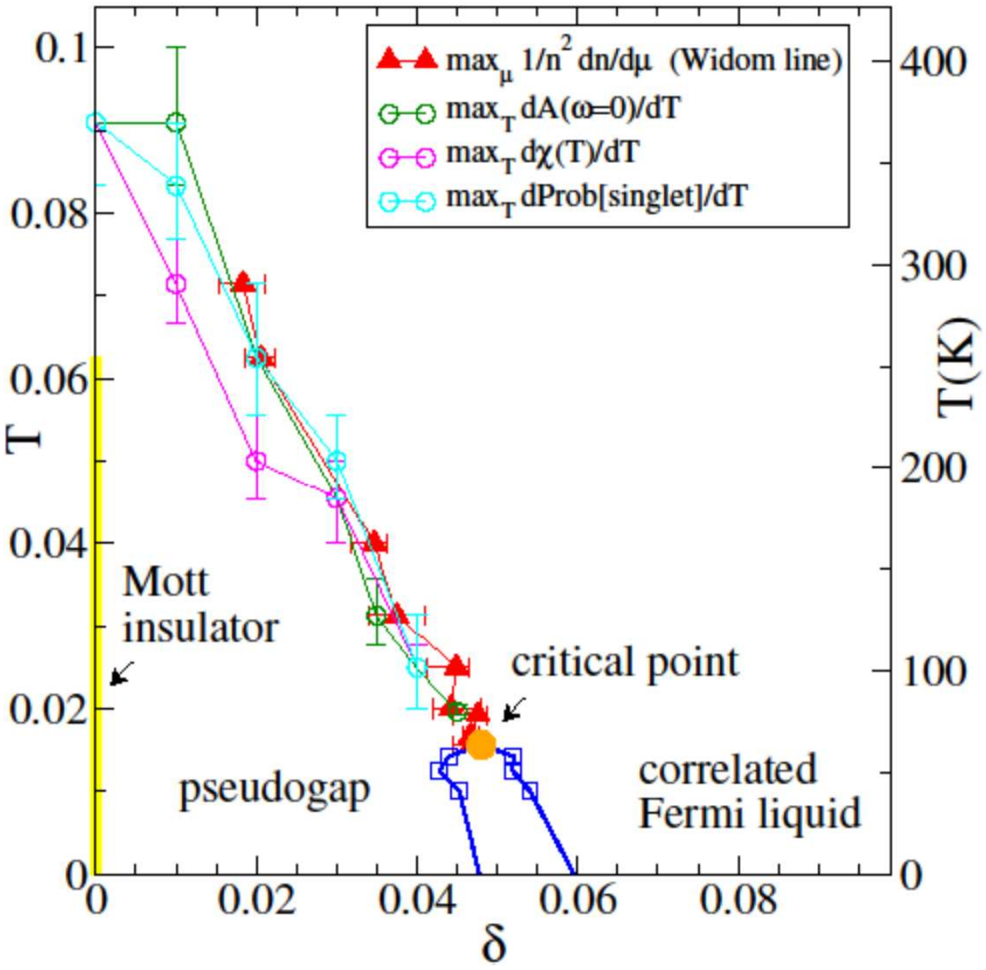
What is the Widom line?



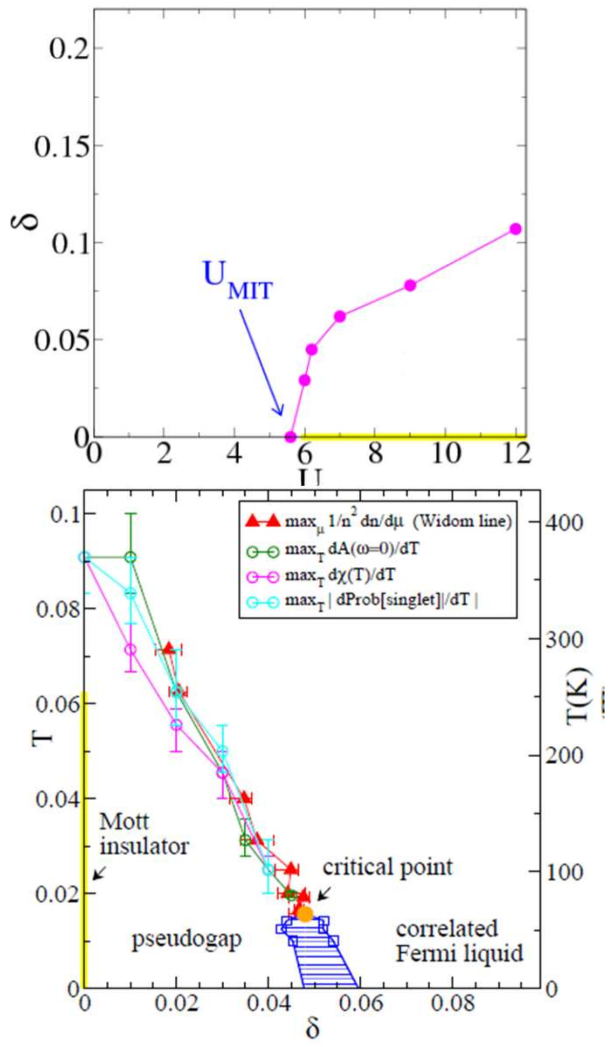
McMillan and Stanley, Nat Phys 2010

- 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 $T \to T_p$
- 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

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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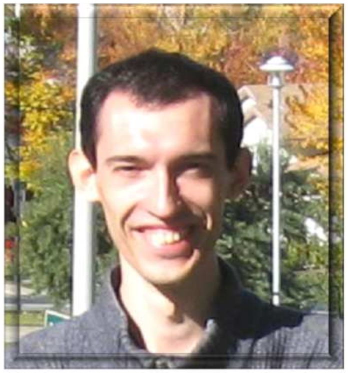


Giovanni Sordi

Patrick Sémon

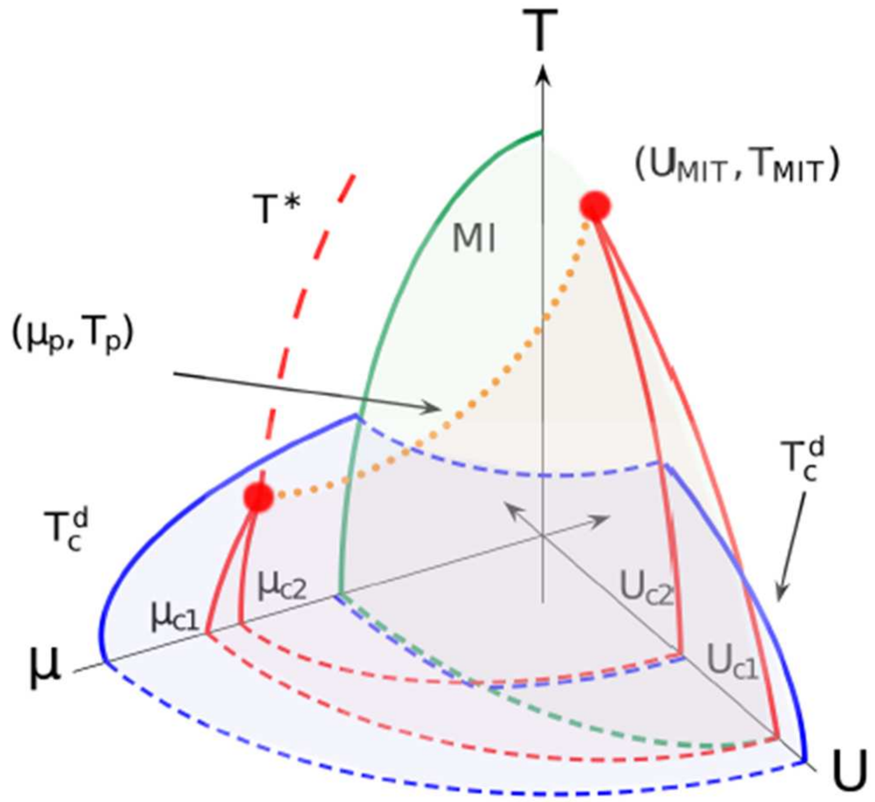
Kristjan Haule

Finite *T* phase diagram

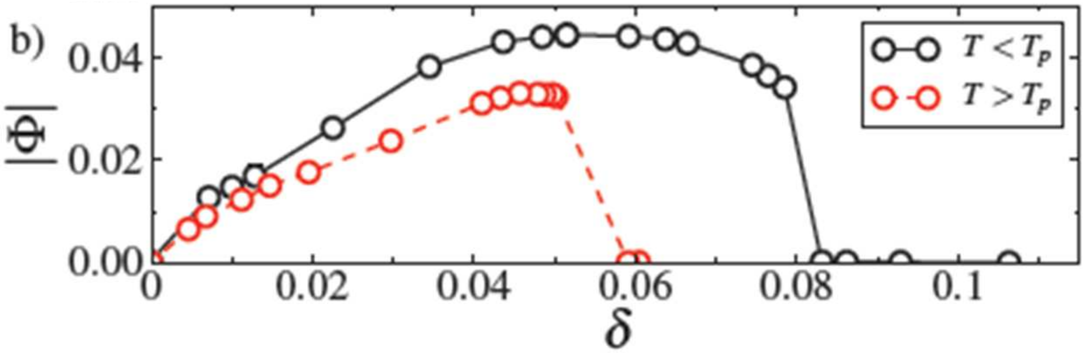
Superconductivity

arXiv:1201.1283v1

Unified phase diagram

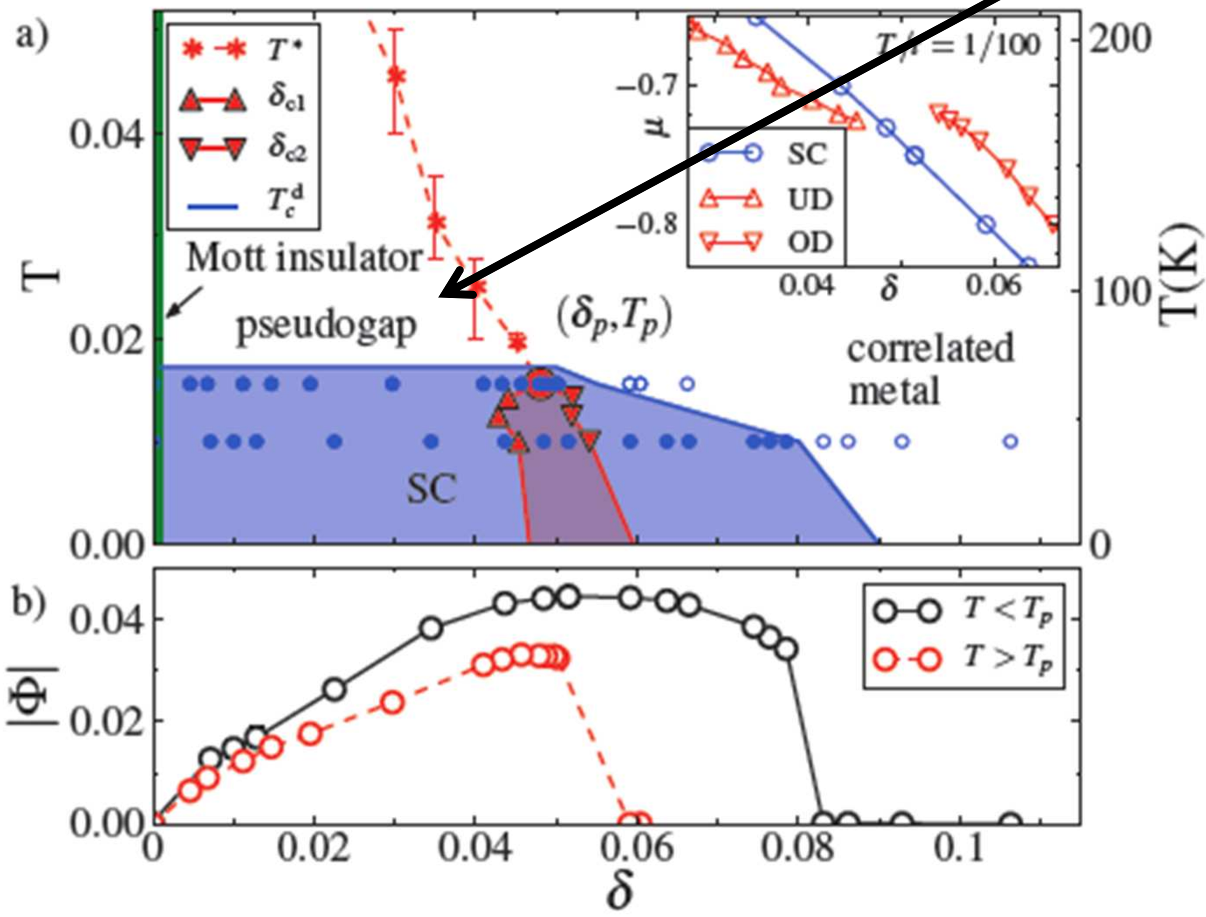


Cuprates (doping driven transition)



Cuprates (doping driven transition)

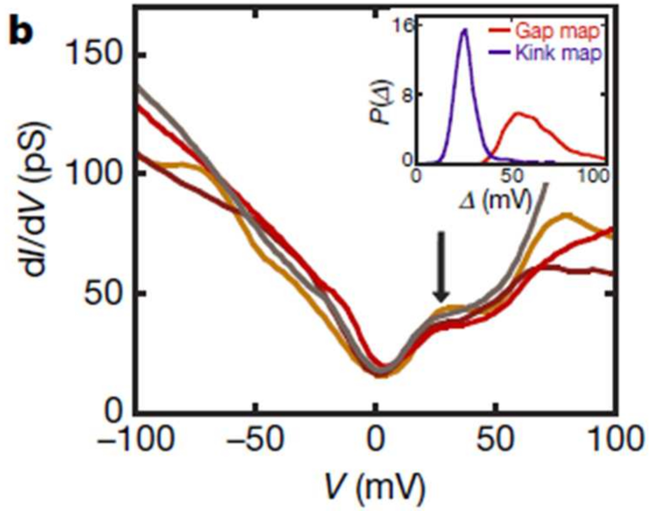
Pseudogap vs pair



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

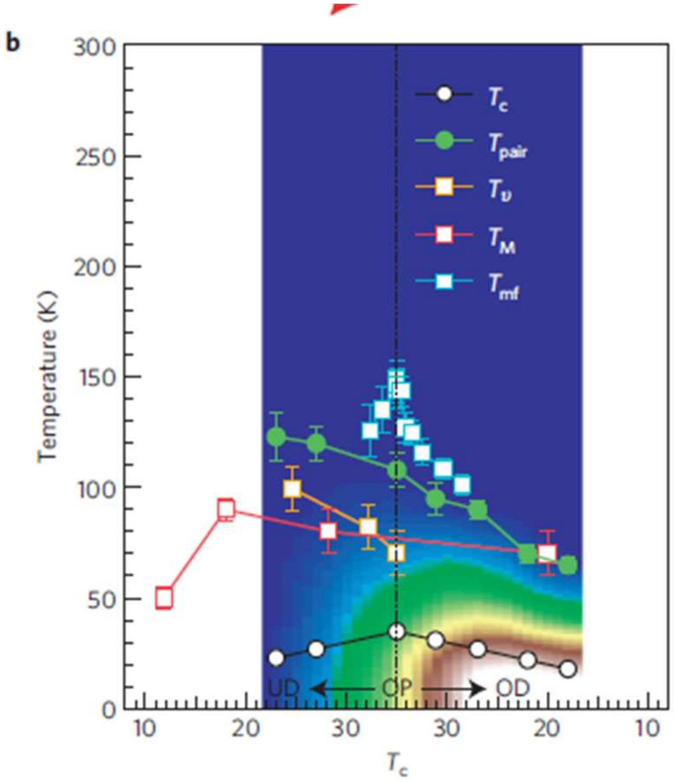
Meaning of T_c^d

- Local pair formation



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

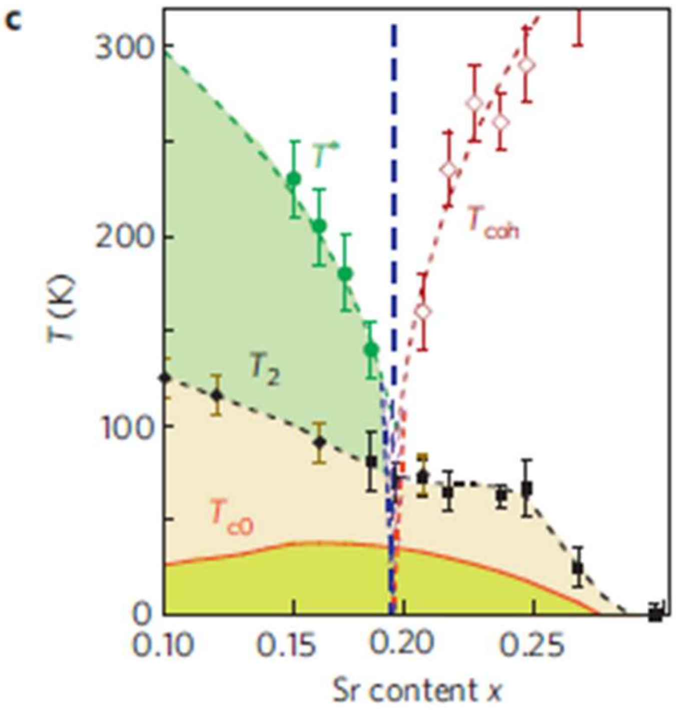
Tpair



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

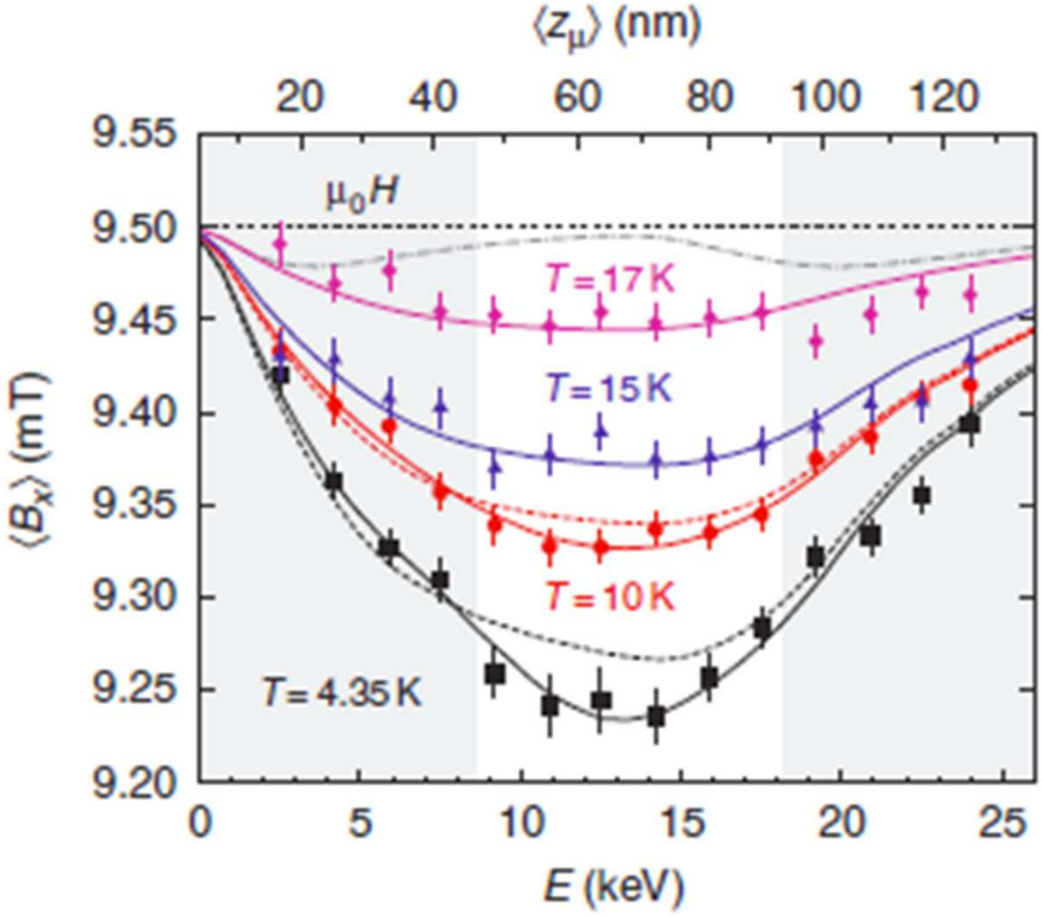


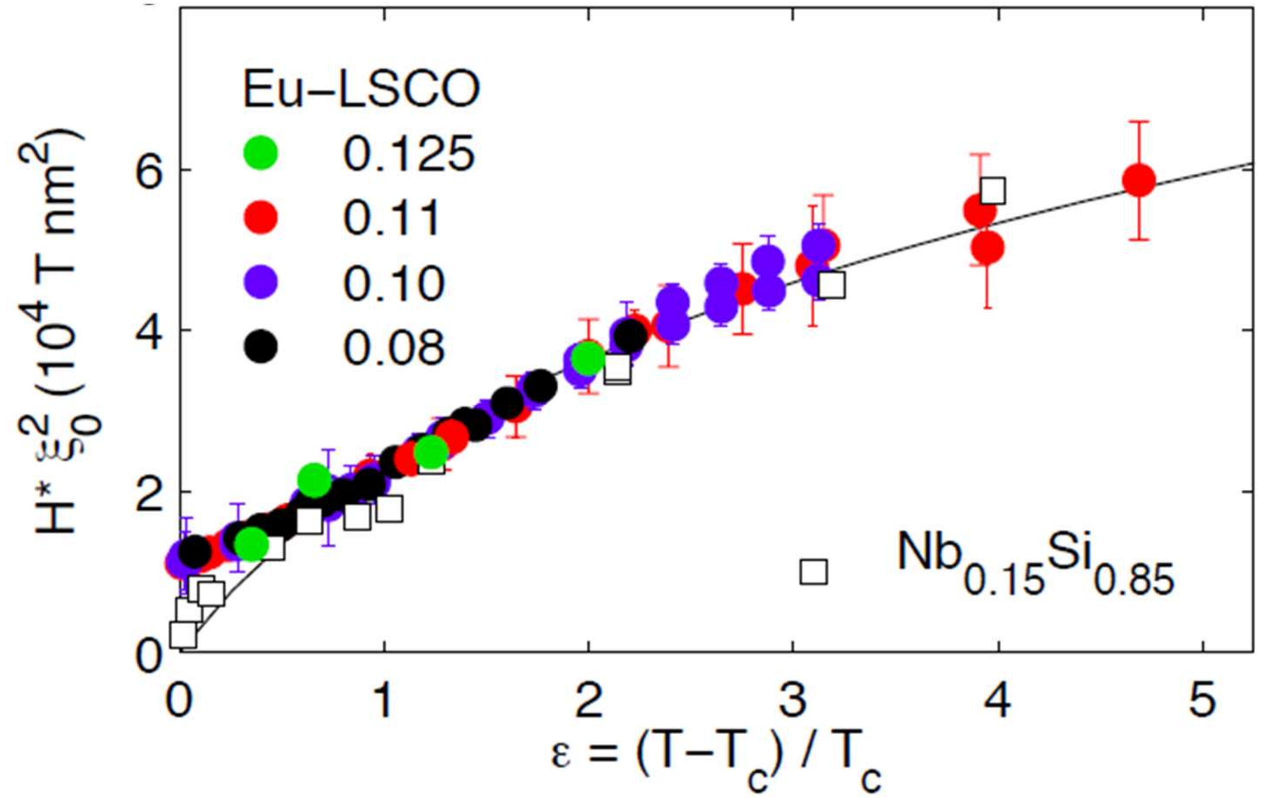
Figure 6 | Depth profile of the local field at different temperatures. The

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

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

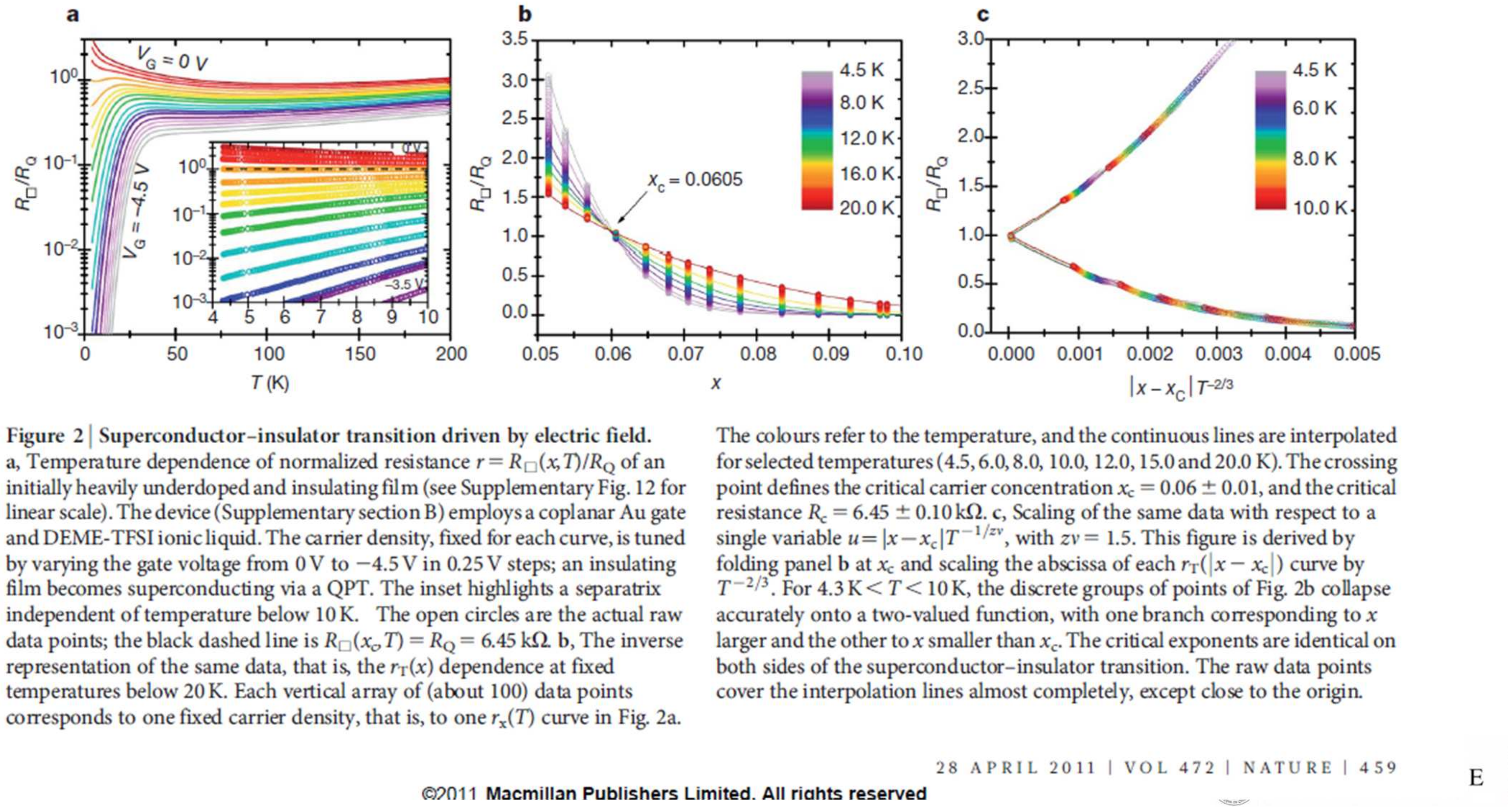
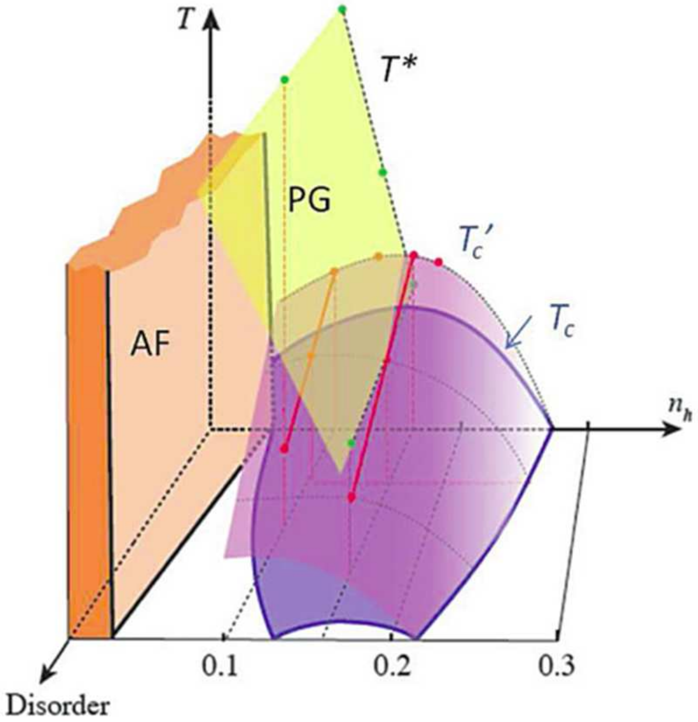


Figure 2 | Superconductor–insulator transition driven by electric field. **a**, Temperature dependence of normalized resistance $r = R_\square(x,T)/R_Q$ of an initially heavily underdoped and insulating film (see Supplementary Fig. 12 for linear scale). The device (Supplementary section B) employs a 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 $4.3\,K < T < 10\,K$, 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.

E

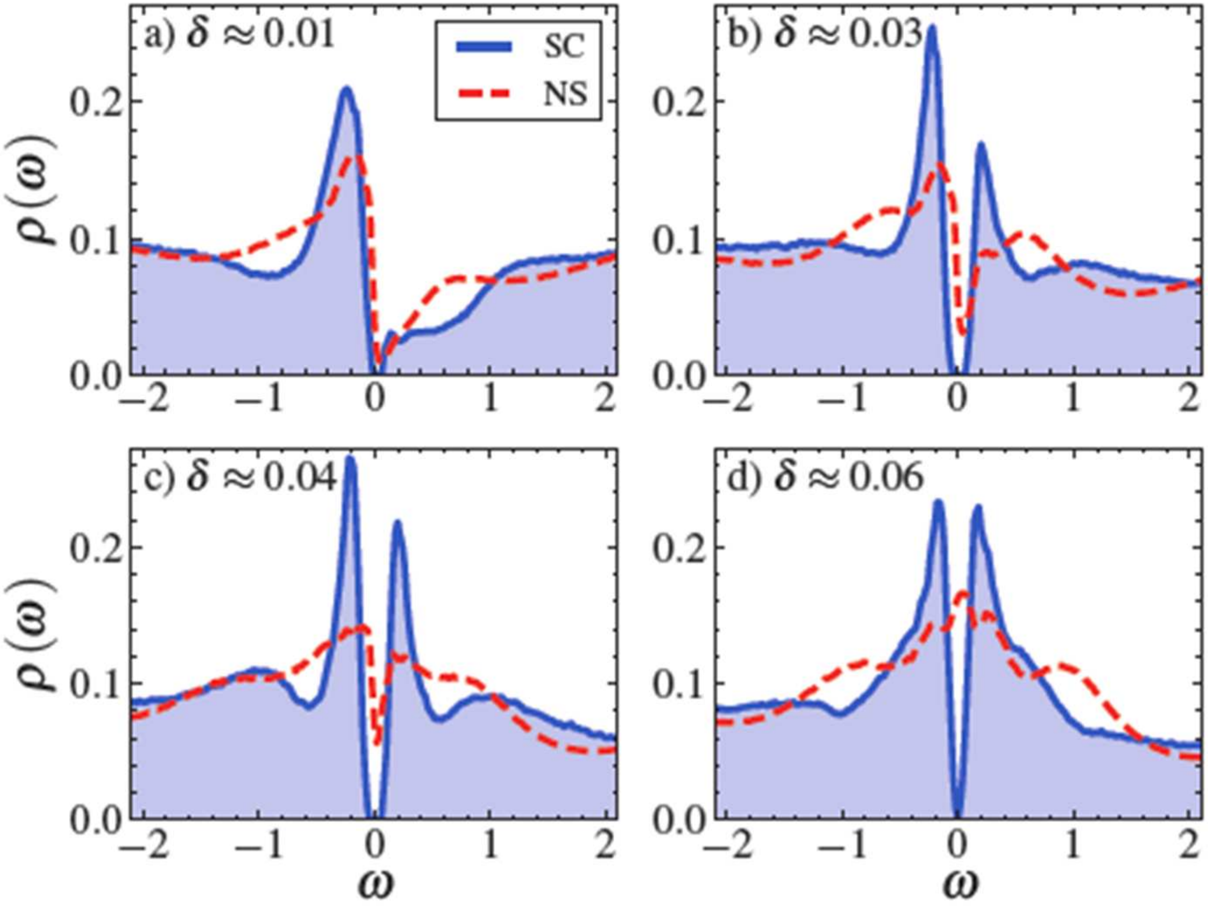
Effect of disorder



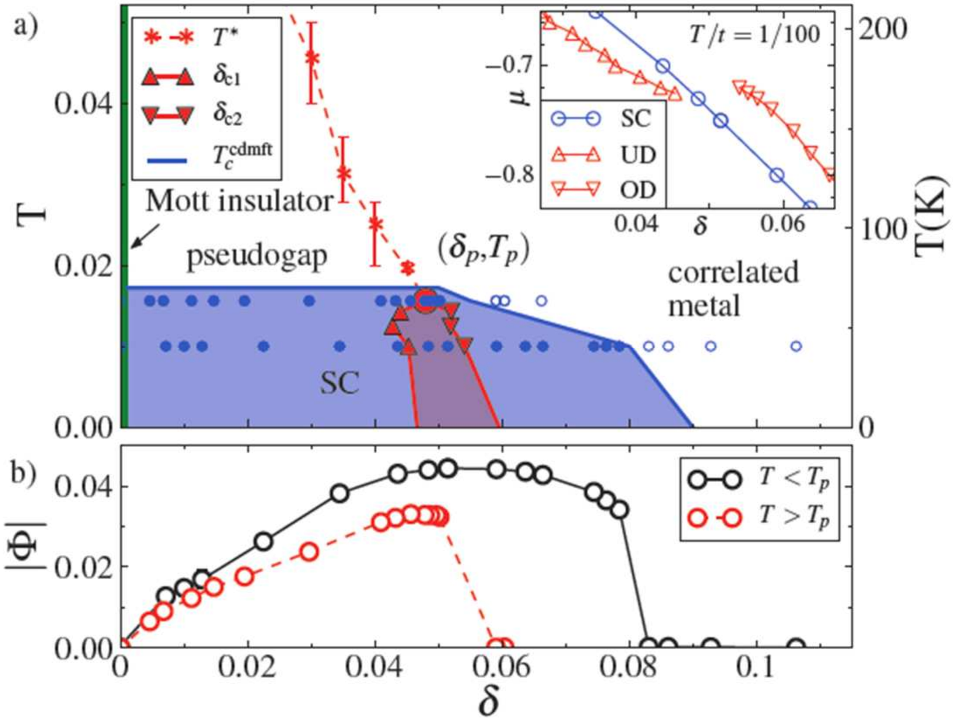
F. Rullier-Albenque, H. Alloul, and G.Rikken,
Phys. Rev. B **84**, 014522 (2011).

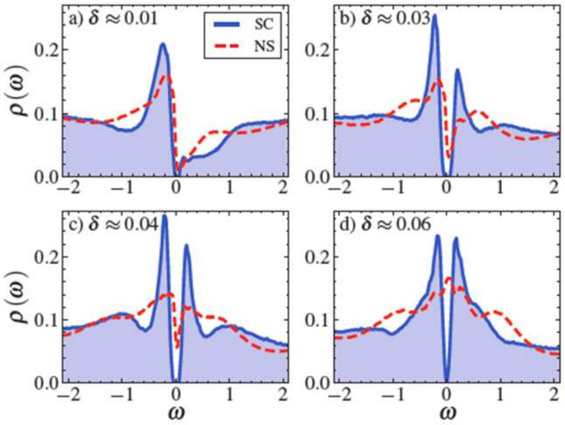
Superconductivity in underdoped vs BCS

First-order transition leaves its mark



Summary: superconductivity





- 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

Projects

High temperature superconductivity

BIG QUESTIONS:

- What is the pairing mechanism in pnictides and cuprates ?
- Is the same fundamental scenario common to all unconventional superconductors ?
- What limits the critical temperature Tc ?
- What is the pseudogap phase of cuprates ?

High temperature superconductivity

- **Collaboration with Rutgers:**
  - – Normal state finite *T* phase diagram of 2d Hubbard model and competition between superconductivity and antiferromagnetism at finite *t'* with CDMFT for more realistic comparisons with experiment.
  - – Competition between antiferromagnetism and pseudogap phase to clearly differentiate the two phenomena at strong coupling.

High temperature superconductivity

- **Collaboration with Rutgers continued-1:**
  - Improved alogorithms
    - Skip list for CT-HYB
  - Compute vertex corrections to obtain
    - The highly non-BCS zero temperature superfluid density
      - High Tc
      - Organics (McKenzie)
    - Resistivity, to verify whether it is linear in temperature.

High temperature superconductivity

- **Collaboration with Rutgers continued-2**
  - Include realistic band structure effects to understand the difference in *Tc* between different compounds: single layer vs multilayer and electron vs hole doped compounds.

High temperature superconductivity

- To understand the mechanism of strongly correlated superconductivity study
  - Effect of near-neighbor repulsion
  - Effect of retardation in three-band model
- Improve the methodology to include long wavelength fluctuations in CDMFT
  - Make the vertex self-consistent to satisfy Pauli principle and achieve consistency between lattice and impurity for double occupancy (à la TPSC).
  - Achieve self-consistency between one- and two-particle quantities

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High temperature superconductivity

- Benchmark CDMFT + DCA against large system calculations by
  - Comparing with results obtained on the Hubbard ladder and also on the square lattice at half-filling where there is no sign problem.

Heterostructures

BIG QUESTION

- Can we create new states of matter at interfaces, or design materials that exhibit desired states such as higher-temperature superconductivity?

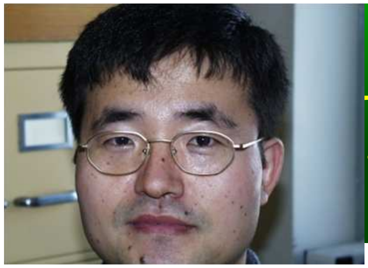
Heterostructures

- Compute with CDMFT and from first-principles (DFT) the charge distribution and ordered-states in the high-Tc *p*-*n* junction (hole-doped on electron-doped high Tc) to look for interface superconductivity arising between two non-superconducting compounds. Project in collaboration with the experimental group of P. Fournier.

Spin liquids

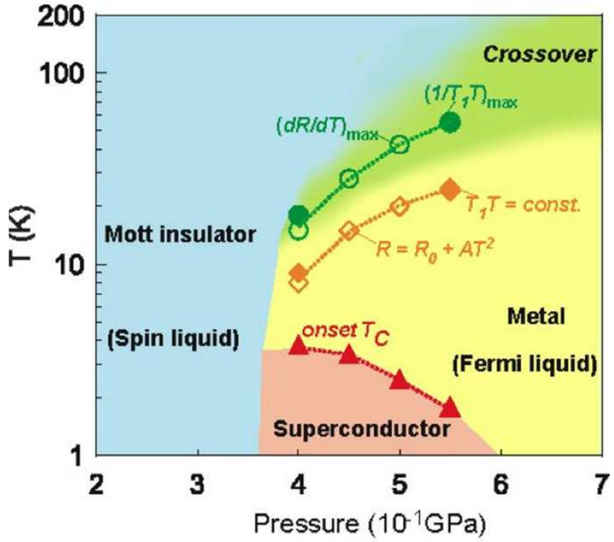
BIG QUESTIONS :

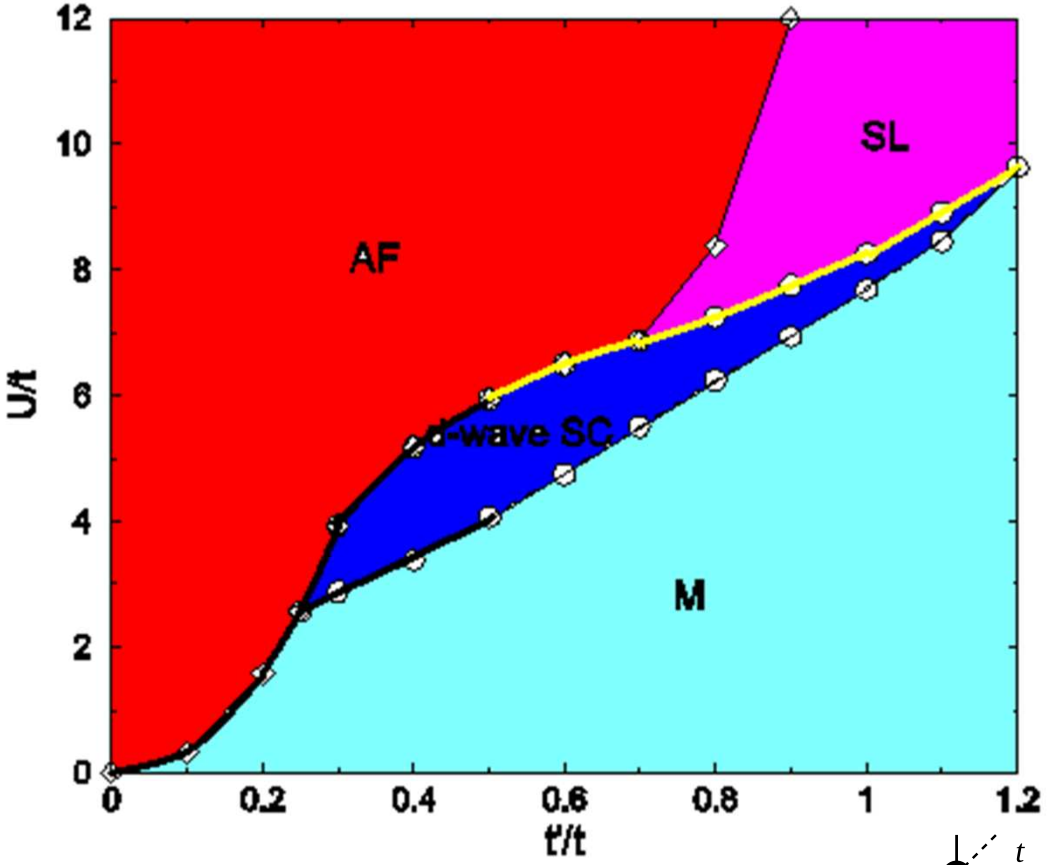
- Is there a quantum spin liquid in nature ?
- What new phenomena exist in frustrated magnetic materials ?
- Can the sign problem be solved for frustrated quantum spin systems ?



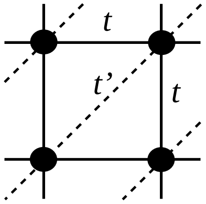
Theoretical phase diagram BEDT

$X = Cu_2(CN)_3$ (t′~ t)





Kyung, A.-M.S.T. PRL 97, 046402 (2006)

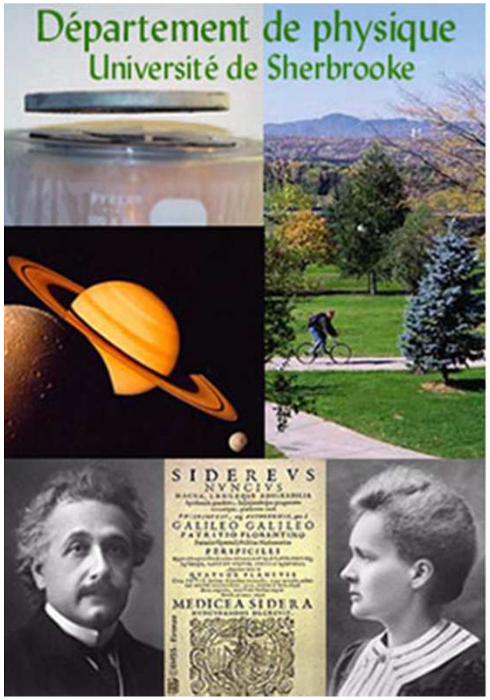


Y. Kurisaki, et al.
Phys. Rev. Lett. **95**, 177001(2005)

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

Spin Liquids

- Obtain the finite temperature phase diagram of the κ-BEDT layered organic superconductors with CDMFT and CTQMC to find how antiferromagnetism leaves room for spin liquid as we move towards the isotropic triangular lattice.
- In the spin-liquid phase, check whether there is a linear specific heat and Pauli susceptibility despite insulating behavior.



André-Marie Tremblay

CANADA RESEARCH CHAIRS
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Merci

Thank you