Insulators, metals, pseudogaps and high-temperature superconductors

A.-M. Tremblay

G. Sordi, K. Haule, D. Sénéchal,

P. Sémon, B. Kyung, G. Kotliar

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CANADIAN INSTITUTE for ADVANCED RESEARCH

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Rice, 16 April, 2012

VERITATEM IN CHARITATE

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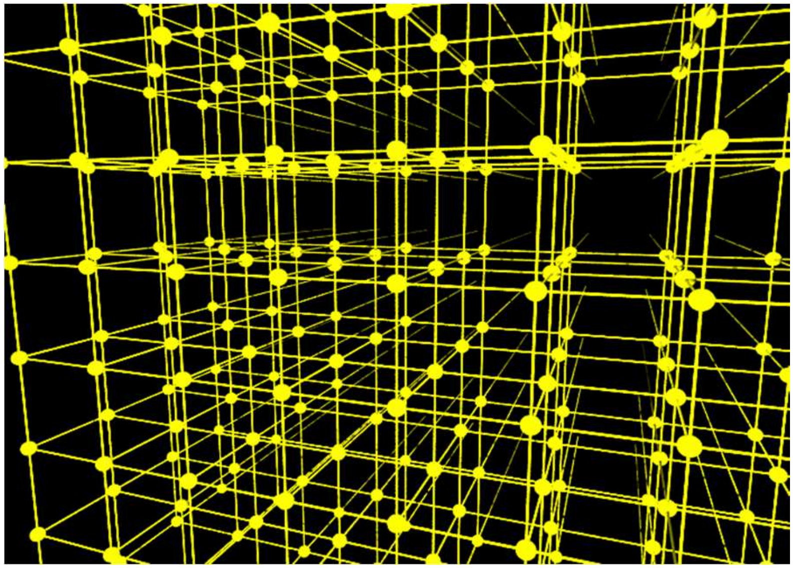
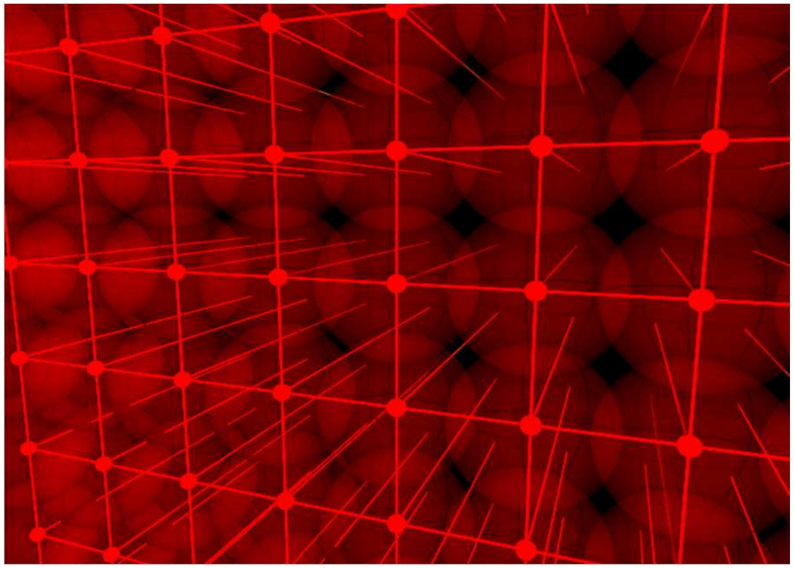
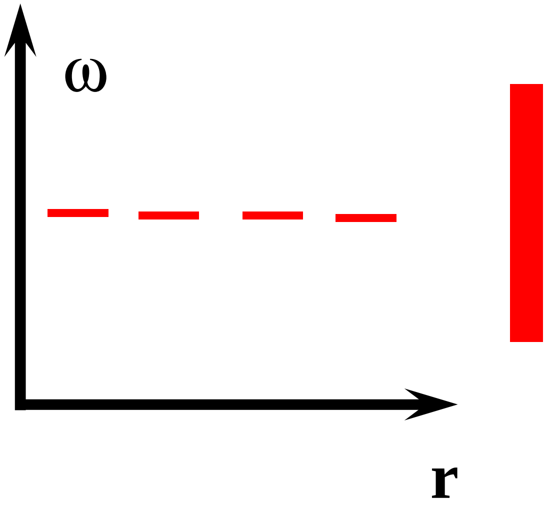
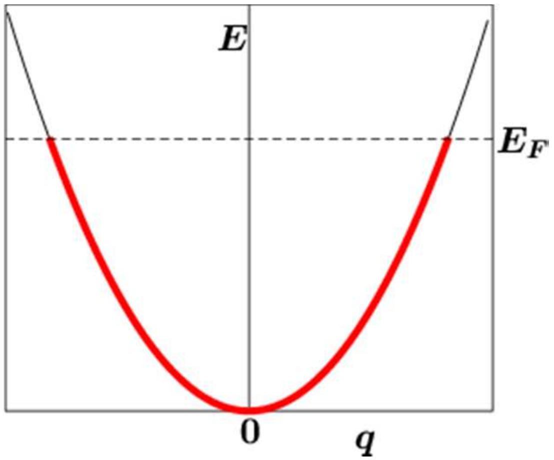
How to make a metal









Courtesy, S. Julian

Superconductivity

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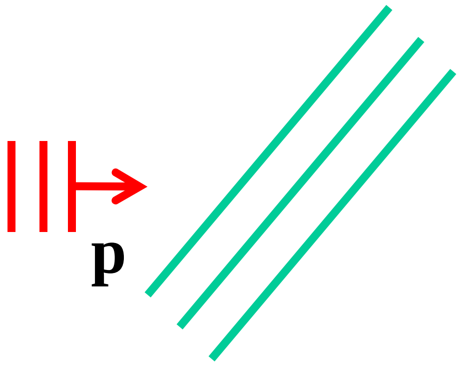
Attraction mechanism in the metallic state



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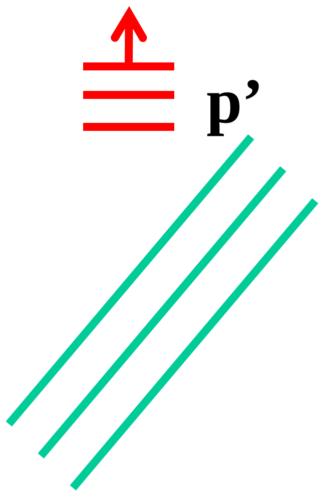
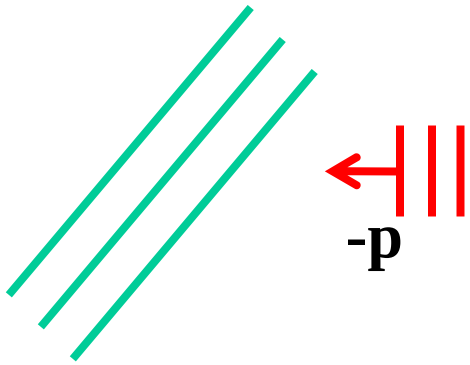
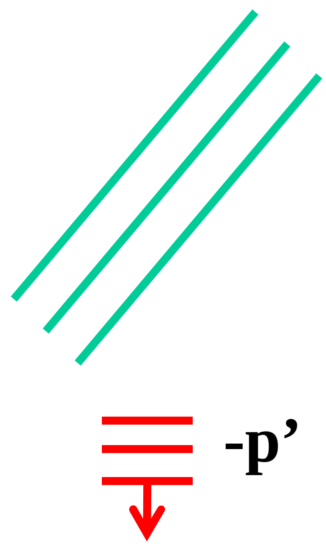
Attraction mechanism in the metallic state



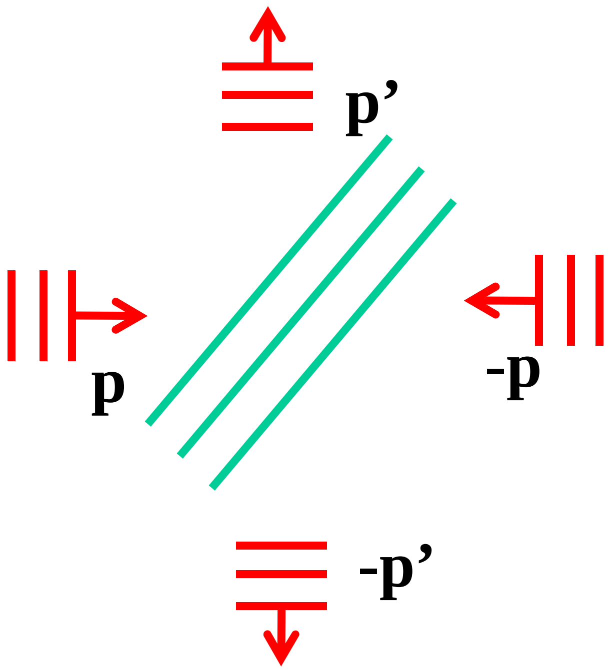
Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



#1 Cooper pair, #2 Phase coherence

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

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

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

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Half-filled band is metallic?

Half-filled band: Not always a metal

NiO, Boer and Verway

Peierls, 1937

Mott, 1949

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« Conventional » Mott transition

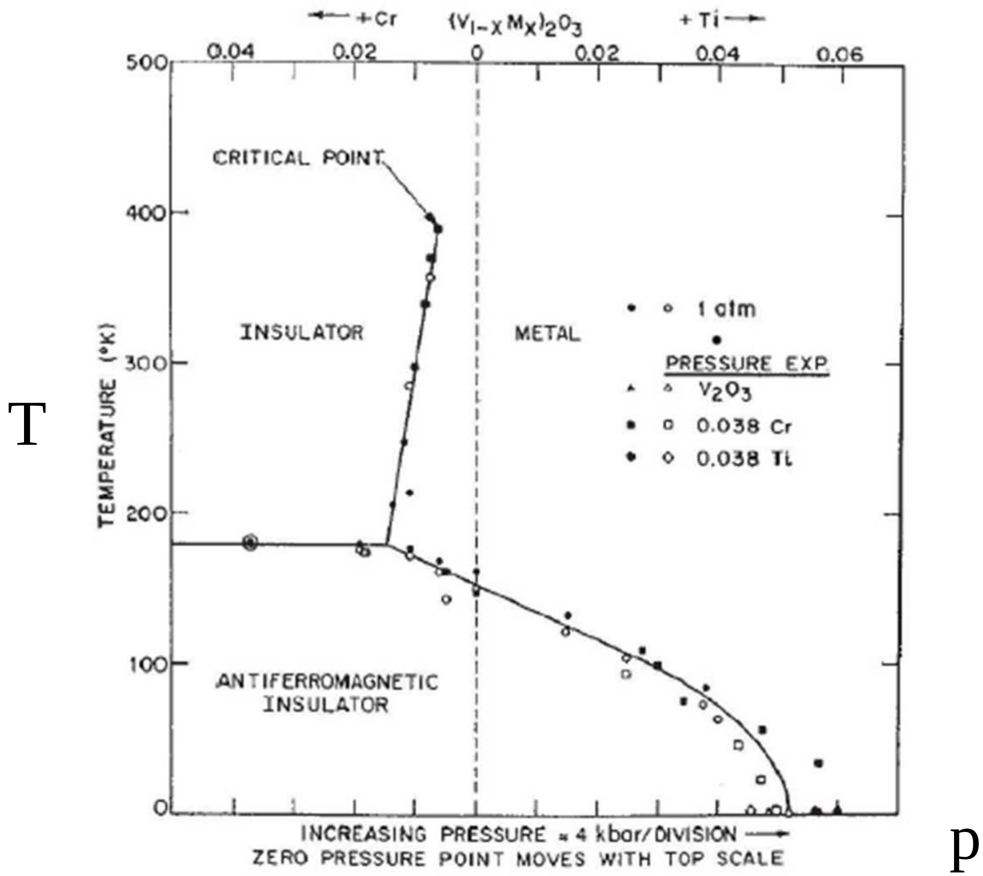
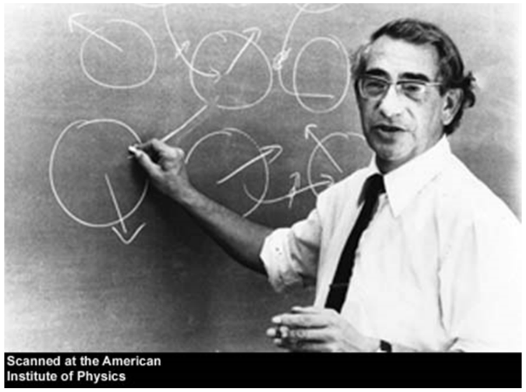


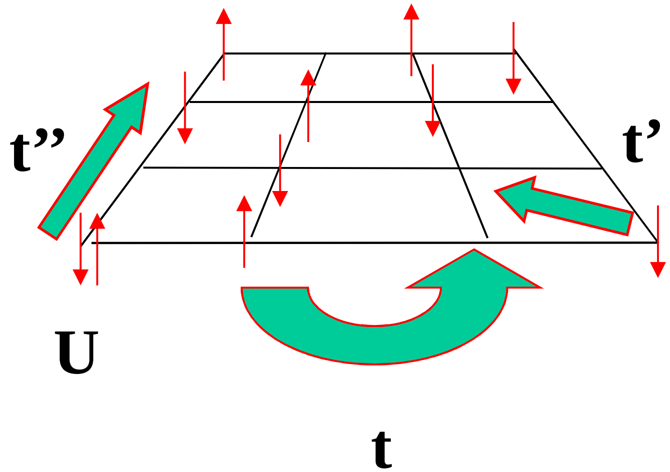
Figure: McWhan, PRB 1970; Limelette, Science 2003

Hubbard model

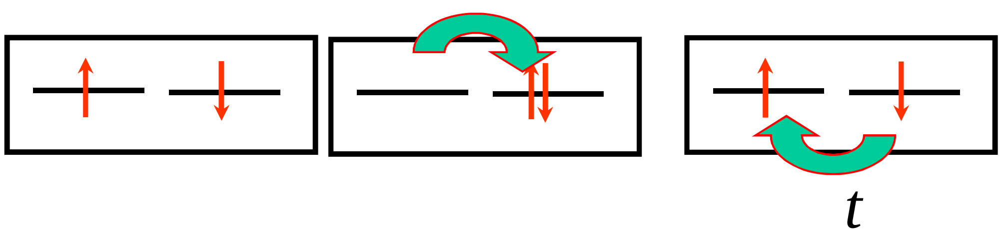


1931-1980

μ



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



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

Superconductivity and attraction?

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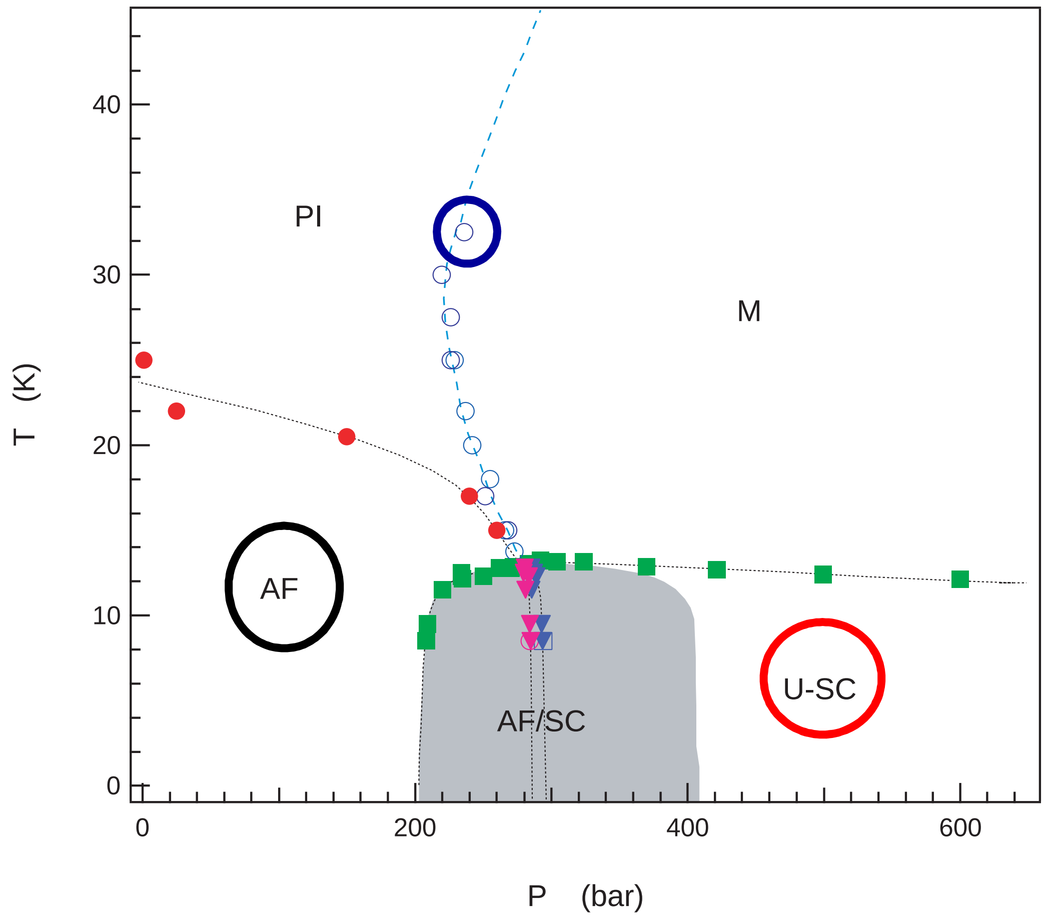
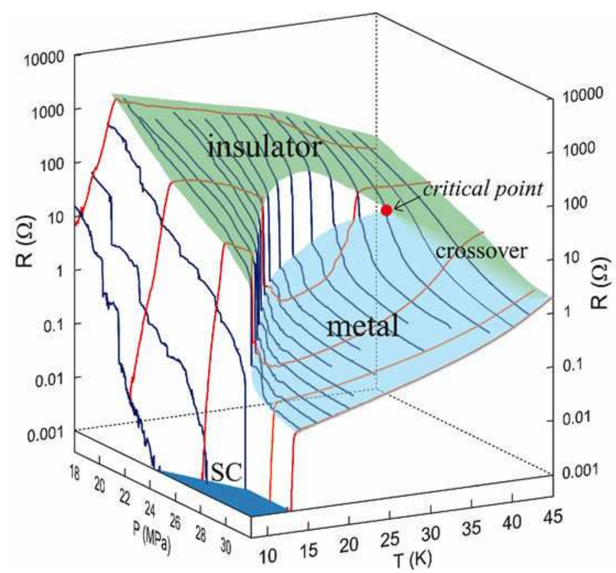
Bare Mott critical point in organics





F. Kagawa, K. Miyagawa, + K. Kanoda
PRB **69** (2004) +Nature **436** (2005)

Phase diagram (X=$Cu[N(CN)_2]Cl$)

S. Lefebvre et al. PRL **85**, 5420 (2000), P. Limelette, et al. PRL **91** (2003)

CIAR The Canadian Institute for Advanced Research

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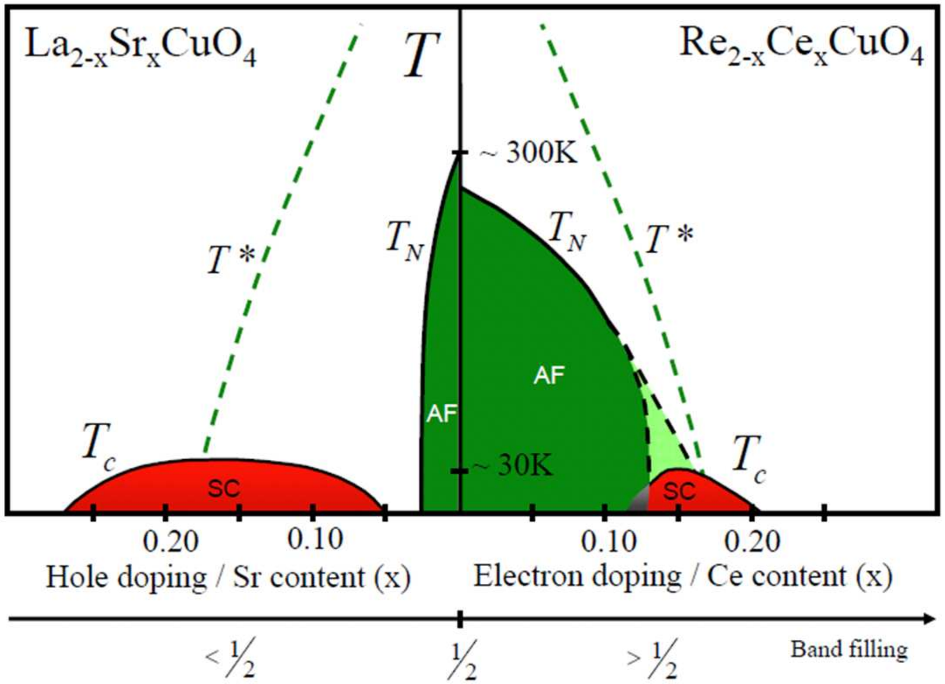
High-temperature superconductors

Armitage, Fournier, Greene, RMP (2009)

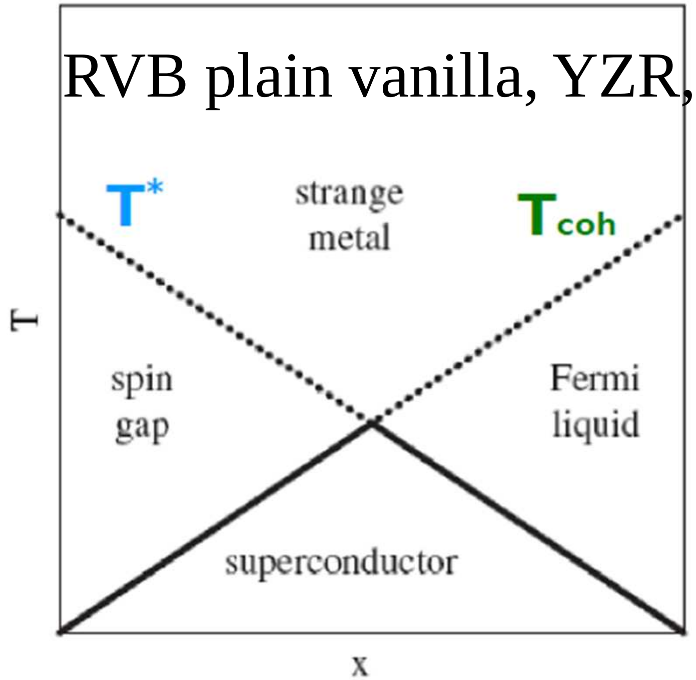


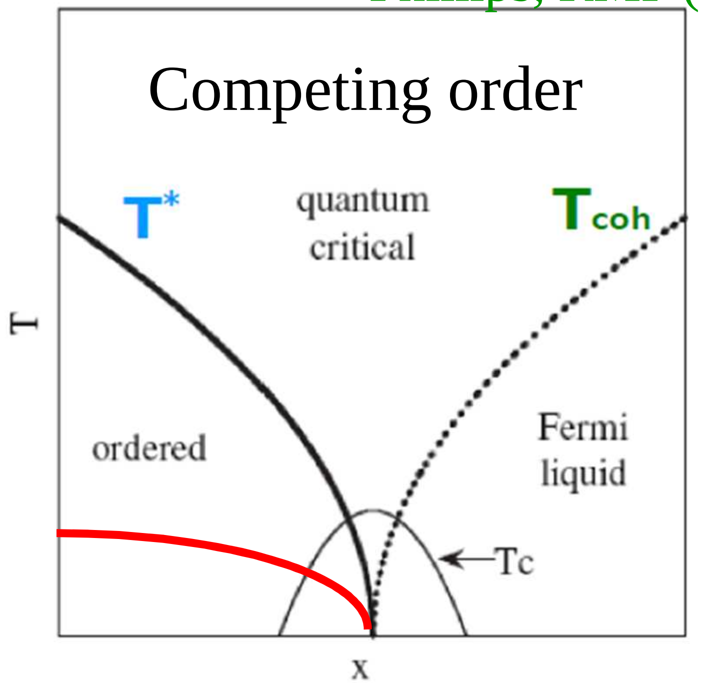
What is under the dome?
Mott Physics away from $n = 1$

- 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)

Two views (caricature)

Norman, Adv. Phys. (2005)
Broun, Nat. Phys. (2006)
Phillips, RMP (2010)





Why T_c decreases?
What is the origin of T^*?
What is the strange metal?

Broken symmetry or not.
What lies beneath the dome.
Mott Physics away from $n = 1$

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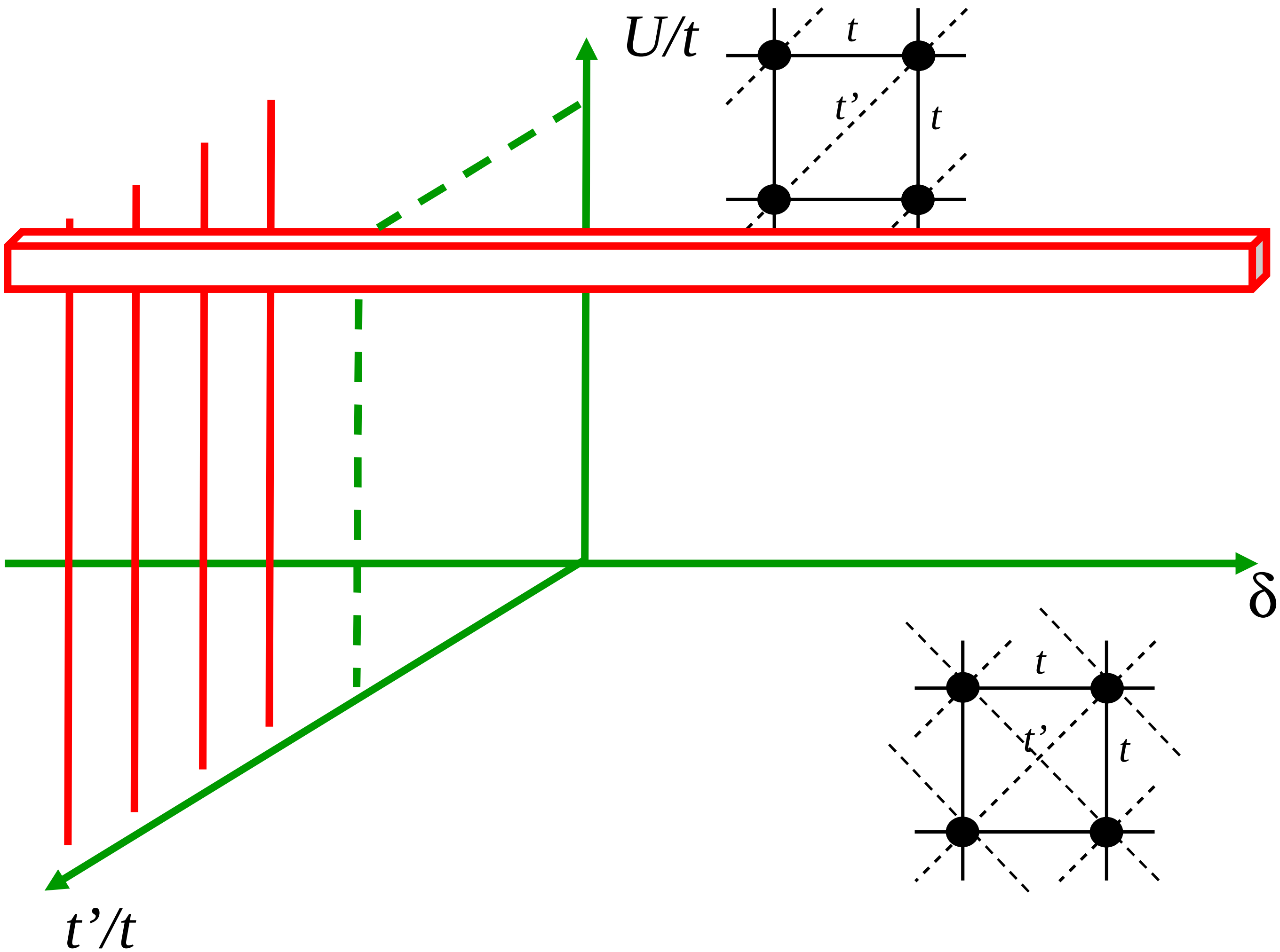
Perspective



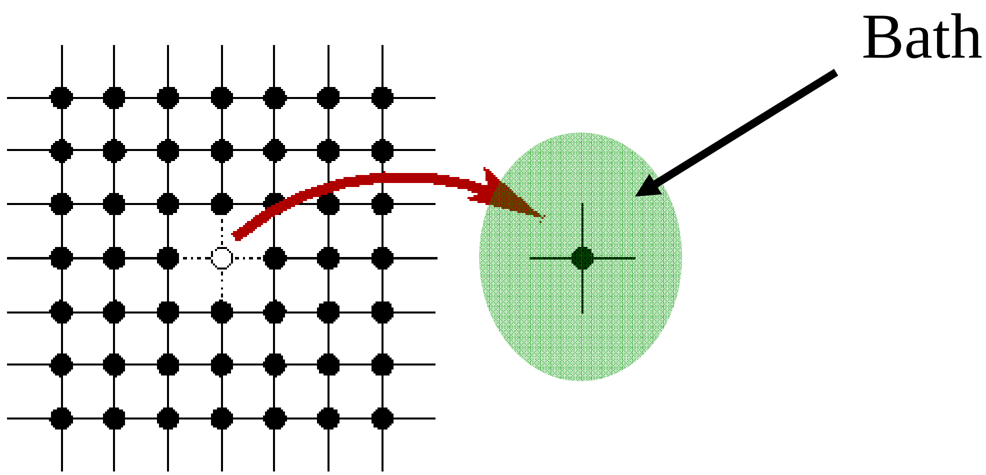
Outline

- Method
- *T=0* phase diagram
  - The « glue »
- Finite *T* phase diagram
  - Normal state
    - First order transition
    - Widom line and pseudogap
  - Superconductivity

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)

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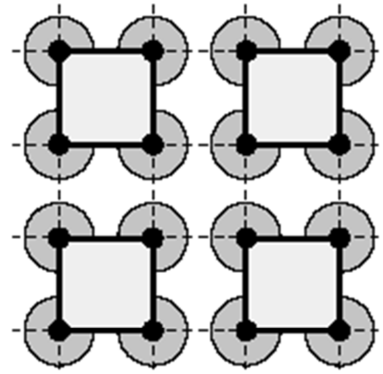
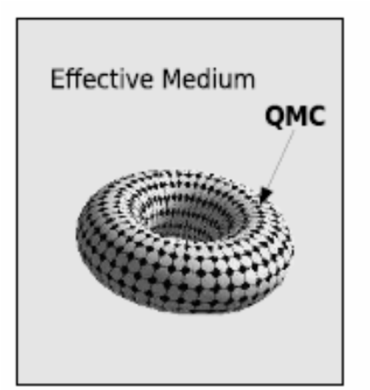
2d Hubbard: Quantum cluster method

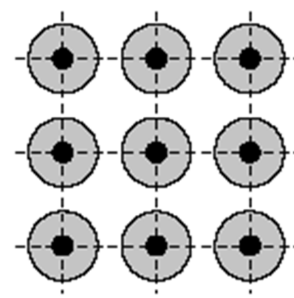
C-DMFT





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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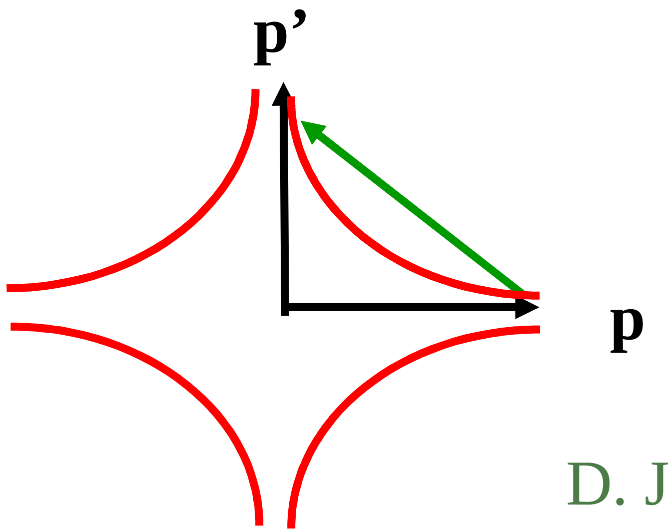
Not perfect!

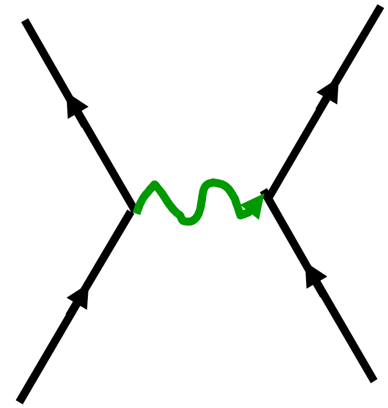
- Long range order:
  - Allow symmetry breaking in the bath (mean-field)
- Missing:
  - Long wavelength fluctuations
- Included:
  - Short-range dynamical and spatial correlations

A bit of physics: superconductivity and repulsion

Cartoon « BCS » weak-coupling picture

$$\Delta_{\mathbf{p}} = -\frac{1}{2V}\sum_{\mathbf{p}'} U(\mathbf{p}-\mathbf{p}')\frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}}\left(1-2n\left(E_{\mathbf{p}'}\right)\right)$$





Exchange of spin waves?
Kohn-Luttinger
T_c with pressure

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

D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch P.R. B **34**, 8190-8192 (1986).
Béal–Monod, Bourbonnais, Emery P.R. B. **34**, 7716 (1986).
Kohn, Luttinger, P.R.L. **15**, 524 (1965).

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A cartoon strong coupling picture

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

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

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

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

Pitaevskii Brückner:

Pair state orthogonal to repulsive core of Coulomb interaction

Kotliar and Liu, P.R. B **38,** 5142 (1988)

Miyake, Schmitt–Rink, and Varma

P.R. B **34**, 6554-6556 (1986)

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d-wave superconductivity

- Weak coupling
  - C. J. Halboth and W. Metzner, Phys. Rev. Lett. 85, 5162 (2000).
  - B. Kyung, J.-S. Landry, and A. M. S. Tremblay, Phys. Rev. B 68, 174502 (2003).
  - C. Bourbonnais and A. Sedeki, Physical Review B 80, 085105 (2009).
  - D. J. Scalapino, Physica C: Superconductivity 470, Supplement 1, S1 (2010), ISSN 0921-4534, proceedings of the 9th International Conference on Materials and Mech anisms of Superconductivity.
- Renormalized Mean-Field Theory
  - P. W. Anderson, P. A. Lee, M. Randeria, T. M. Rice, N. Trivedi, and F. C. Zhang, Journal of Physics: Condensed Matter 16, R755 (2004).
  - K.-Y. Yang, T. M. Rice, and F.-C. Zhang, Phys. Rev. B 73, 174501 (2006).
- Slave particles
  - P. A. Lee, N. Nagaosa, and X.-G. Wen, Rev. Mod. Phys. 78, 17 (2006).
  - M. Imada, Y. Yamaji, S. Sakai, and Y. Motome, Annalen der Physik 523, 629 (2011)
- Variational approaches
  - T. Giamarchi and C. Lhuillier, Phys. Rev. B 43, 12943 (1991).
  - A. Paramekanti, M. Randeria, and N. Trivedi, Phys. Rev. B 70, 054504 (2004).

d-wave superconductivity

- Quantum cluster methods
  - T. Maier, M. Jarrell, T. Pruschke, and J. Keller, Phys. Rev. Lett. 85, 1524 (2000).
  - David Sénéchal, P.-L. Lavertu, M.-A. Marois and A.-M. S. Tremblay, PRL **94**, 156404 (2005).
  - T. A. Maier, M. Jarrell, T. C. Schulthess, P. R. C. Kent, and J. B. White, Phys. Rev. Lett. 95, 237001 (2005).
  - K. Haule and G. Kotliar, Phys. Rev. B 76, 104509 (2007).
  - Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST , Phys. Rev. B (2008)
  - Many more…

But…

QMC constrained path

S. Zhang, Carlson, Gubernatis Phys. Rev. Lett. 78, 4486 (1997)

Refined variational approach: no

Aimi and Imada, J. Phys. Soc. Jpn (2007)

T = 0 phase diagram: cuprates

Phase diagram

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

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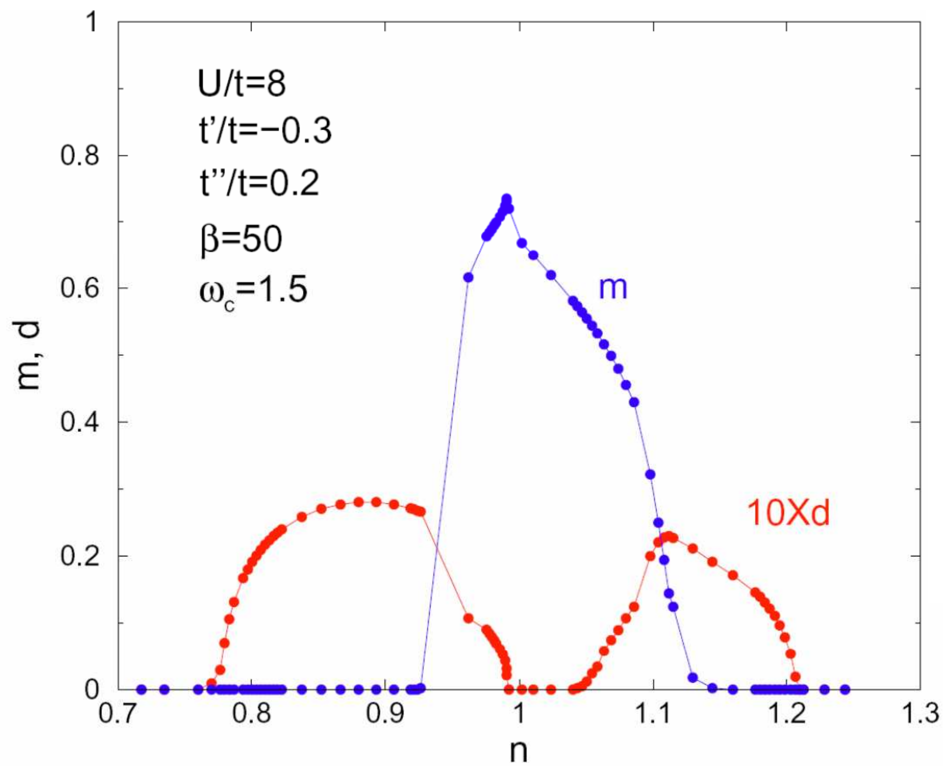
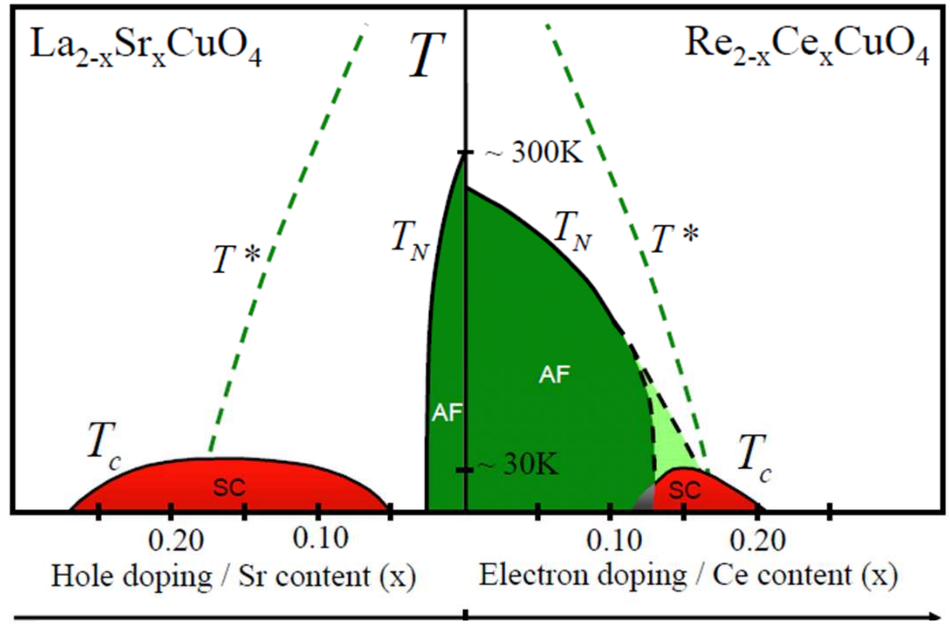
CDMFT global phase diagram



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



Armitage, Fournier, Greene, RMP (2009)



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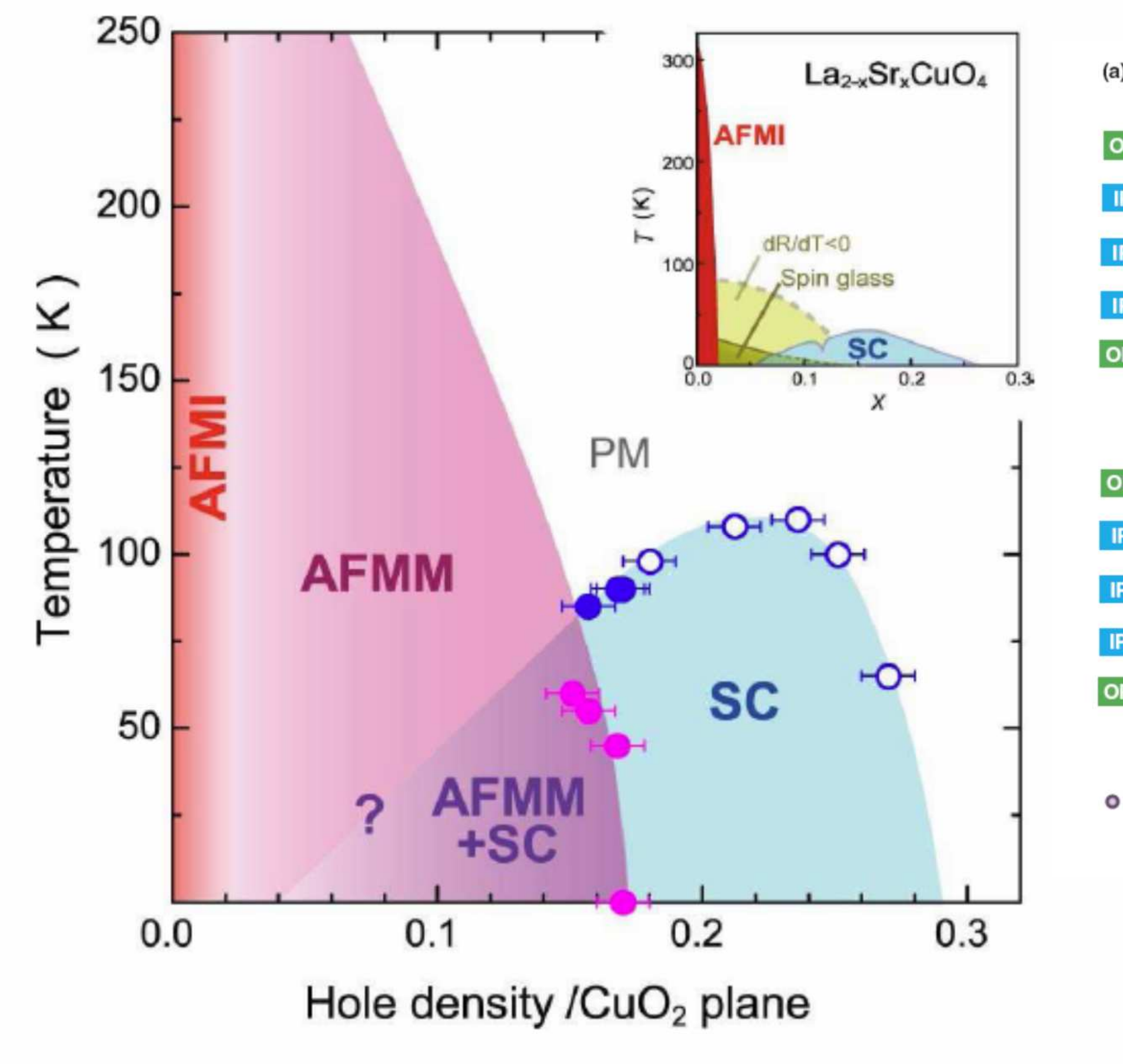
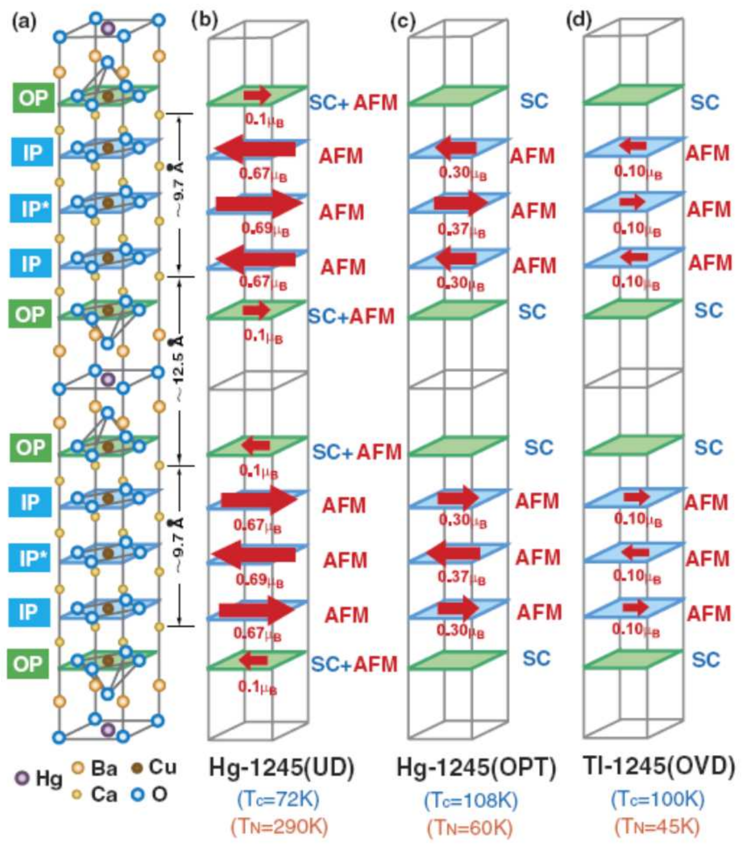
Consistent with following experiments

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





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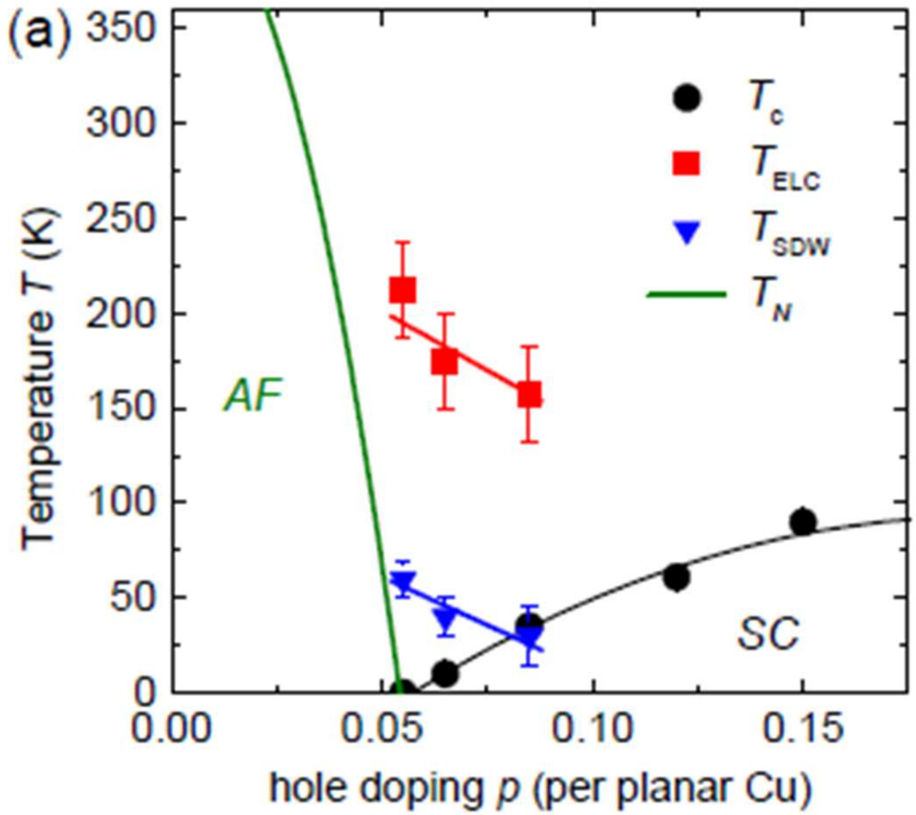
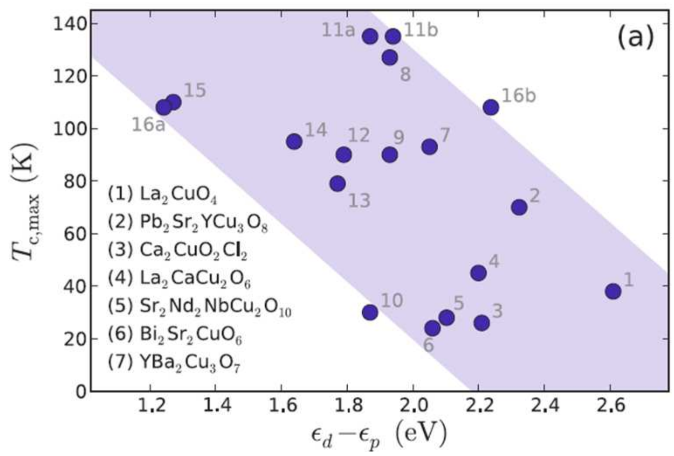
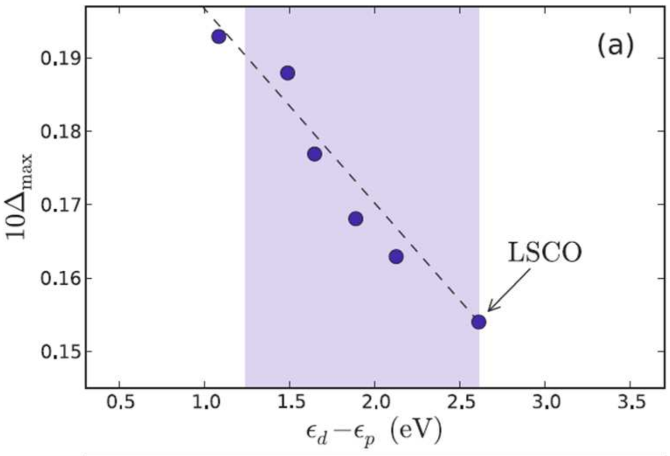
Magnetic phase diagram of YBCO



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

Materials dependent properties





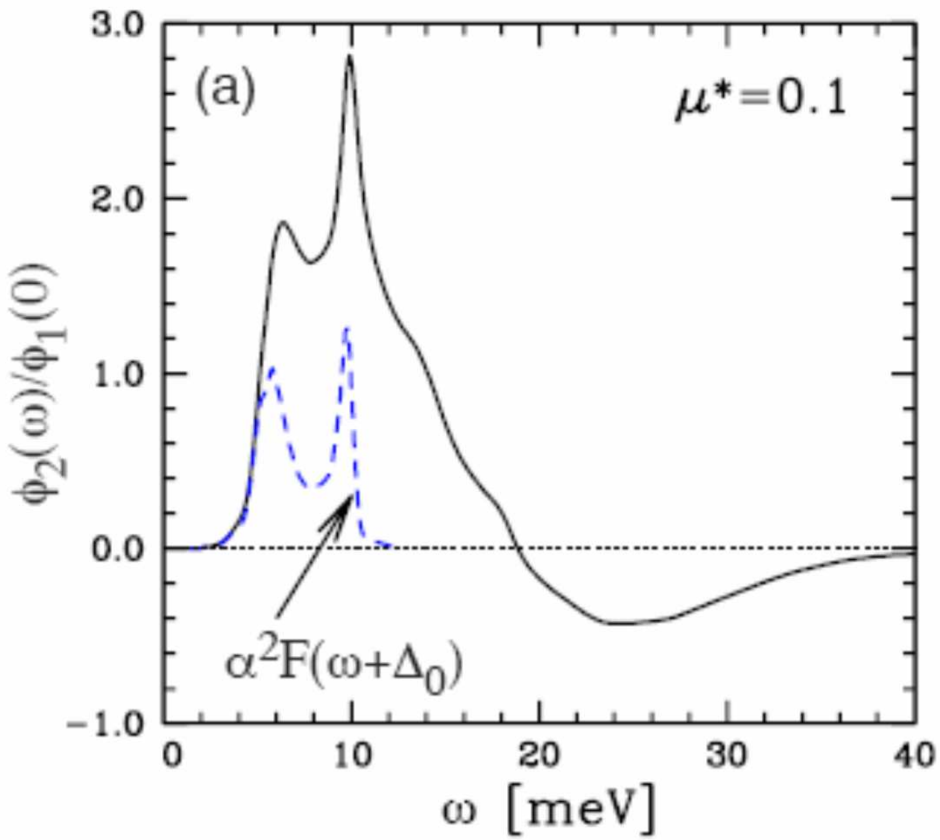
C. Weber, C.-H. Yee, K. Haule, and G. Kotliar, ArXiv e-prints (2011), 1108.3028.

$T = 0$ phase diagram

The glue

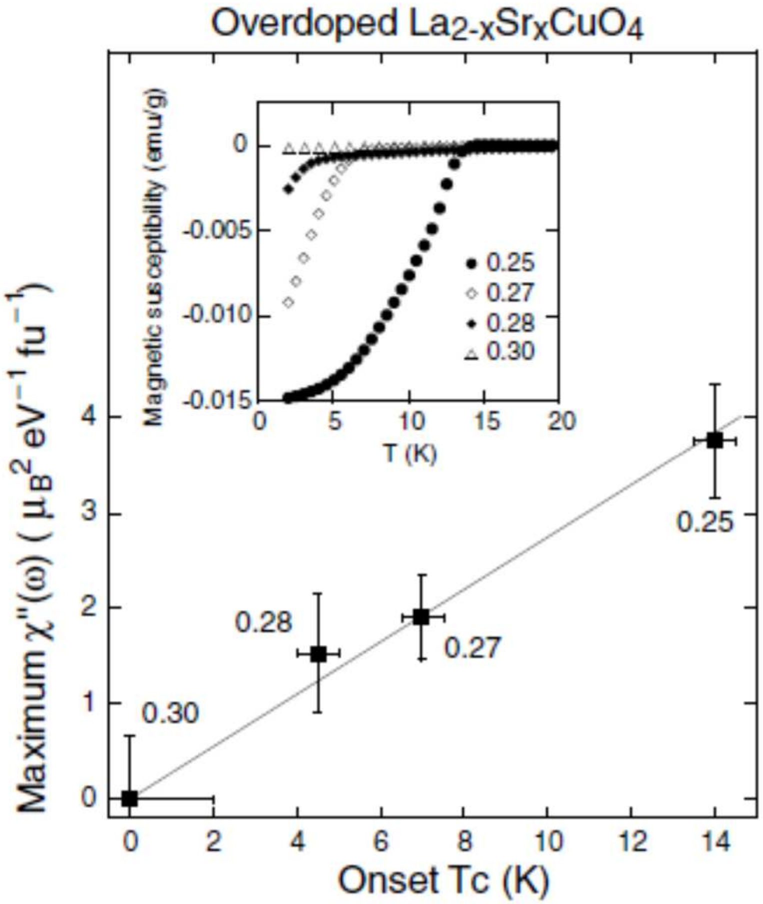
Im Σ_{an} and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

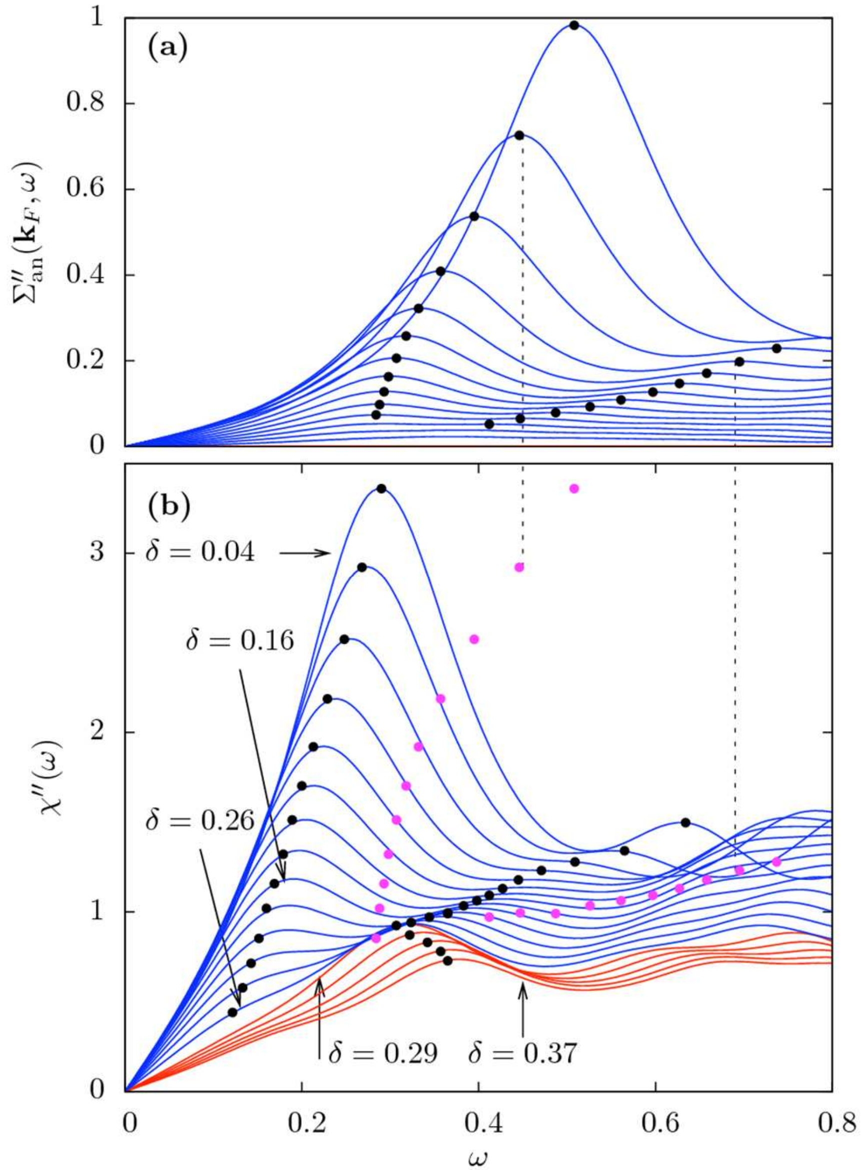


The glue

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



Wakimoto … Birgeneau PRL (2004)



The glue and neutrons

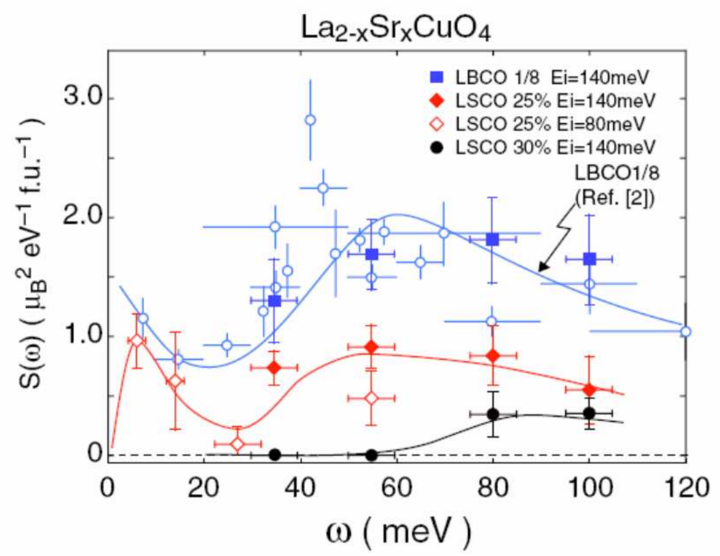
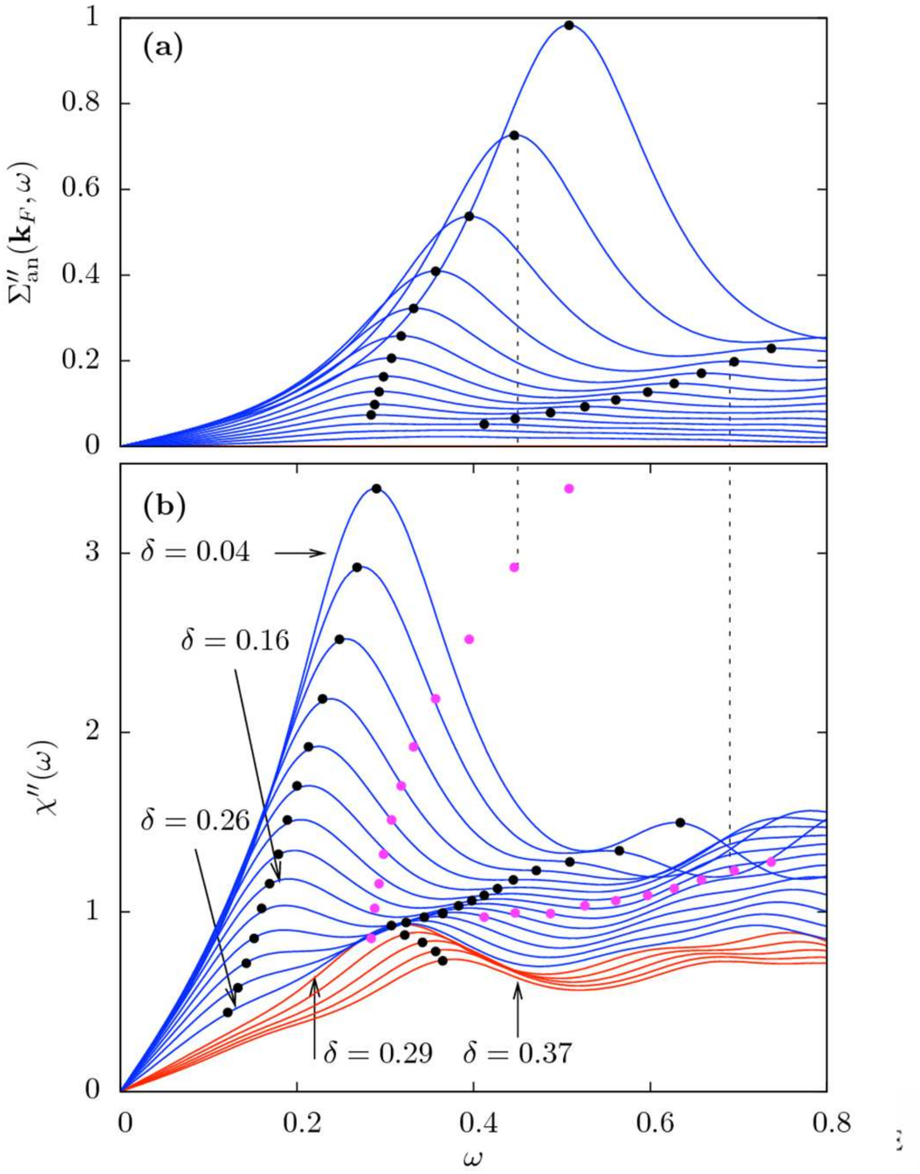


FIG. 3 (color online). **Q**-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i = 140$ meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO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



Outline

- Method
- *T=0* phase diagram
  - The « glue »
- Finite *T* phase diagram
  - Normal state
    - First order transition
    - Widom line and pseudogap
  - Superconductivity

Finite *T* phase diagram

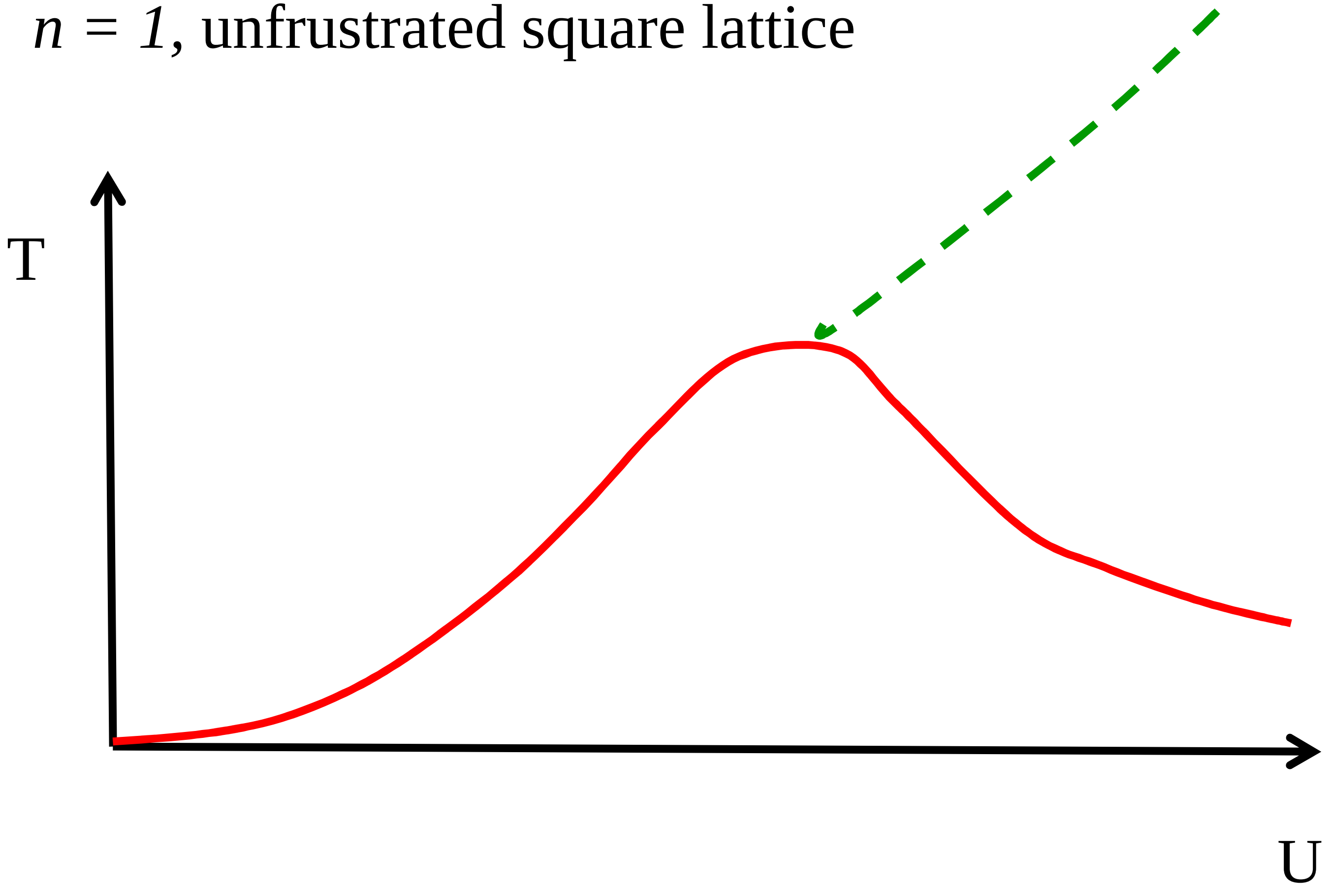
Normal state of the cuprates

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

- Fermi liquid
  - Start from Fermi sea
  - Self-energy analytical
  - One to one correspondence of elementary excitations
  - Landau parameters
  - Long-wavelength collective modes can become unstable
- Mott insulator
  - Hubbard model
  - Atomic limit
  - Self-energy singular
  - DMFT
  - How many sites in the cluster determines how low in temperature your description of the normal state is valid.
  - Long-wavelength collective modes can become unstable

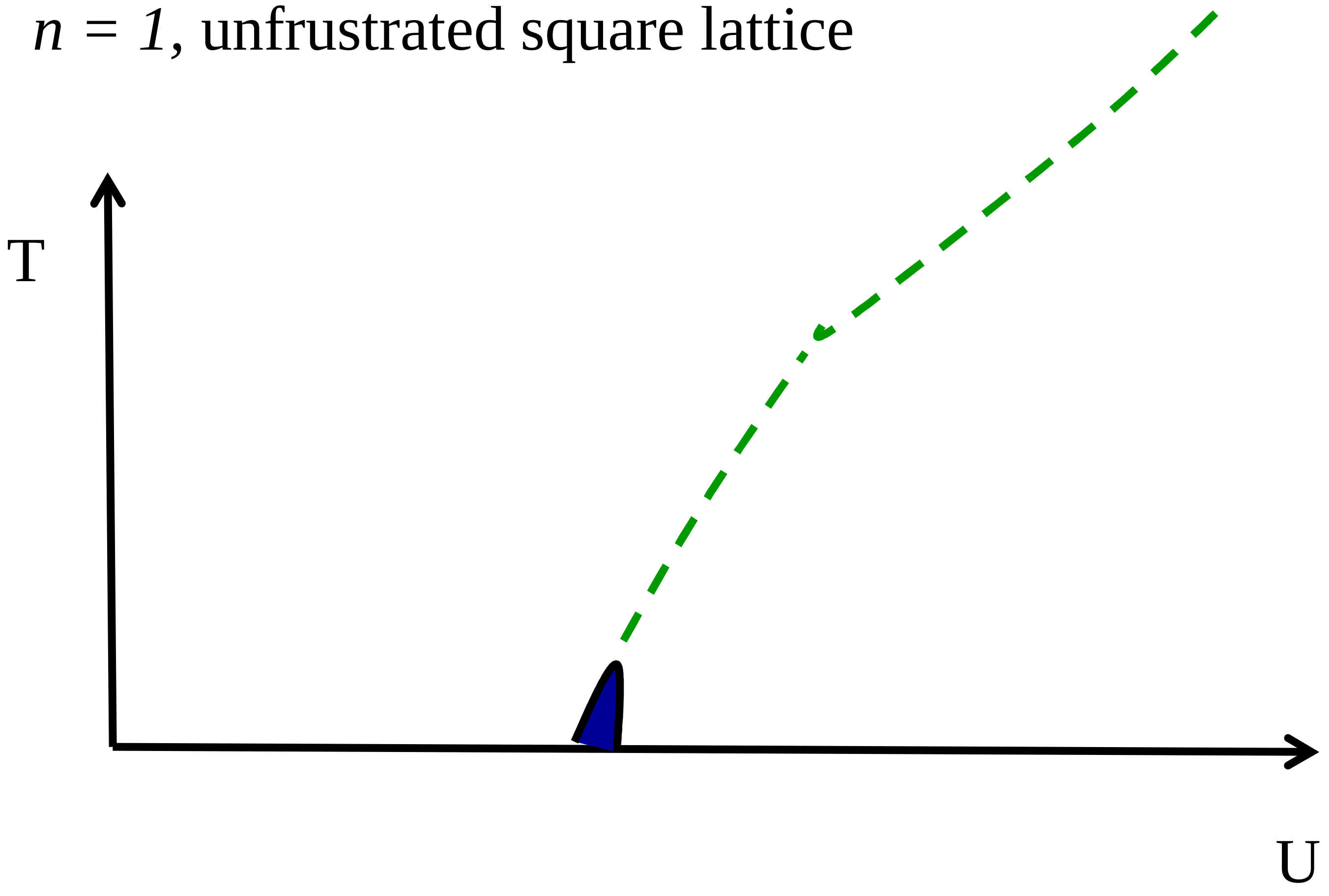
Local moment and Mott transition

n = 1, unfrustrated square lattice

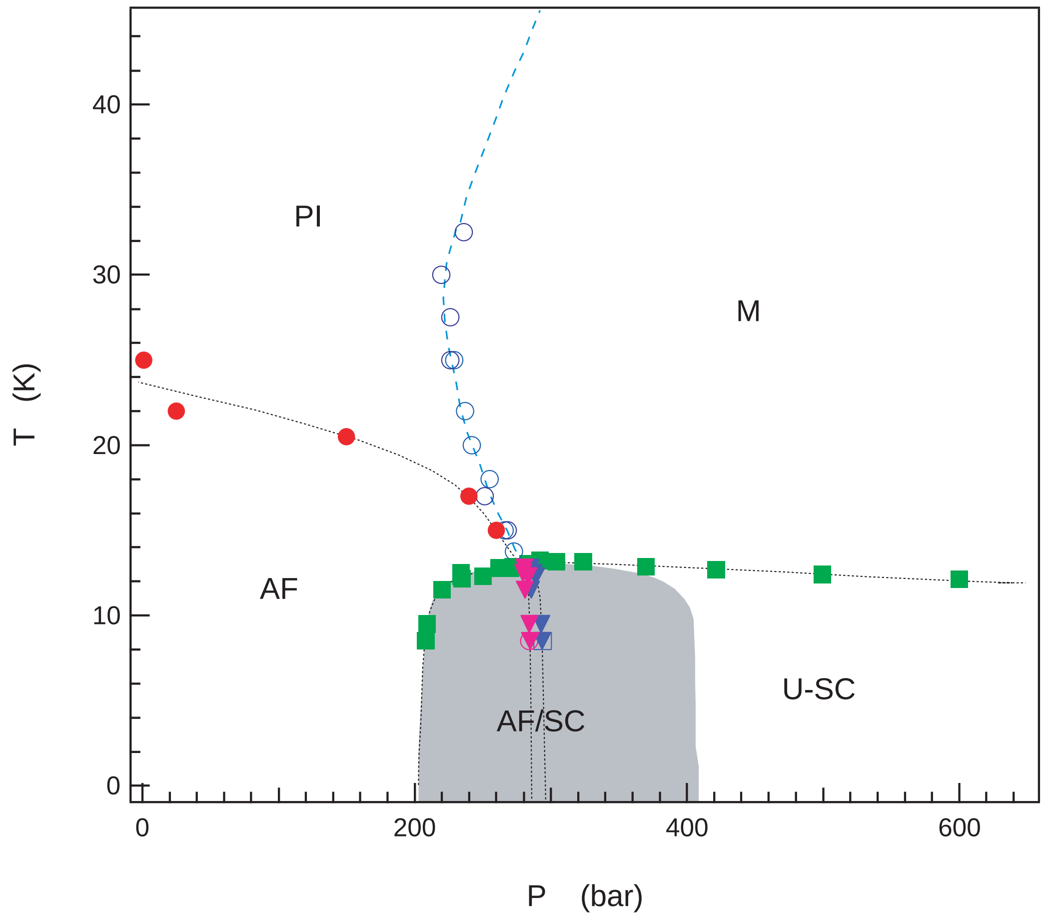


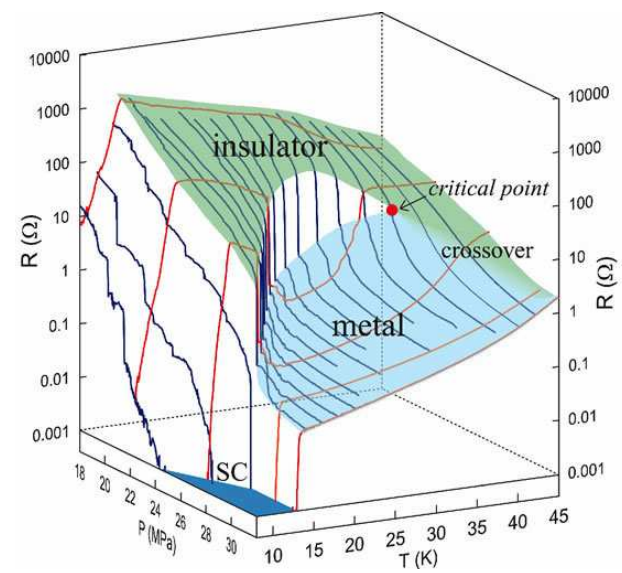
Local moment and Mott transition

n = 1, unfrustrated square lattice



Bare Mott critical point in organics





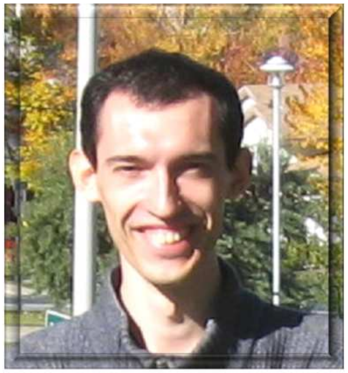
F. Kagawa, K. Miyagawa, + K. Kanoda
PRB **69** (2004) +Nature **436** (2005)

Phase diagram (X=Cu[N(CN)$_2$]Cl)

S. Lefebvre et al. PRL **85**, 5420 (2000), P. Limelette, et al. PRL **91** (2003)

Finite *T* phase diagram

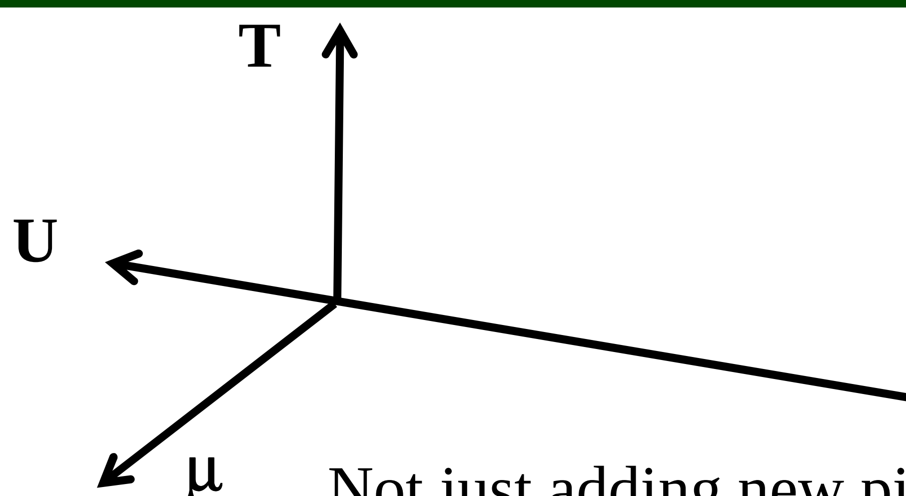
Normal state of the cuprates



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

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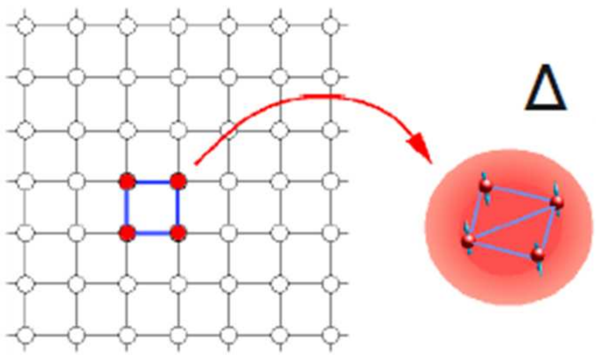
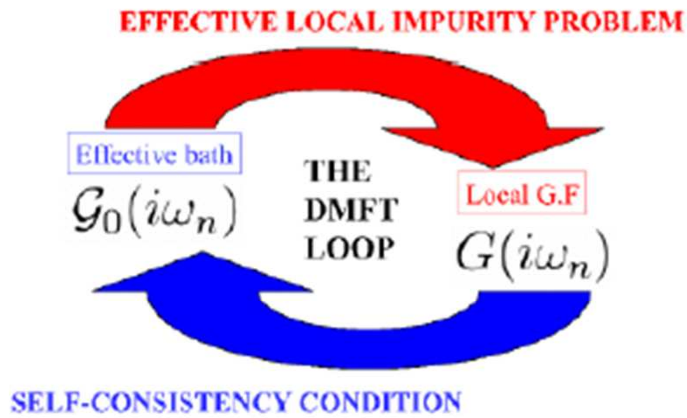
C-DMFT



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



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

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

Solving cluster in a bath problem

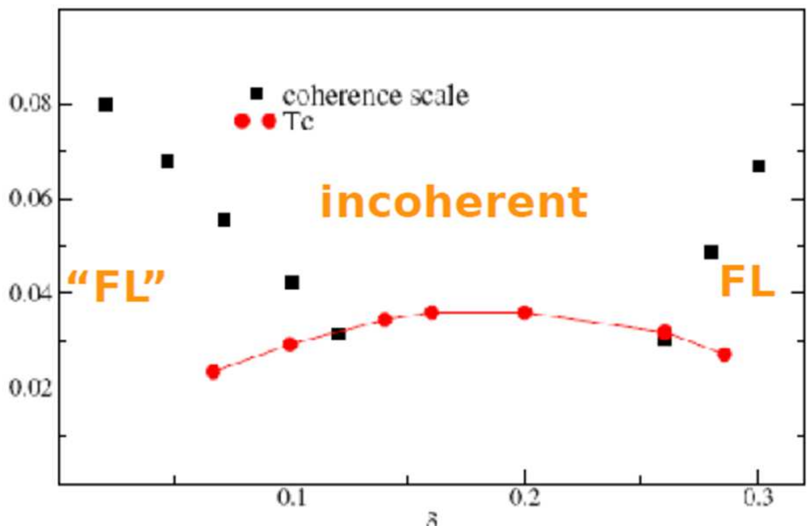
- Continuous-time Quantum Monte Carlo calculations to sum all diagrams generated from expansion in powers of hybridization.

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

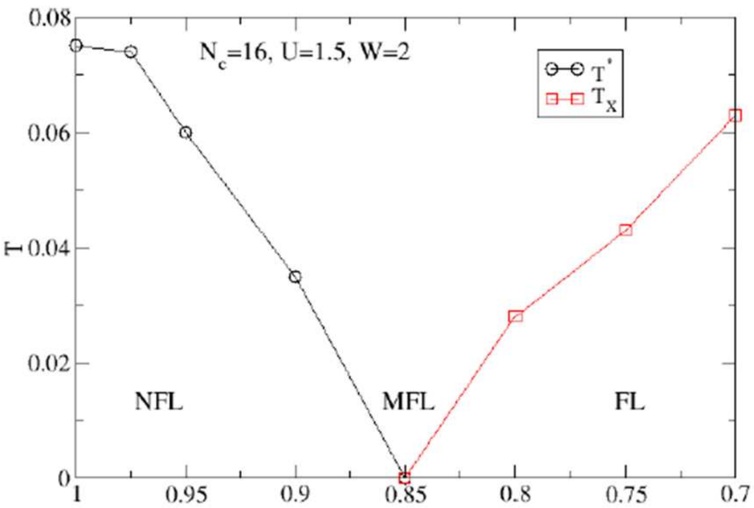
  – K. Haule, Phys. Rev. B **75**, 155113 (2007).

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)

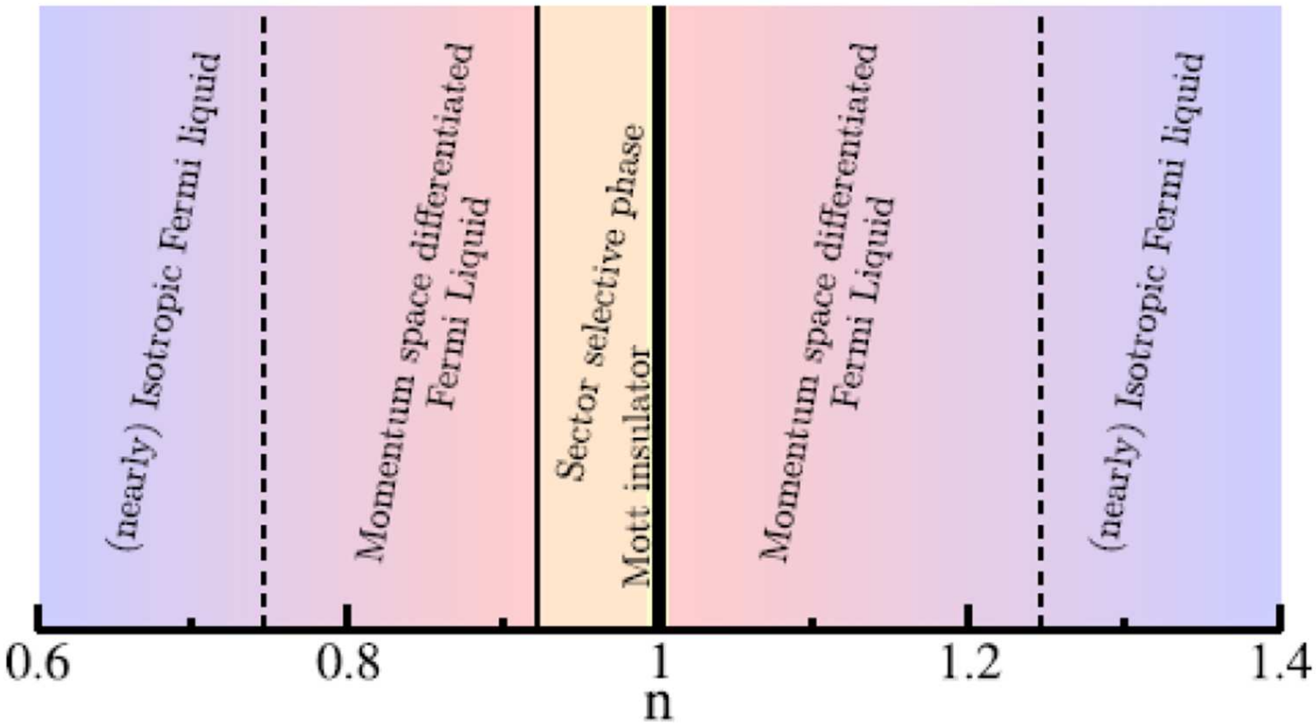


K. Haule, G. Kotliar, PRB (2008)



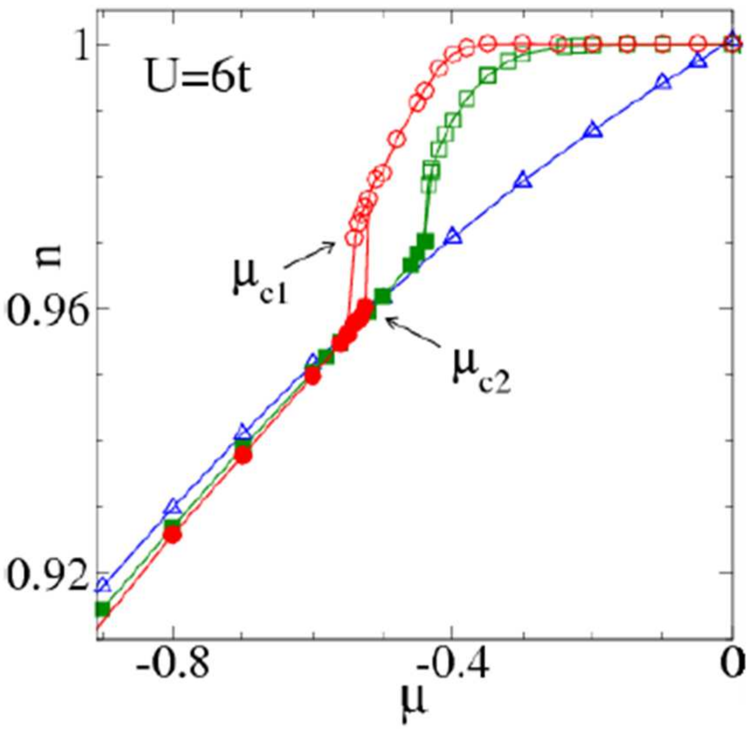
Vildhyadhiraja, PRL (2009)

Doping driven Mott transition



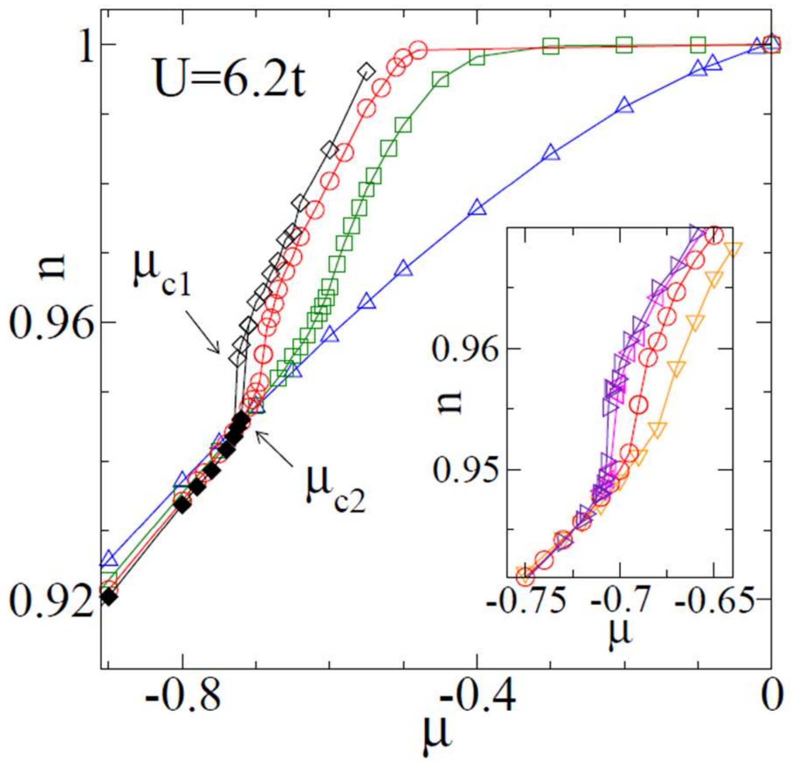
Gull, Werner, Millis, (2009)

First order transition at finite doping

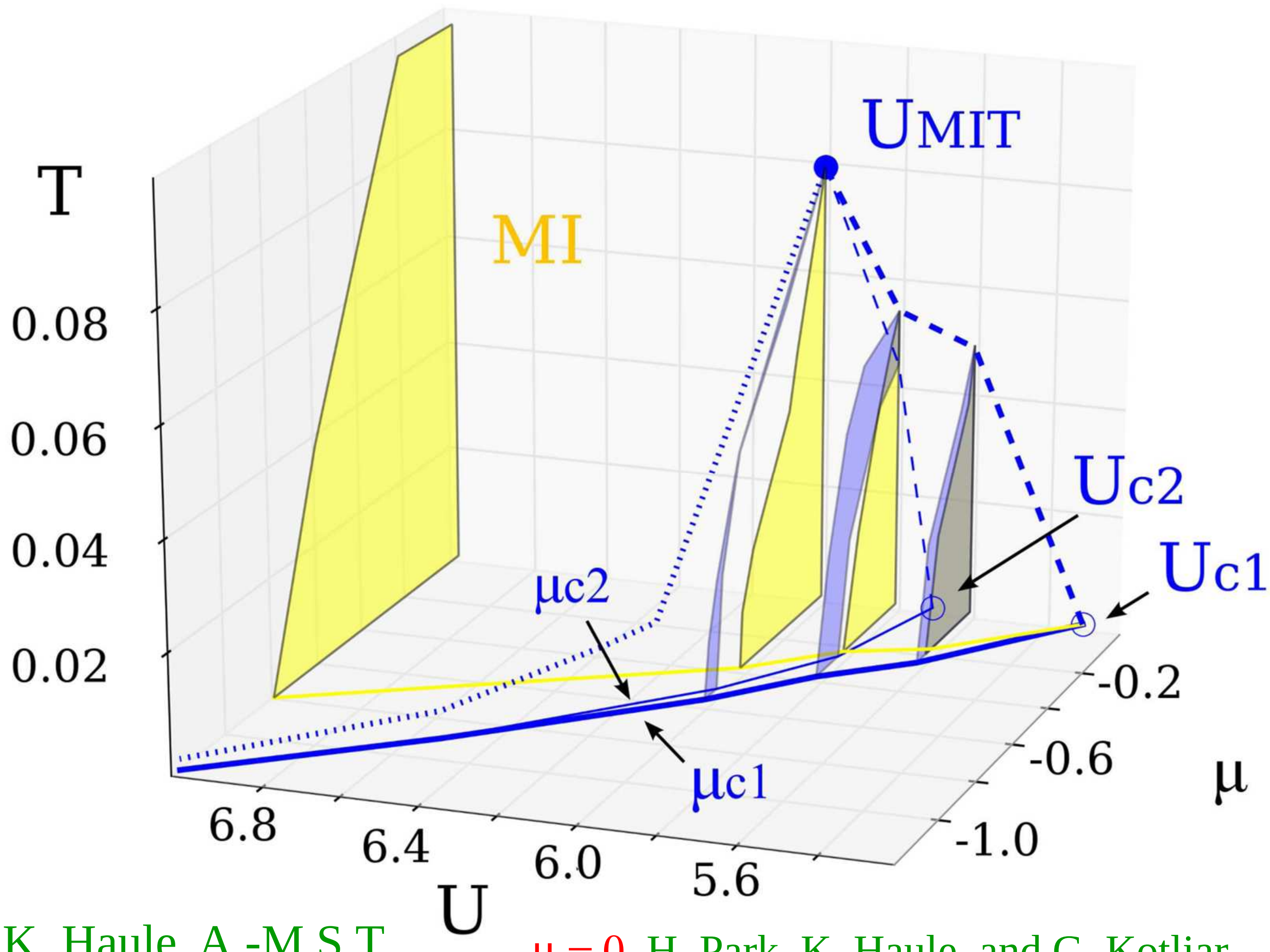


$n(\mu)$ for several temperatures:
$T/t =$1/10, 1/25, 1/50

The critical point



Normal state phase diagram



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

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

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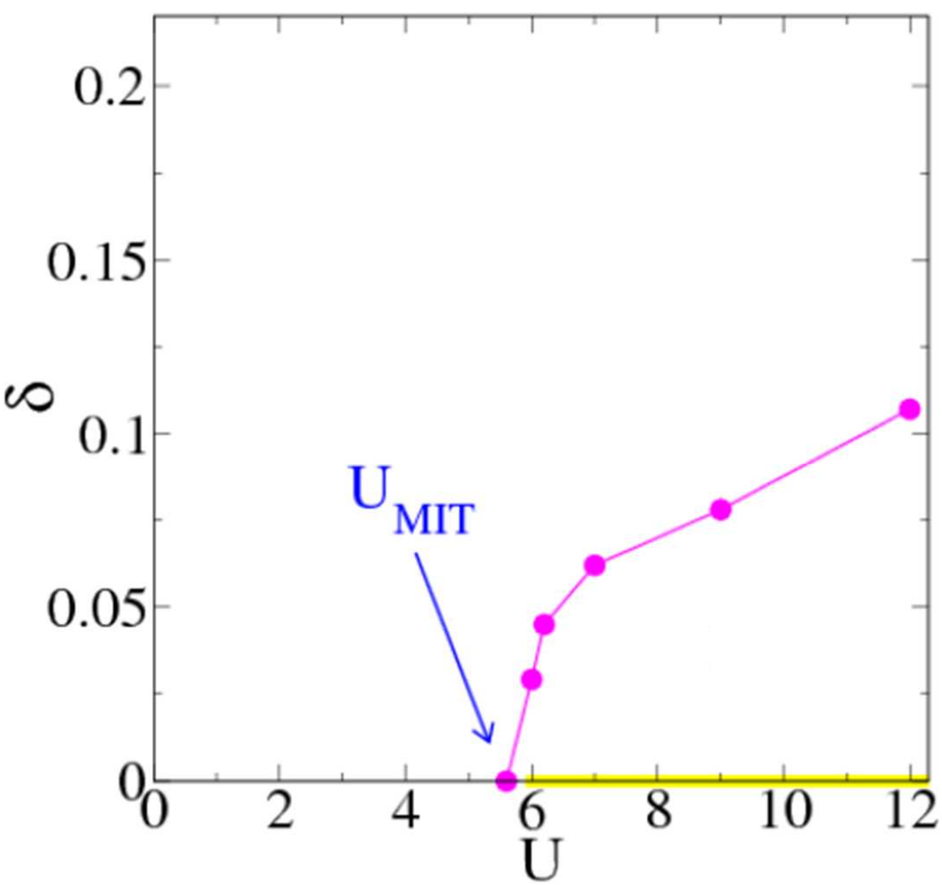
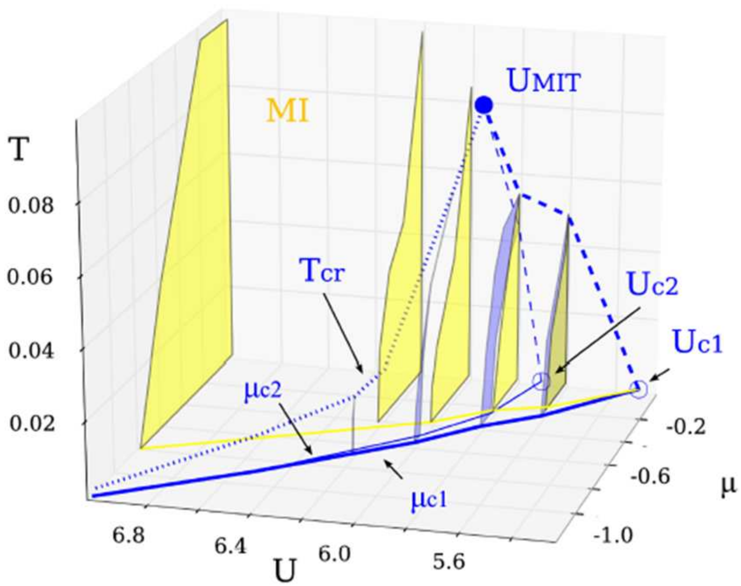
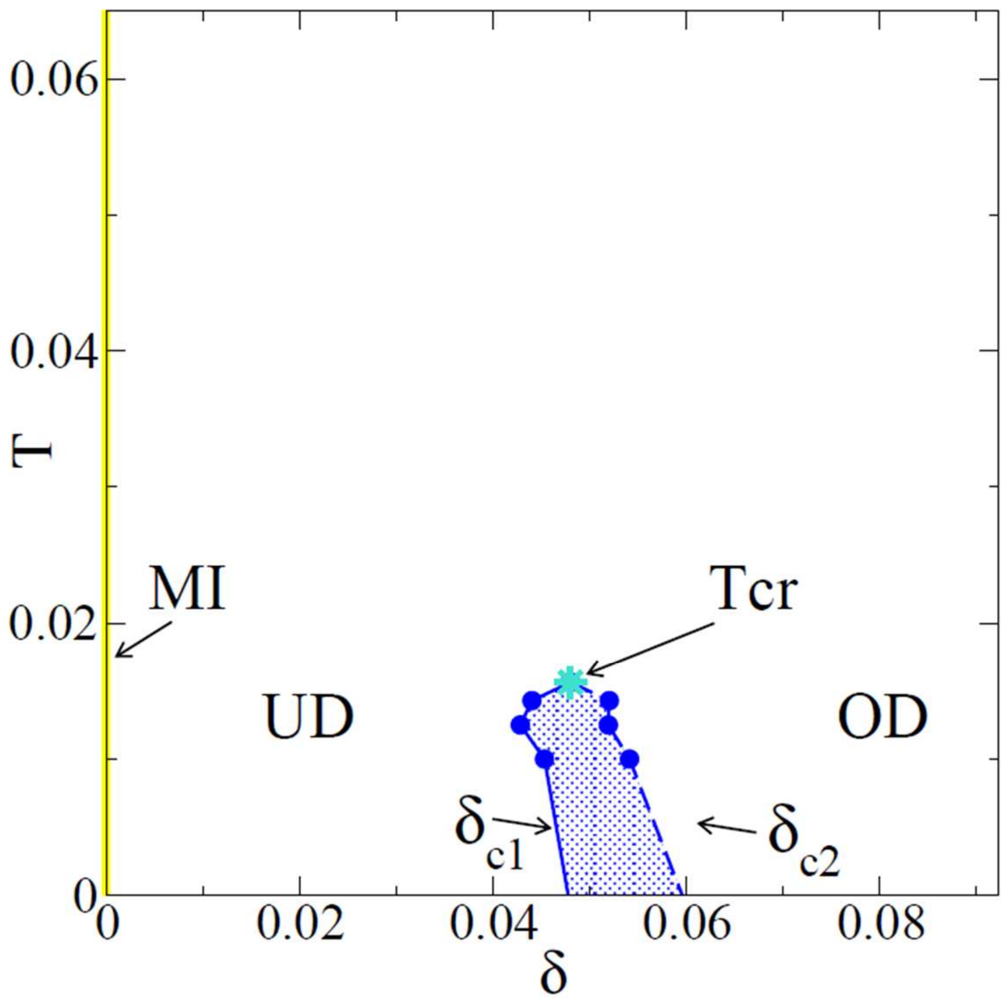
Link to Mott transition up to optimal doping

Doping dependence of critical point as a function of U





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



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

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

Here "optimal doping" $\delta_{\mathrm{c}} =$ doping at which the 1st order transition occurs

How does the UD phase differ from the OD phase?

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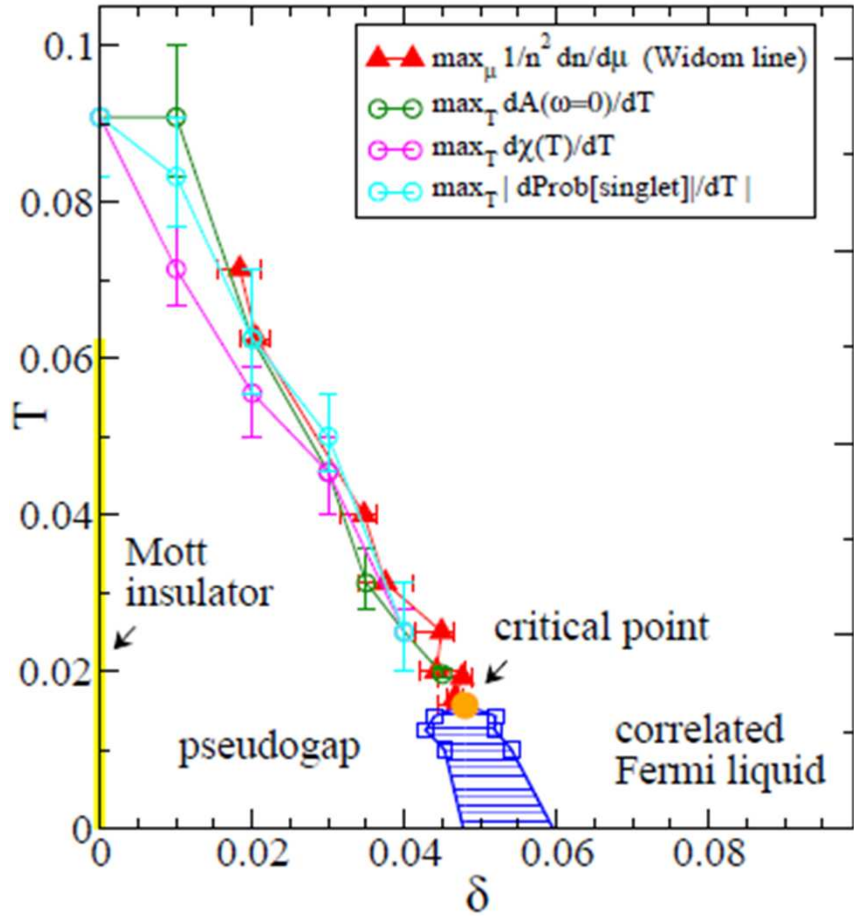
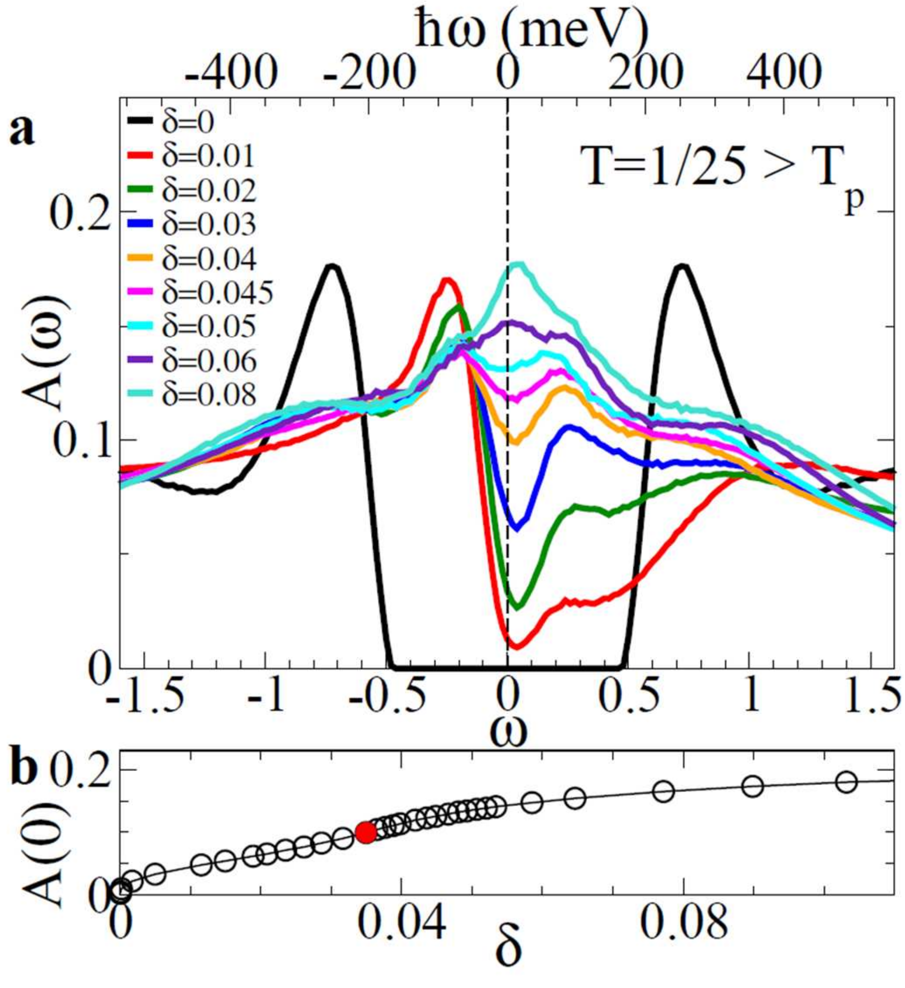
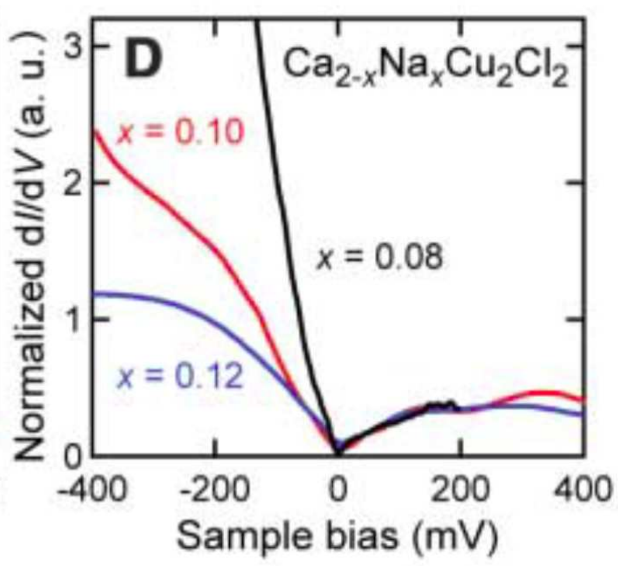
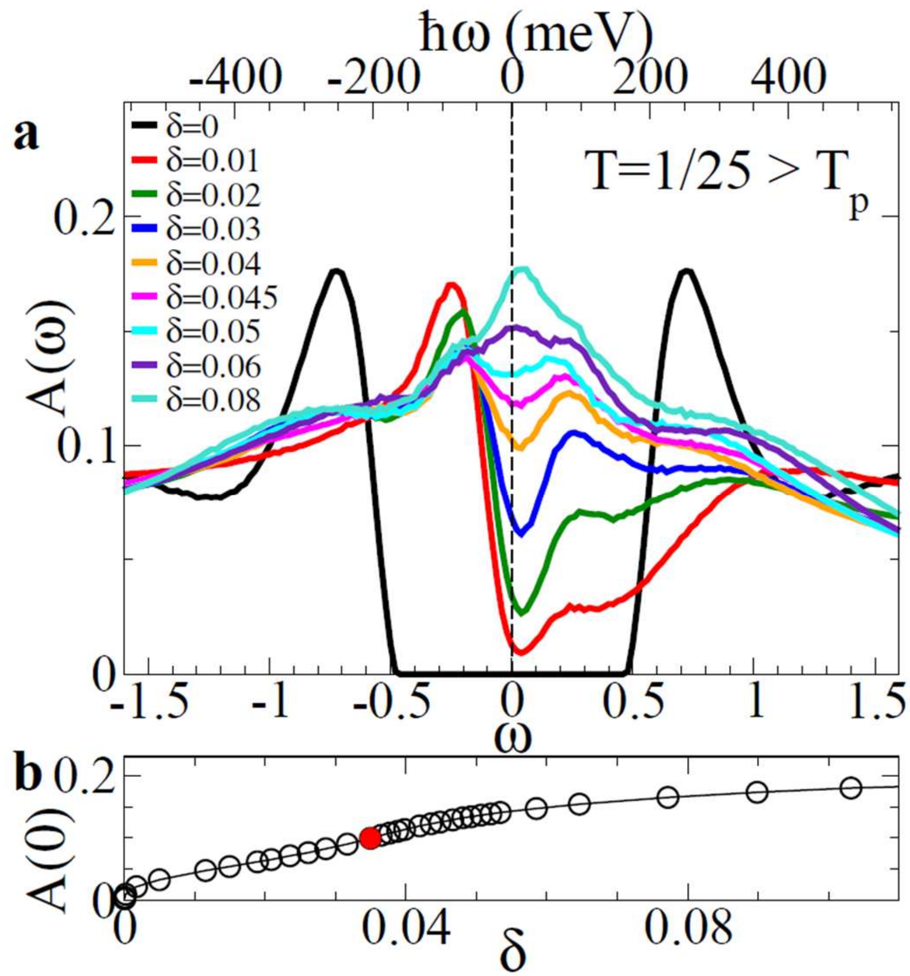
Density of states





Density of states





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

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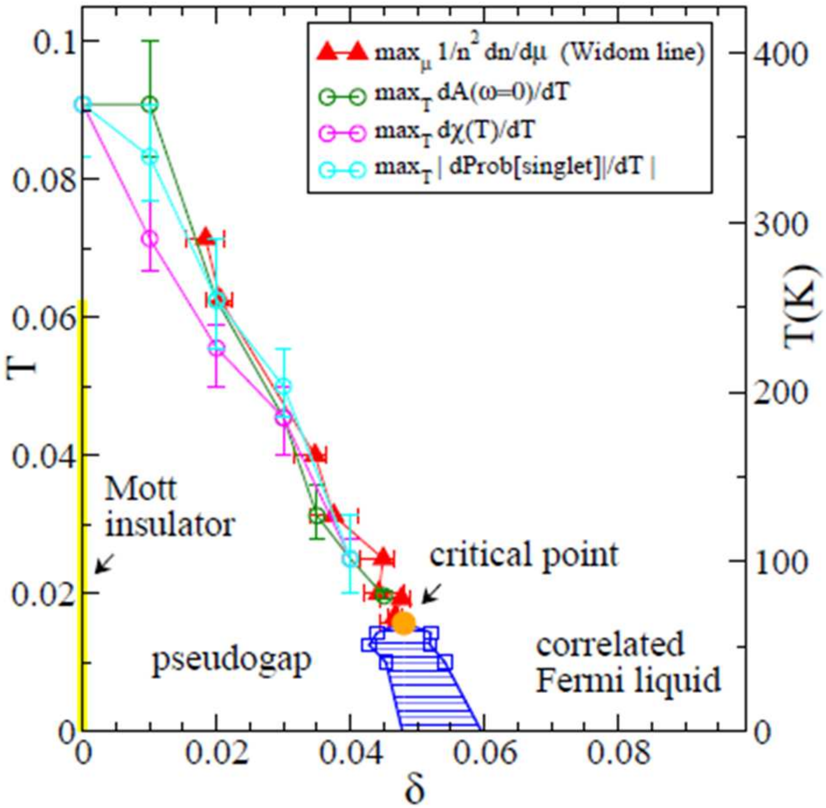
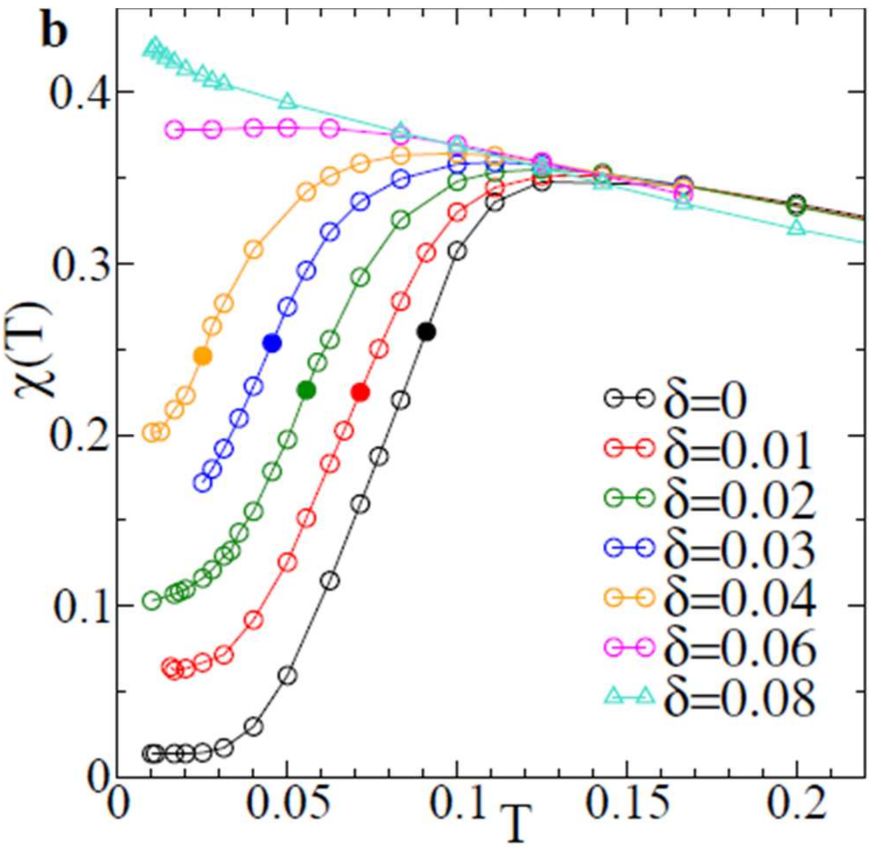
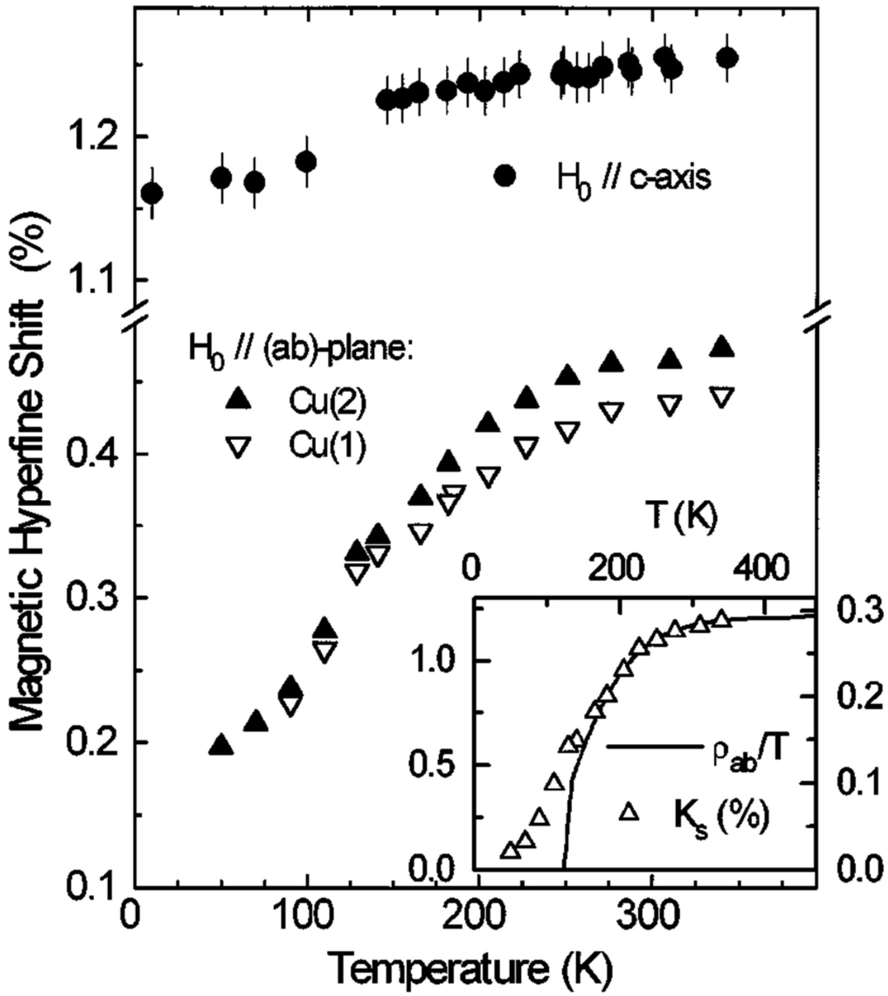
Spin susceptibility



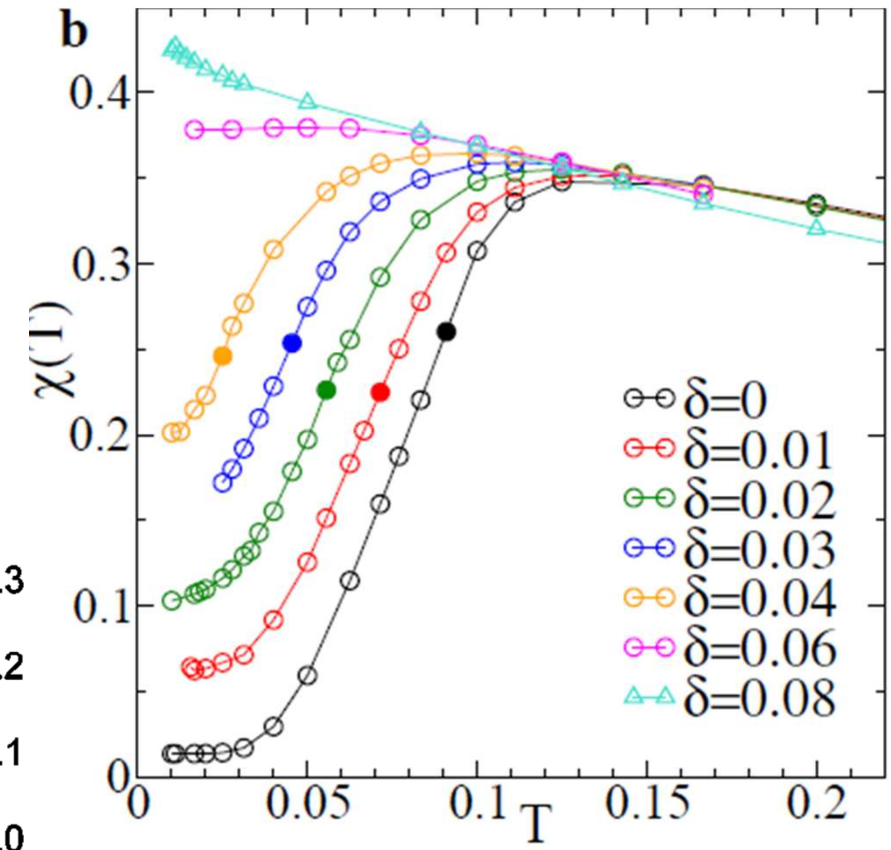


Spin susceptibility



Underdoped Hg1223

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



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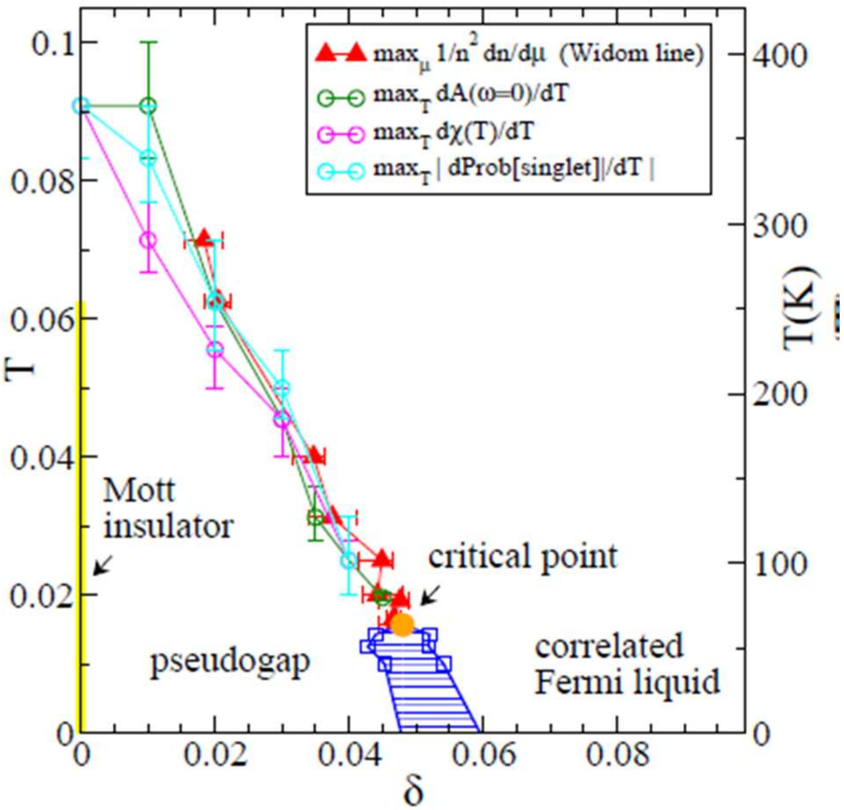
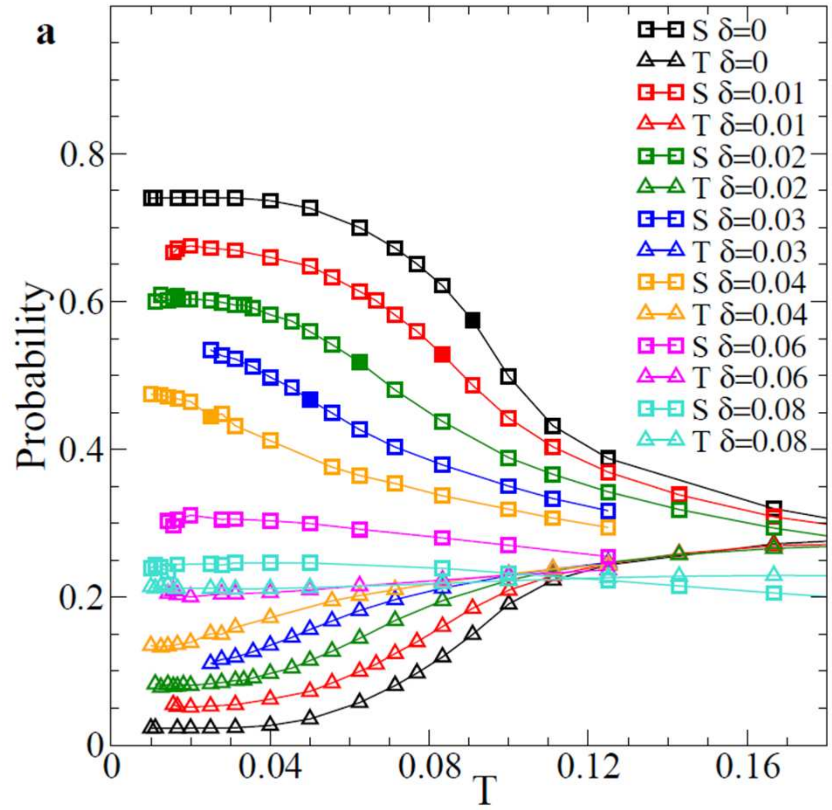
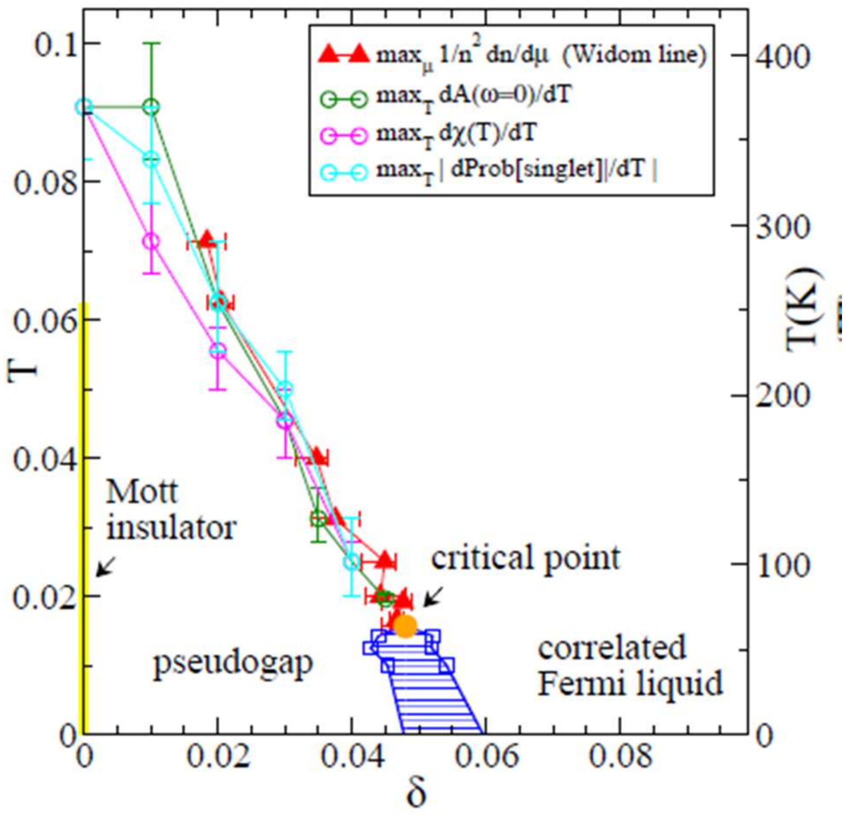
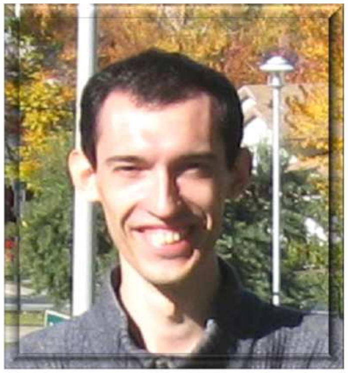
Plaquette eigenstates





Pseudogap *T** along the Widom line





Giovanni Sordi

Patrick Sémon

Kristjan Haul

Finite *T* phase diagram

Pseudogap in the normal state and the Widom line

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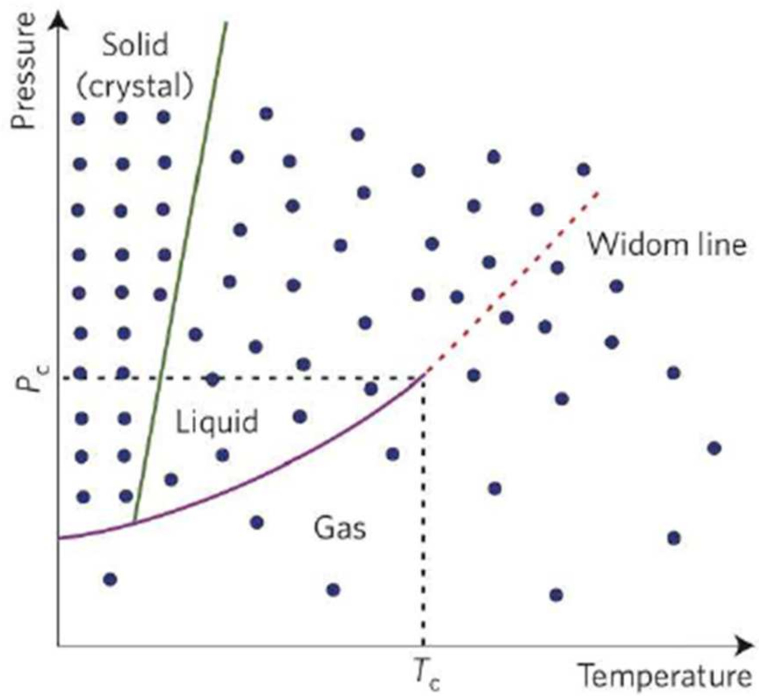
What is the Widom line?



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

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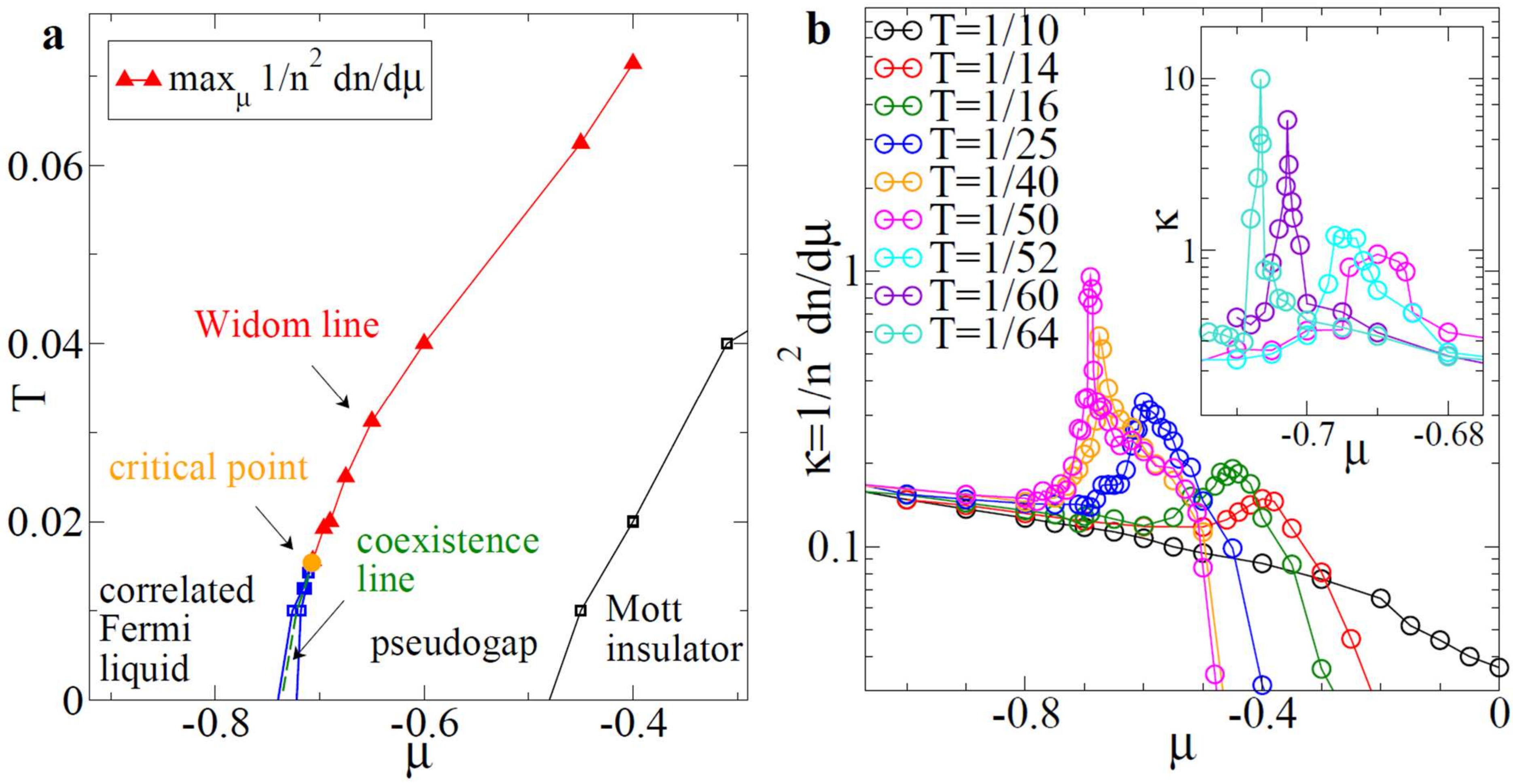
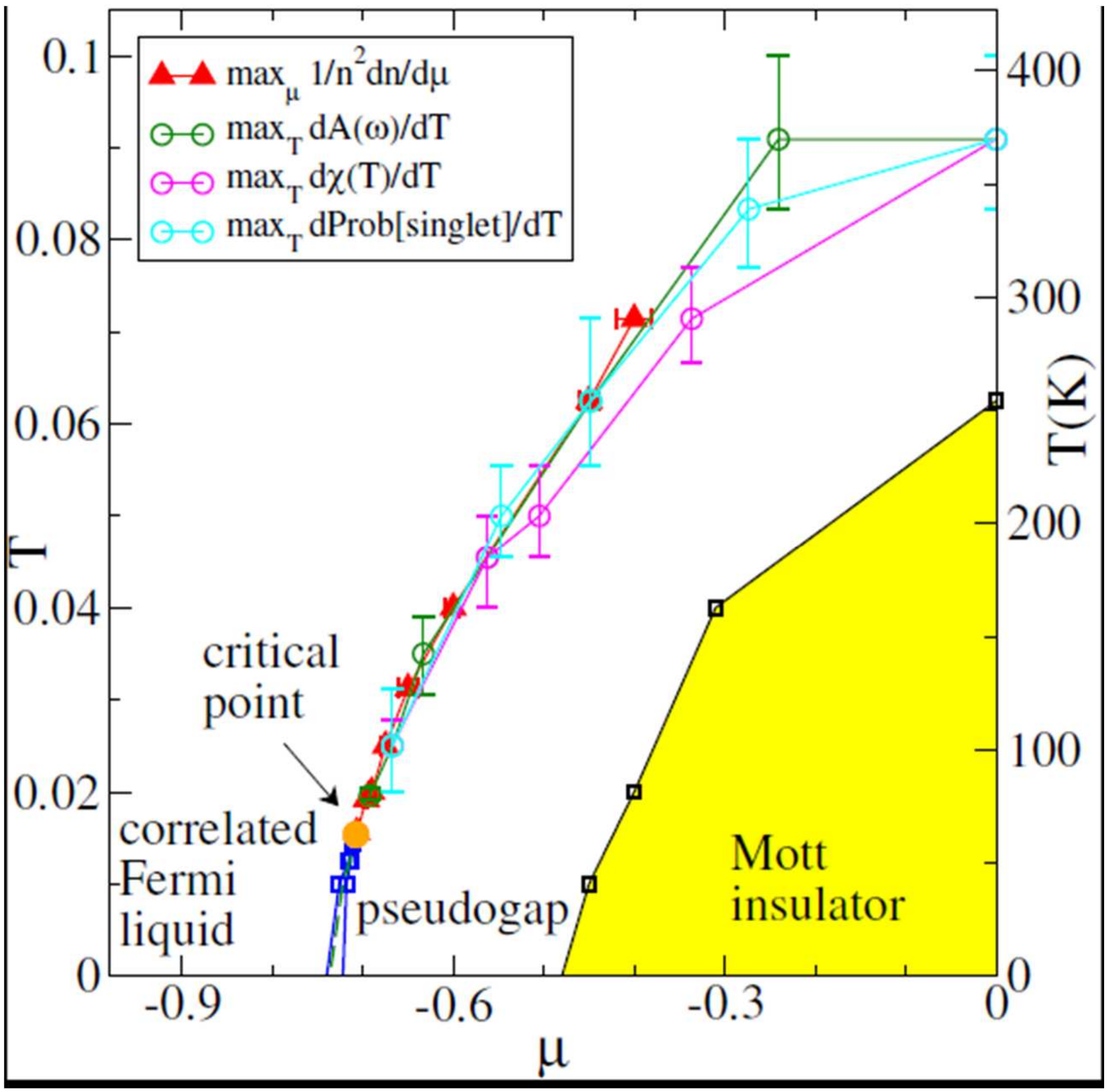
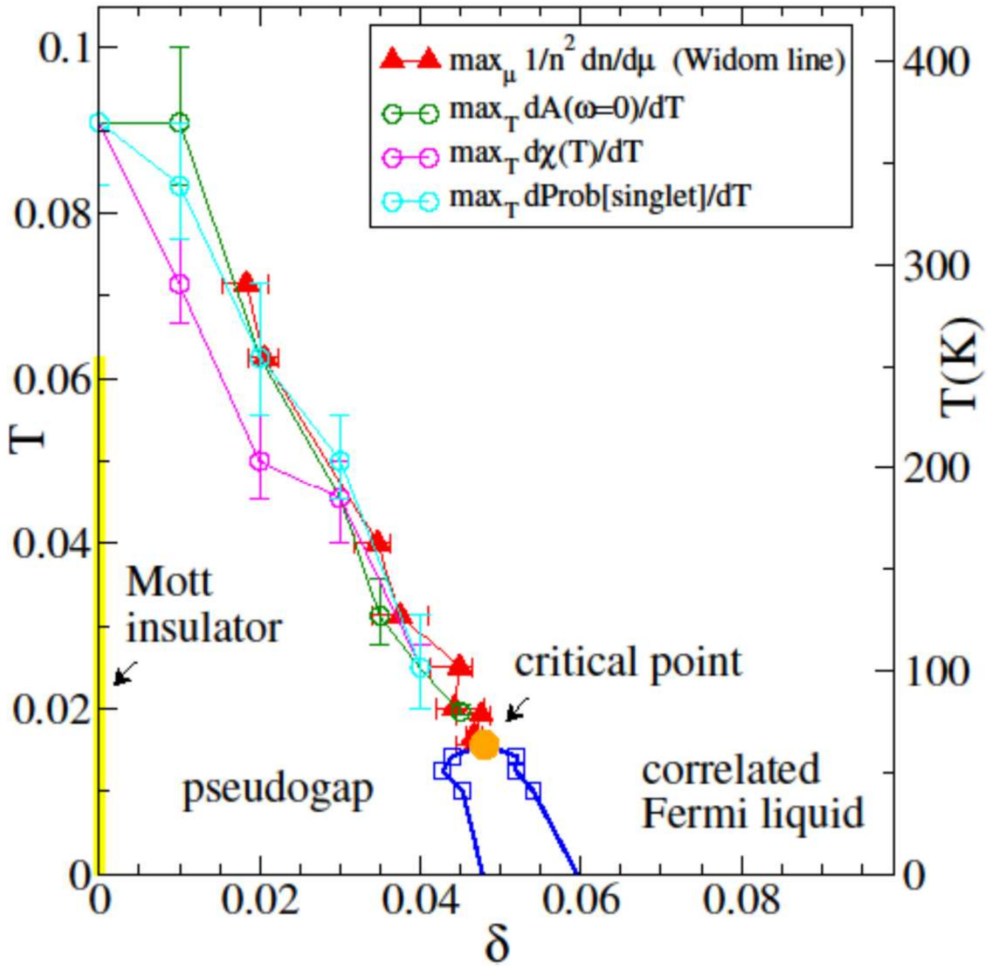
The Widom line

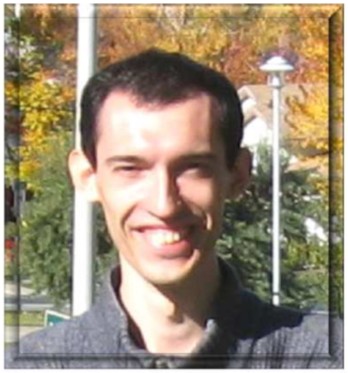


Rapid change also in dynamical quantities



Phase diagram





Giovanni Sordi

Patrick Sémon

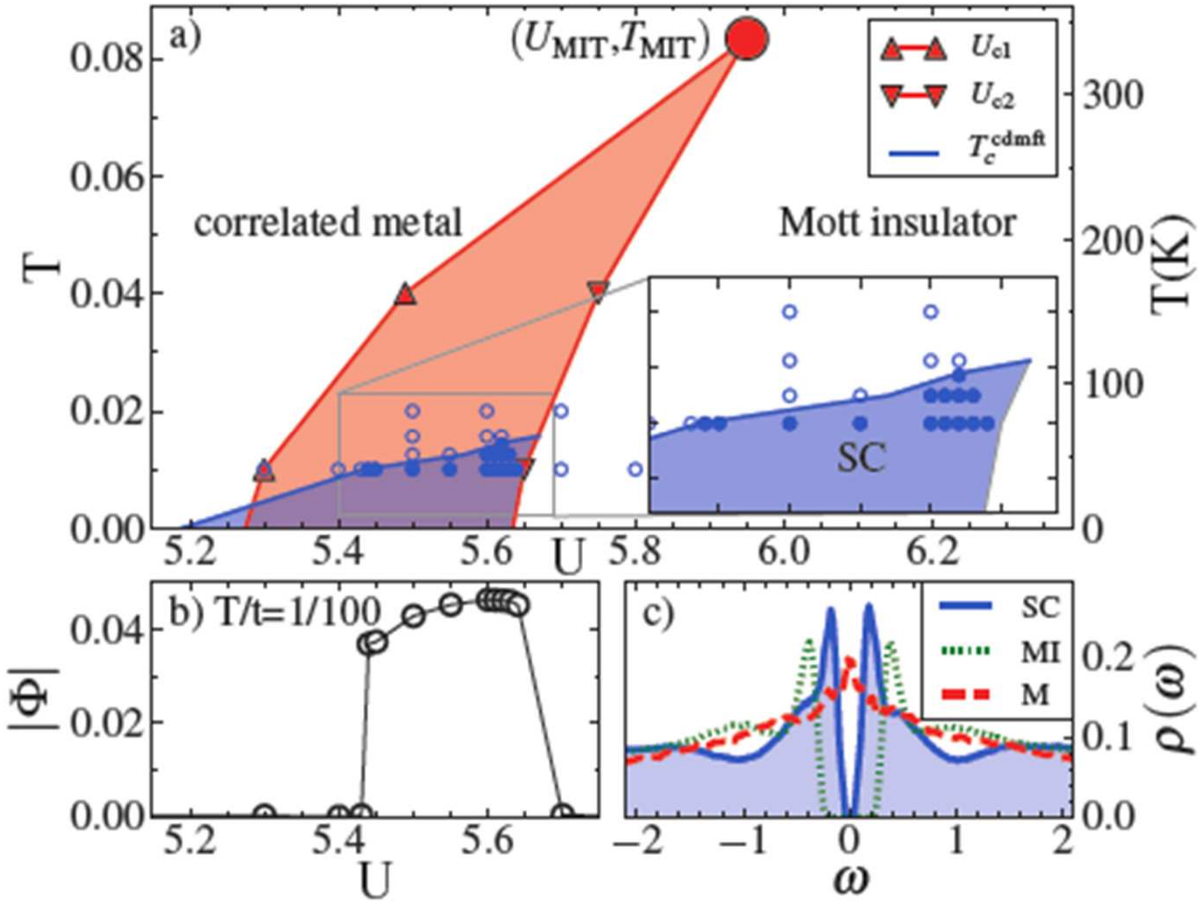
Kristjan Haul

Finite *T* phase diagram

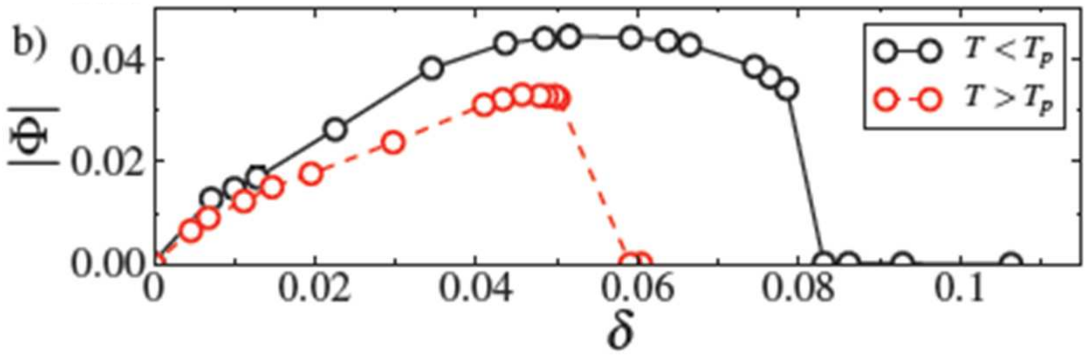
Superconductivity

arXiv:1201.1283v1

$n = 1$, Almost layered organics BEDT

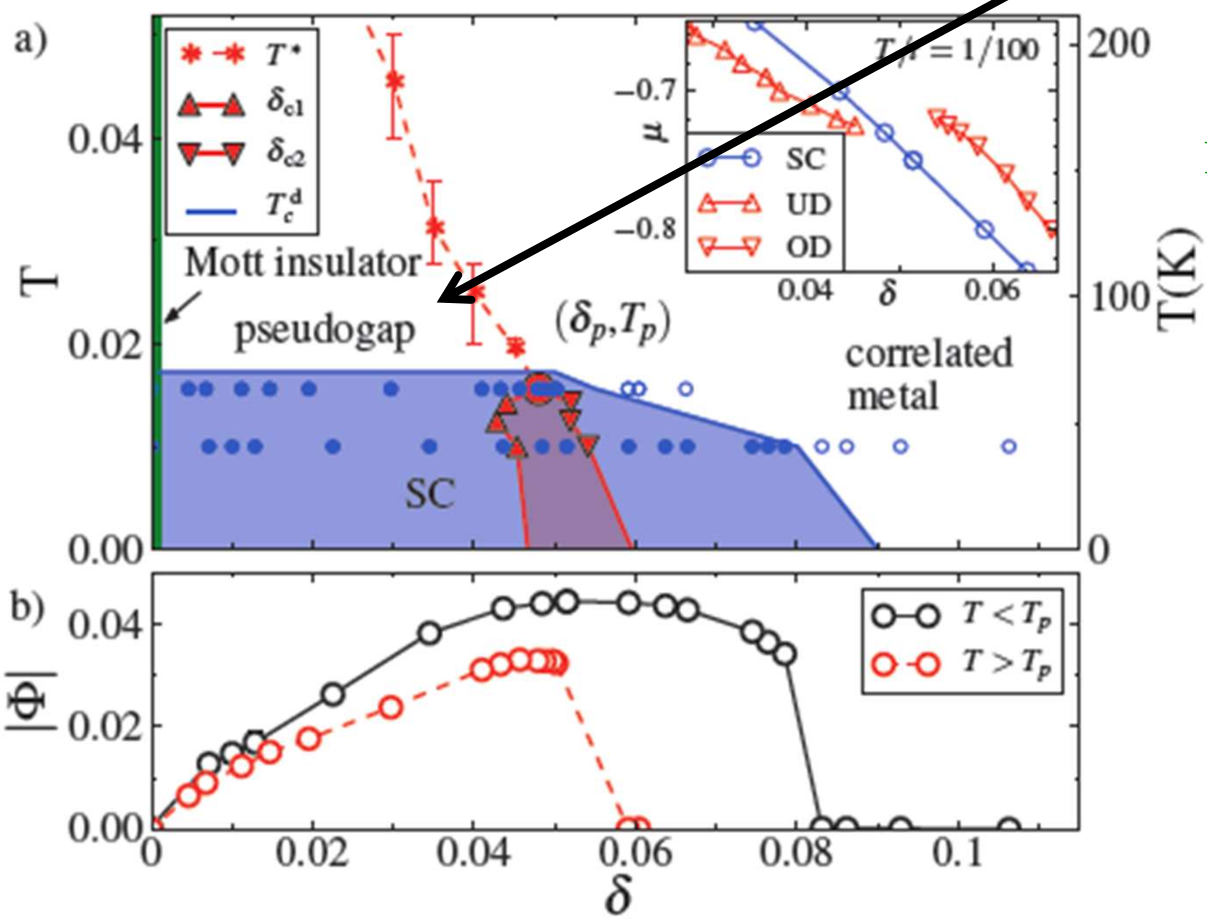


Cuprates (doping driven transition)



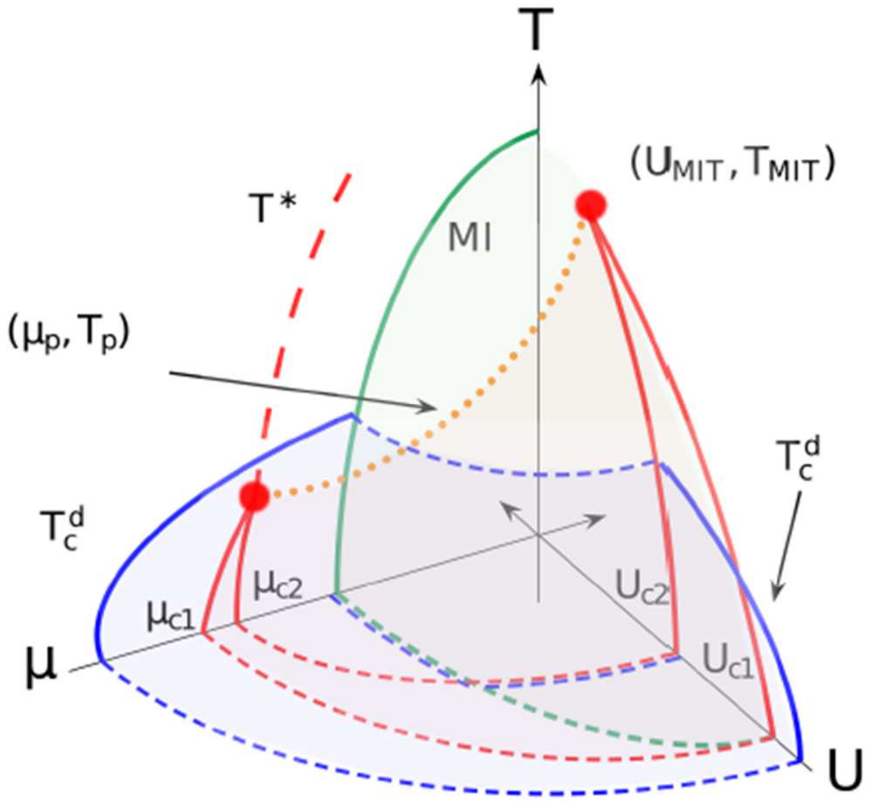
Cuprates (doping driven transition)

Pseudogap vs pair



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

Unified phase diagram



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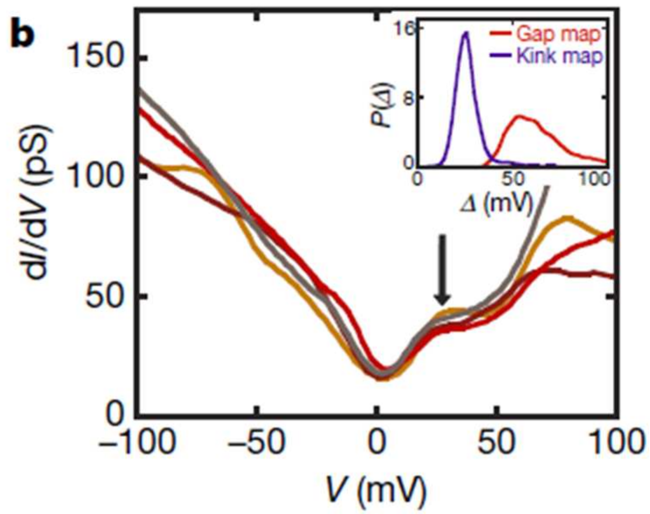
Meaning of T_c^d

- Local pair formation



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

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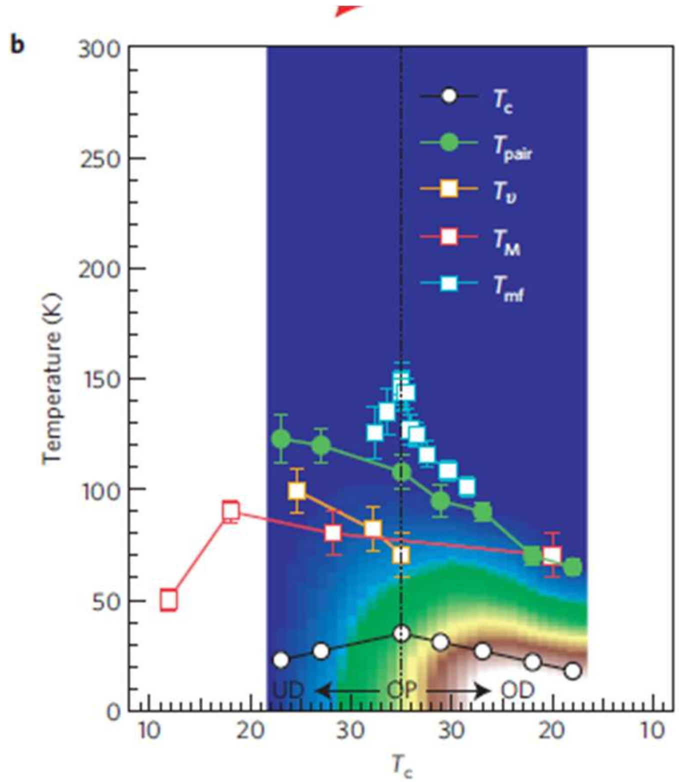
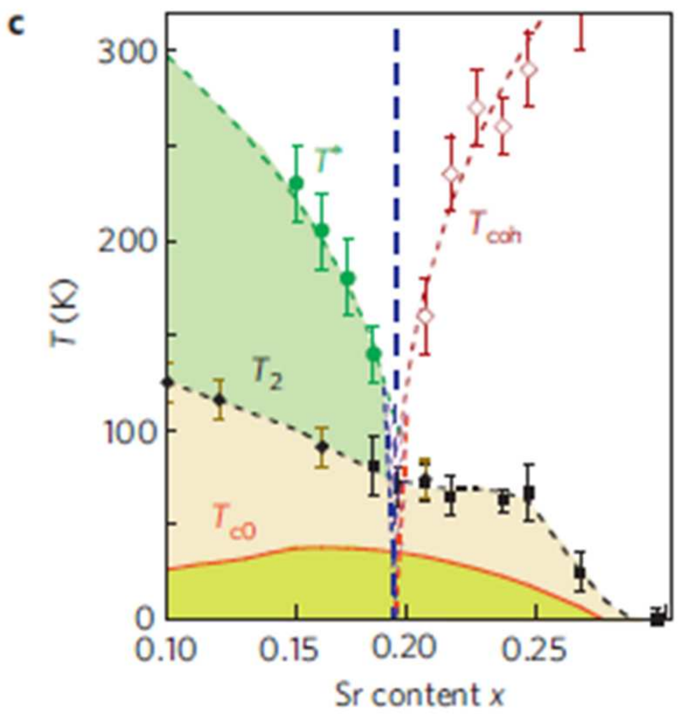
T_{pair}



ARPES
Bi2212

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

T_2



Magnetoresistance, LSCO
Fluctuating vortices

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

Phase fluctuations and disorder?

Monolayer LSCO, field doped

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

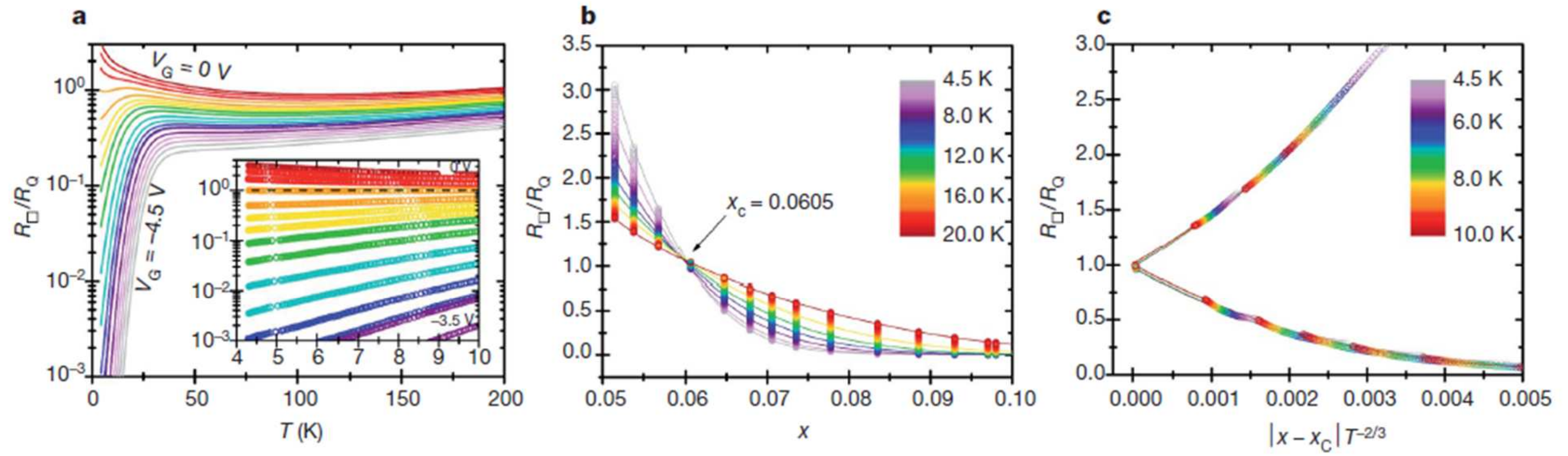
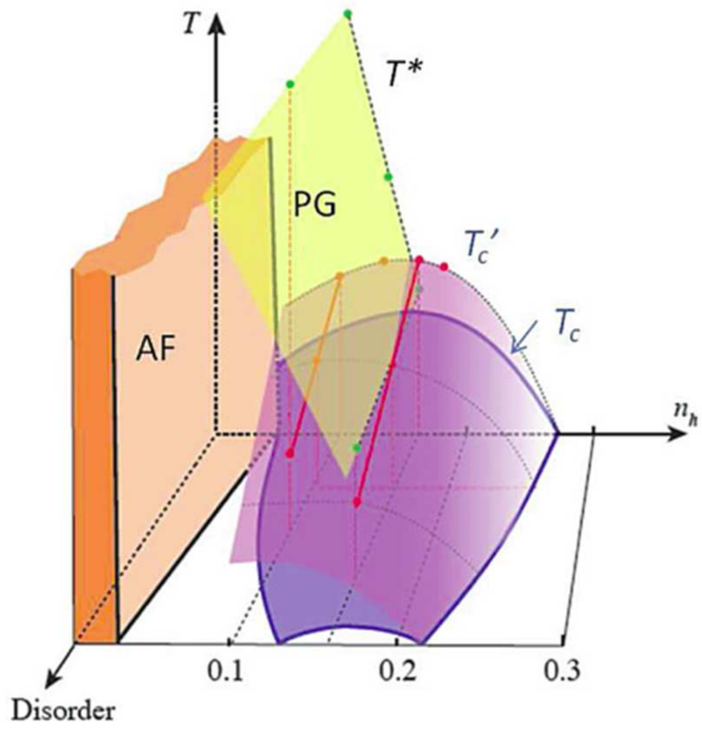


Figure 2 | Superconductor–insulator transition driven by electric field. **a**, Temperature dependence of normalized resistance $r = R_\square(x,T)/R_Q$ of an initially heavily underdoped and insulating film (see Supplementary Fig. 12 for linear scale). The device (Supplementary section B) employs a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

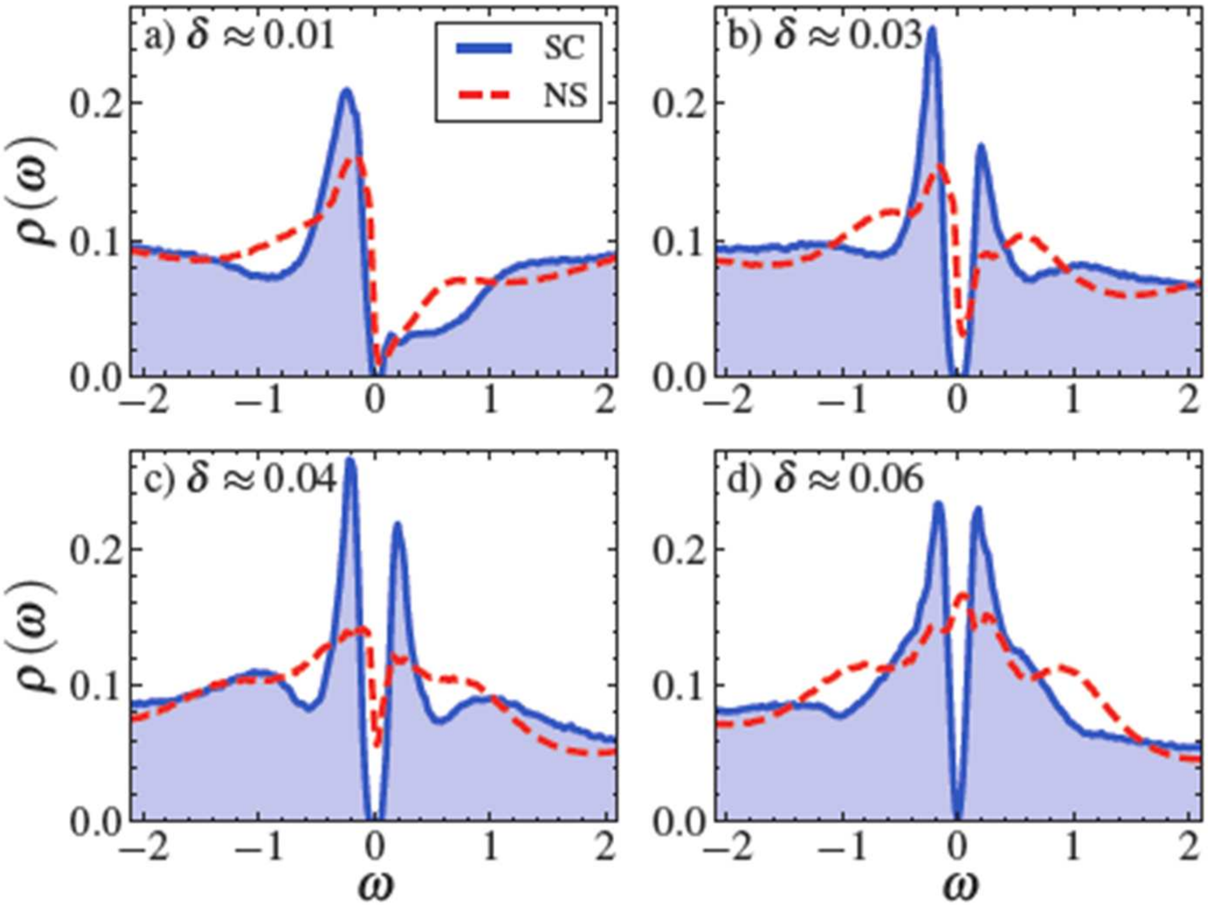
Effect of disorder



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



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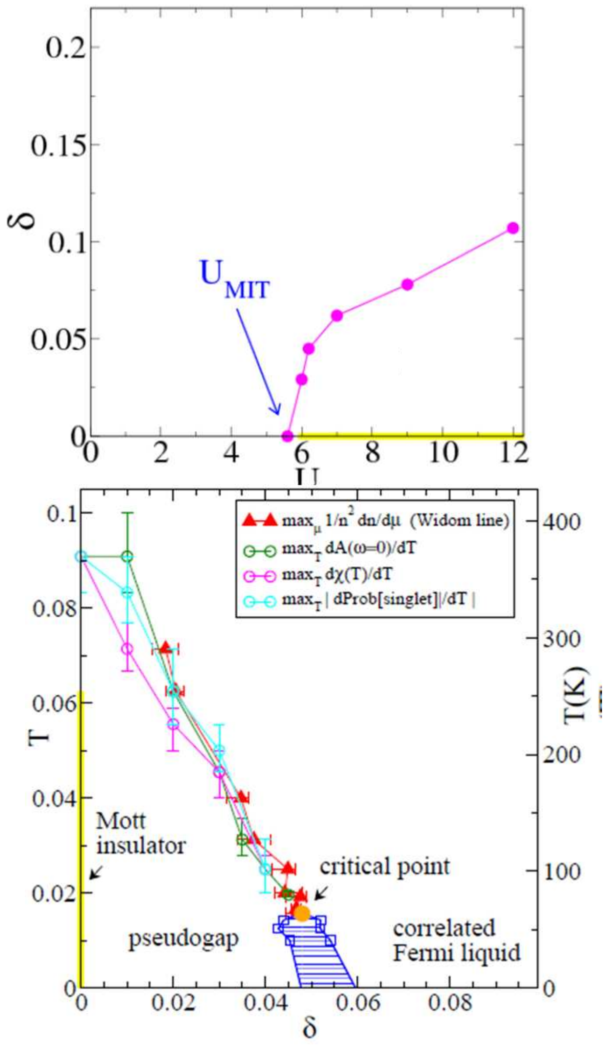
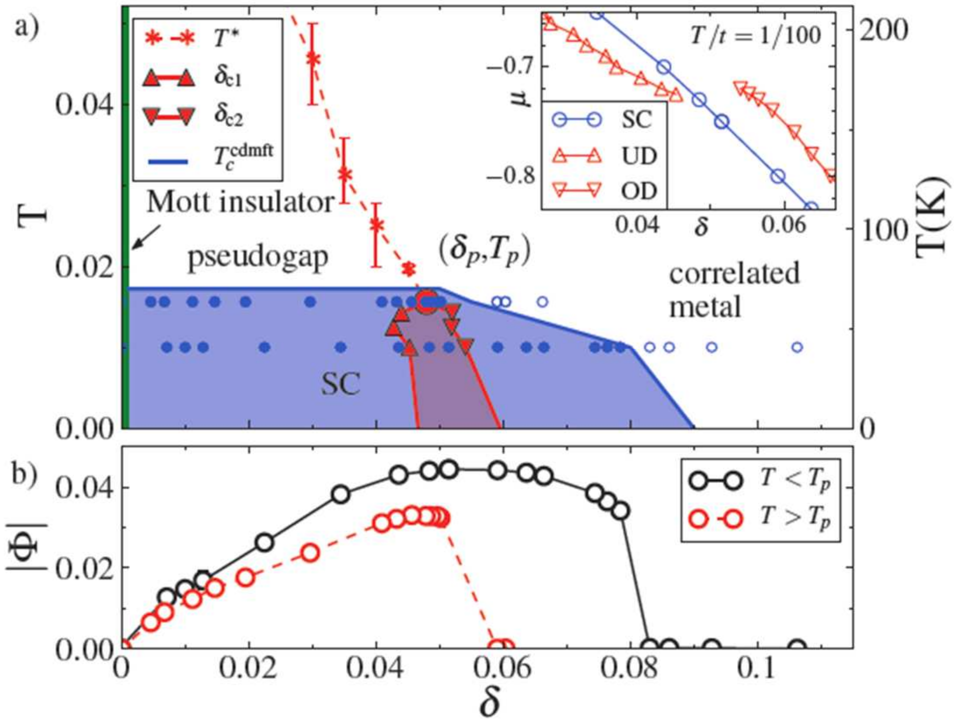
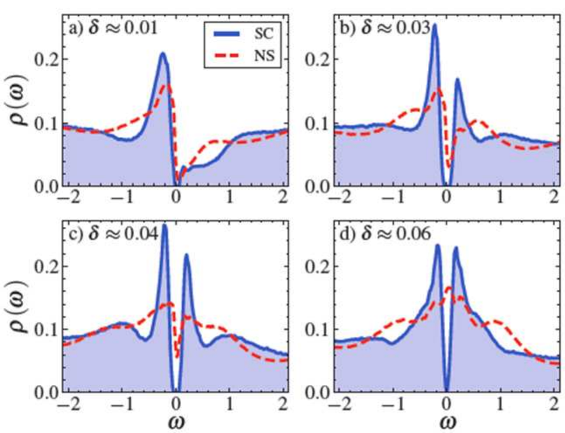
Summary



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

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

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Merci

Thank you