Mott Physics in Superconductors

A.-M. Tremblay

G. Sordi, D. Sénéchal, K. Haule,

S. Okamoto, B. Kyung, M. Civelli

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CANADIAN INSTITUTE for ADVANCED RESEARCH

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Harvard, 15 September 2011

VERITATEM IN CHARITATE

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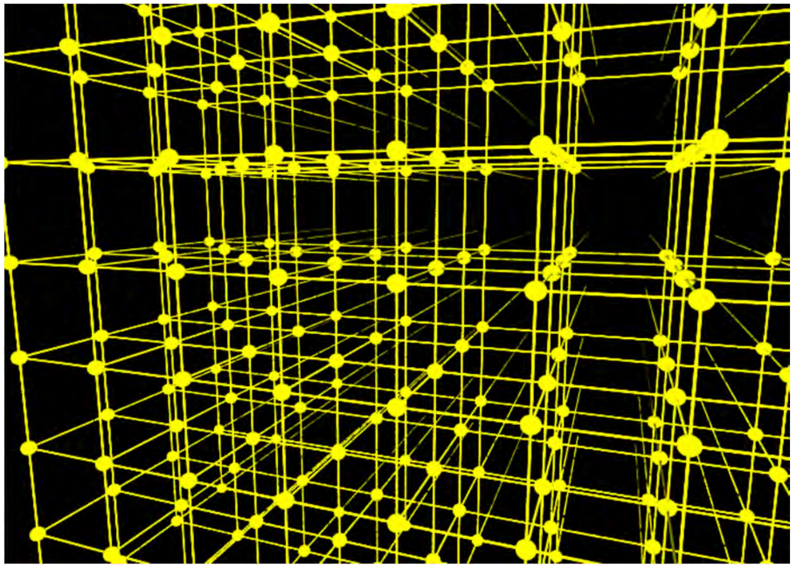
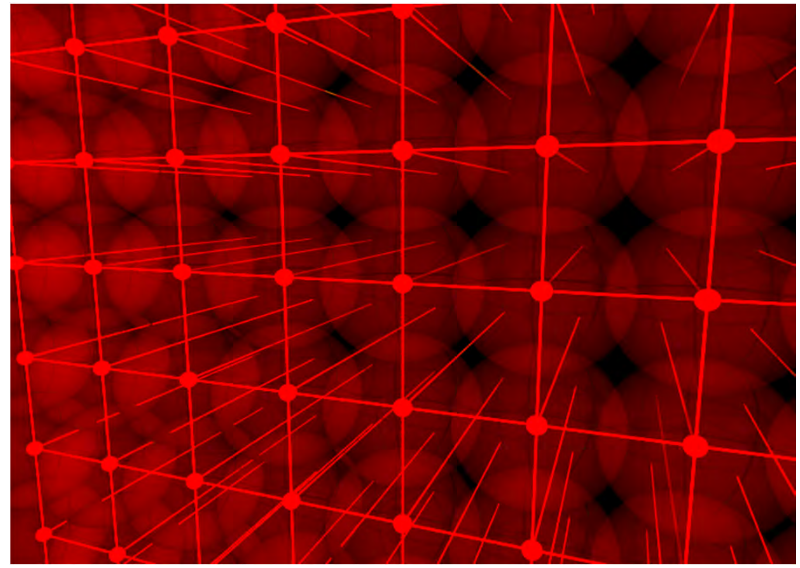
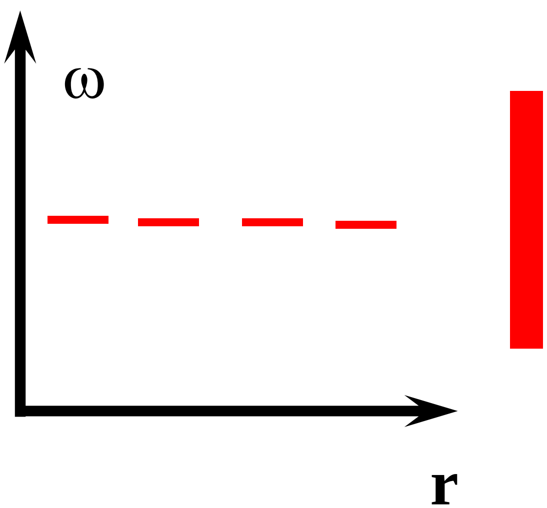
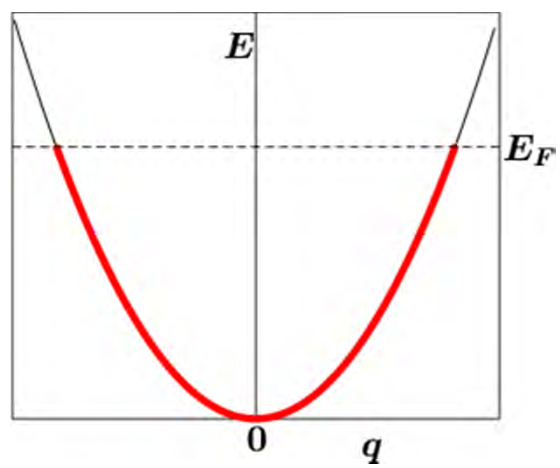
How to make a metal





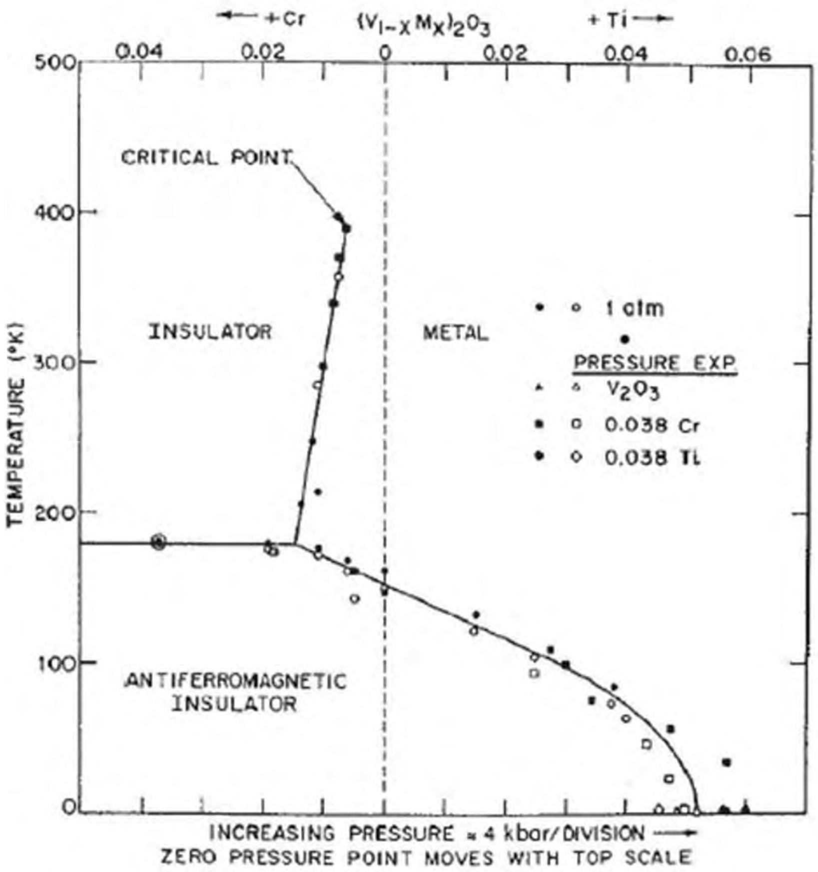




Courtesy, S. Julian

« Conventional » Mott transition

T



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Understood from Hubbard model and dynamical mean field theory

Figure: McWhan, PRB 1970; Limelette, Science 2003

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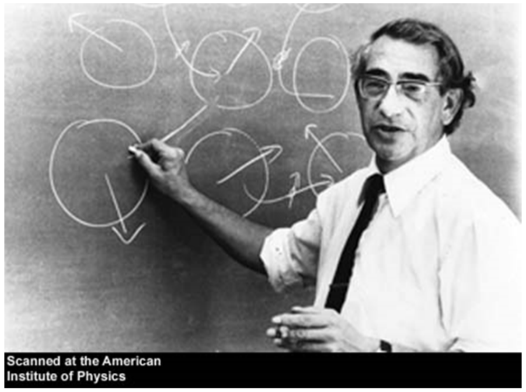
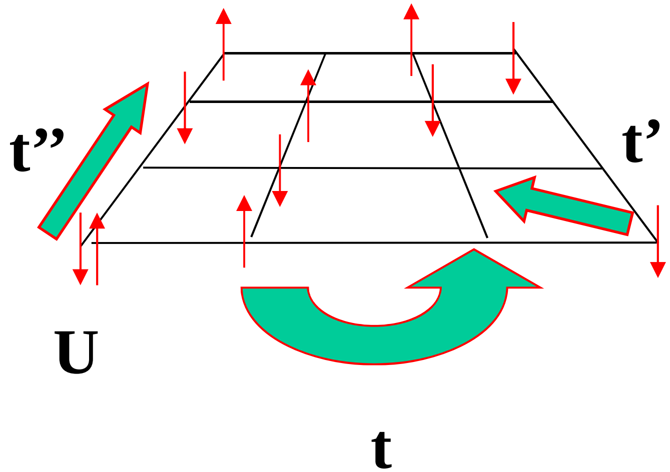
Hubbard model

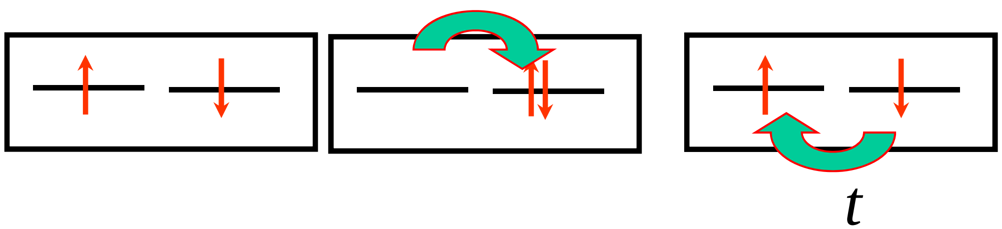


1931-1980

μ

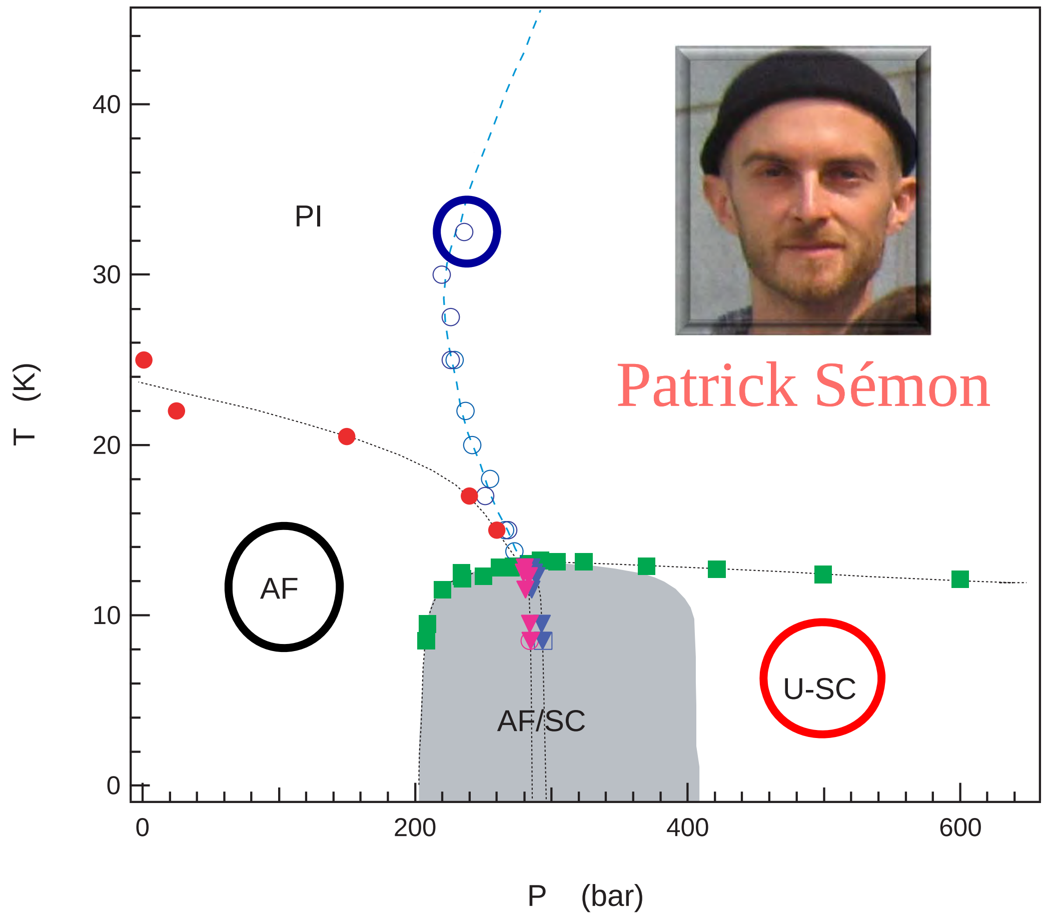


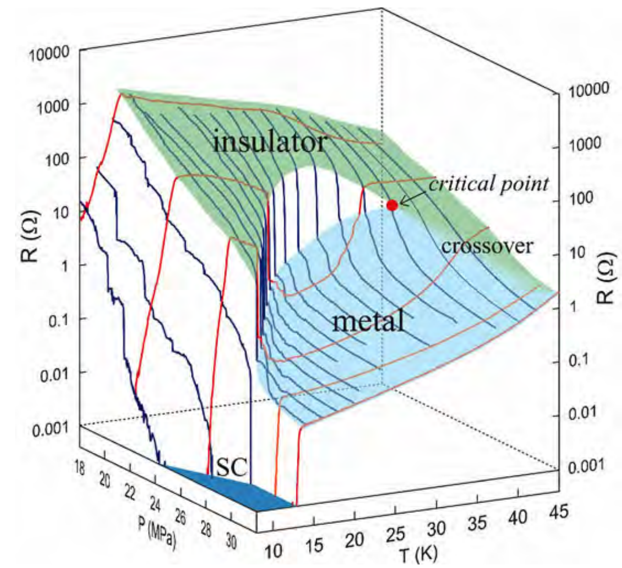
$$H = -\sum_{<ij>\sigma} t_{i,j} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



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

Bare Mott critical point in organics



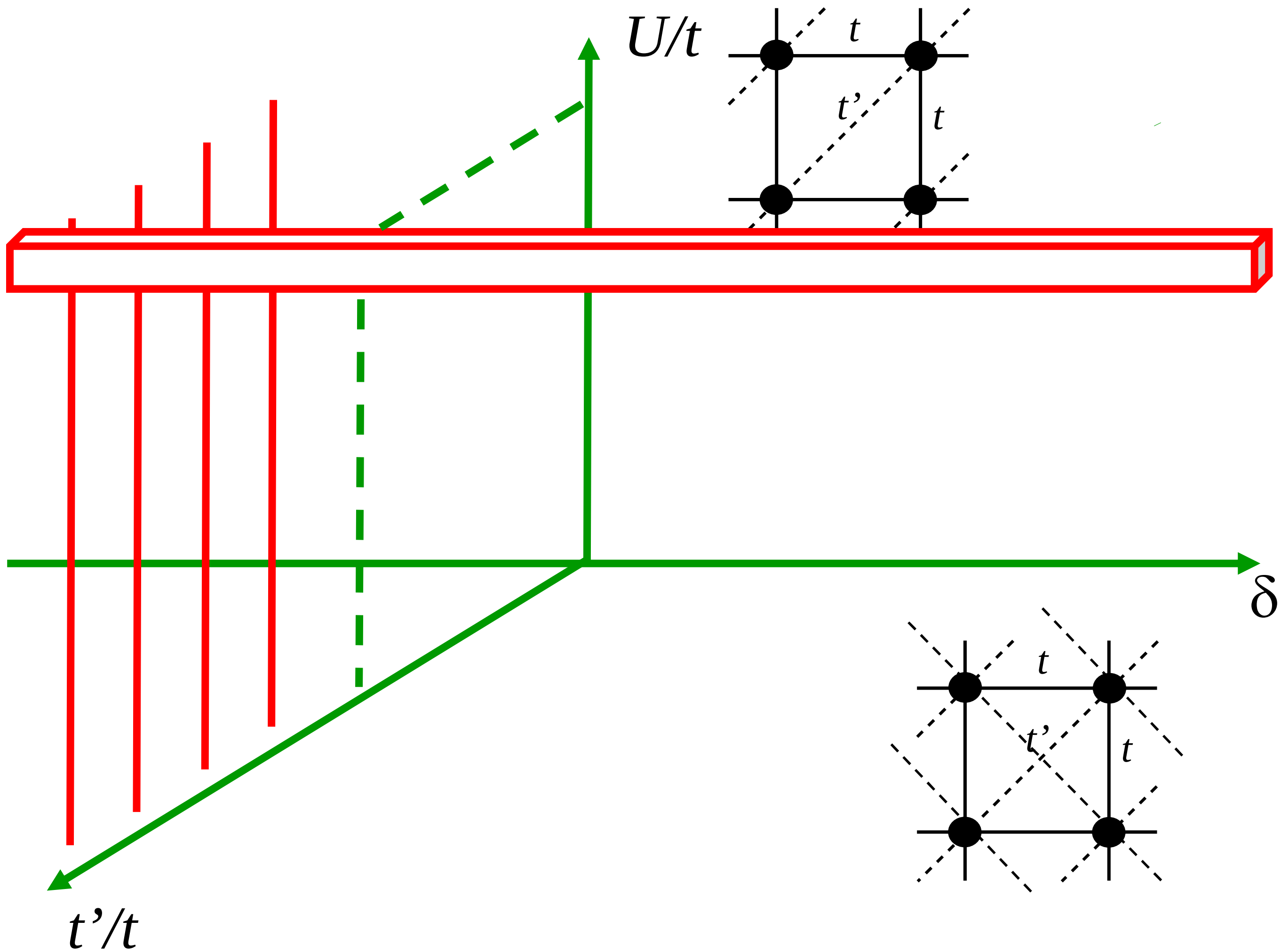


F. Kagawa, K. Miyagawa, + K. Kanoda
PRB **69** (2004) +Nature **436** (2005)

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

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

Perspective



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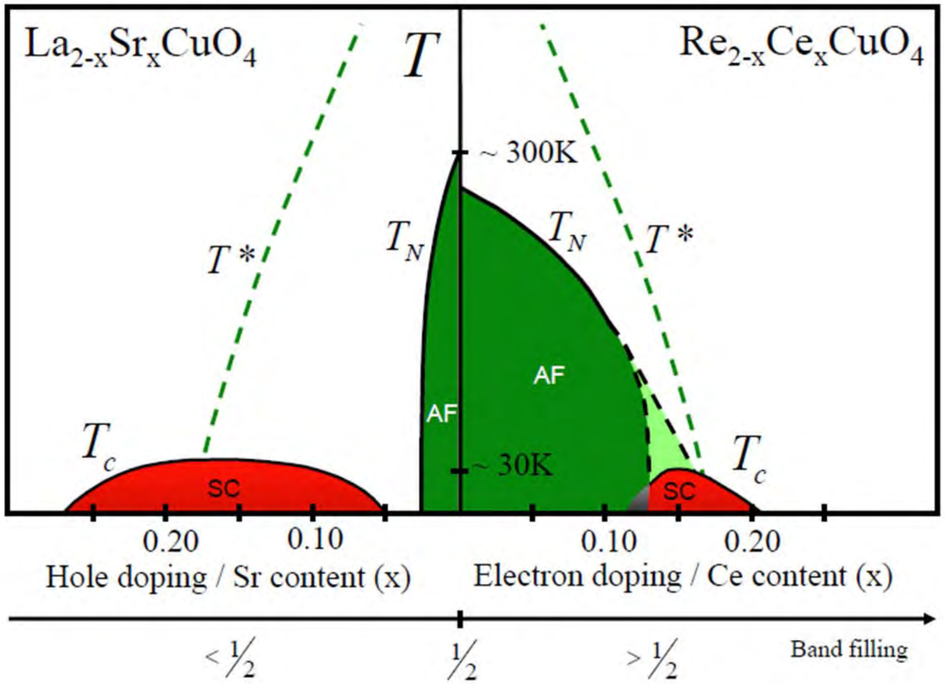
Normal state of high-temperature superconductors

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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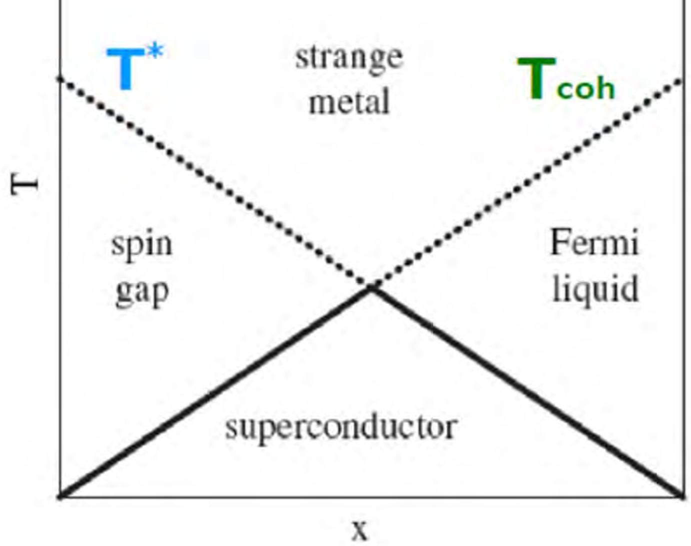
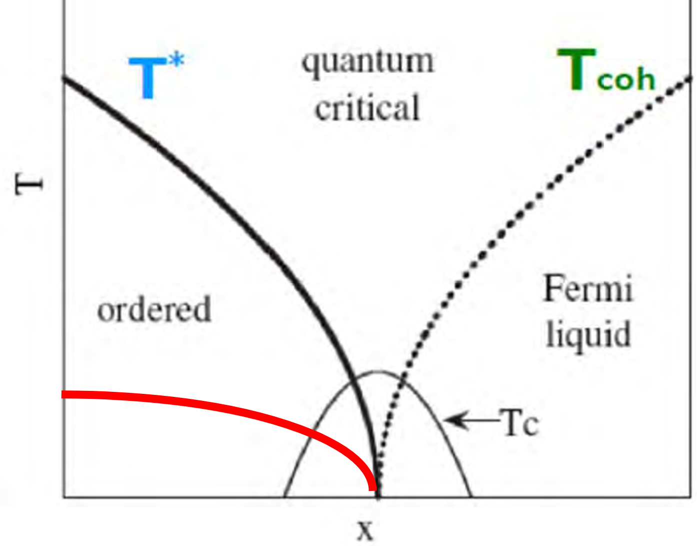
Two views (caricature)

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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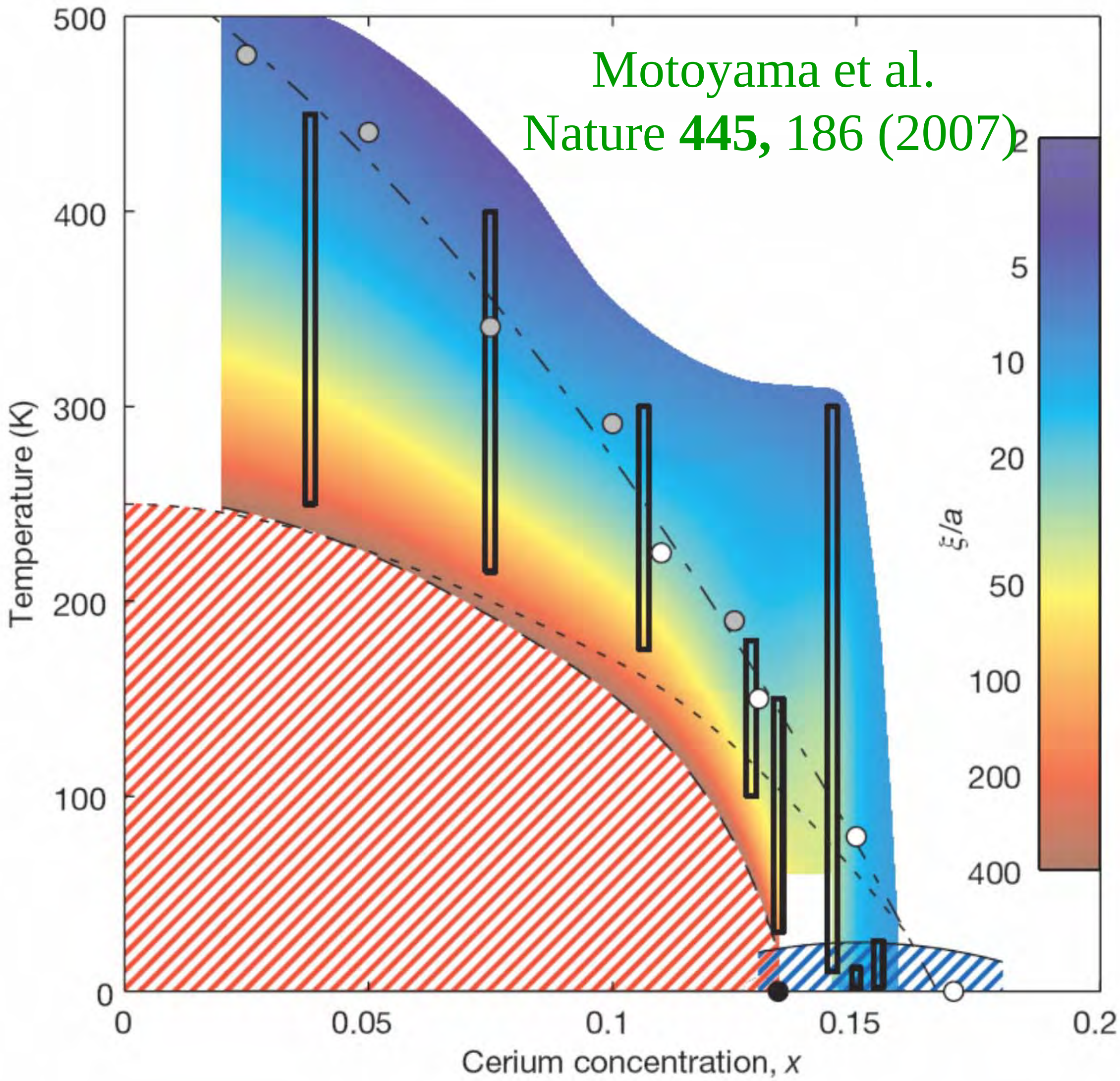
$d = 2$ precursors, e-doped



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

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

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

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

Semi-quantitative fits of both ARPES and neutron

TPSC: general ideas

- General philosophy
  - Drop diagrams
  - Impose constraints and sum rules
    - Conservation laws
    - Pauli principle ($\langle n_\sigma^2 \rangle = \langle n_\sigma \rangle$)
    - Local moment and local density sum-rules
- Get for free:
    - Mermin-Wagner theorem
    - Kanamori-Brückner screening
    - Consistency between one- and two-particle $\Sigma G = U\langle n_\sigma n_{-\sigma} \rangle$

Vilk, AMT J. Phys. I France, **7**, 1309 (1997);
Theoretical methods for strongly correlated electrons also (Mahan, 3rd)

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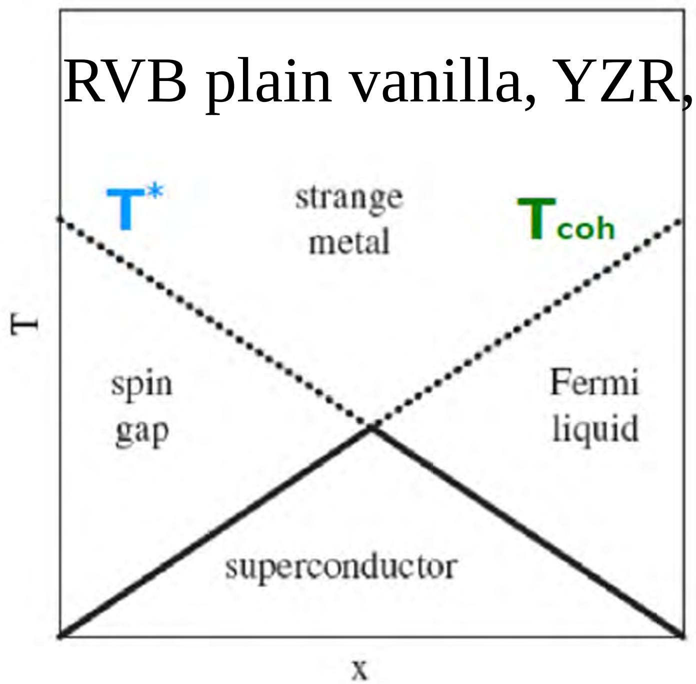
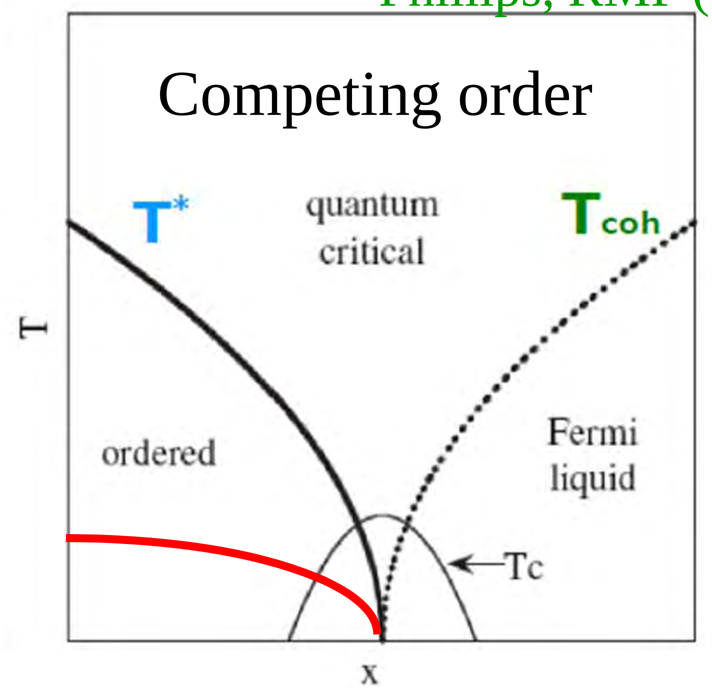
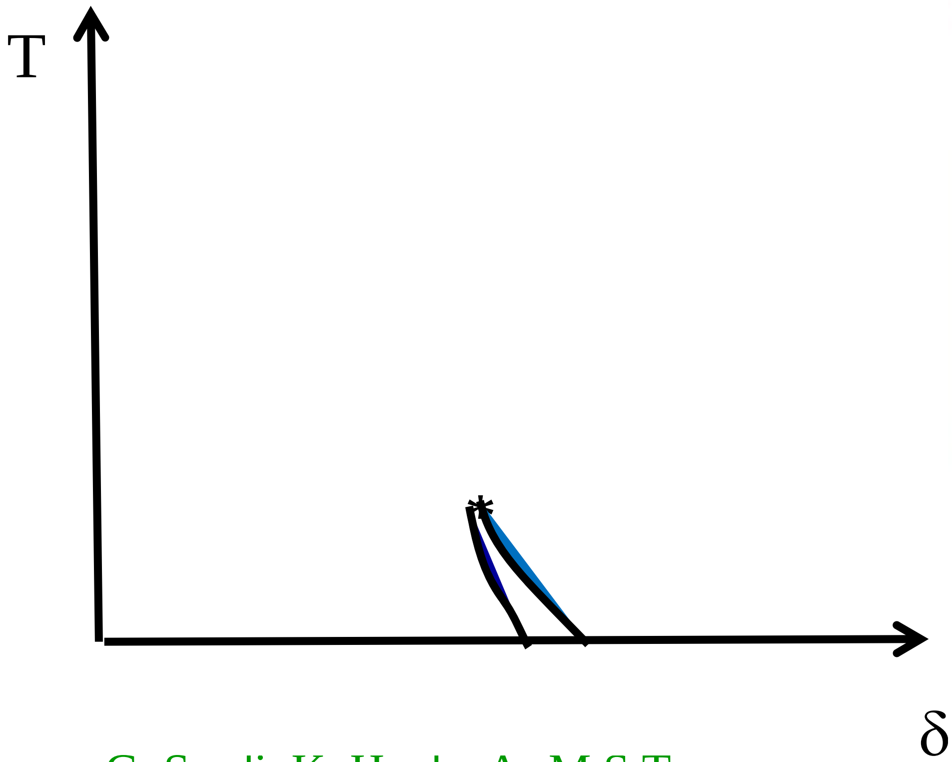
Two views (caricature)

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

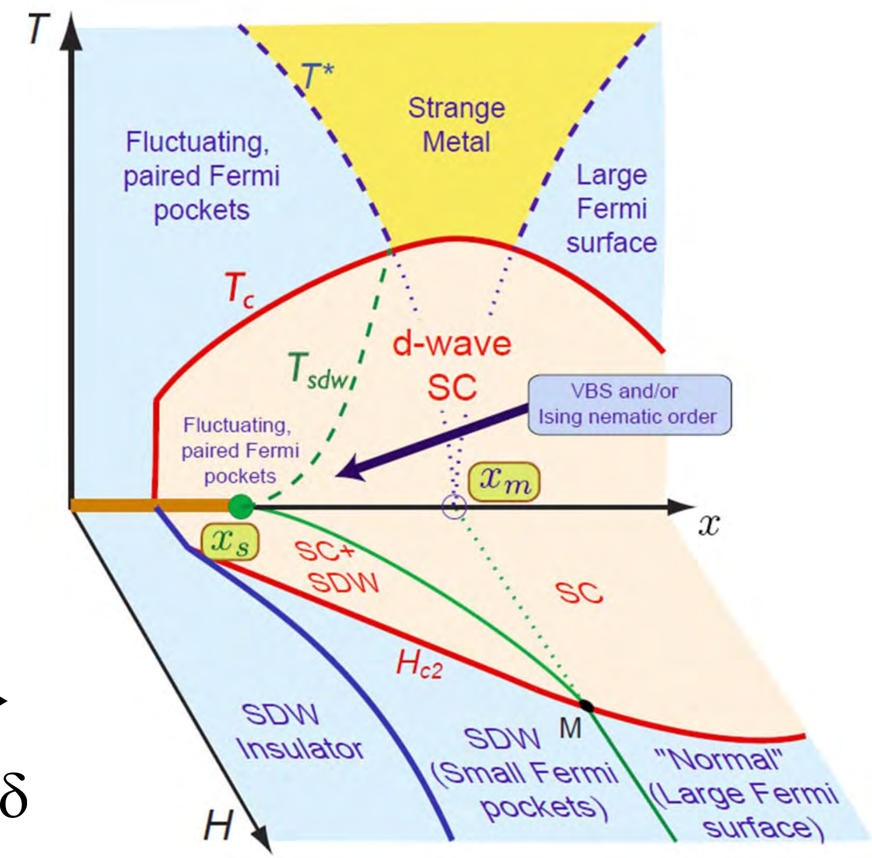




An alternate view (a bit of both)



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



S. Sachdev, Physica C **470**, S4 (2010)
Matthias Punk + Subir Sachdev (unpublished)
T. C. Ribeiro and X.-G. Wen,
PRL (2005) and Phys. Rev. B 74, 155113 (2006)

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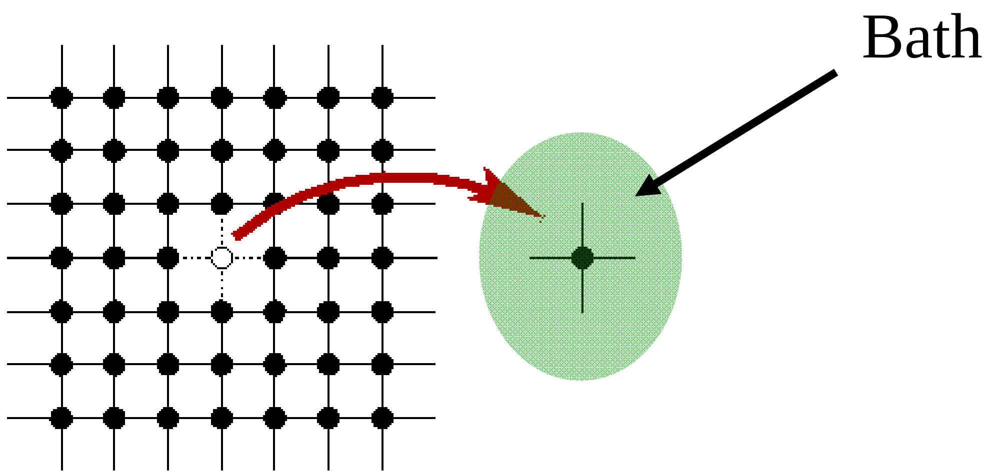
Outline

- Method
- Normal state
  - First order transition
  - Widom line and pseudogap
- Superconducting state
  - Glue

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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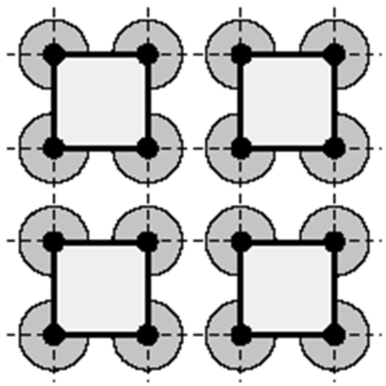
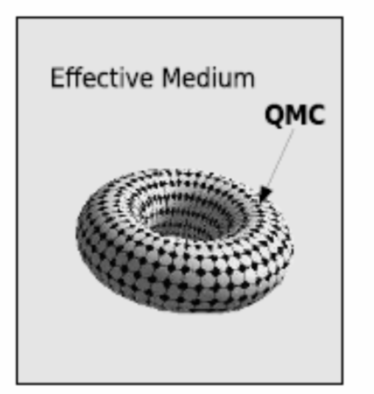
2d Hubbard: Quantum cluster method

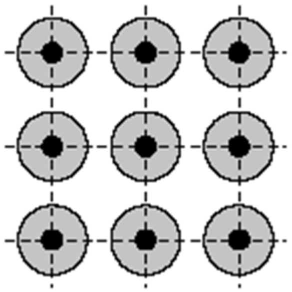
C-DMFT





DCA

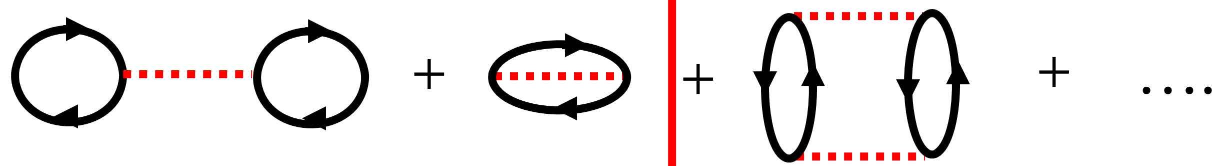
DMFT



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

Dynamical "variational" principle

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

$\Phi[G] =$ 

Universality

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

$$\frac{\delta\Omega_{\mathbf{t}}[G]}{\delta G} = \Sigma - G_{0\mathbf{t}}^{-1} + G^{-1} = 0$$

$$G = \frac{1}{G_{0\mathbf{t}}^{-1} - \Sigma}$$

Then Ω is grand potential

Related to dynamics (cf. Ritz)

H.F. if approximate Φ by first order

FLEX higher order

Luttinger and Ward 1960, Baym and Kadanoff (1961)

Another way to look at this (Potthoff)

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

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

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

Still stationary (chain rule)

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

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

SFT : Self-energy Functional Theory

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

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

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

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

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

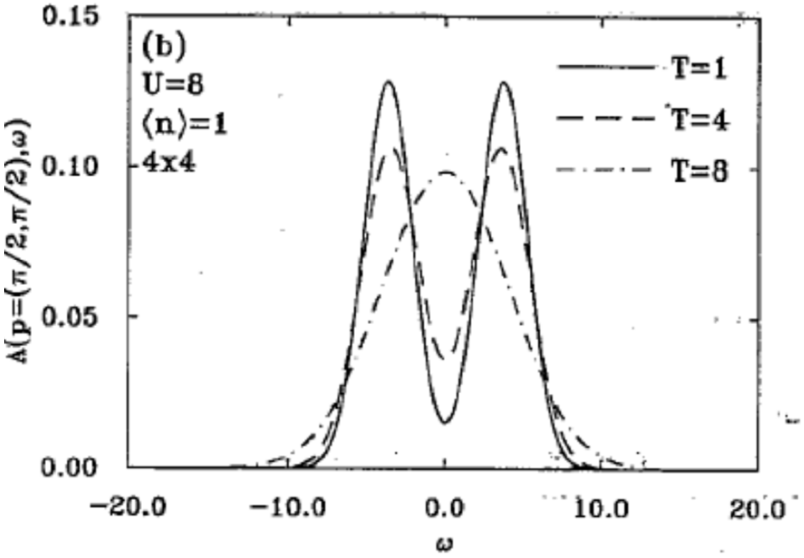
Variation of the self-energy, through parameters in $H_0(\mathbf{t'})$

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

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.

Mott insulator at finite T



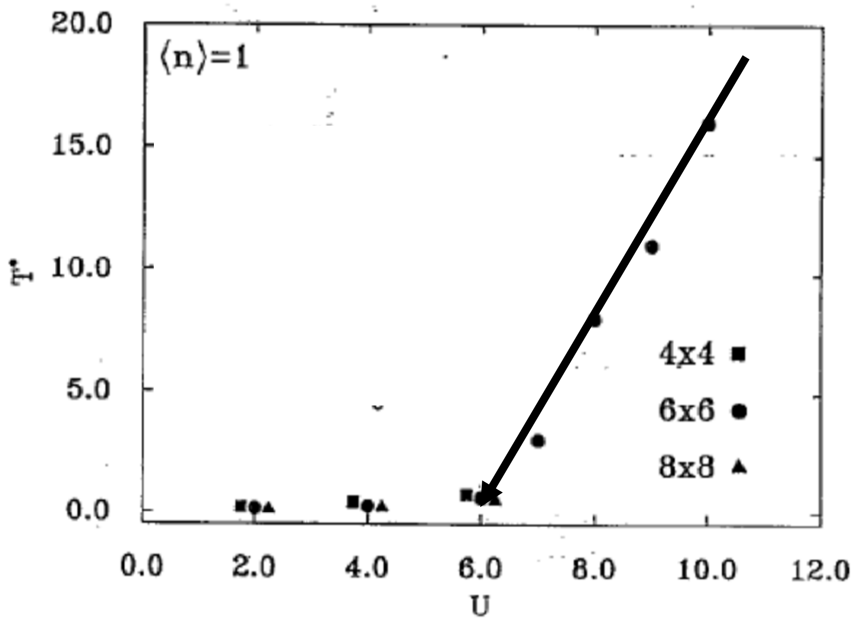


FIG. 5. The temperature T^* at which the gap develops vs U for 4×4, 6×6, and 8×8 lattices.

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)

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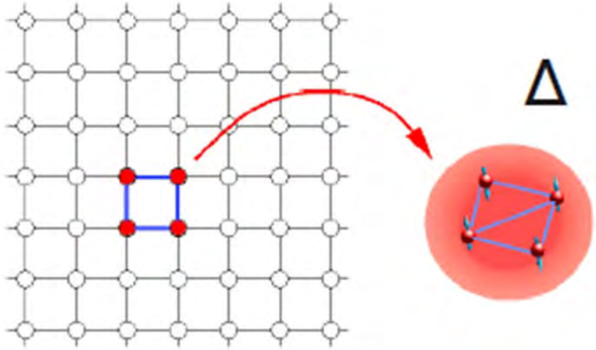
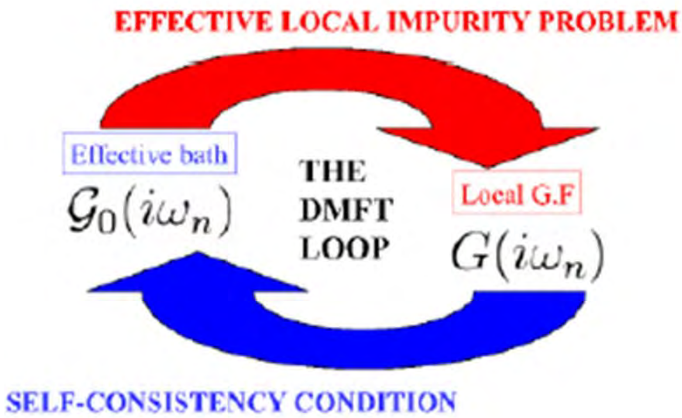
C-DMFT

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





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

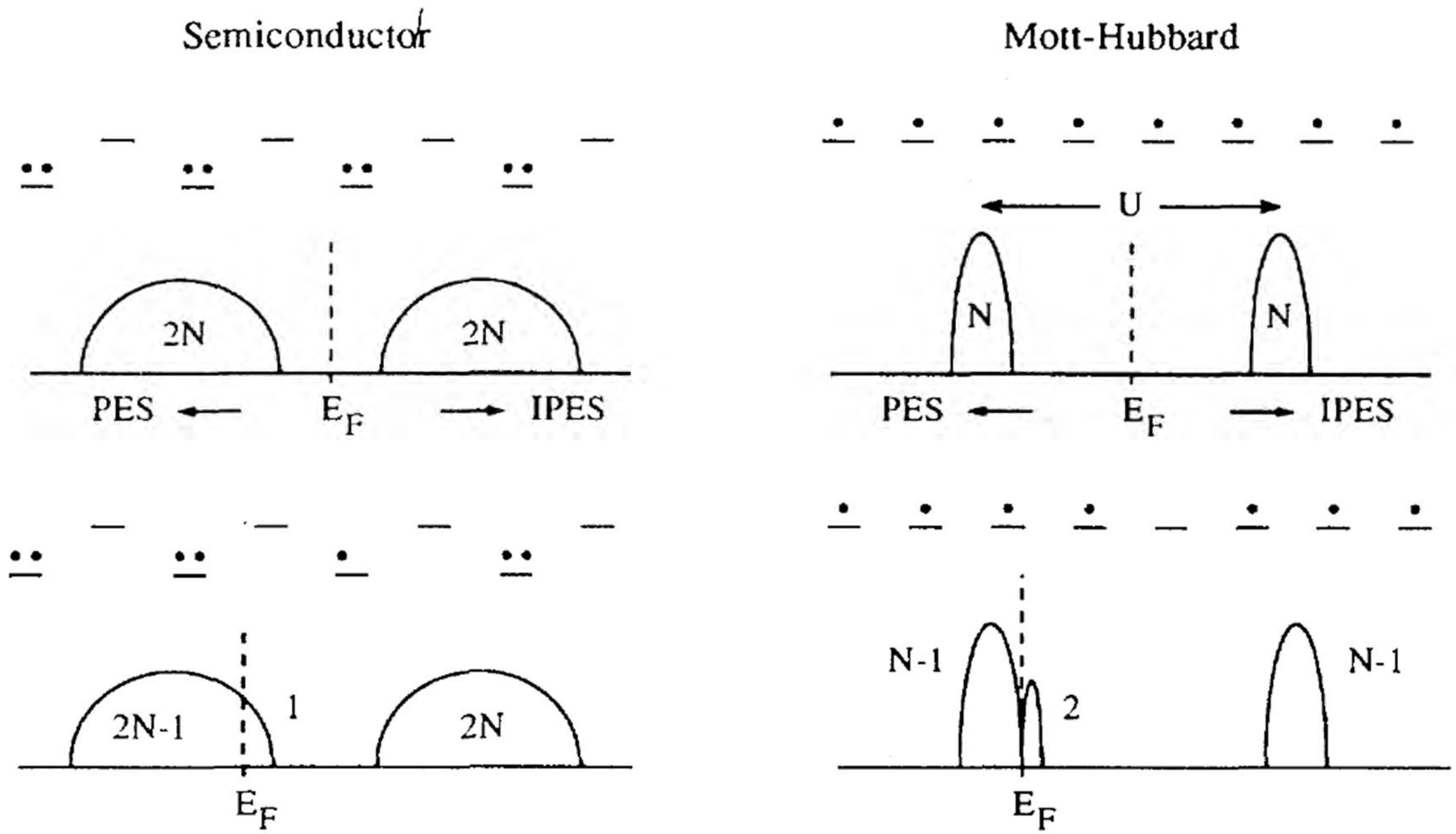
$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n) - \left[\sum_{\tilde{k}} \frac{1}{i\omega_n + \mu - t_c(\tilde{k}) - \Sigma_c(i\omega_n)}\right]^{-1}$$

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).

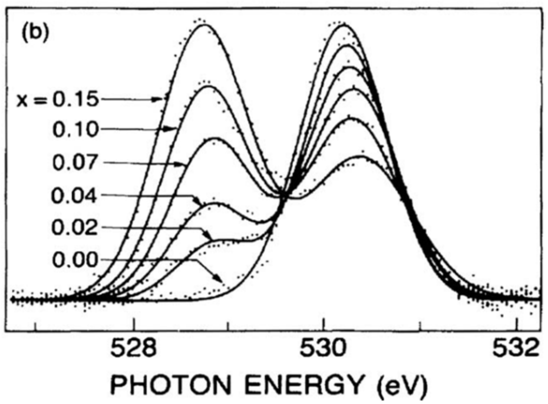
Cuprates as doped Mott insulators

Spectral weight transfer

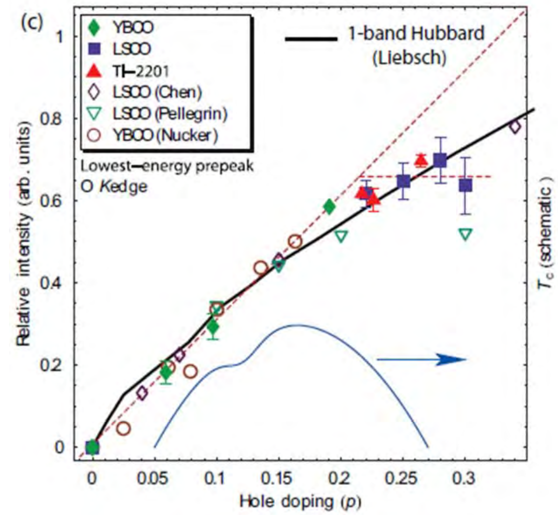


Meinders *et al.* PRB **48**, 3916 (1993)

Experiment: X-Ray absorption



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



Peets et al. PRL **103**, (2009),
Phillips, Jarrell PRL , vol. **105**, 199701 (2010)

Number of low energy states above ω = 0 scales as *2x* +
Not as 1+x as in Fermi liquid

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

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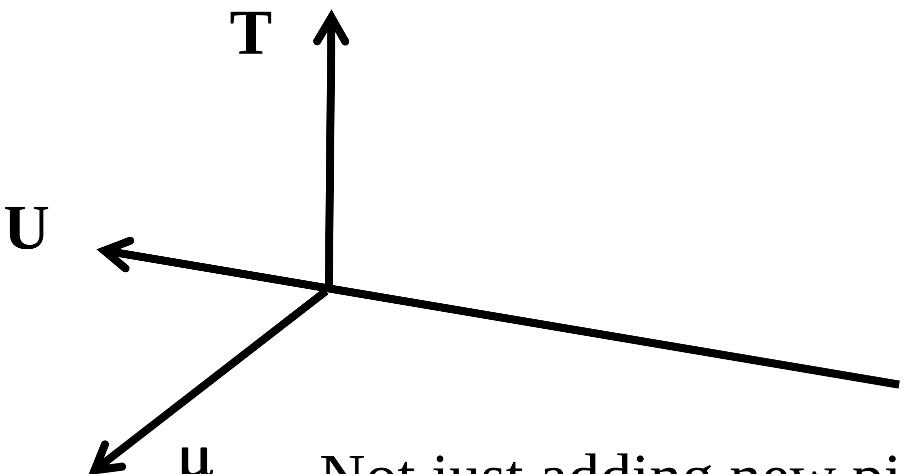
Giovanni Sordi

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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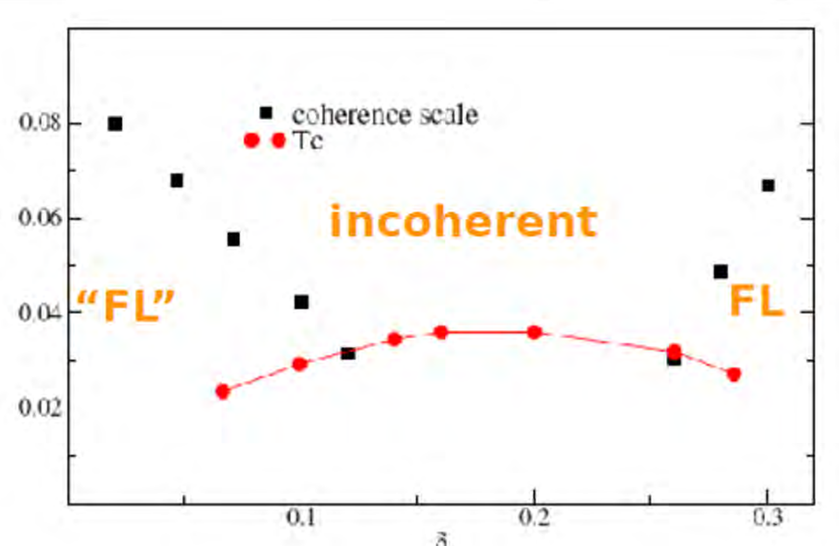
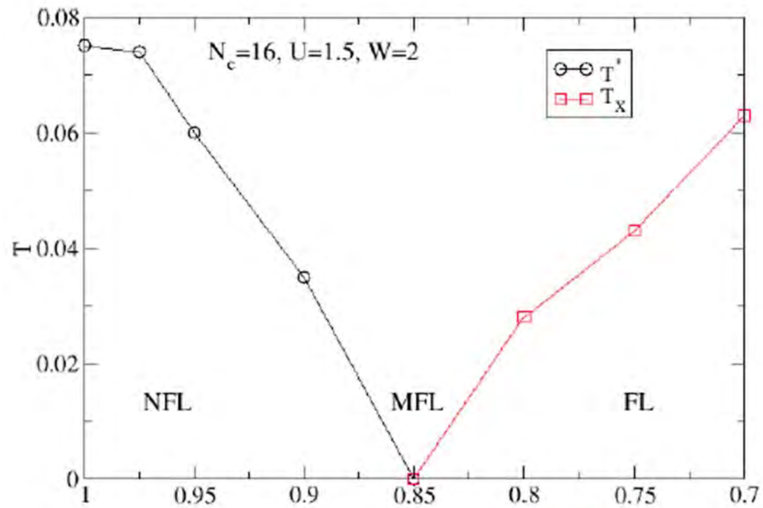
Doping driven Mott transition, *t' = 0*

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)

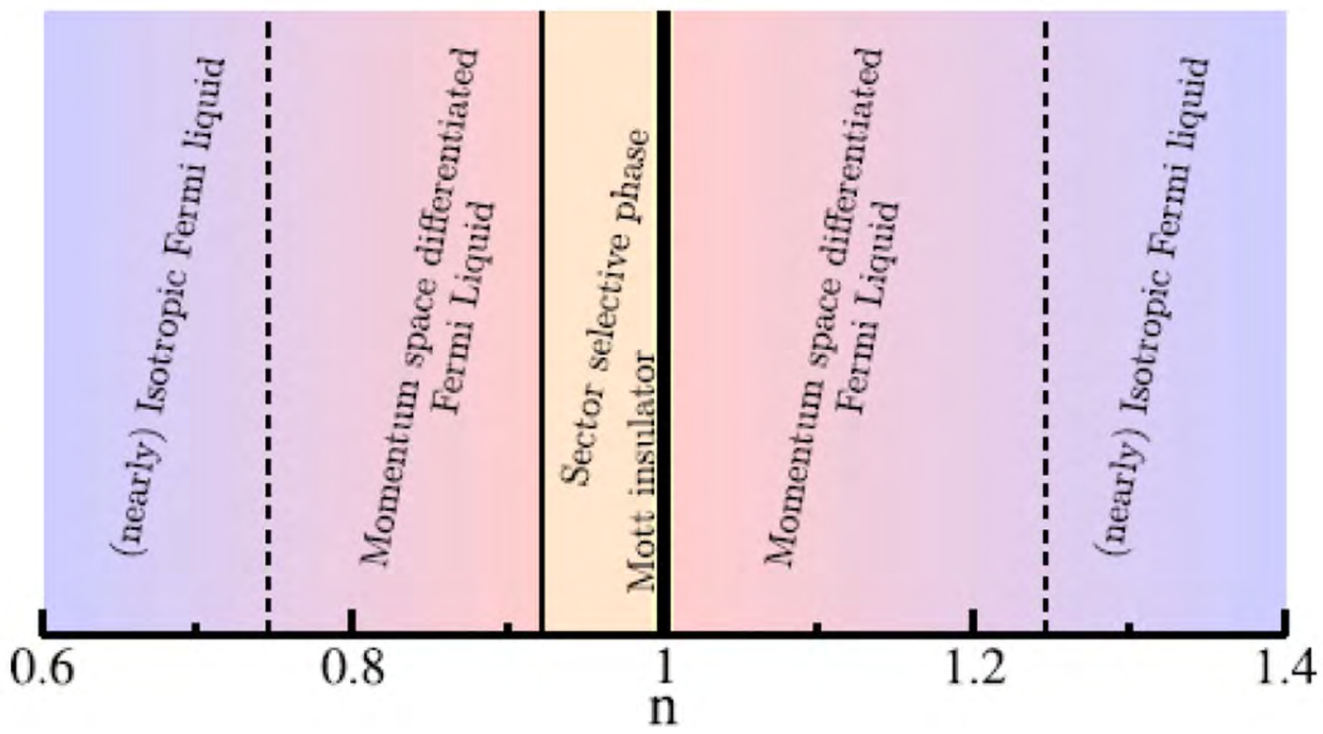


K. Haule, G. Kotliar, PRB (2008)



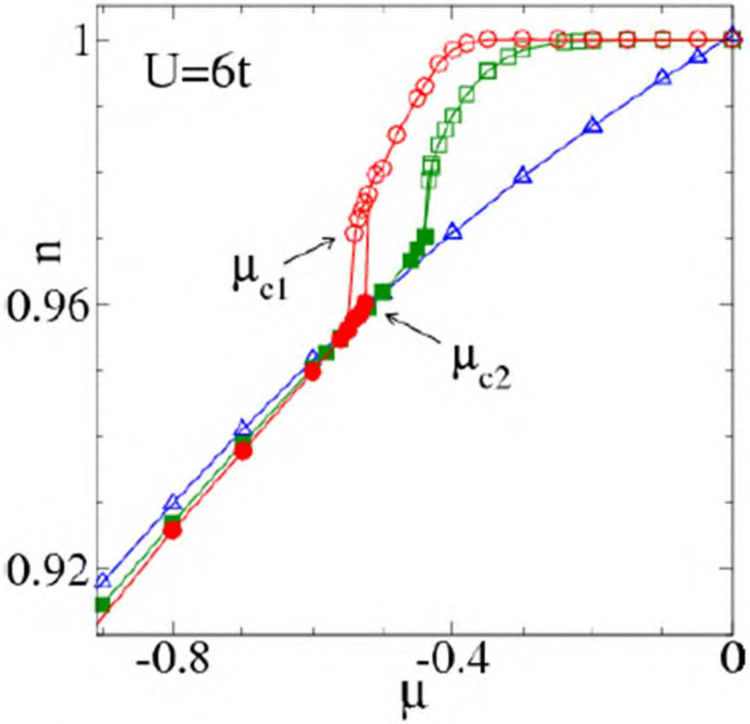
Vildhyadhiraja, PRL (2009)

Doping driven Mott transition



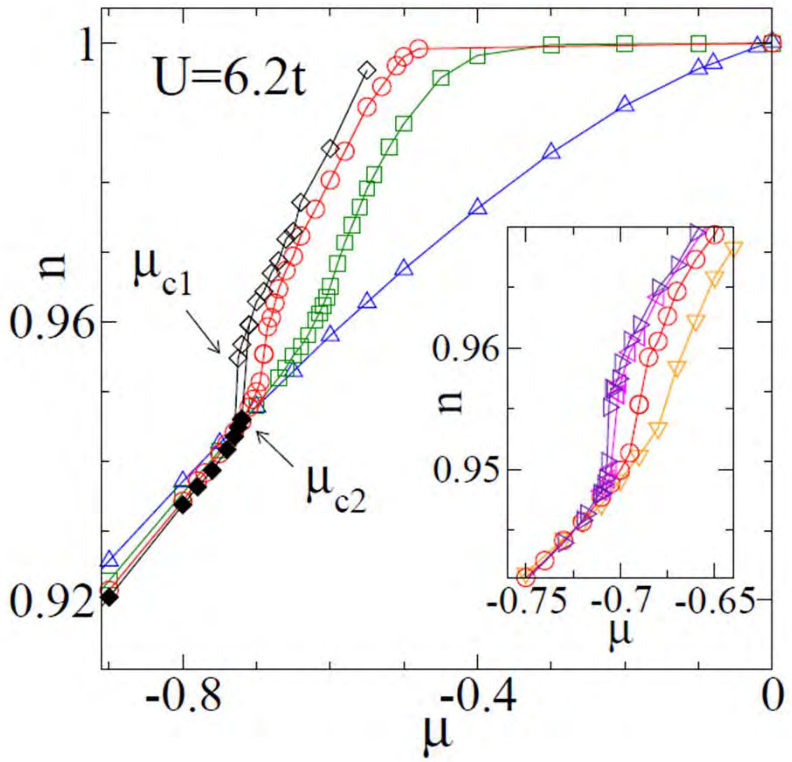
Gull, Werner, Millis, (2009)

First order transition at finite doping

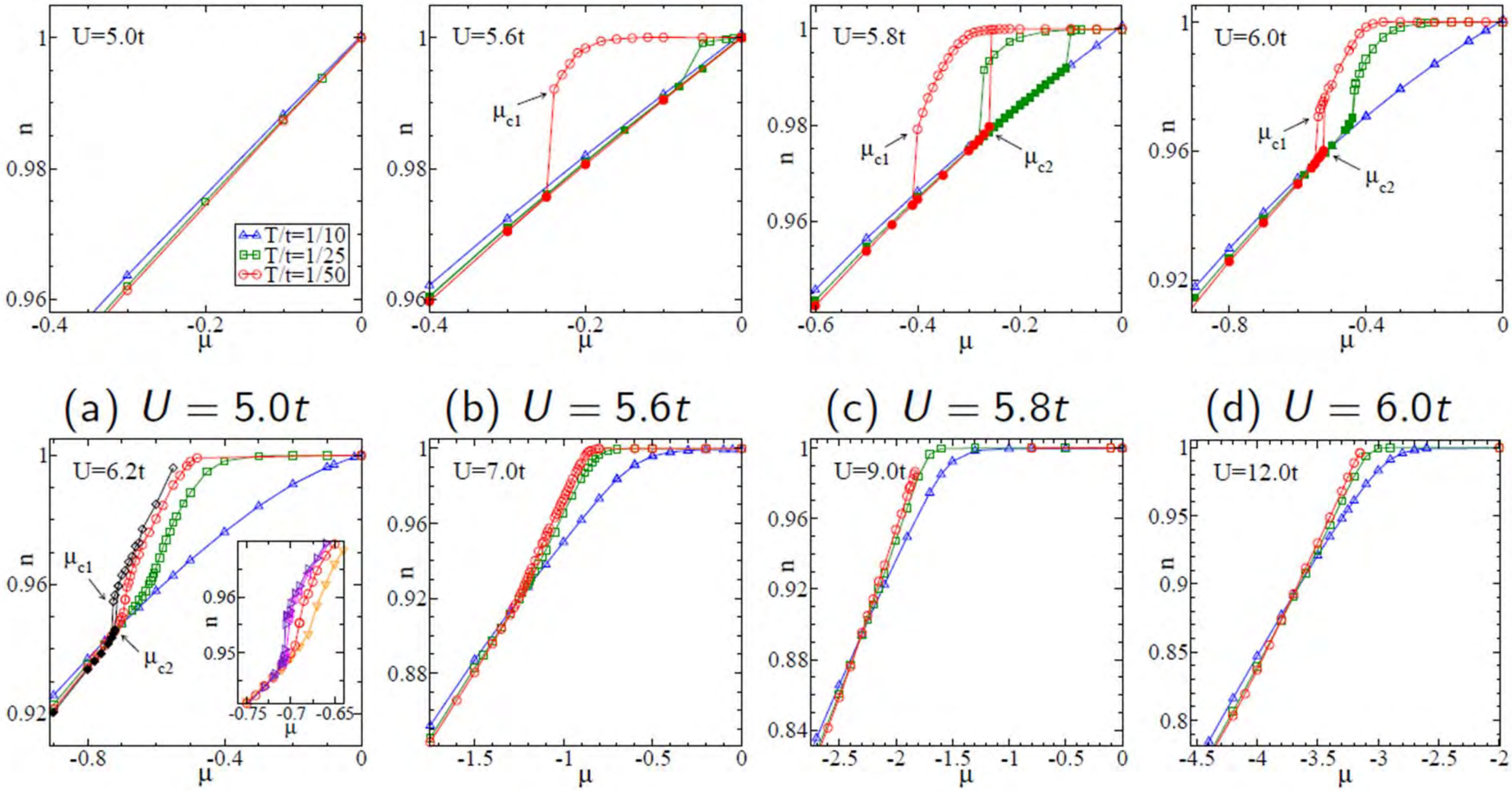


$n(\mu)$ for several temperatures:
$T/t =$ 1/10, 1/25, 1/50

The critical point



Systematic exploration $n(\mu)$



(a) $U = 5.0t$ (b) $U = 5.6t$ (c) $U = 5.8t$ (d) $U = 6.0t$

(e) $U = 6.2t$ (f) $U = 7.0t$ (g) $U = 9.0t$ (h) $U = 12.0t$

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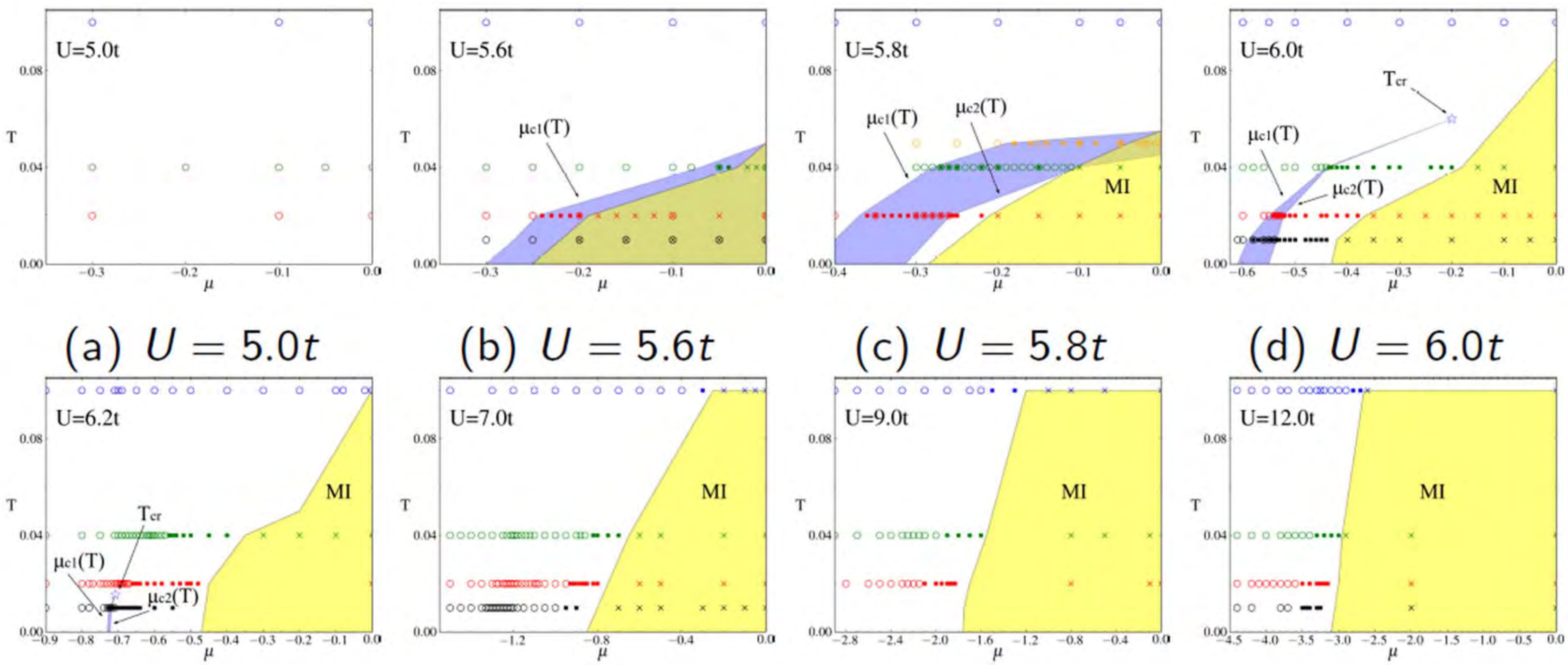
Systematic exploration of the phase diagram

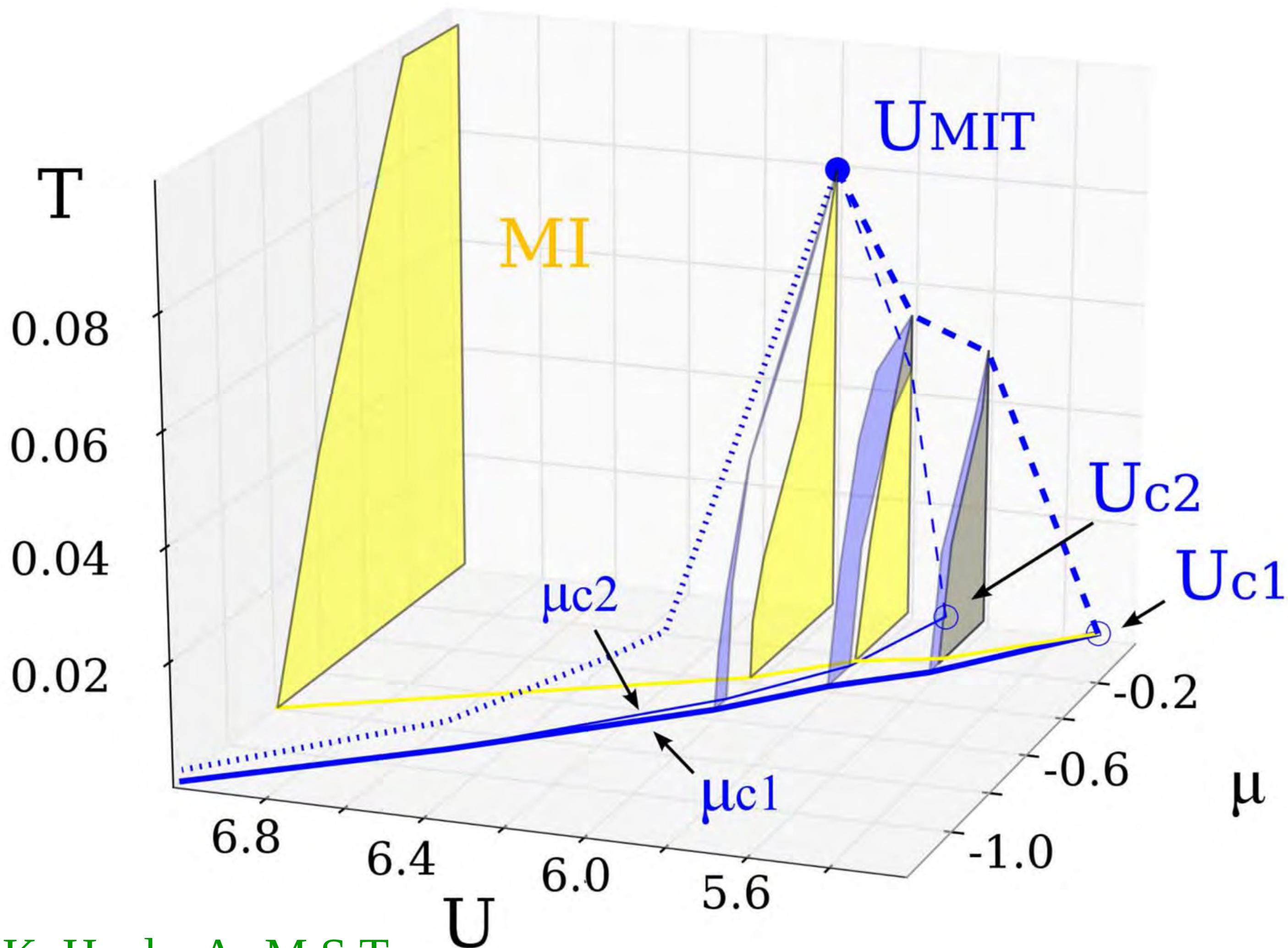


(a) $U = 5.0t$ (b) $U = 5.6t$ (c) $U = 5.8t$ (d) $U = 6.0t$

(e) $U = 6.2t$ (f) $U = 7.0t$ (g) $U = 9.0t$ (h) $U = 12.0t$

Yellow region: Mott insulator ($n(\mu) = 1$, $dn/d\mu = 0$)
White region: metal ($dn/d\mu = 0$)
Blue region: coexistence region

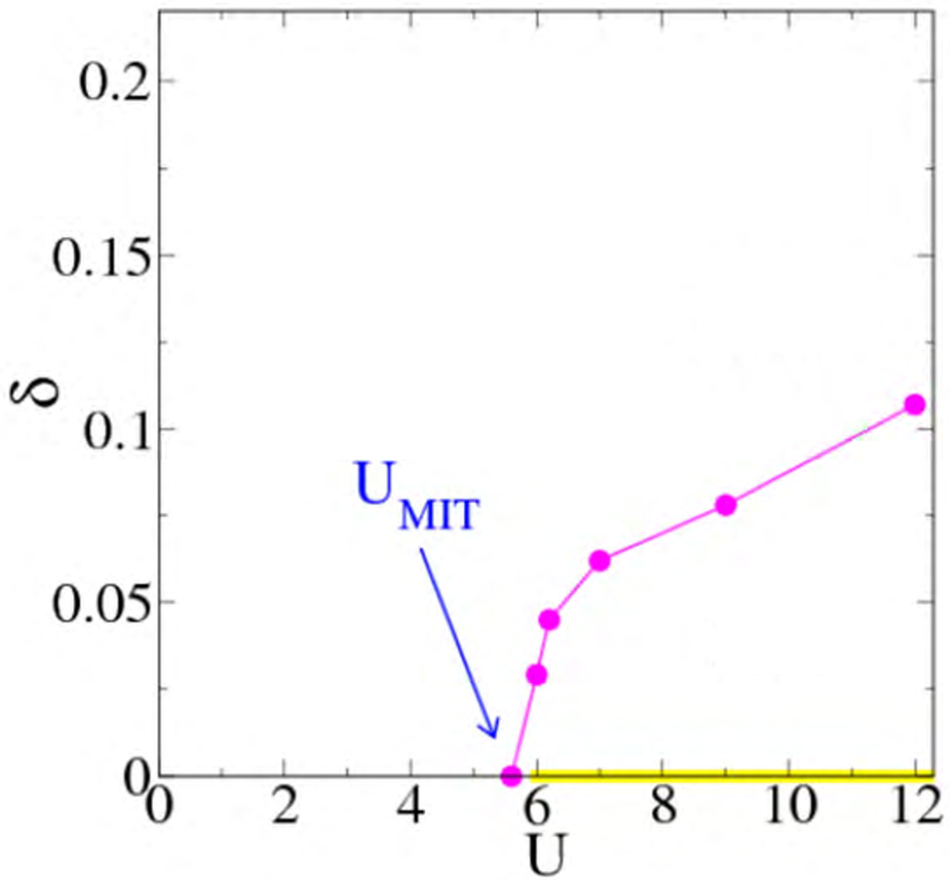
Normal state phase diagram

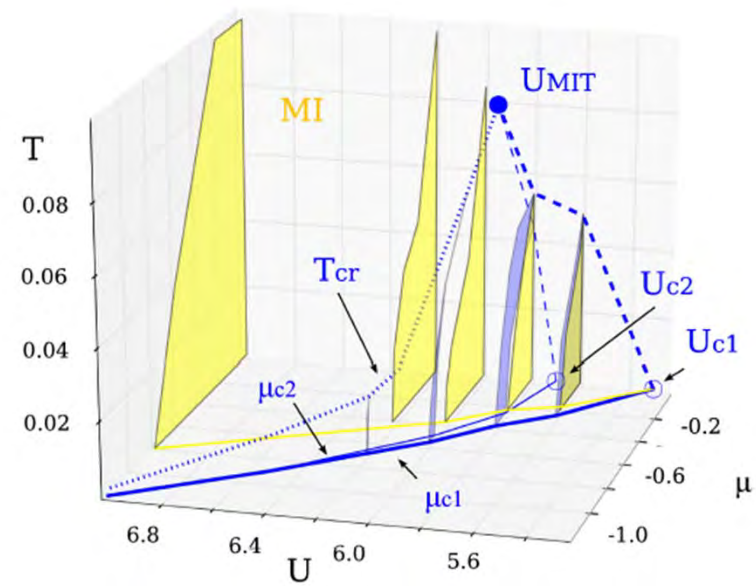


G. Sordi, K. Haule, A.-M.S.T
PRL, **104**, 226402 (2010)

Link to Mott transition up to optimal doping

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





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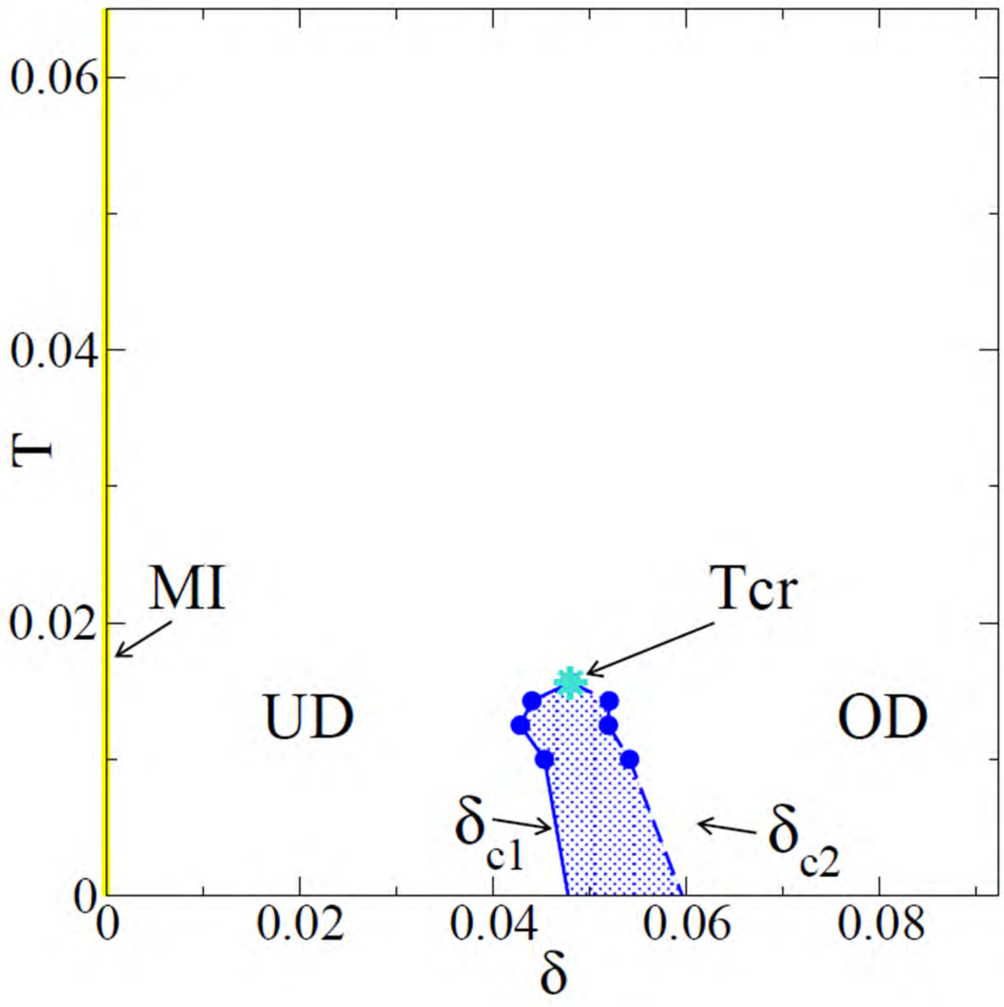
Characterisation of the phases (U=6.2t)



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

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?

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Patrick Sémon

Kristjan Haul

Pseudogap and the Widom line

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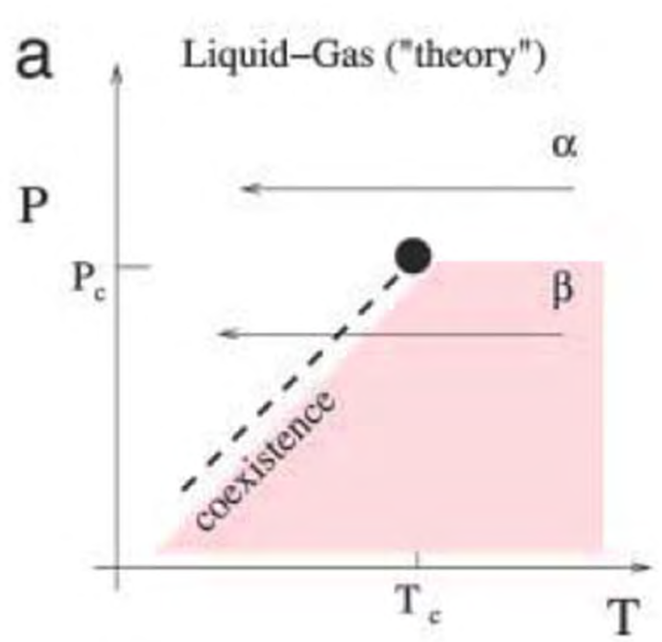
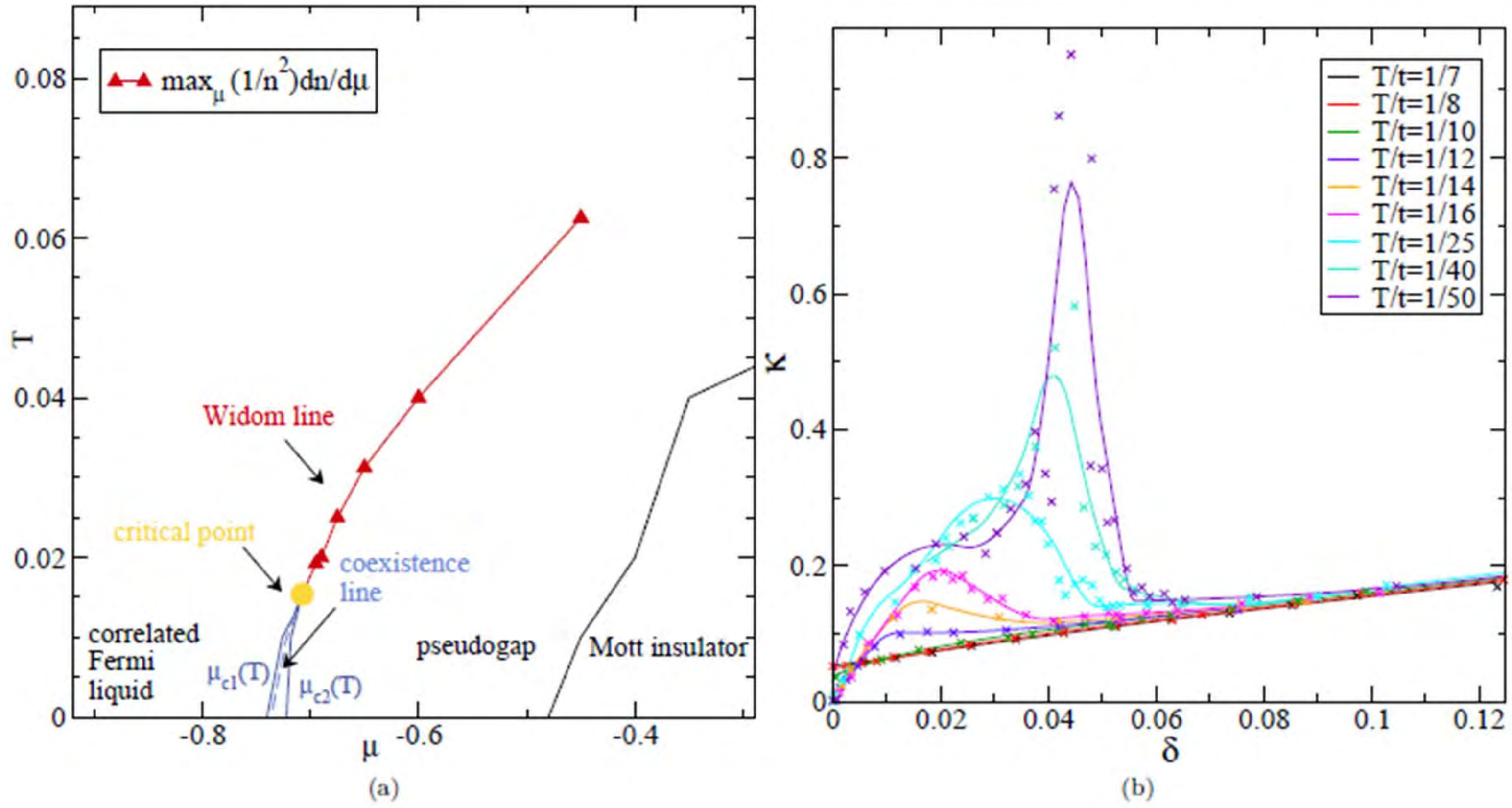
The Widom line



Xu et al. PNAS, **102**, 46 (2005)
Simeoni et al., Nature Physics **6**, 503 (2010)

The Widom line



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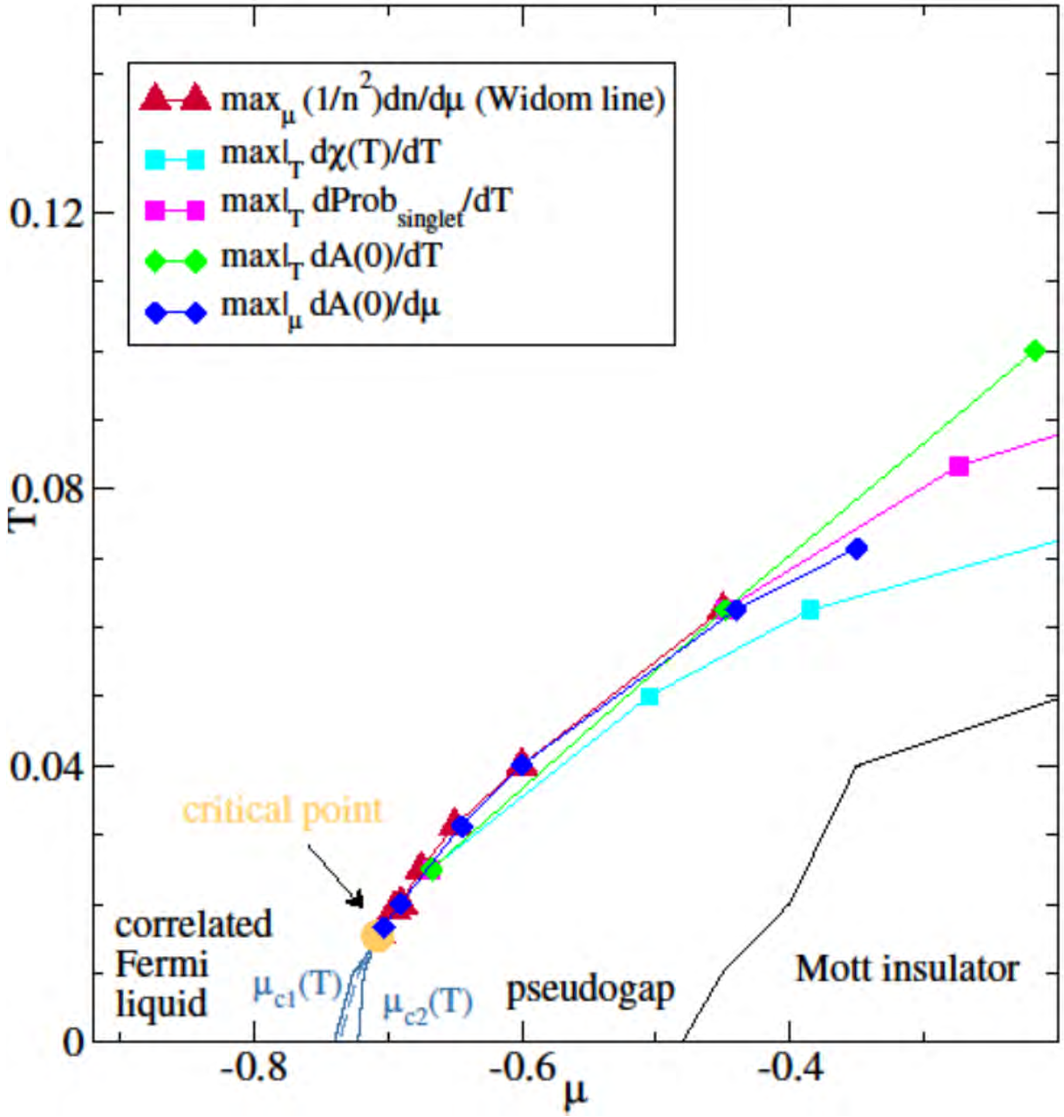
Rapid change also in dynamical quantities



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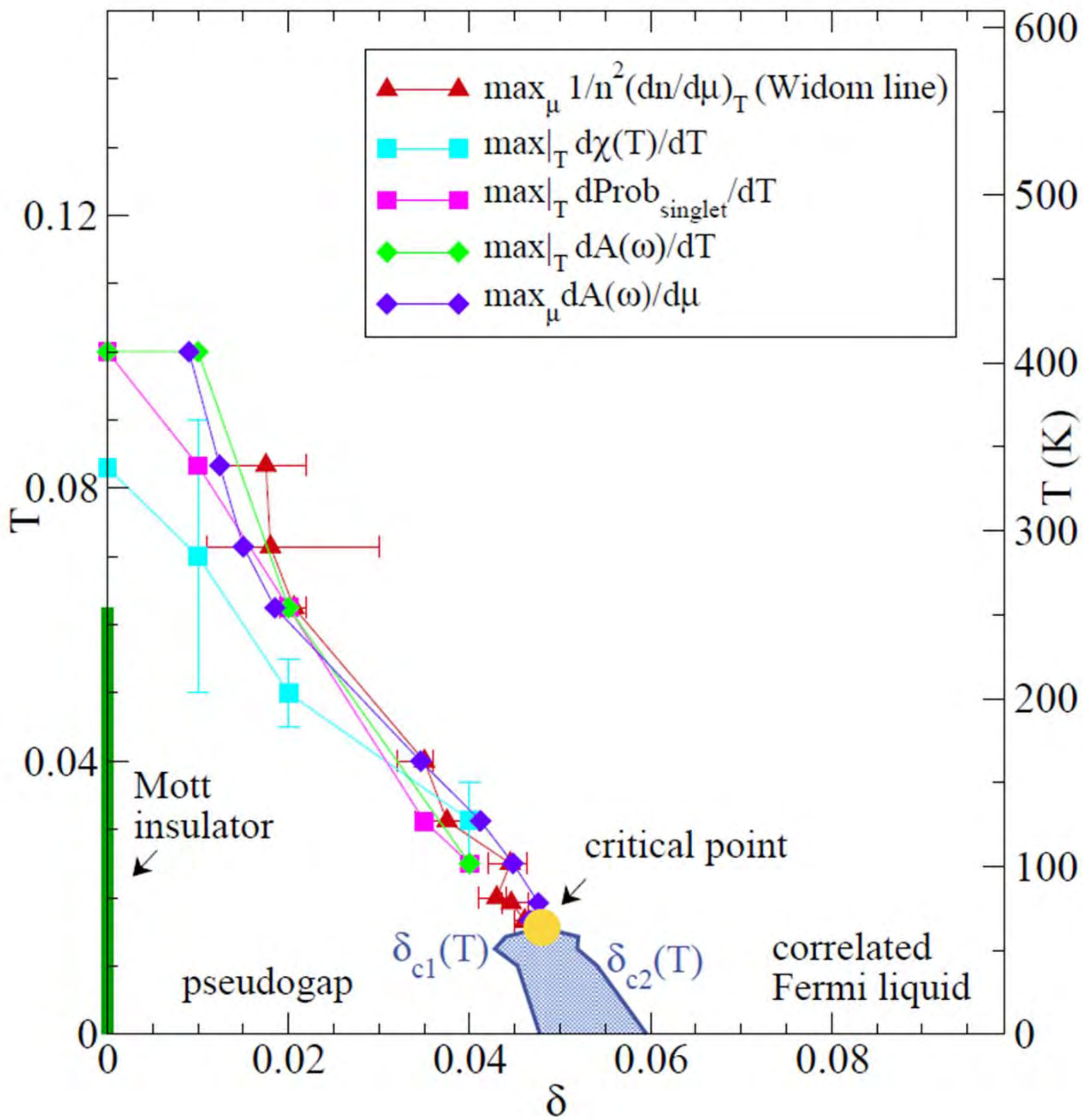
Phase diagram



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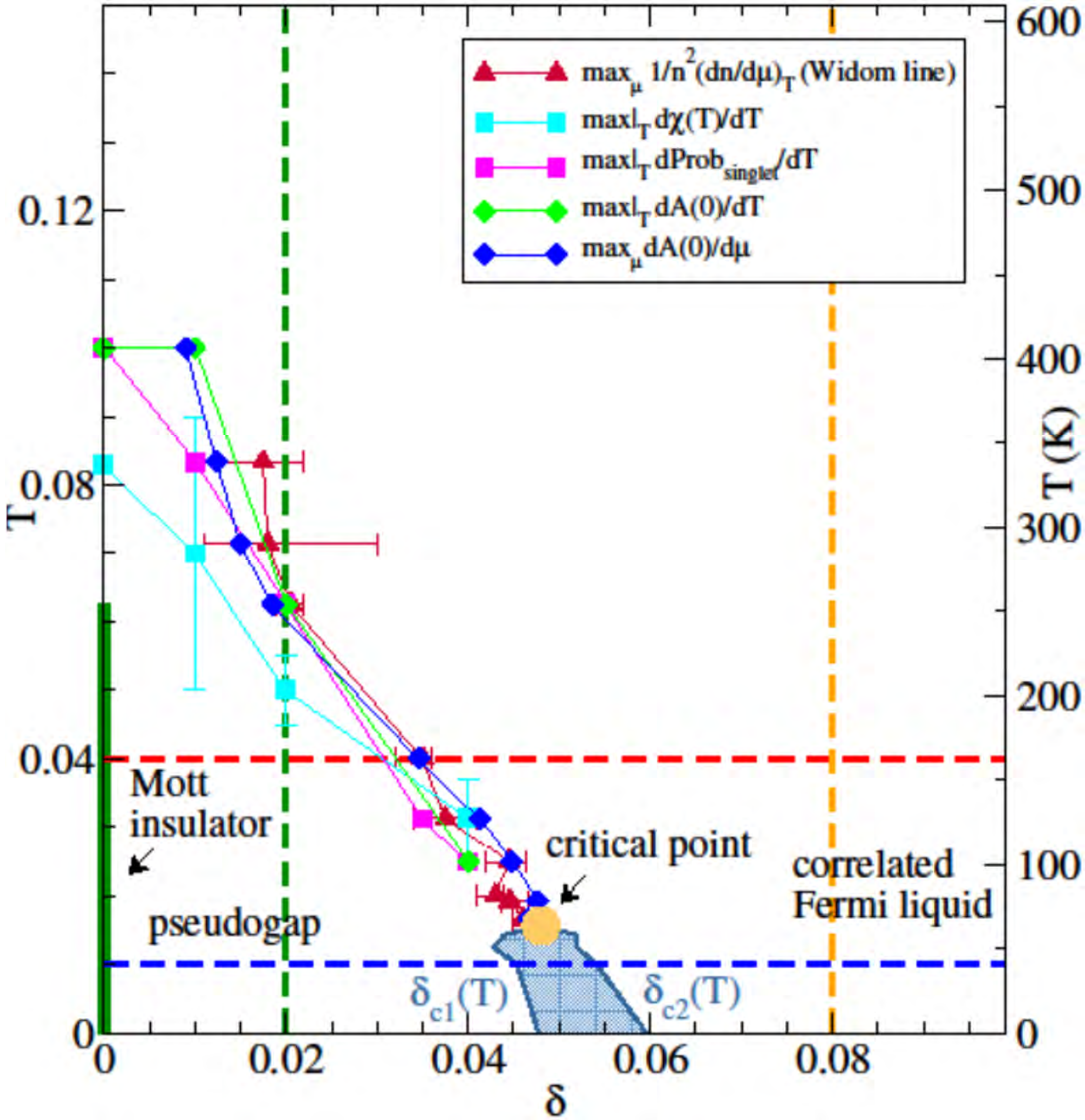
As a function of doping



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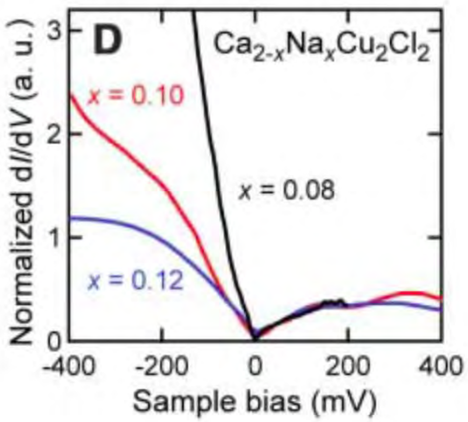
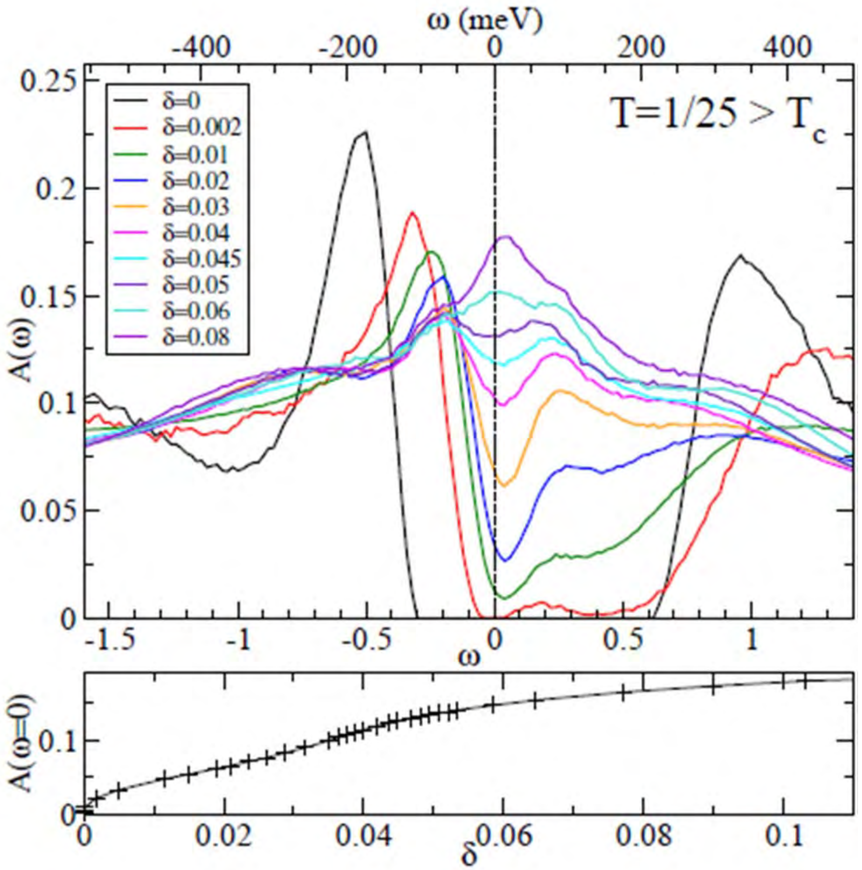
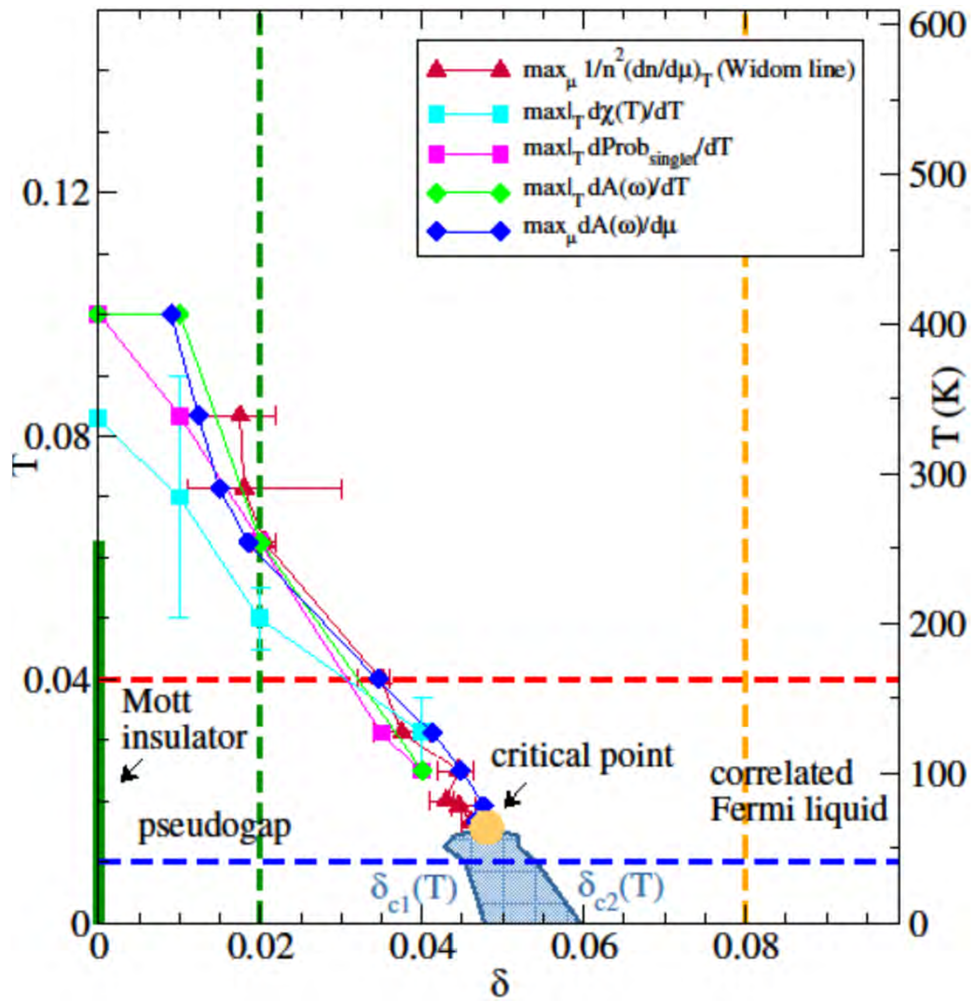
Tunneling DOS





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

As a function of doping



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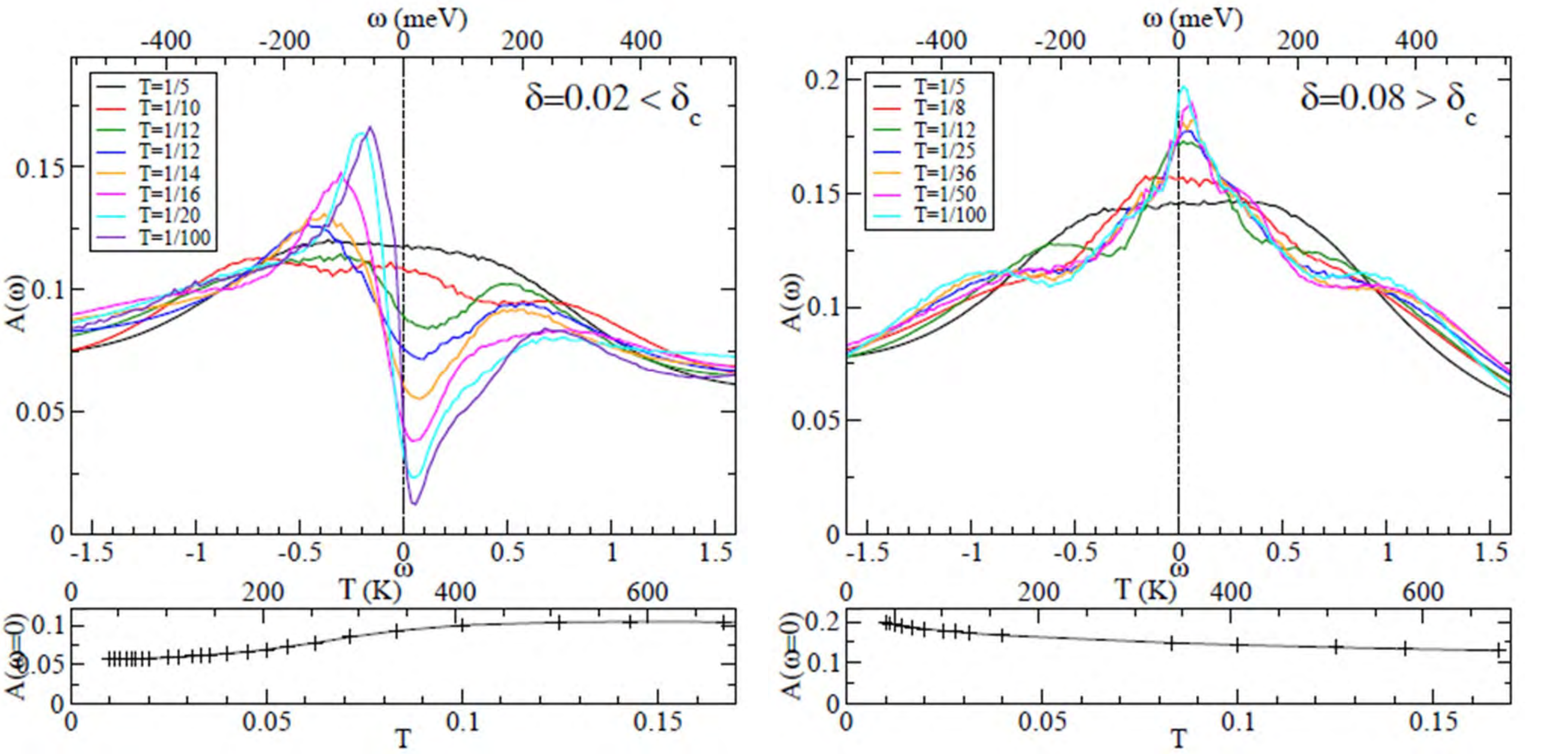
T dependence of the DOS



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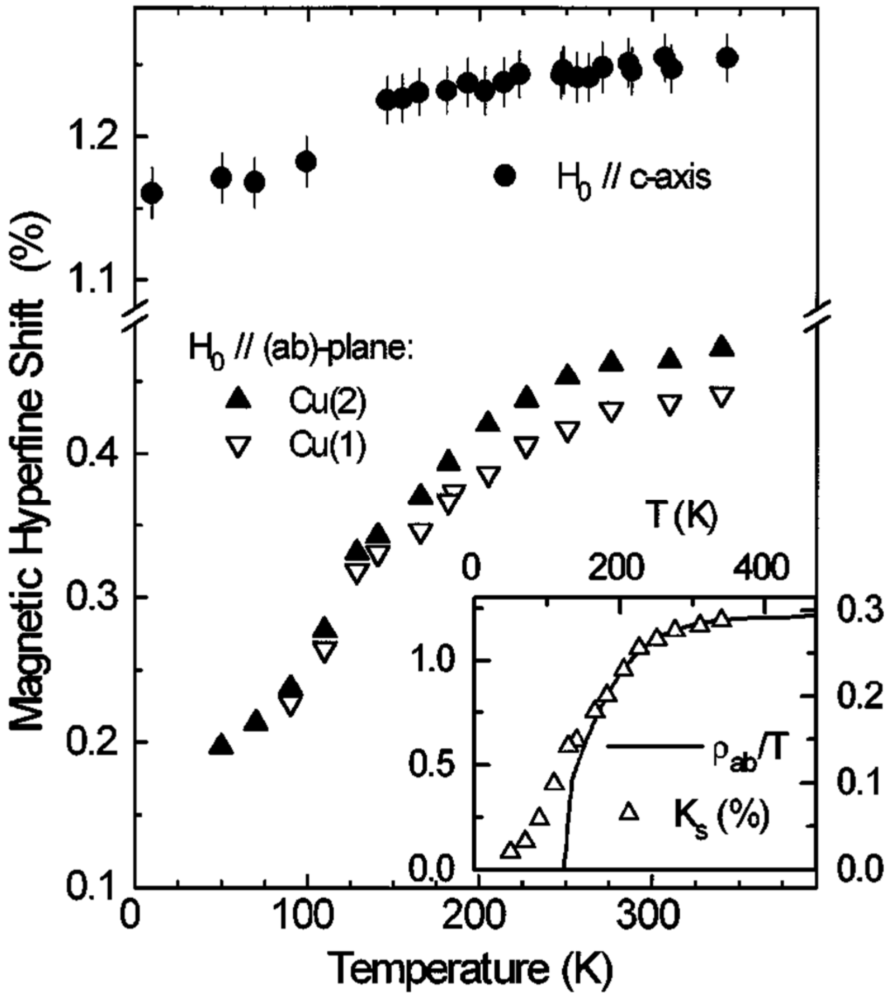
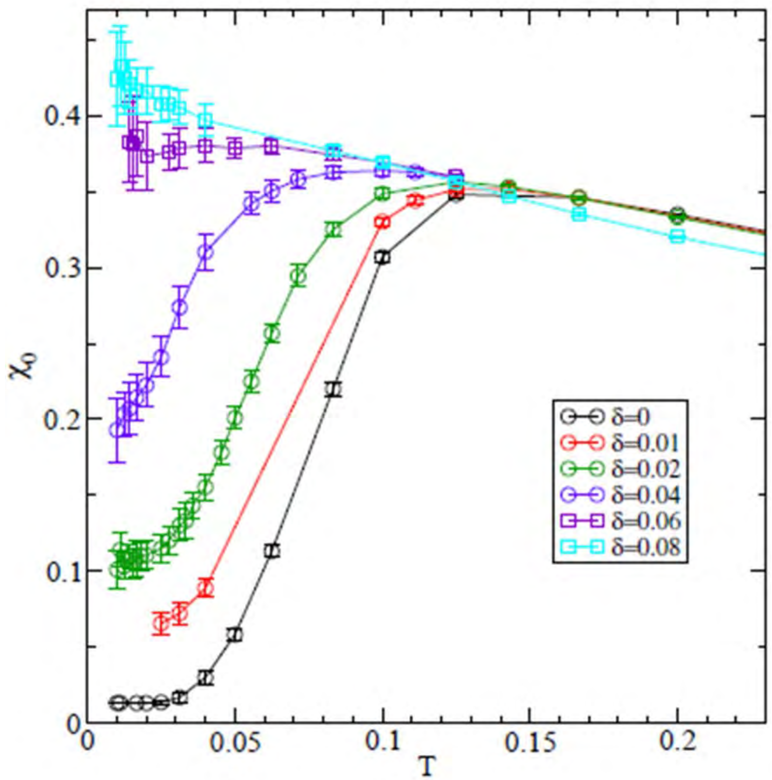
Spin susceptibility

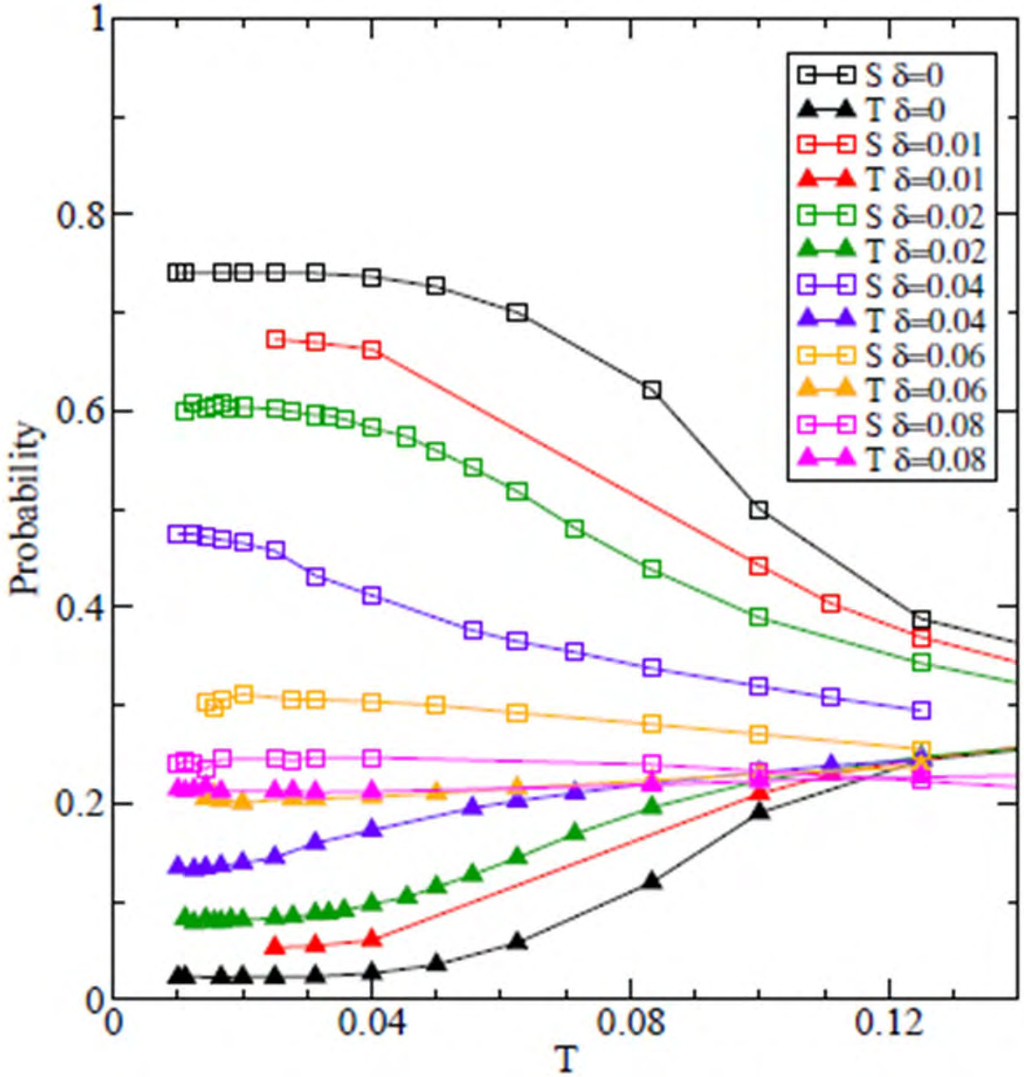


Underdoped Hg1223

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



Plaquette eigenstates



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Pseudogap and the Widom line

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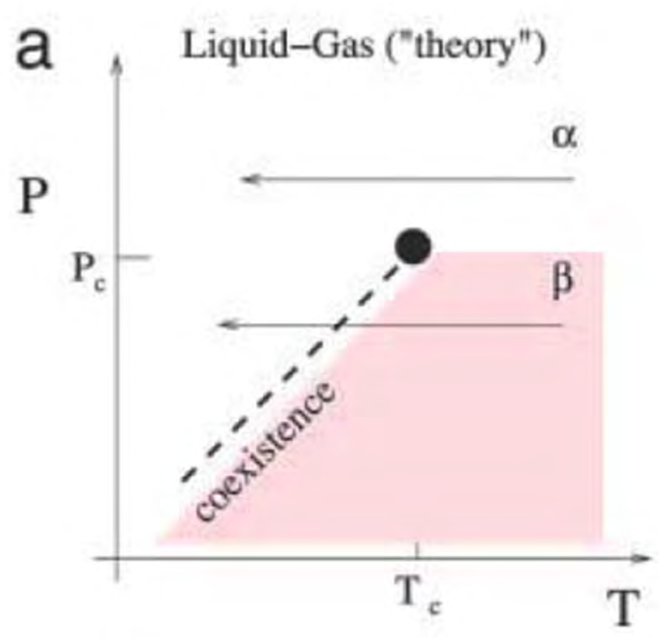
The Widom line



Xu et al. PNAS, **102**, 46 (2005)
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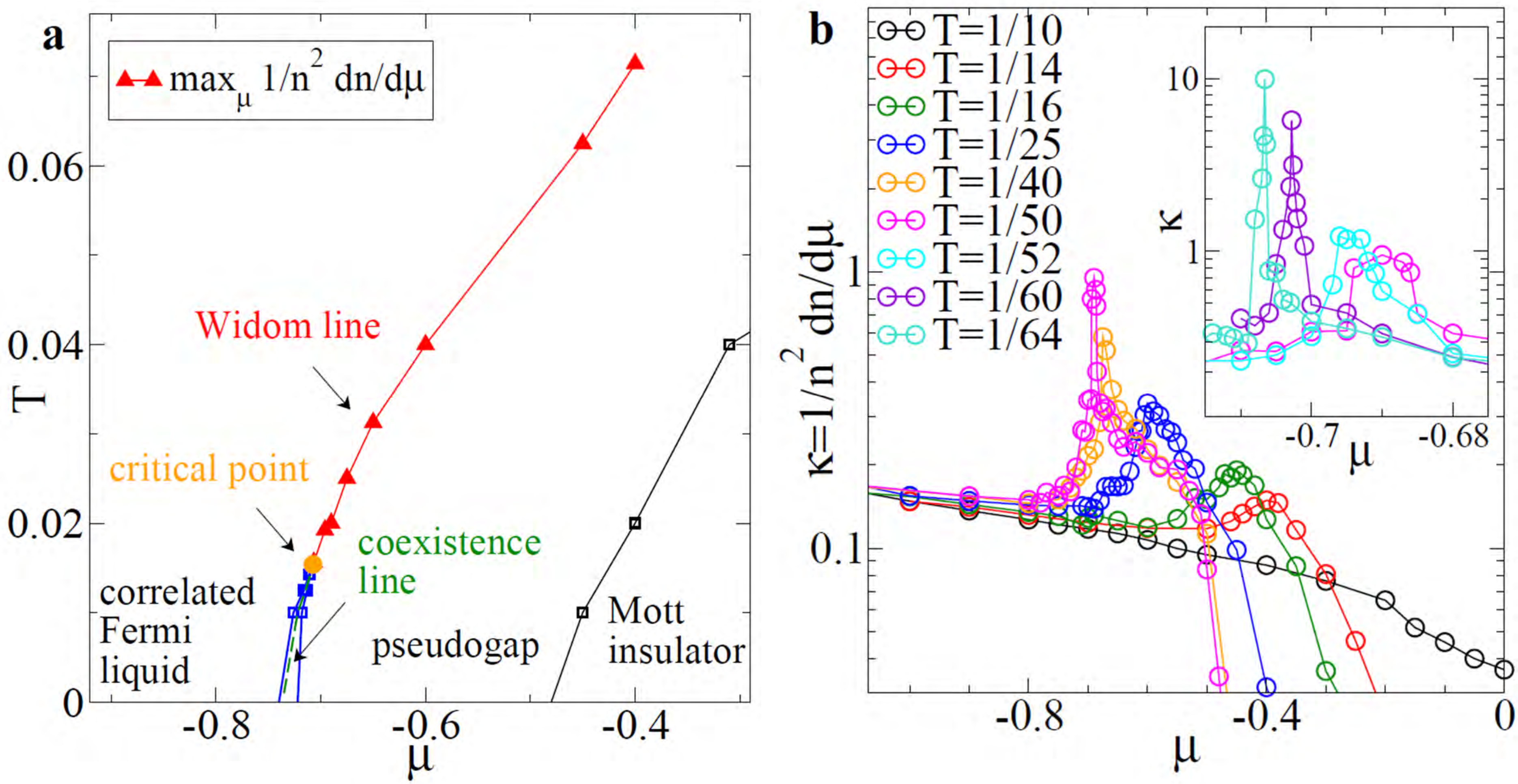
The Widom line



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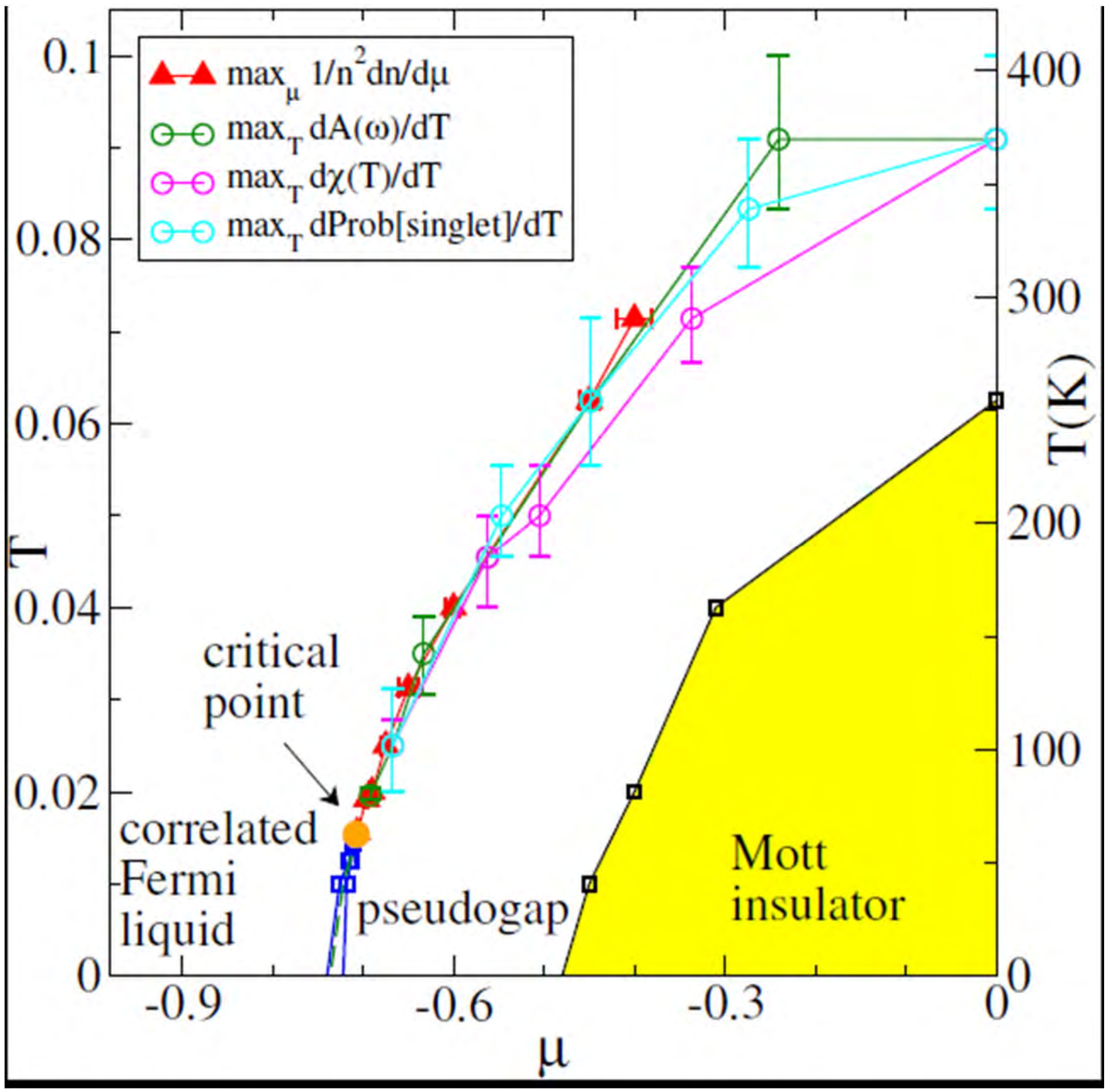
Rapid change also in dynamical quantities



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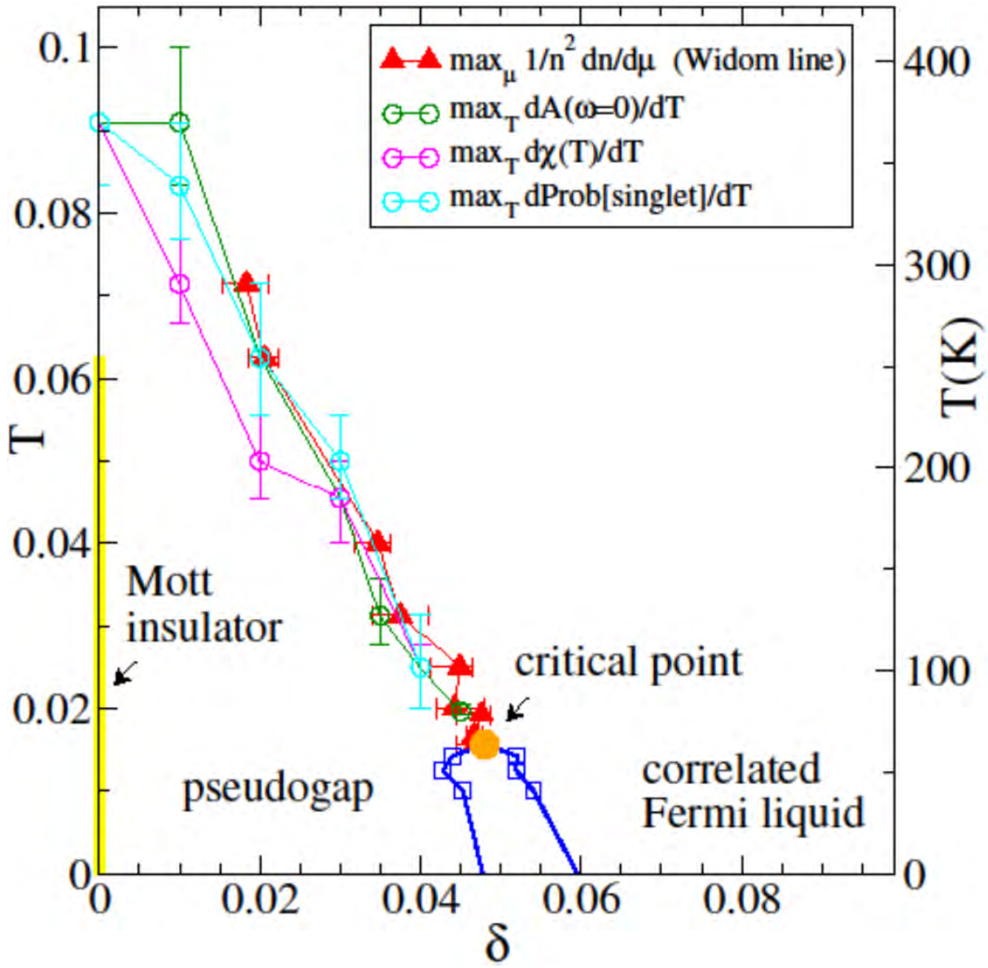
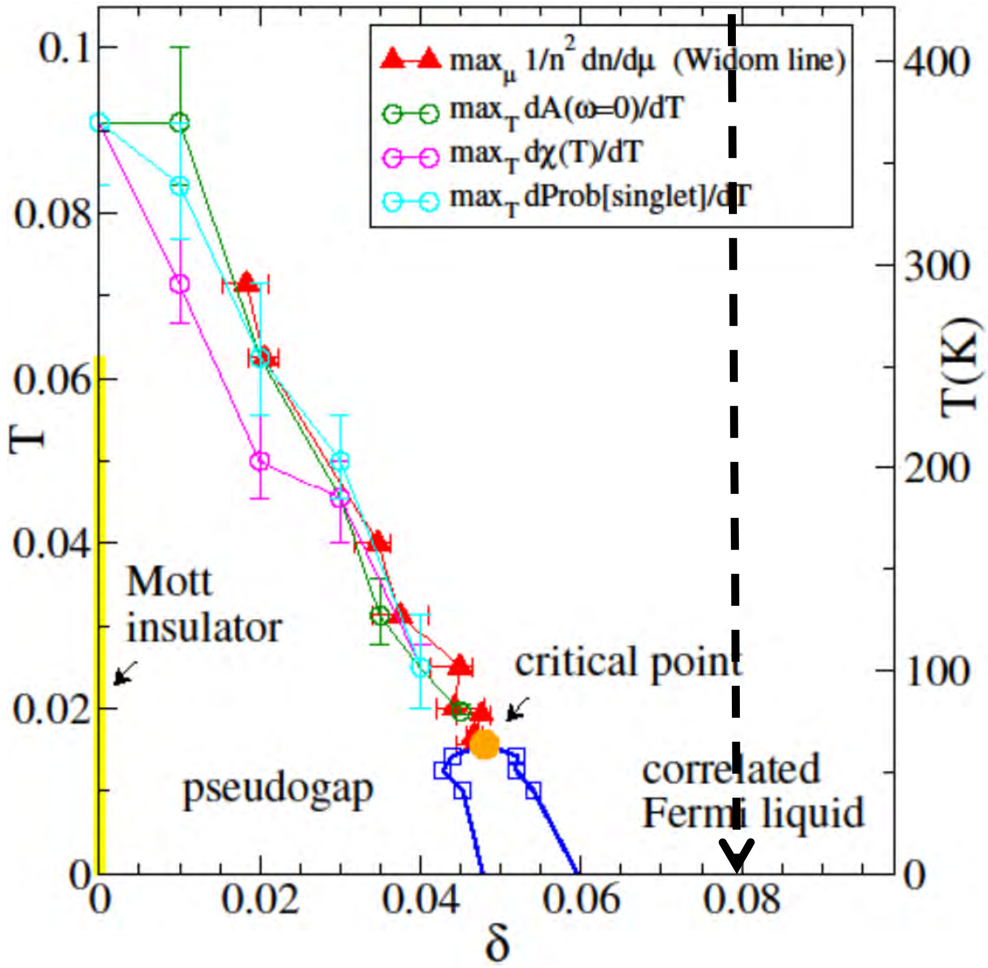
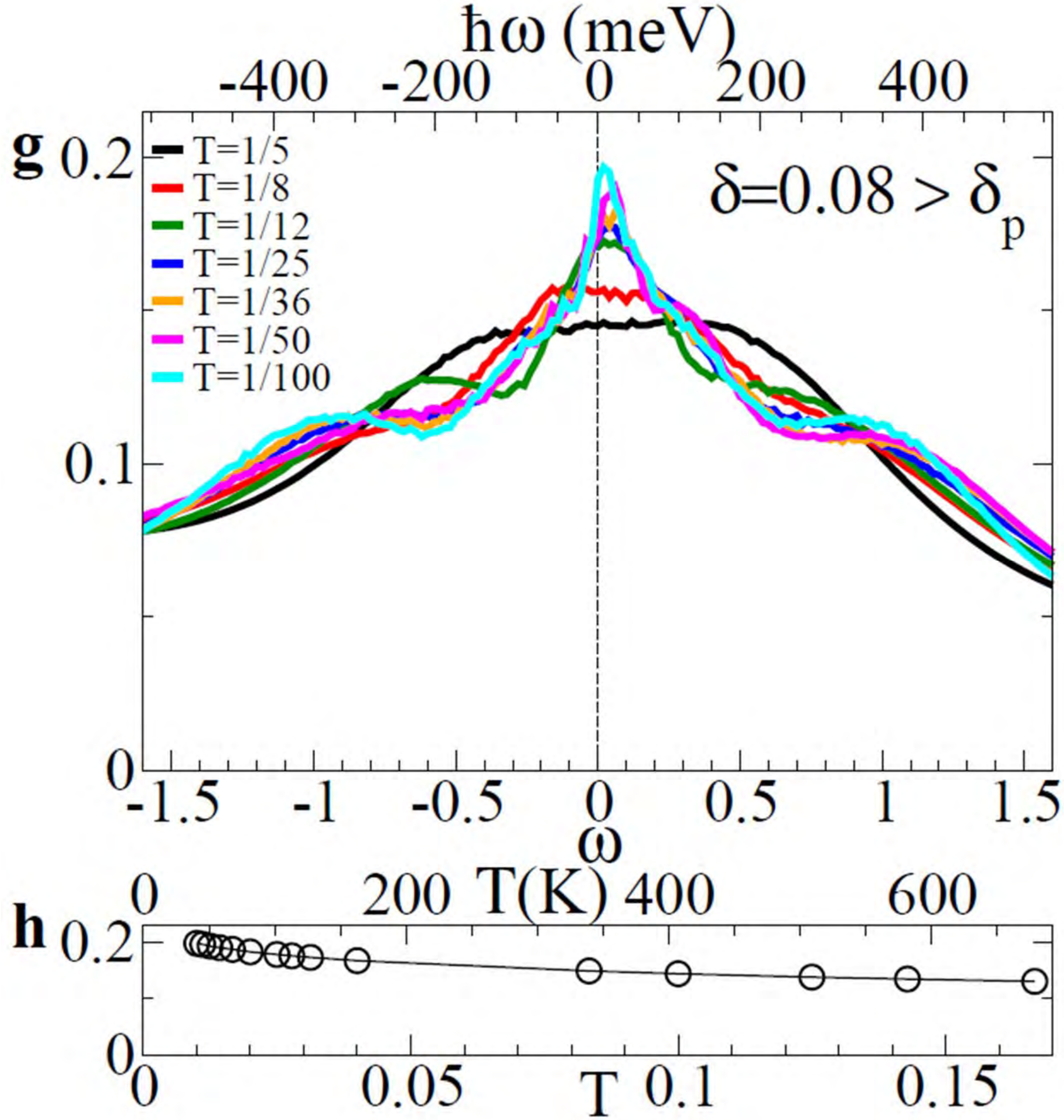
Phase diagram



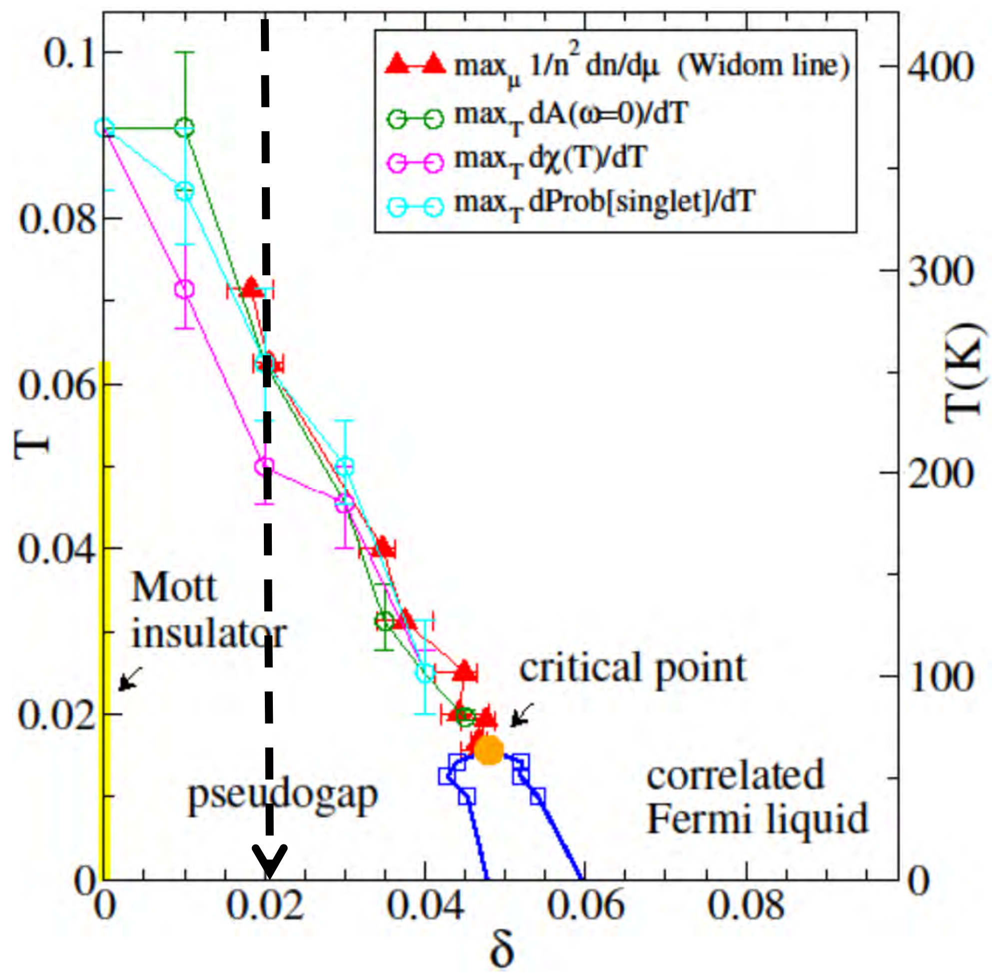
Phase diagram



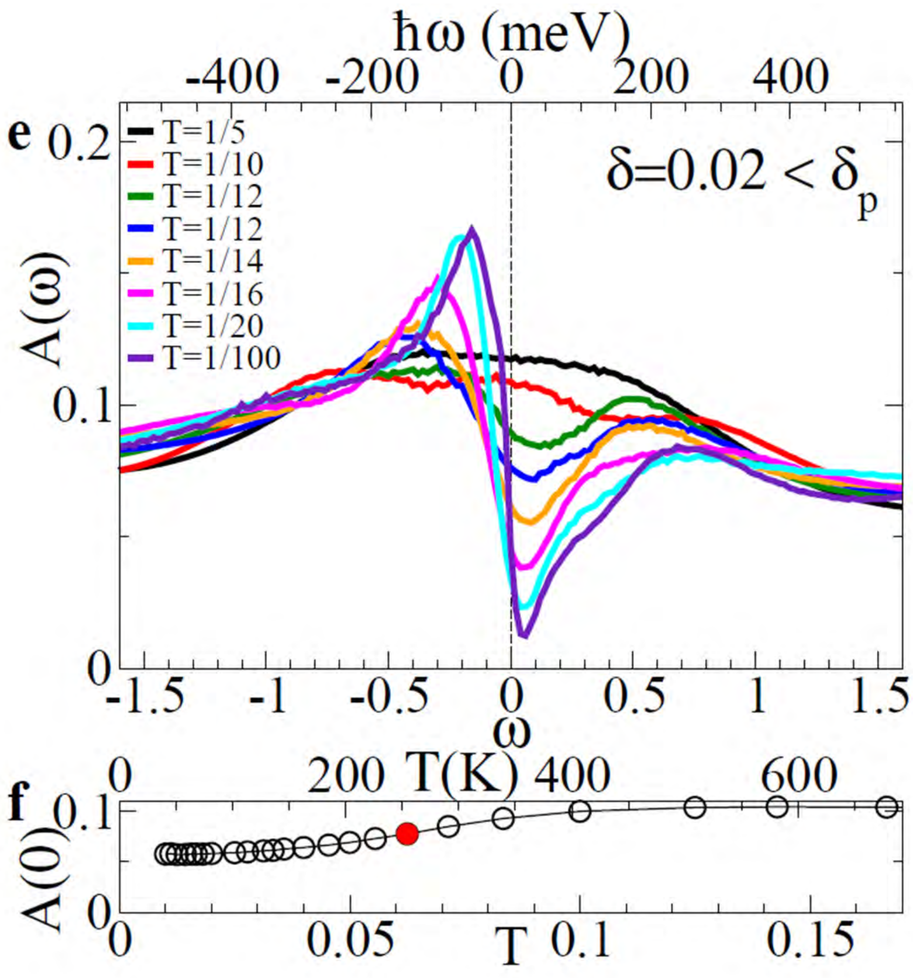


ħω (meV)
-400 -200 0 200 400
g
0.2
0.1
0
T=1/5
T=1/8
T=1/12
T=1/25
T=1/36
T=1/50
T=1/100
δ=0.08 > δ_p
-1.5 -1 -0.5 0 0.5 1 1.5
ω
0 200 T(K) 400 600
h
0.2
0
0 0.05 T 0.1 0.15

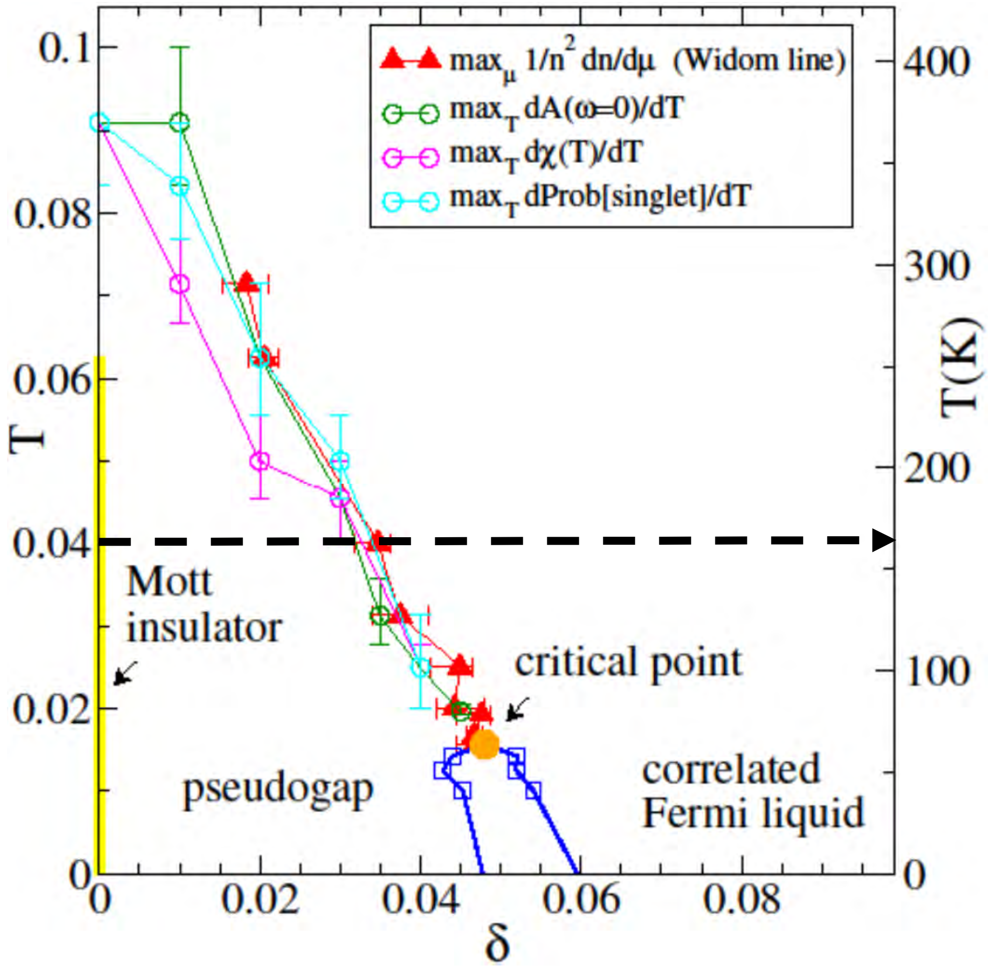
Phase diagram



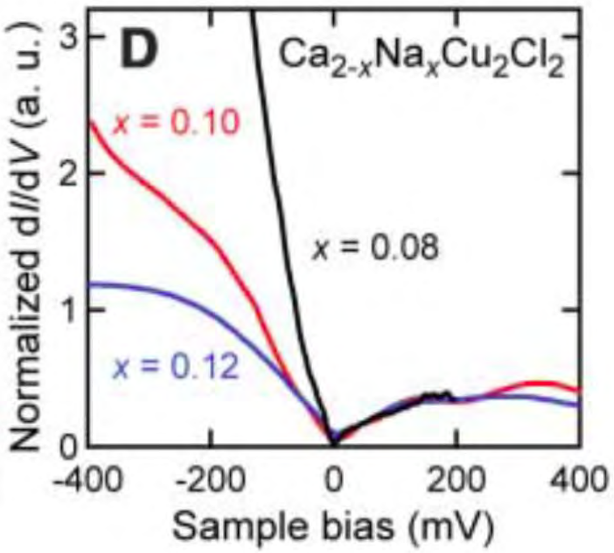
T dependence of the DOS

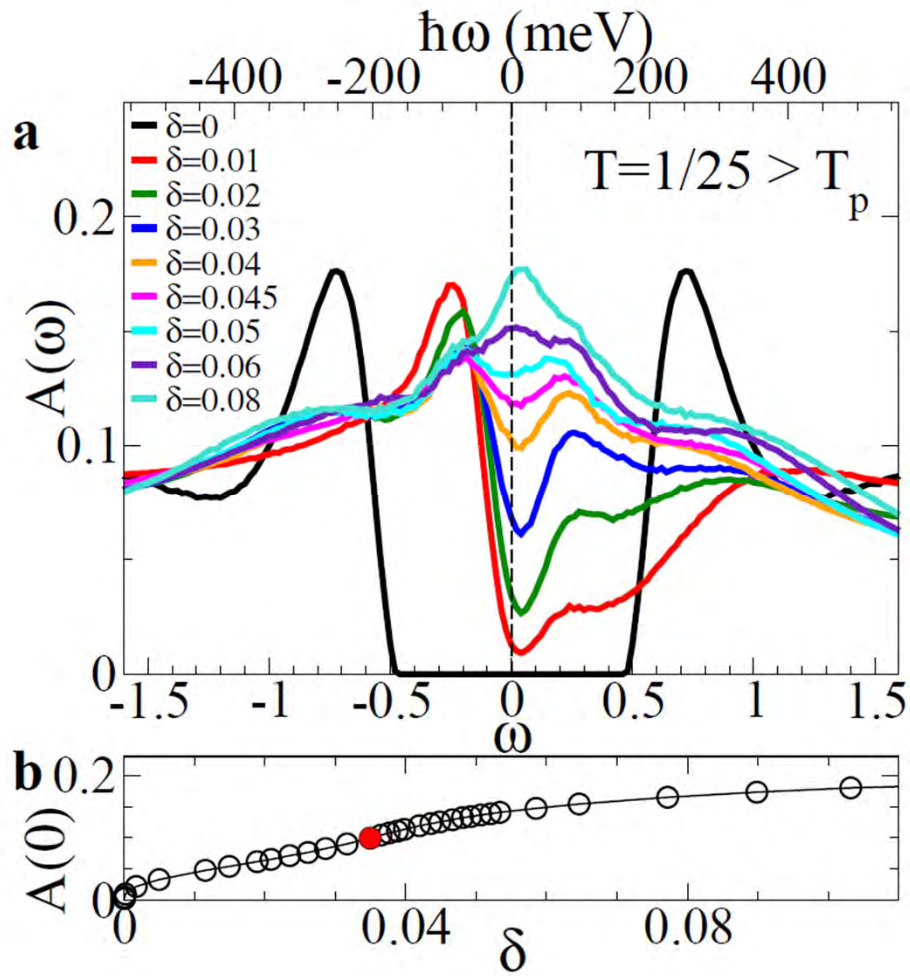


Phase diagram



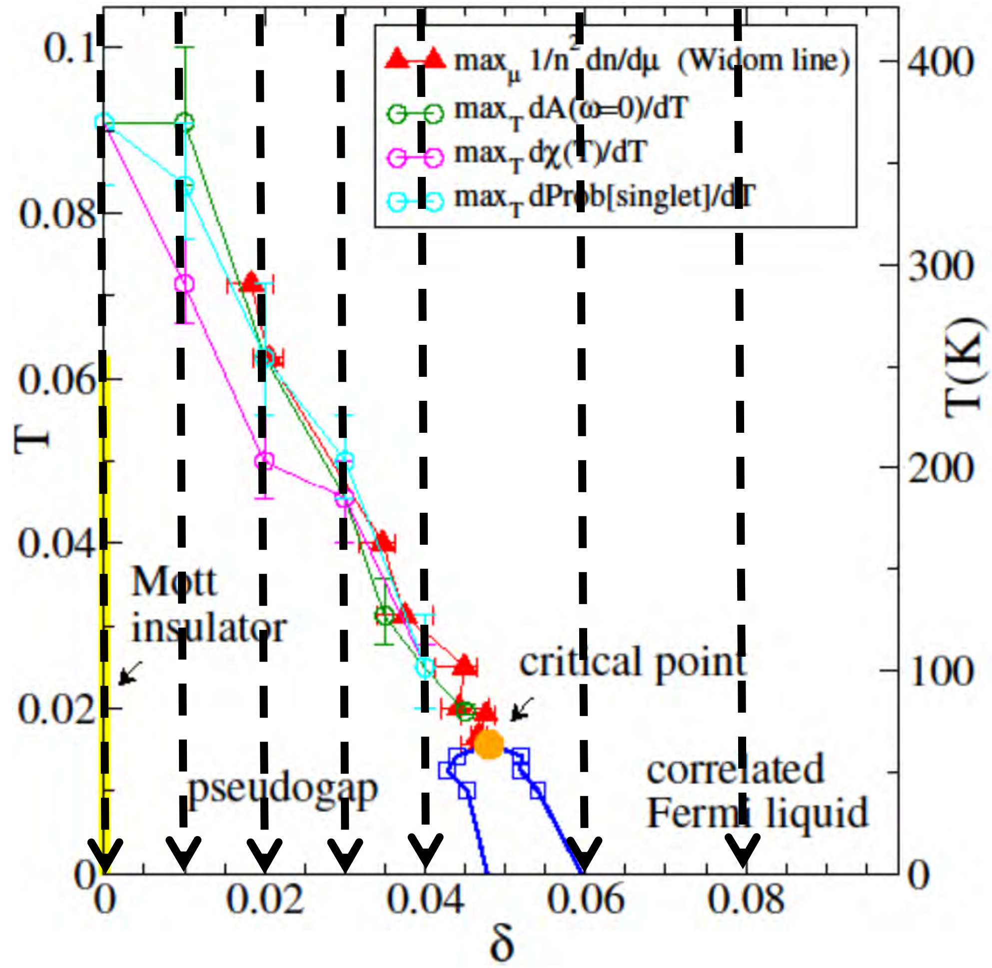
Tunneling DOS



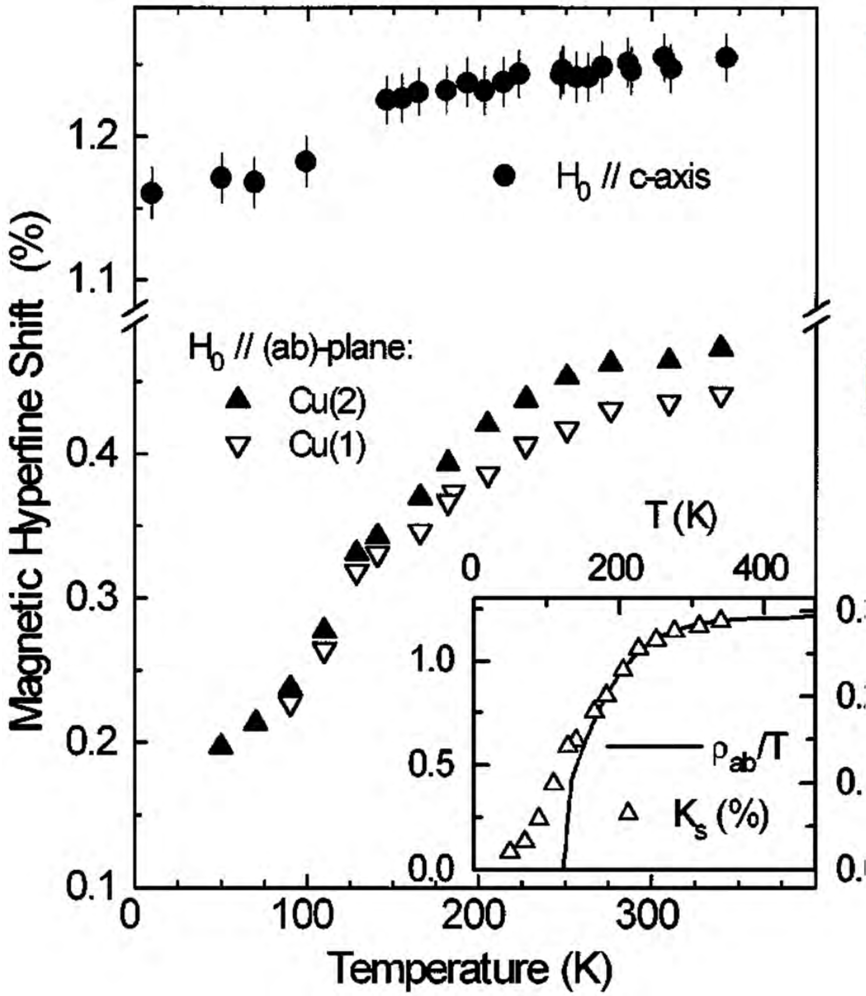


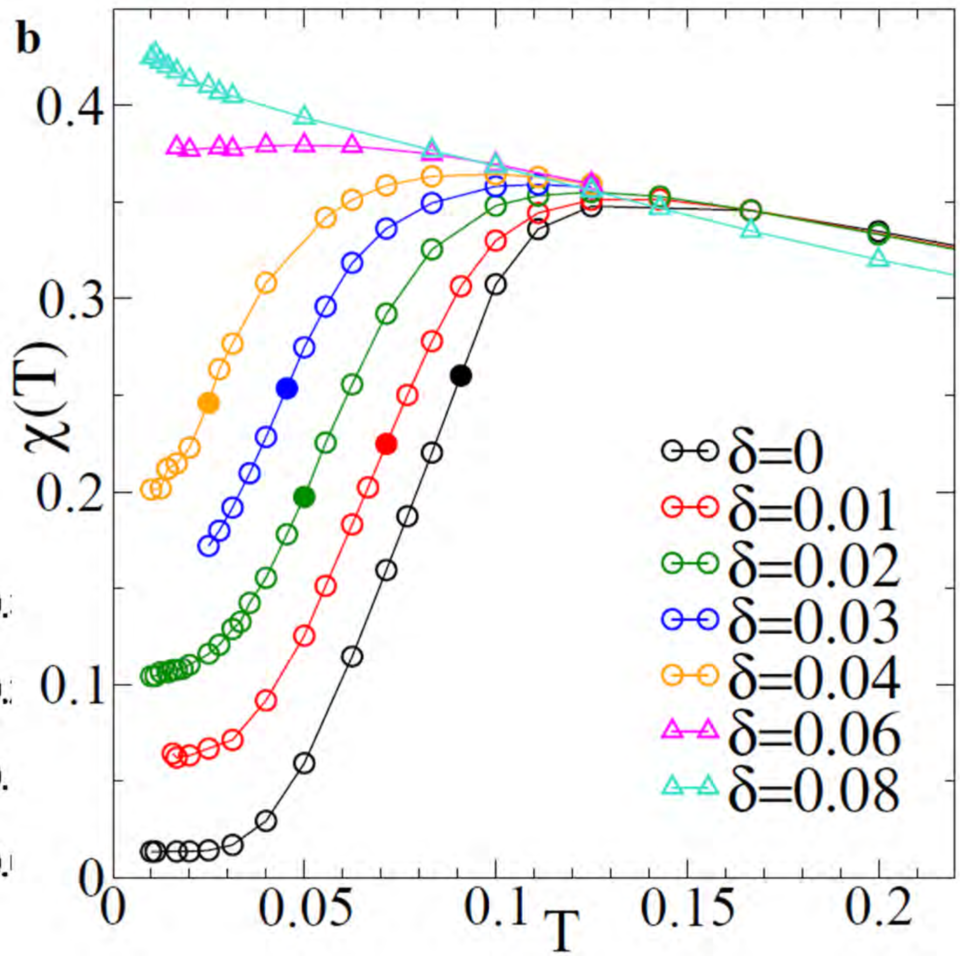
Khosaka et al. *Science* **315**, 1380 (2007);

Phase diagram



Spin susceptibility

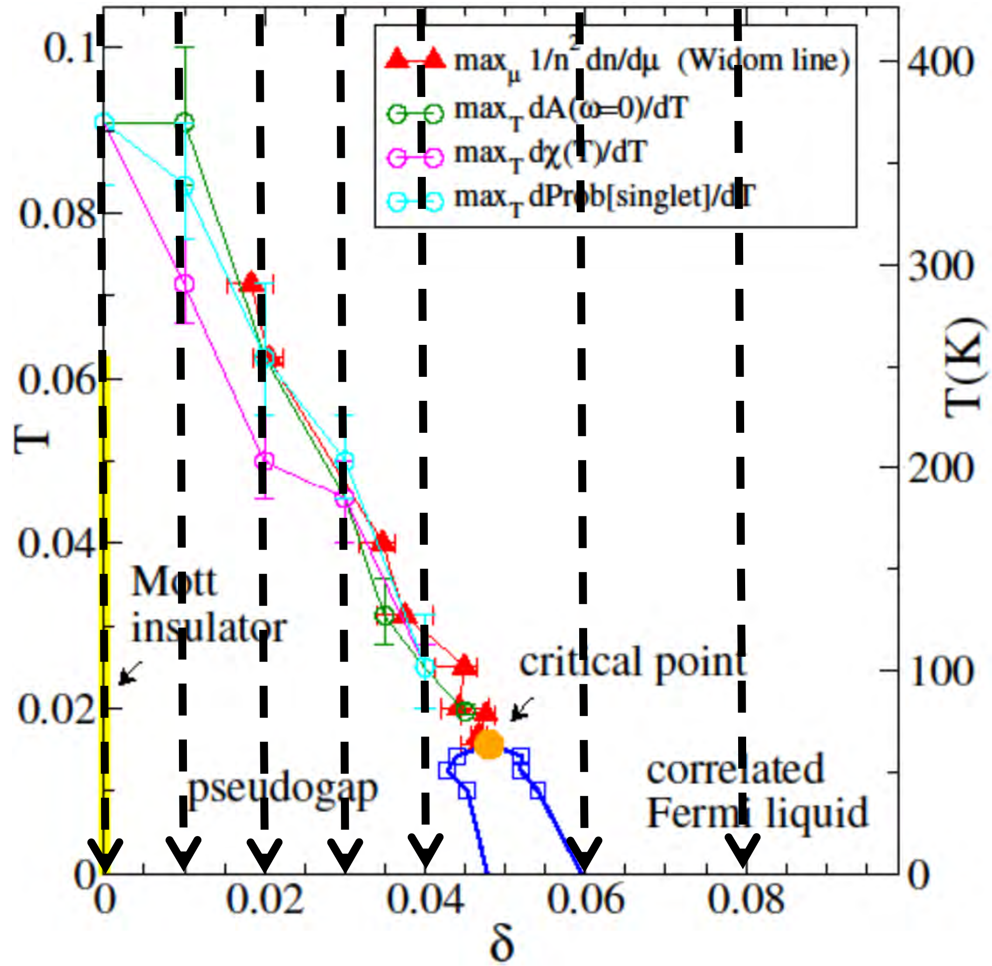




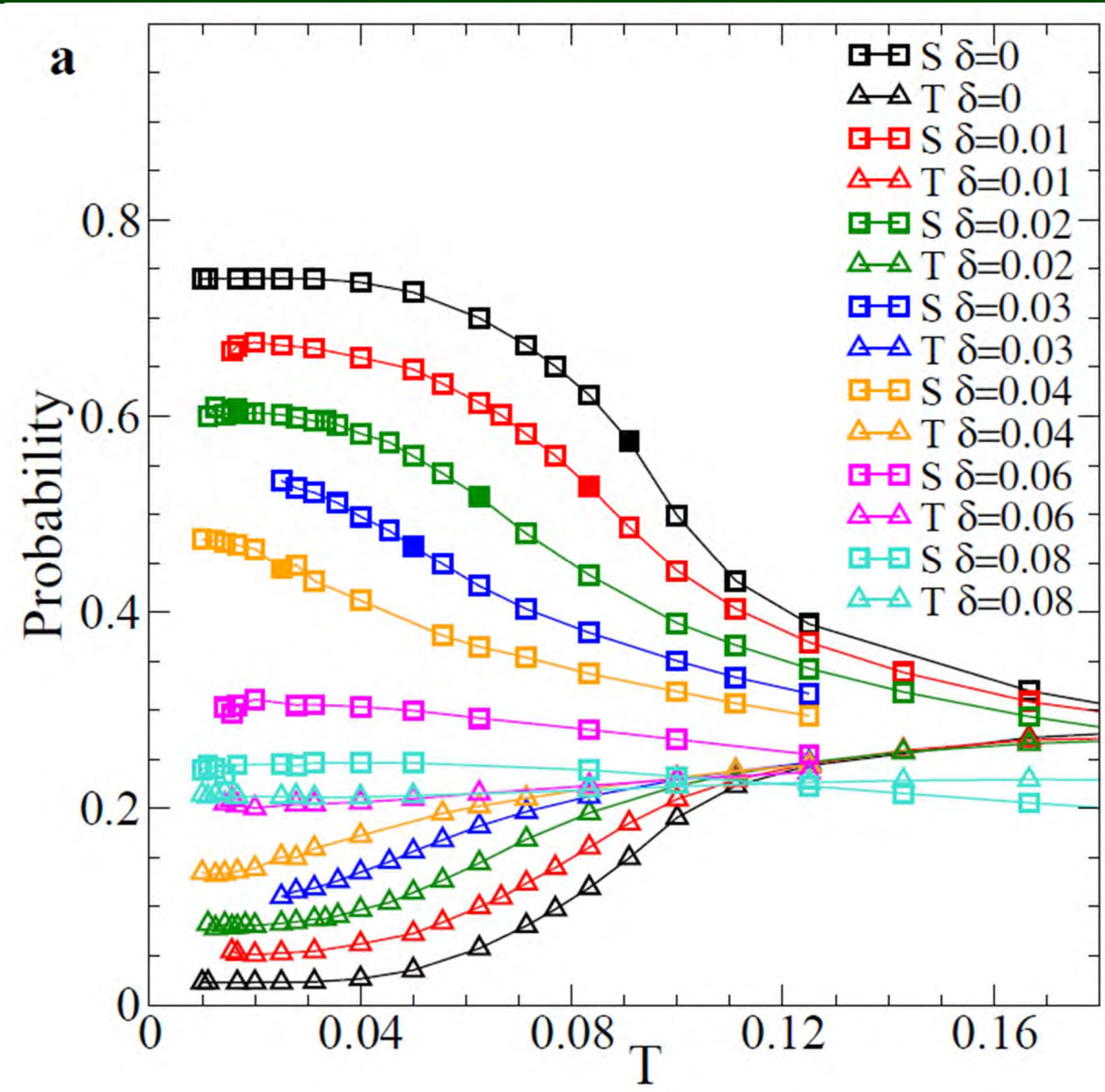
Underdoped Hg1223

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

Phase diagram



Plaquette eigenstates



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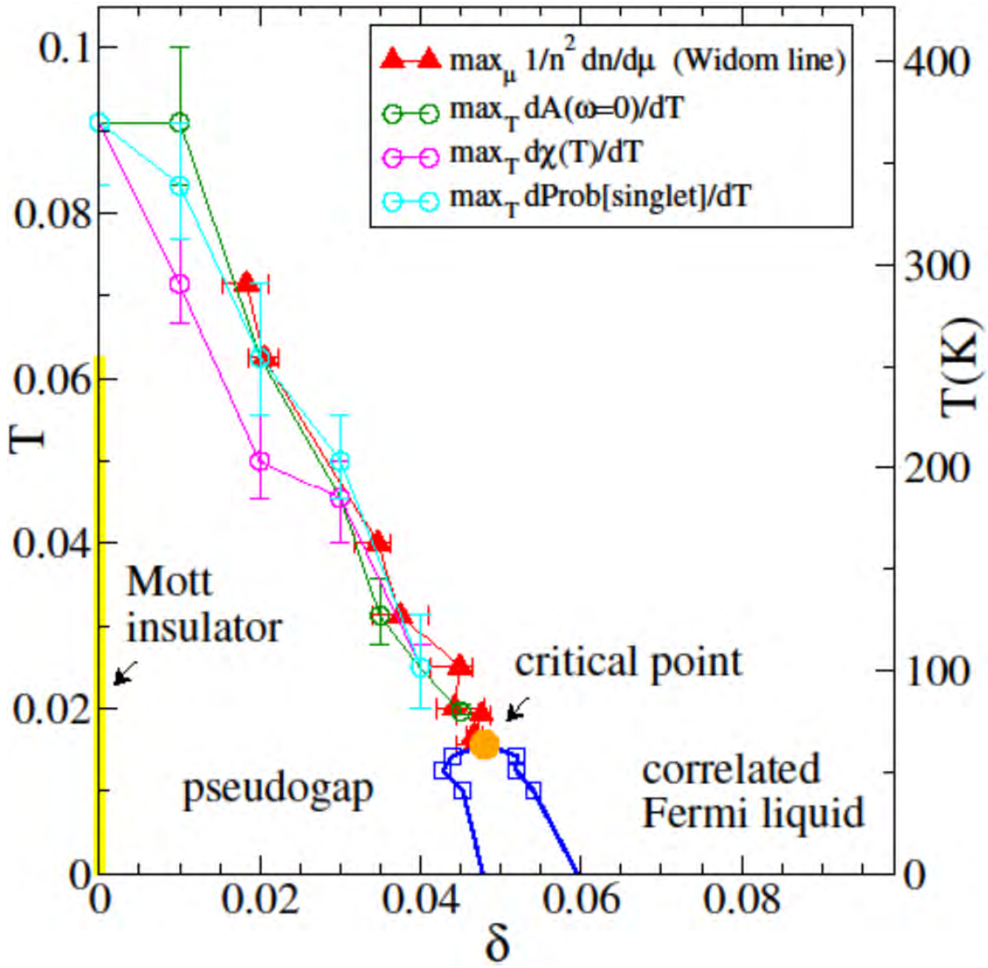
Phase diagram



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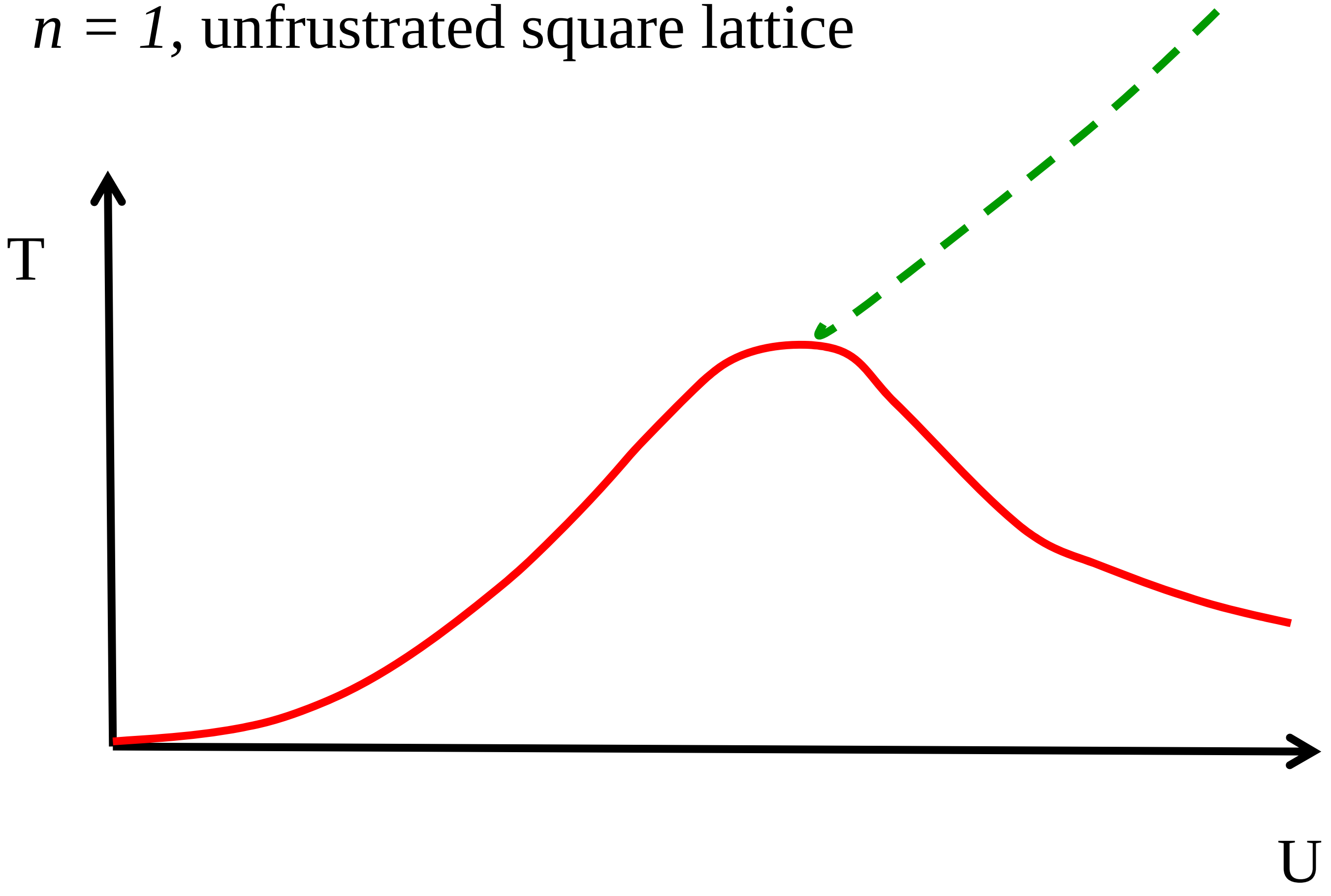
Local moment and Mott transition

n = 1, unfrustrated square lattice



Local moment and Mott transition

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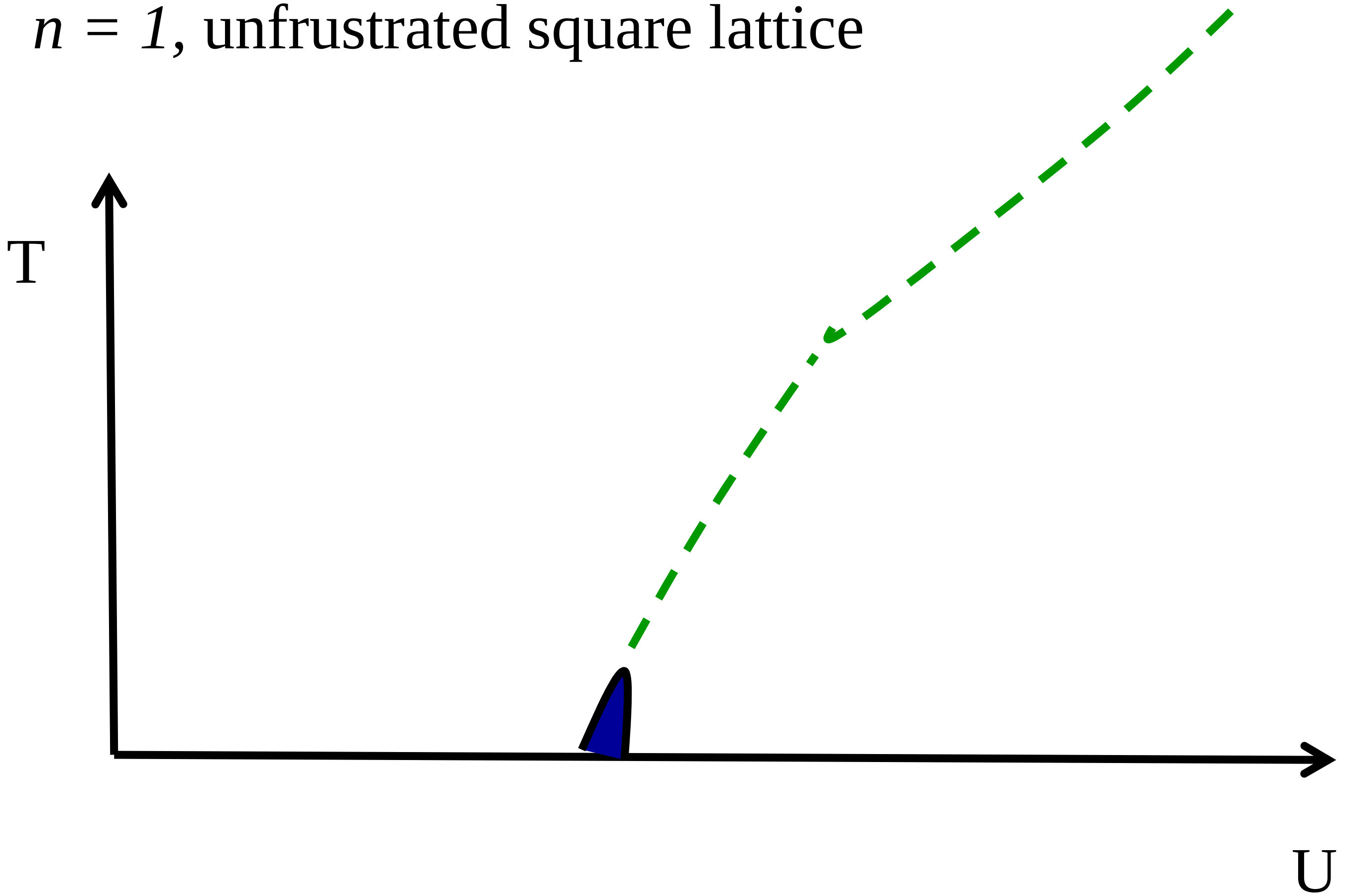
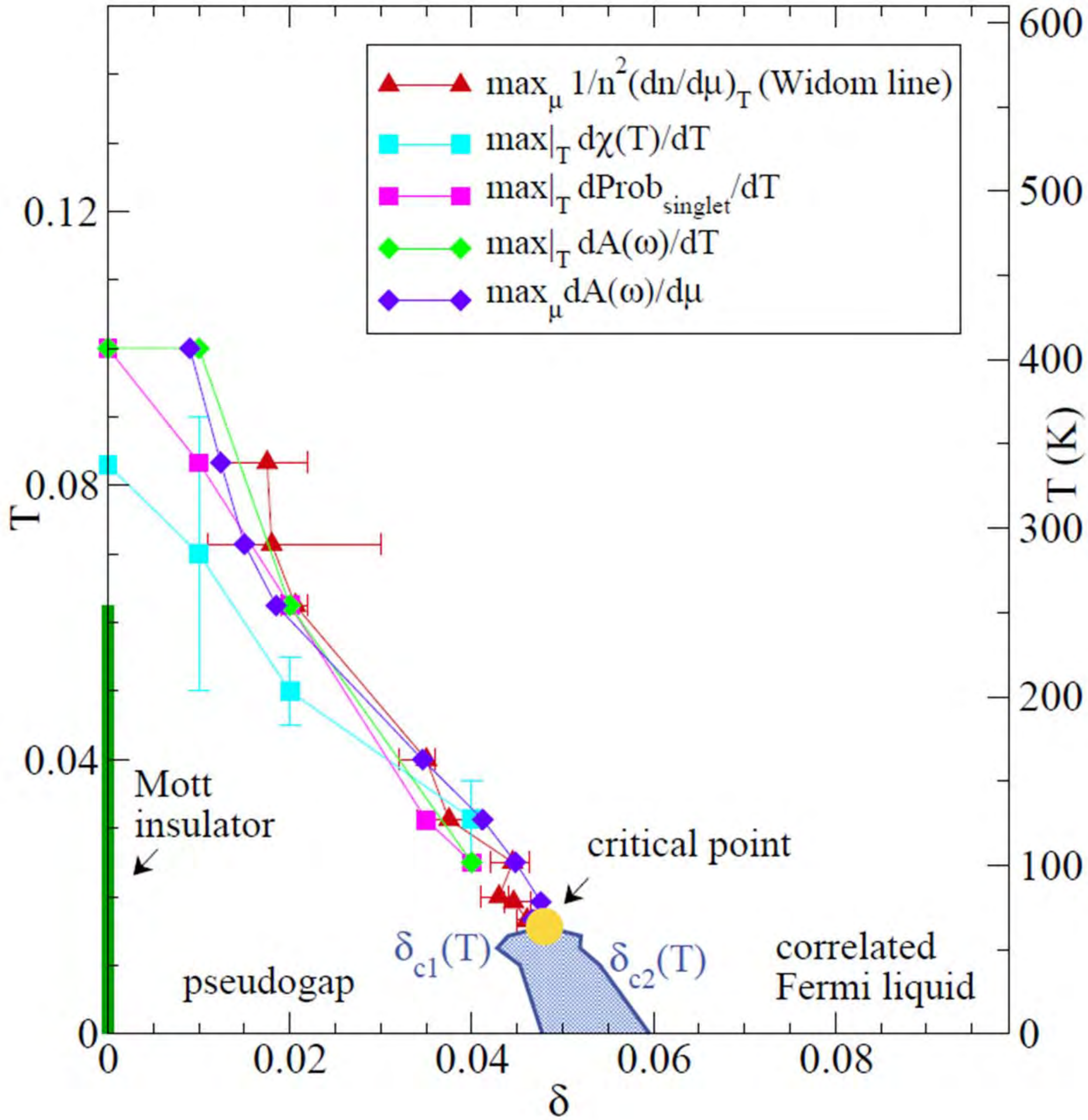


Local singlet and pseudogap transition



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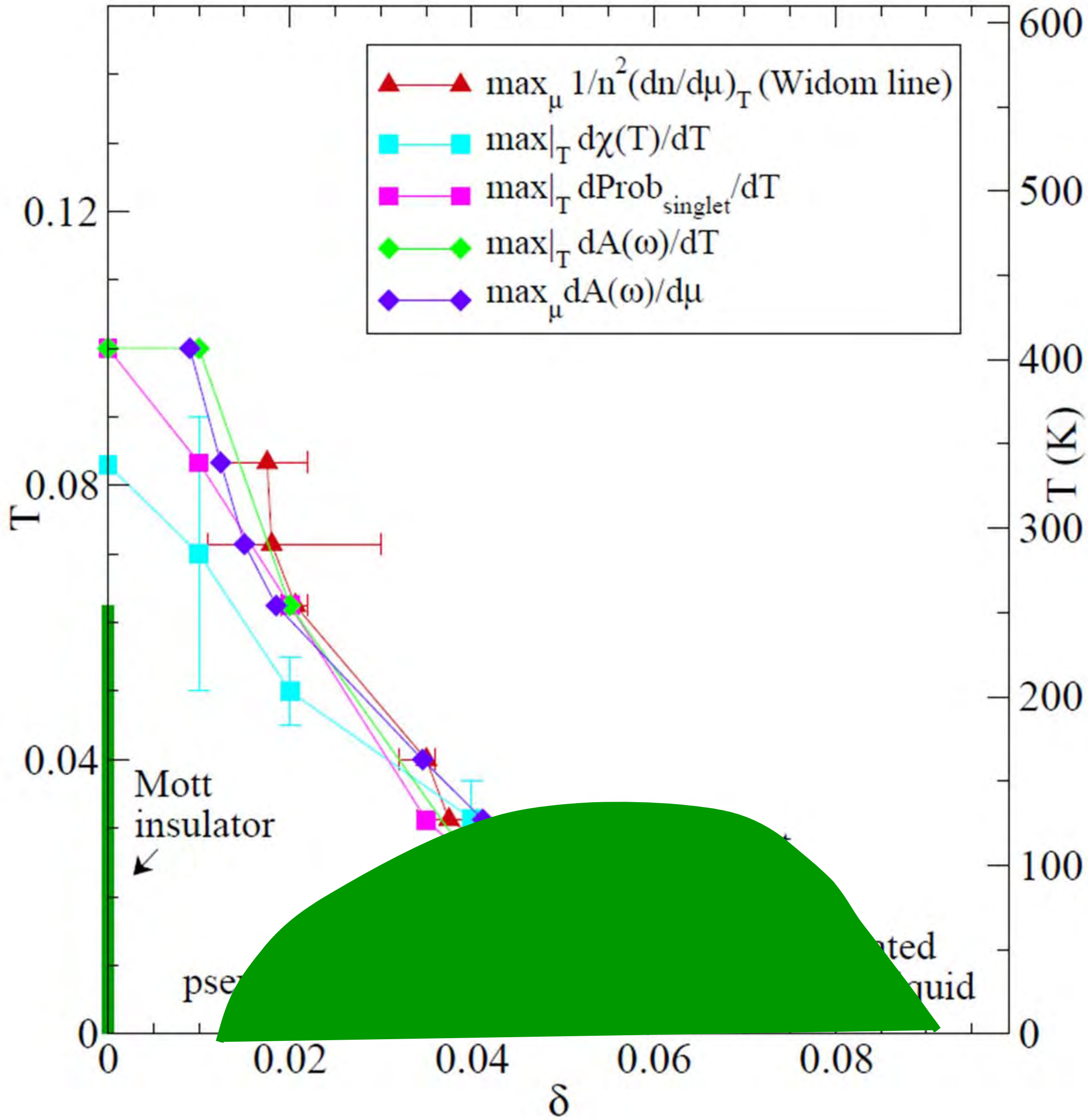
Local singlet and pseudogap transition



Another property of the UD phase

Underdoped metal very sensitive to anisotropy

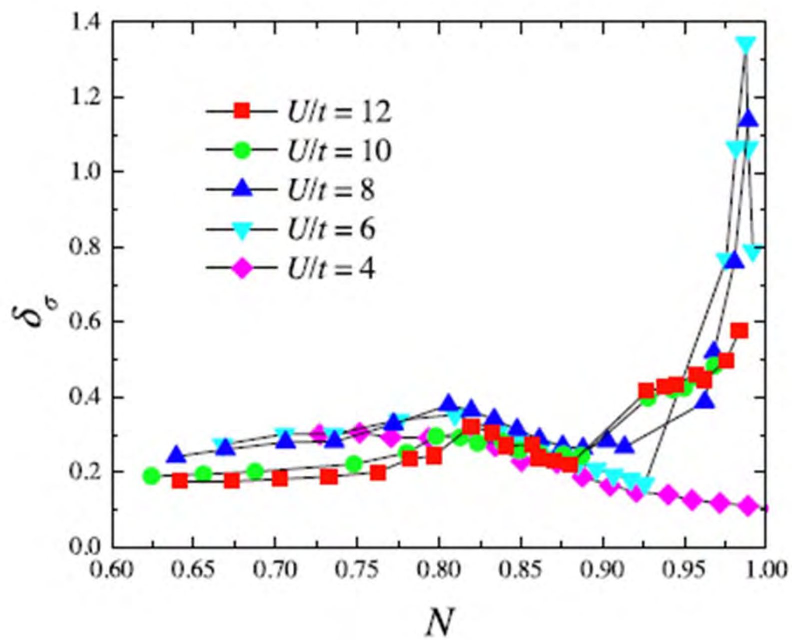
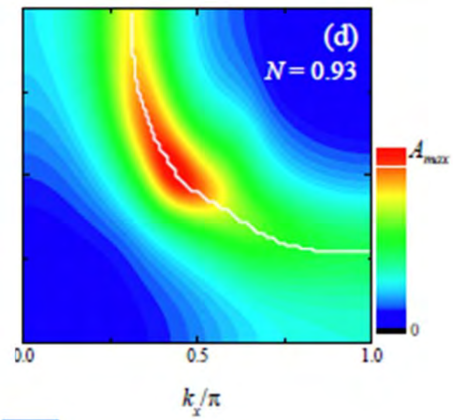
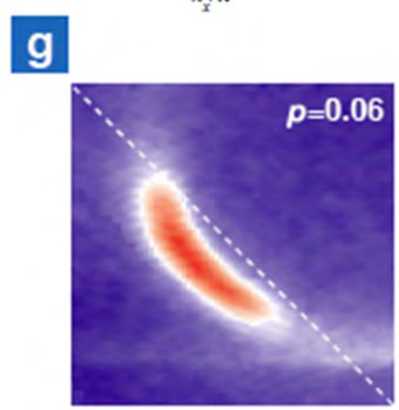


FIG. 3: (Color online) Anisotropy in the CDMFT conductivity $\delta_\sigma = 2\,[\sigma_x(0) - \sigma_y(0)]\,/\,[\sigma_x(0) + \sigma_y(0)]$ as a function of filling N for various values of U and $\eta = 0.1$, $\delta_0 = 0.04$.





Satoshi Okamoto

David Sénéchal

Okamoto, Sénéchal, Civelli, AMST
Phys. Rev. B **82**, 180511R 2010

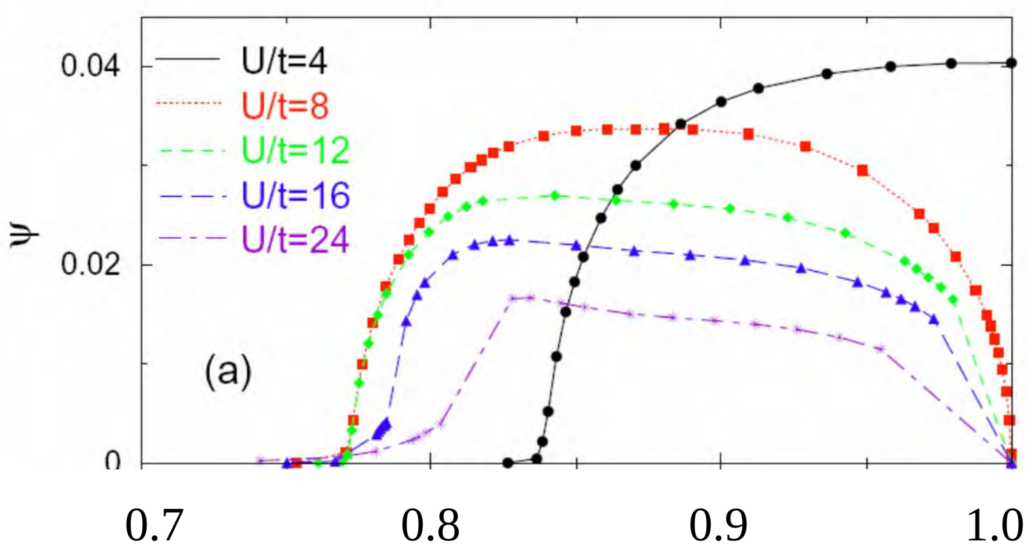
D. Fournier *et al.* Nature Physics (Marcello Civelli

Superconductivity

Phase diagram

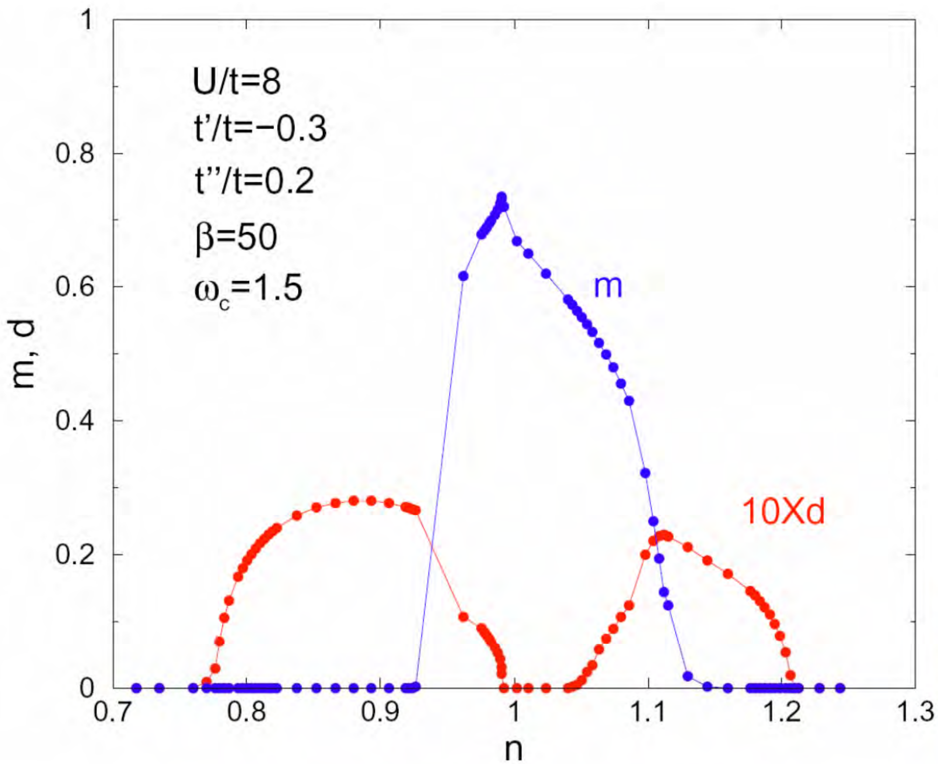
Exact diagonalization as impurity solver ($T=0$).

Dome vs Mott (CDMFT)

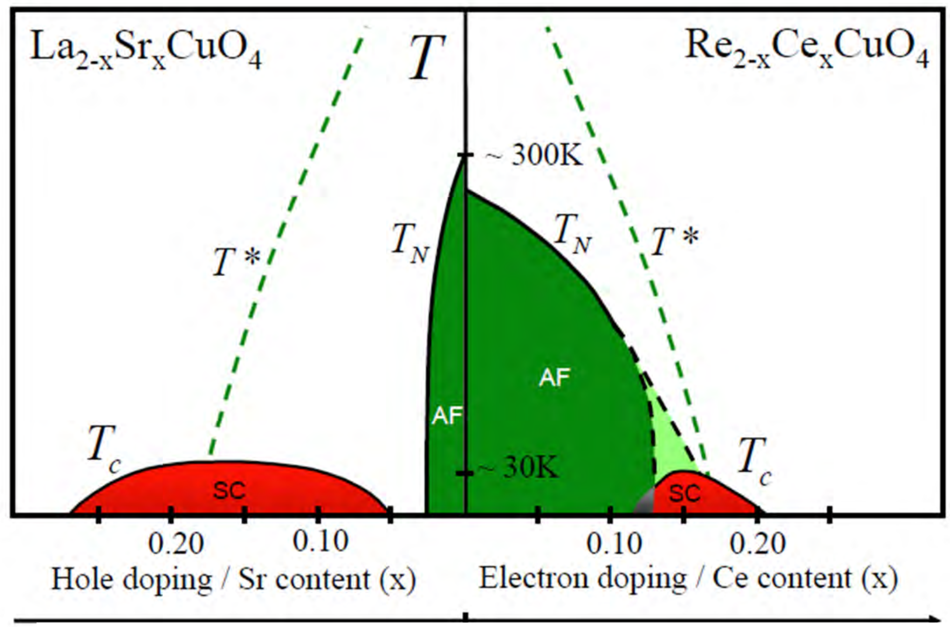


Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008)

CDMFT global phase diagram



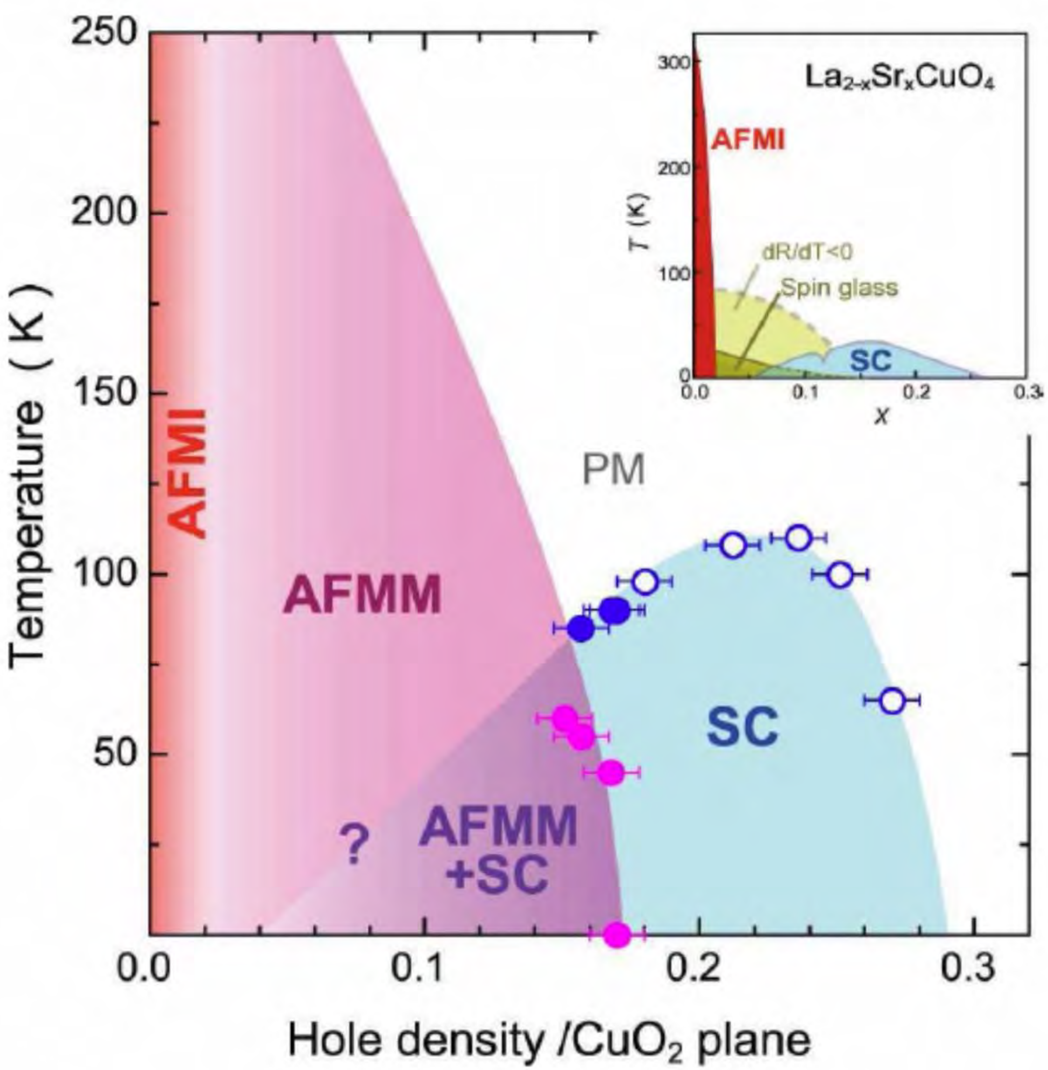
Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008)

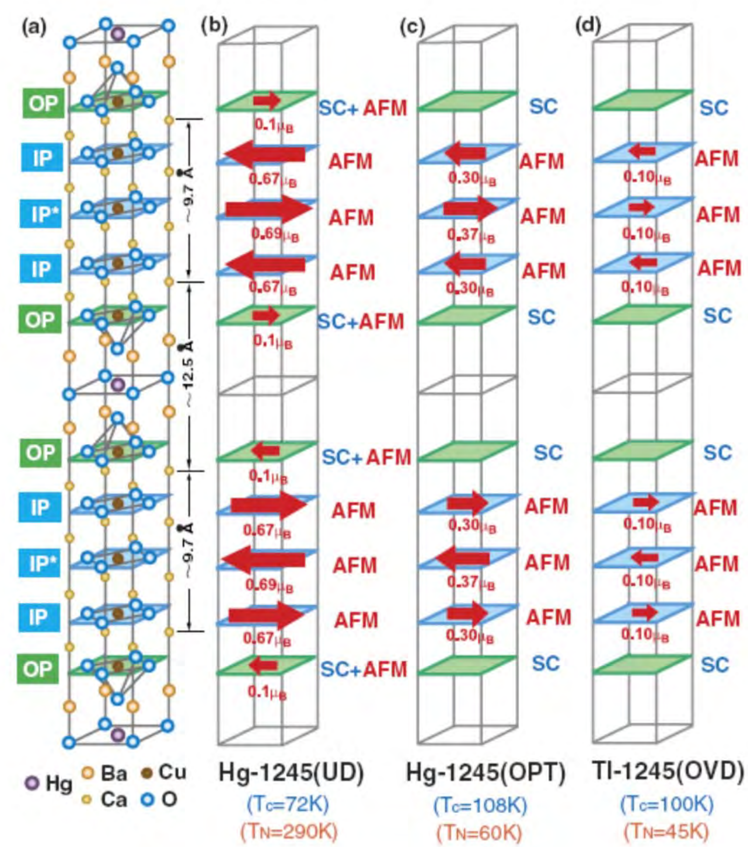


Armitage, Fournier, Greene, RMP (2009)

Consistent with following experiment

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





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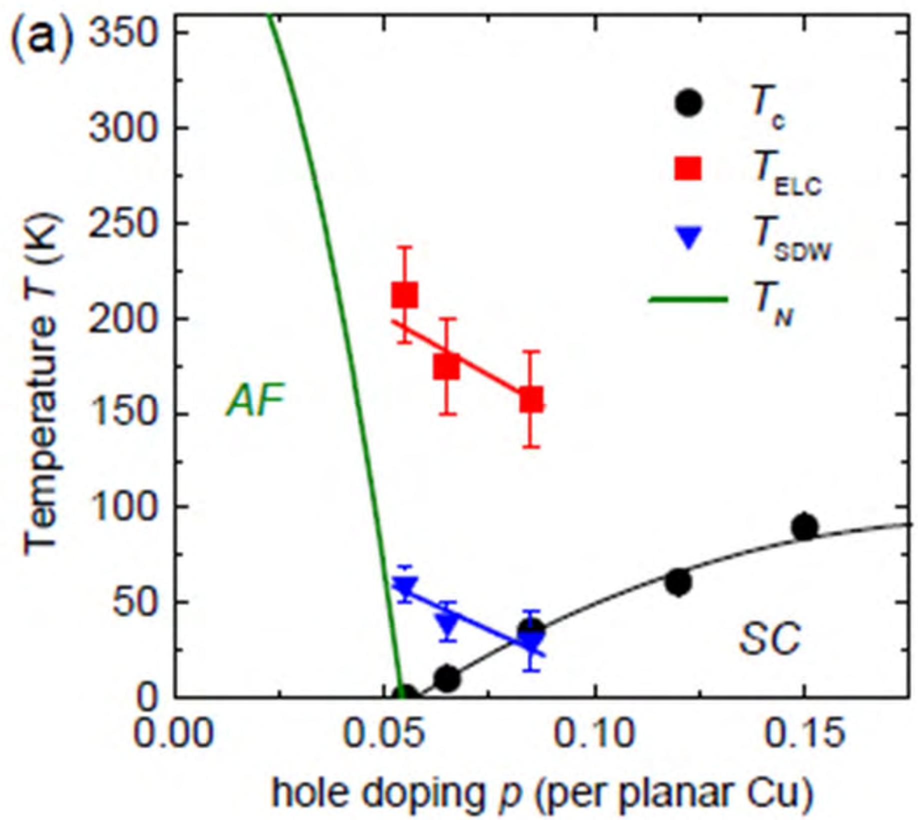
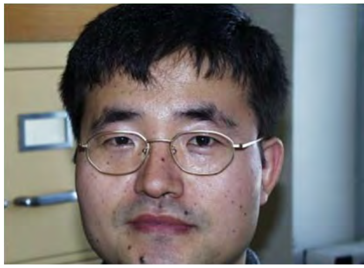
Magnetic phase diagram of YBCO

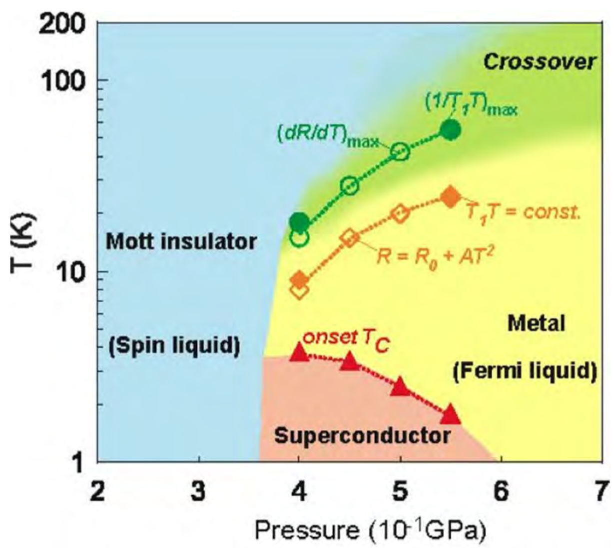


Haug, … Keimer, New J. Phys. 12, 105006 (2010)



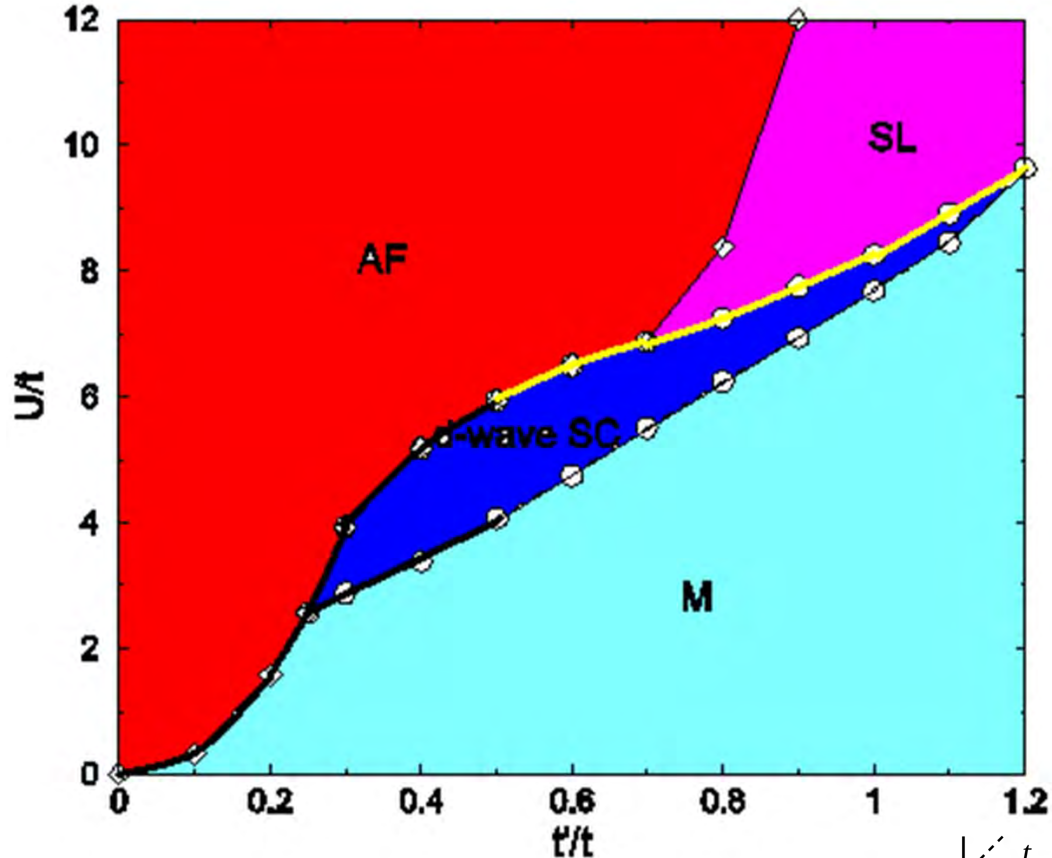
Theoretical phase diagram BEDT

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

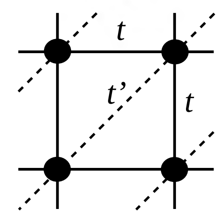


Y. Kurisaki, et al.

Phys. Rev. Lett. **95**, 177001(2005)



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

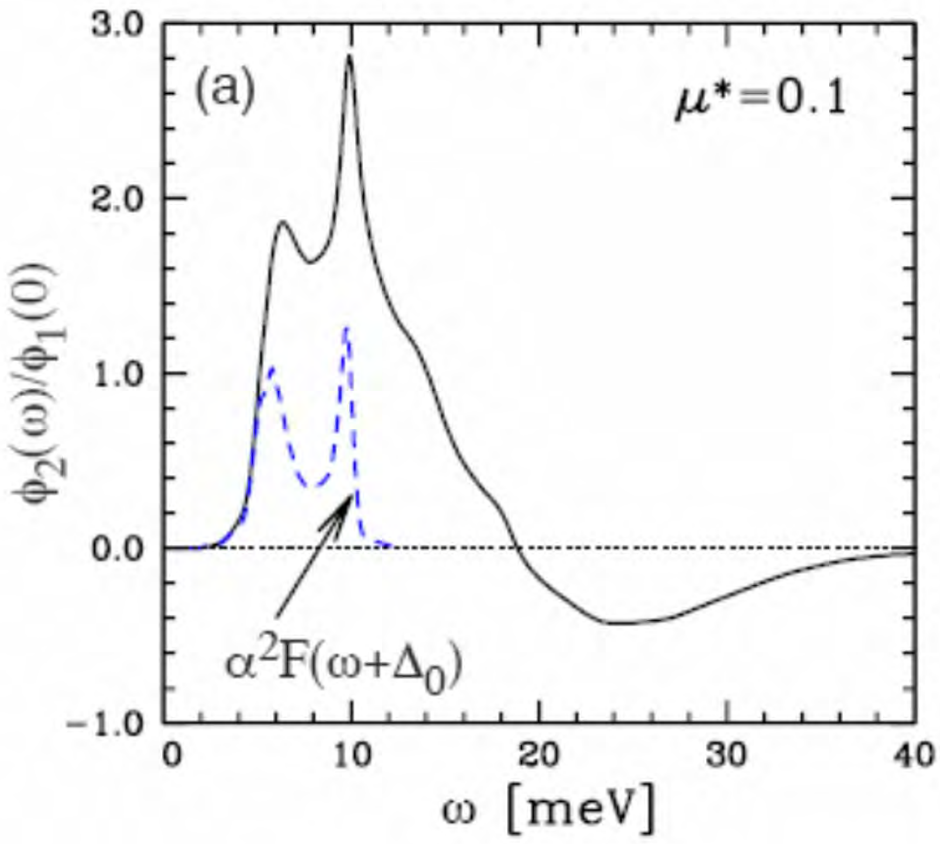


Y. Shimizu, et al. Phys. Rev. Lett. **91**, (2003)

The glue

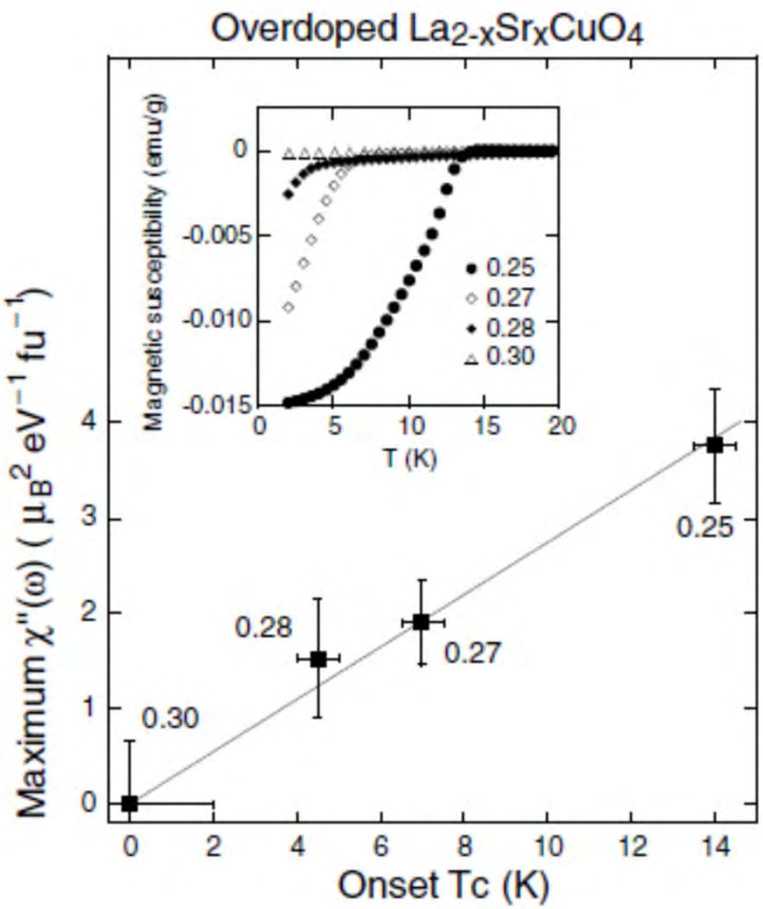
Im Σ_{an} and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

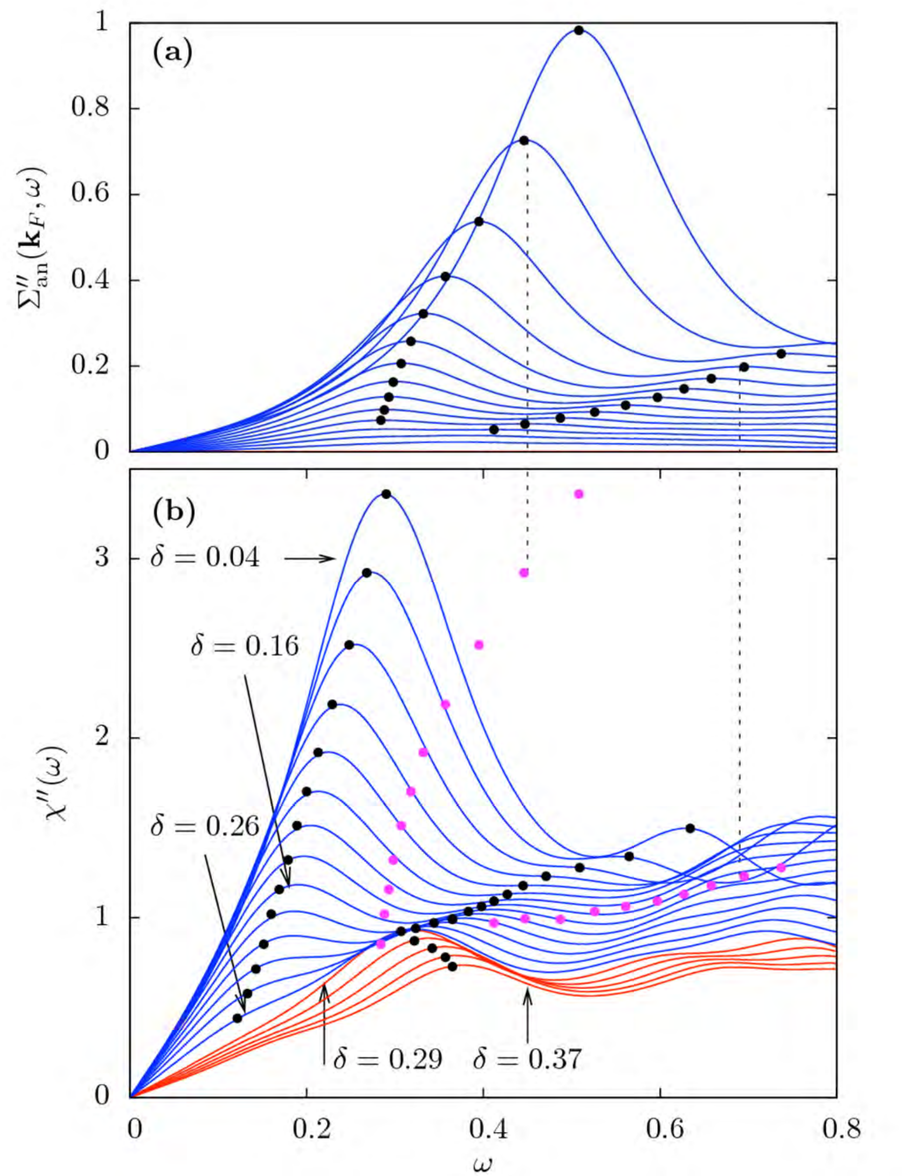


The glue

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



Wakimoto … Birgeneau PRL (2004)



The glue and neutrons

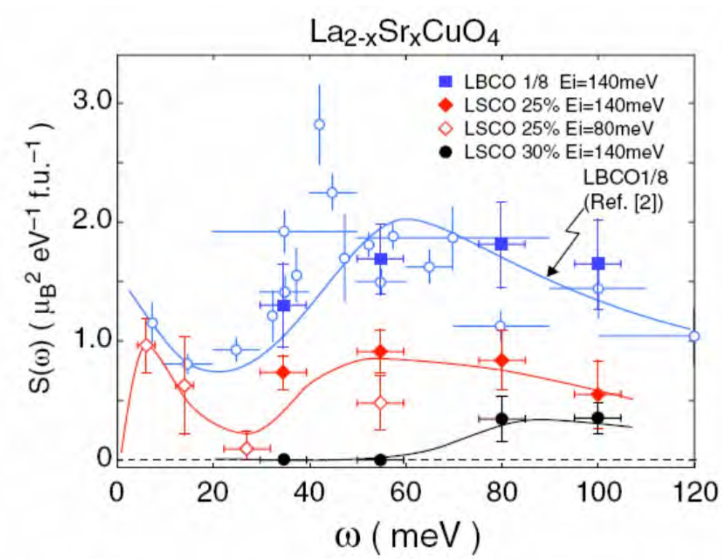
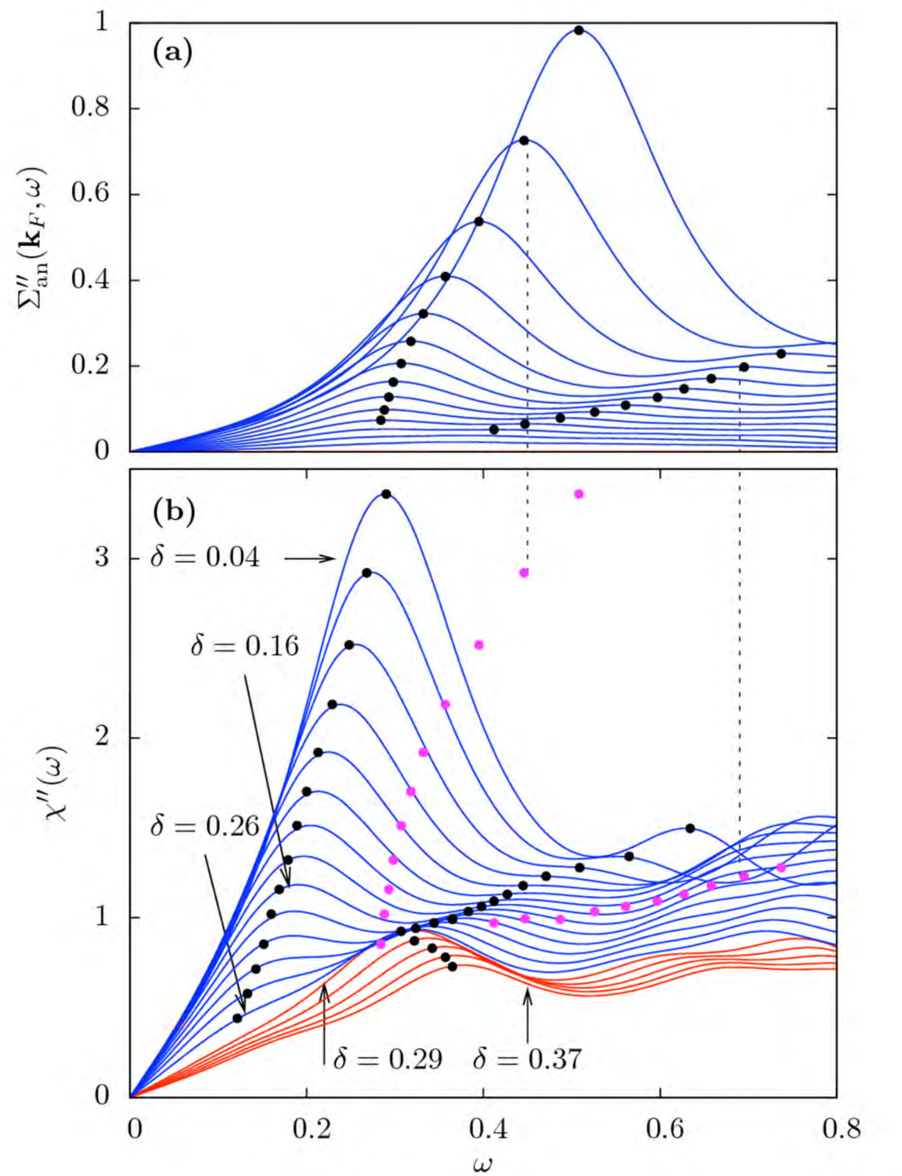


FIG. 3 (color online). **Q**-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i = 140$ meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO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

Main collaborators


Giovanni Sordi


David Sénéchal


Kristjan Haule


Bumsoo Kyung


Marcello Civelli


Satoshi Okamoto

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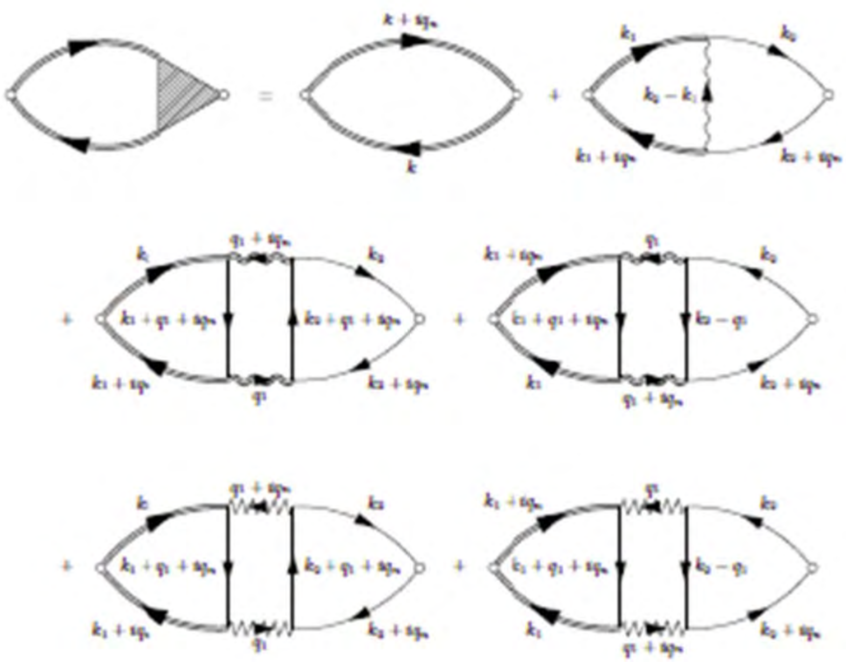
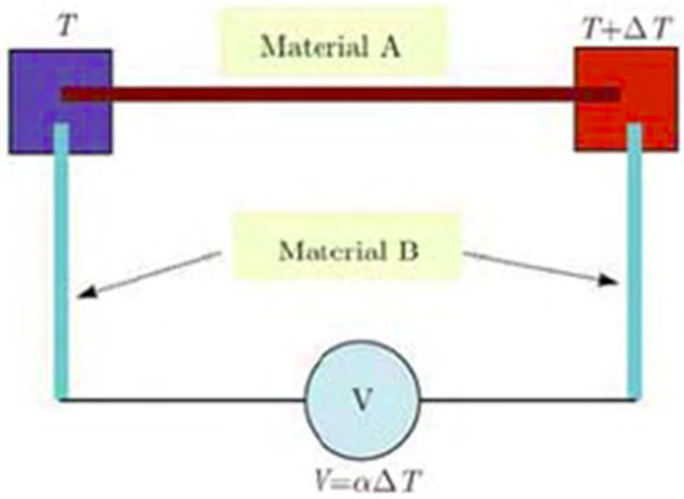
Resistivity (TPSC)



Dominic Bergeron

Thermoelectric power



Louis-François Arsenault

Sriram Shastry

Patrick Sémon

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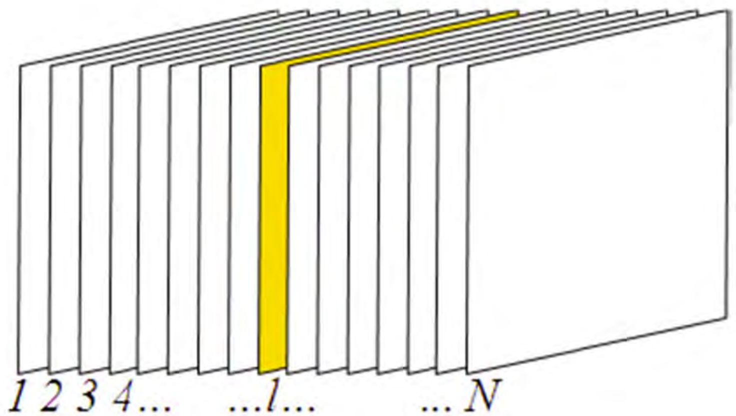
Heterostructures



Maxime Charlebois

Syed Hassan

David Sénéchal

Patrick Fournier

Maxime Dion

Simon Verret

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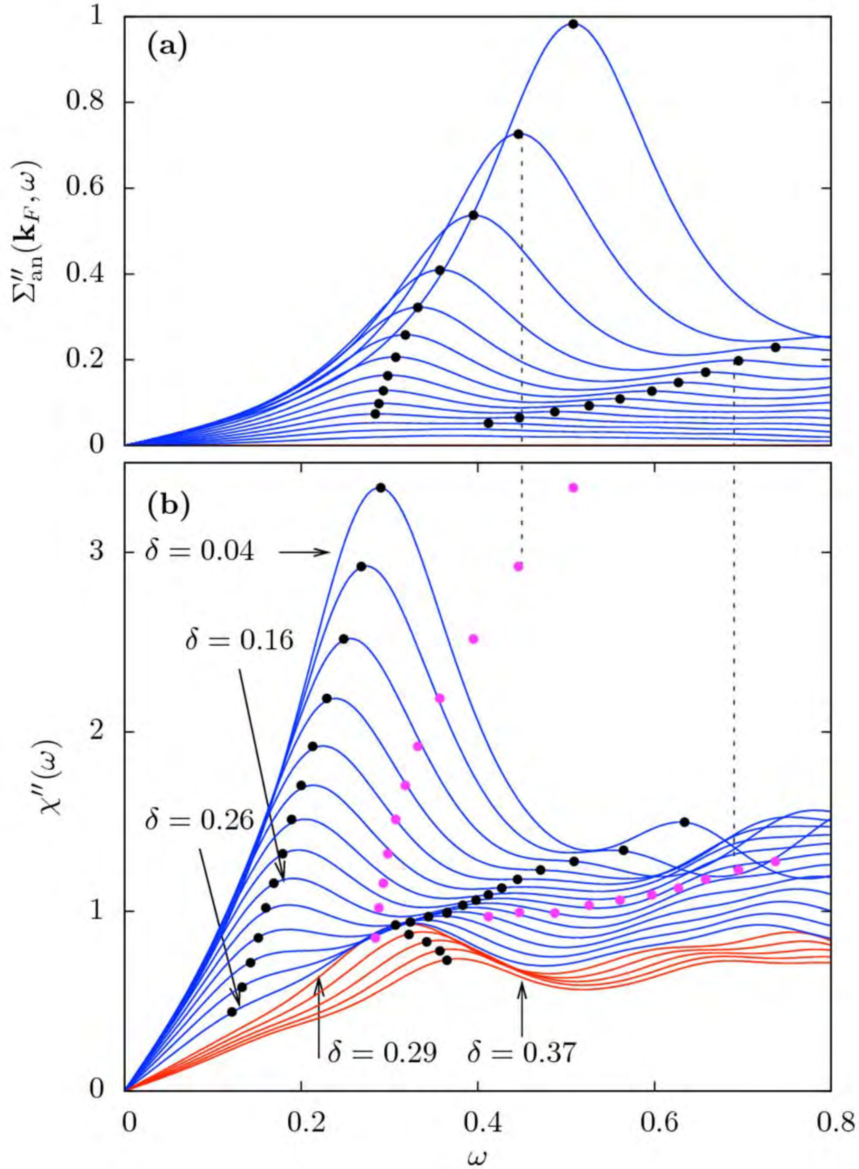
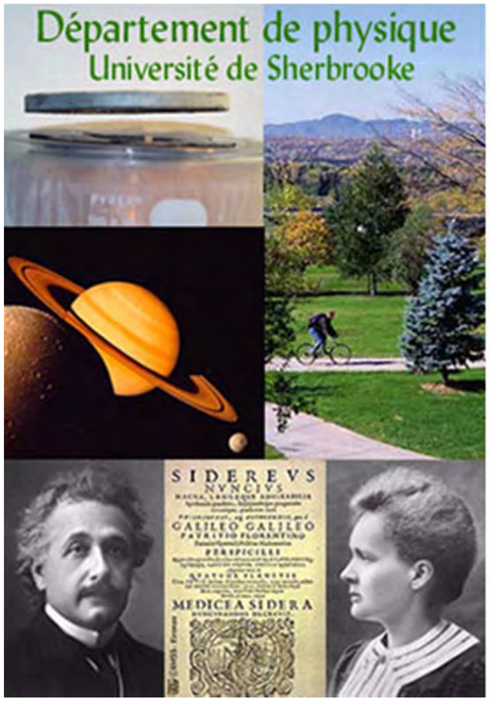
Retardation effects



David Sénéchal



André-Marie Tremblay

CANADA RESEARCH CHAIRS
CHAIRES DE RECHERCHE DU CANADA

RQMP
Le regroupement québécois sur les matériaux de pointe

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Conclusions

- Tools for Hubbard model, high Tc.
- The influence of Mott Physics extends way beyond half-filling
  - Pseudogap as a phase
  - Effects of critical point at high temperature (Widom line)
  - Superconductivity
    - Dome
    - Retardation effects in pairing come from spin fluctuations.

Merci

Thank you