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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Rutgers, 24 January, 2012

VERITATEM IN CHARITATE

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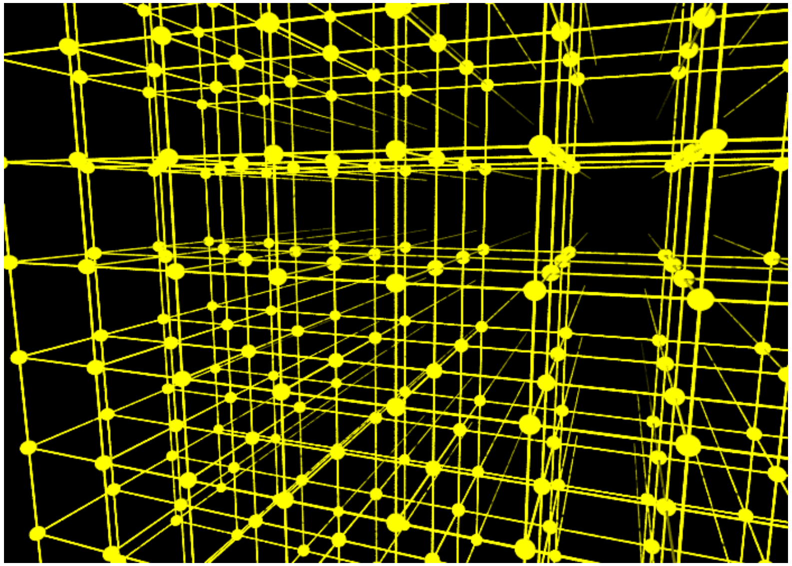
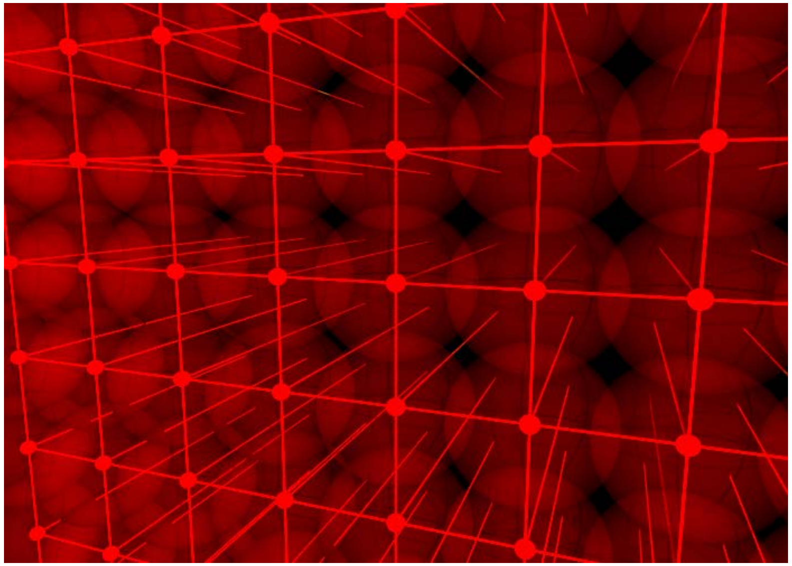
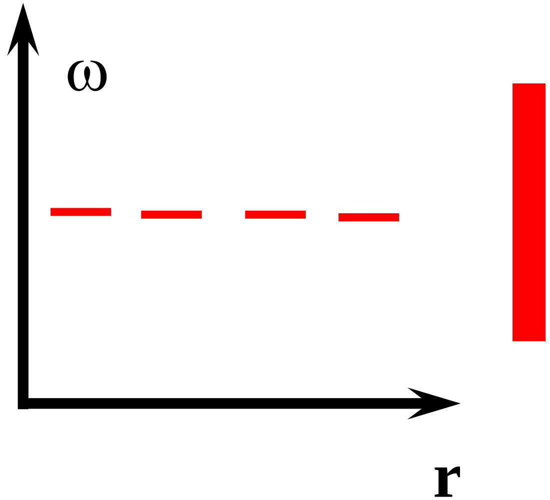
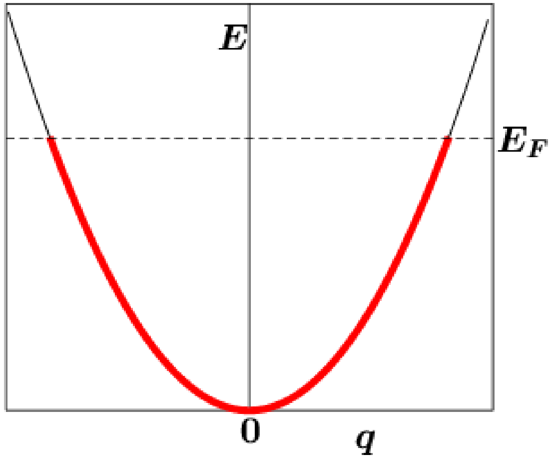
How to make a metal





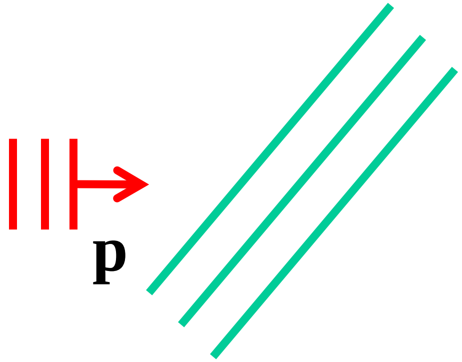




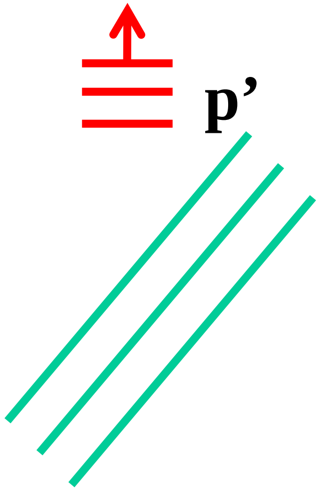
Courtesy, S. Julian

Superconductivity

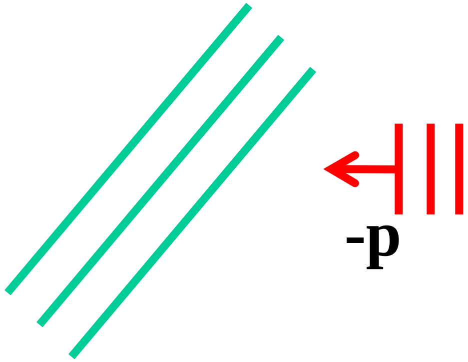
Attraction mechanism in the metallic state



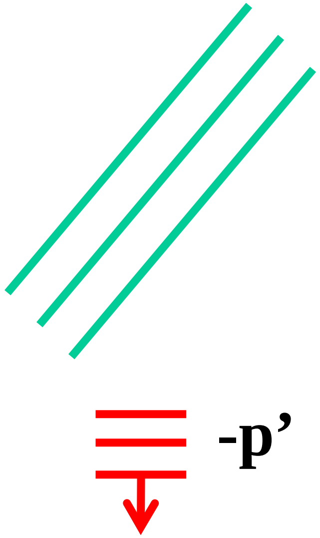
Attraction mechanism in the metallic state



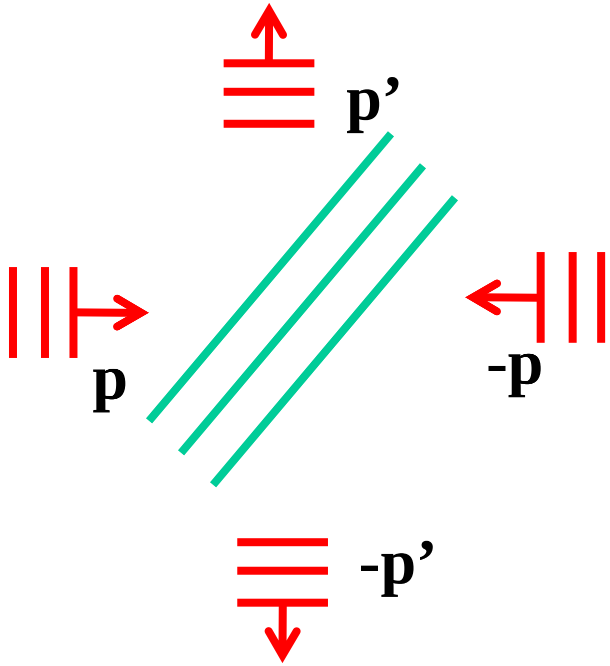
Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



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#1 Cooper pair, #2 Phase coherence

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

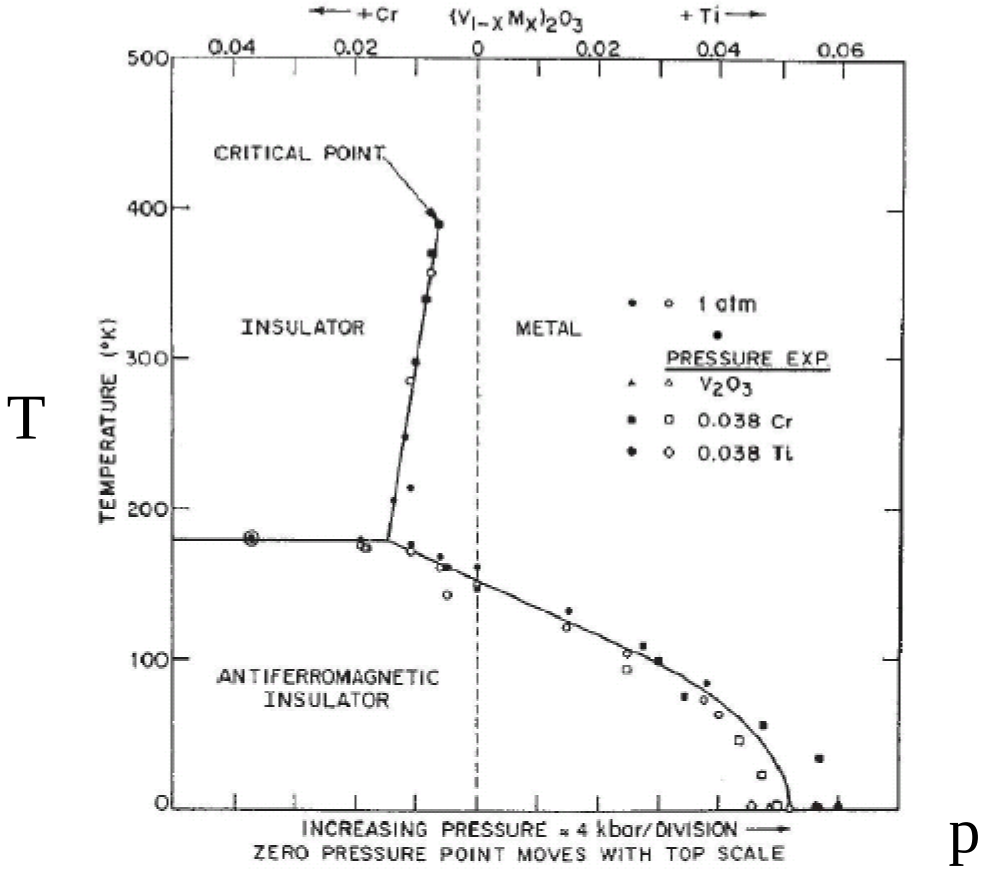
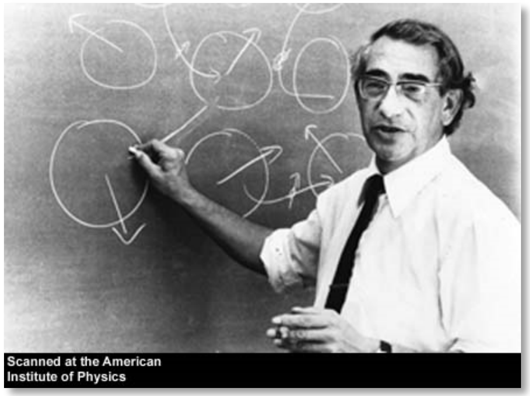
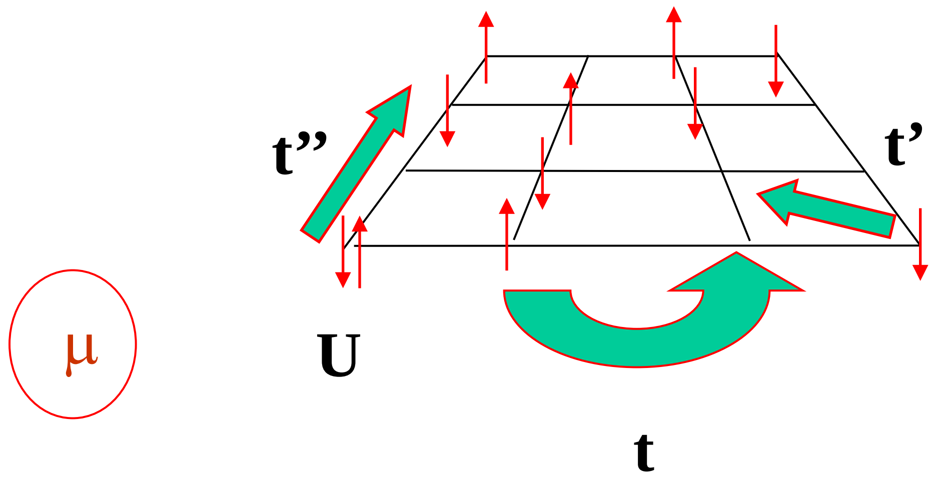


Figure: McWhan, PRB 1970; Limelette, Science 2003

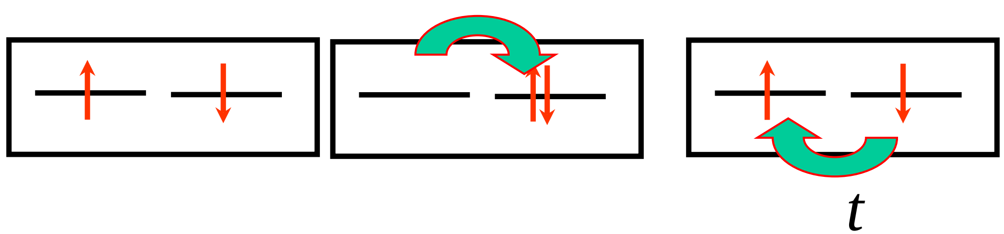
Hubbard model



1931-1980



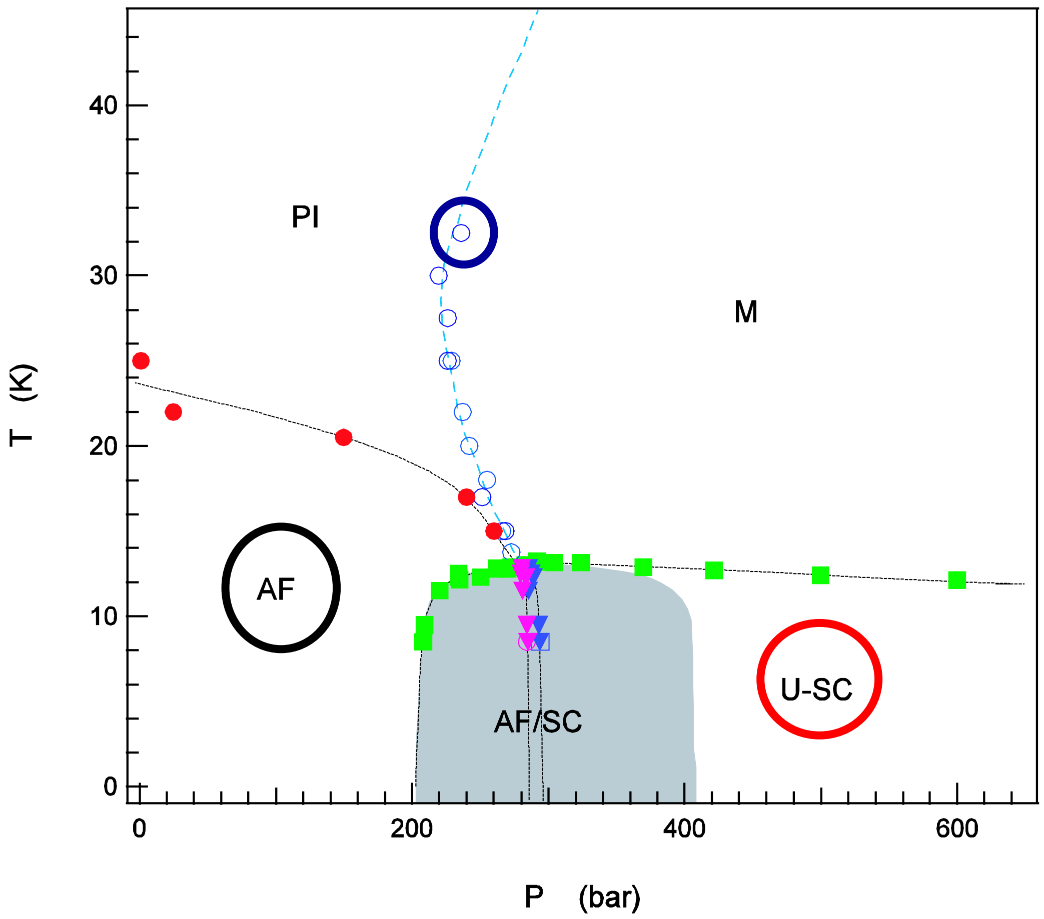
$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

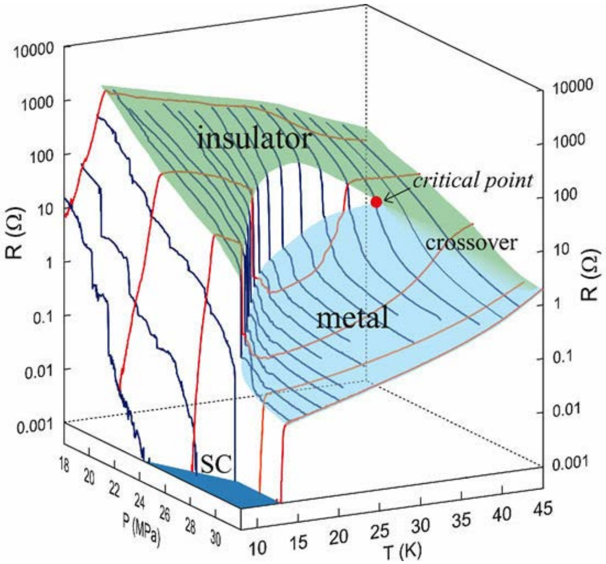


Effective model, Heisenberg: $J = 4t^2/U$

Superconductivity and attraction?

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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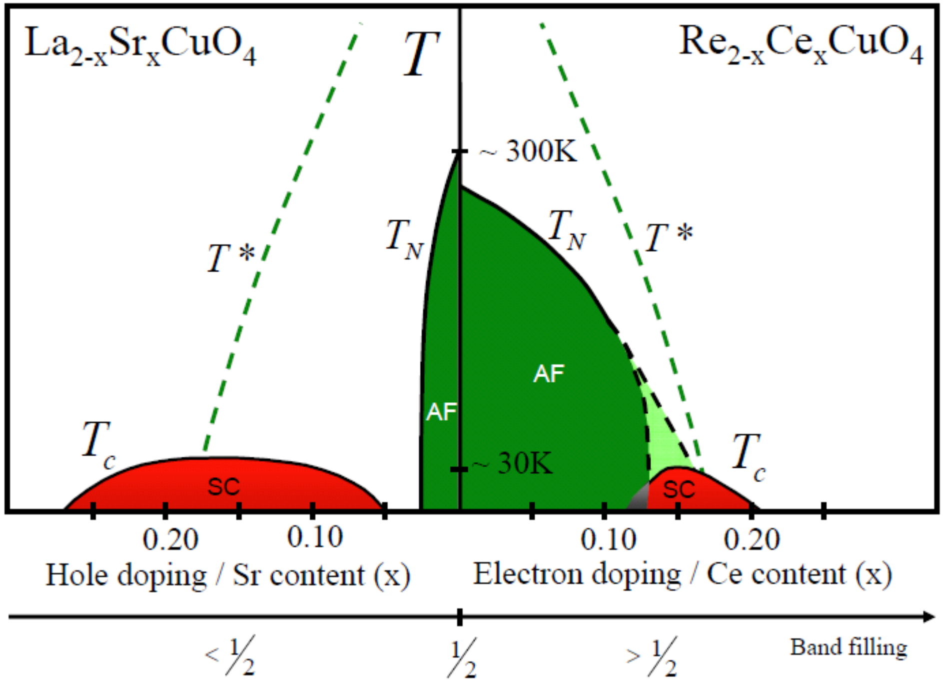
High-temperature superconductors

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)

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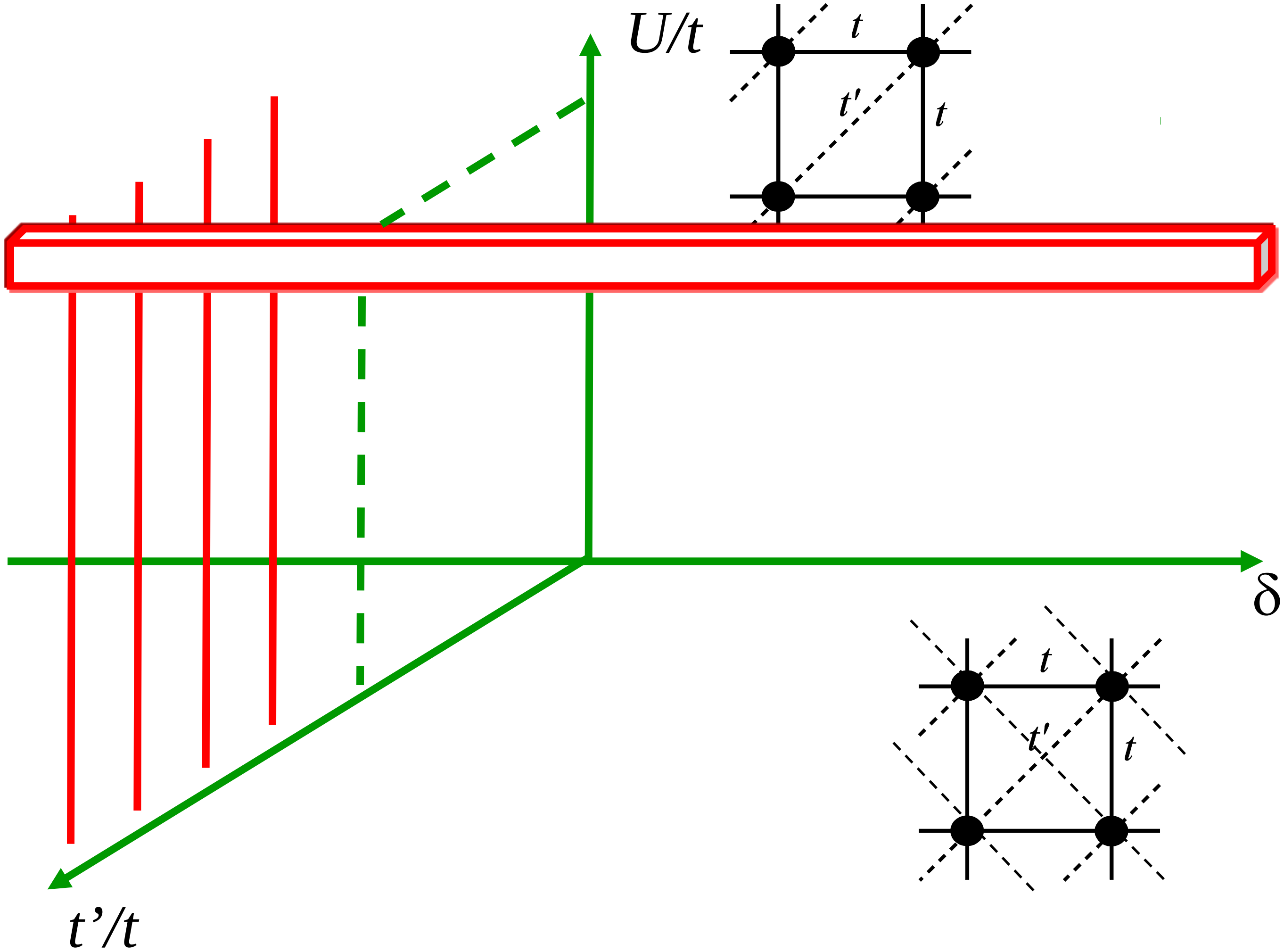
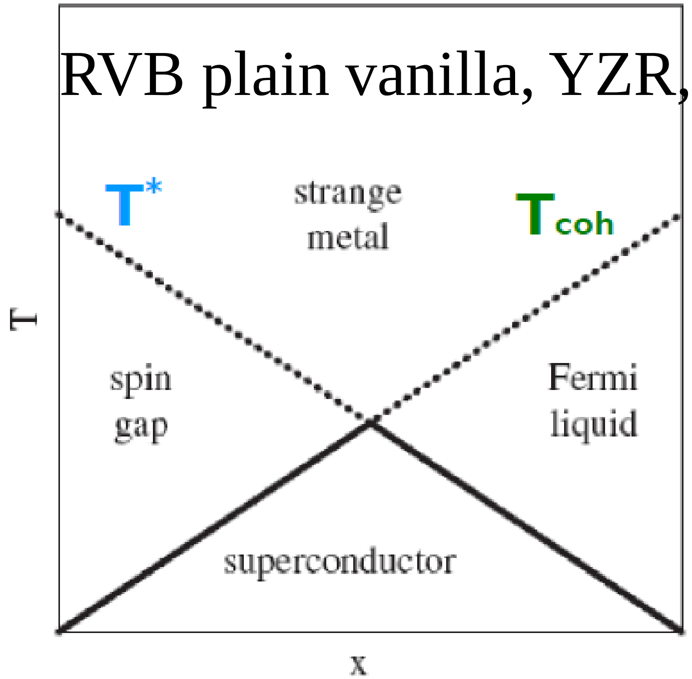
Perspective



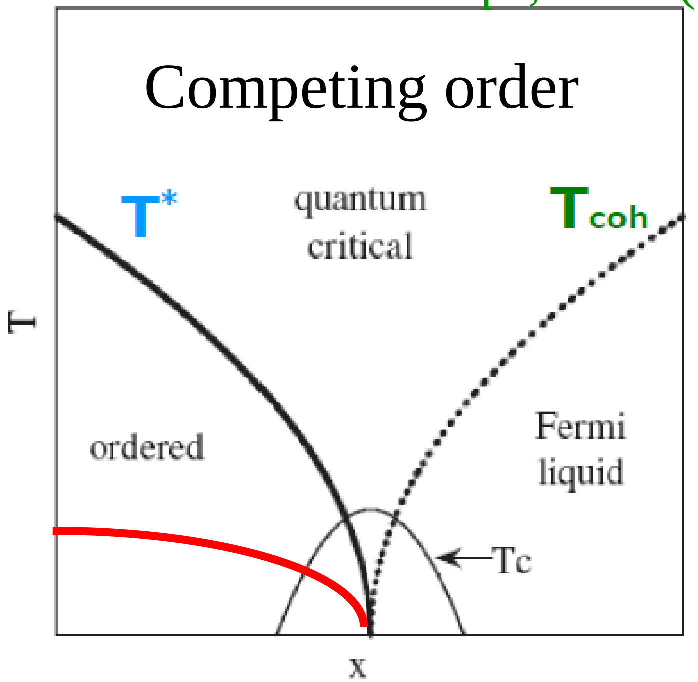
Two views (caricature)

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

RVB plain vanilla, YZR,



Competing order



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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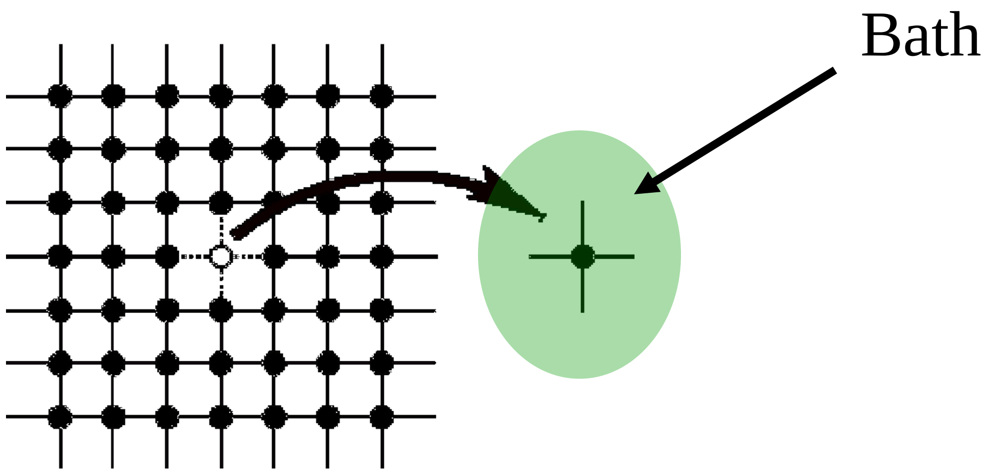
Outline

- 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*

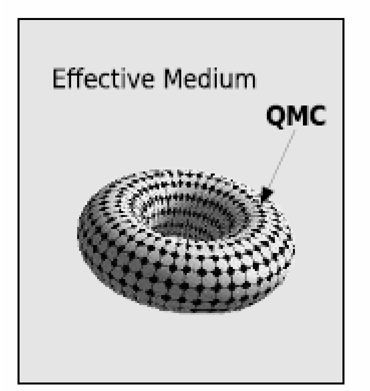
- Compute scattering rate (self-energy) of impurity problem.
- Use that self-energy (ω dependent) for lattice.
- Project lattice on single-site and adjust bath so that single-site DOS obtained both ways be equal.



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

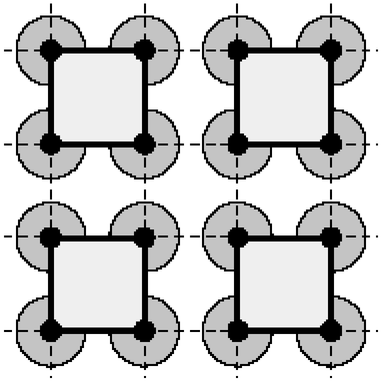
DMFT, (*d = 3)*

2d Hubbard: Quantum cluster method

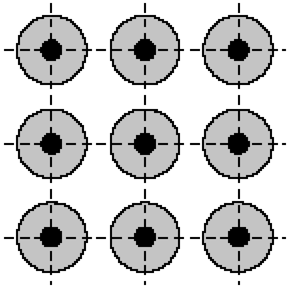


DCA

C-DMFT



DMFT



Hettler …Jarrell…Krishnamurty PRB **58** (1998)
Kotliar et al. PRL **87** (2001)
M. Potthoff *et al.* PRL **91,** 206402 (2003).
Maier, Jarrell et al., Rev. Mod. Phys. **77**, 1027 (2005)

Another way to look at this (Potthoff)

Still stationary (chain rule)

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

SFT : Self-energy Functional Theory

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

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

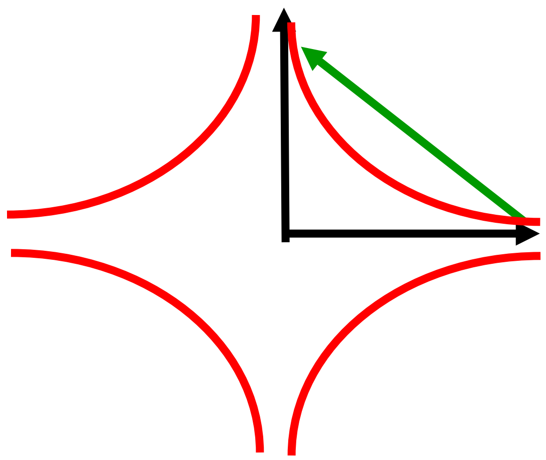
Vary with respect to parameters of the cluster (including Weiss fields)

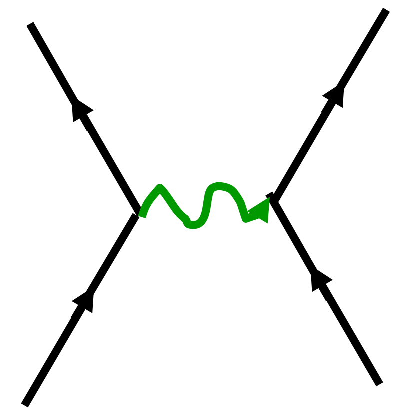
Variation of the self-energy, through parameters in $H_0(\mathbf{t'})$

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

A bit of physics: superconductivity and repulsion

Cartoon « BCS » weak-coupling picture





Exchange of spin waves?
Kohn-Luttinger
T_c with pressure

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).

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

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A cartoon strong coupling picture

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

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).
  - 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).

But…

QMC constrained path

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

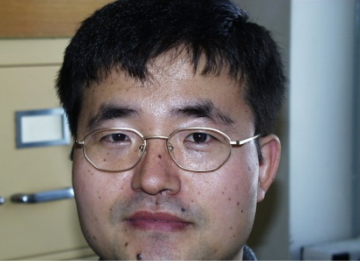
Refined variational approach: no

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

$T = 0$ phase diagram $n = 1$

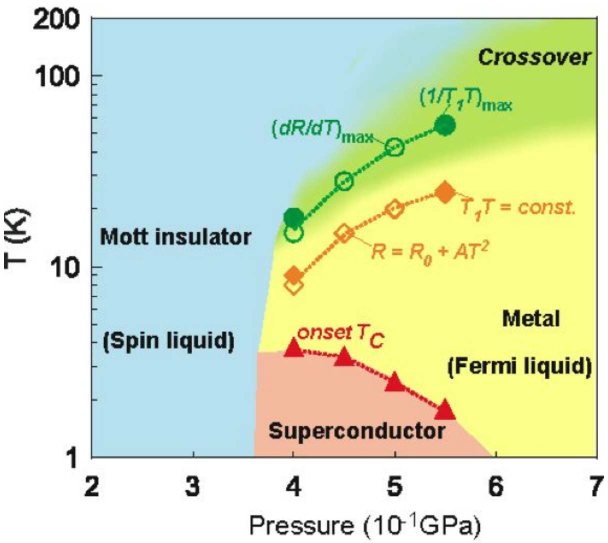
Phase diagram

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

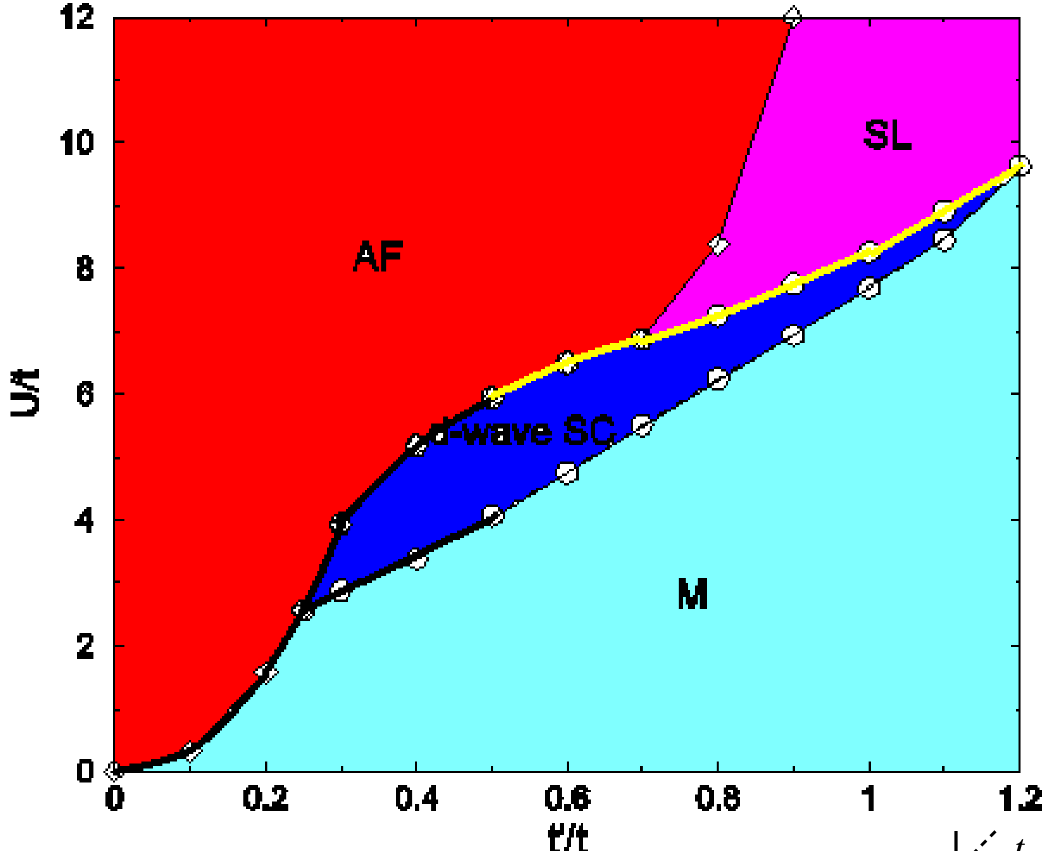


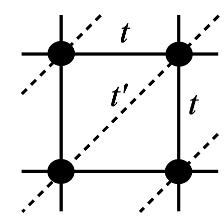
Theoretical phase diagram BEDT

X= $Cu_2(CN)_3$ (t'~ t)



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





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

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

T = 0 phase diagram: cuprates

Phase diagram

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

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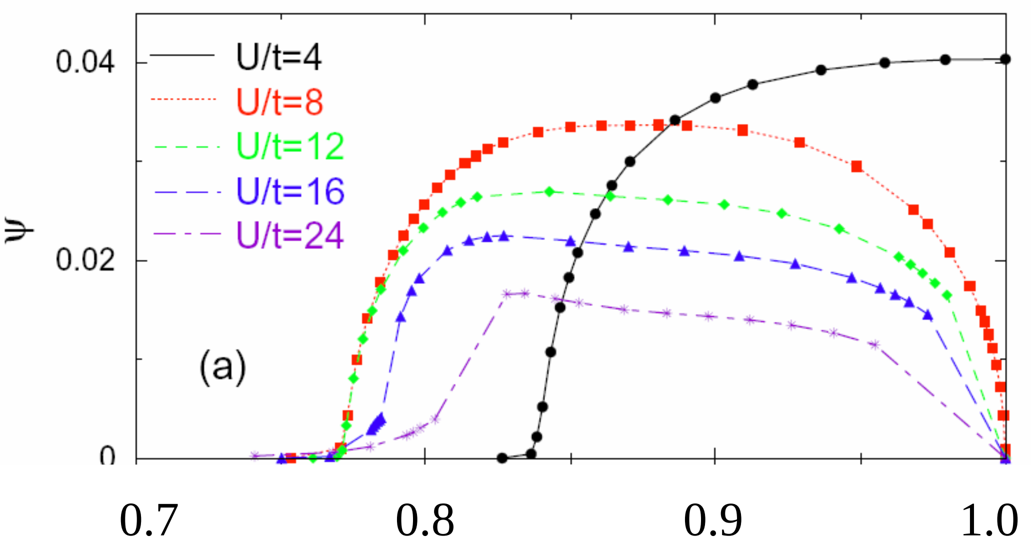
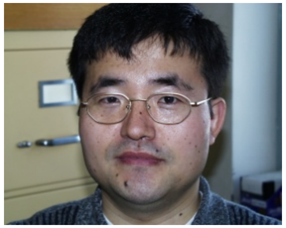
Dome vs Mott (CDMFT)



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



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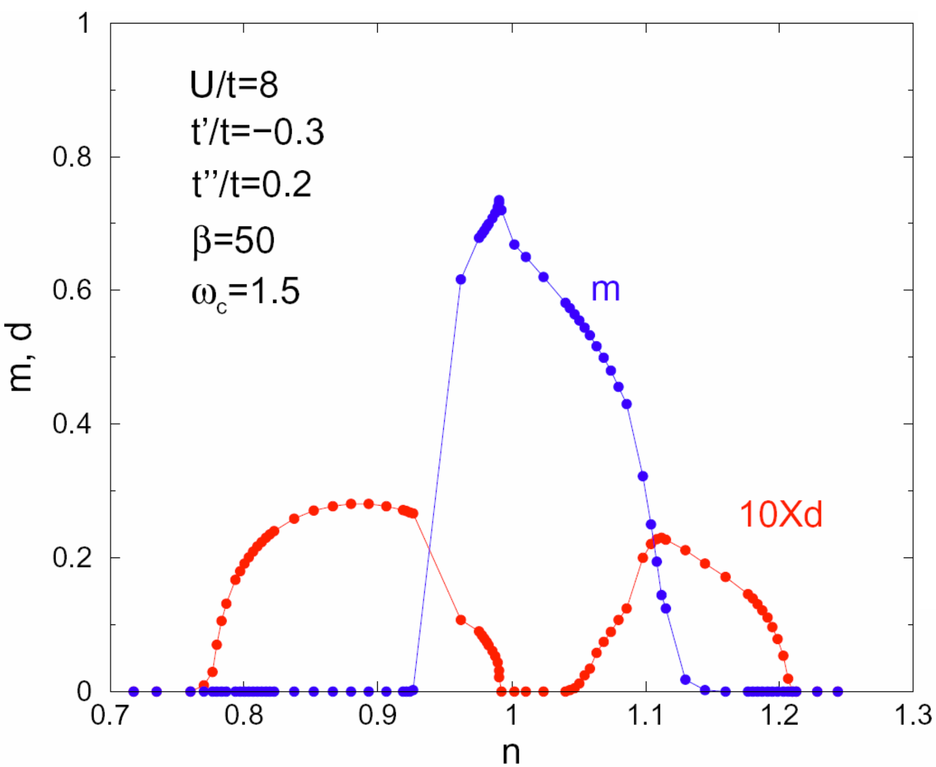
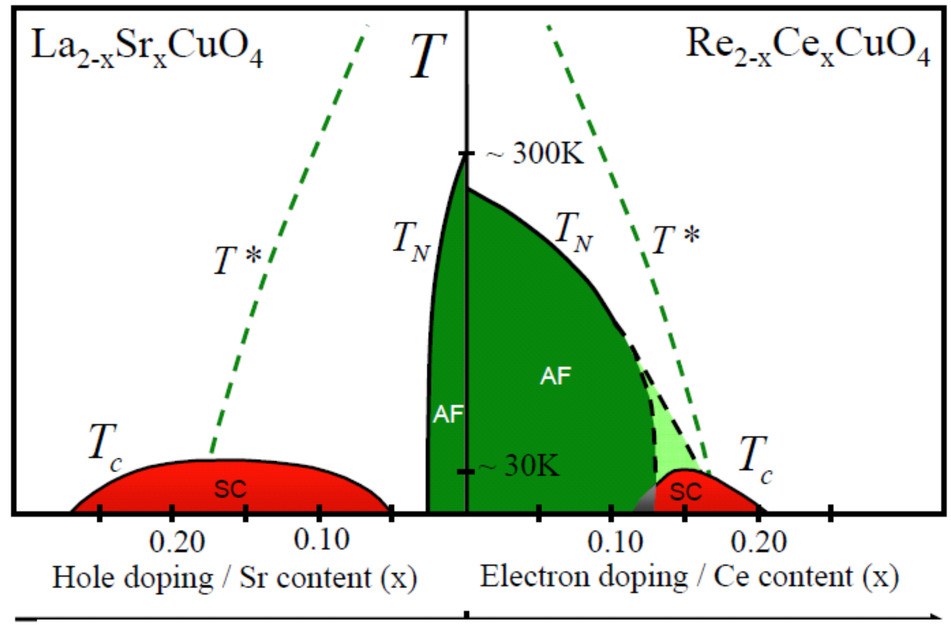
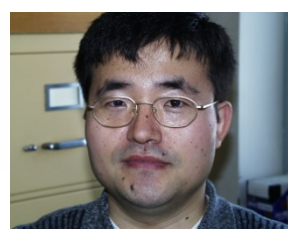
CDMFT global phase diagram



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



Armitage, Fournier, Greene, RMP (2009)



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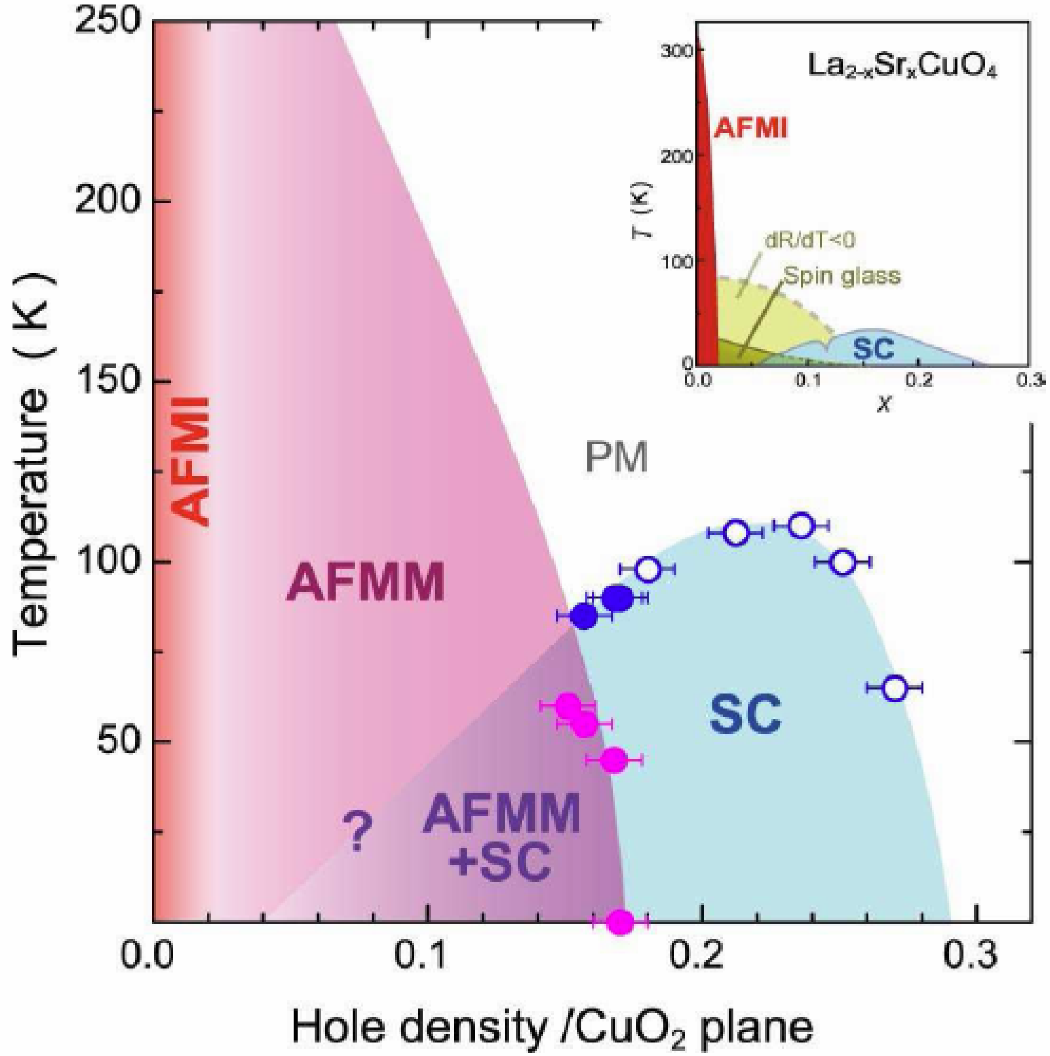
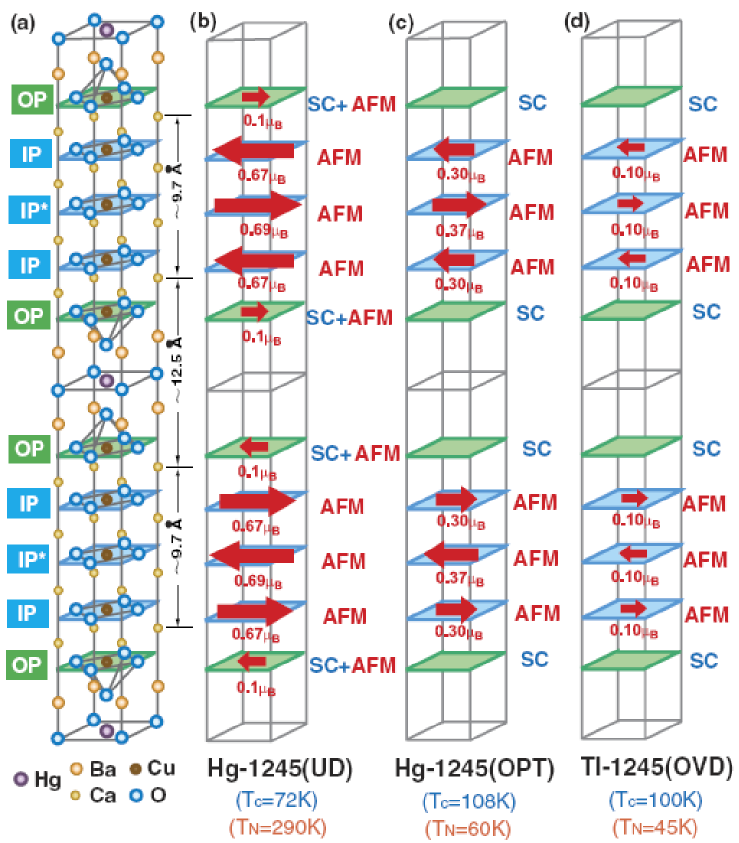
Consistent with following experiments

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





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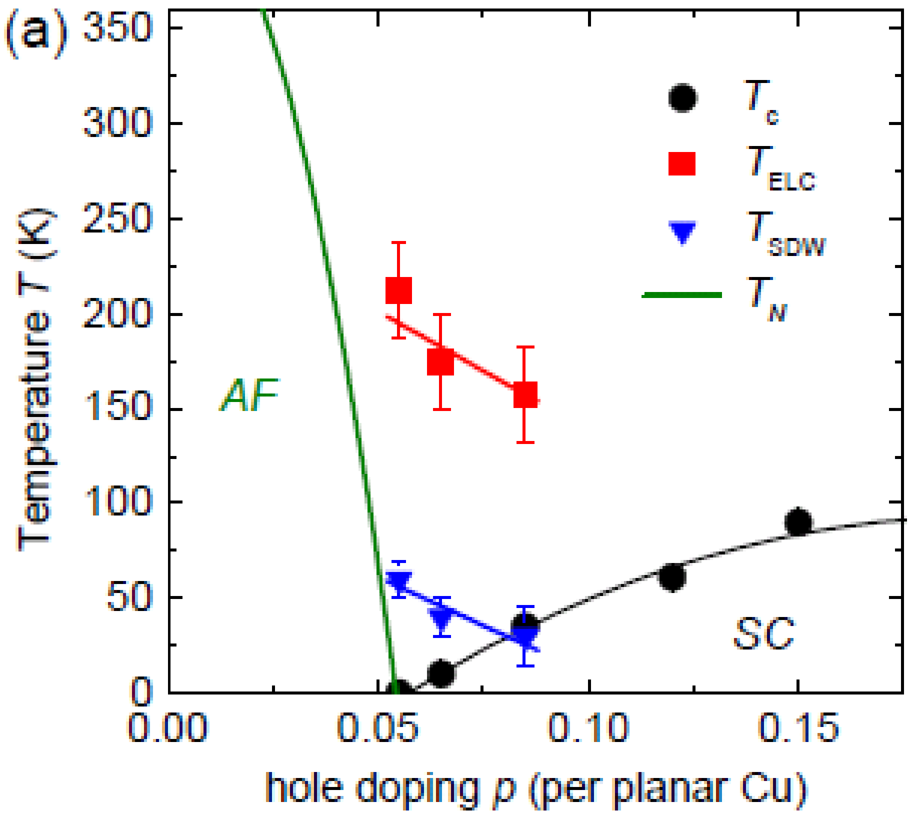
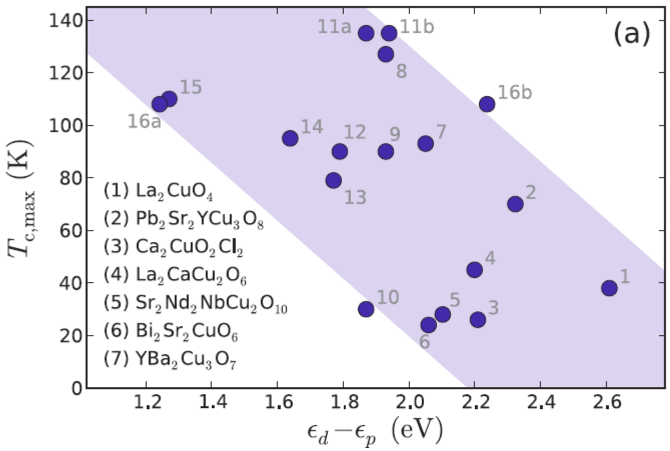
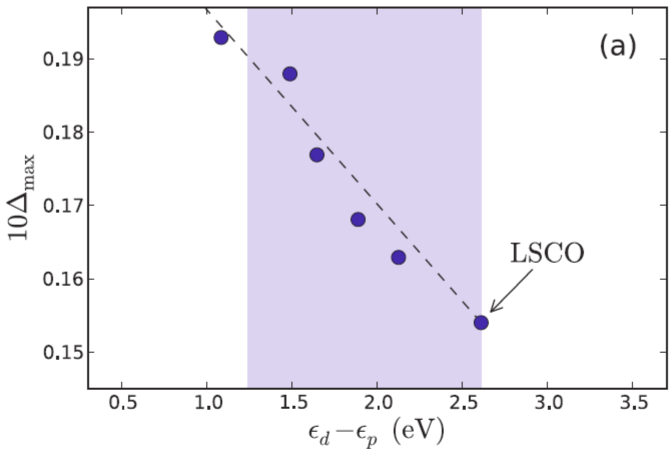
Magnetic phase diagram of YBCO



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

Materials dependent properties





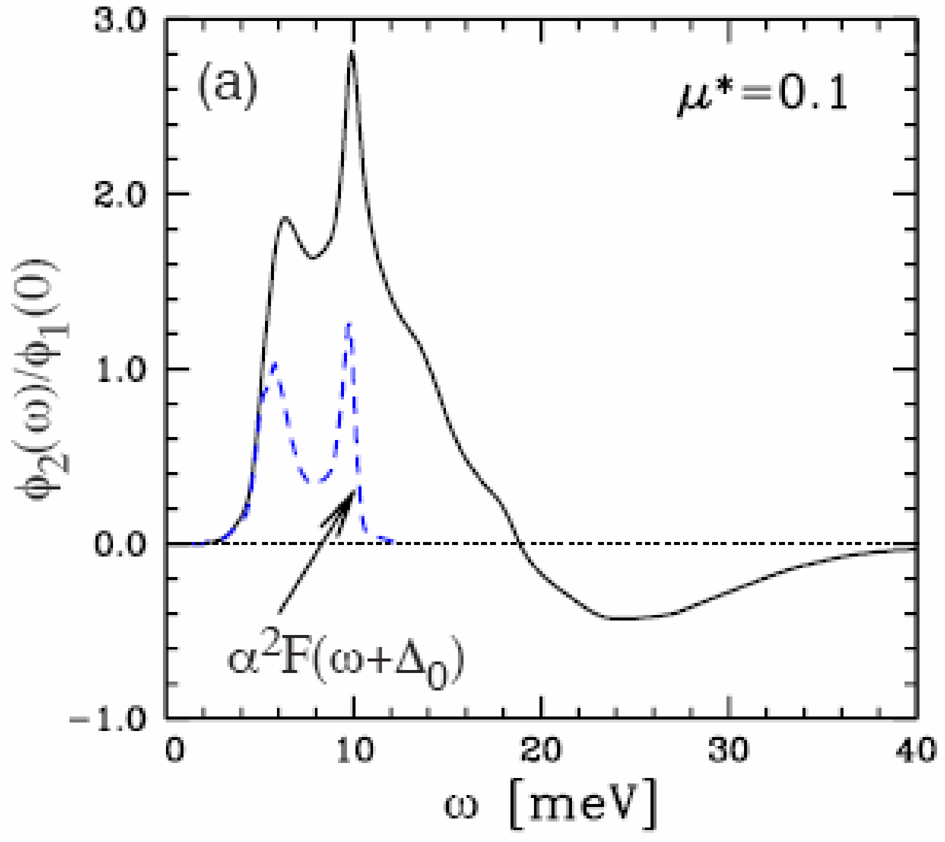
C. Weber, C.-H. Yee, K. Haule, and G. Kotliar, ArXiv e-prints (2011), 1108.3028.

T = 0 phase diagram

The glue

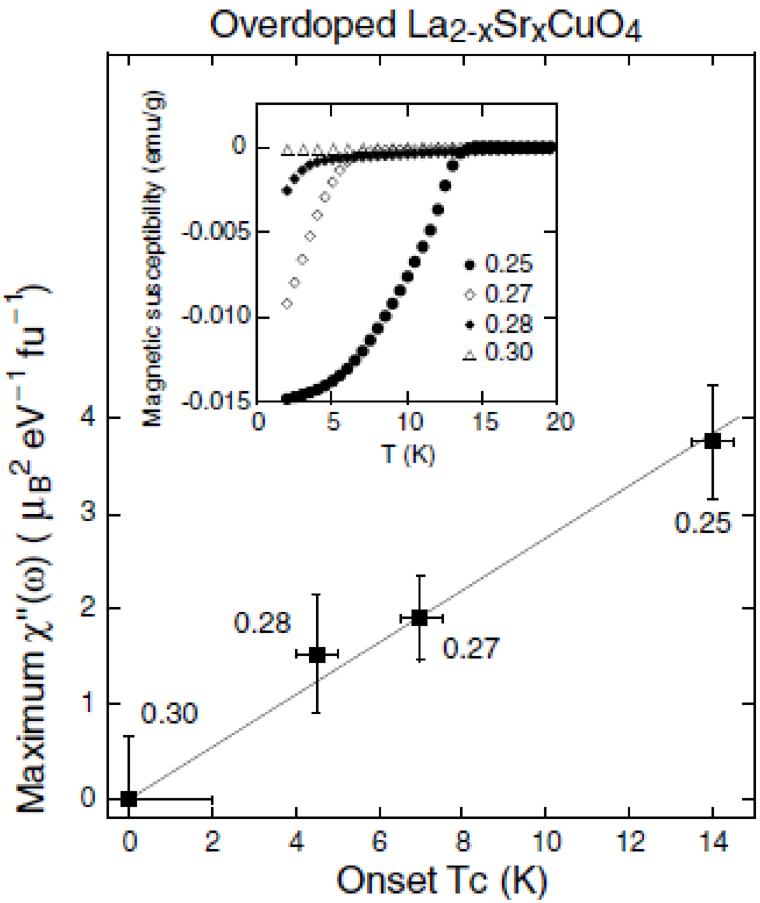
Im Σ_{an} and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

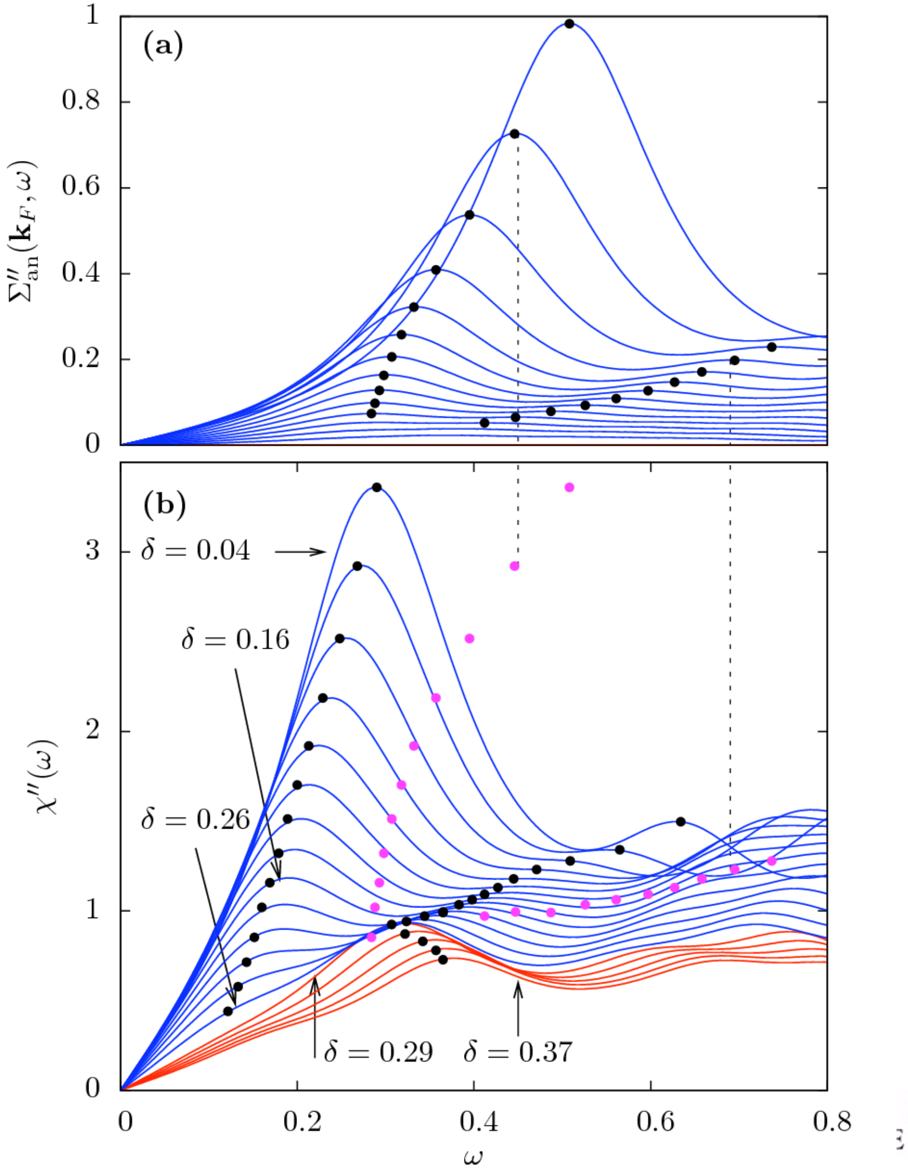


The glue

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



Wakimoto … Birgeneau PRL (2004)



The glue and neutrons

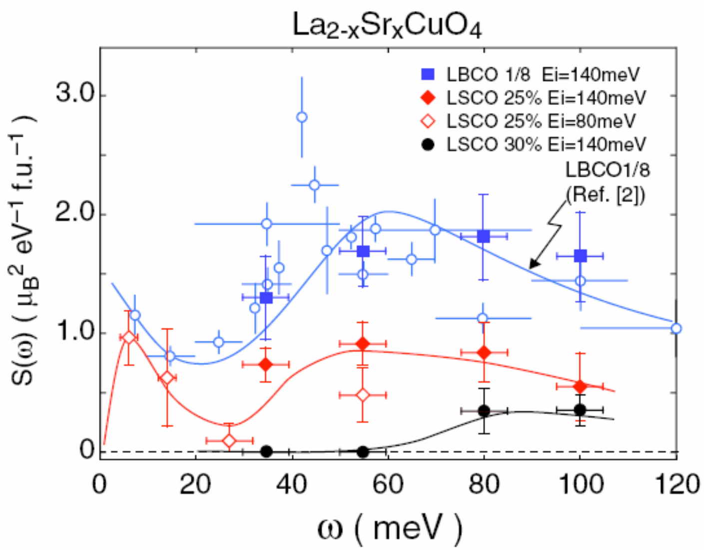
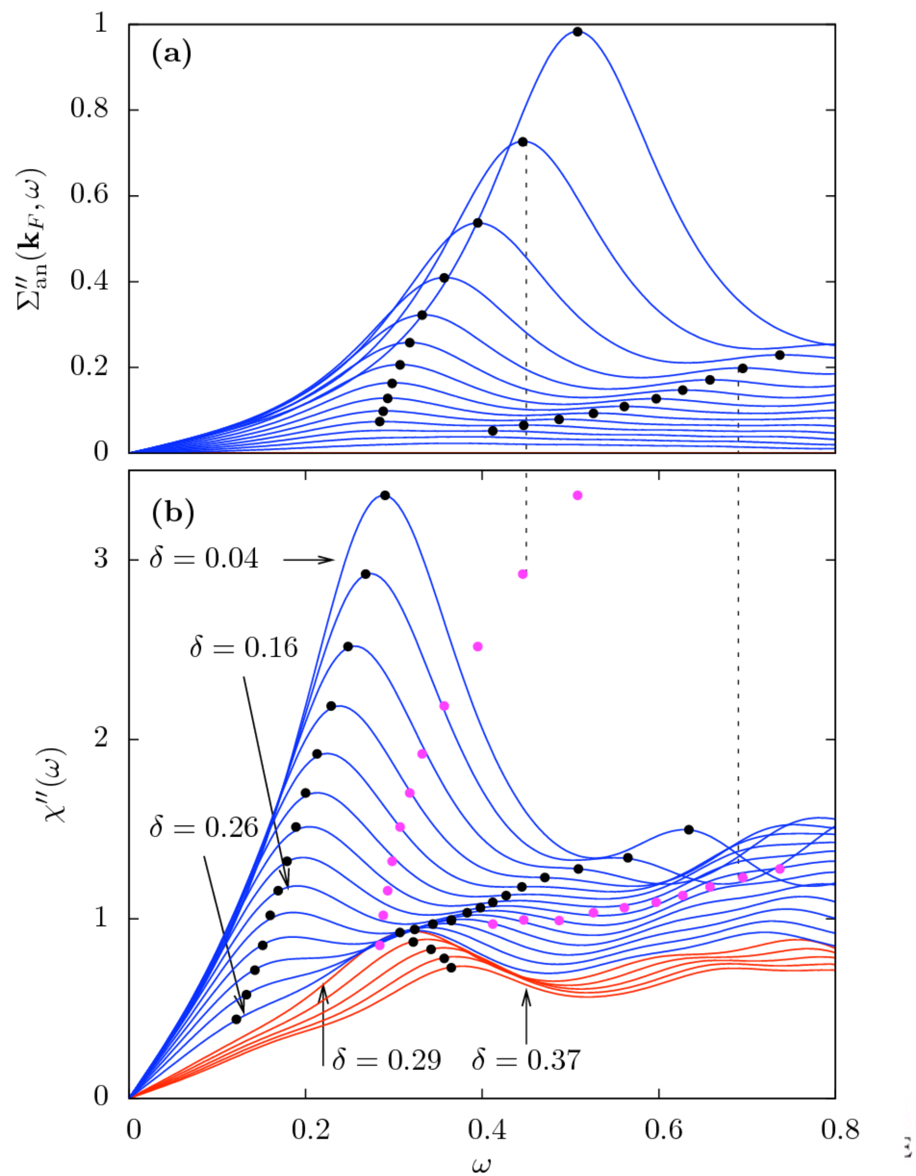


FIG. 3 (color online). **Q**-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for E_i = 140 meV, open for E_i = 80 meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO 1/8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

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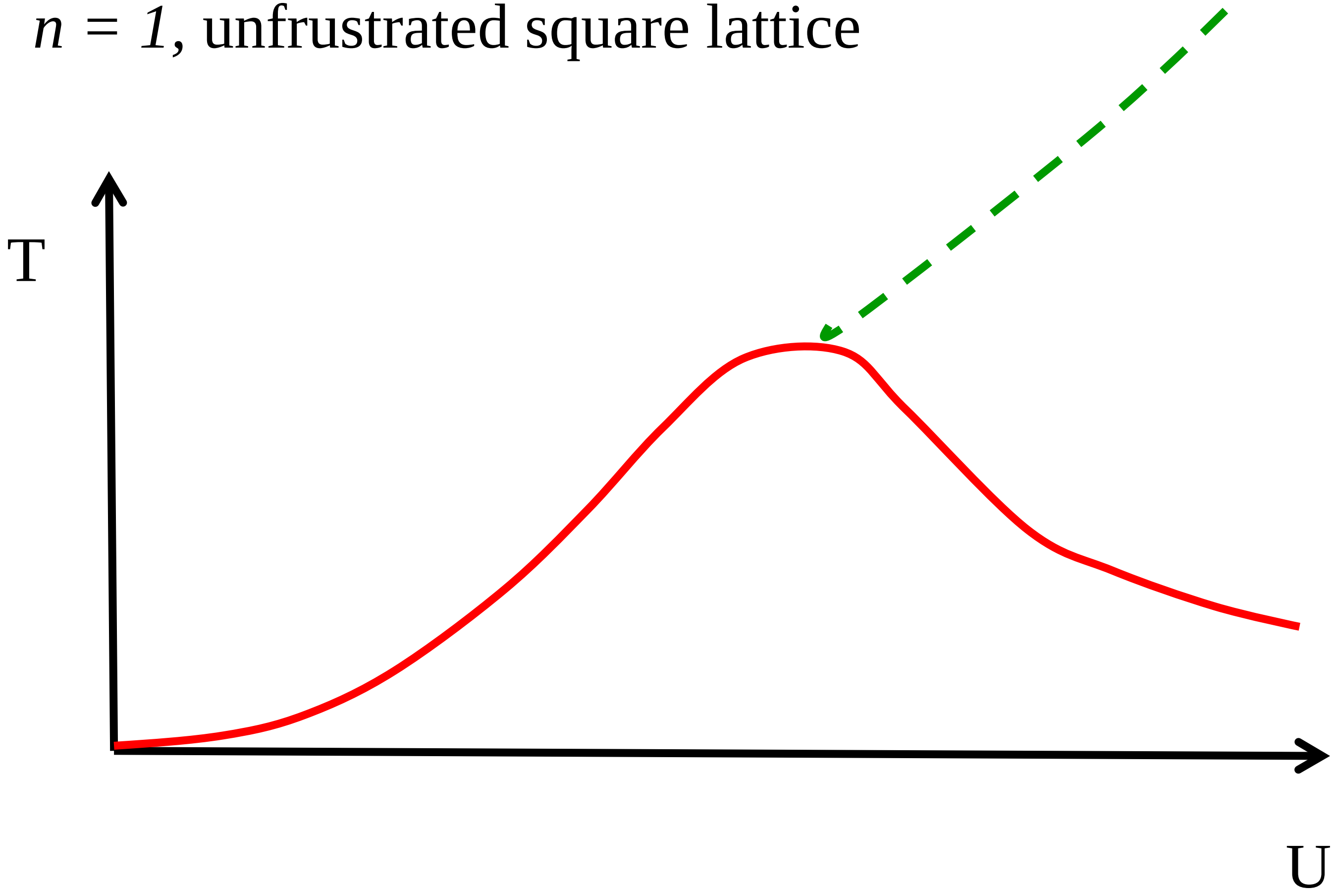
Understanding finite temperature phase from a *mean-field theory* down to $T = 0$

- Fermi liquid
  - Start from Fermi sea
  - Self-energy analytical
  - One to one correspondence of elementary excitations
  - Landau parameters
- 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.

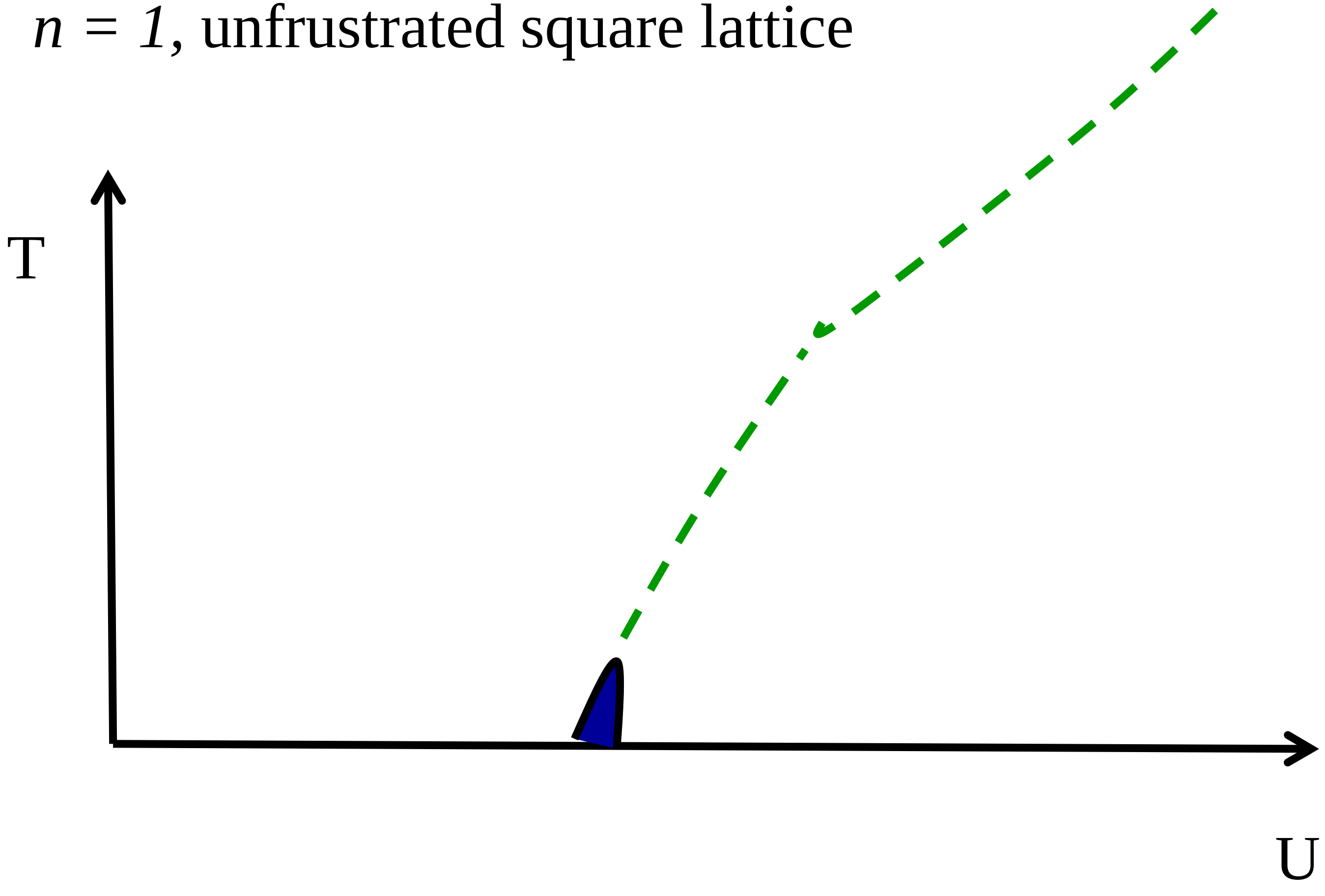
Local moment and Mott transition

n = *1*, unfrustrated square lattice



Local moment and Mott transition

n = *1*, unfrustrated square lattice



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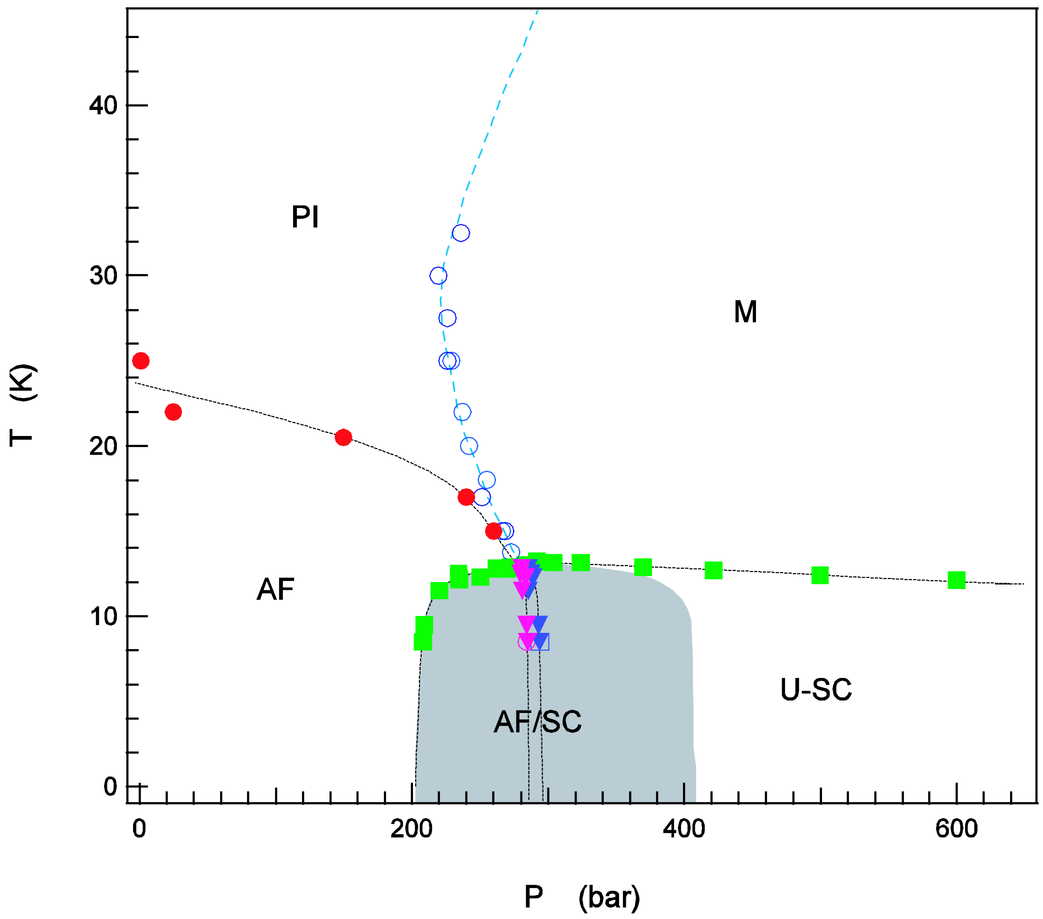
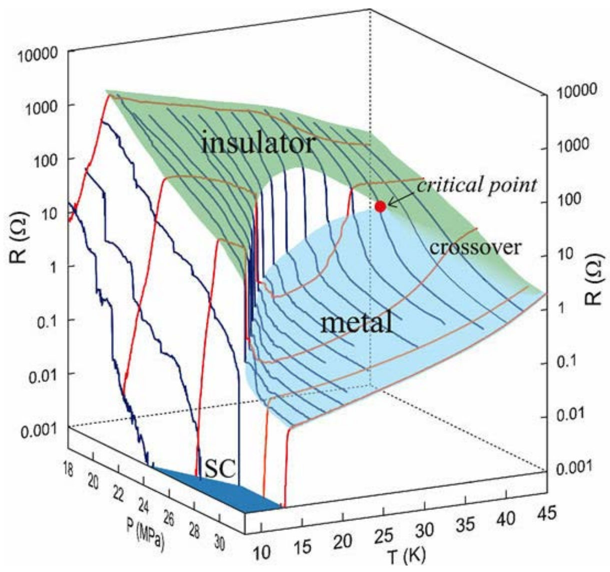
Bare Mott critical point in organics





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)

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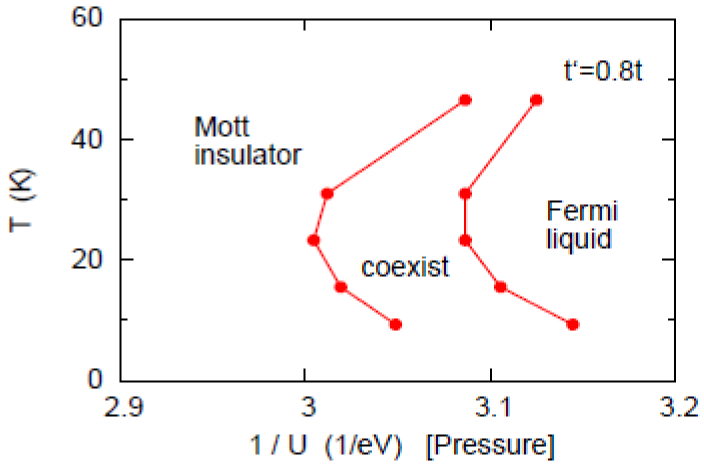
Interaction-induced Mott transition theory



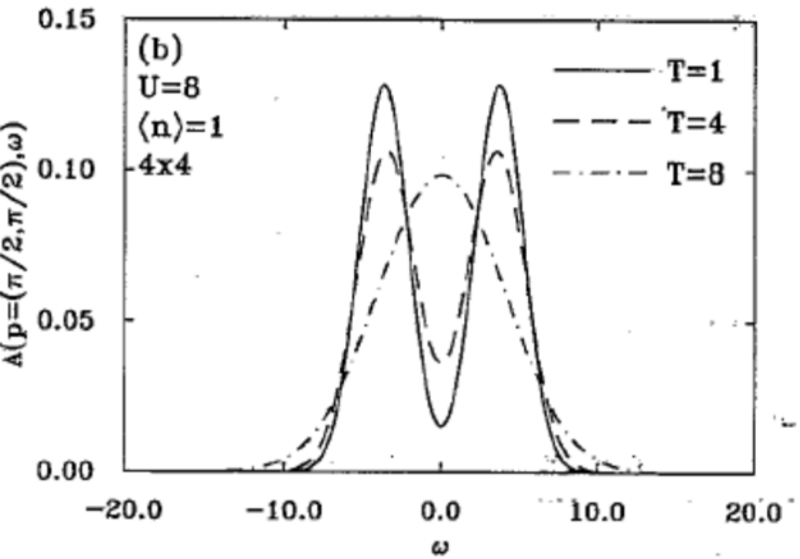
κ–BEDT-Cl

κ–BEDT-CN

Liebsch Phys. Rev. B **79**, 195108 (2009)

See also: Ohashi et al. PRL **100**, 076402 (2008)

Mott insulator at finite T



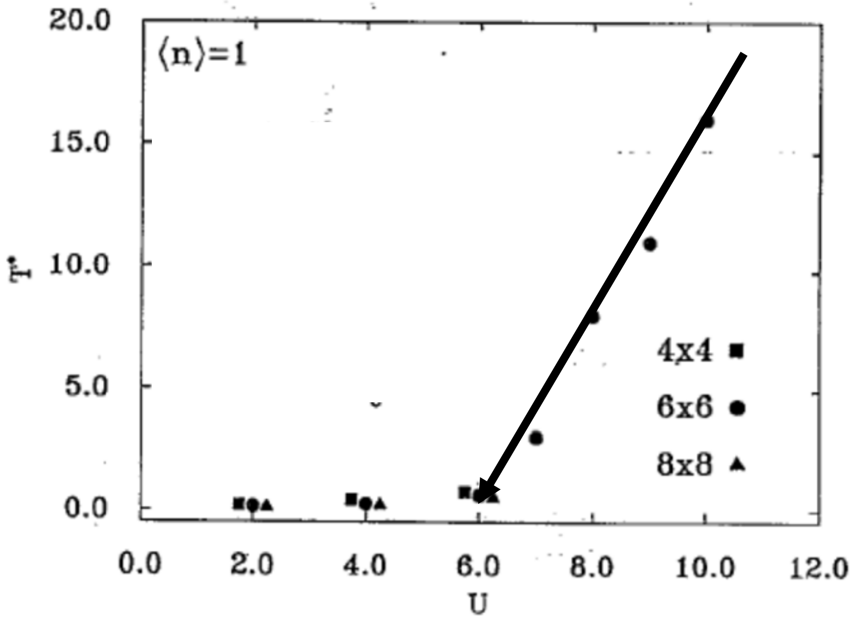


FIG. 5. The temperature T^* at which the gap develops vs U for 4×4, 6×6, and 8×8 lattices.

M. Vekic and S.R. White, PRB 47, 1160 (1993)

Interaction-induced Mott transition, *n* = *1*

Method	U_{c1}	U_c	U_{c2}	Ref.
VCA+ED 2 x 2 + 8b	5.25	5.5	6.37	Balzer et al. EPL (2009)
CDMFT+CTQMC+H 2 x 2	5.3		5.7	Park et al. PRL (2008)
DCA+CTQMC+H 8	5.7		6.4	Gull et al. cond-mat (2009)
DCA+CTQMC+H 4	!	~4.2	!	Gull et al. EPL (2008)
Dual fermions	!	~6.5	!	Hafermann et al. (2008)
CDMFT+ED 2 x 2 + 8b 15 parameters	?	~5.6	?	Liebsch, Merino… (2008)
CDMFT+ED 2,3,4		~4		Zhang et al. PRB (2007) (3d also)
QMC 6 x 6		6		Vekic et al. (1993)

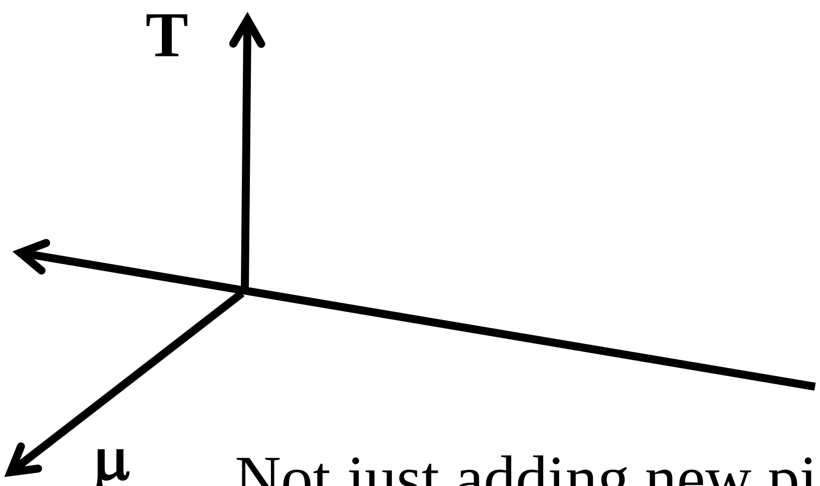
Finite *T* phase diagram

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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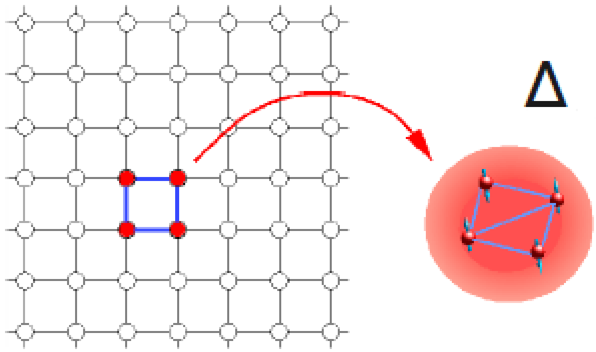
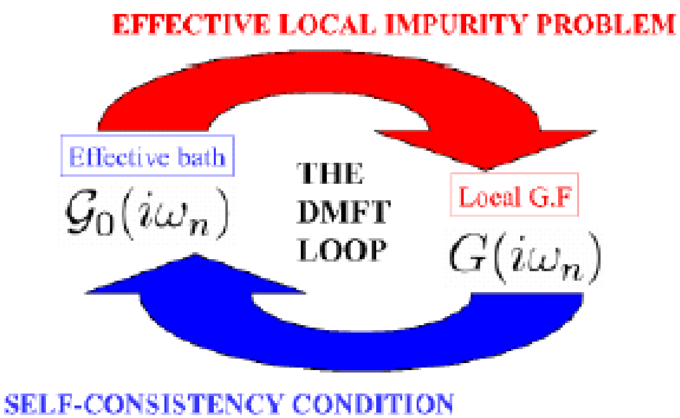
C-DMFT



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



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

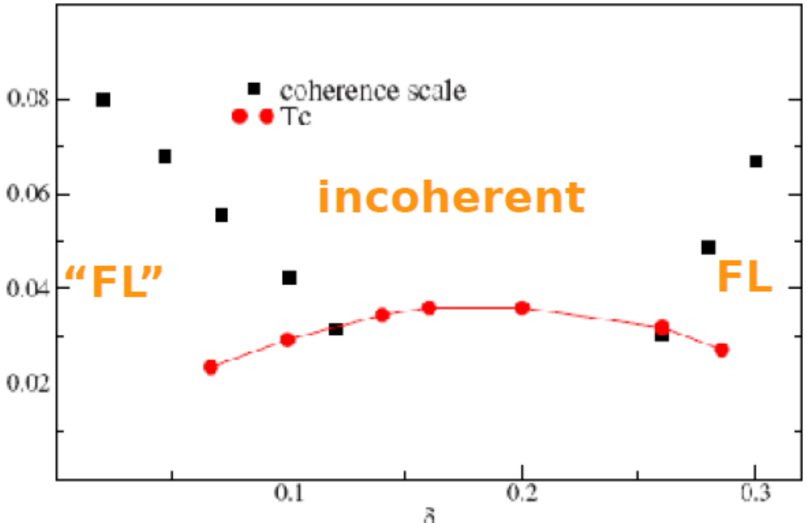
$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n) - \left[\sum_{\tilde{k}} \frac{1}{i\omega_n + \mu - t_c(\tilde{k}) - \Sigma_c(i\omega_n)} \right]^{-1}$$

Solving cluster in a bath problem

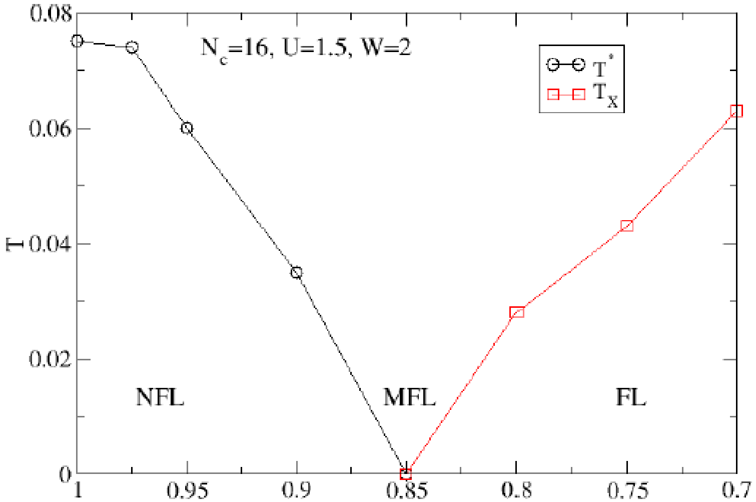
- Continuous-time Quantum Monte Carlo calculations to sum all diagrams generated from expansion in powers of hybridization.
  - P. Werner, A. Comanac, L. de' Medici, M. Troyer, and A. J. Millis, Phys. Rev. Lett. **97**, 076405 (2006).
  - K. Haule, Phys. Rev. B **75**, 155113 (2007).

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)

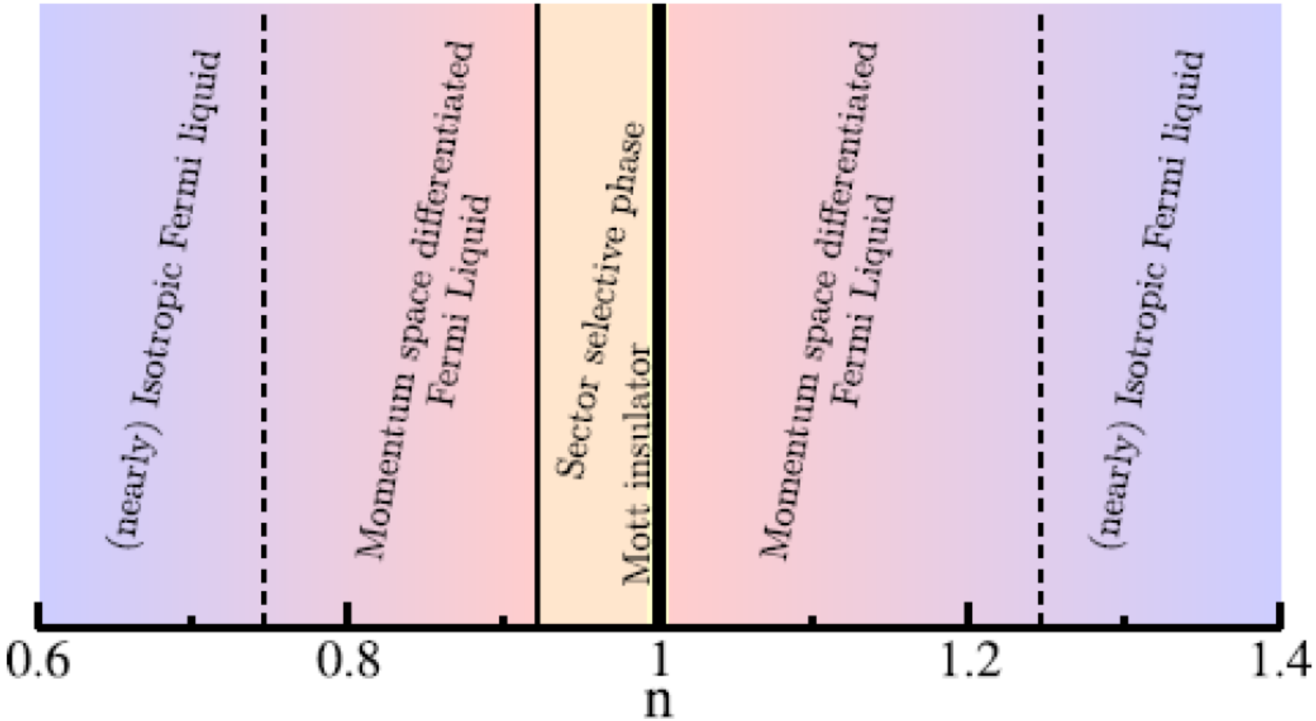


K. Haule, G. Kotliar, PRB (2008)



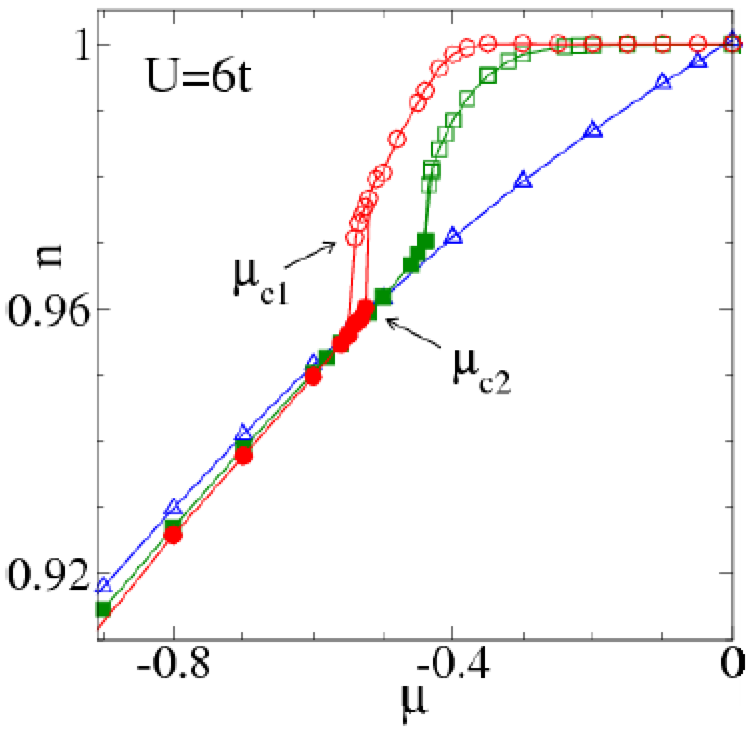
Vildhyadhiraja, PRL (2009)

Doping driven Mott transition



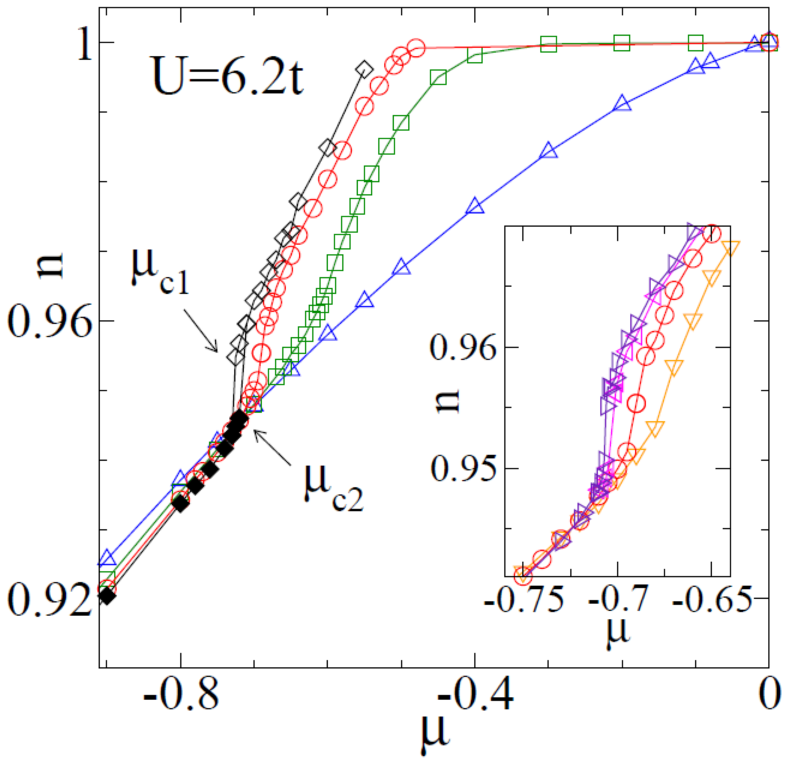
Gull, Werner, Millis, (2009)

First order transition at finite doping

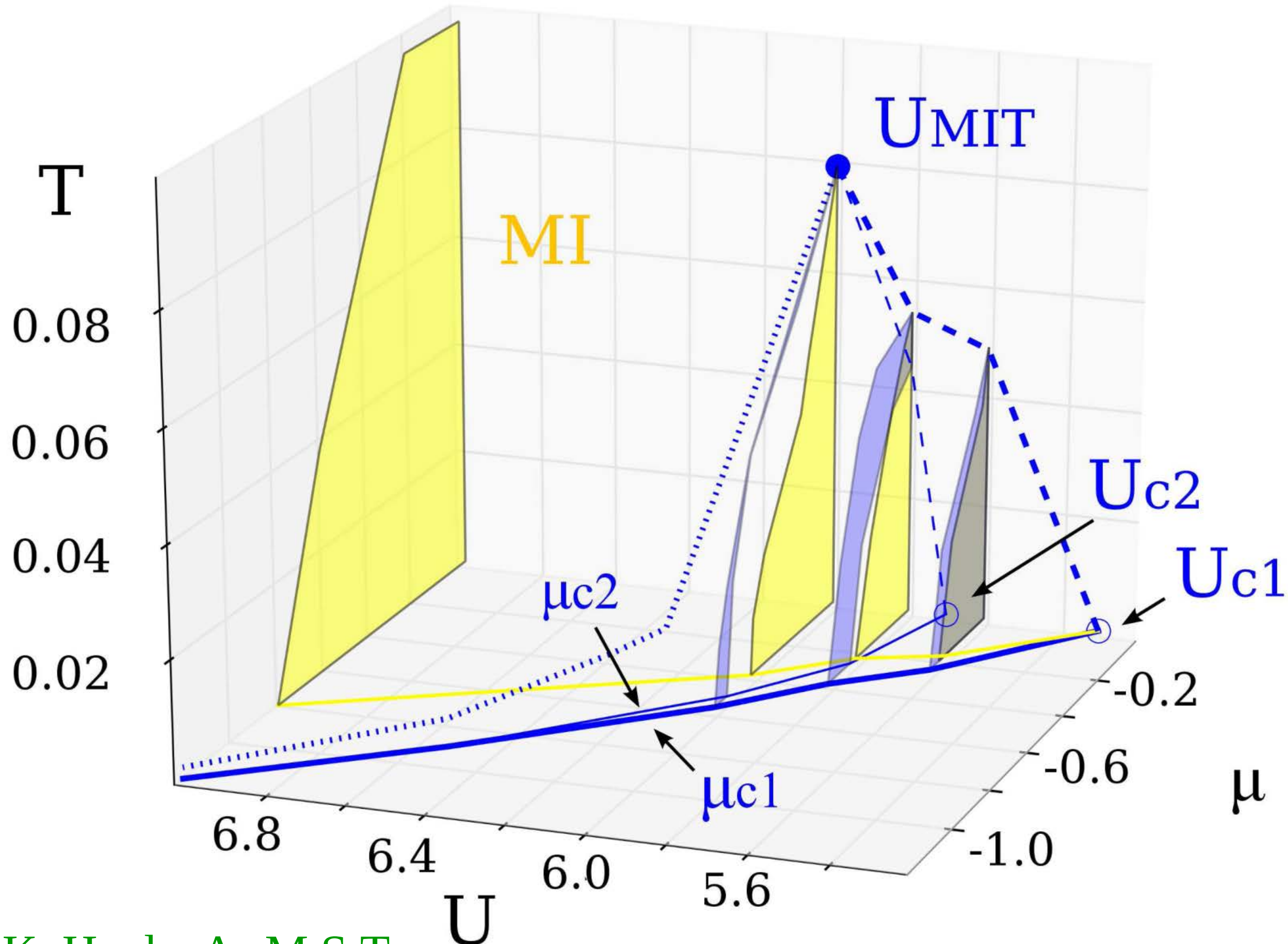


$n(\mu)$ for several temperatures:
$T/t =$ 1/10, 1/25, 1/50

The critical point



Normal state phase diagram



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

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

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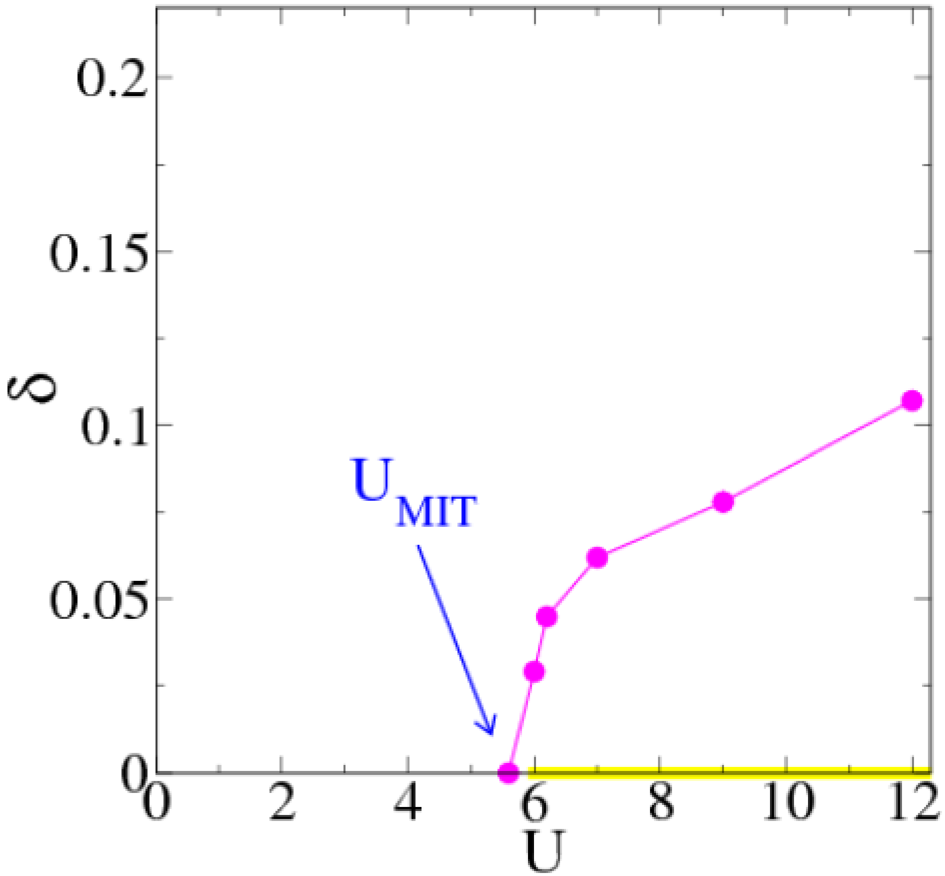
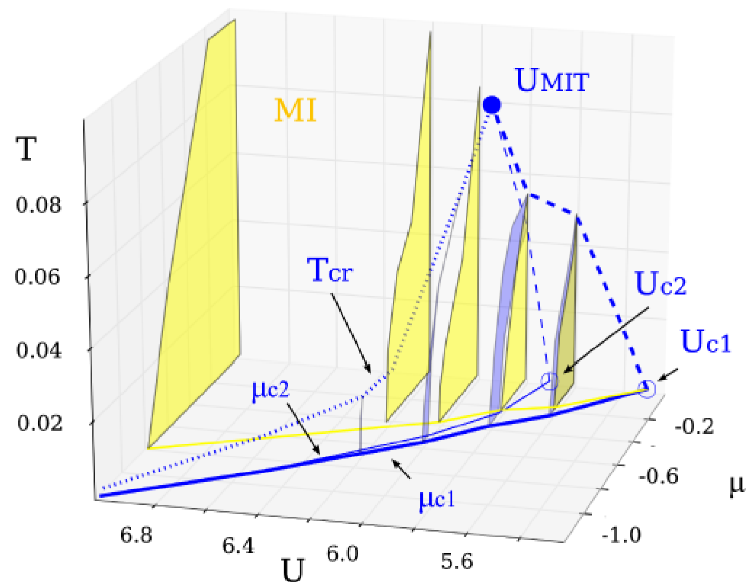
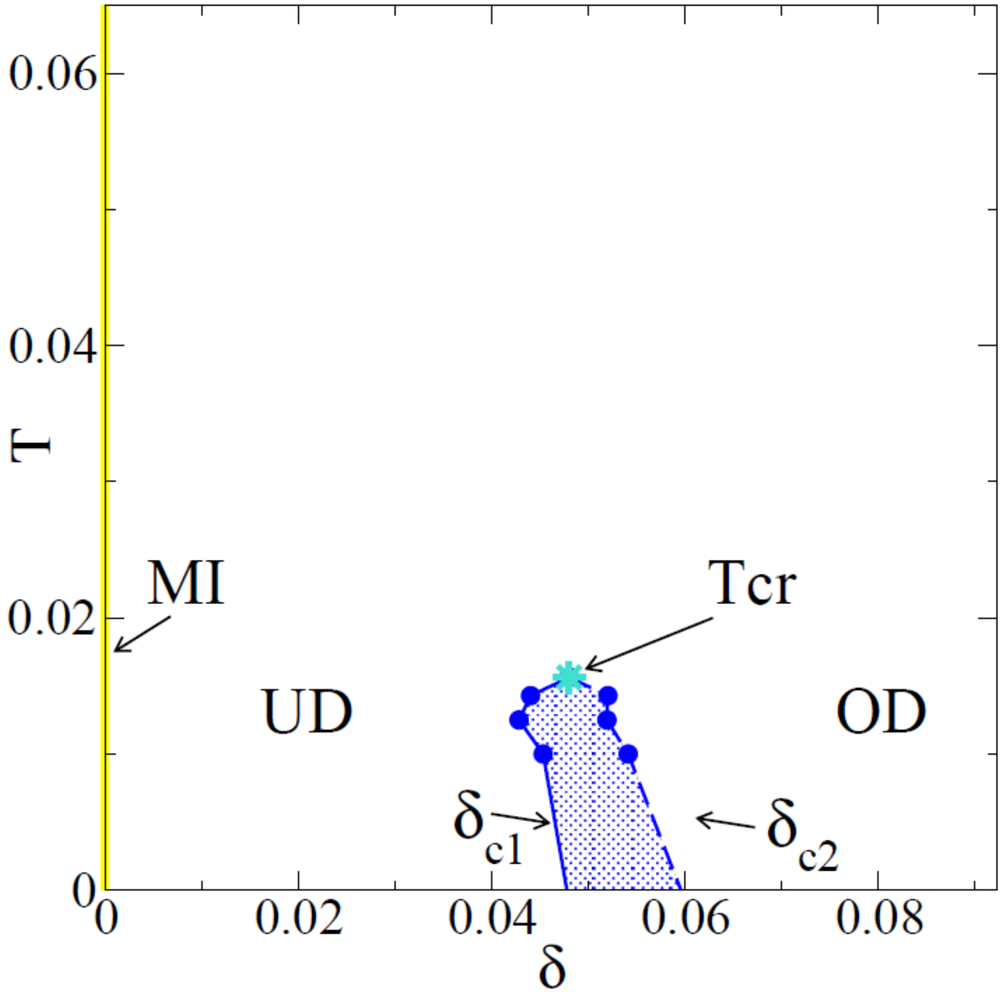
Link to Mott transition up to optimal doping

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





Characterisation of the phases (U=6.2t)



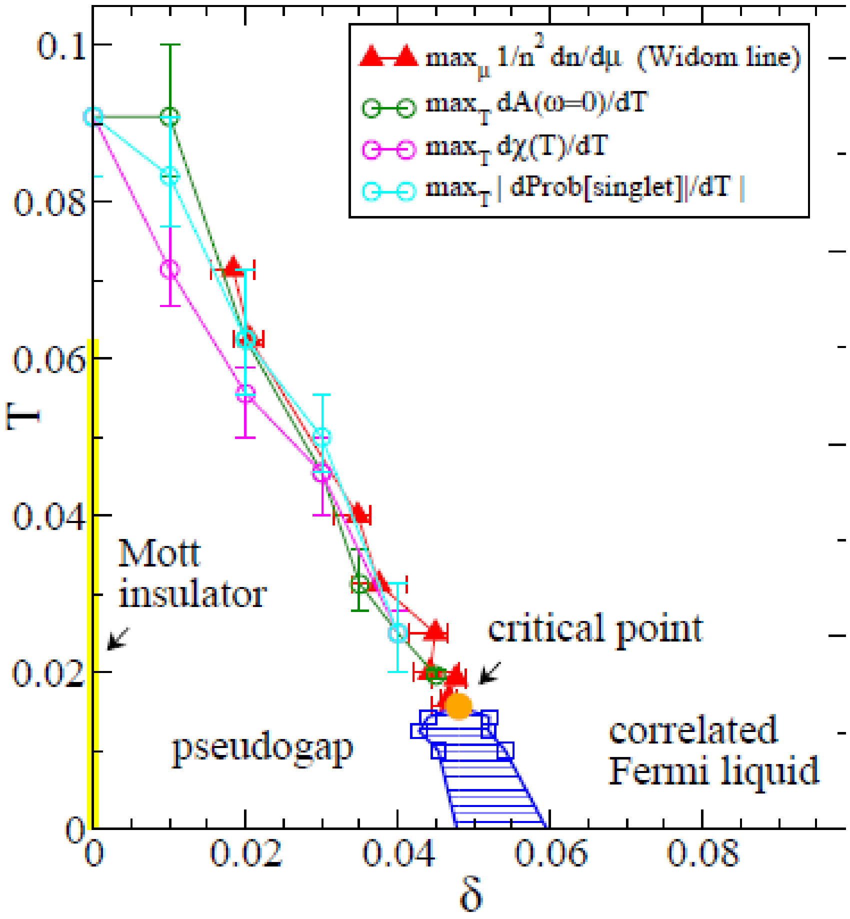
$U > U_{\mathrm{MIT}}$:

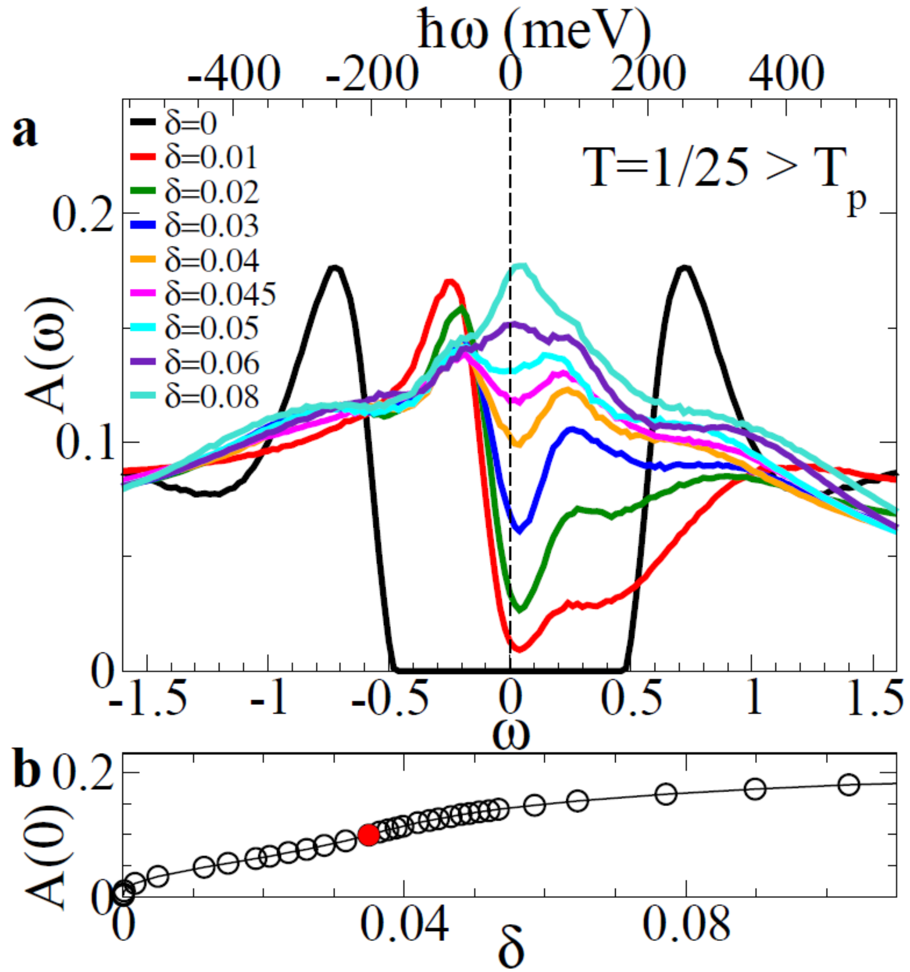
1. Mott insulator (MI)
2. Underdoped phase (UD): $\delta < \delta_c$
3. Overdoped phase (OD): $\delta > \delta_c$
4. Coexistence/forbidden region

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

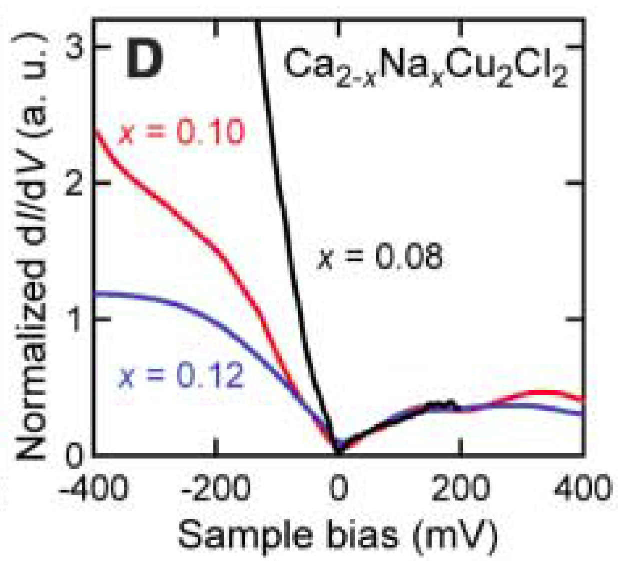
How does the UD phase differ from the OD phase?

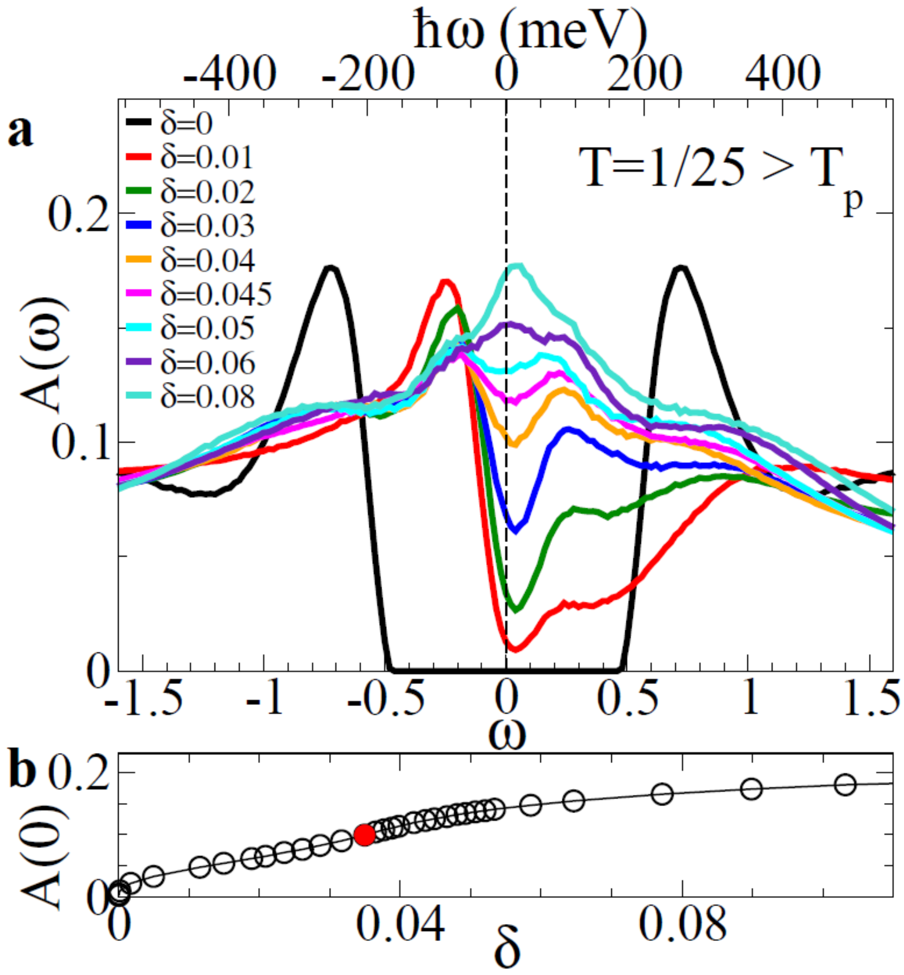
Density of states





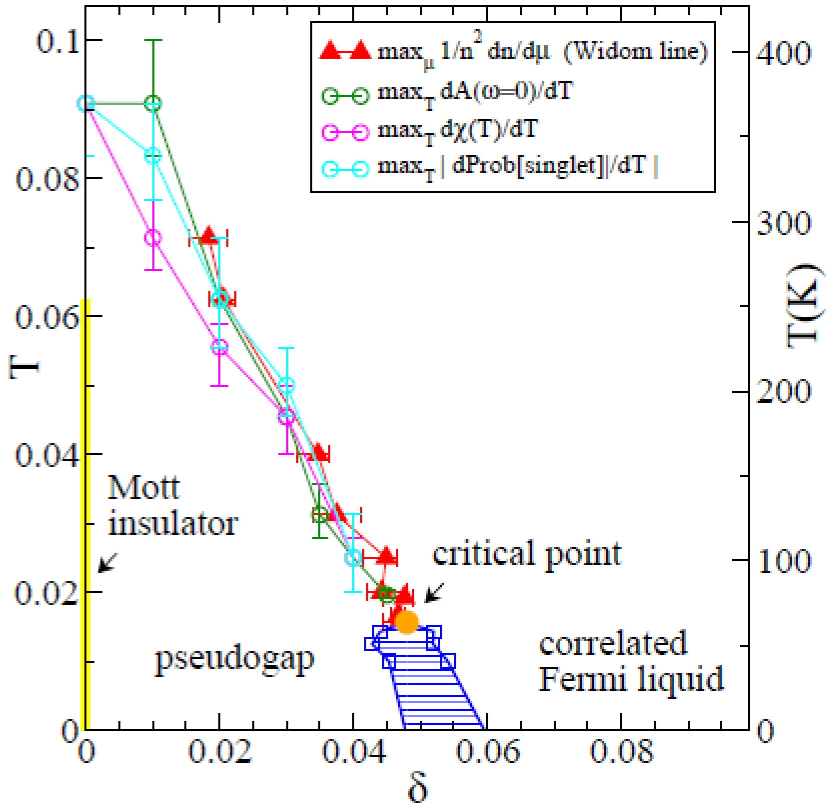
Density of states

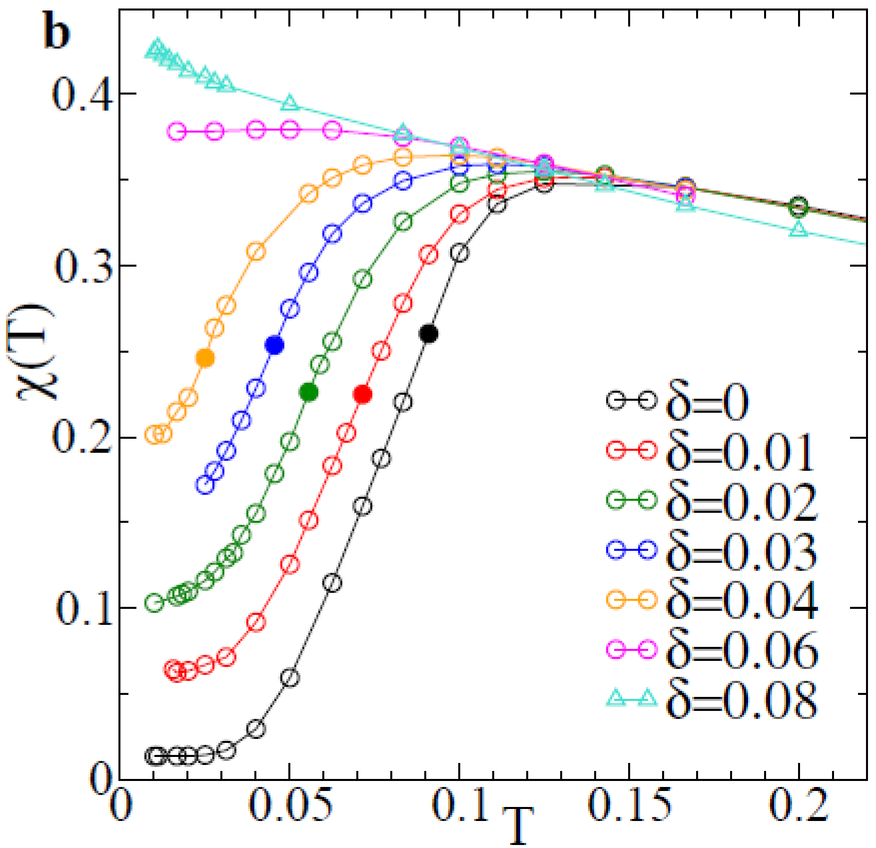




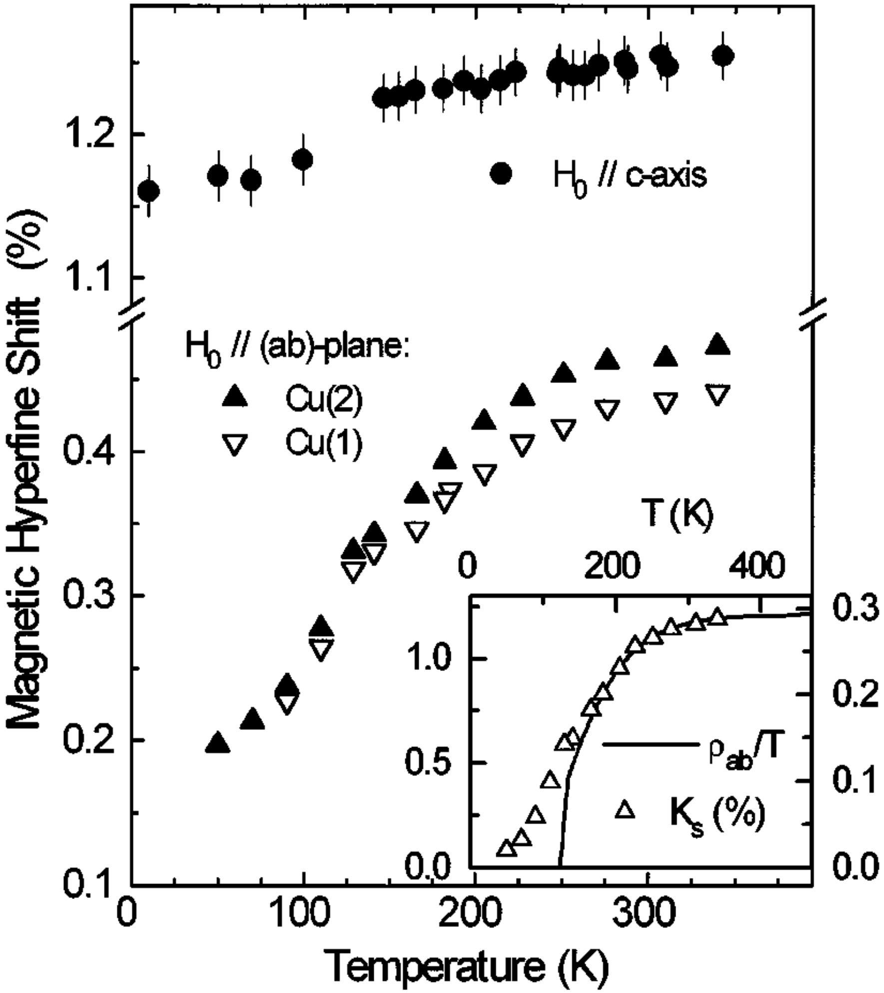
Khosaka et al. *Science* **315**, 1380 (2007);

Spin susceptibility



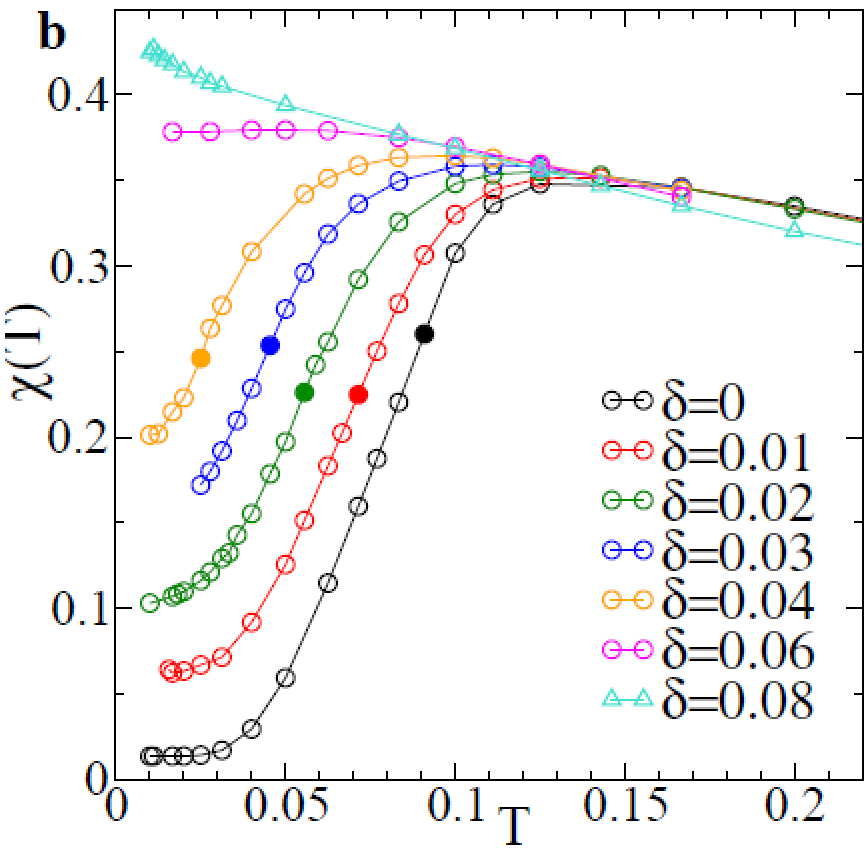


Spin susceptibility



Underdoped Hg1223

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



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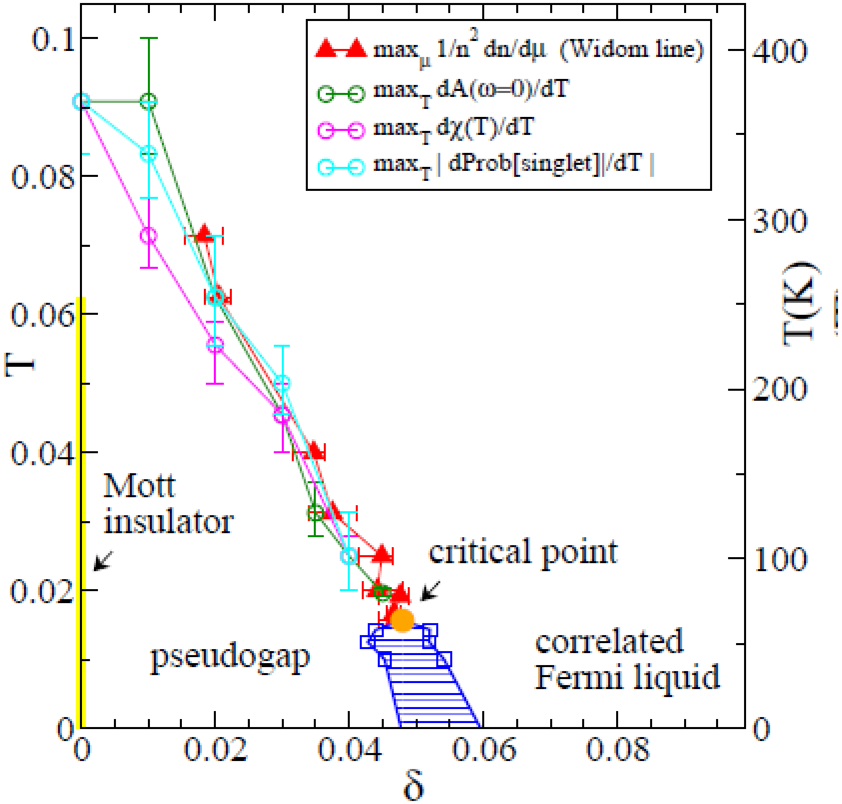
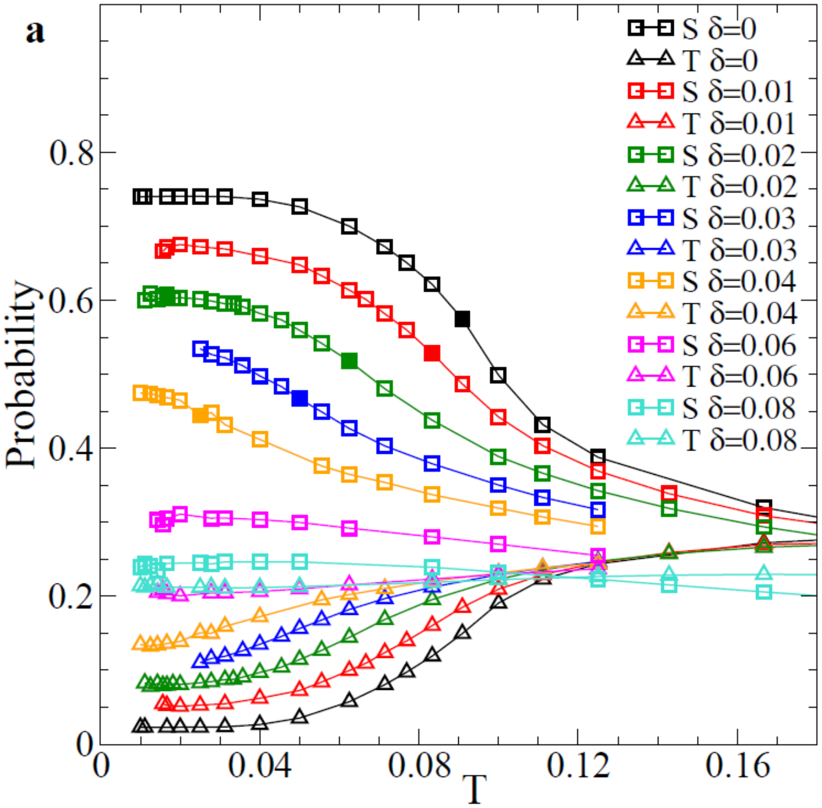
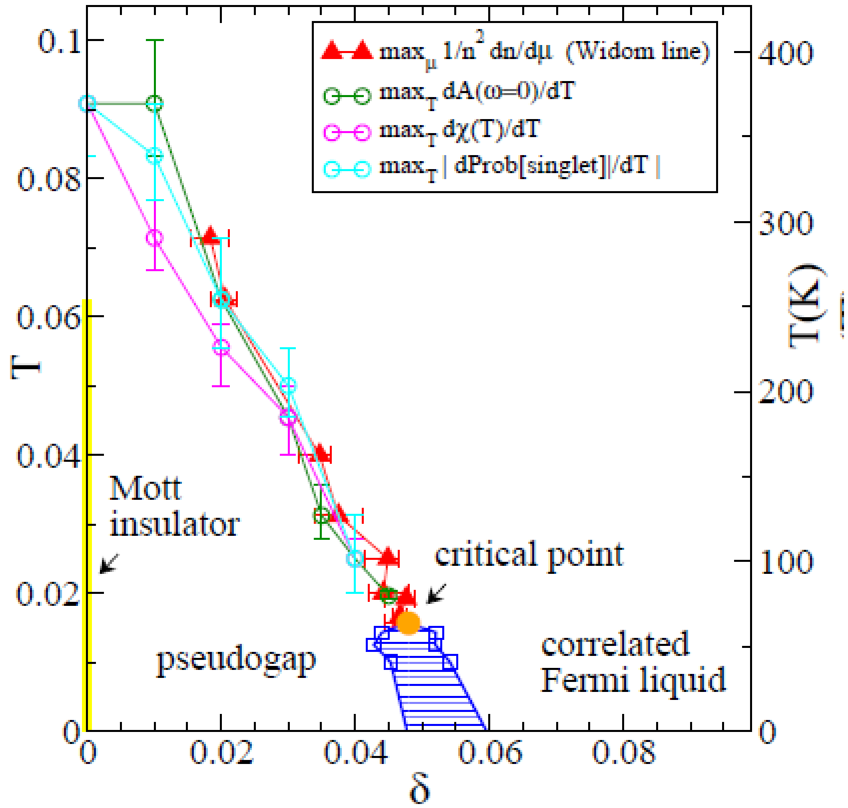
Plaquette eigenstates





Pseudogap T^* along the Widom line



Giovanni Sordi

Patrick Sémon

Kristjan Haule

Finite *T* phase diagram

Pseudogap in the normal state and the Widom line

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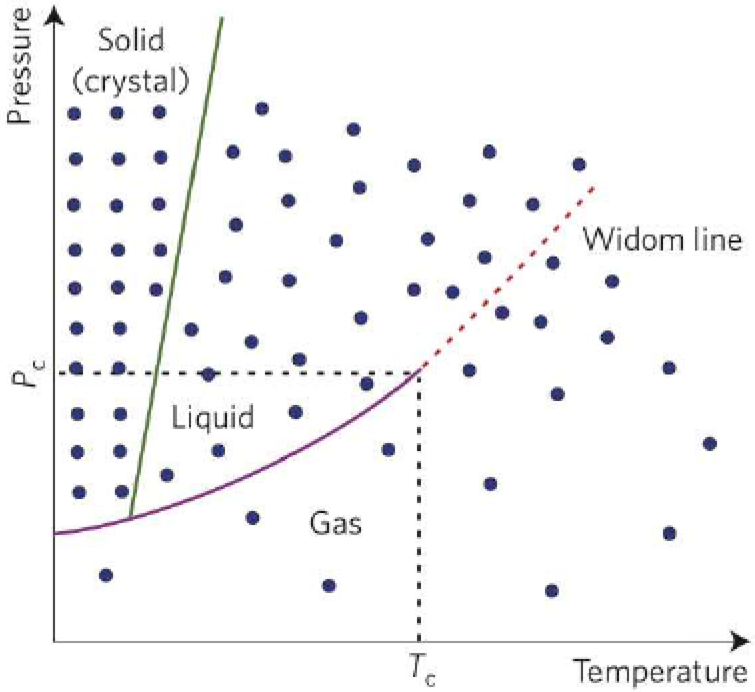
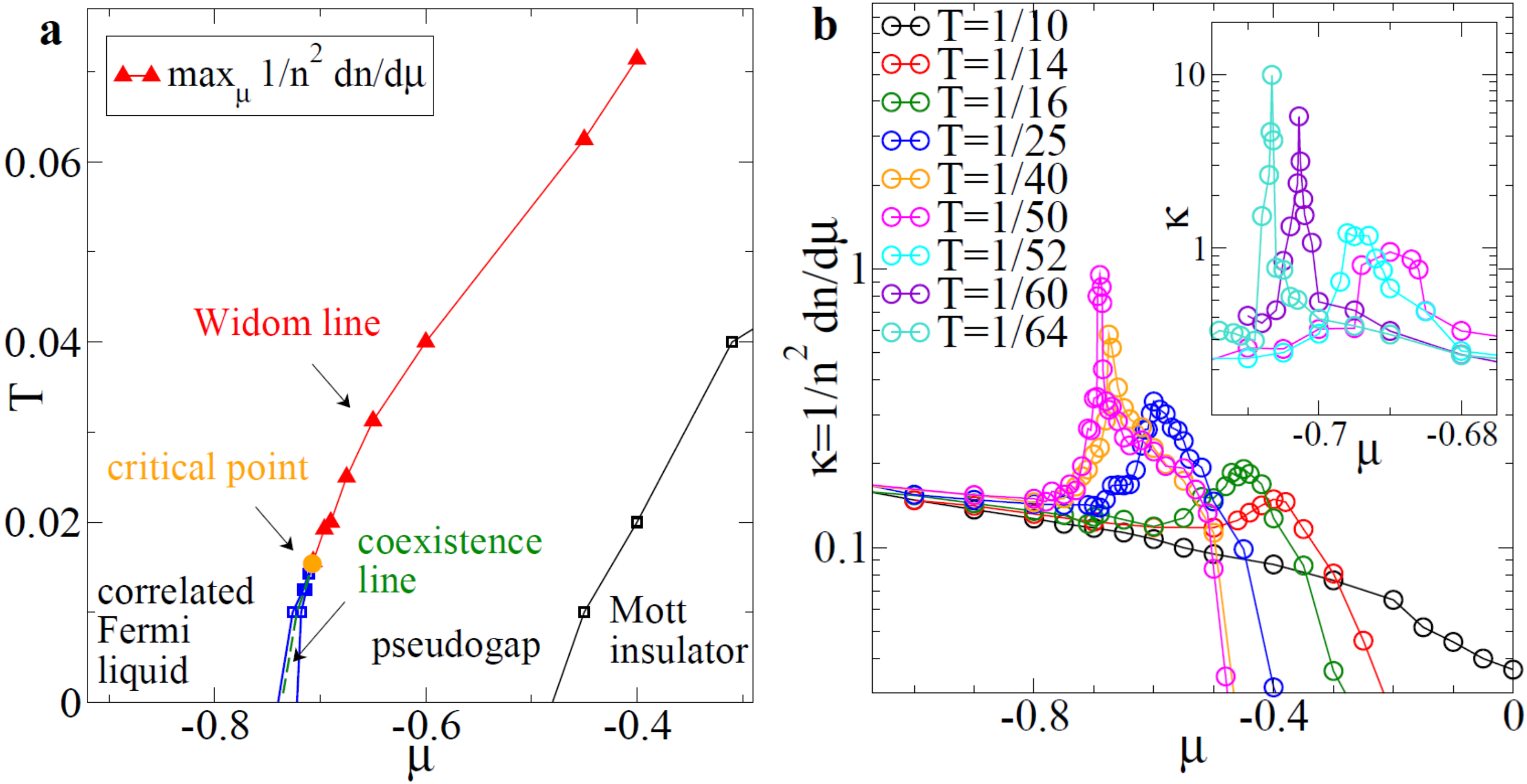
What is the Widom line?



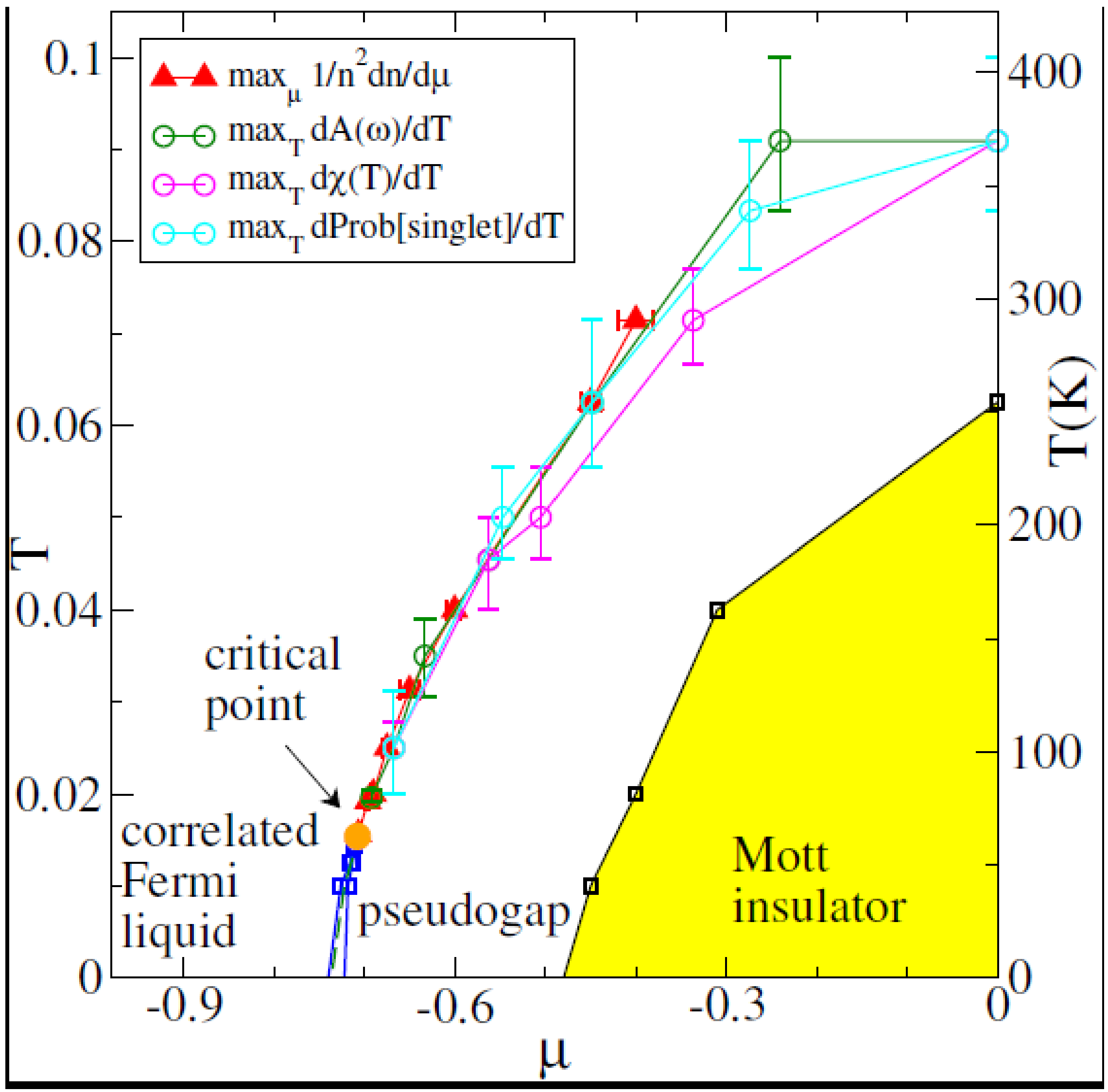
McMillan and Stanley, Nat Phys 2010

- 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 $T \rightarrow T_p$
- 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

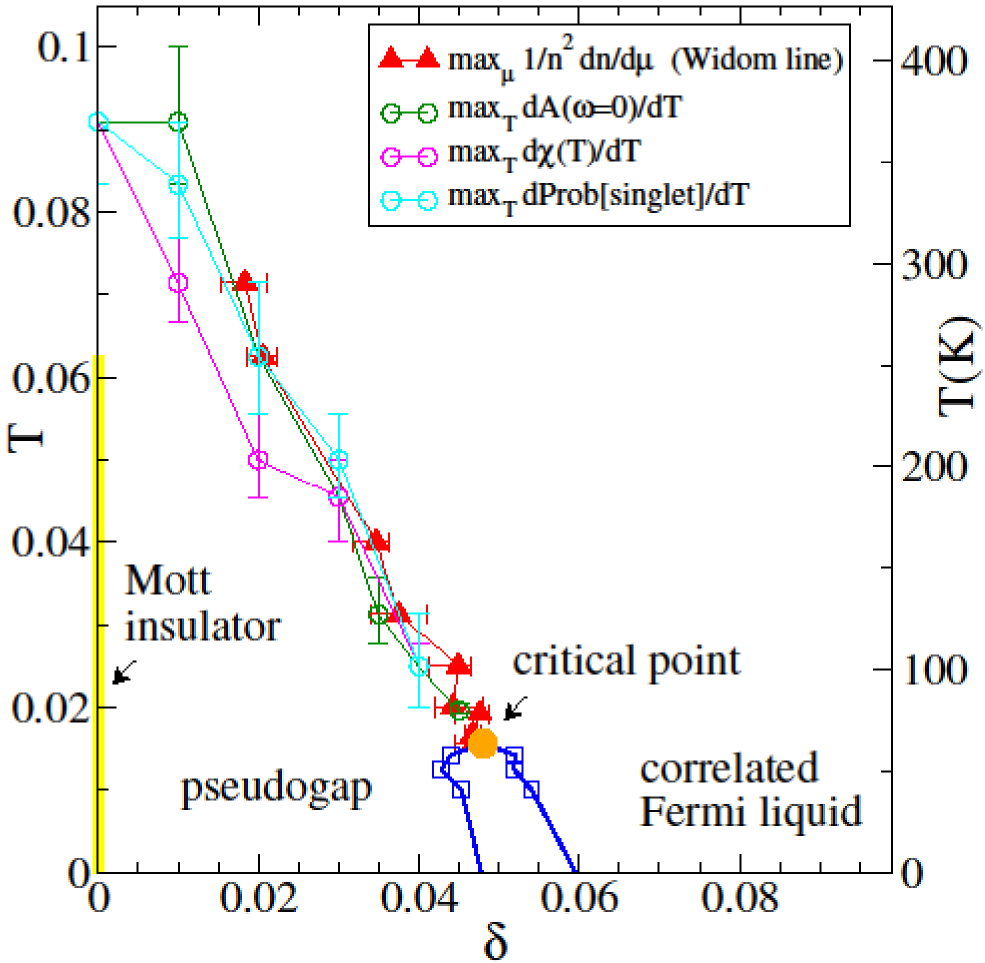
The Widom line



Rapid change also in dynamical quantities



Phase diagram



Giovanni Sordi

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Kristjan Haul

Finite *T* phase diagram

Superconductivity

arXiv:1201.1283v1

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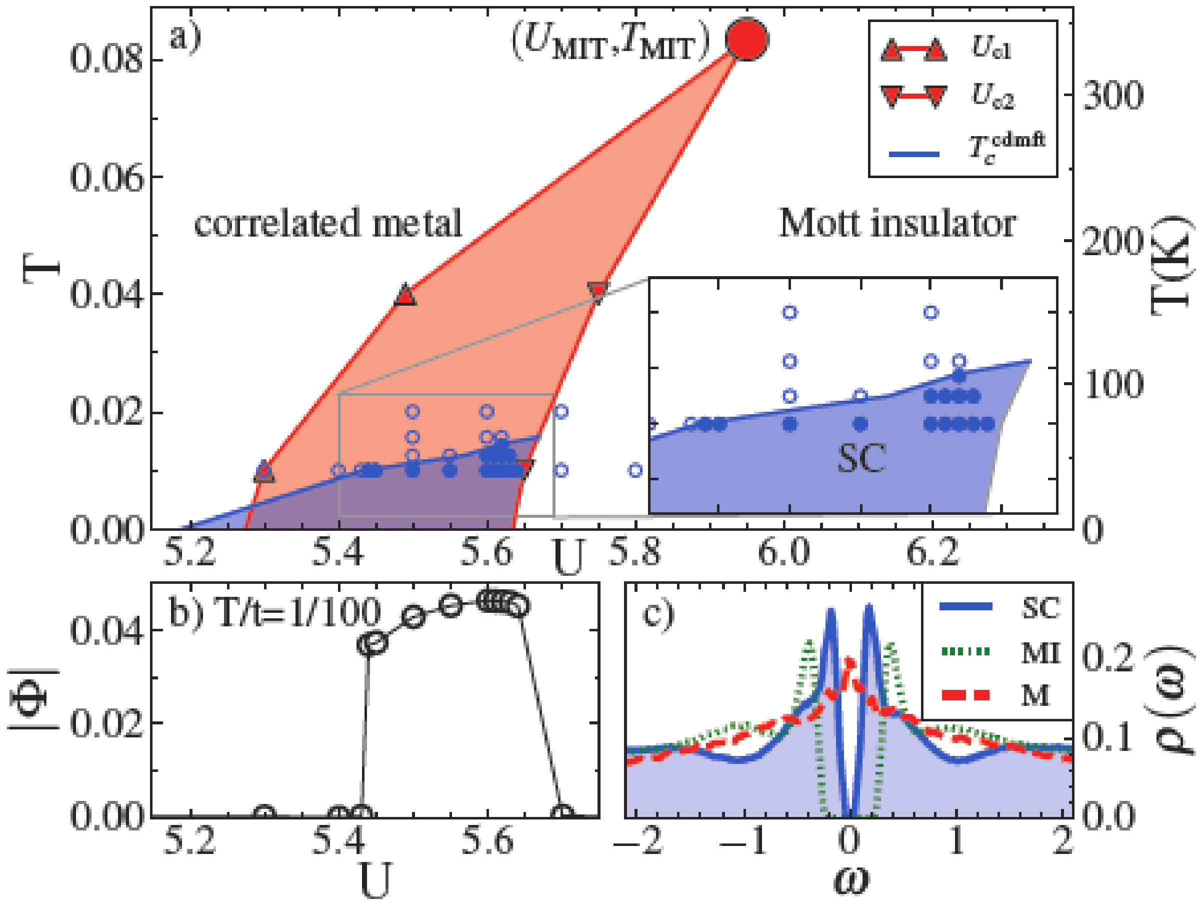
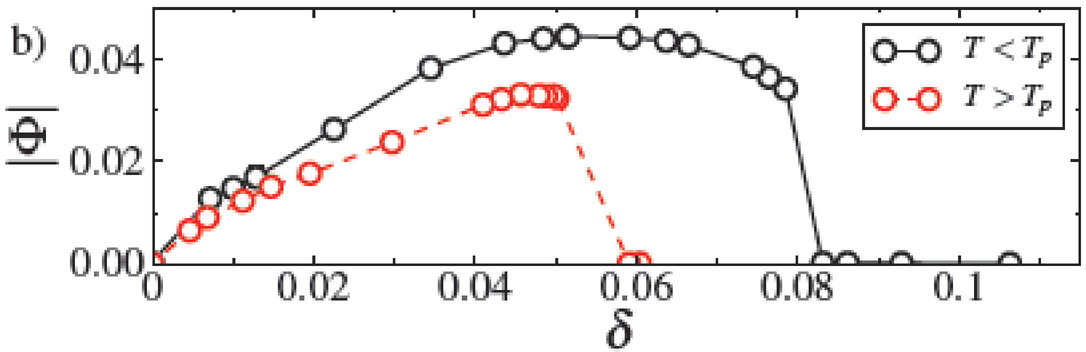
n = 1, Almost layered organics BEDT

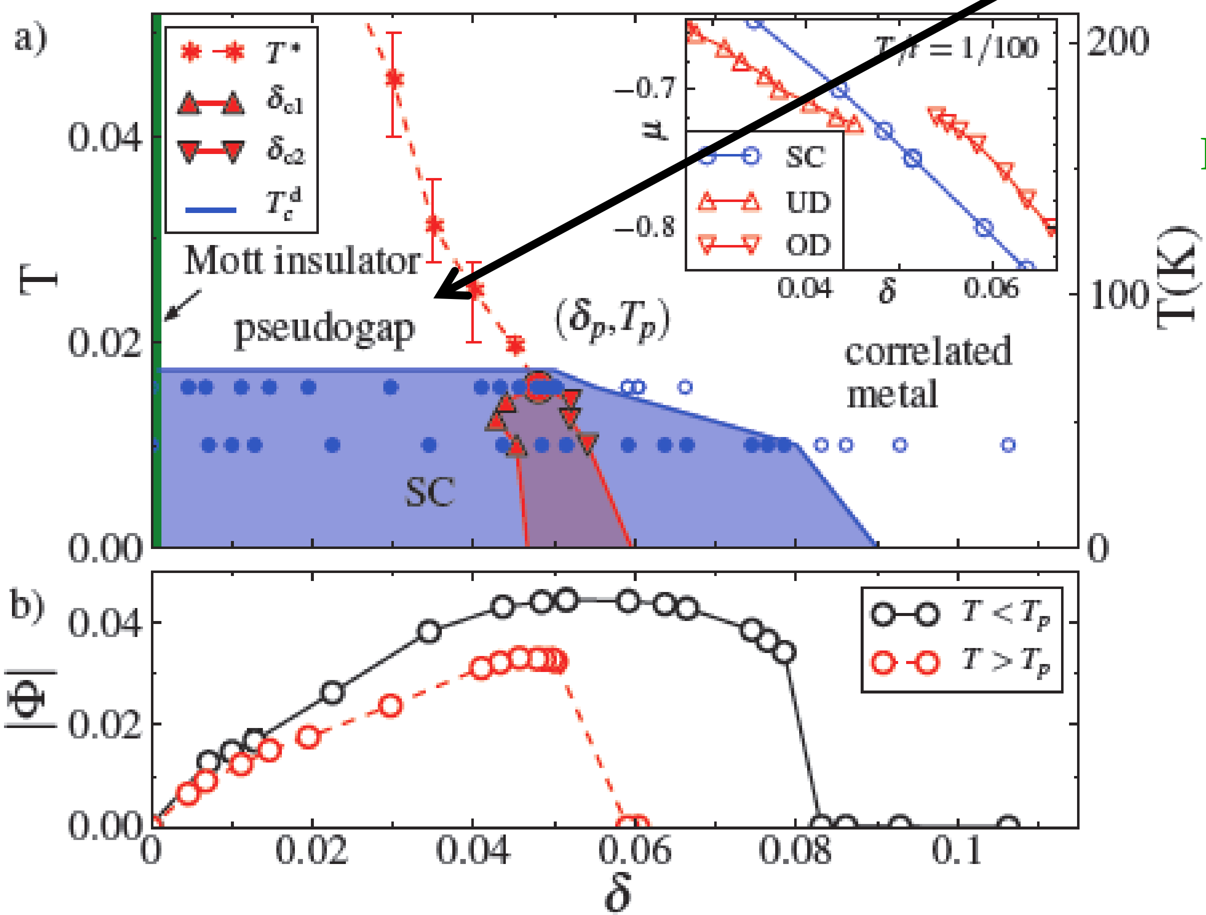


Cuprates (doping driven transition)



Cuprates (doping driven transition)

Pseudogap vs pair



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

Contrast Tc and order parameter even at large U

Haule&Kotliar PRB 76 104509: t-J model (J/t=0.3)

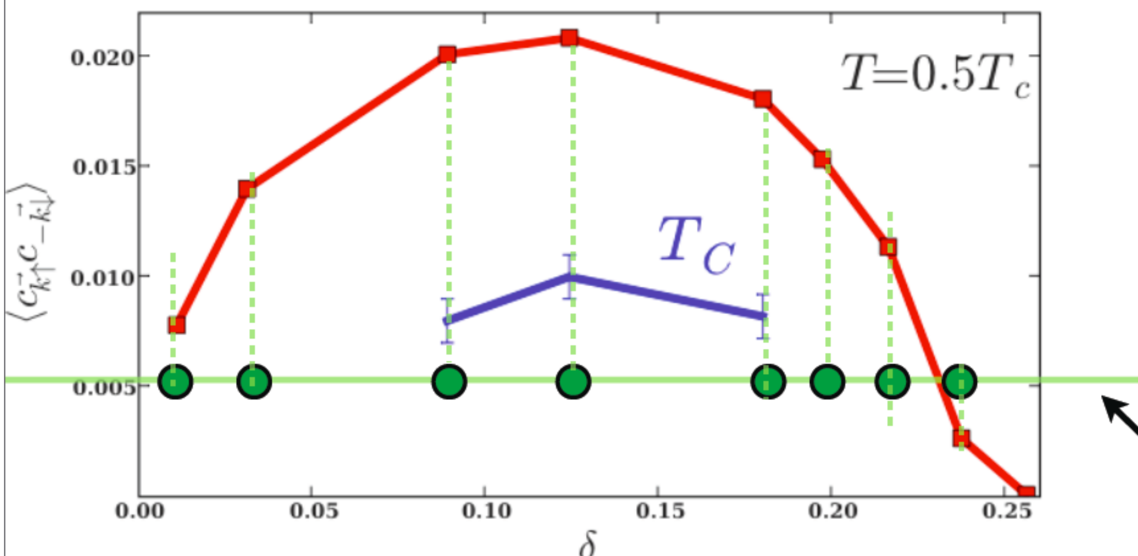
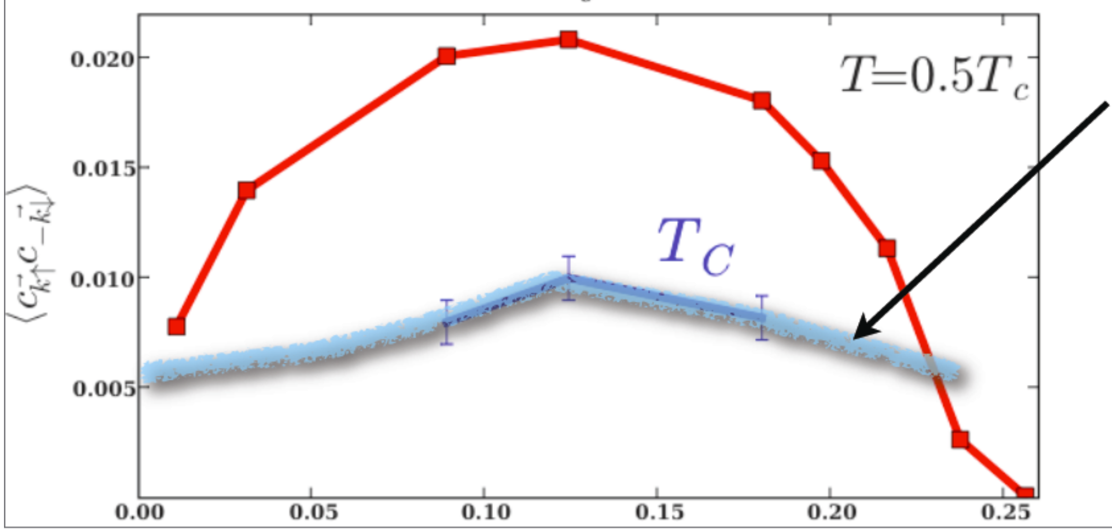


FIG. 20. (Color online) Order parameter in C-DMFT computed with CTQMC at T=0.5T_{cmax}. The critical temperature (in units of t) for a few doping values is also displayed.

Tc^max/2

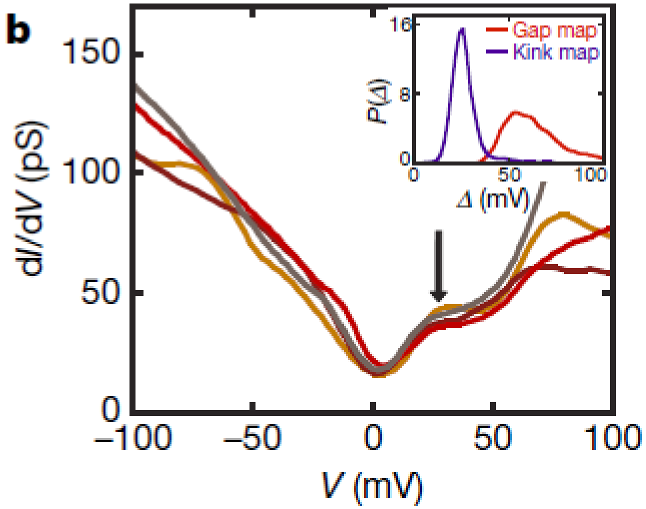


Lower bound

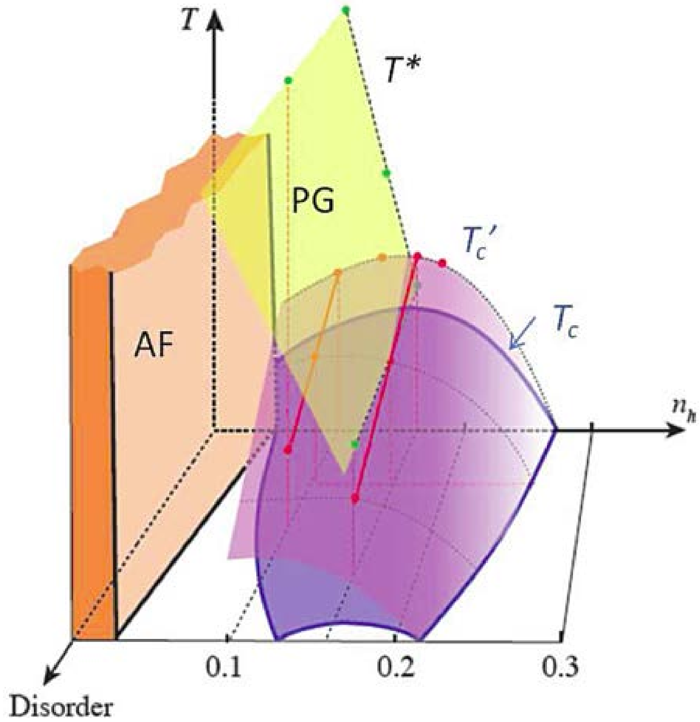
FIG. 20. (Color online) Order parameter in C-DMFT computed with CTQMC at T=0.5T_{cmax}. The critical temperature (in units of t) for a few doping values is also displayed.

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)

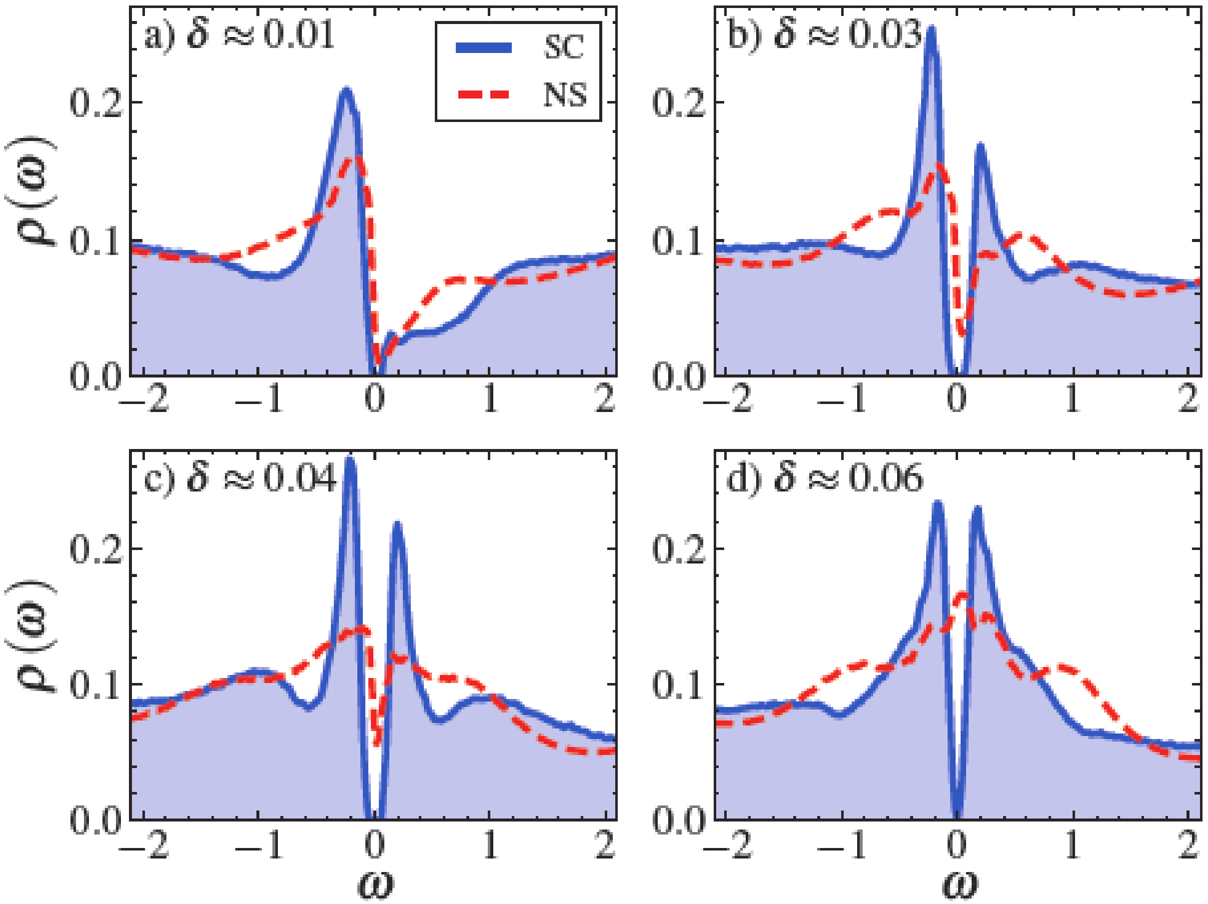


F. Rullier-Albenque, H. Alloul, and G.Rikken, Phys. Rev. B **84**, 014522 (2011).

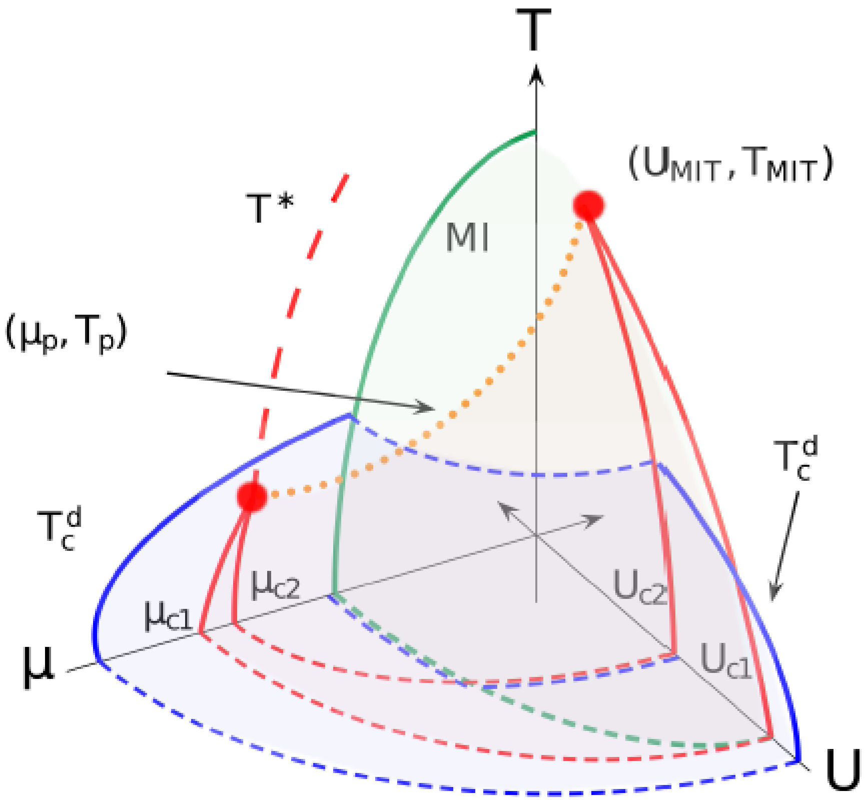
Actual T_c in underdoped

- 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).

First-order transition leaves its mark



Unified phase diagram



Other topics

Main collaborators

Giovanni Sordi

Kristjan Haule

David Sénéchal

Bumsoo Kyung

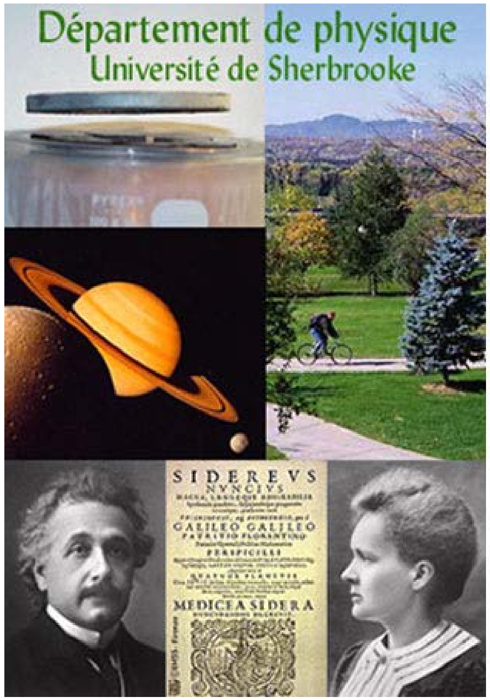
Patrick Sémon

Massimo Capone

Sarma Kancharla

Marcello Civelli

Gabriel Kotliar



André-Marie Tremblay

CANADA RESEARCH CHAIRS
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RQMP
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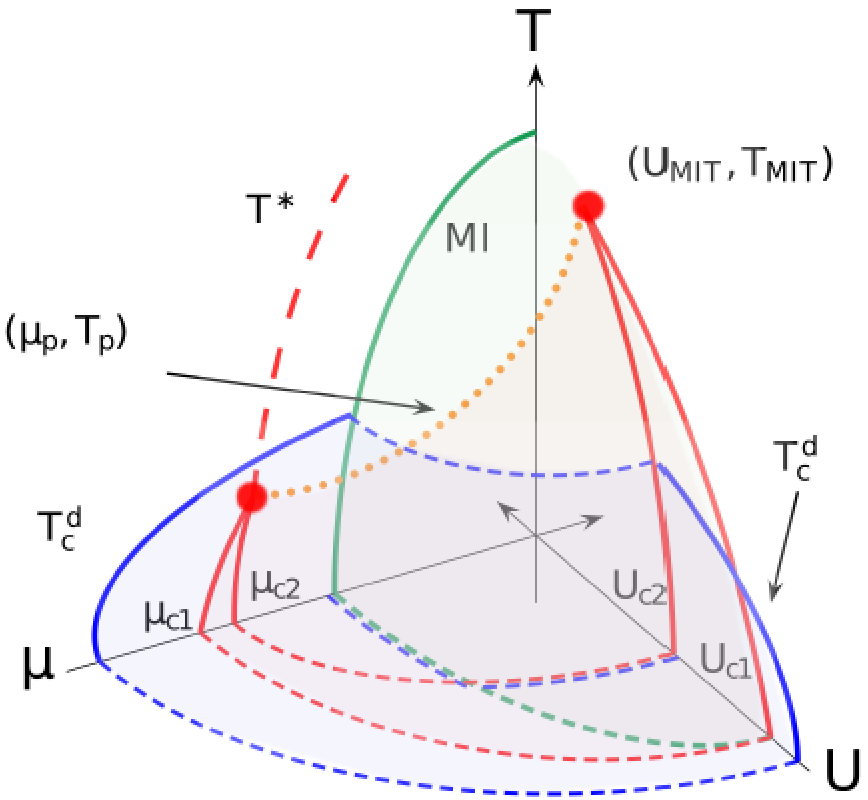
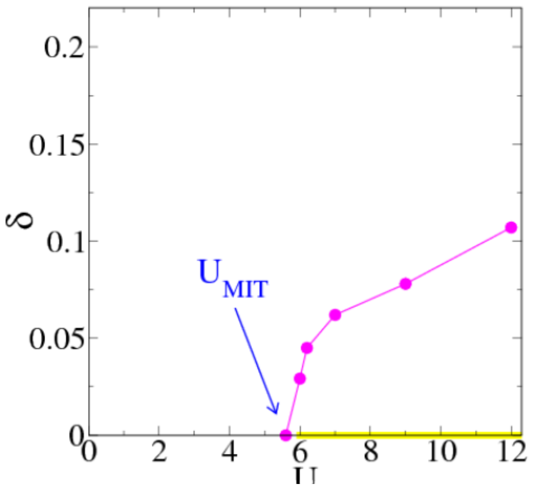
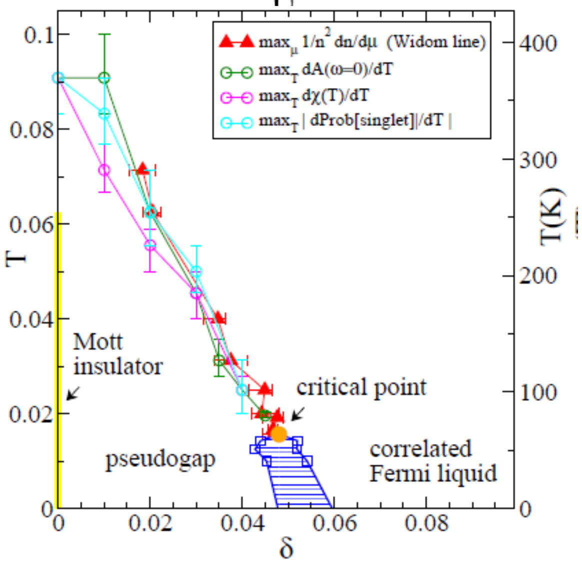
Summary



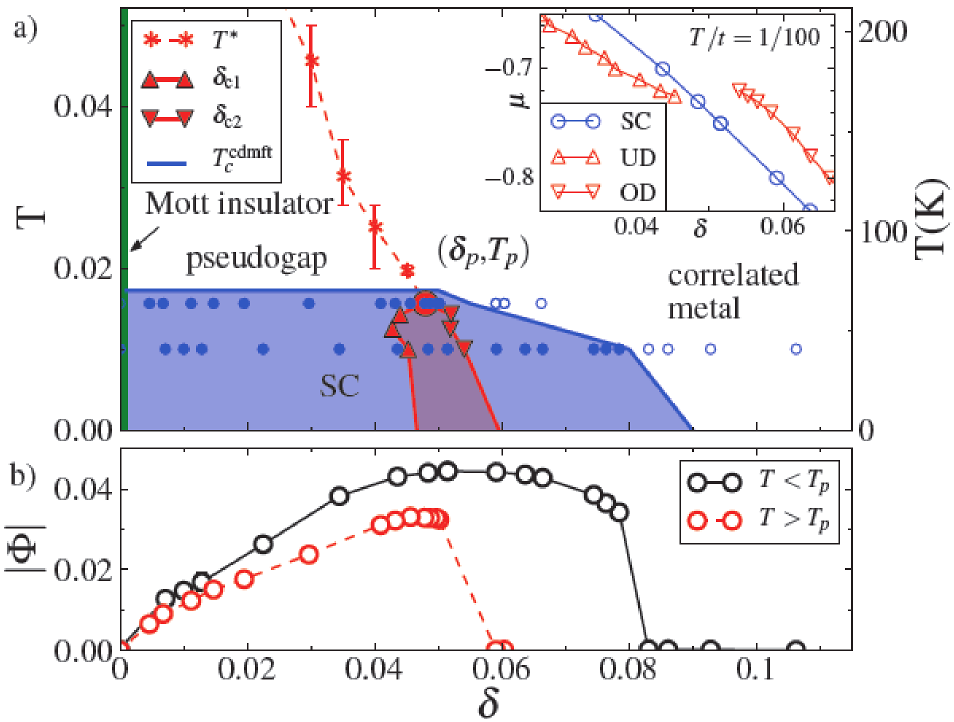
Summary

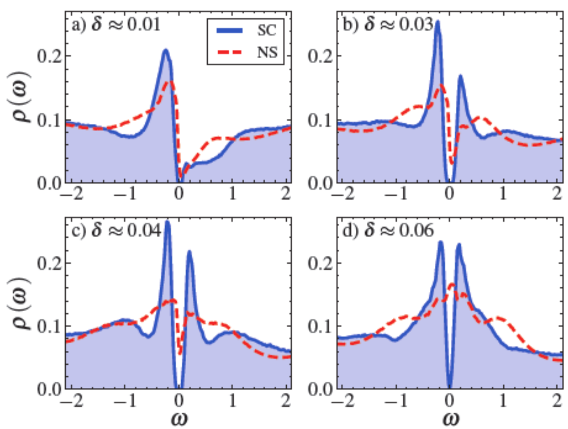




- Mott physics extends way beyond half-filling
- Pseudogap is a phase
- Pseudogap *T** is a Widom line
- High compressibility (stripes?)

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