Superconductivity in doped or pressurized insulators : cuprates and organics

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G. Sordi, K. Haule, D. Sénéchal, C.-D. Hébert

P. Sémon, B. Kyung, G. Kotliar,

M. Civelli, S. Kancharla,

CIFAR
CANADIAN INSTITUTE for ADVANCED RESEARCH

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Grenoble, 13 March, 2015

VERITATEM IN CHARITATE

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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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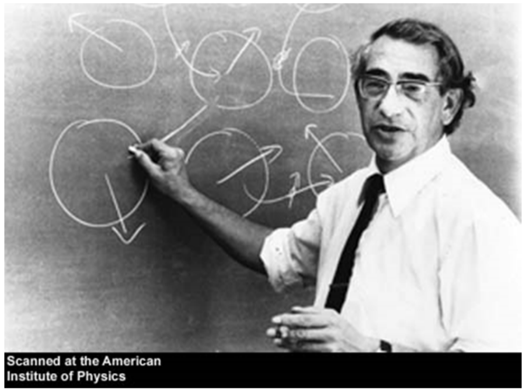
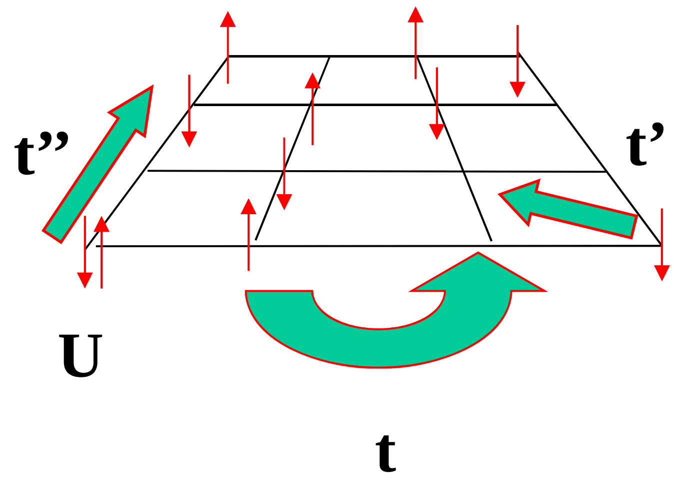
Hubbard model

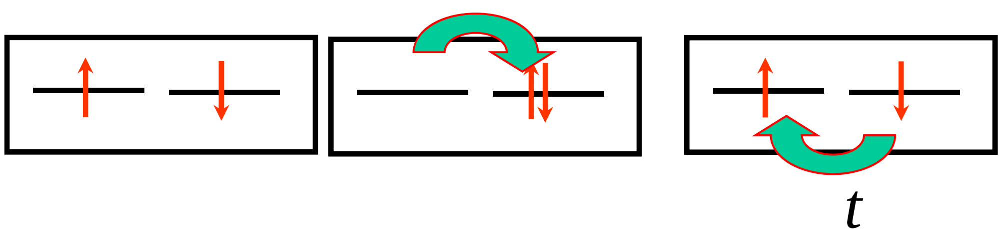


1931-1980

μ



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



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

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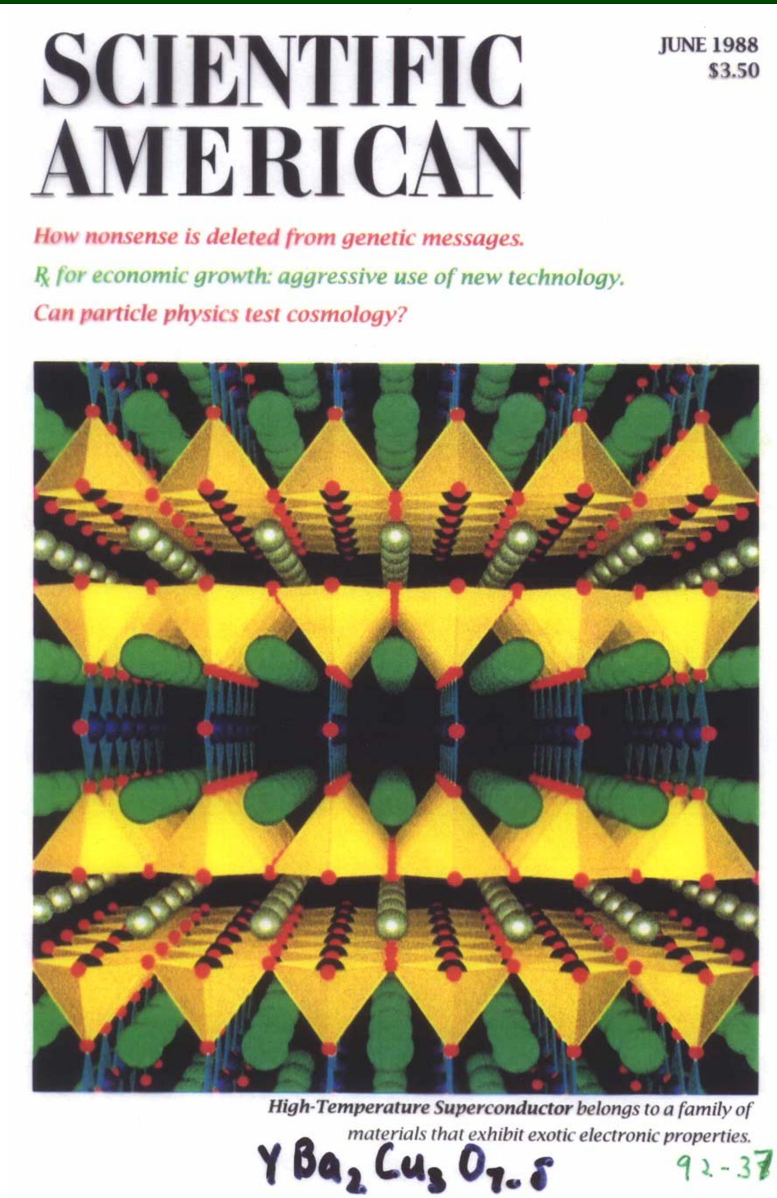
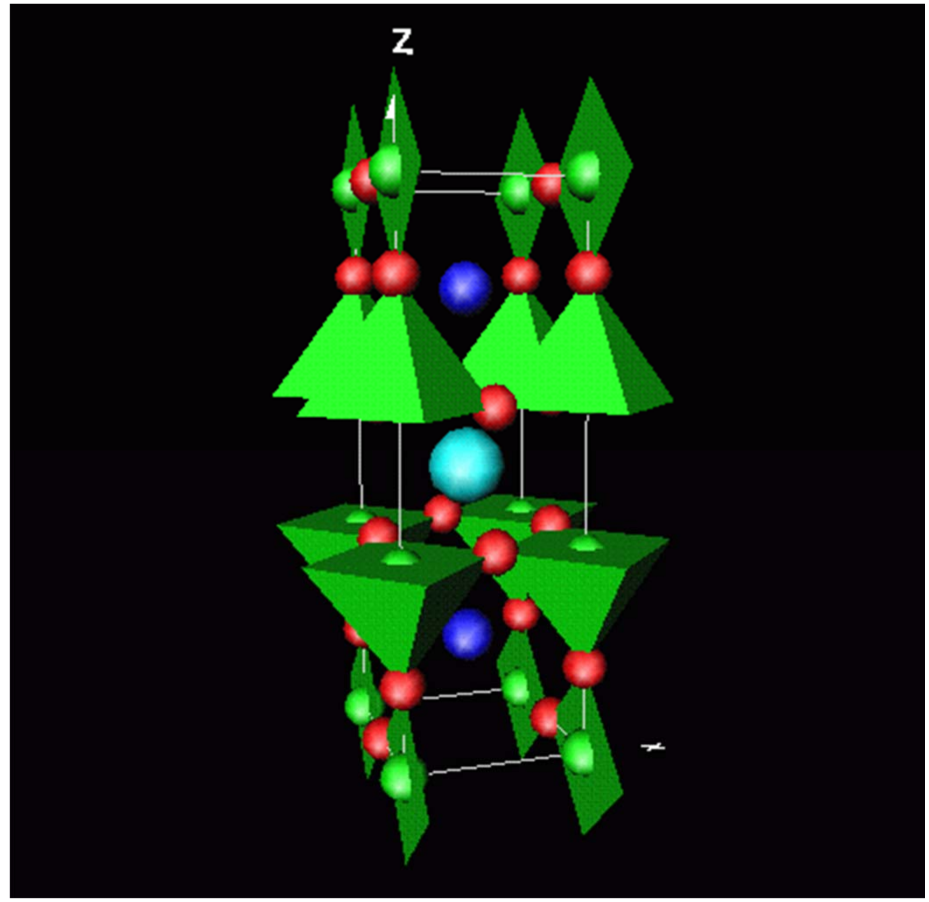
Superconductivity and attraction?

Cuprates



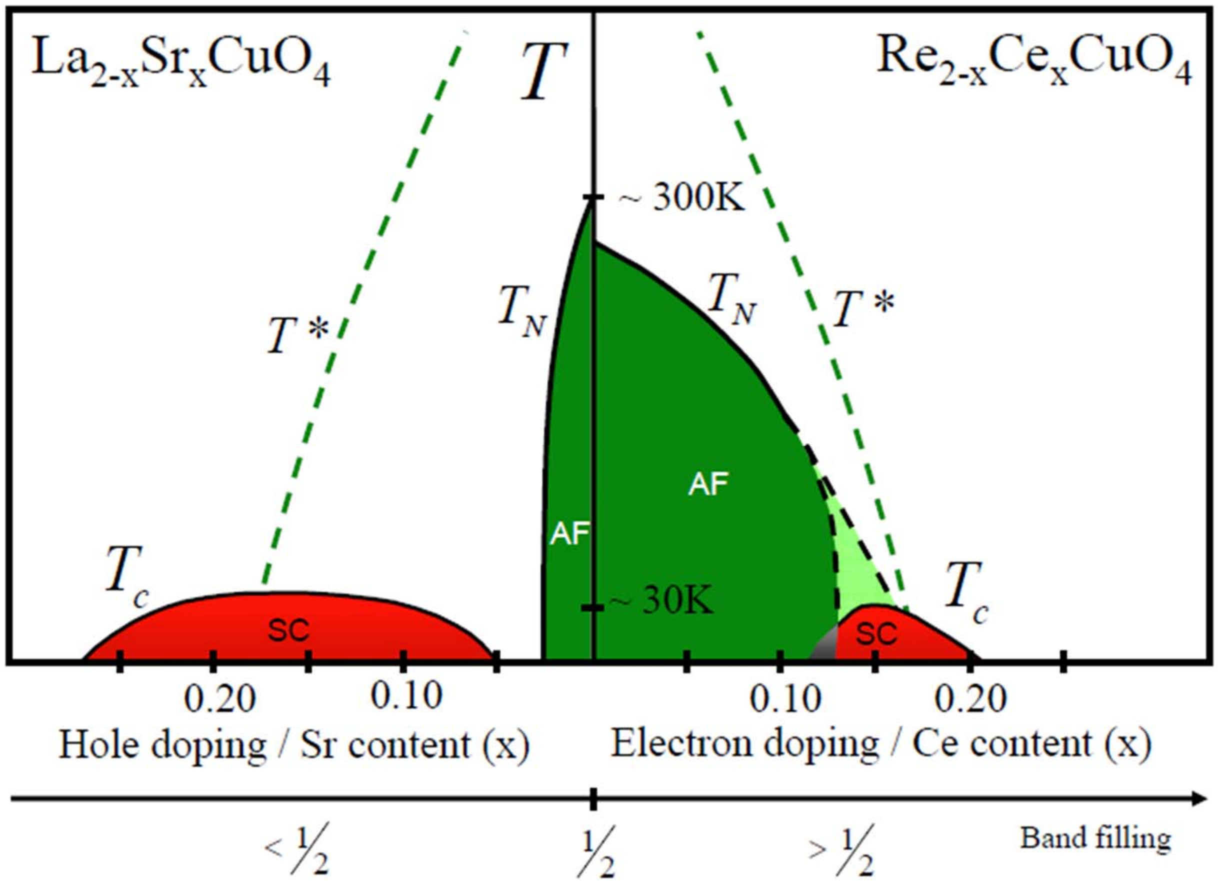
SCIENTIFIC AMERICAN
JUNE 1988
$3.50
How nonsense is deleted from genetic messages.
Rx for economic growth: aggressive use of new technology.
Can particle physics test cosmology?
High-Temperature Superconductor belongs to a family of materials that exhibit exotic electronic properties.
Y Ba2 Cu3 O7-δ
92-37



z

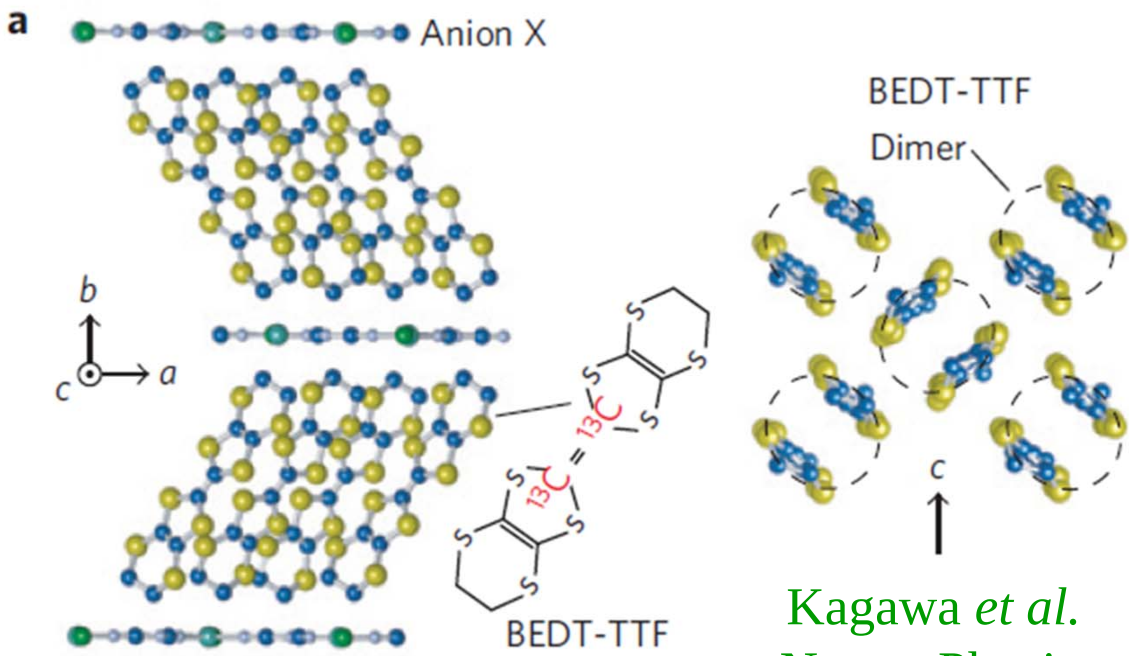
High-temperature superconductors

Armitage, Fournier, Greene, RMP (2009)

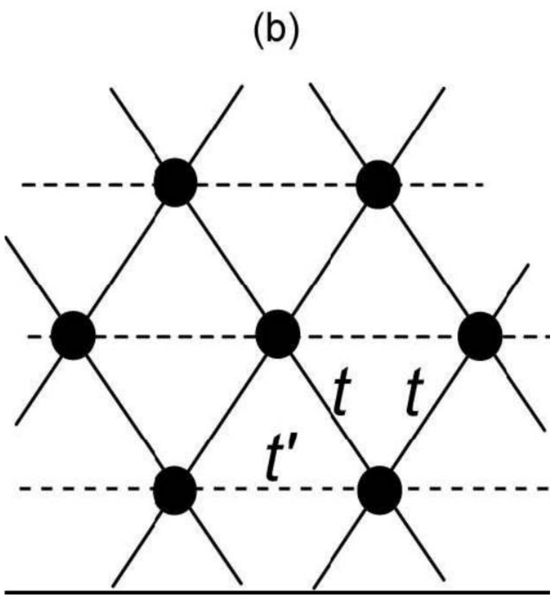


Hubbard on anisotropic triangular lattice

H. Kino + H. Fukuyama, J. Phys. Soc. Jpn **65** 2158 (1996),
R.H. McKenzie, Comments Condens Mat Phys. **18**, 309 (1998)



Kagawa *et al.* Nature Physics **5,** 880 (2009)



n=1, varying *t'/t*

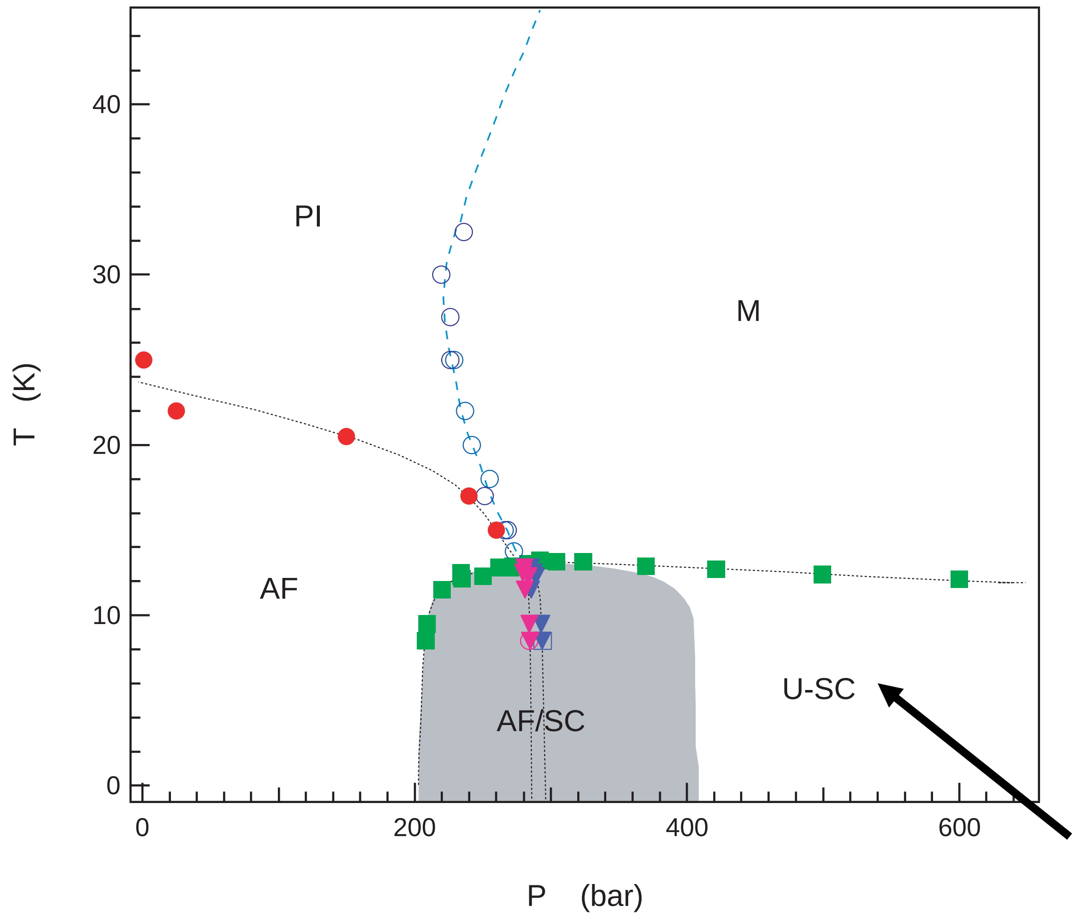
$$H = \sum_{ij\sigma} (t_{ij} - \delta_{ij}\mu) c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

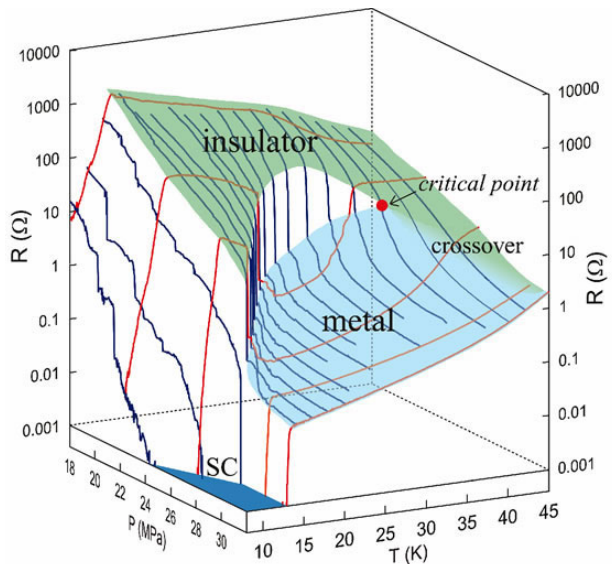
$t \approx 50\,\mathrm{meV}$

$\Rightarrow U \approx 400\,\mathrm{meV}$

t'/t ~ 0.6 - 1.1

Phase diagram for organics





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

B_g for C_{2h} and B_{2g} for D_{2h}

Powell, McKenzie cond-mat/0607078

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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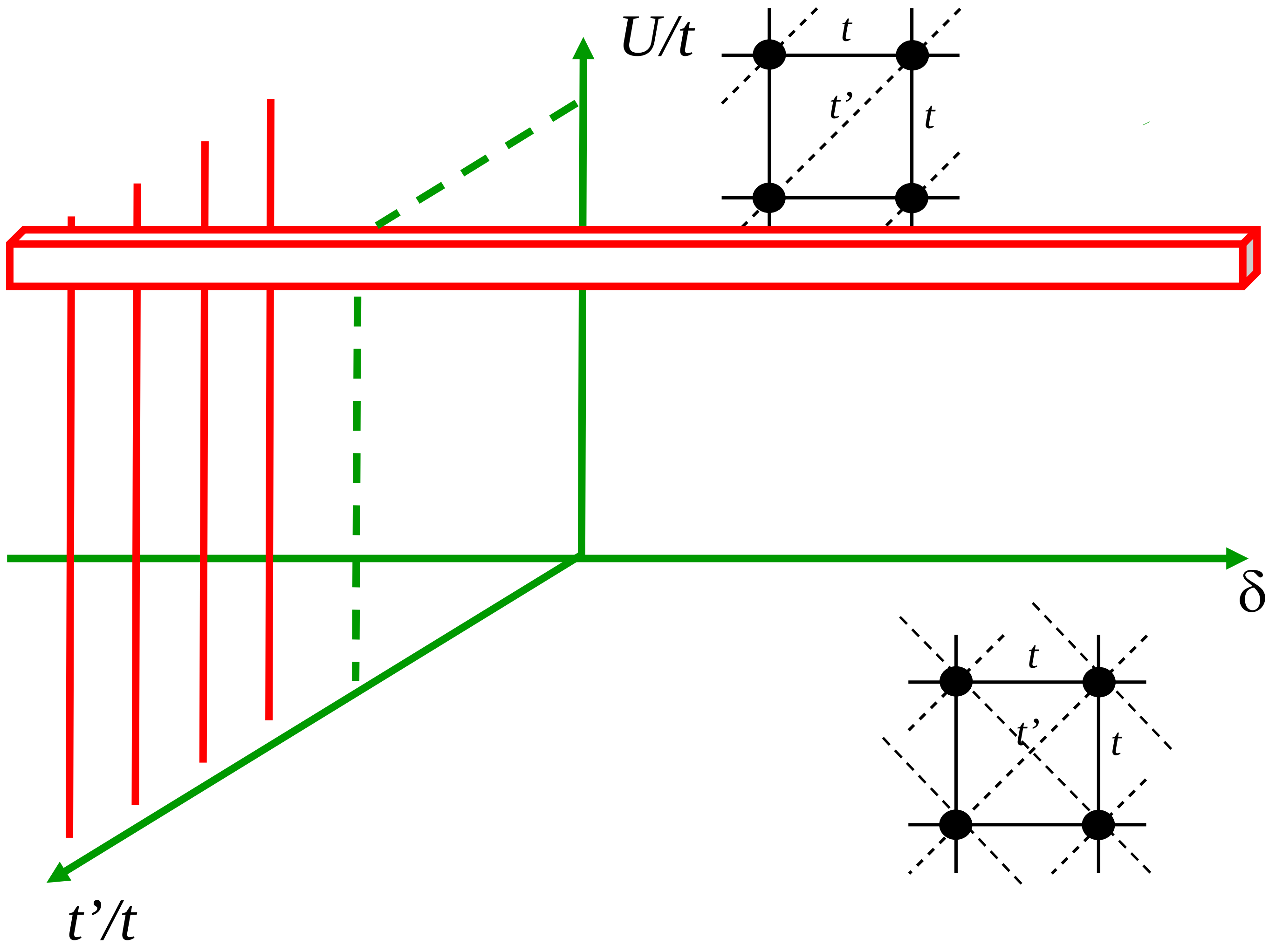
Perspective



Outline

- Method
- $T=0$ phase diagram
- Finite T phase diagram
  - Normal state
    - First order transition
    - Widom line and pseudogap
  - Superconductivity

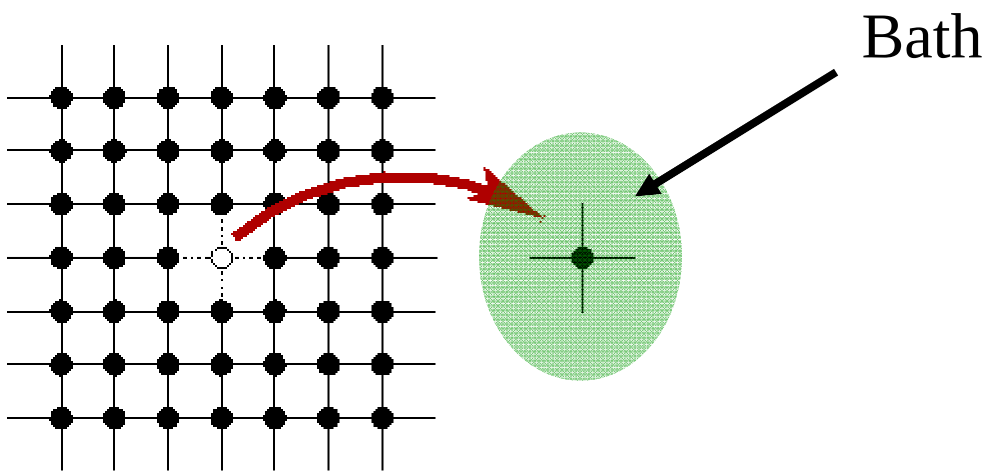
Method

"The effect of concept-driven revolution is to explain old things in new ways. The effect of tool-driven revolution is to discover new things that have to be explained."

Freeman Dyson *Imagined Worlds*

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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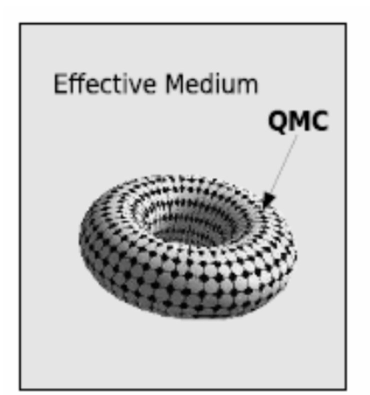
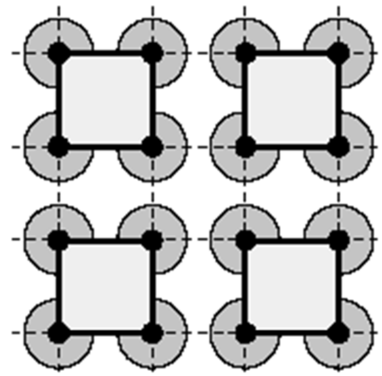
2d Hubbard: Quantum cluster method

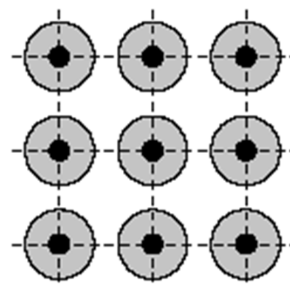


DCA

C-DMFT



DMFT



Hettler …Jarrell…Krishnamurty PRB **58** (1998)
Kotliar et al. PRL **87** (2001)
M. Potthoff *et al.* PRL **91,** 206402 (2003).

REVIEWS

Maier, Jarrell et al., RMP. (2005)
Kotliar *et al.* RMP (2006)
AMST *et al.* LTP (2006)

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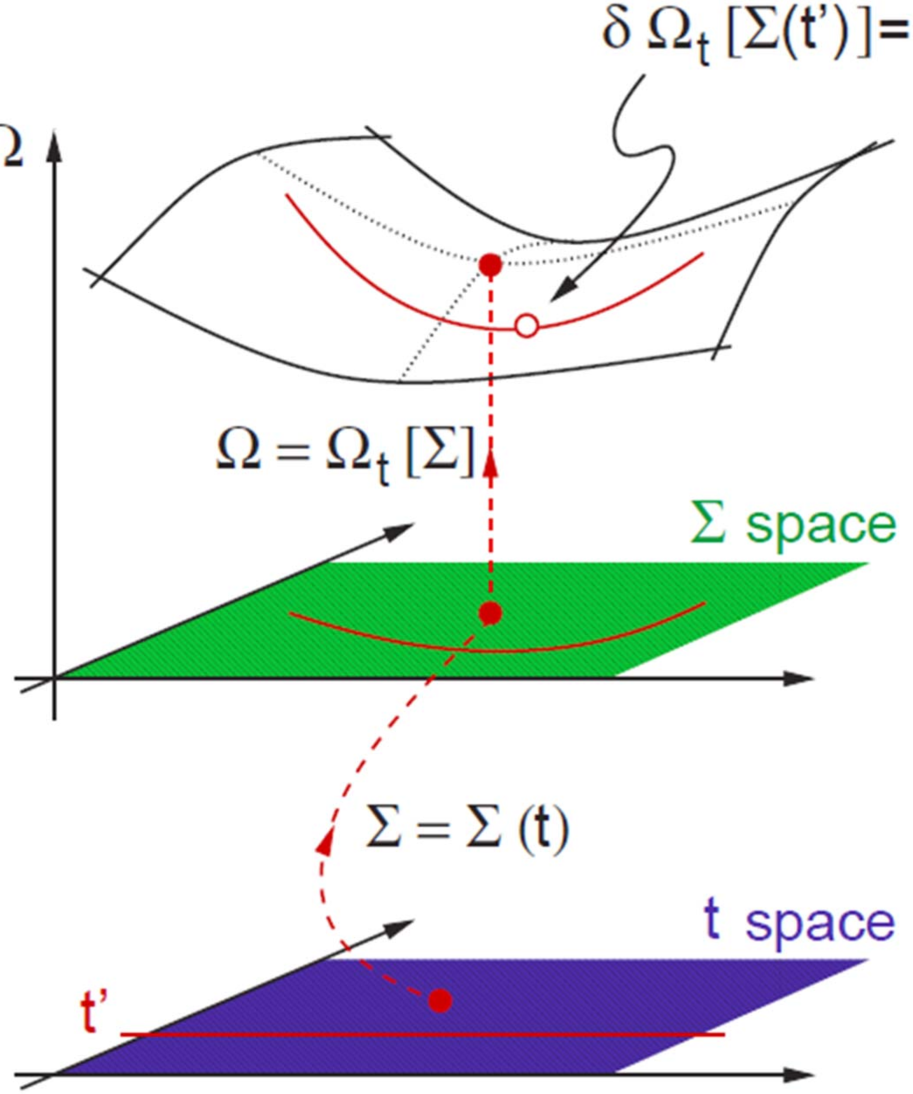
DMFT as a stationnary point



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

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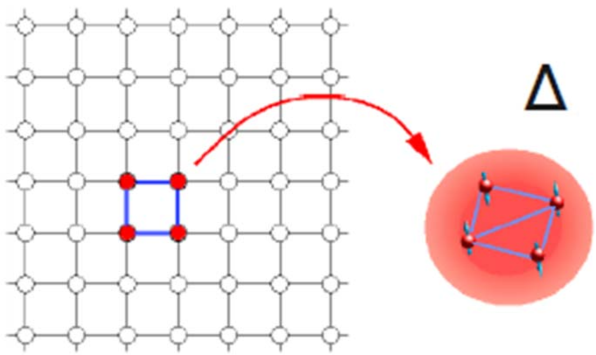
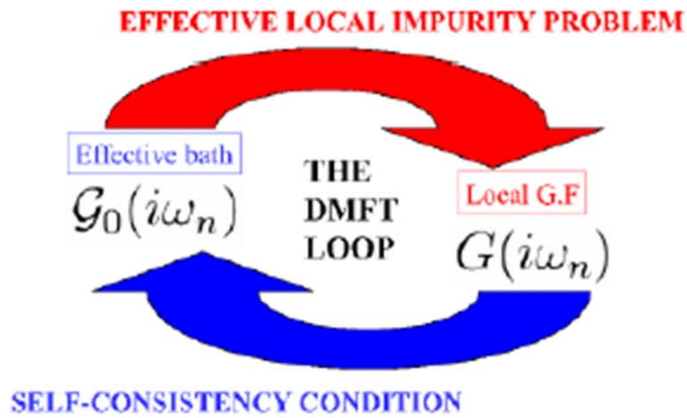
+ and -

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

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

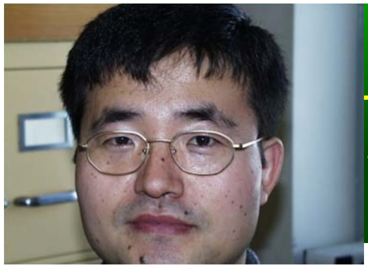
Why important

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

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

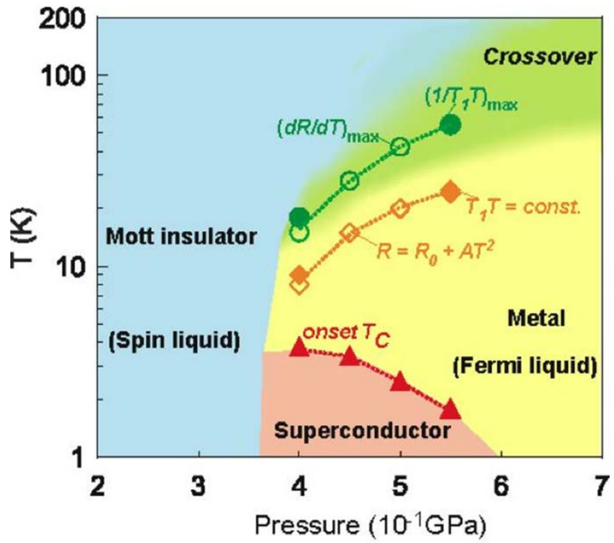
Phase diagram

Exact diagonalization as impurity solver (T=0).



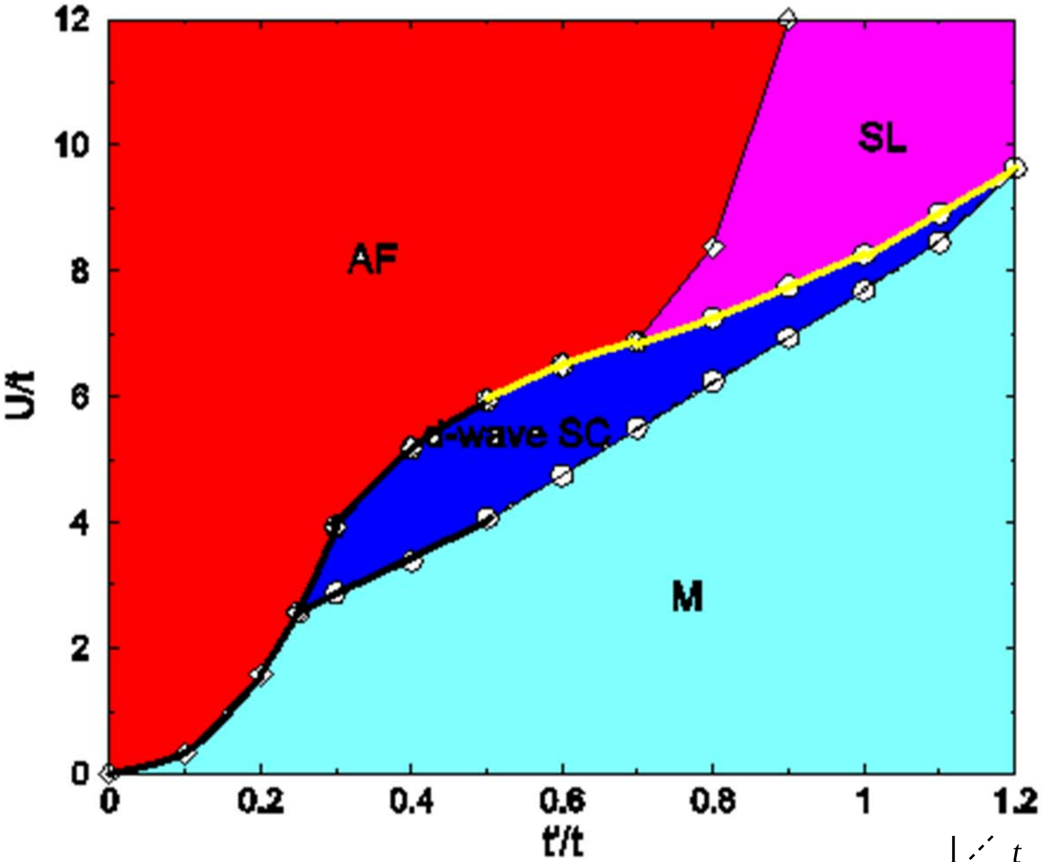
Theoretical phase diagram BEDT

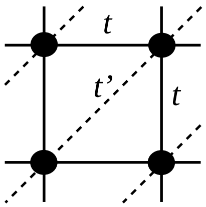
X= $Cu_2(CN)_3$ (t'~ t)



Y. Kurisaki, et al.

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





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

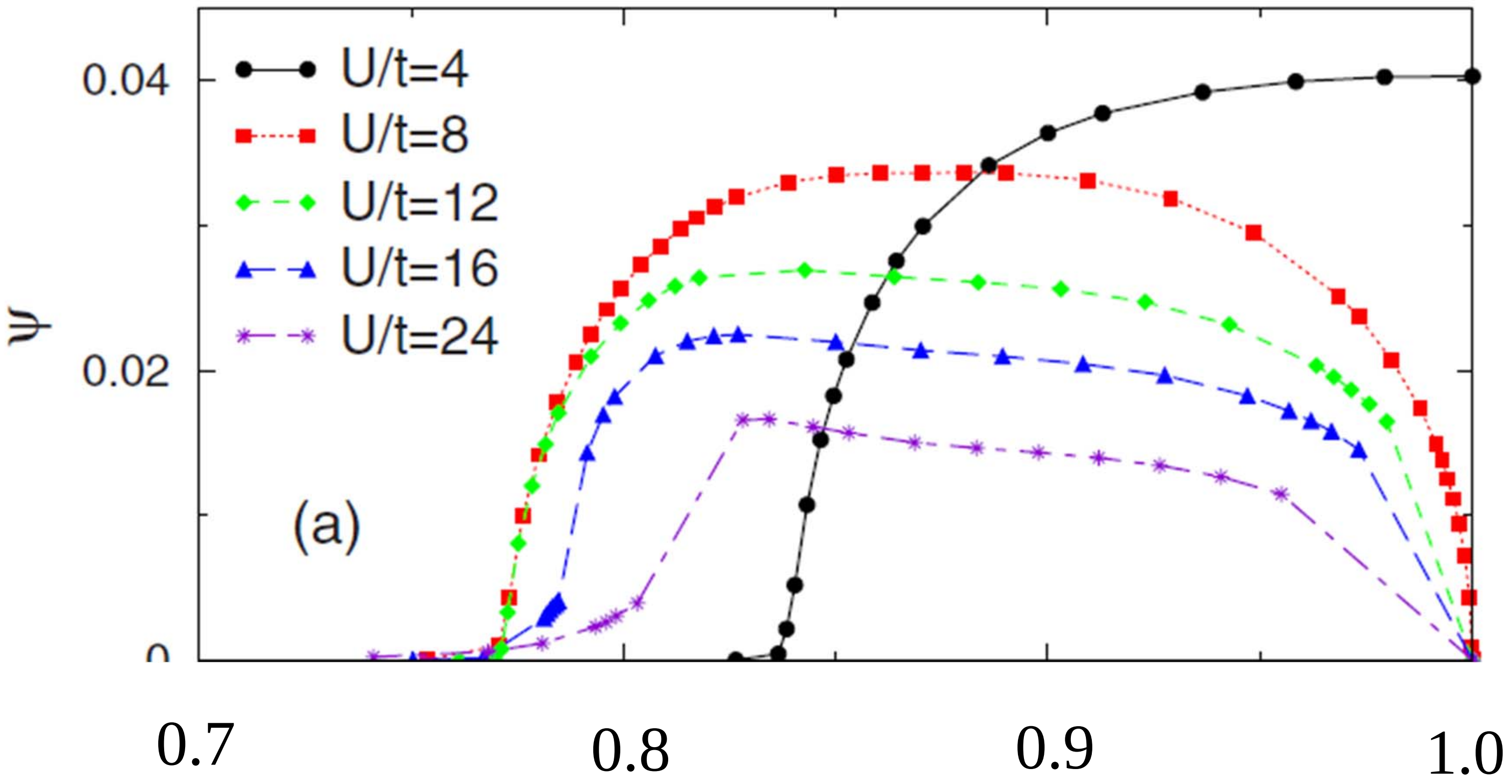
Y. Shimizu, et al. Phys. Rev. Lett. **91**, (2003)

T = 0 phase diagram: cuprates

Phase diagram

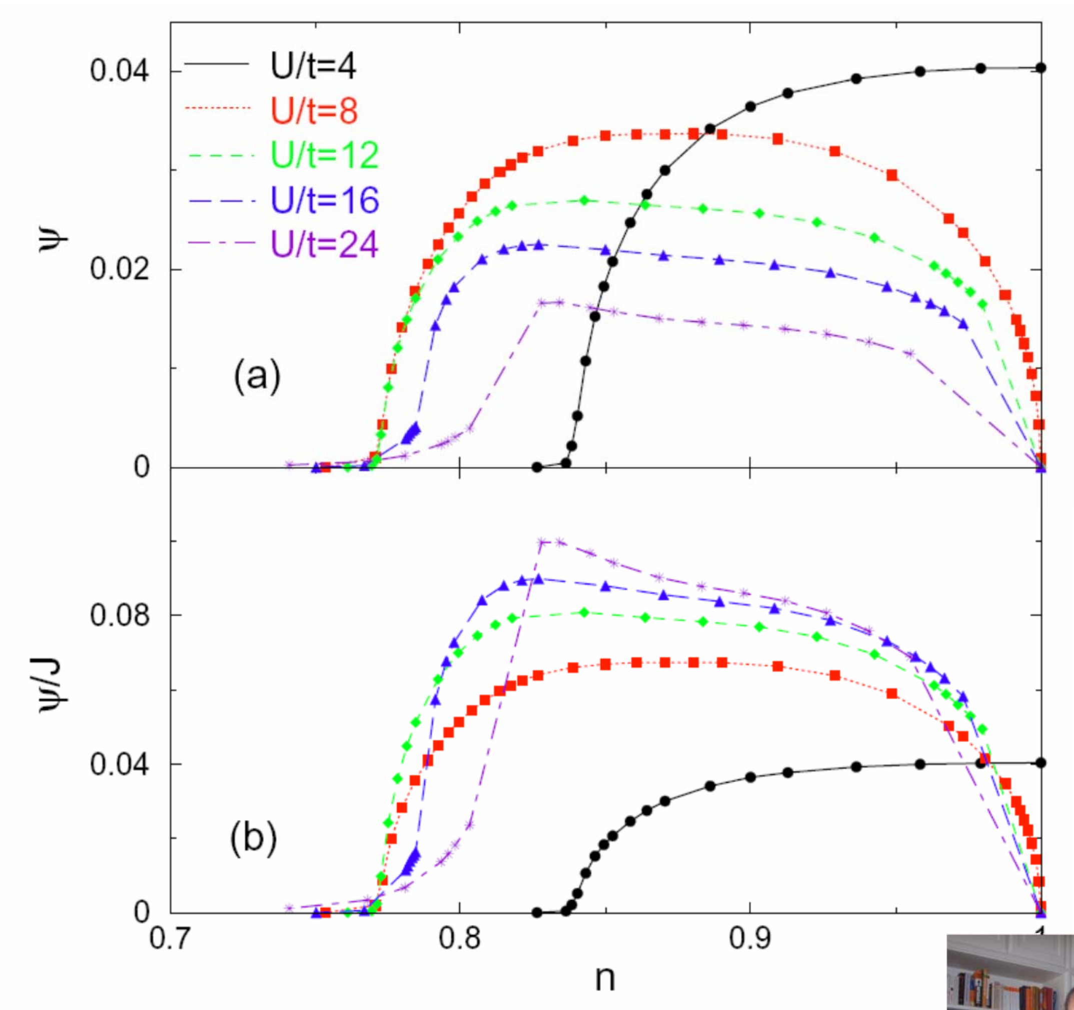
Exact diagonalization as impurity solver (*T=0*).

Theory: T_c down vs Mott

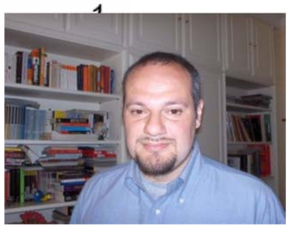


S. Kancharla *et al.* Phys. Rev. B (2008)

Dome vs Mott (CDMFT)



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



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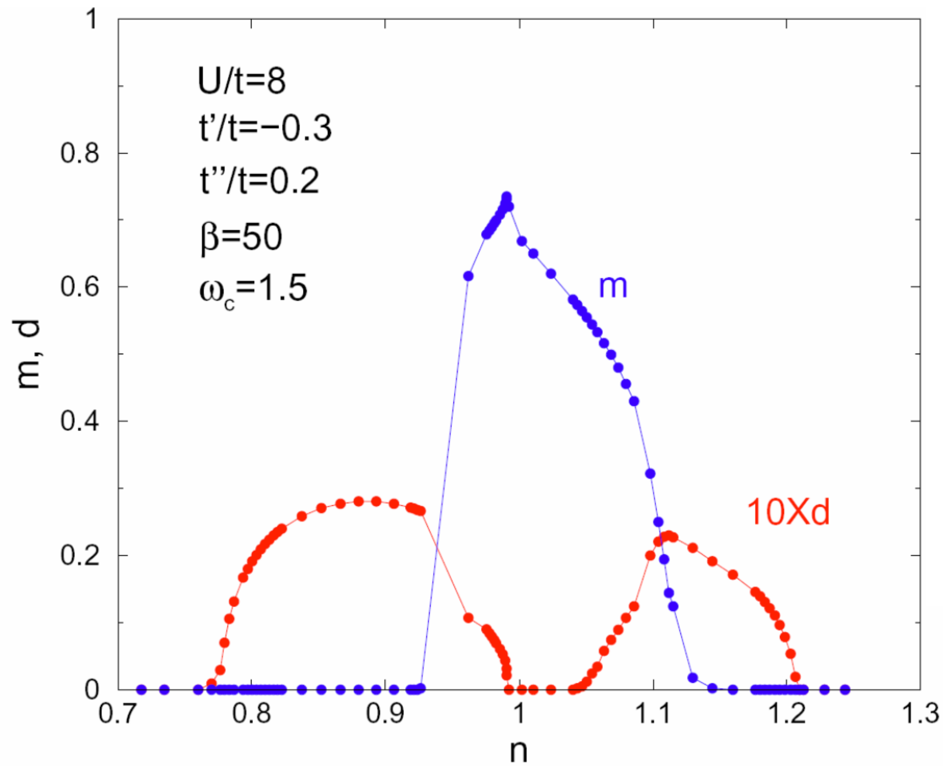
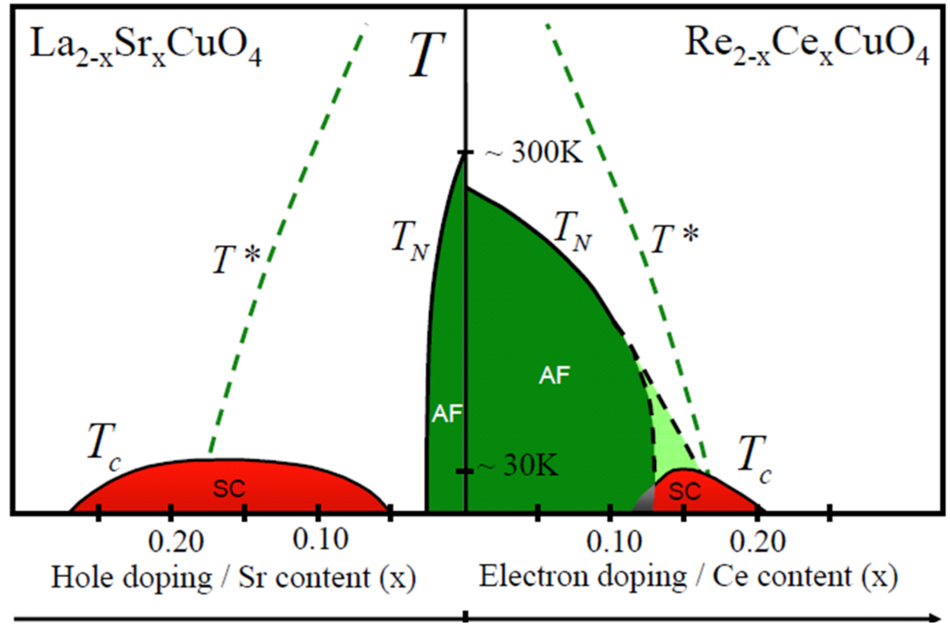
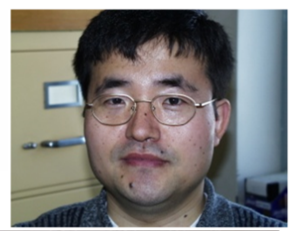
CDMFT global phase diagram



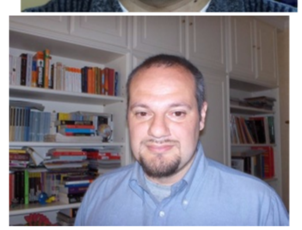
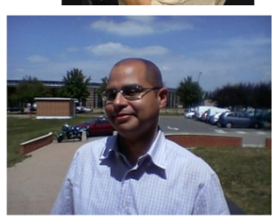
Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008)
AND Capone, Kotliar PRL (2006)



Armitage, Fournier, Greene, RMP (2009)





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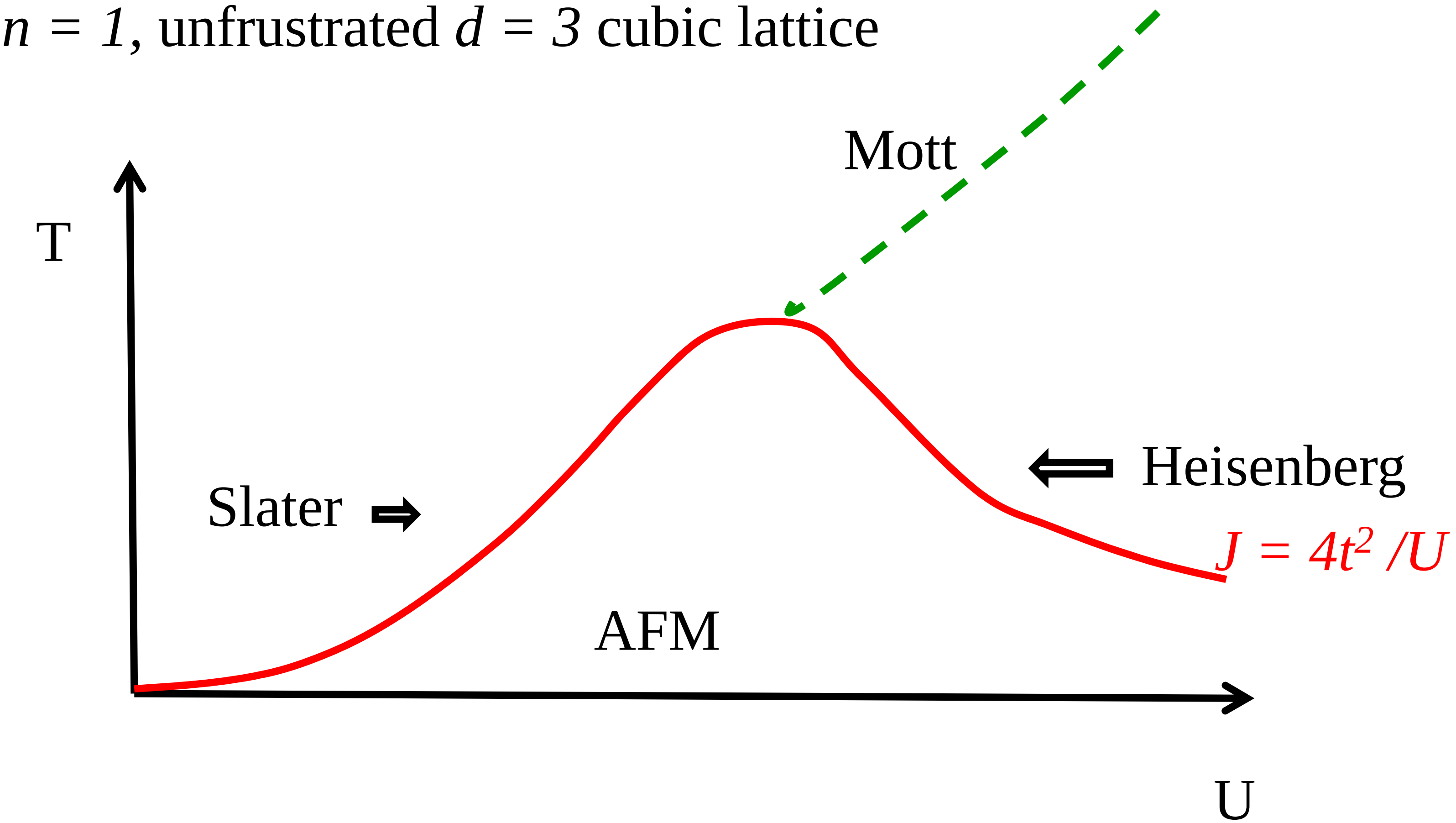
Finite *T* phase diagram

Normal state of the cuprates

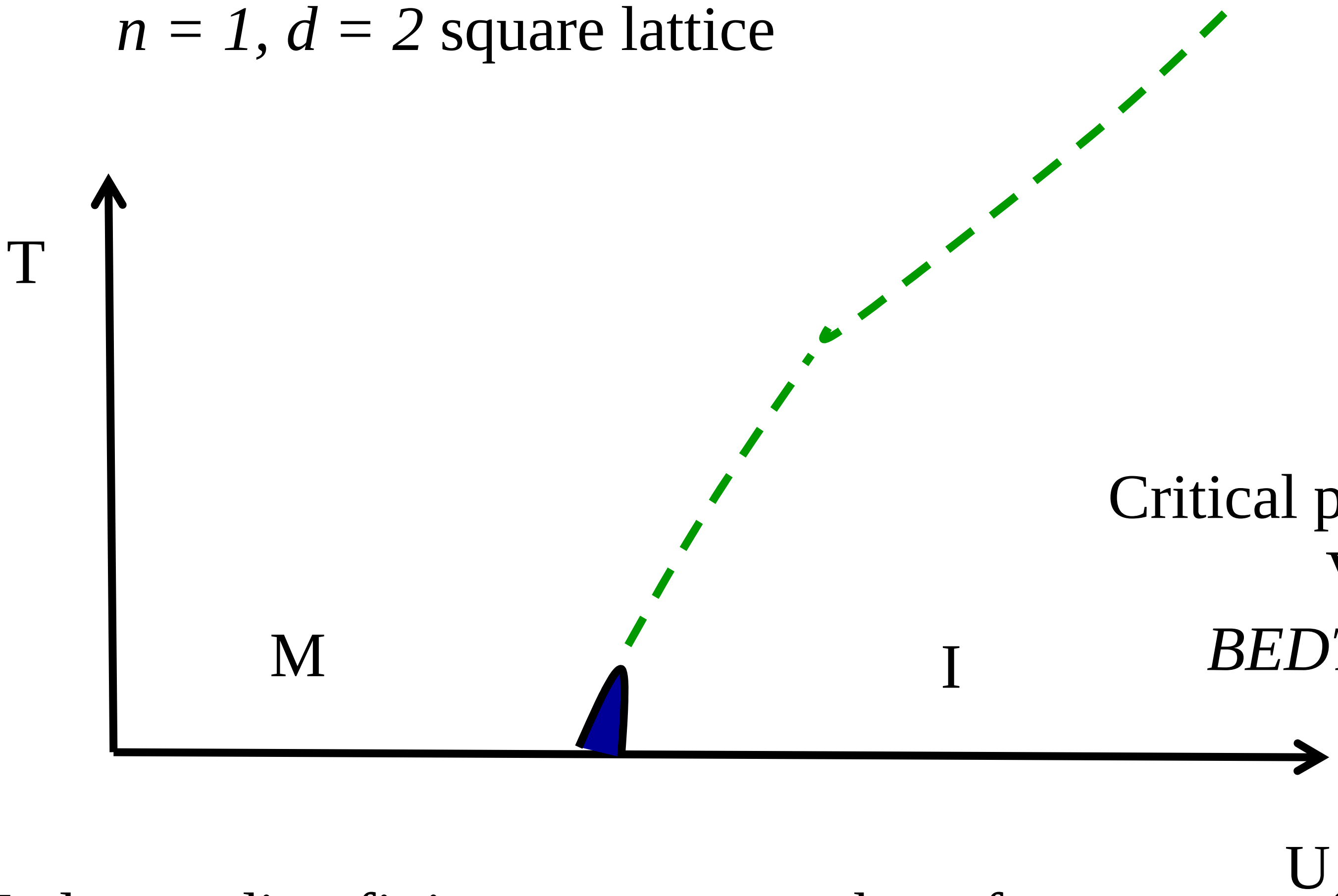
Preliminary: Weak vs Strong correlations

$n = 1$, unfrustrated $d = 3$ cubic lattice



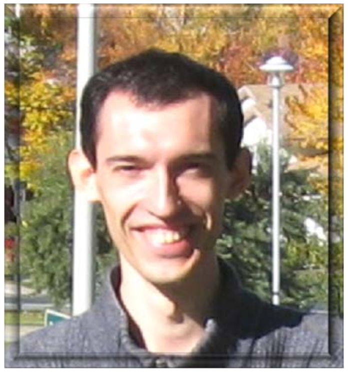
Local moment and Mott transition

n = 1, d = 2 square lattice



Critical point visible in V_2O_3, *BEDT* organics

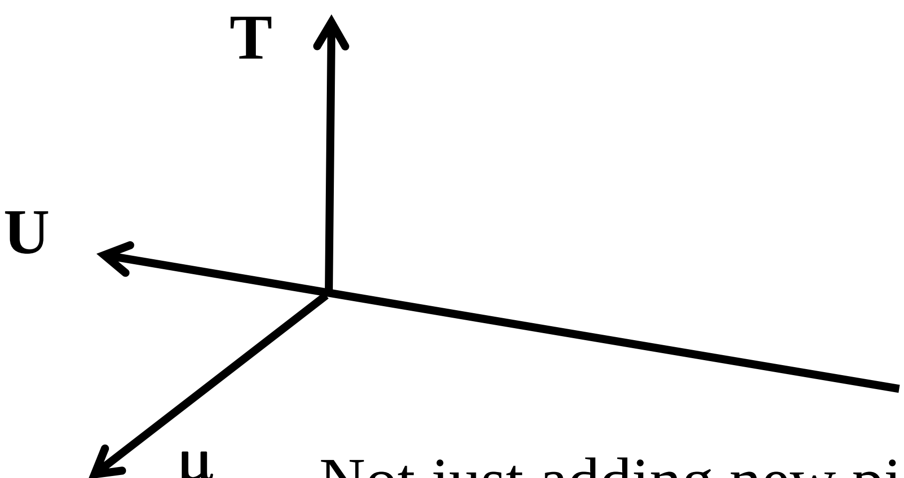
Understanding finite temperature phase from a *mean-field theory* down to *T = 0*



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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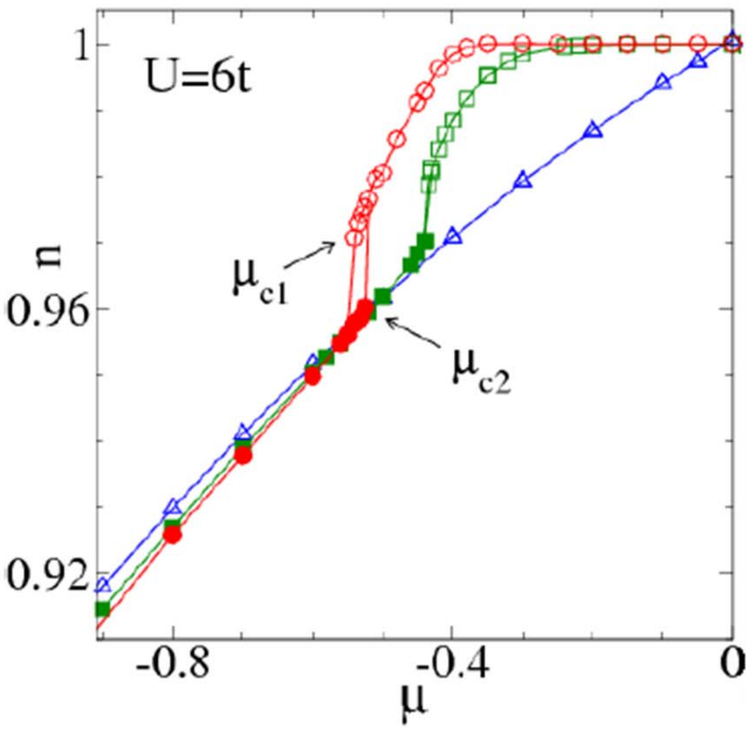
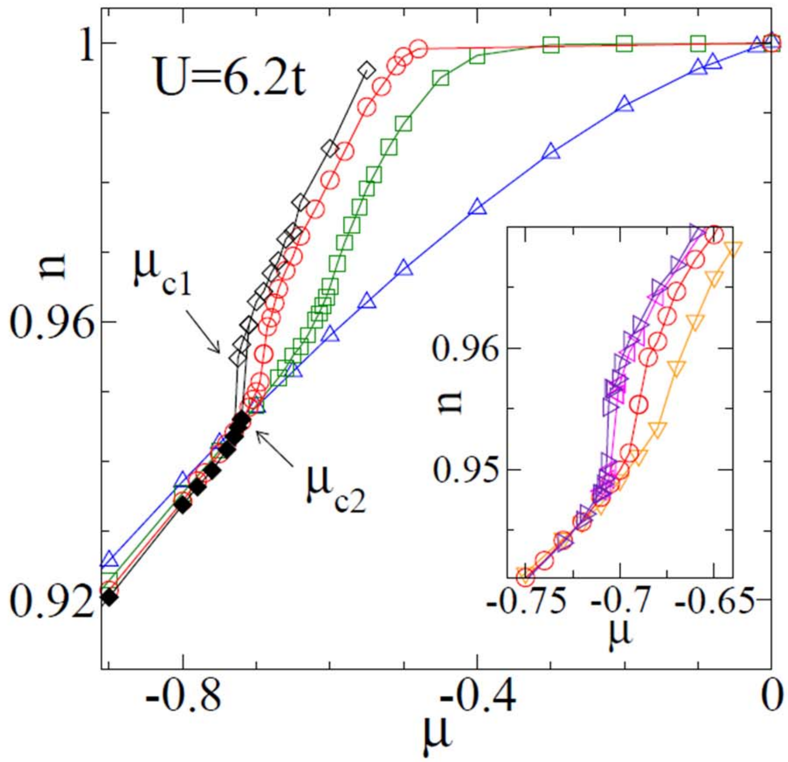
First order transition at finite doping

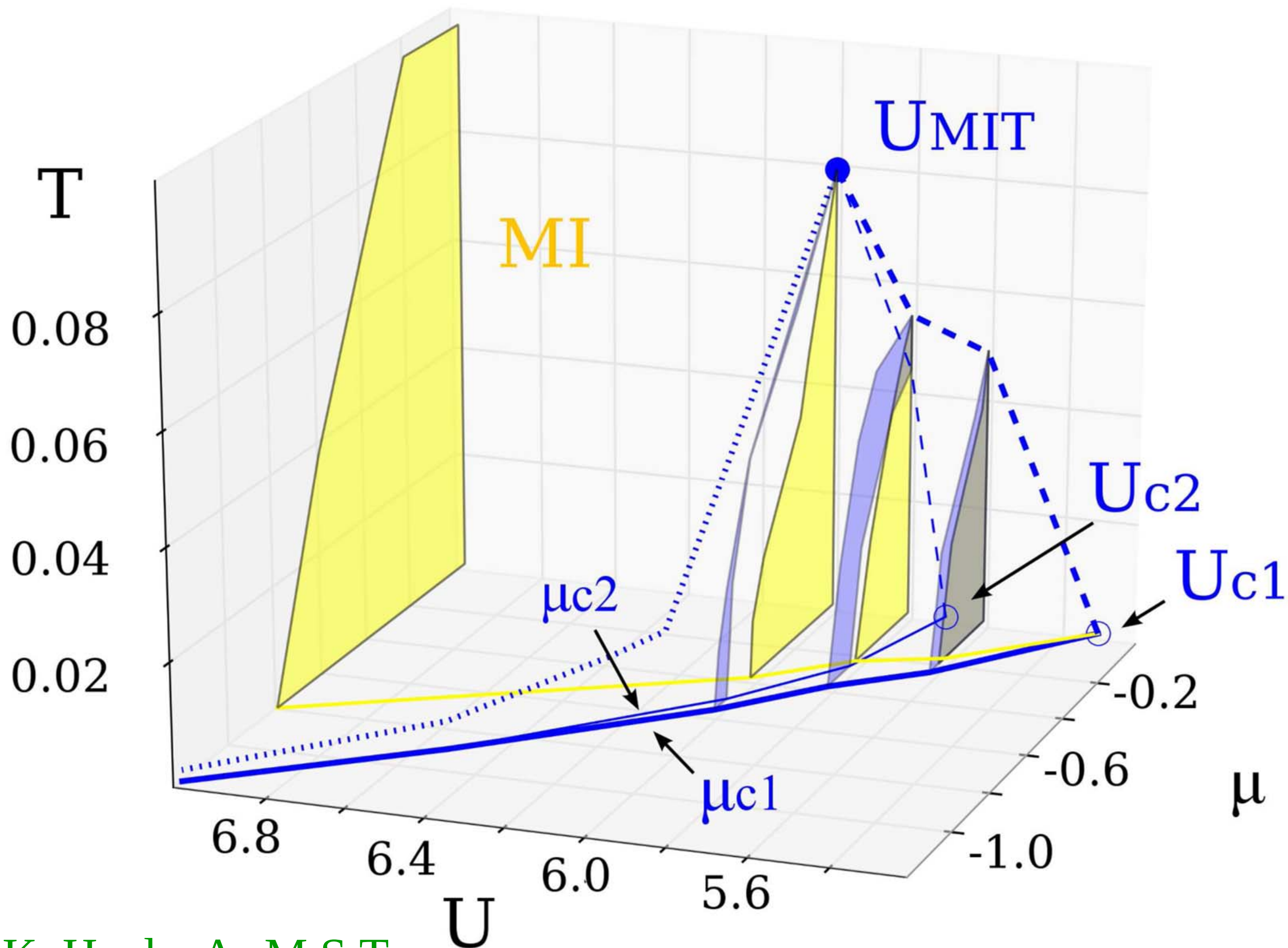


$n(\mu)$ for several temperatures:
$T/t =$1/10, 1/25, 1/50

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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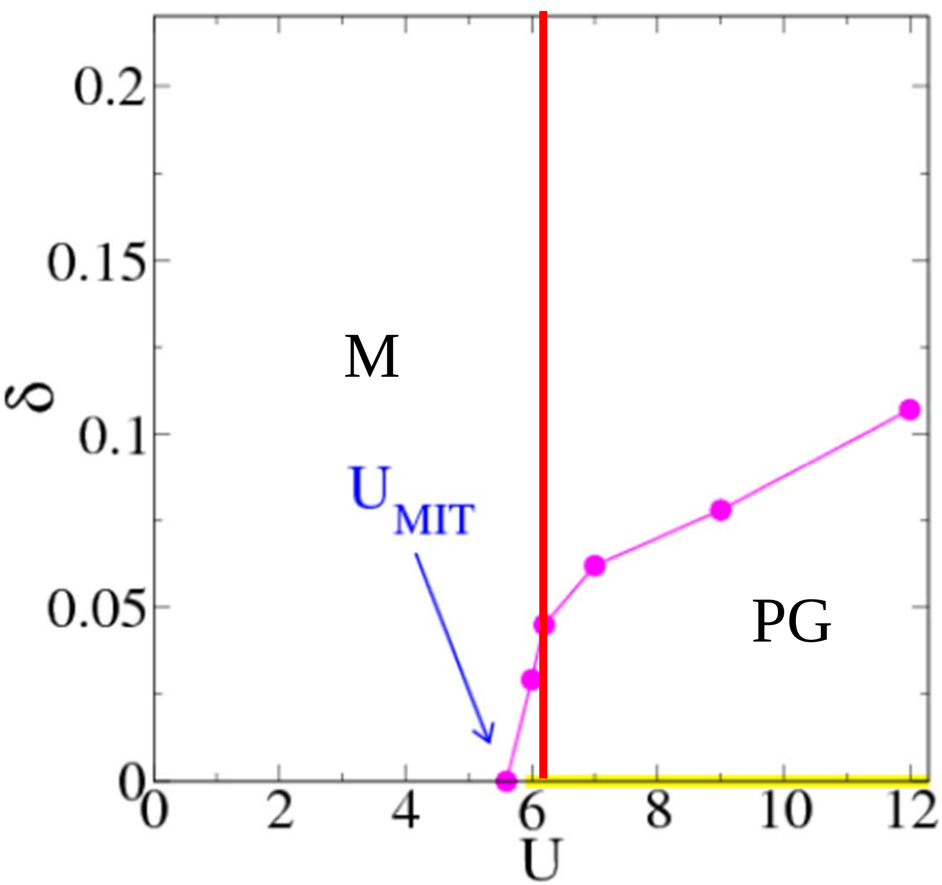
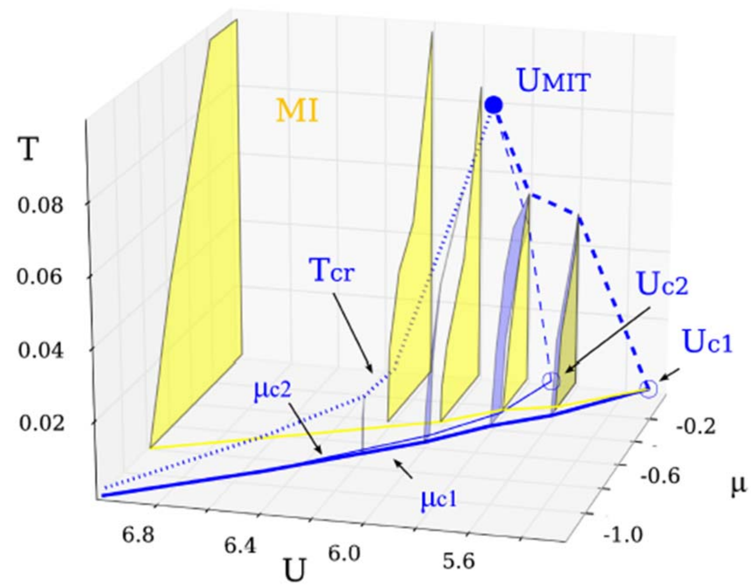
Link to Mott transition up to optimal doping

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



Smaller *D* and *S*



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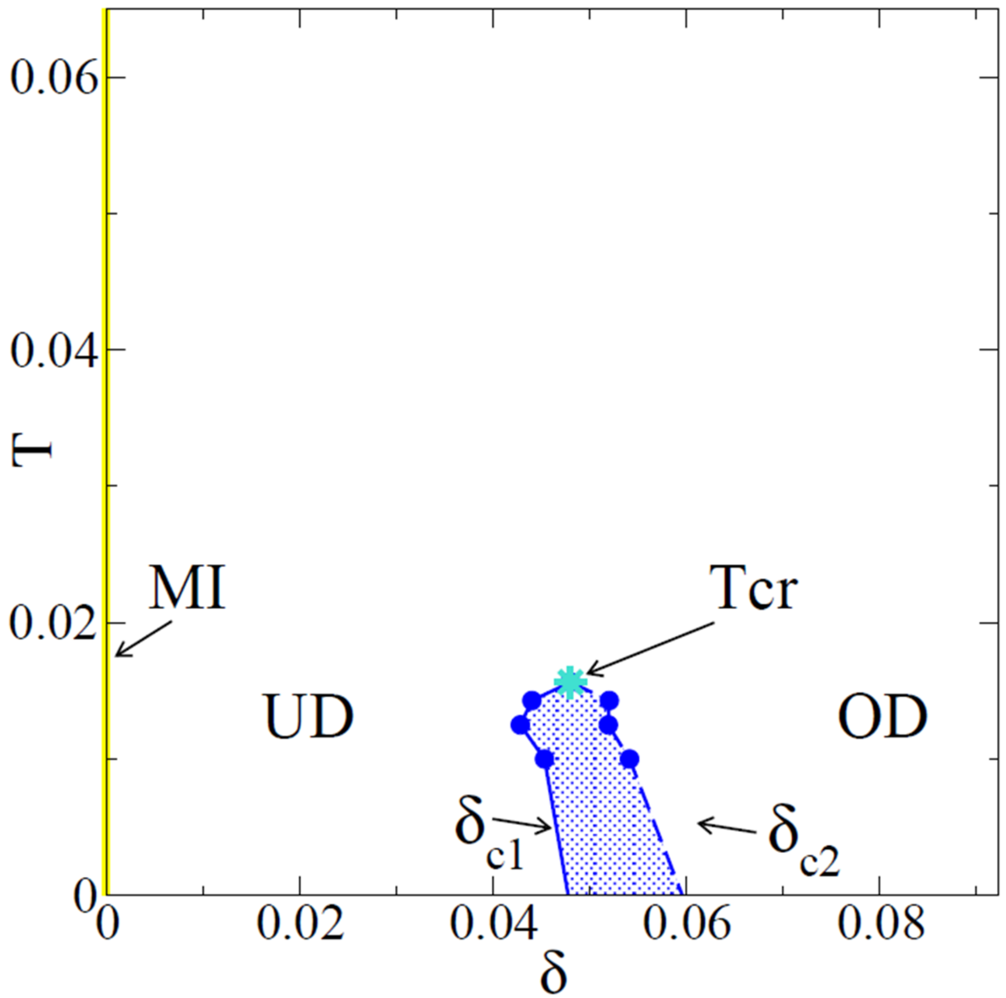
Characterisation of the phases (U=6.2t)



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

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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Giovanni Sordi

Patrick Sémon

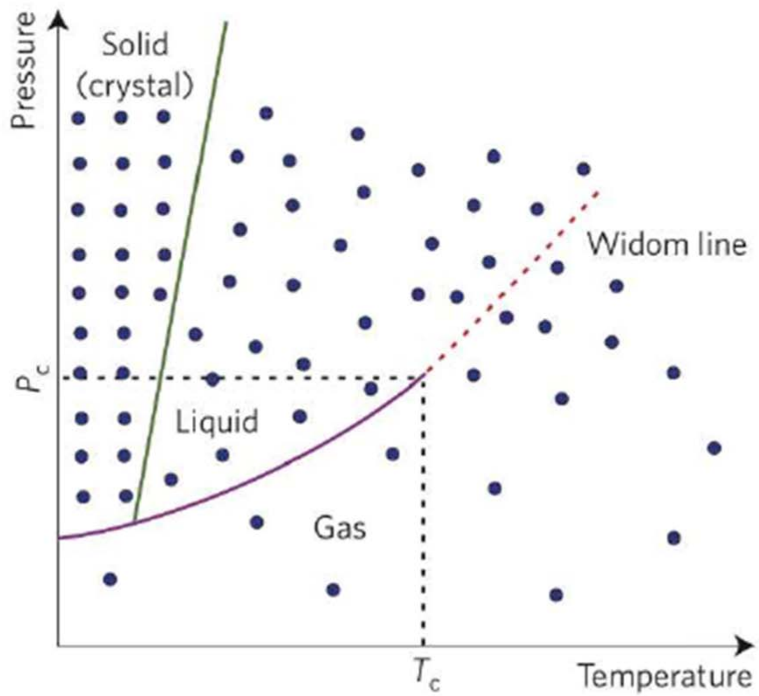
Kristjan Haul

Widom line *(t' = 0)*

Pseudogap in the normal state and the Widom line

Université de Sherbrooke

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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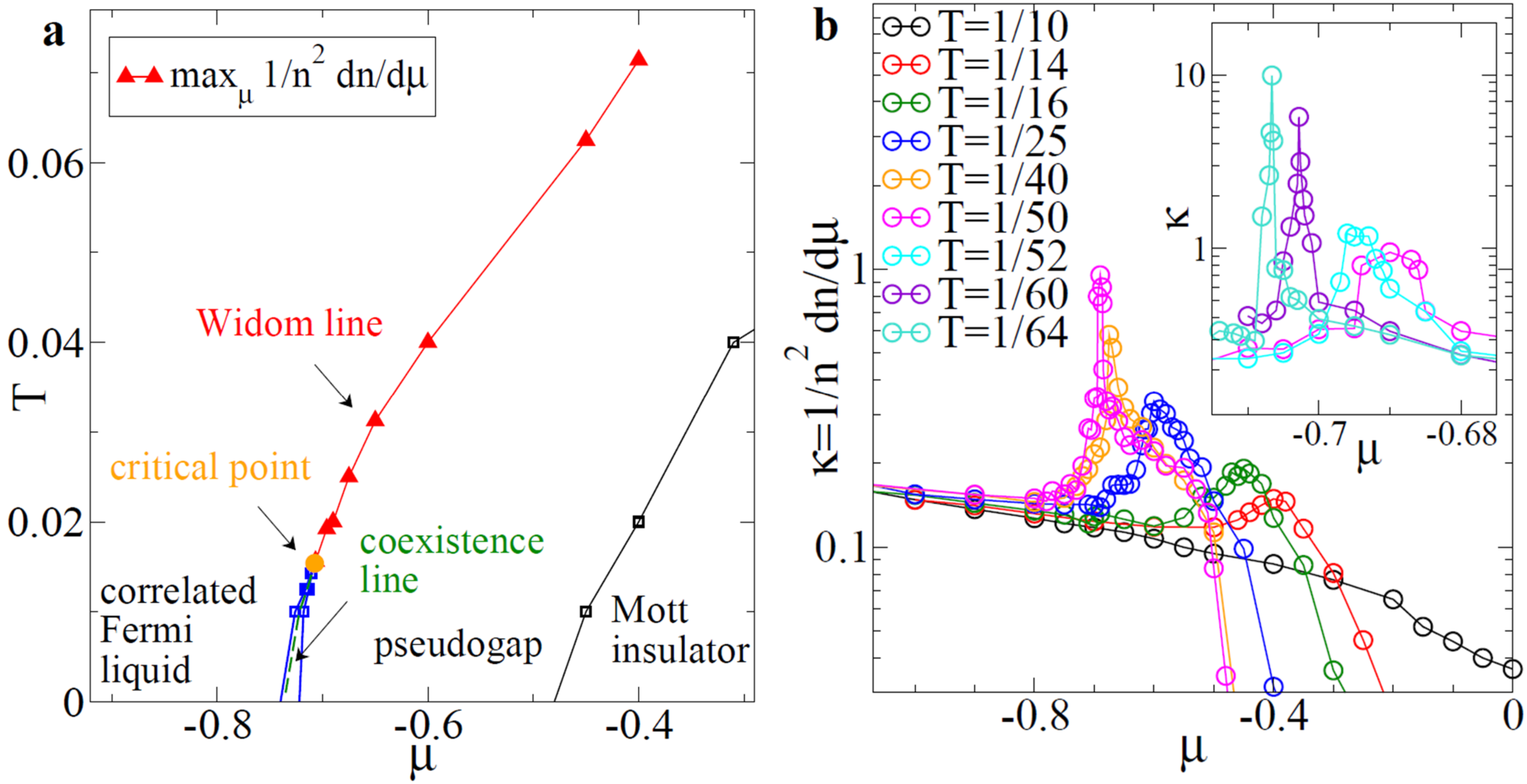
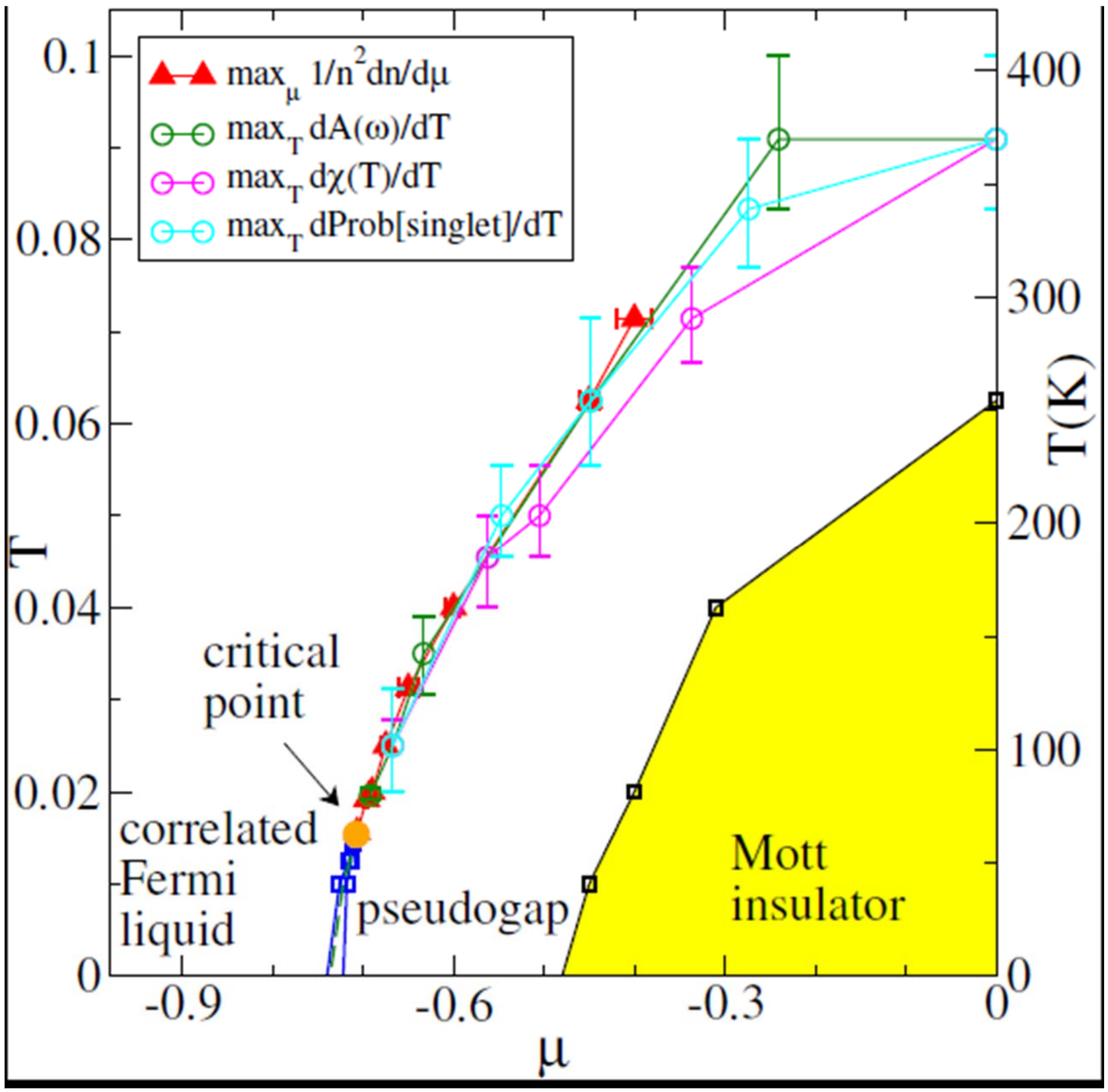
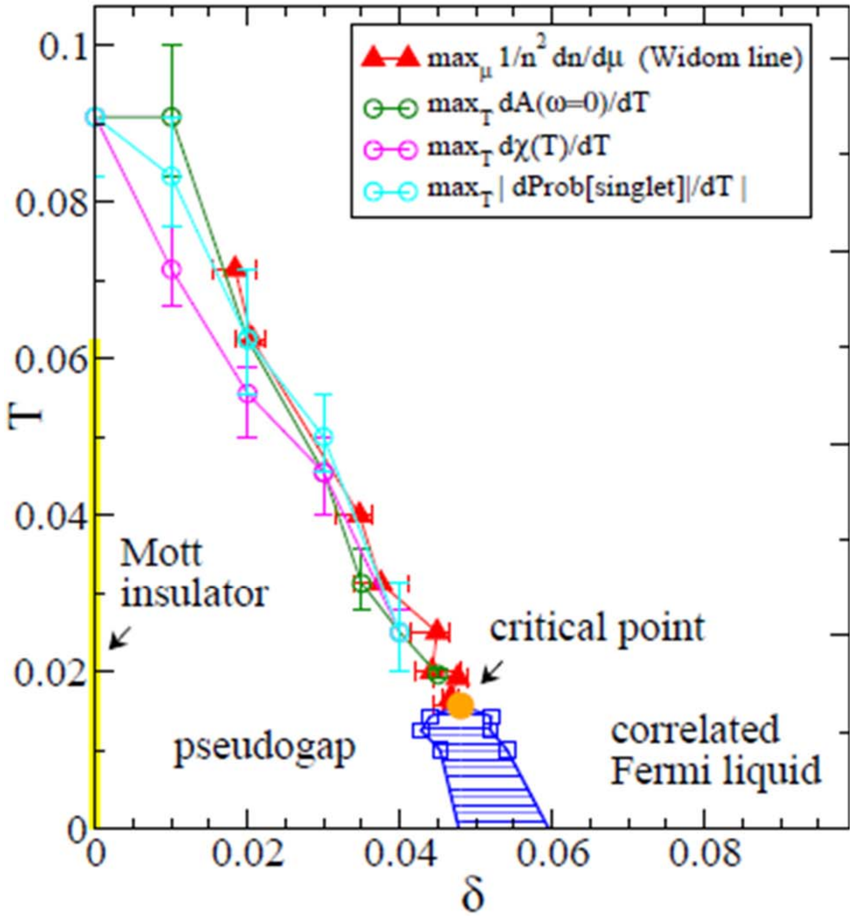
The Widom line

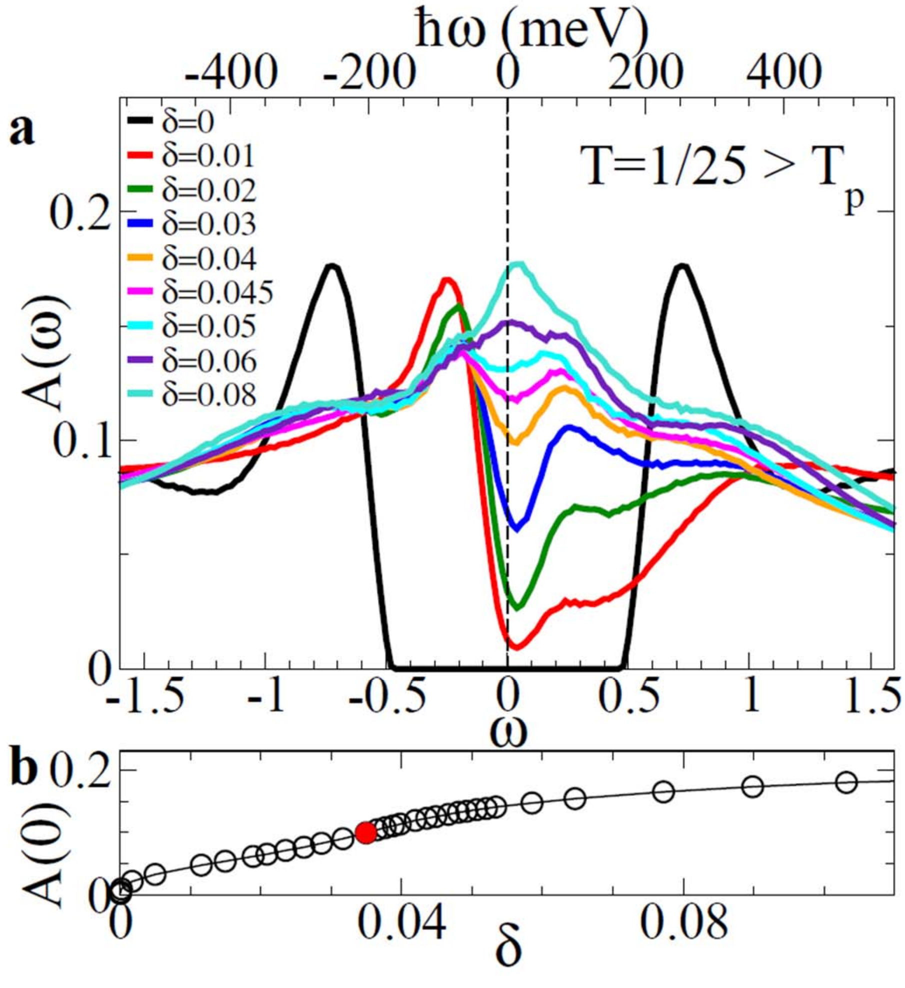


Rapid change also in dynamical quantities

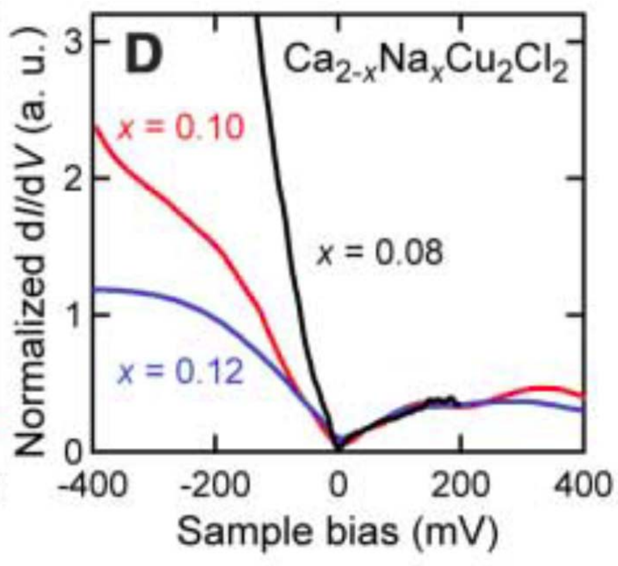


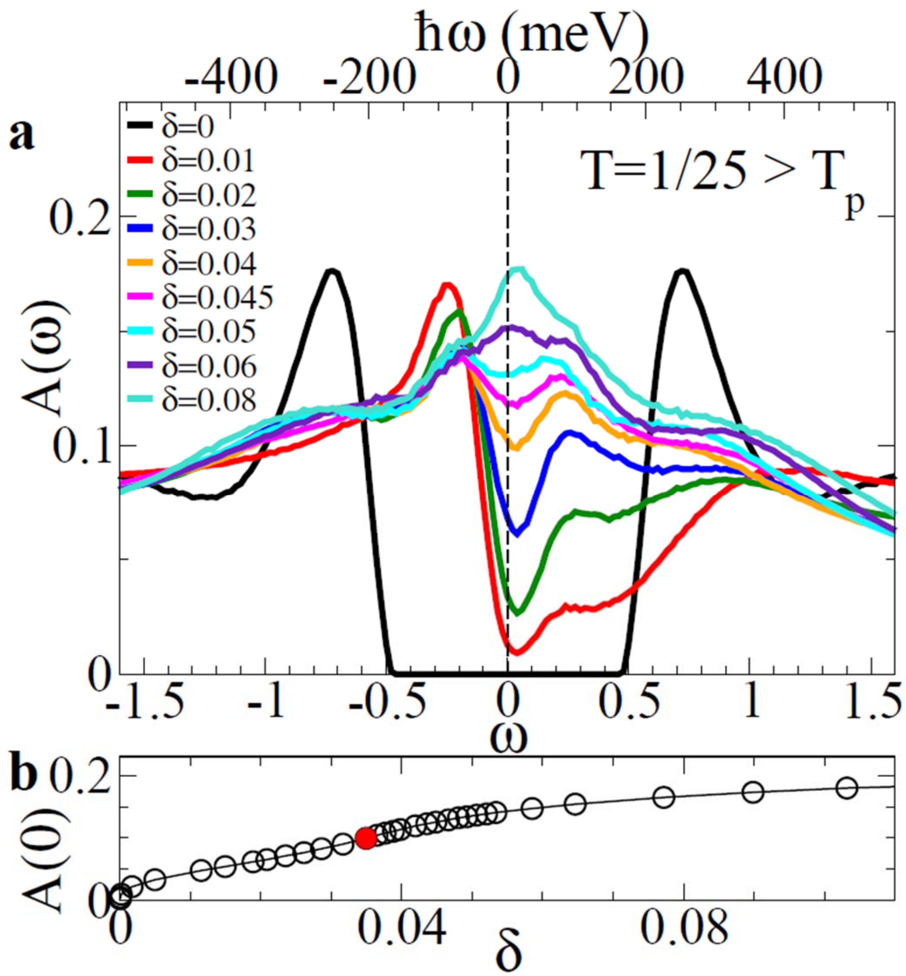
Density of states





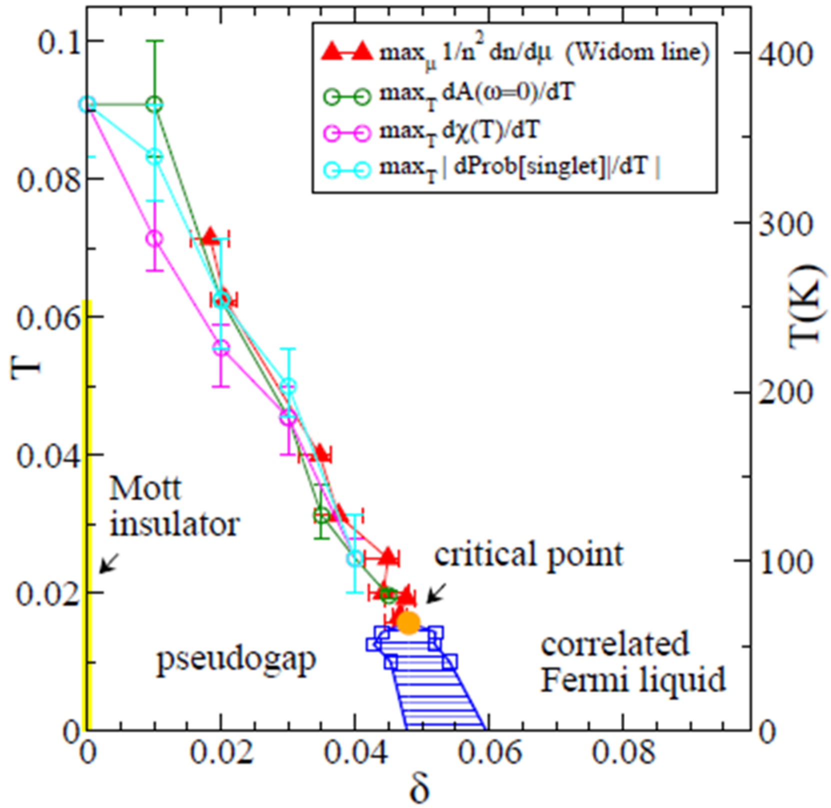
Density of states

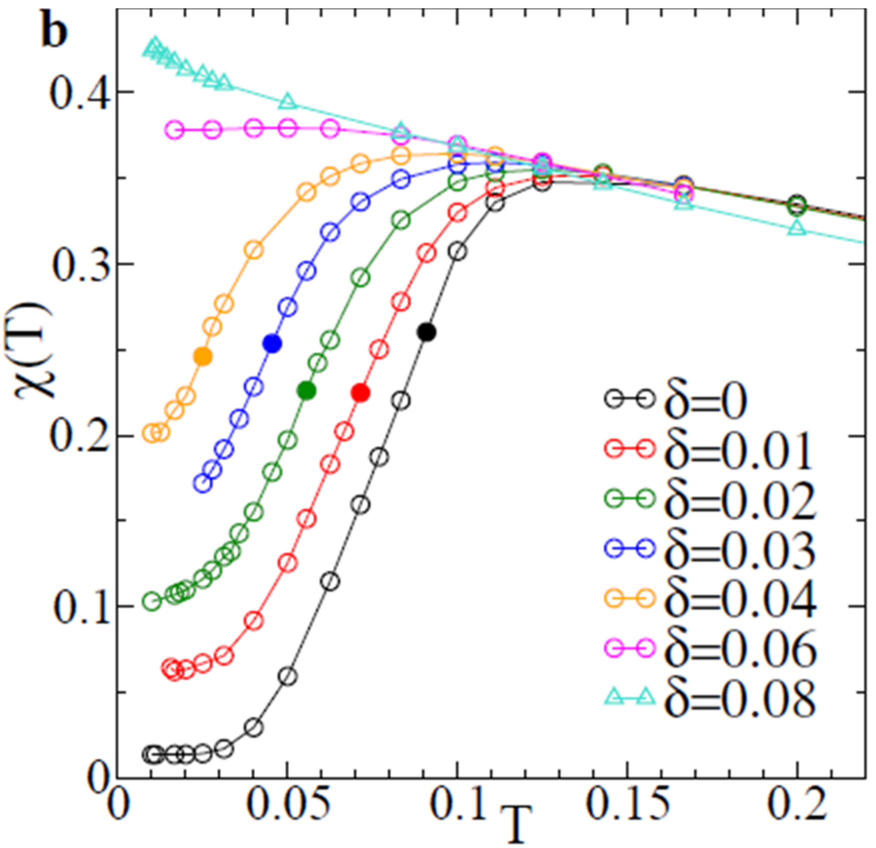




Khosaka et al. *Science* **315**, 1380 (2007);

Spin susceptibility





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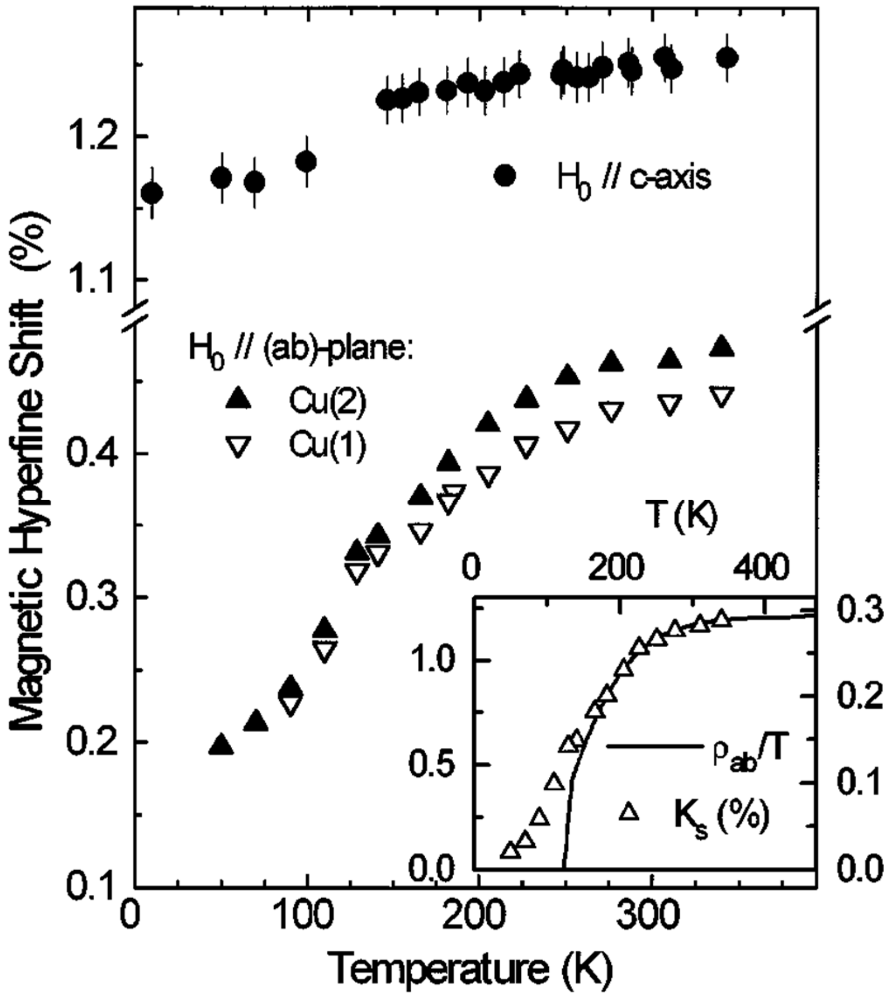
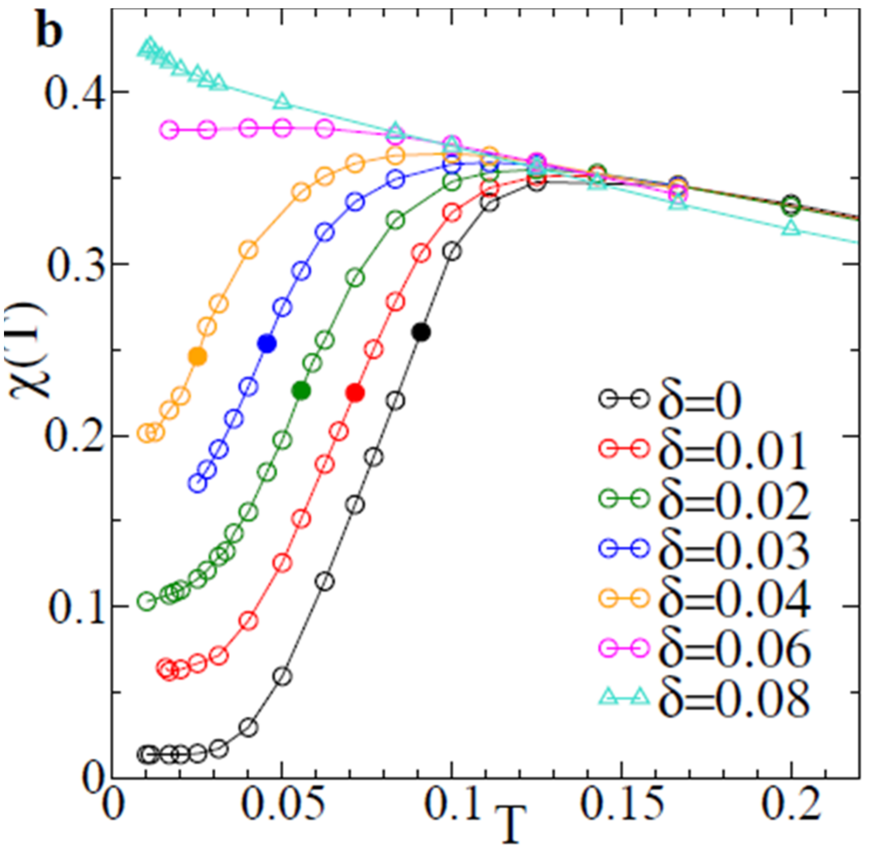
Spin susceptibility



Underdoped Hg1223

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



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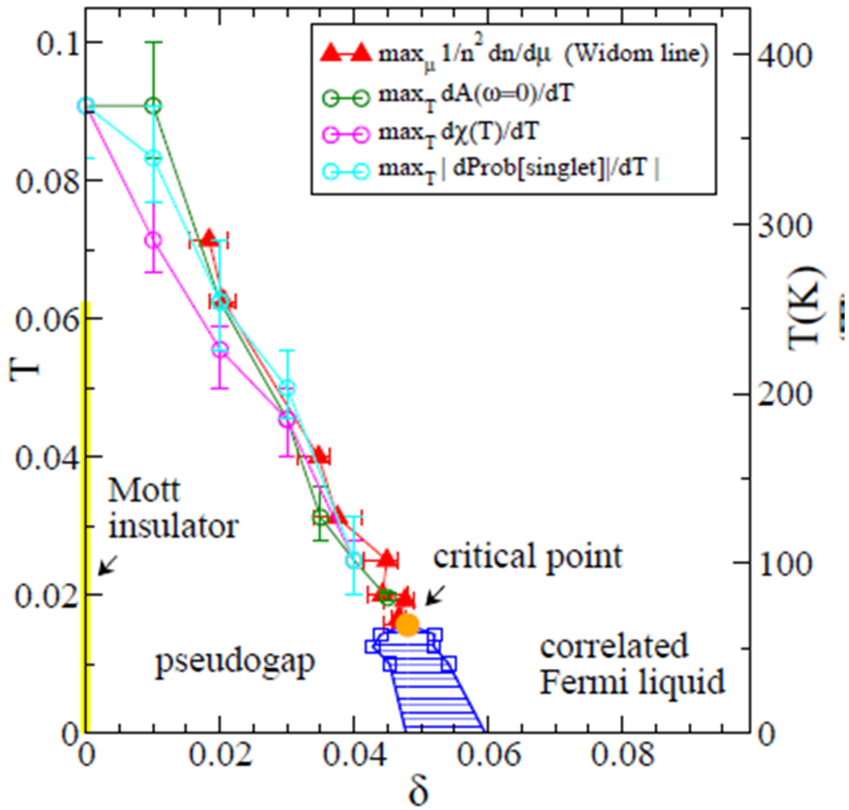
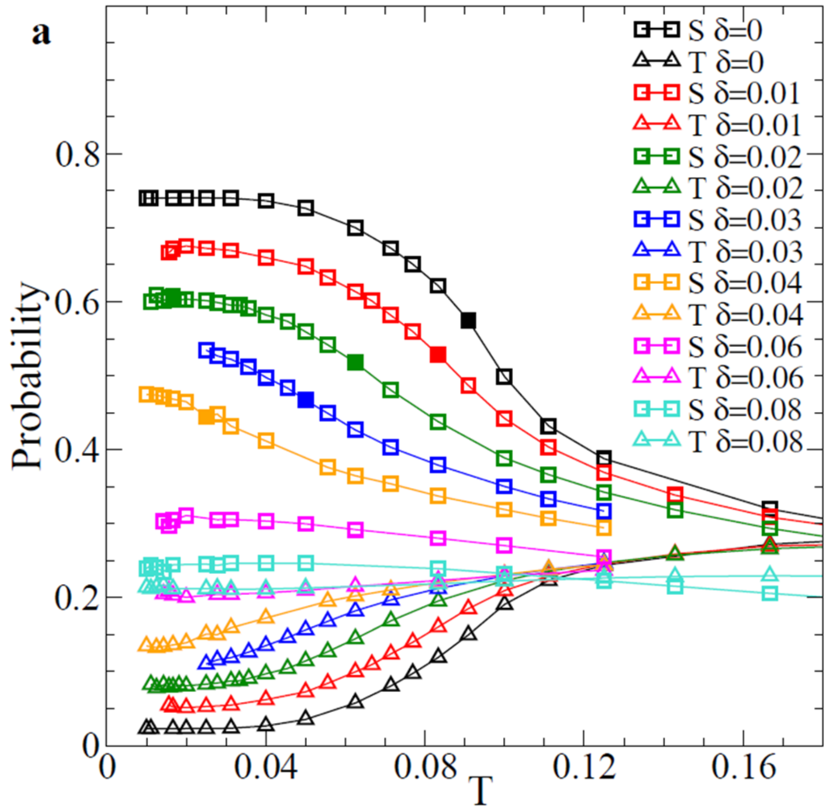
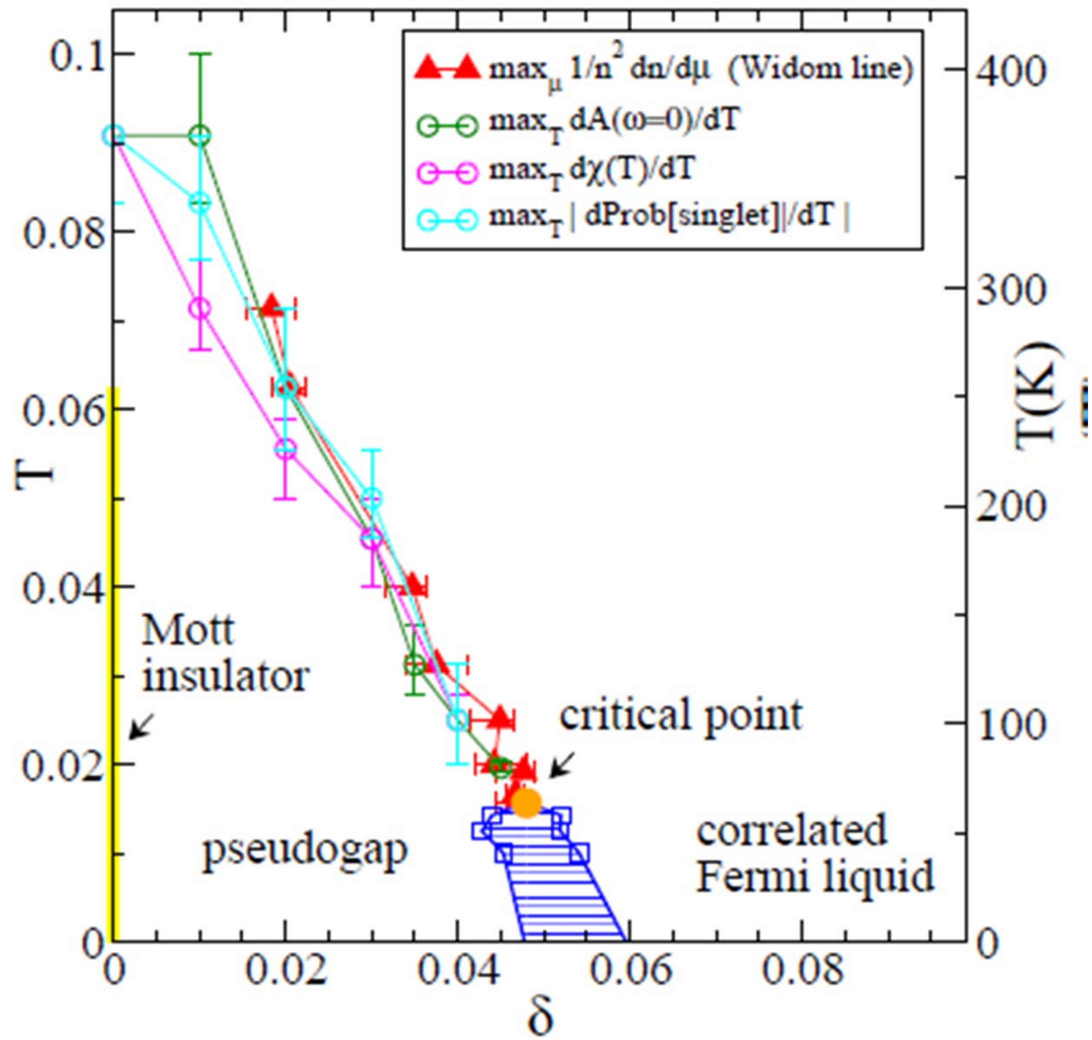
Plaquette eigenstates





Pseudogap along the Widom line T_W



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What is the minimal model?

H. Alloul arXiv:1302.3473

C.R. Académie des Sciences, (2014)

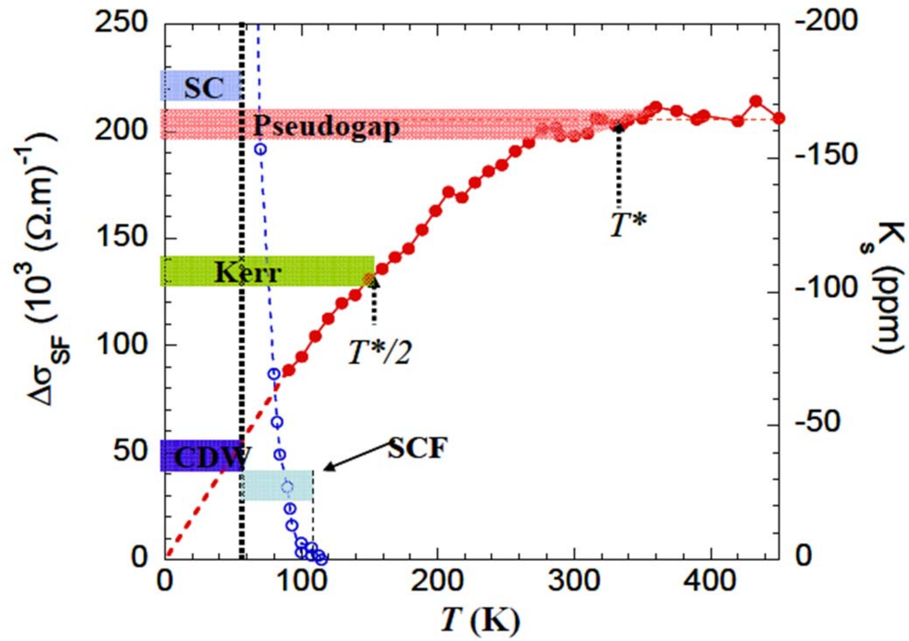

Fig 1 Spin contribution K_s to the ^{89}Y NMR Knight shift [11] for $YBCO_{6.6}$ permit to define the PG onset T^*. Here K_s is reduced by a factor two at $T \sim T^*/2$. The sharp drop of the SC fluctuation conductivity (SCF) is illustrated (left scale) [23]. We report as well the range over which a Kerr signal is detected [28], and that for which a CDW is evidenced in high fields from NMR quadrupole effects [33] and ultrasound velocity data [30]. (See text).

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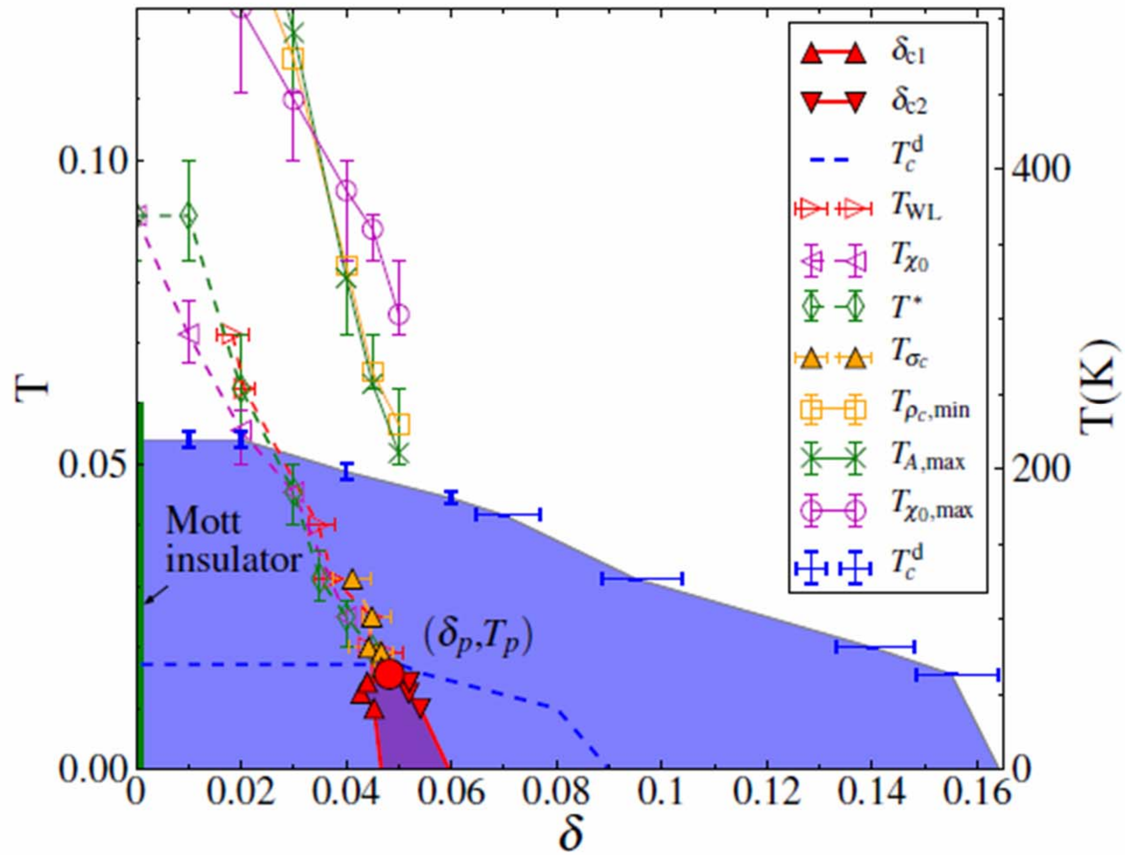
Two crossover lines

Giovanni Sordi

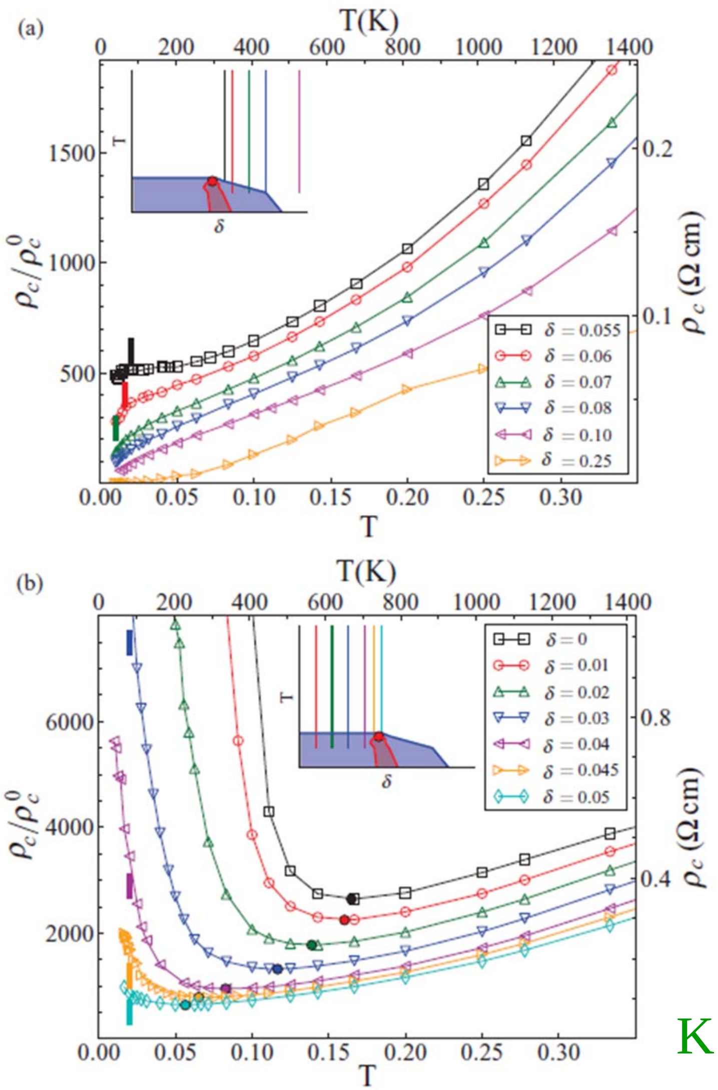
Patrick Sémon

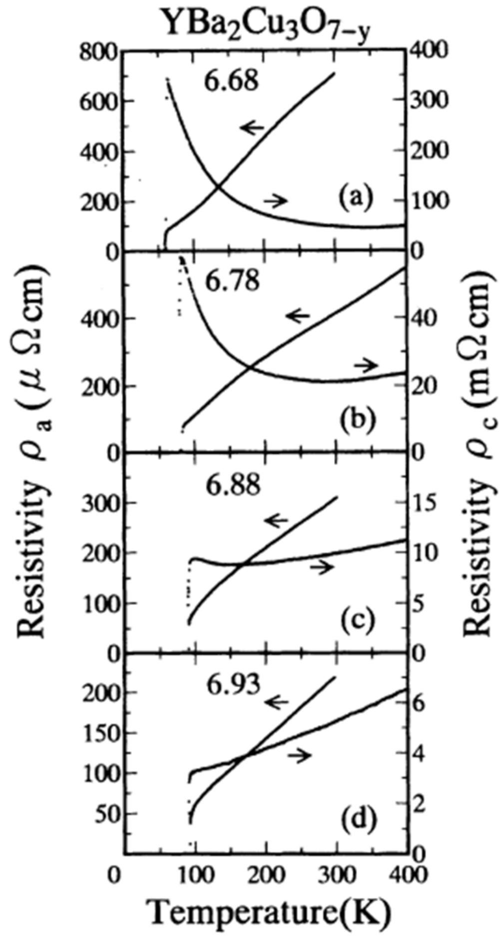


G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)

P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B **89**, 165113/1-6 (2014)

C-axis resistivity





K. Takenaka, K. Mizuhashi, H. Takagi, and S. Uchida, Phys. Rev.B 50, 6534 (1994).

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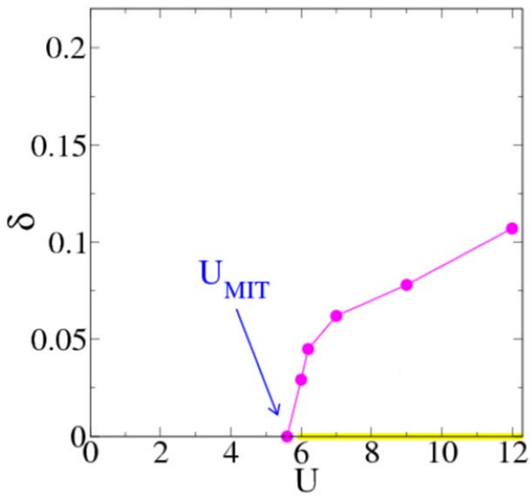
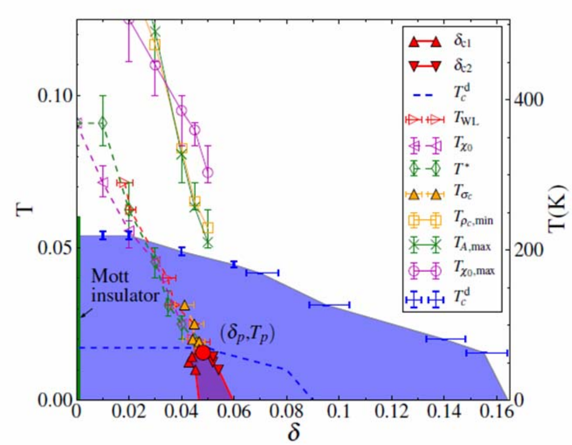
Summary: normal state



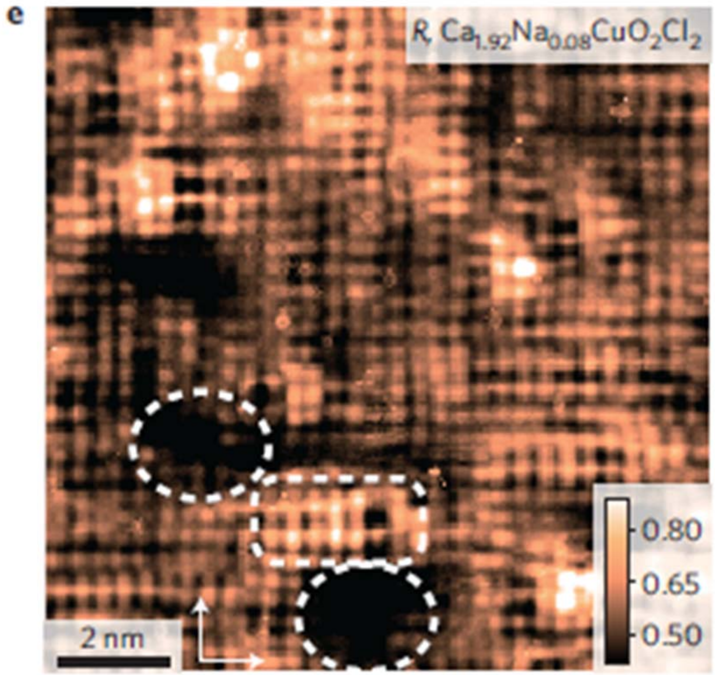


- Mott physics extends way beyond half-filling
- Pseudogap is a phase
- Pseudogap *T* controlled by a Widom line and its precursor
- High compressibility (stripes?)

Charge Density Wave

h-doped

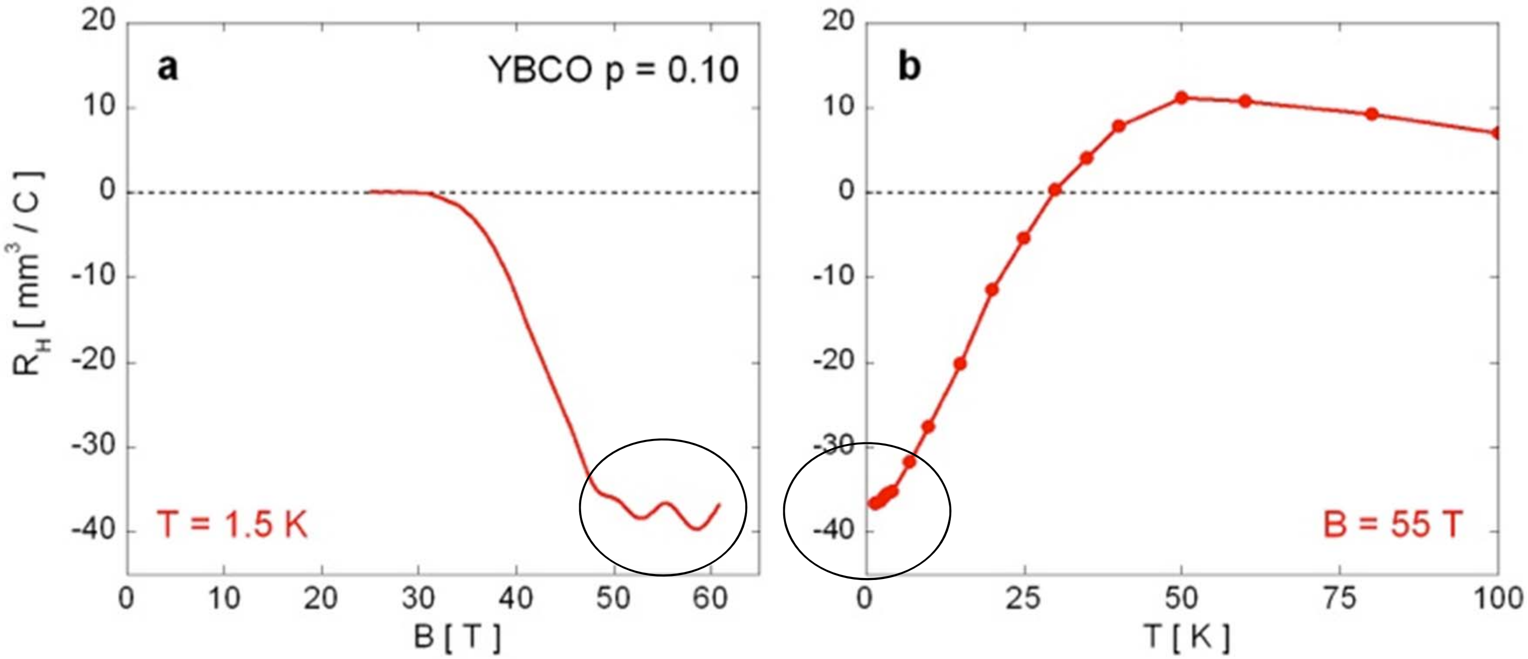
Intra-unit cell nematic order: STM

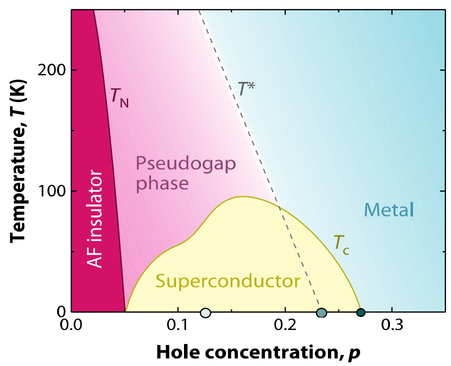


Kohsaka et al. Nature Physics 2012

Quantum oscillations in cuprates: 2007

N. Doiron-Leyraud et al., Nature 2007 *D. LeBoeuf et al., Nature 2007*





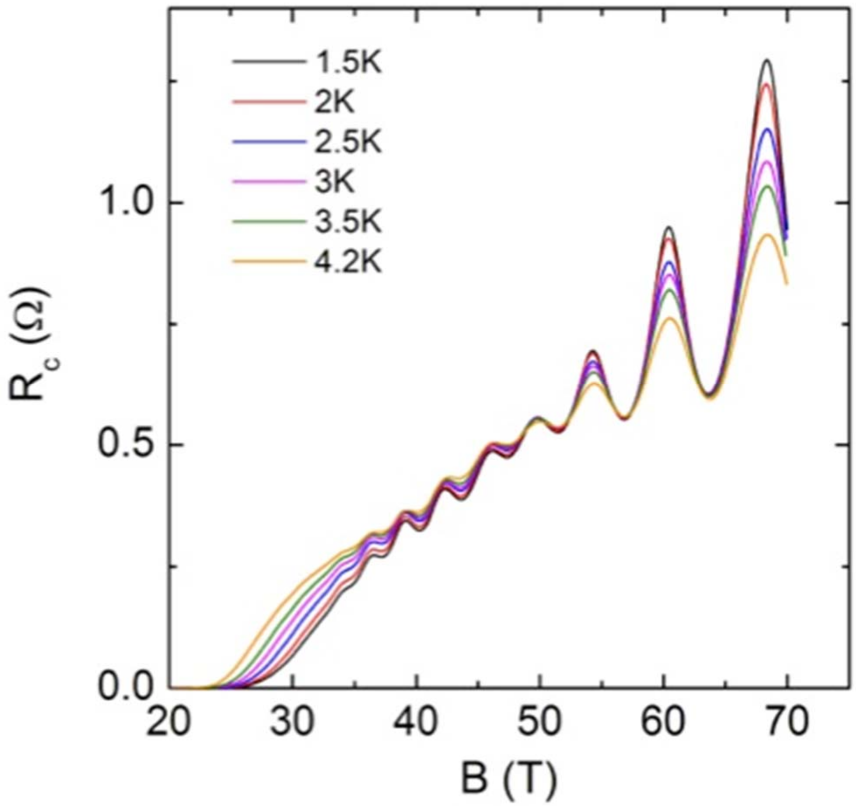
Quantum oscillations ***R_H < 0***

Fermi surface includes a small *electron* pocket !

Université de Sherbrooke

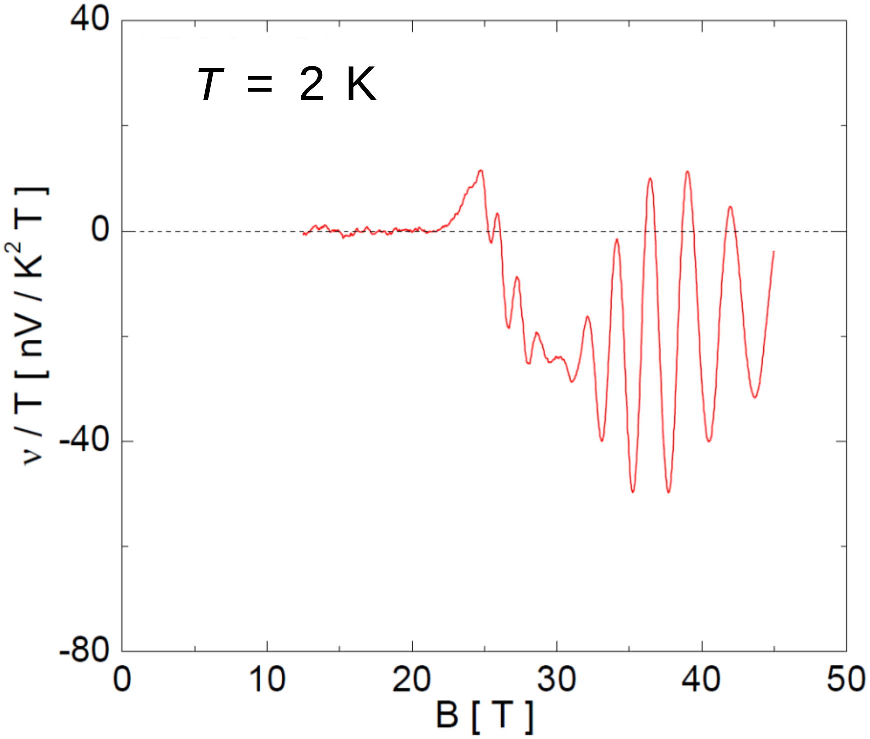
Quantum oscillations in cuprates: 2013

Resistance



LNCMI, Toulouse

Nernst



NHMFL, Tallahassee

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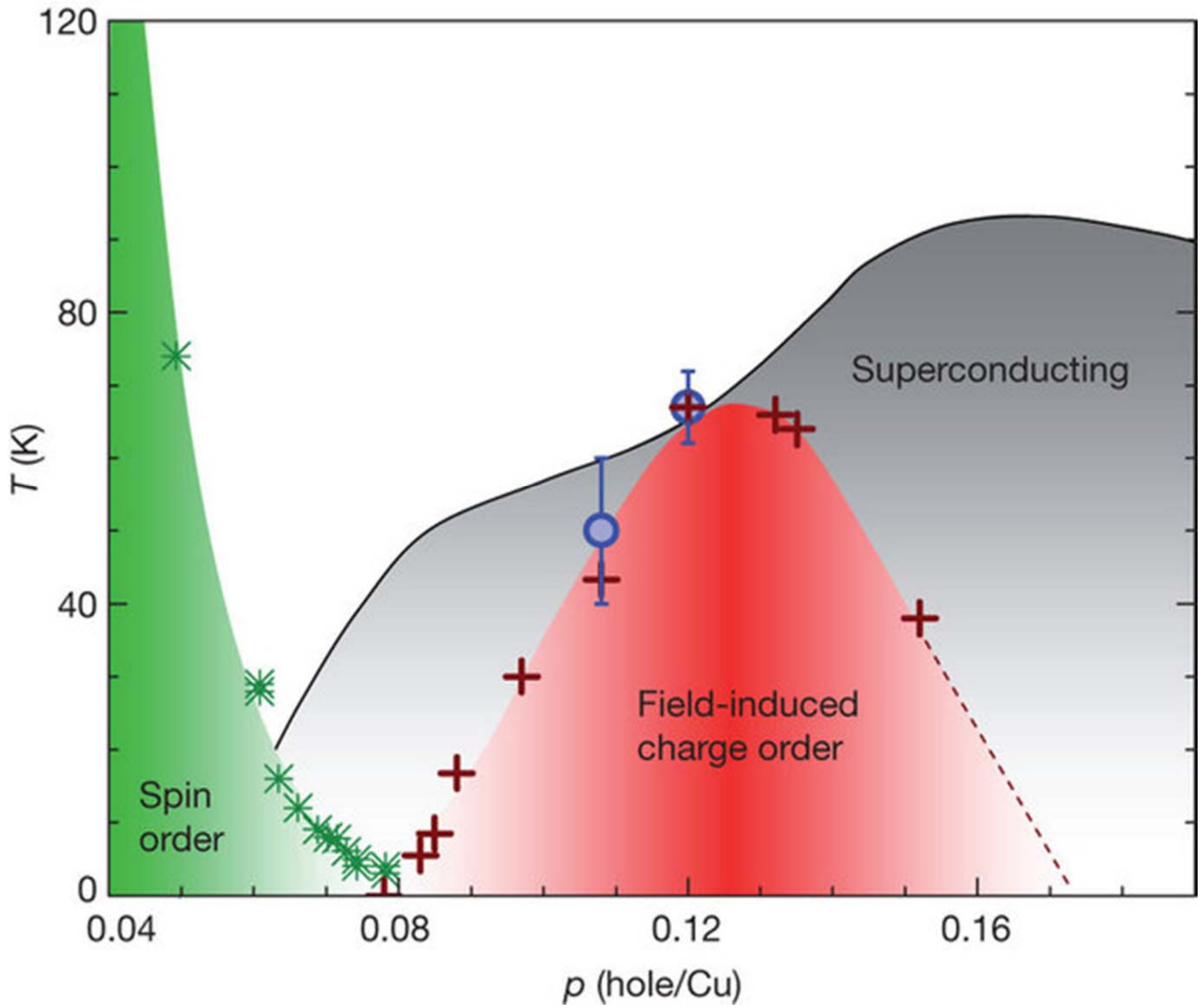
Stripes and reconstructed Fermi surface



Wu et al. Julien, Nature **477**, 191–194 (2011)

Competing CDW order

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- Lawler, M. J. et al. Intra-unit-cell electronic nematicity of the high-Tc copper-oxide pseudogap states. Nature 466, 347351 (2010).
- Parker, C. V. et al. Fluctuating stripes at the onset of the pseudogap in the high-Tc superconductor B2Sr2CaCu2O8Cx. Nature 468, 677680 (2010).
- Chang, J. et al. Direct observation of competition between superconductivity and charge density wave order in YBa2Cu3O6:67. Nature Phys. 8, 871876 (2012).
- Ghiringhelli, G. et al. Long-range incommensurate charge fluctuations in (Y;Nd)Ba2Cu3O6Cx. Science 337, 821825 (2012).
- Achkar, A. J. et al. Distinct charge orders in the planes and chains of ortho-III-ordered YBa2Cu3O6C superconductors identified by resonant elastic X-ray scattering. Phys. Rev. Lett. 109, 167001 (2012).
- Wu, T. et al. Magnetic-field-induced charge-stripe order in the high-temperature superconductor YBa2Cu3Oy. Nature 477, 192194 (2011).
- LeBoeuf, D. et al. Thermodynamic phase diagram of static charge order in underdoped YBa2Cu3Oy. Nature Phys. 9, 7983 (2013).

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nature physics

LETTERS

PUBLISHED ONLINE: 14 OCTOBER 2012 | DOI: 10.1038/NPHYS2456

Direct observation of competition between superconductivity and charge density wave order in $YBa_2Cu_3O_{6.67}$

J. Chang[1,2]*, E. Blackburn[3], A. T. Holmes[3], N. B. Christensen[4], J. Larsen[4,5], J. Mesot[1,2], Ruixing Liang[6,7], D. A. Bonn[6,7], W. N. Hardy[6,7], A. Watenphul[8], M. v. Zimmermann[8], E. M. Forgan[3] and S. M. Hayden[9]

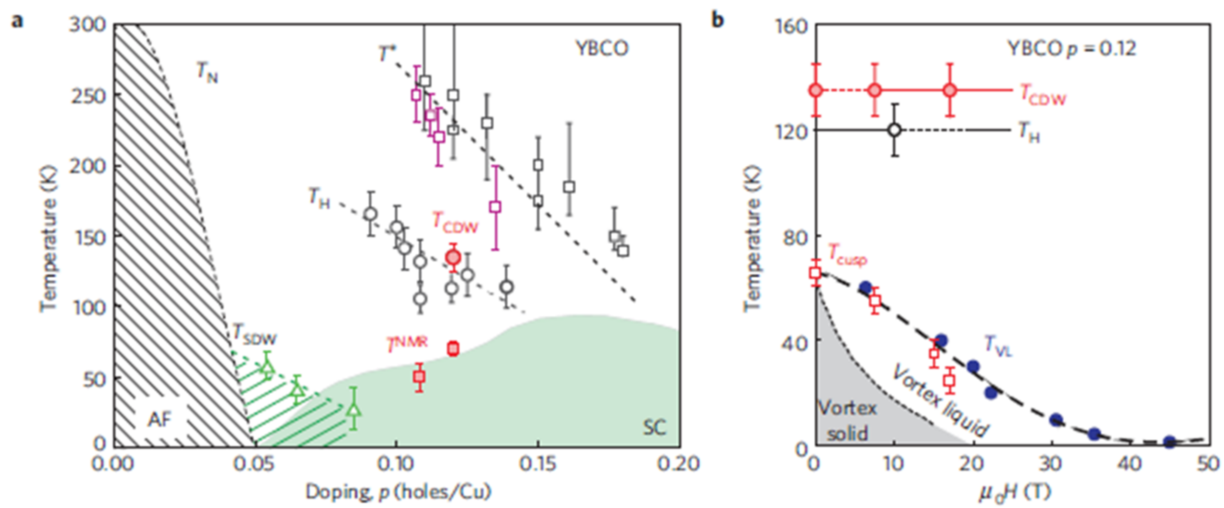
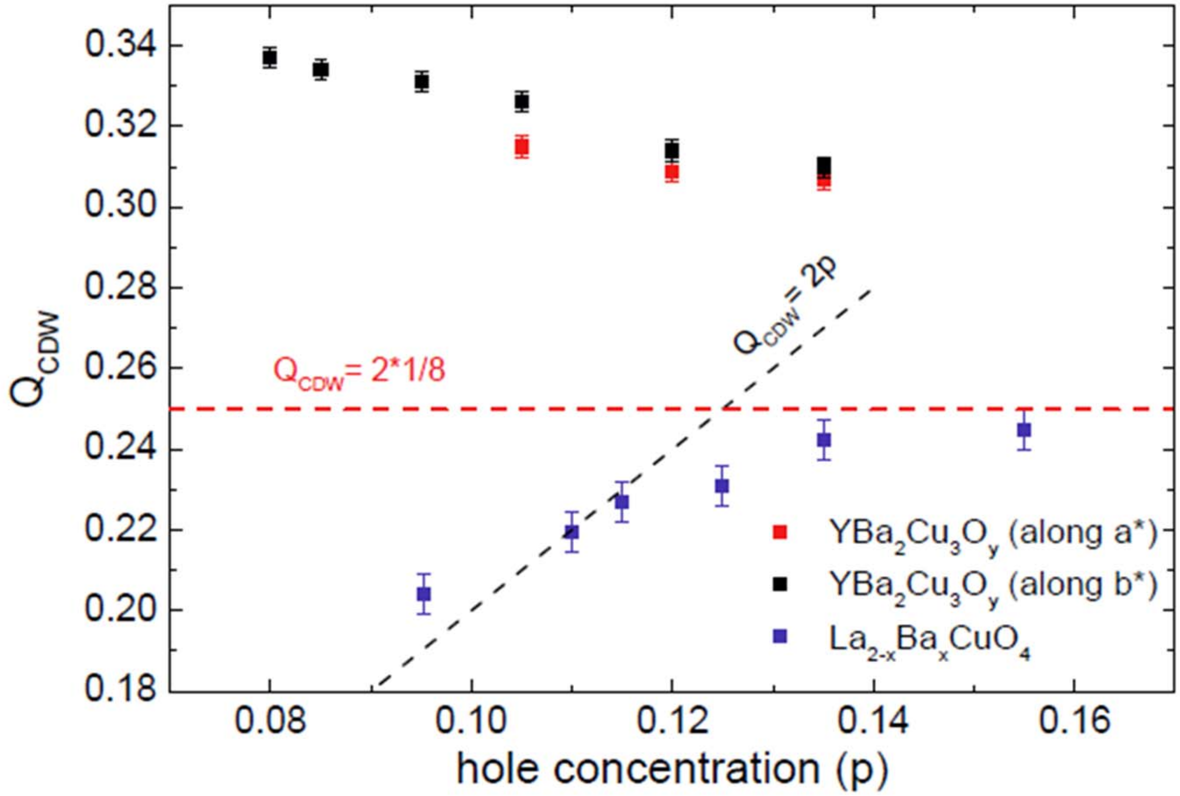


Figure 4 | Phase diagram of $YBa_2Cu_3O_{7-x}$. a, Doping dependence of the antiferromagnetic ordering temperature T_N, the incommensurate spin-density wave order T_{SDW} (green triangles; ref. 21), the superconducting temperature T_c and the pseudogap temperature T^* as determined from the Nernst effect[30] (black squares) and neutron diffraction[29] (purple squares). Notice that the Nernst effect[30] indicates a broken rotational symmetry inside the pseudogap region, whereas a translational symmetry preserving magnetic order is found by neutron scattering[29]. Below temperature scale T_H (black circles), a larger and negative Hall coefficient was observed[26] and interpreted in terms of a Fermi surface reconstruction. Our X-ray diffraction experiments show that in YBCO $p = 0.12$ incommensurate CDW order spontaneously breaks the crystal translational symmetry at a temperature T_{CDW} that is twice as large as T_c. T_{CDW} is also much larger than T^{NMR} (red squares), the temperature scale below which NMR observes field-induced charge order[13]. **b**, Field dependence of T_{CDW} (filled red circles) and T_{cusp} (open squares), the temperature below which the CDW is suppressed by superconductivity, compared with T_H (open black circle) and T_{VL} (filled blue circles), the temperature where the vortex liquid state forms[26]. Error bars on T_{SDW}, T_H, T_{NMR}, and T^* are explained in refs 21,26,30,33. The error bars on T_{CDW} and T_{cusp} reflect the uncertainty in determining the onset and suppression temperature of CDW order from Fig. 2.

KE

Wave vector



Keimer, Julich summer school 2013

Theories

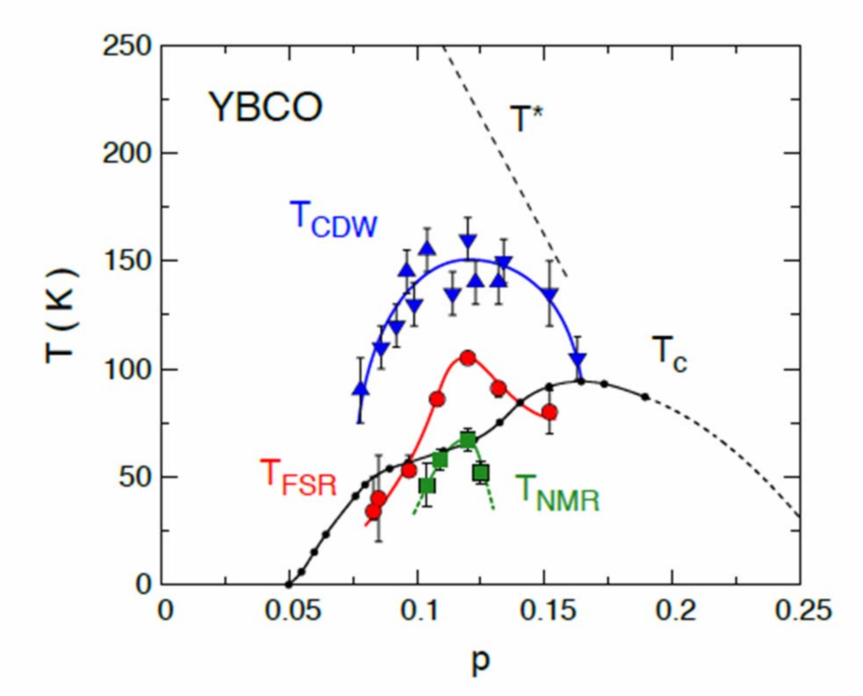
S. Sachdev and R. La Placa Phys. Rev. Lett. **111**, 027202 (2013)
D. Chowdhury, S. Sachdev arxiv. 1501.00002

K. B. Efetov, H. Meier, and C. Pepin, Nat Phys **9**, 442 (2013).

Y. Wang and A. Chubukov, Phys. Rev. B 90, 035149 (2014).

…

Phase diagram with CDW



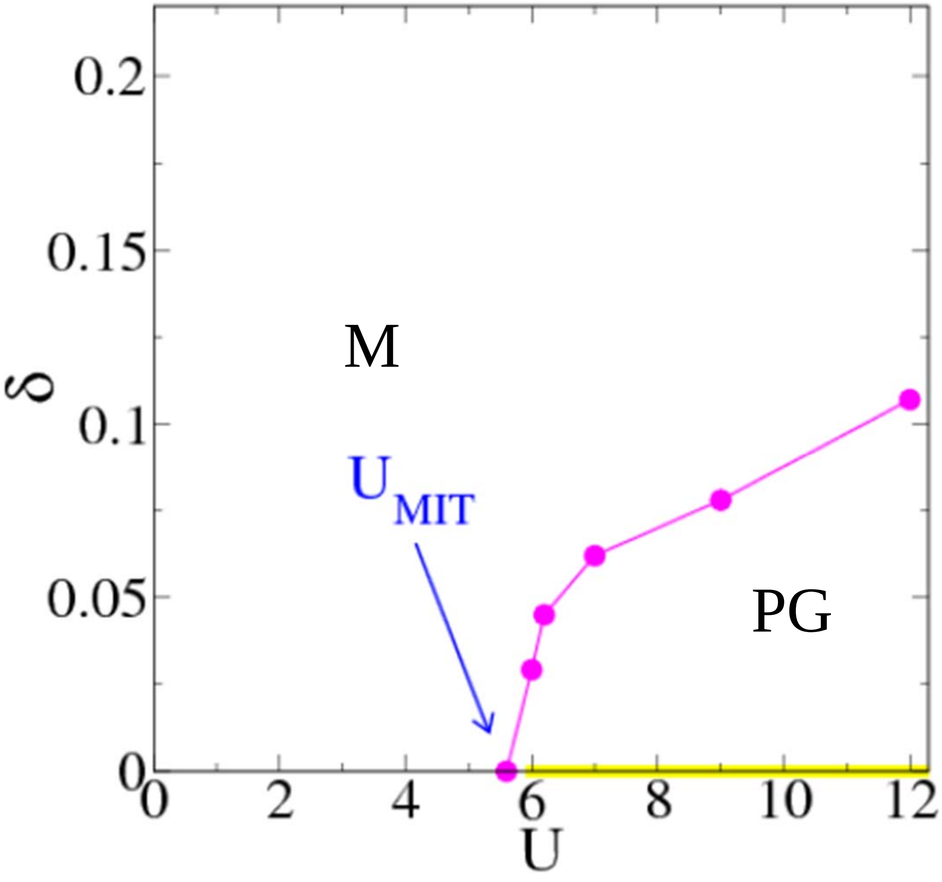
Cyr-Choinière et al, arxiv1503.02033

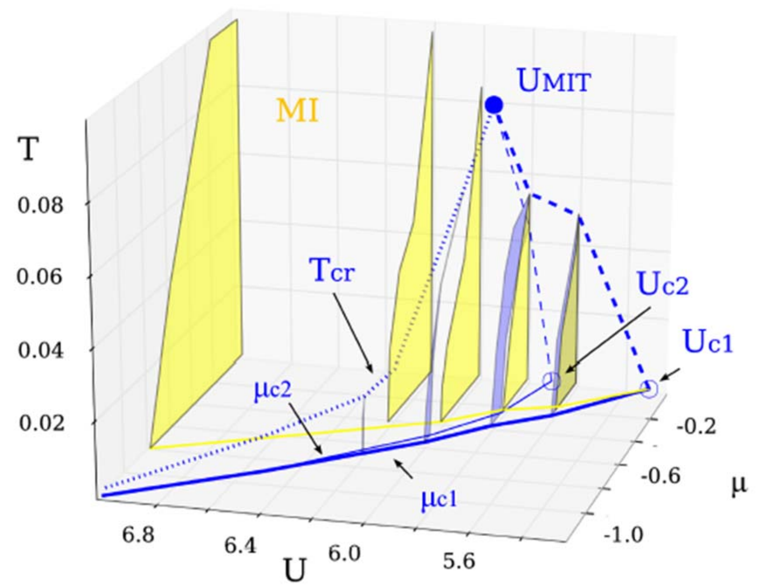
$T = 0$ phase diagram

Normal state and large anisotropy

Recall phase diagram

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





Underdoped metal very sensitive to anisotropy

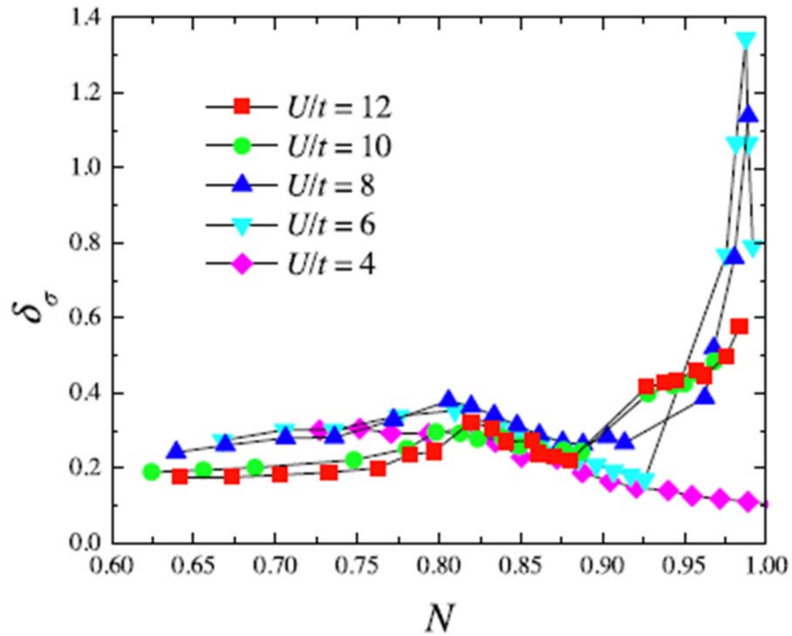
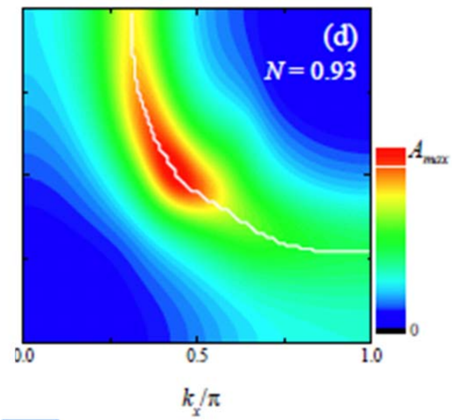
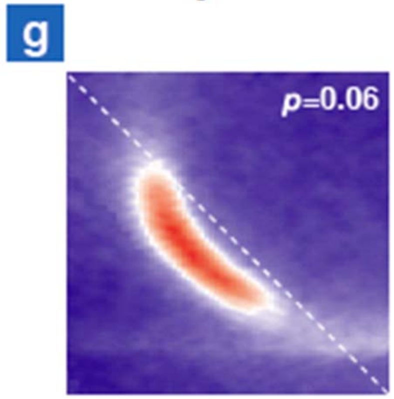


FIG. 3: (Color online) Anisotropy in the CDMFT conductivity $\delta_\sigma = 2\,[\sigma_x(0) - \sigma_y(0)]\,/\,[\sigma_x(0) + \sigma_y(0)]$ as a function of filling N for various values of U and $\eta = 0.1$, $\delta_0 = 0.04$.

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



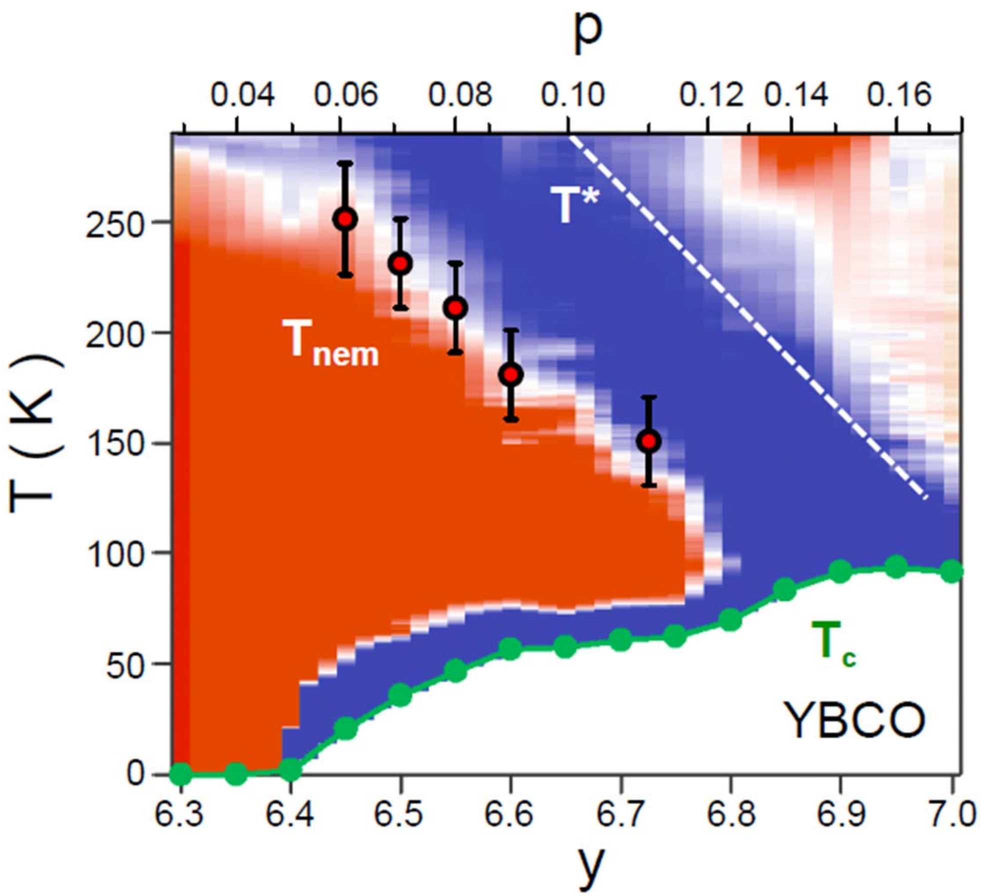


Satoshi Okamoto

David Sénéchal

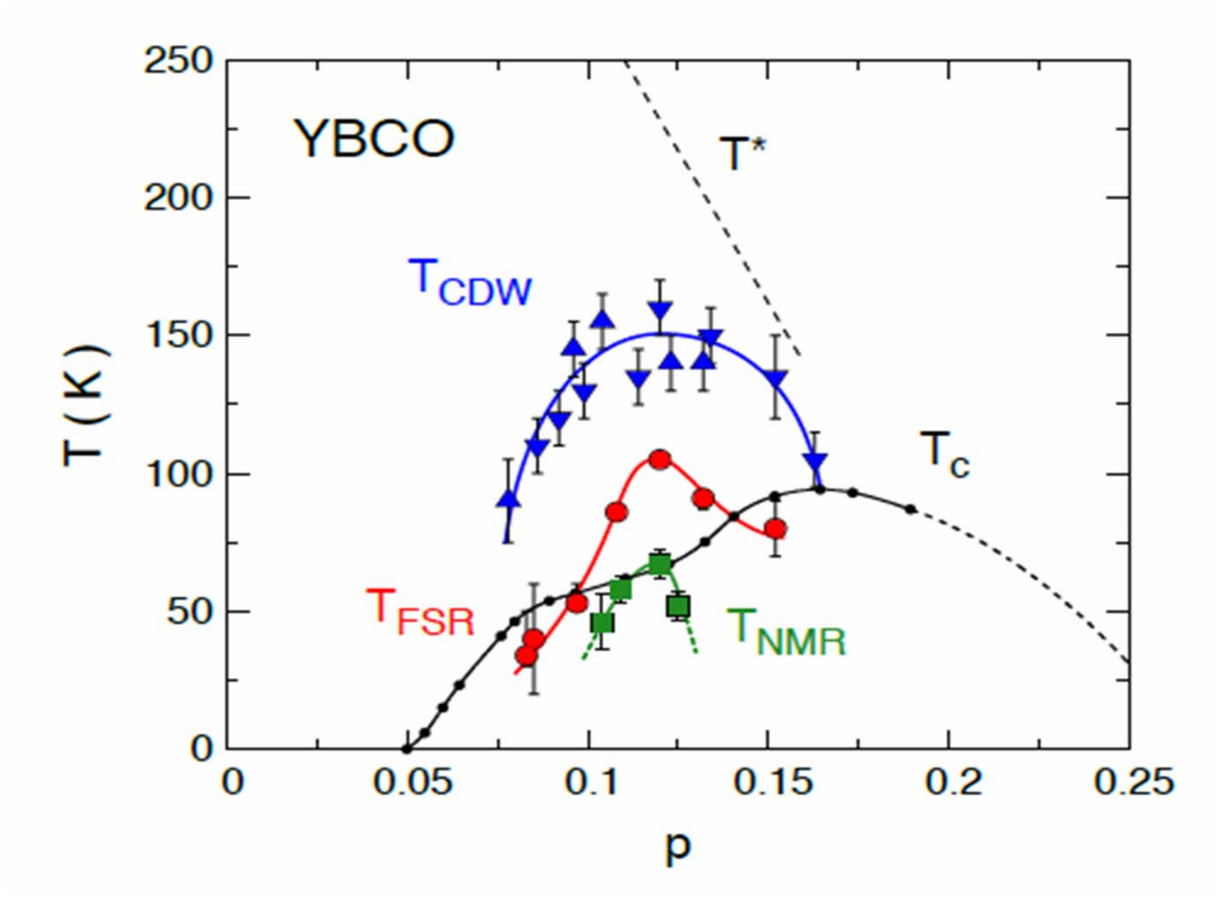
D. Fournier *et al.* Nature Physics (Marcello Civelli

Resistivity anisotropy and curvature map



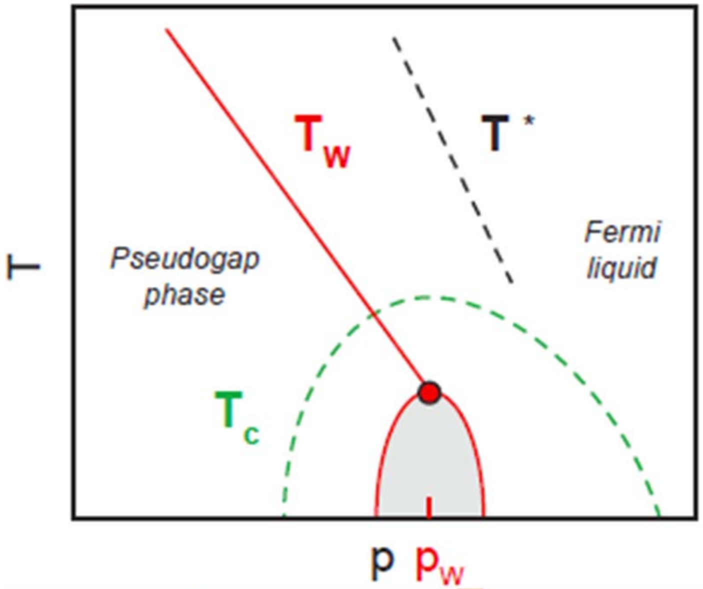
Y. Ando *et al.*, *Phys. Rev. Lett.* **93**, 267001 (2004).

Phase diagram, including CDW

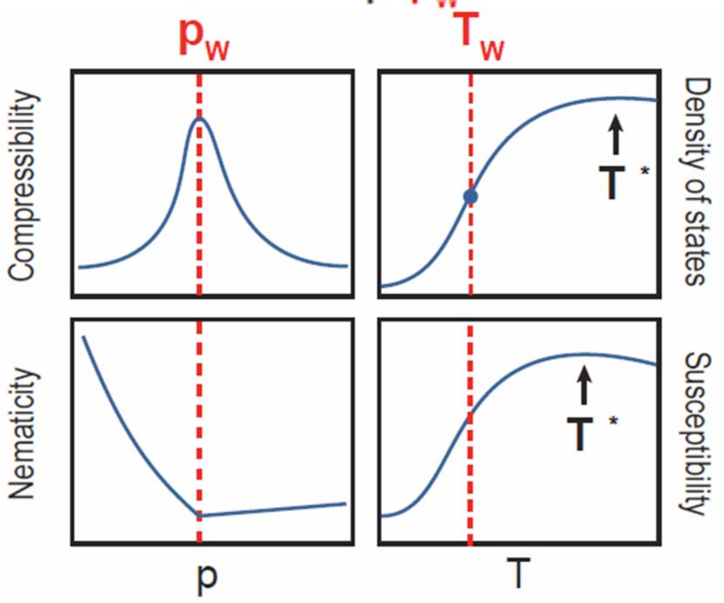


Cyr-Choinière et al, arxiv1503.02033

Summary



T
T_W
T^*
Pseudogap phase
Fermi liquid
T_c
p
p_W



p_W
T_W
Compressibility
Density of states
T^*
Nematicity
Susceptibility
T^*
p
T

Giovanni Sordi

Patrick Sémon

Kristjan Haul

Finite *T* phase diagram

Superconductivity

G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)
P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B **89**, 165113/1-6 (2014)

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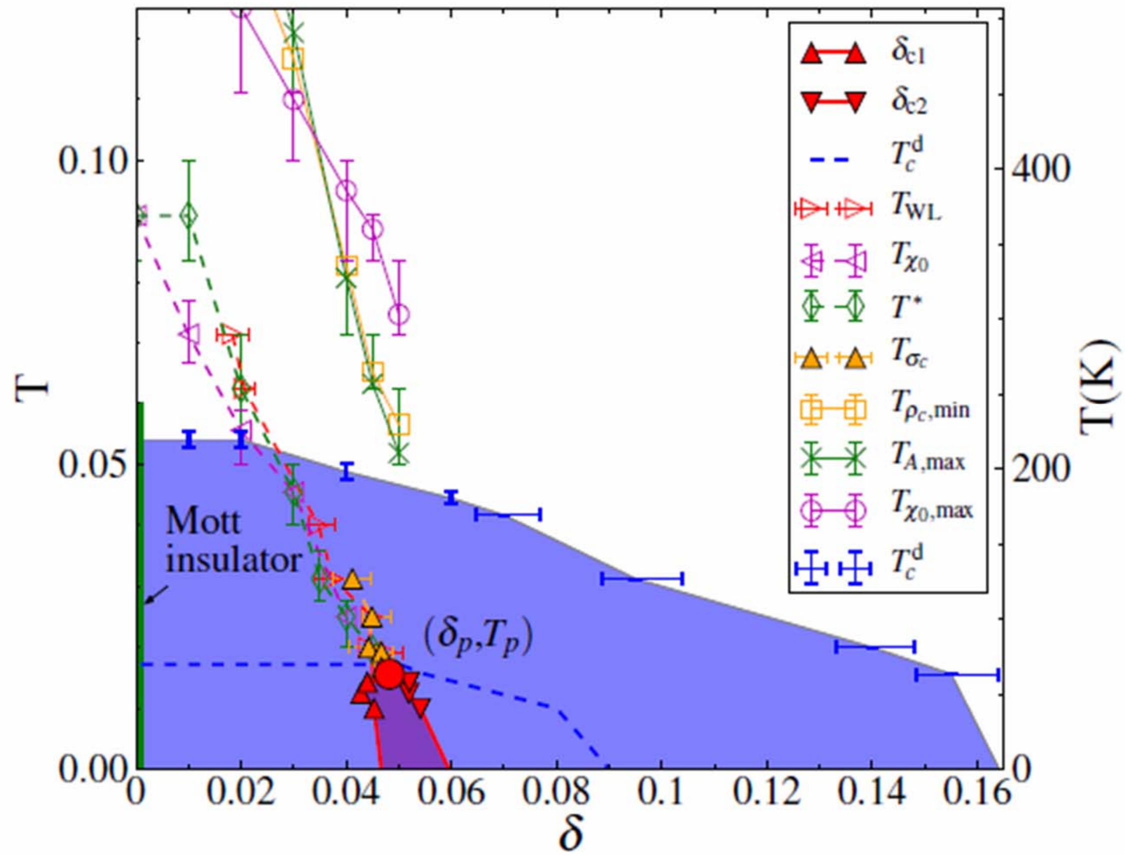
Dôme?

Giovanni Sordi

Patrick Sémon



G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)

P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B **89**, 165113/1-6 (2014)

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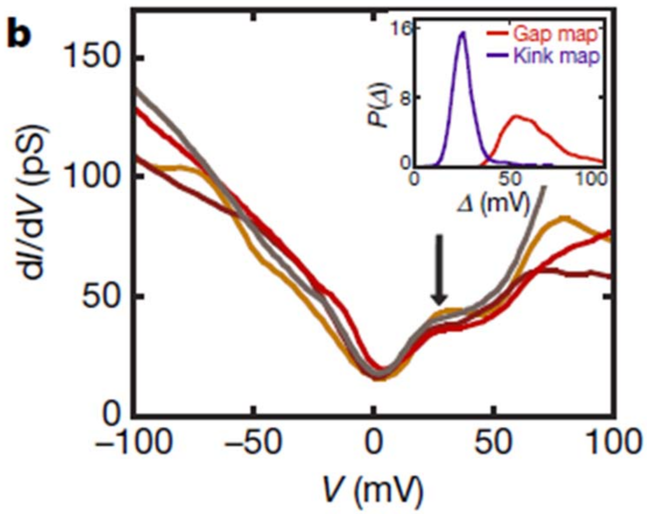
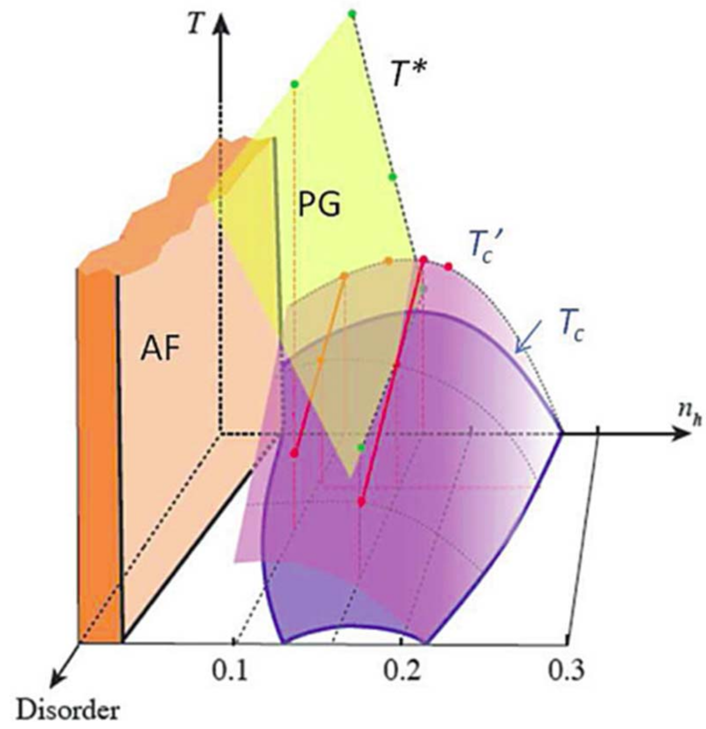
Meaning of T_c^d

- Local pair formation

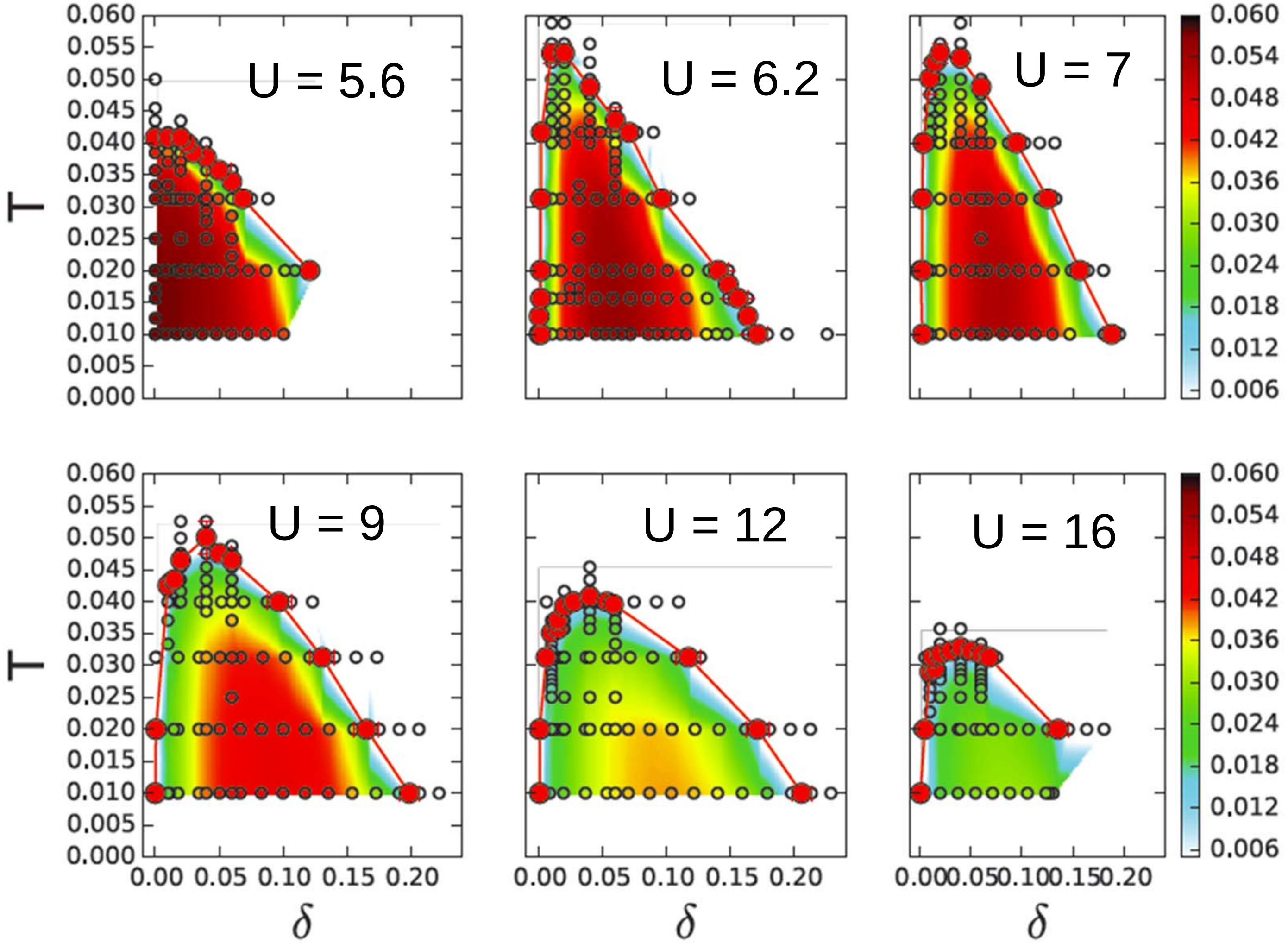


K. K. Gomes, A. N. Pasupathy, A. Pushp, S. Ono, Y. Ando, and A. Yazdani, Nature **447**, 569 (2007)



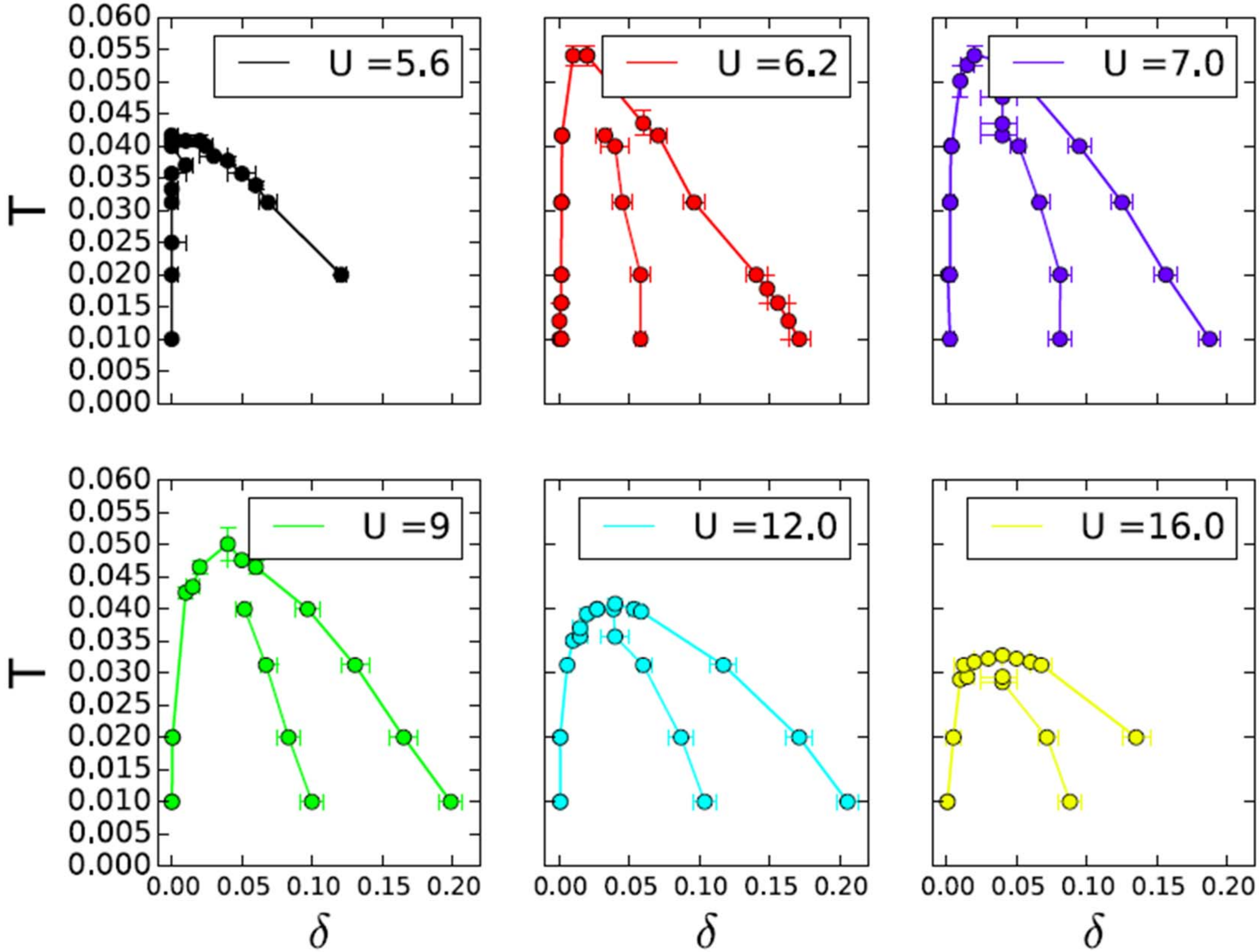
F. Rullier-Albenque, H. Alloul, and G.Rikken, Phys. Rev. B **84**, 014522 (2011).

Order parameter (color) and T_c



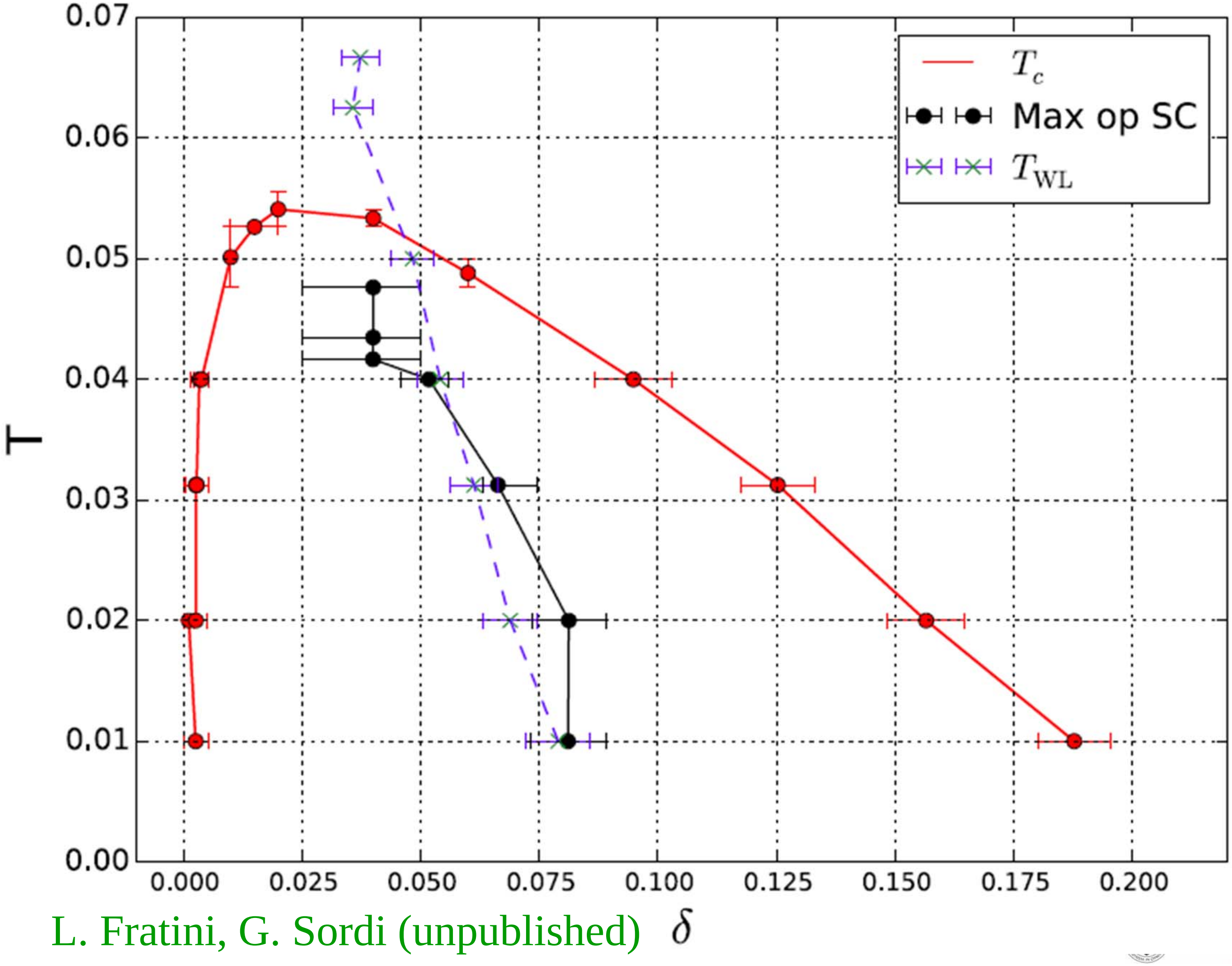
L. Fratini, G. Sordi (unpublished)

T_c vs $T_{max\ order\ parameter}$



L. Fratini, G. Sordi (unpublished)

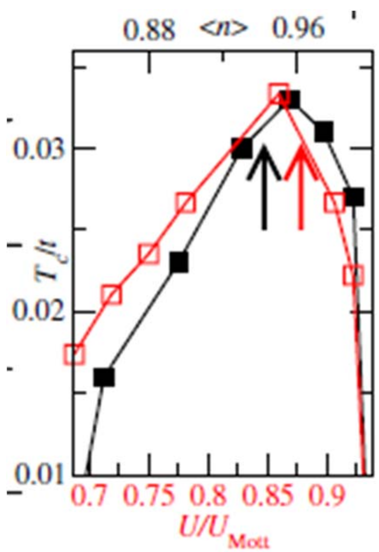
U=7, T_W vs T_c vs $T_{\text{max order parameter}}$



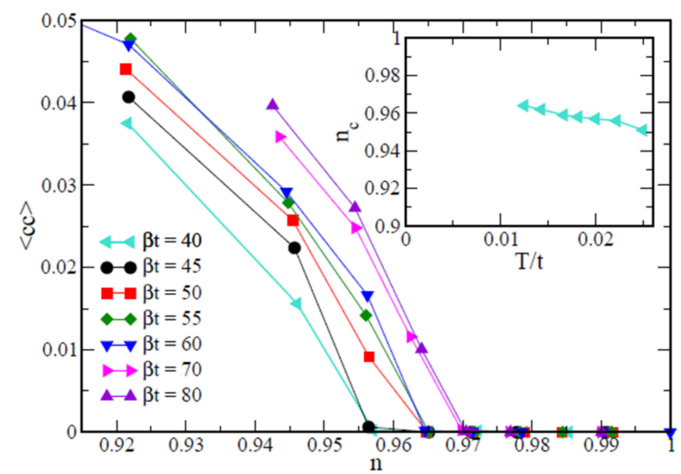
L. Fratini, G. Sordi (unpublished)

Larger clusters

- In 2x2 T_c vanishes extremely close to half-filling. In larger cluster, earlier.
- Local pairs in underdoped (2x2)



8 site DCA, $U=6t$



8 site DCA, $U=6.5t$

Gull Parcollet Millis,
PRL **110**, 216405 (2013)

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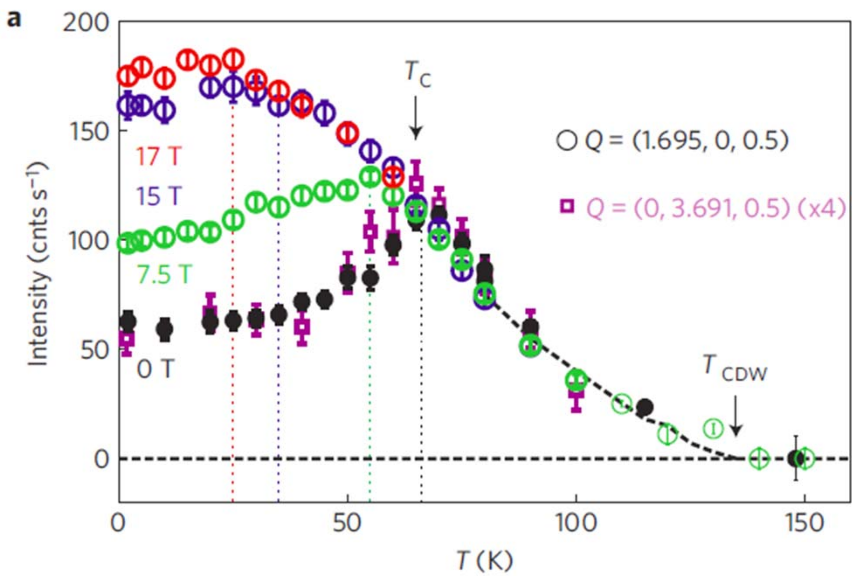
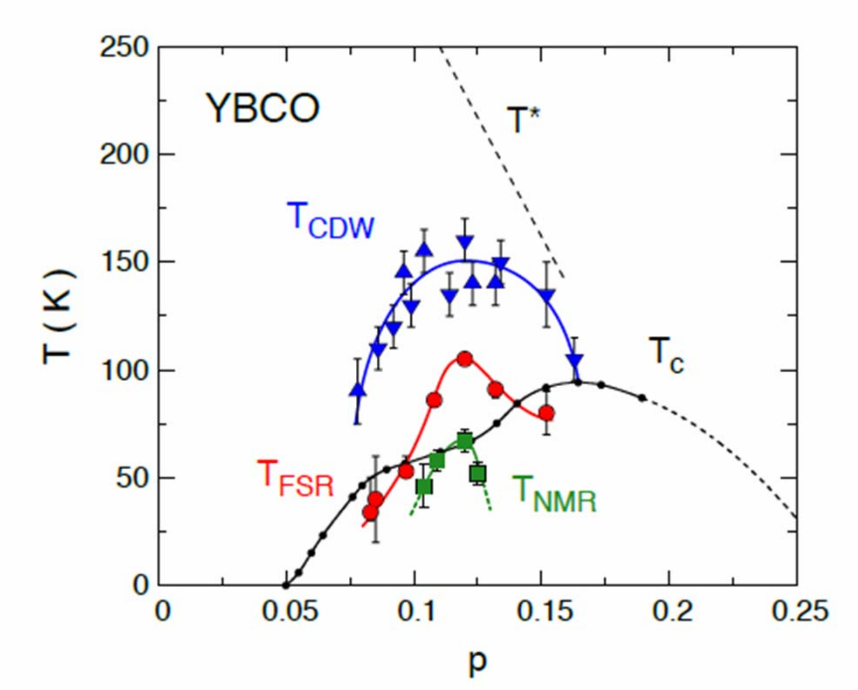
Competition between CDW and SC

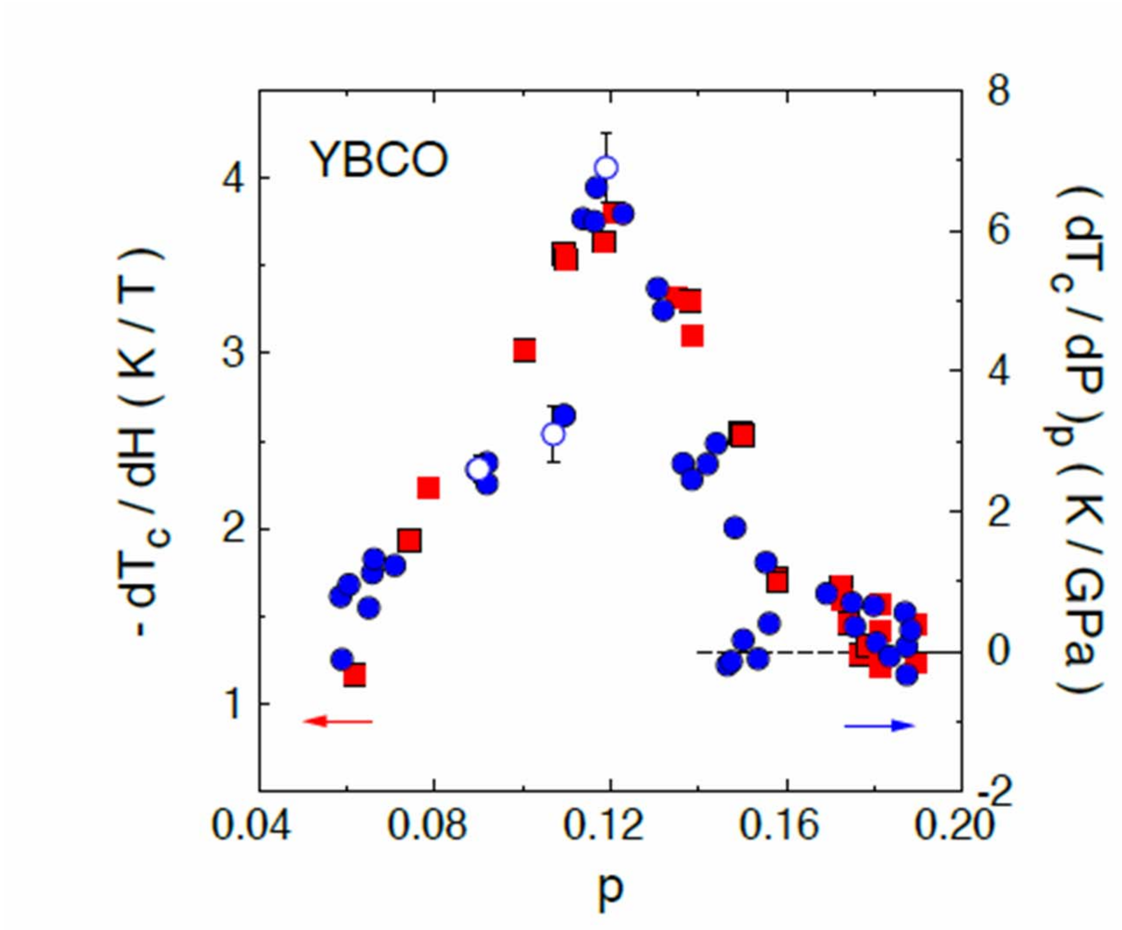


J. Chang *et al.*, *Nat. Phys.* **8**, 871-876 (2012).



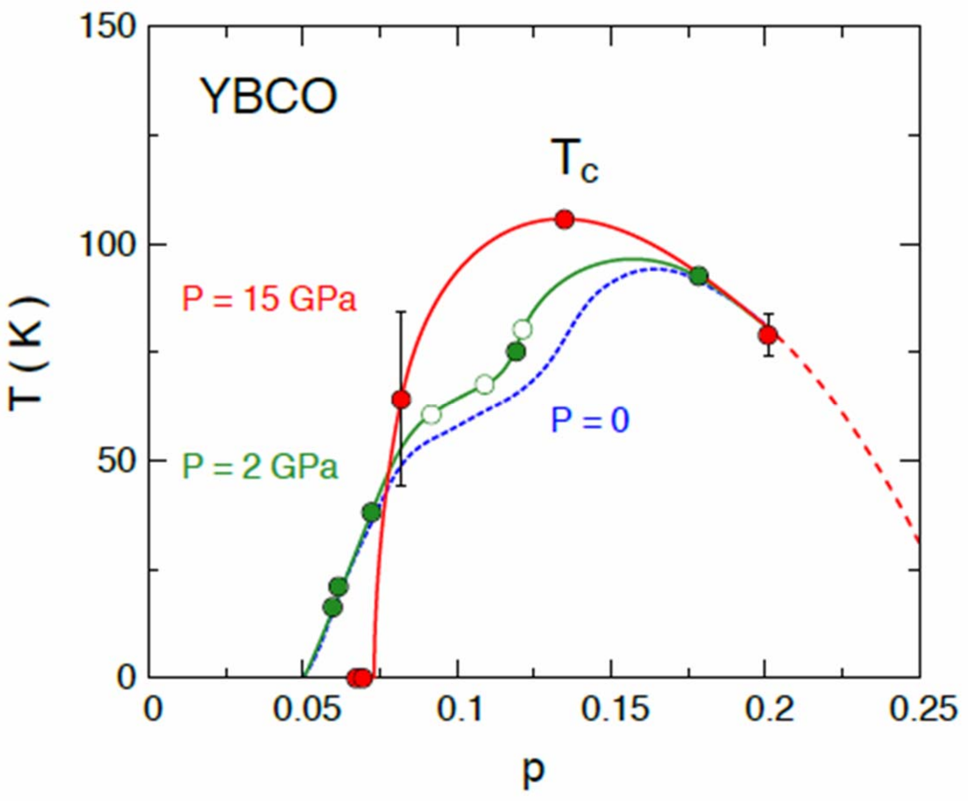
Cyr-Choinière et al, arxiv1503.02033

Tuning SC and CDW



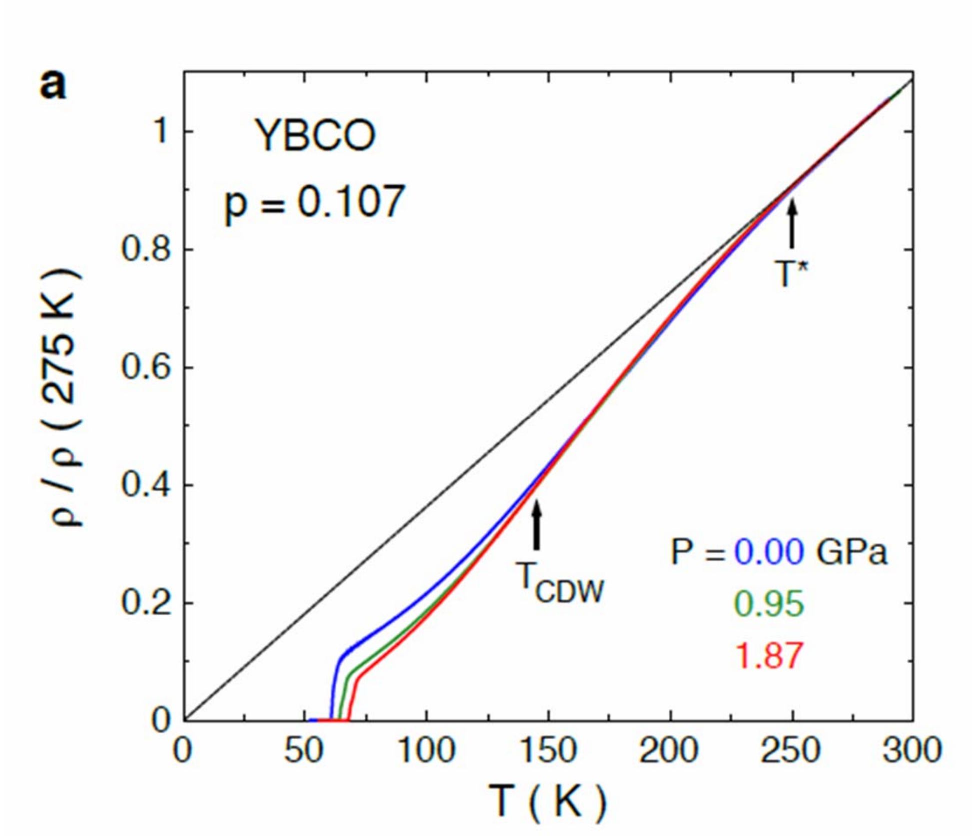
Cyr-Choinière et al, arxiv1503.02033

Getting rid of the CDW



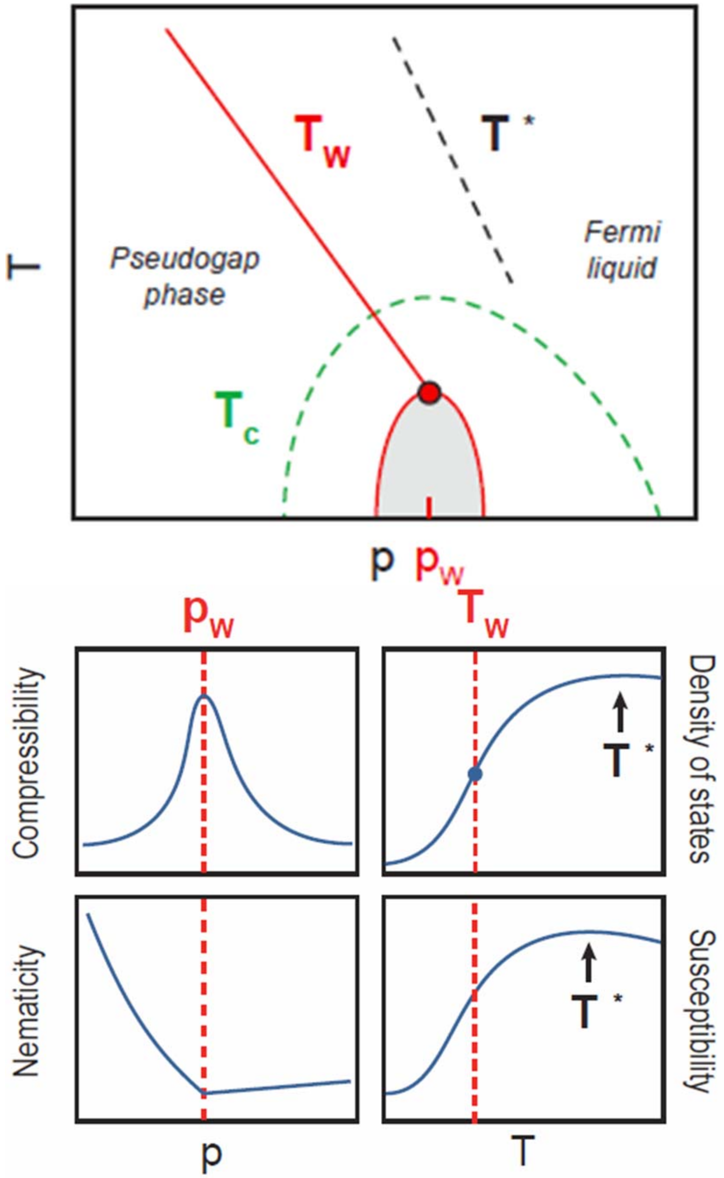
Cyr-Choinière et al, arxiv1503.02033

T* not affected



Cyr-Choinière et al, arxiv1503.02033

An alternate point of view



- - Is the pseudogap (PG) a crossover or a phase transition ?
- - Relation between CDW and the PG ?
- - Why CDW peaked at 12% doping ?
- - Origin of nematicity ?
- - Why superconducting ?
- - Why a dome of SC ?
- - Does a one-band model capture the key physics ?
- AFM QCP important?
- Lessons from other SC?

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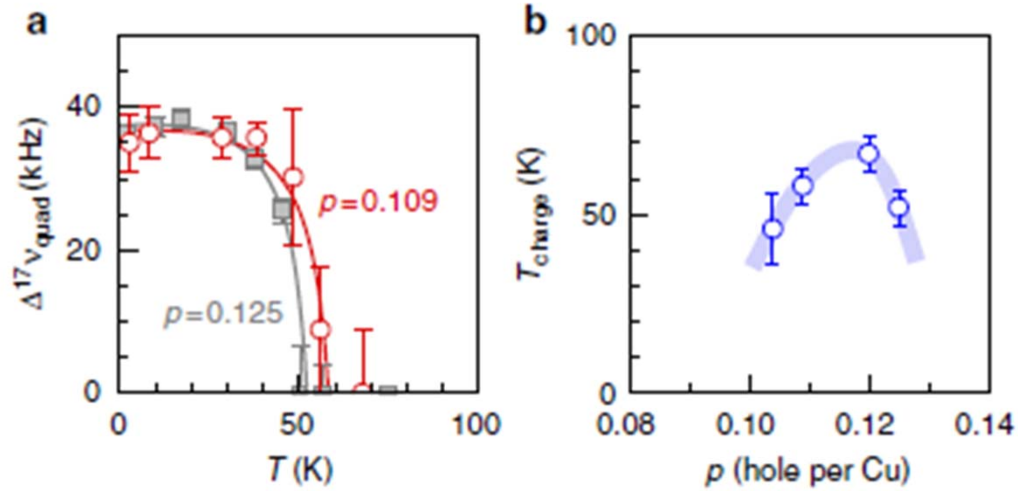
A first order transition?



Tao Wu, H. Mayaffre, … & M.-H. Julien
Nat. Commun. **4**, 2113 (2013).

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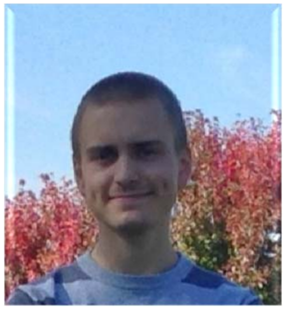

Charles-David Hébert

Patrick Sémon

Bandwidth control and doping control of the Mott transition in organics

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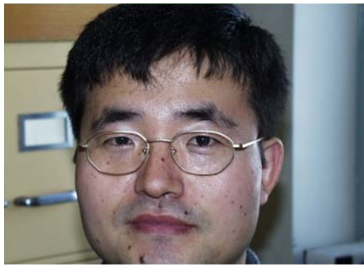
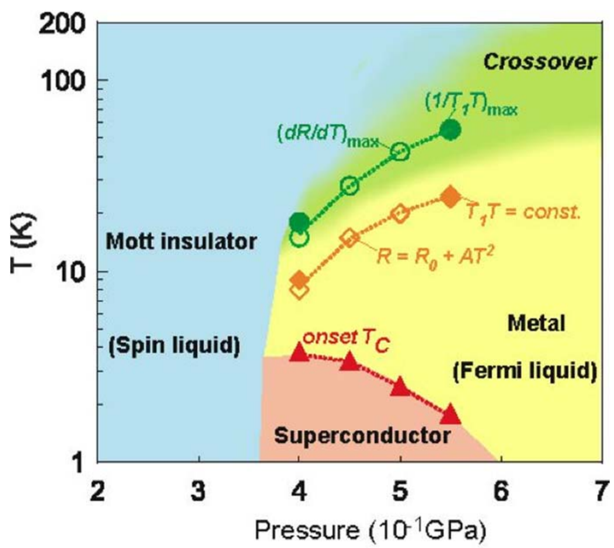


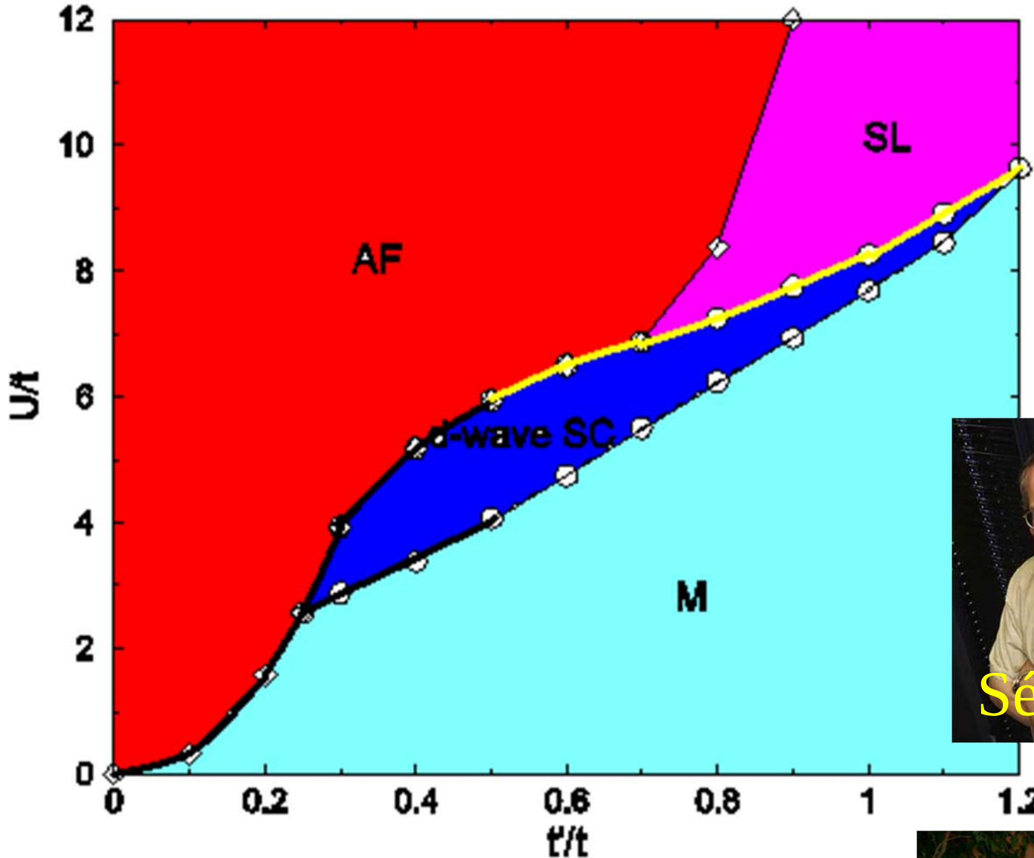
Theoretical phase diagram BEDT

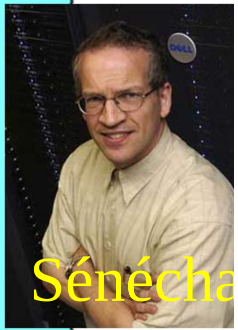
$X = Cu_2(CN)_3$ (t'~ t)



Y. Kurisaki, et al.

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



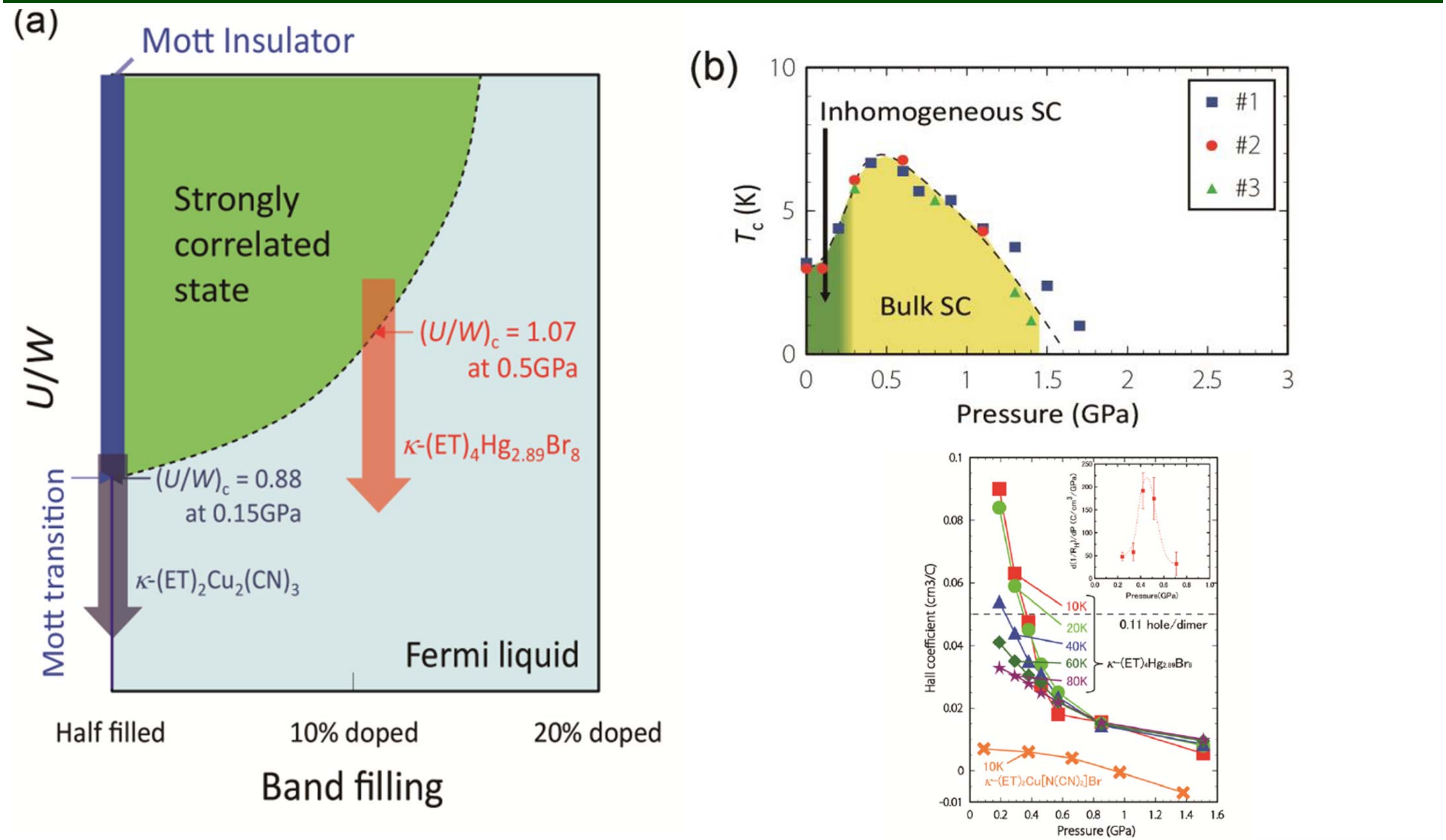


Kyung, A.-M.S.T. PRL 97, 046402 (2006)

Sénéchal, Sahebsara, Phys. Rev. Lett. **97**, 257004

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

Doped BEDT



H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

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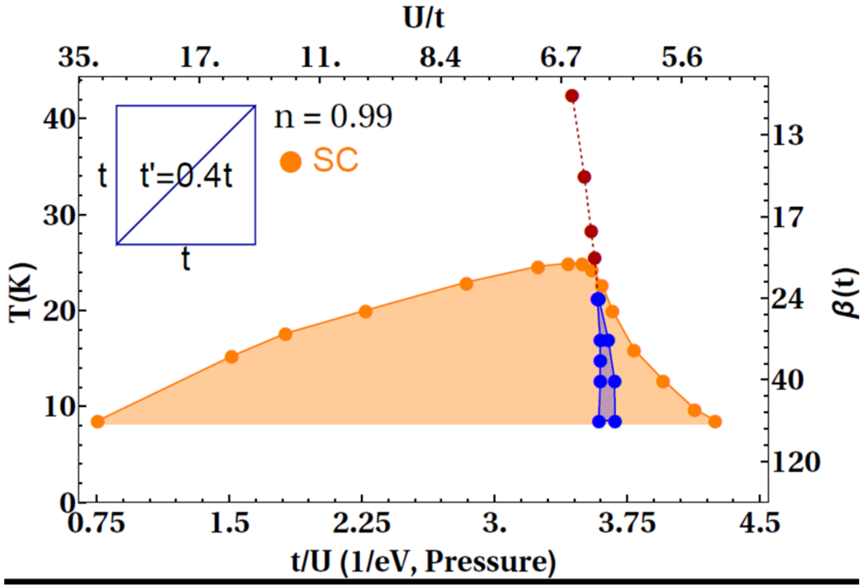
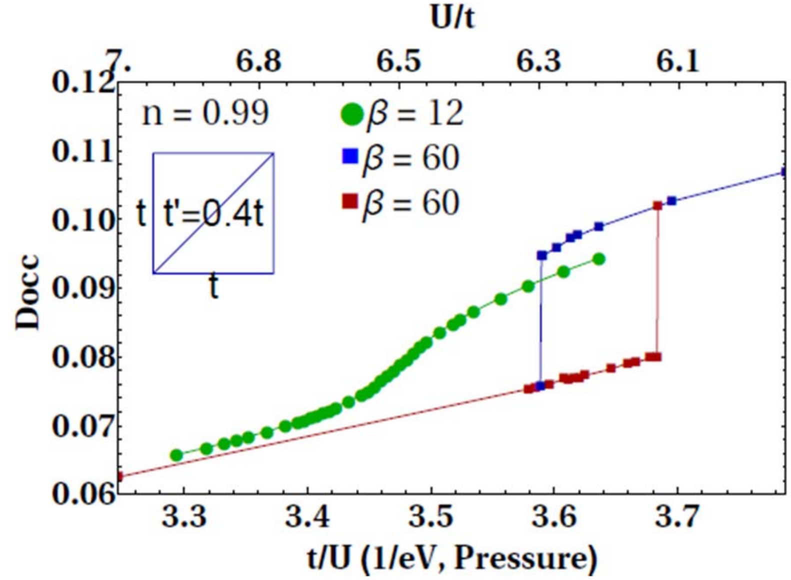
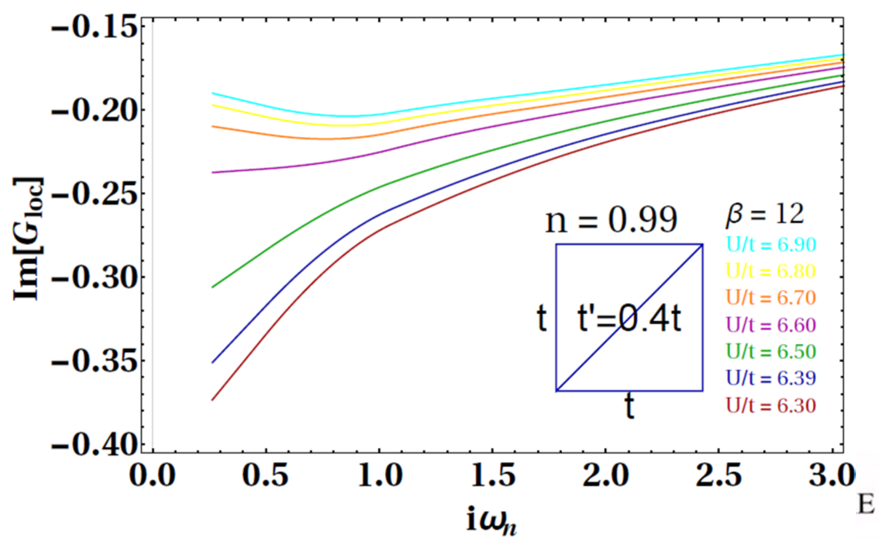
Widom line in organics

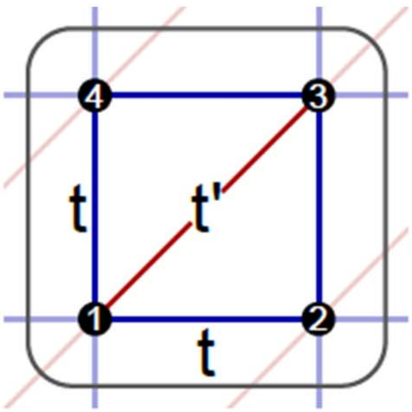


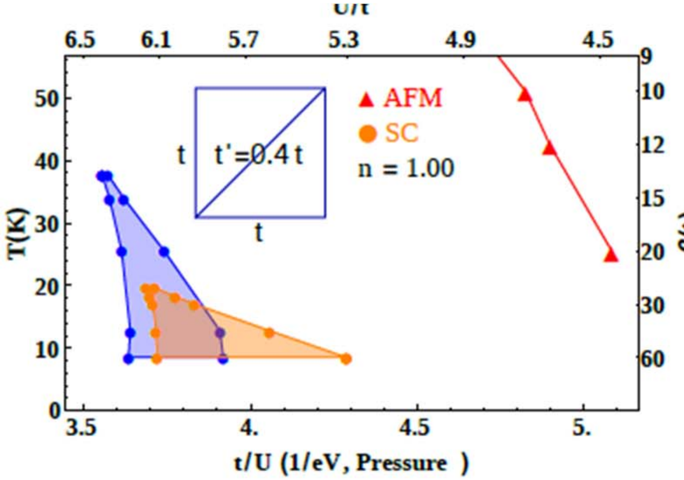




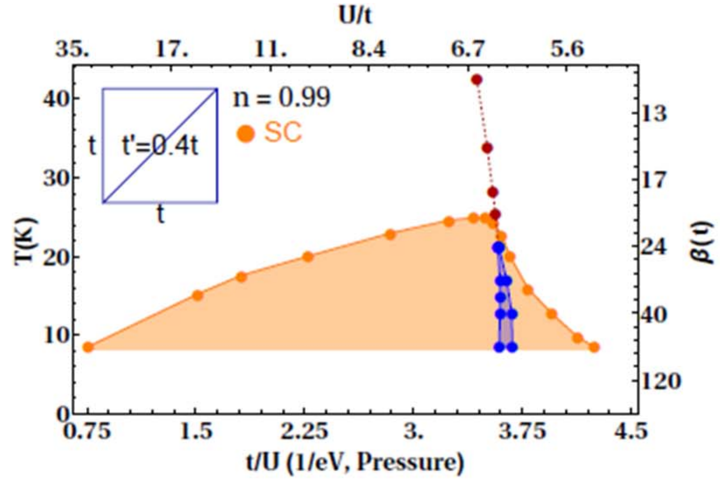
Charles-David Hébert, Patrick Sémon , AMT

t’=0.4t

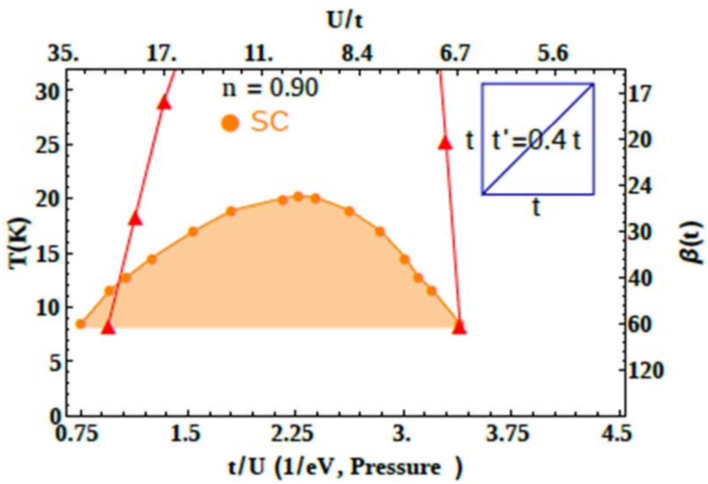


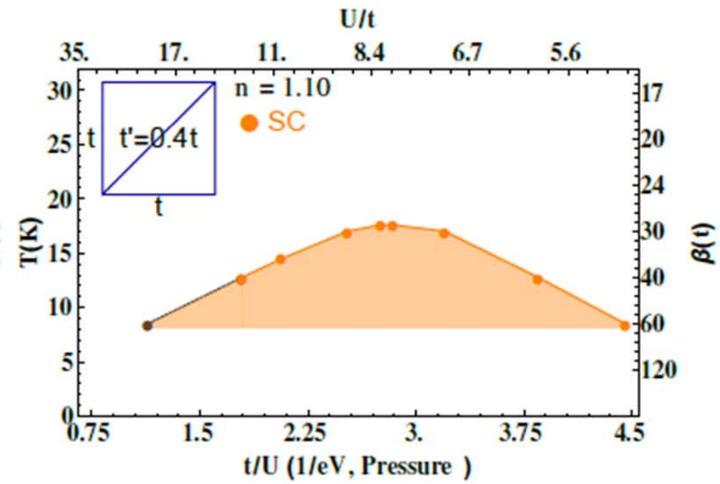


(a)



(b)





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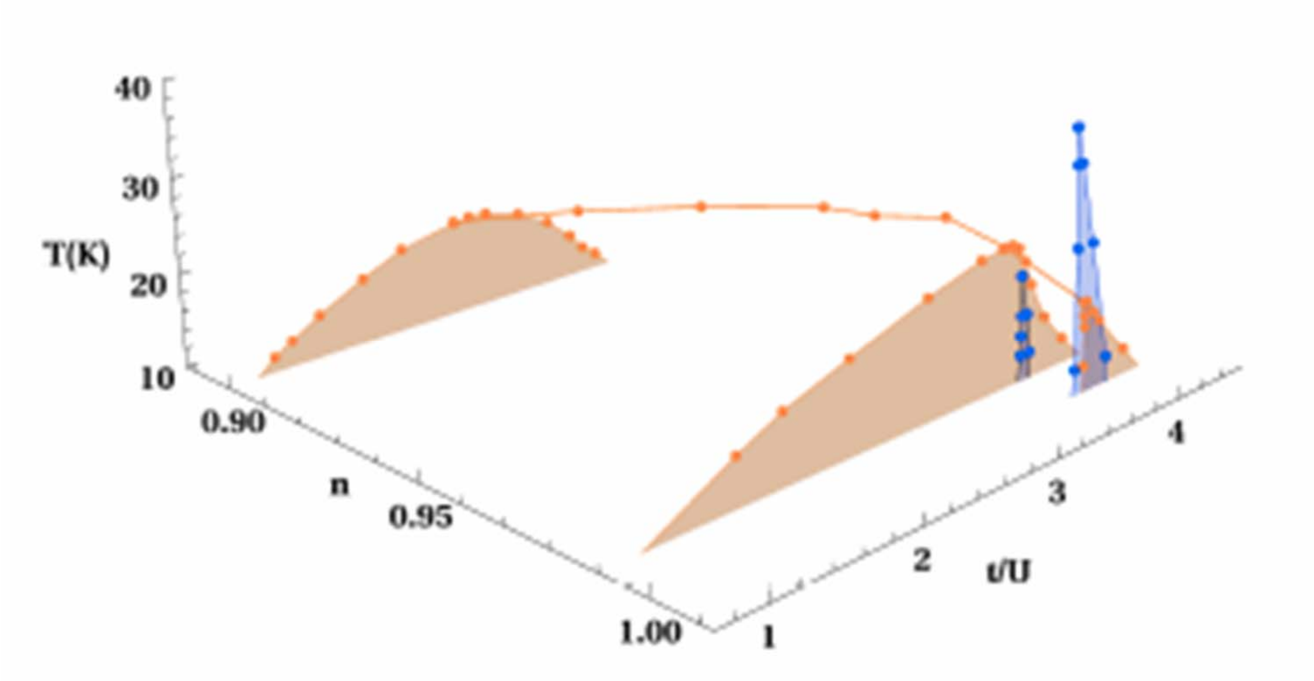
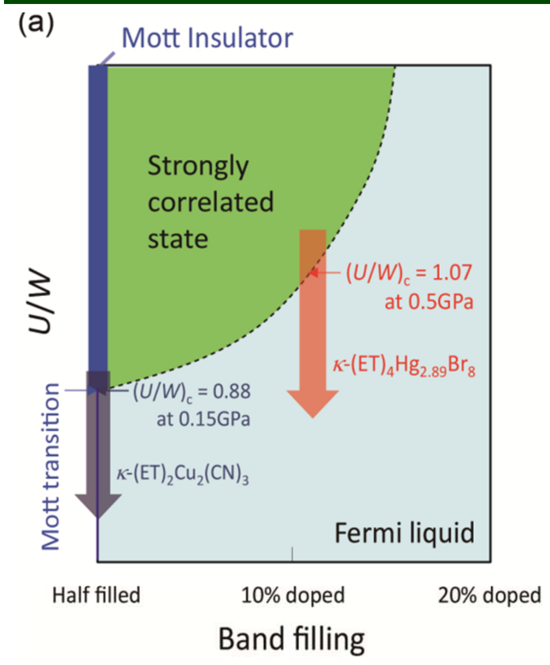
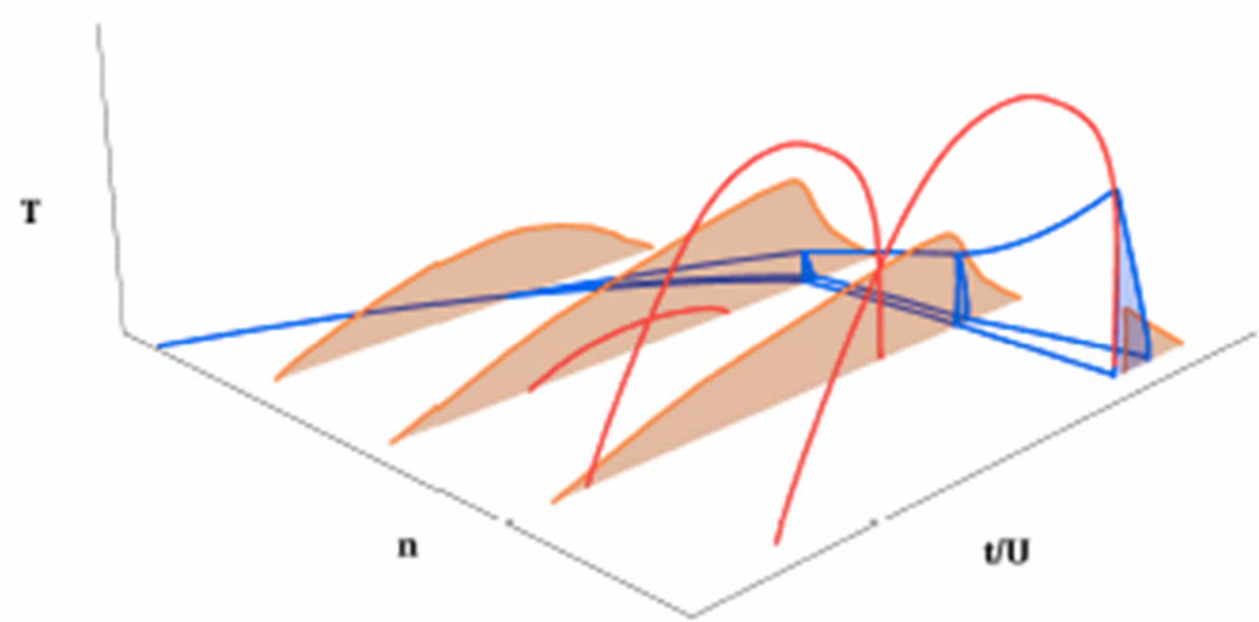
t’ = 0.4t overview



Generic case





Summary : organics

- Agreement with experiment
  - SC: larger T_c and broader P range if doped
  - Larger frustration: Decrease T_N and T_c
  - Normal state metal to pseudogap crossover
- Predictions
  - First order transition at low T in normal state (or remnants in SC state)
- Physics
  - SC dome without a AFM-QCP. Follows first-order.
  - SC from short range J.
  - T_c decreases at Widom line

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Main collaborators

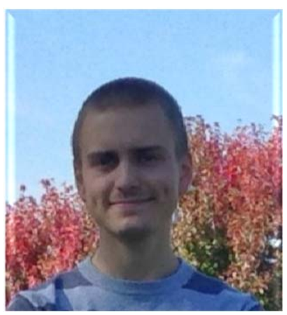

Giovanni Sordi


Kristjan Haule


David Sénéchal

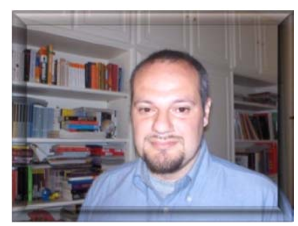

Bumsoo Kyung


Patrick Sémon


Charles-David Hébert


Sarma Kancharla


Marcello Civelli


Massimo Capone


Gabriel Kotliar

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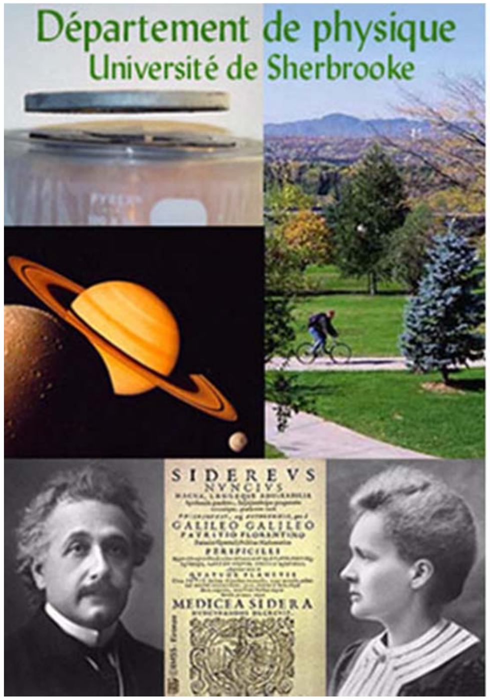

André-Marie Tremblay

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Merci

Thank you

A.-M.S. Tremblay

"Strongly correlated superconductivity"

Chapt. 10 : *Emergent Phenomena in Correlated Matter Modeling and Simulation, Vol. 3*, E. Pavarini, E. Koch, and U. Schollwöck (eds.)

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