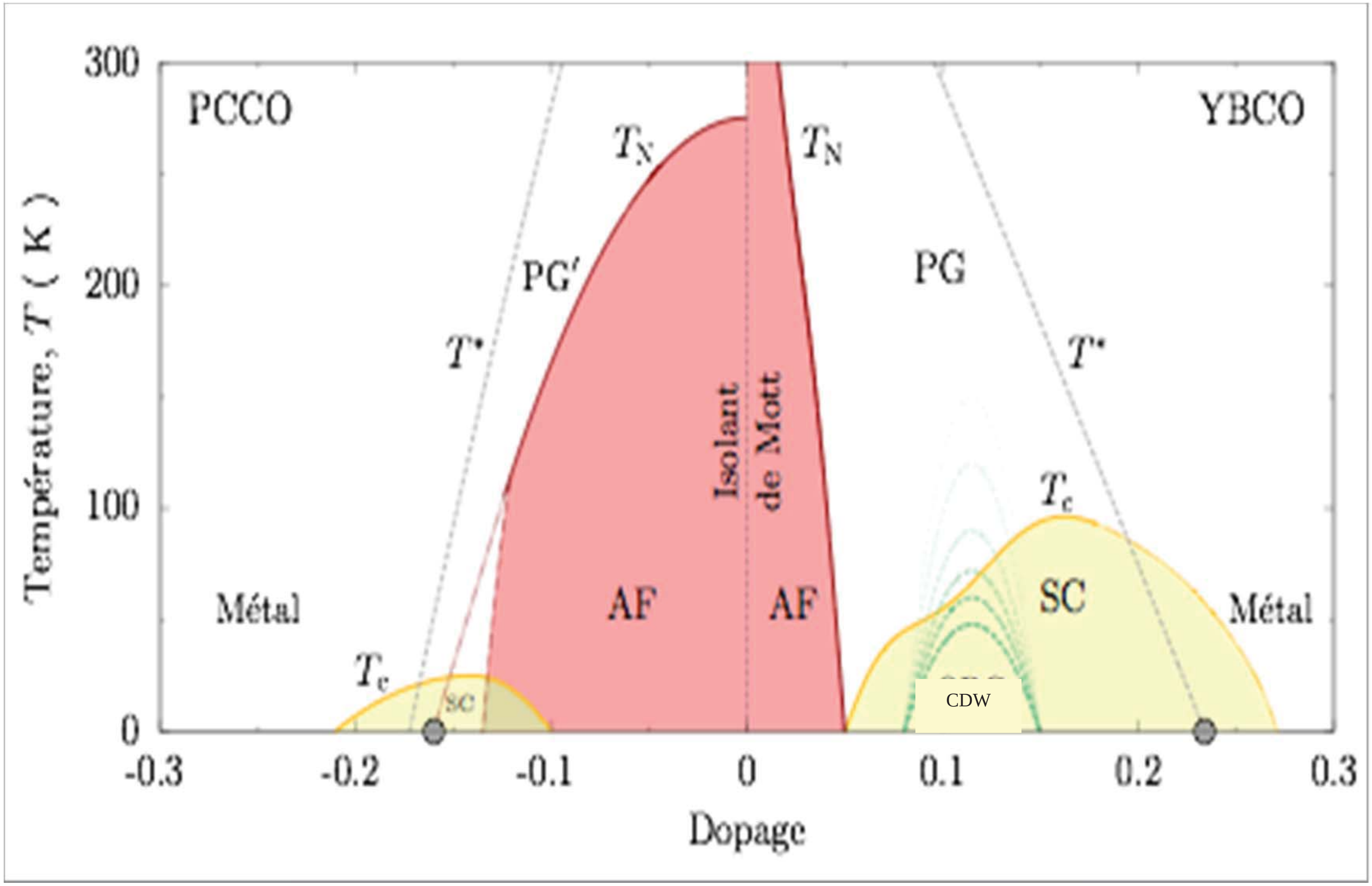
6. Charge Density Wave

h-doped

Our road map



Thèse de Francis Laliberté,
Université de Sherbrooke

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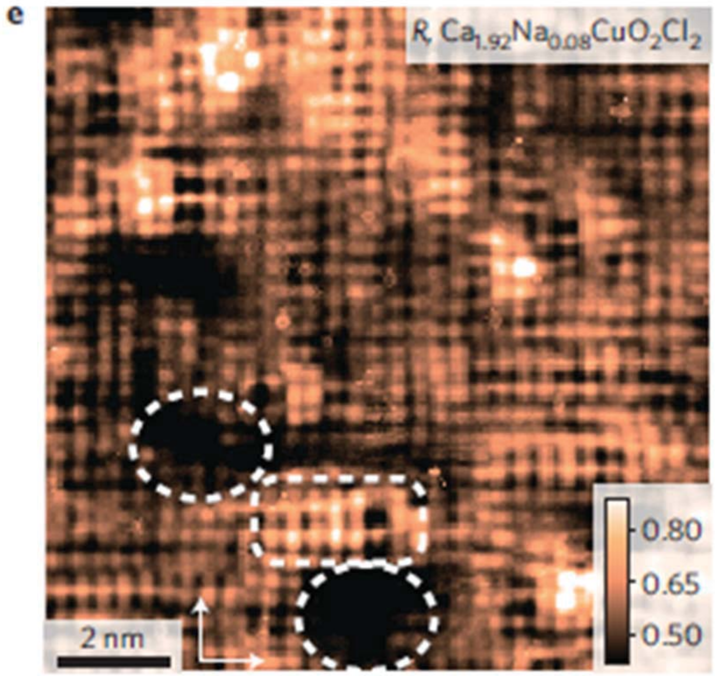
Intra-unit cell nematic order: STM



Kohsaka et al. Nature Physics 2012

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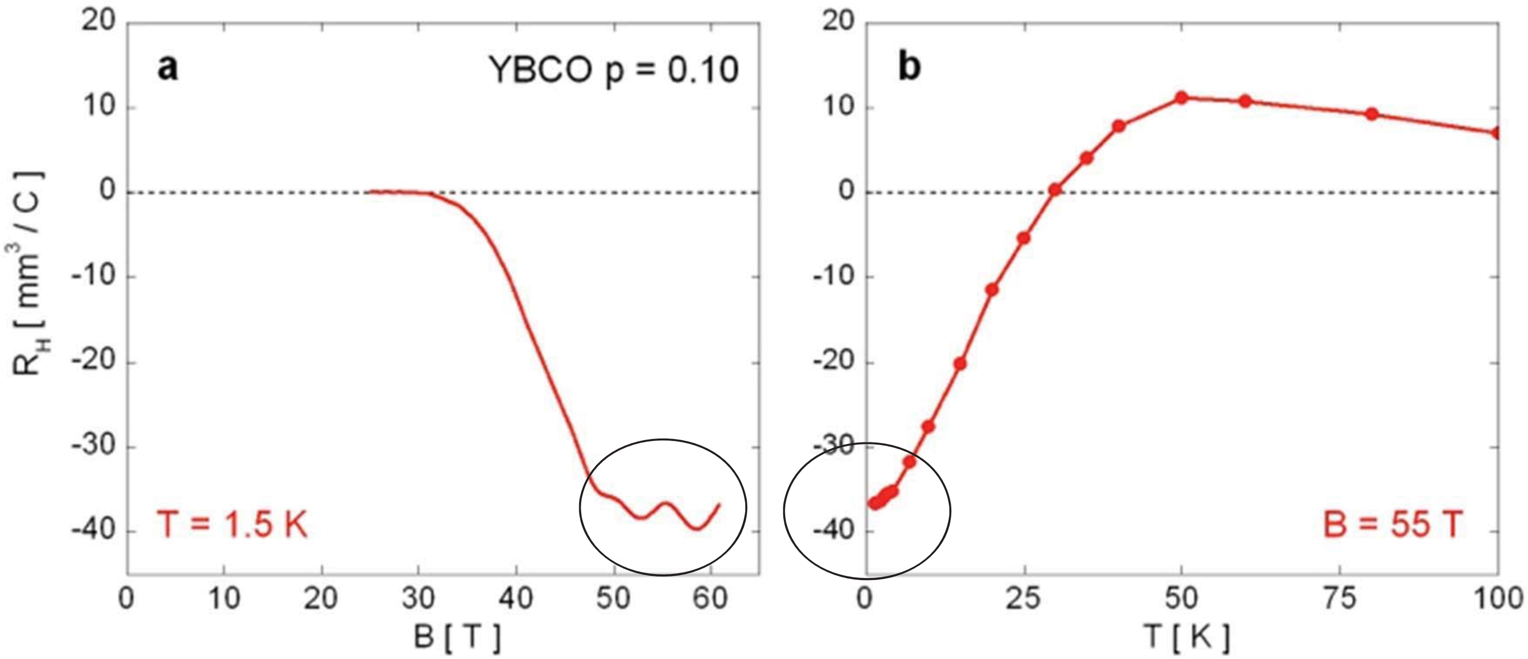
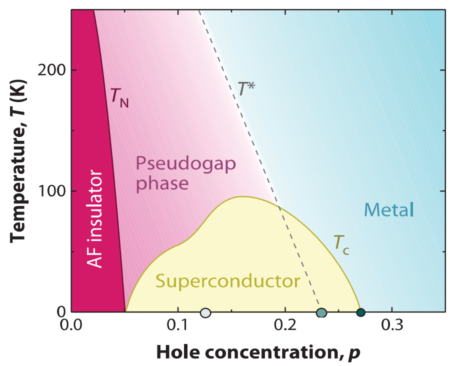
Quantum oscillations in cuprates: 2007

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 !

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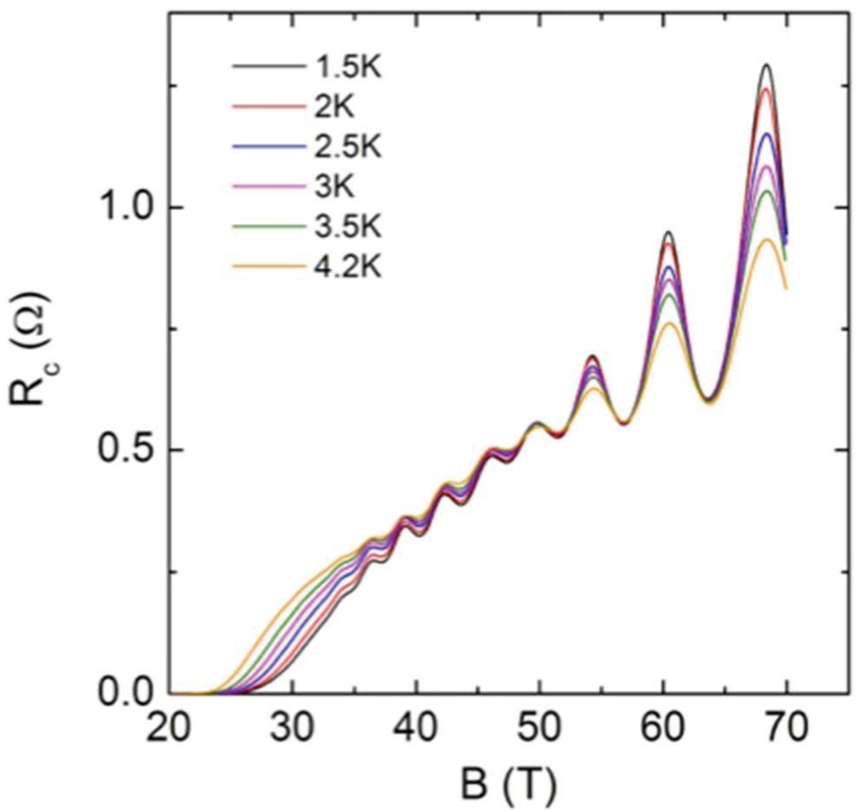
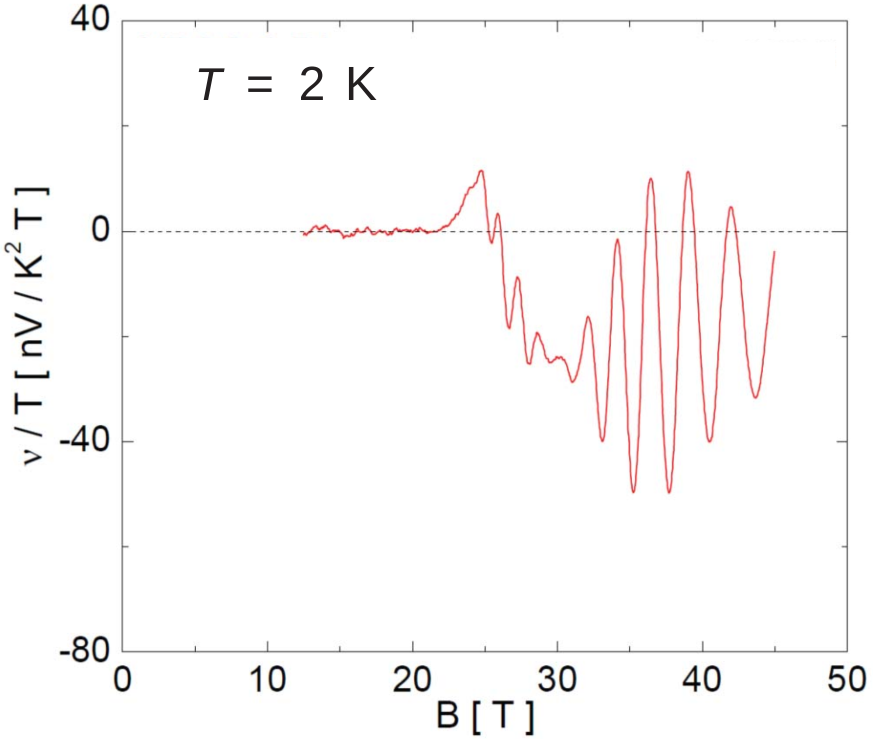
Quantum oscillations in cuprates: 2013

Resistance



LNCMI, Toulouse

Nernst



NHMFL, Tallahassee

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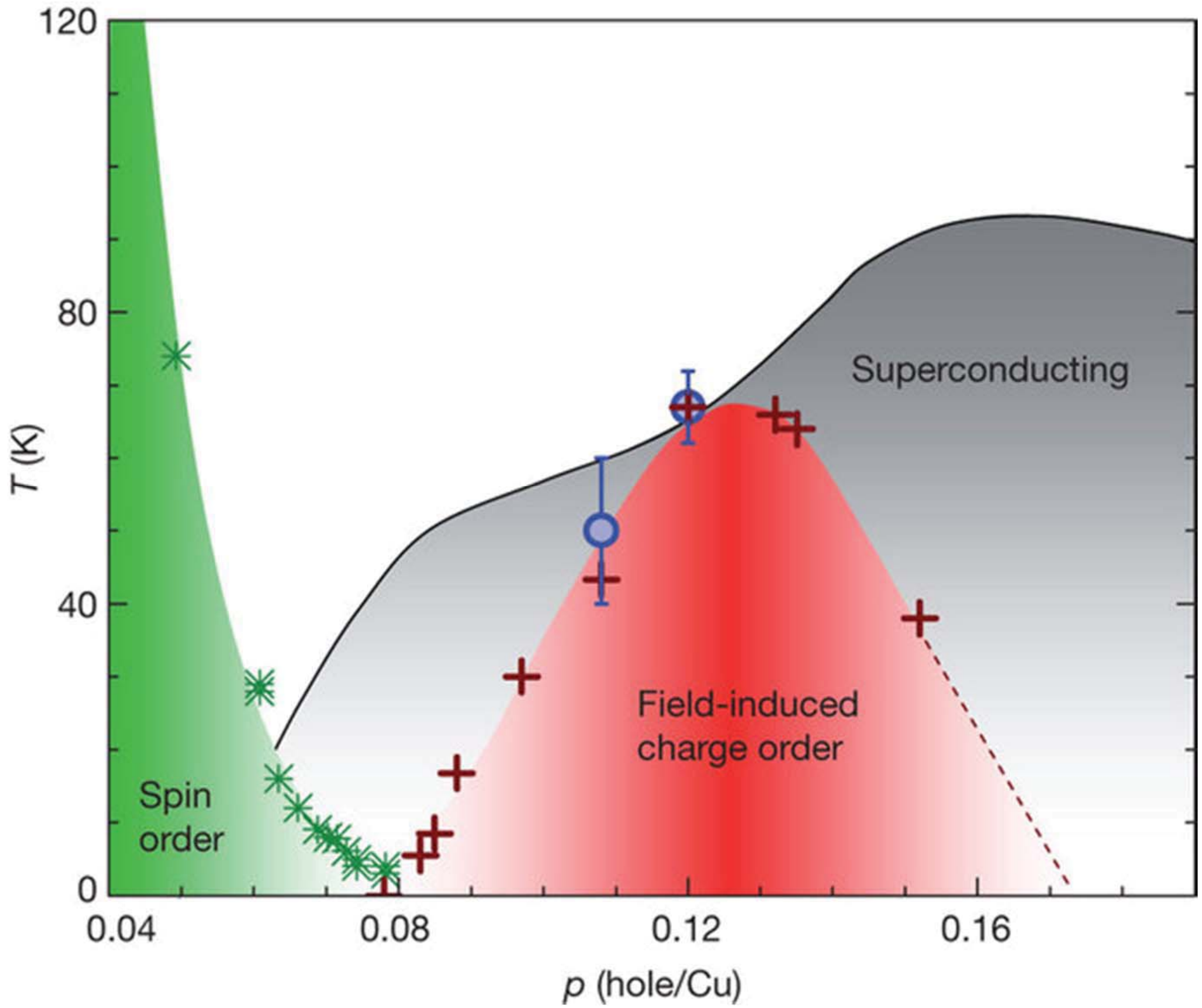
Stripes and reconstructed Fermi surface



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

Competing CDW order

- Wise, W. D. et al. Charge-density-wave origin of cuprate checkerboard visualized by scanning tunnelling microscopy. Nature Phys. 4, 696699 (2008).
- 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]

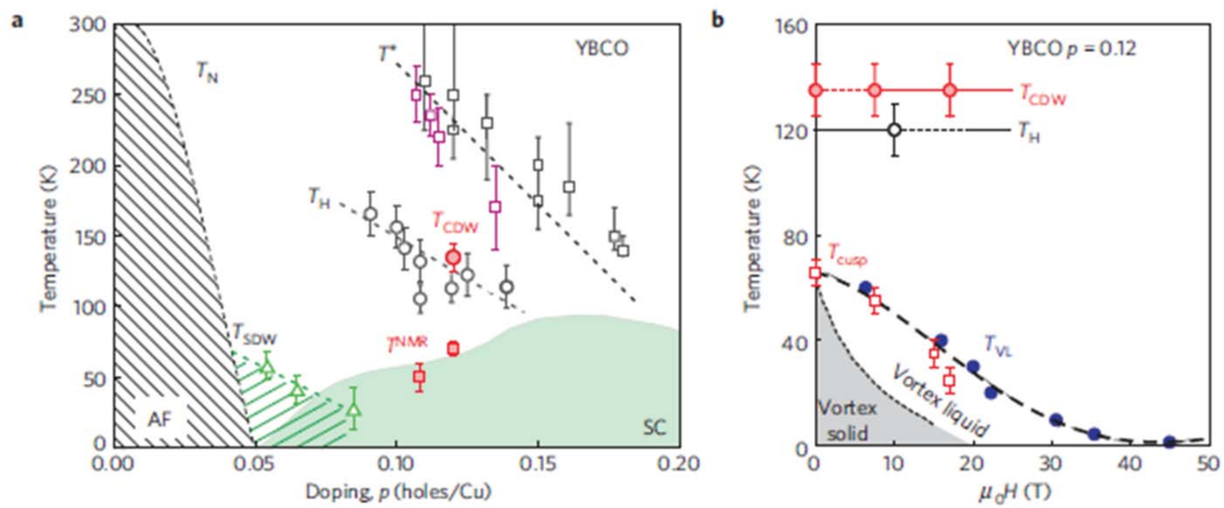
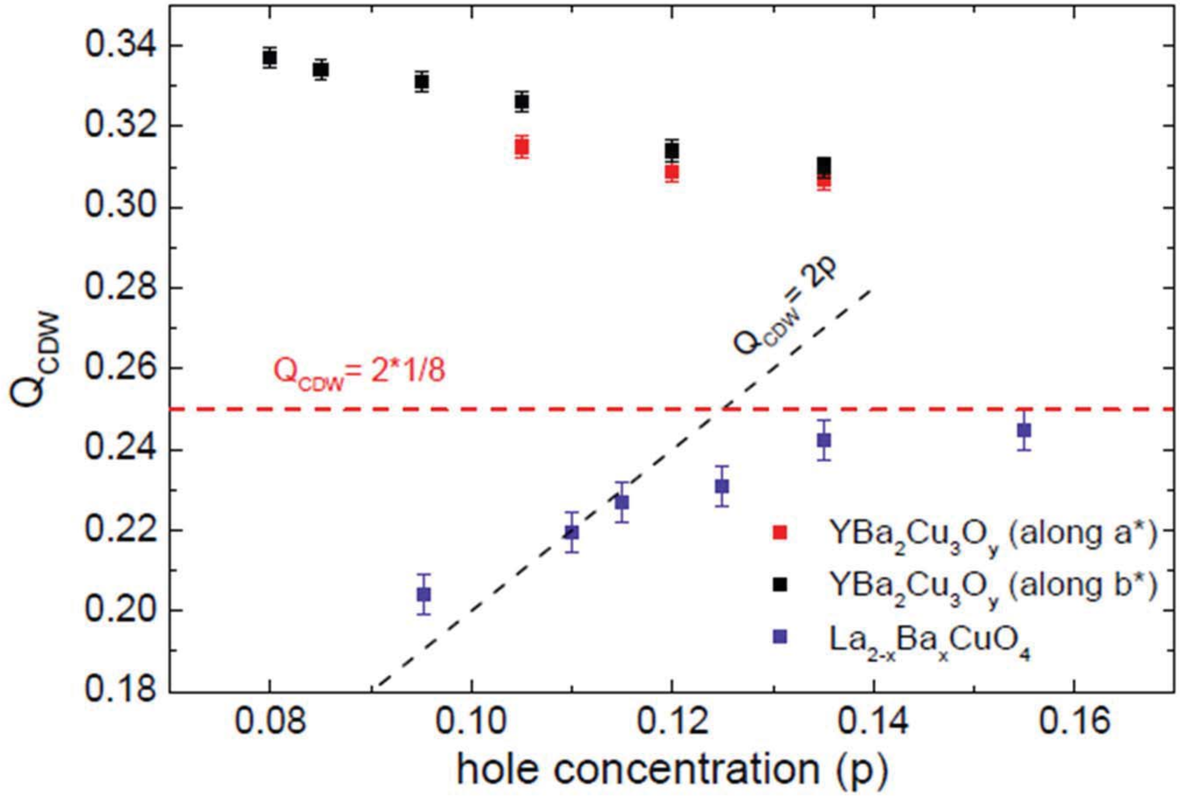


Figure 4 | Phase diagram of $YBa_2Cu_3O_{7-x}$. a, Doping dependence of the antiferromagnetic ordering temperature T_N, the incommensurate spin-density wave order T_{SDW} (green triangles; ref. 21), the superconducting temperature T_c and the pseudogap temperature T^* as determined from the Nernst effect[30] (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

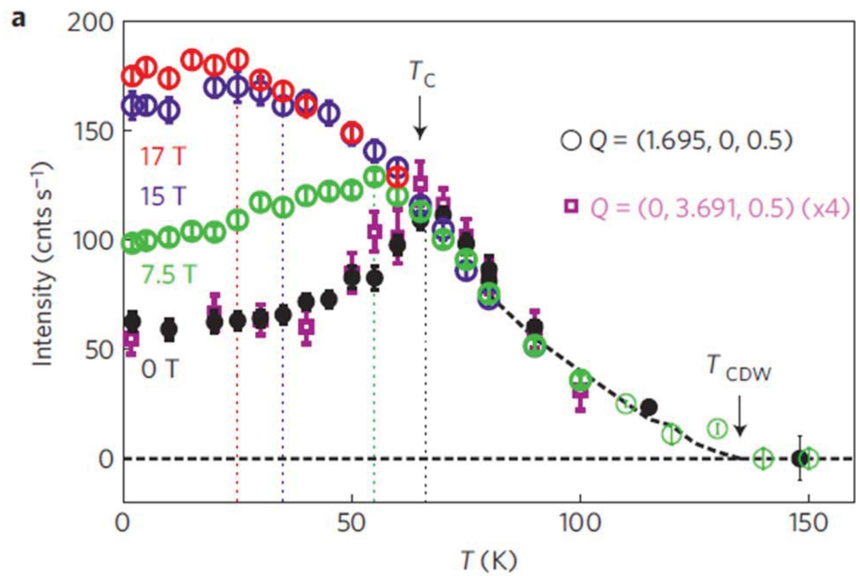
S. Sachdev and R. La Placa Phys. Rev. Lett. **111**, 027202 (2013)
D. Chowdhury, S. Sachdev arxiv. 1501.00002

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

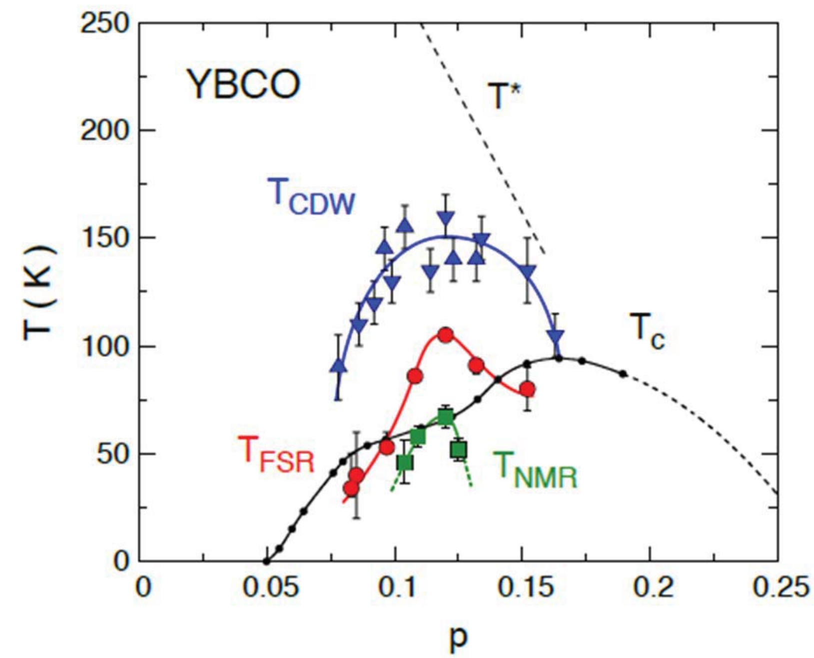
Y. Wang and A. Chubukov, Phys. Rev. B 90, 035149 (2014).

…

Competition between CDW and SC

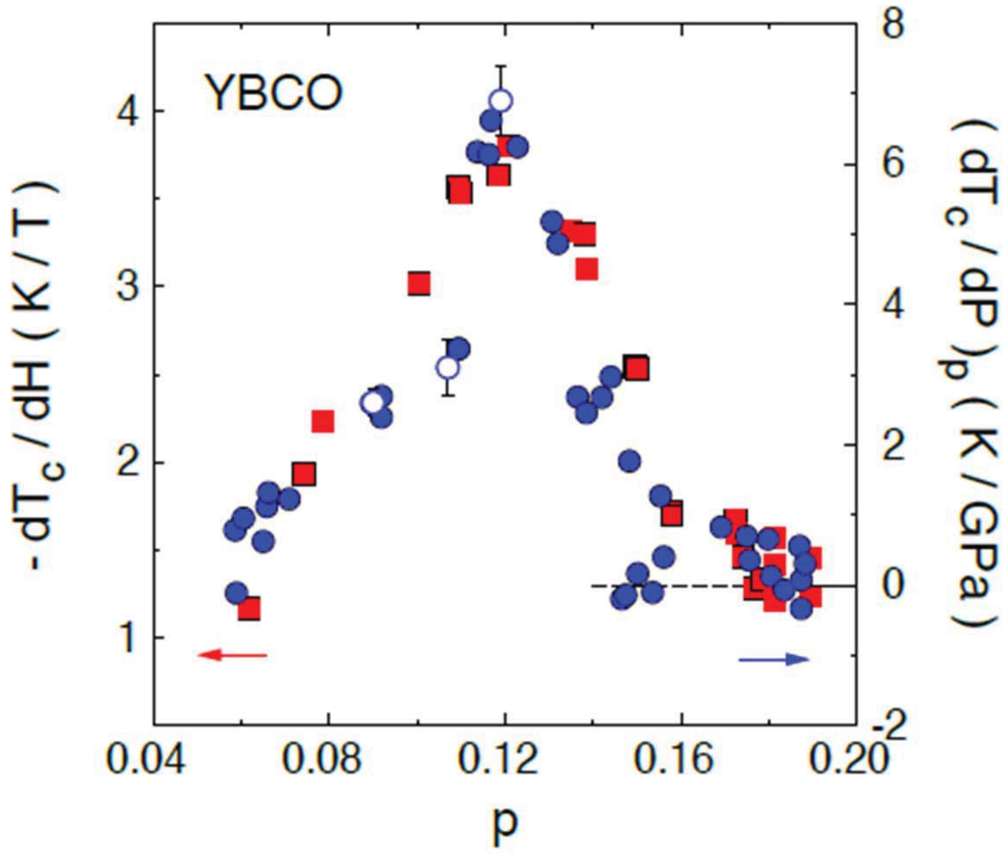


J. Chang *et al.*, *Nat. Phys.* **8**, 871-876 (2012).



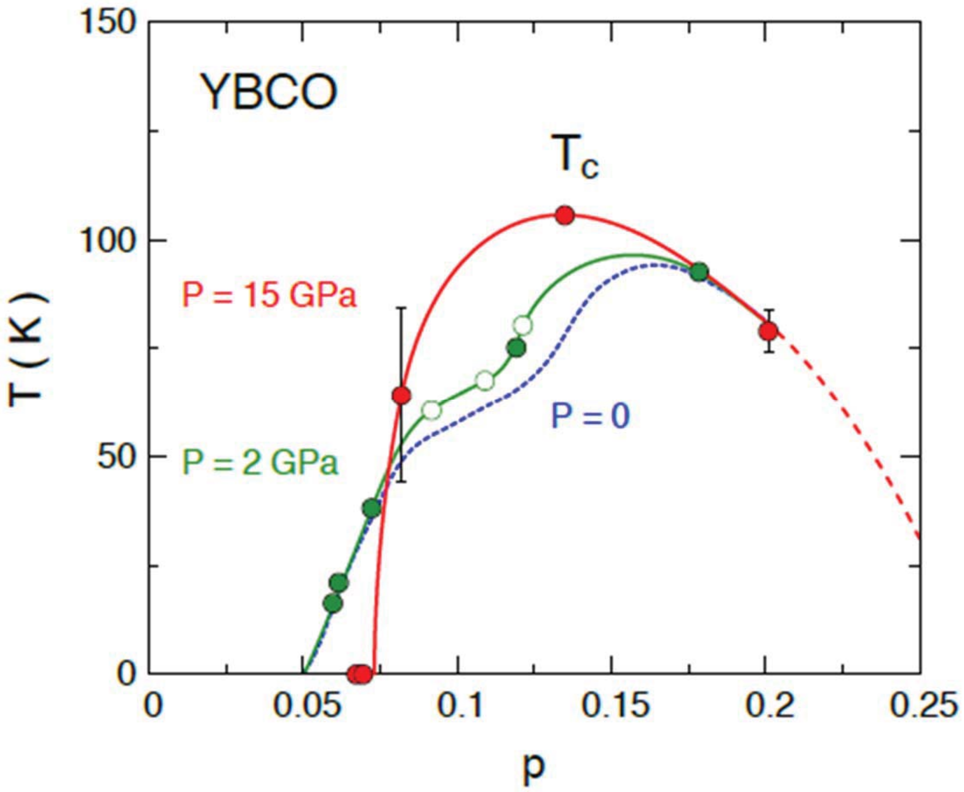
Cyr-Choinière et al, arxiv1503.02033

Tuning SC and CDW



Cyr-Choinière et al, arxiv1503.02033

Getting rid of the CDW



Cyr-Choinière et al, arxiv1503.02033

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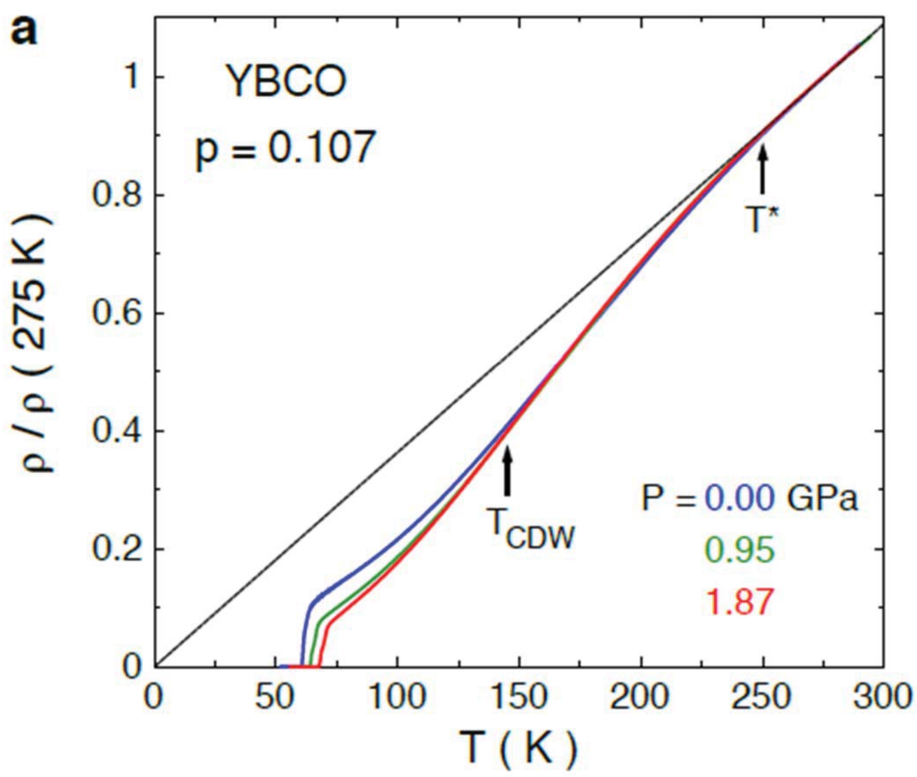
T* not affected

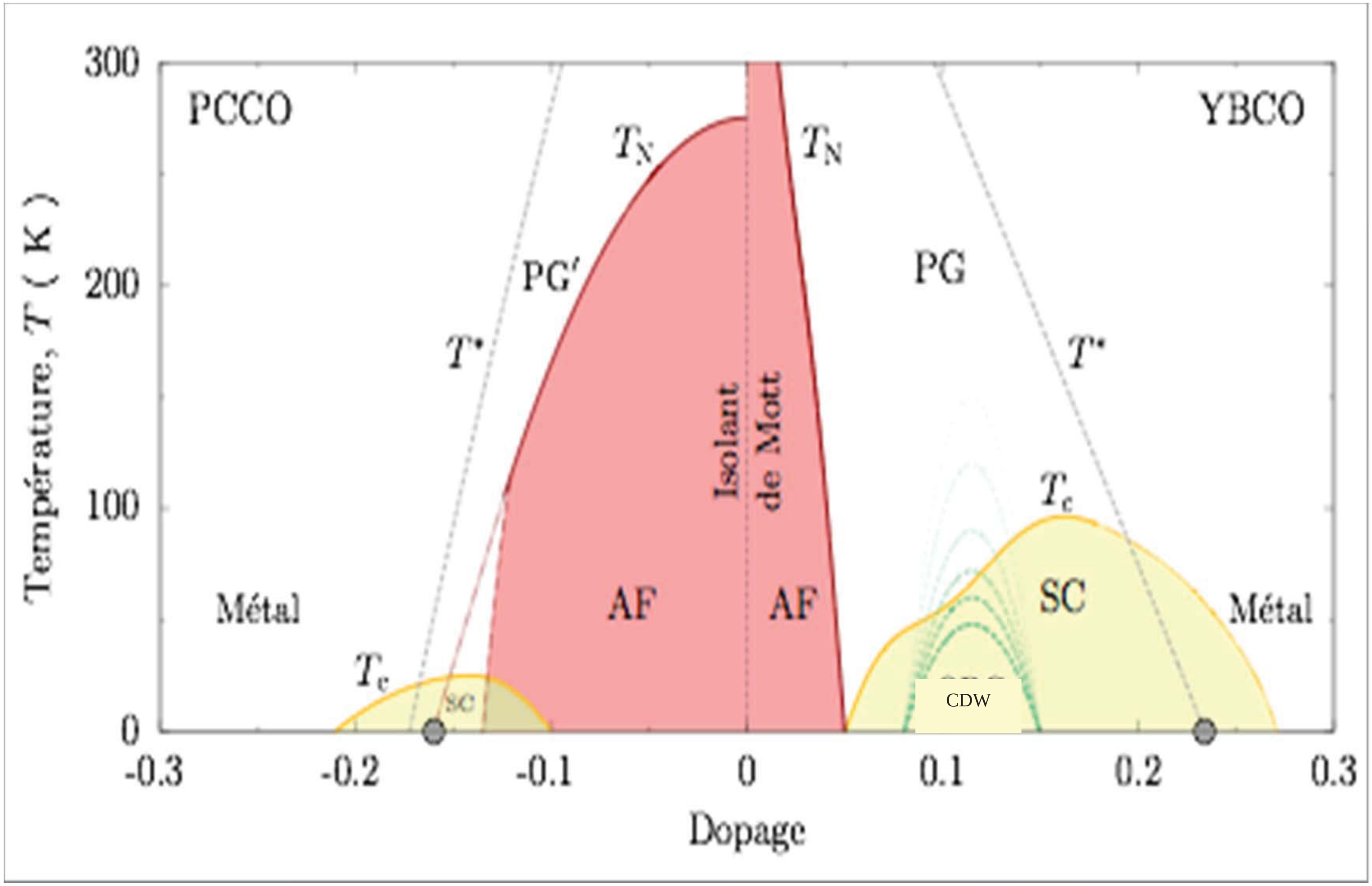


Cyr-Choinière et al, arxiv1503.02033

7. Pseudogap

h-doped

Our road map



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Université de Sherbrooke

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Three classes of mechanisms

- Rounded first order transition
- *d* =*2* precursor to a lower temperature broken symmetry phase (e-doped)
- Mott physics (h-doped)

Consider first this Mott hypothesis (Cannot be CDW)

- 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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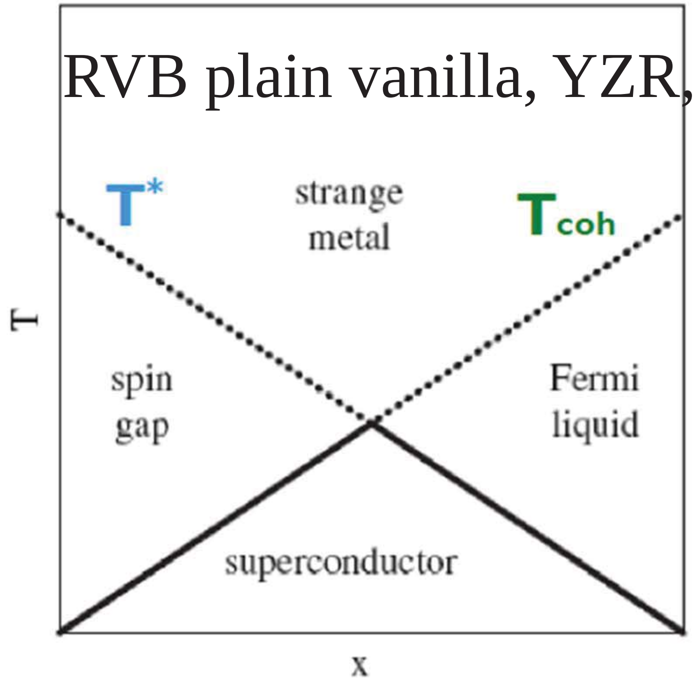
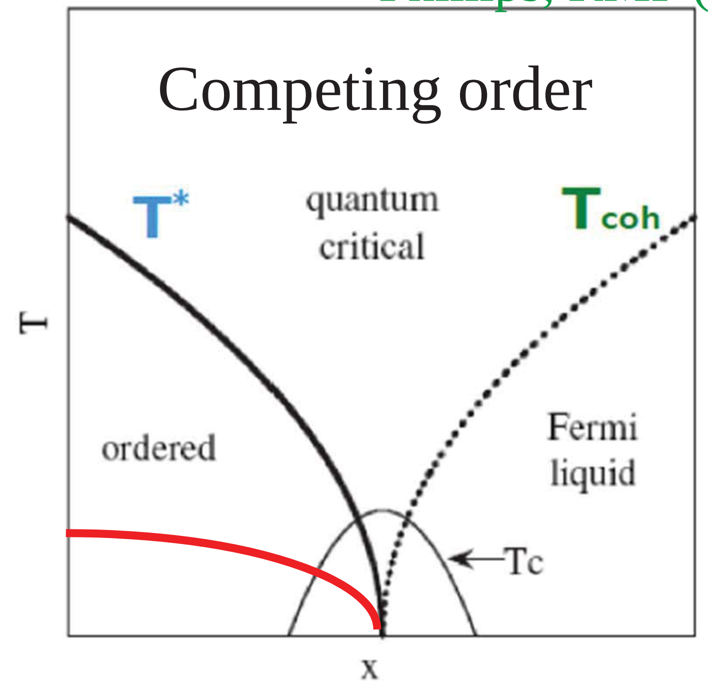
Three views (caricature)

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





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

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

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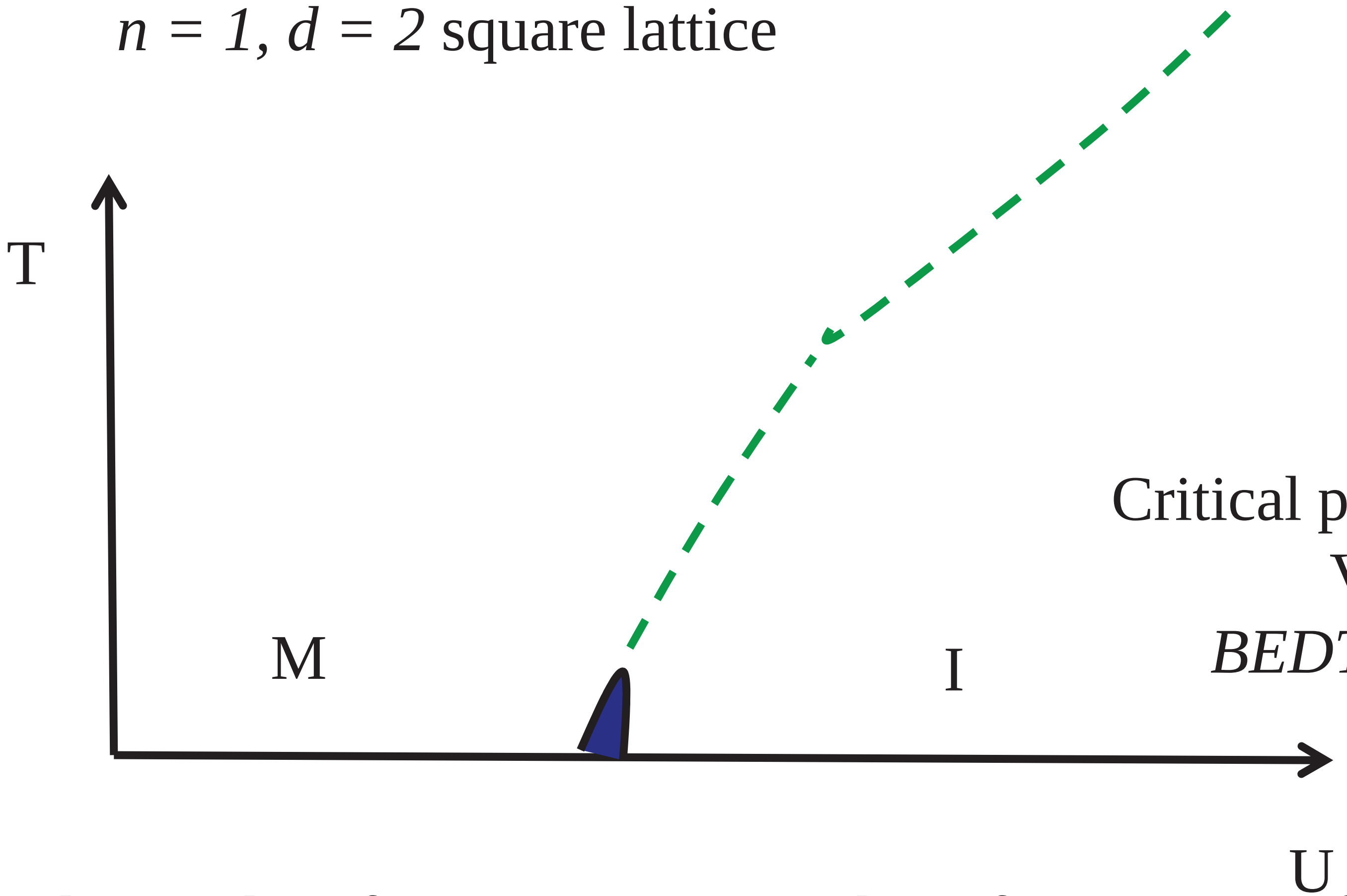
Local moment and Mott transition

n = 1, d = 2 square lattice



Critical point visible in
V_2O_3,
BEDT organics

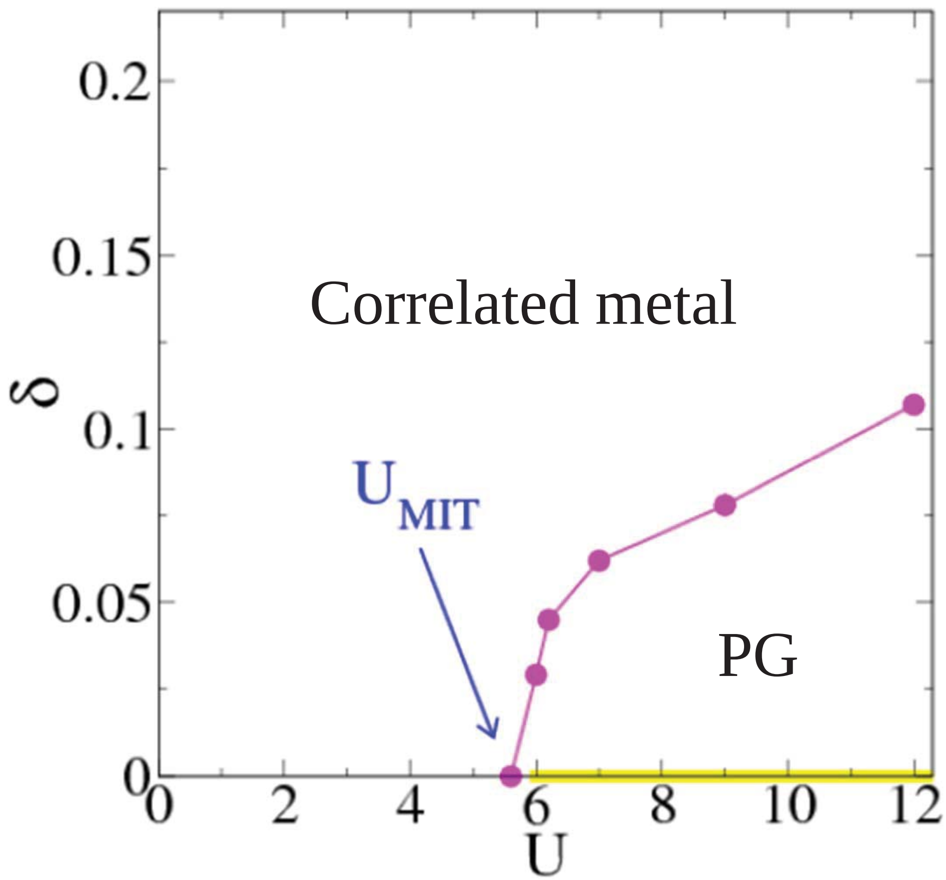
Understanding finite temperature phase from a *mean-field theory* down to $T = 0$

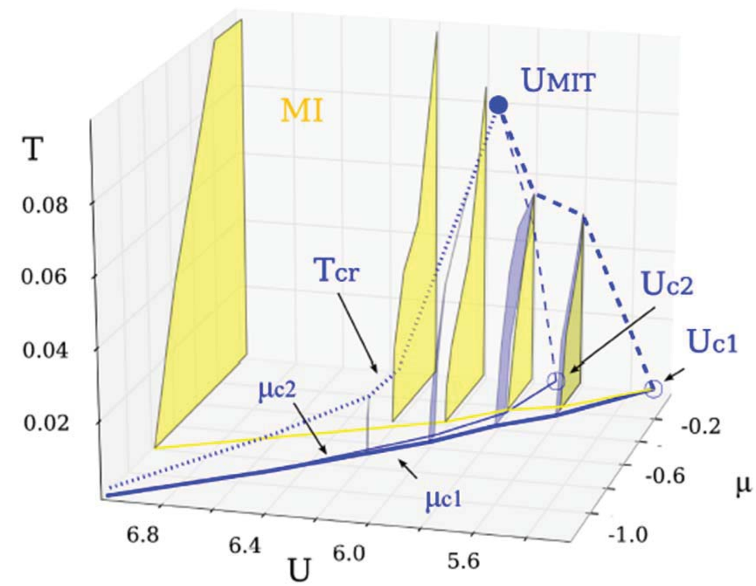
Interaction-induced Mott transition, *n = 1*

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)

Link to Mott transition up to optimal doping

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





Sordi et al. PRL 2010, PRB 2011

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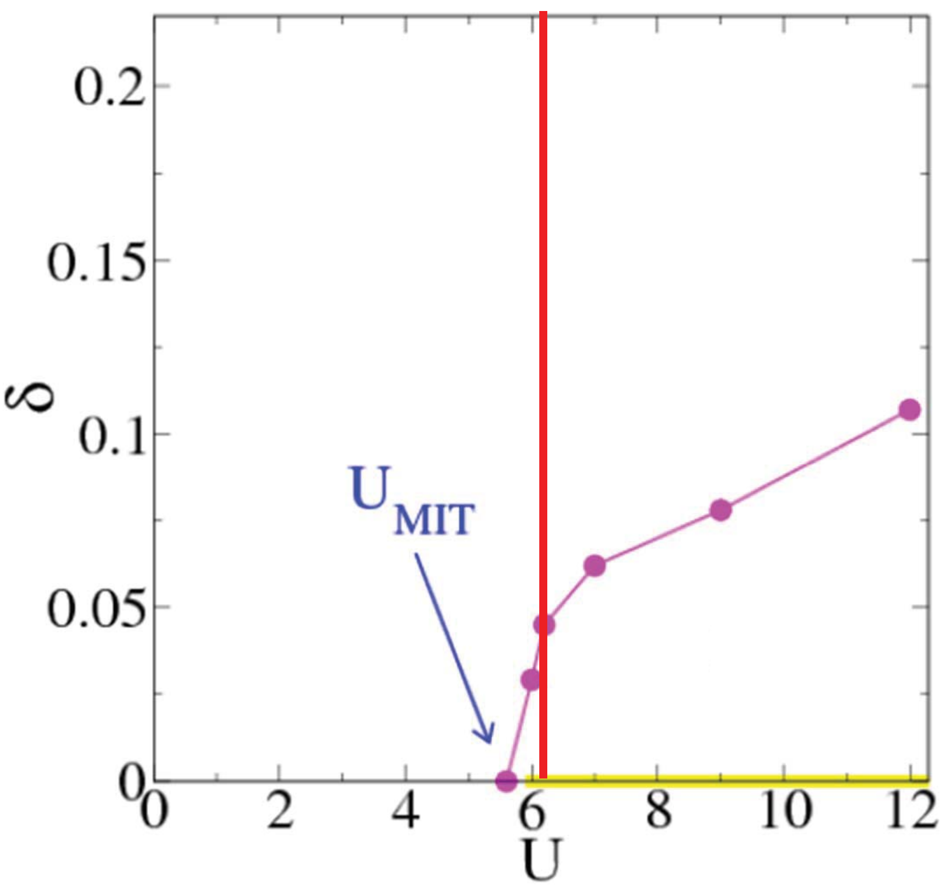
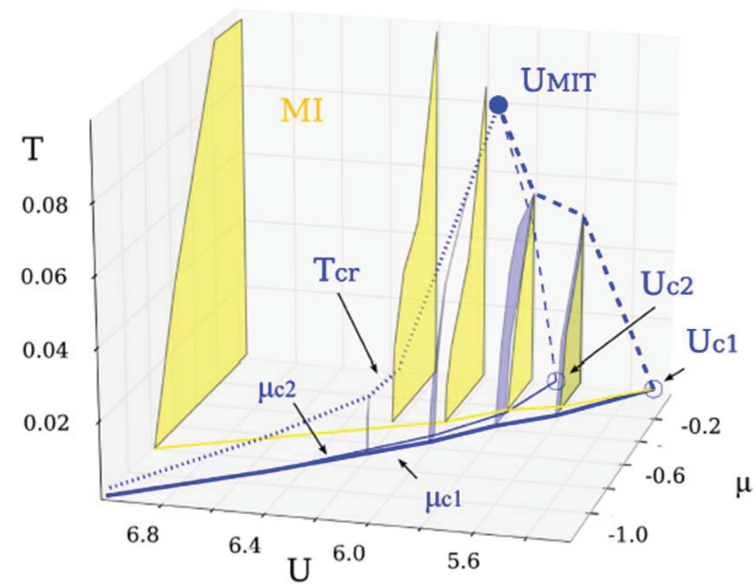
Link to Mott transition up to optimal doping
Another emergent transition

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



Smaller *D* and *S*



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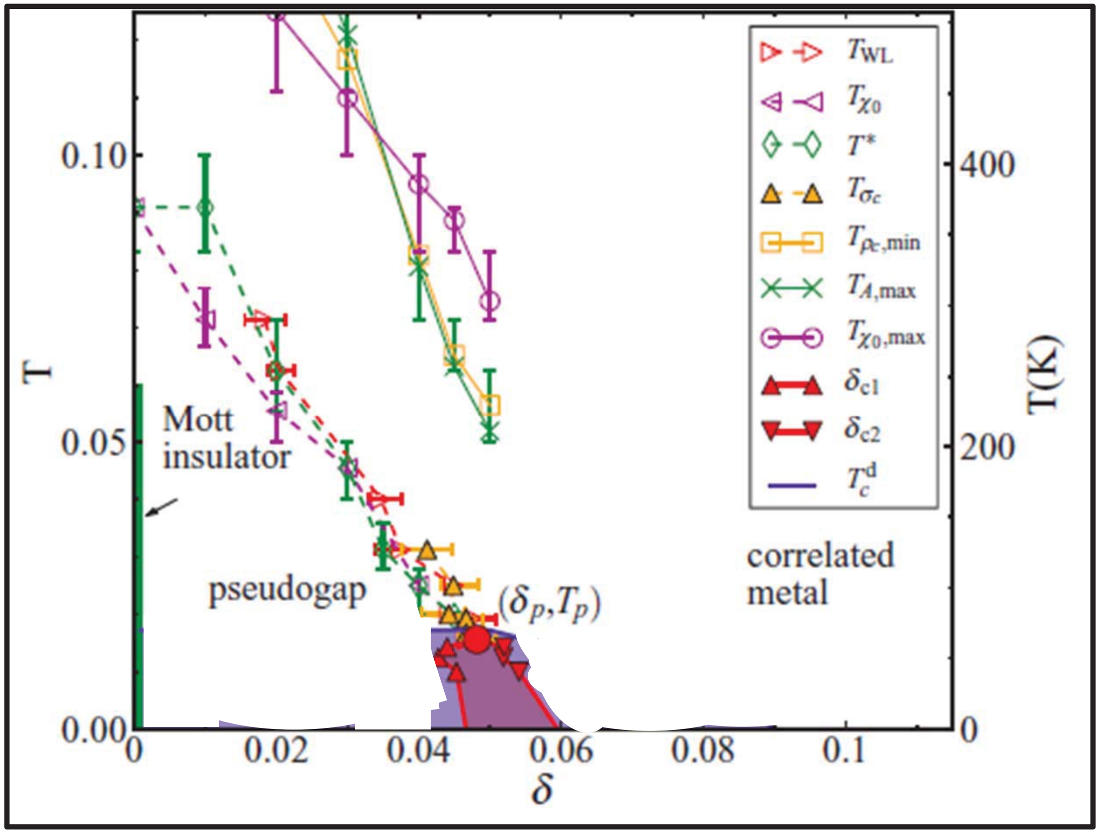
Two crossover lines



Sordi et al. PRL 108, 216401 (2012)
PRB **87**, 041101(R) (2013)

What is the minimal model?

Noninteracting case:

$$\chi^{0R}_{nn}(\mathbf{q},\omega) = -2\int \frac{d^3\mathbf{k}}{(2\pi)^3}\frac{f(\zeta_{\mathbf{k}})-f(\zeta_{\mathbf{k+q}})}{\omega+i\eta+\zeta_{\mathbf{k}}-\zeta_{\mathbf{k+q}}}$$

H. Alloul
Comptes Rendus Physique,
15, 519 (2014)

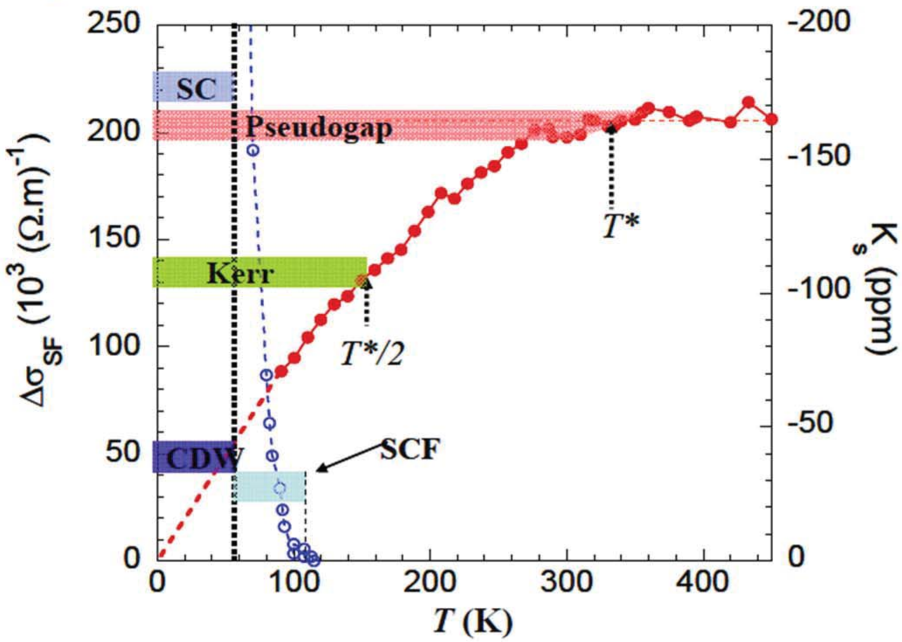


Fig 1 Spin contribution K_s to the ^{89}Y NMR Knight shift [11] for $YBCO_{6.6}$ permit to define the PG onset T^*. Here K_s is reduced by a factor two at $T \sim T^*/2$. The sharp drop of the SC fluctuation conductivity (SCF) is illustrated (left scale) [23]. We report as well the range over which a 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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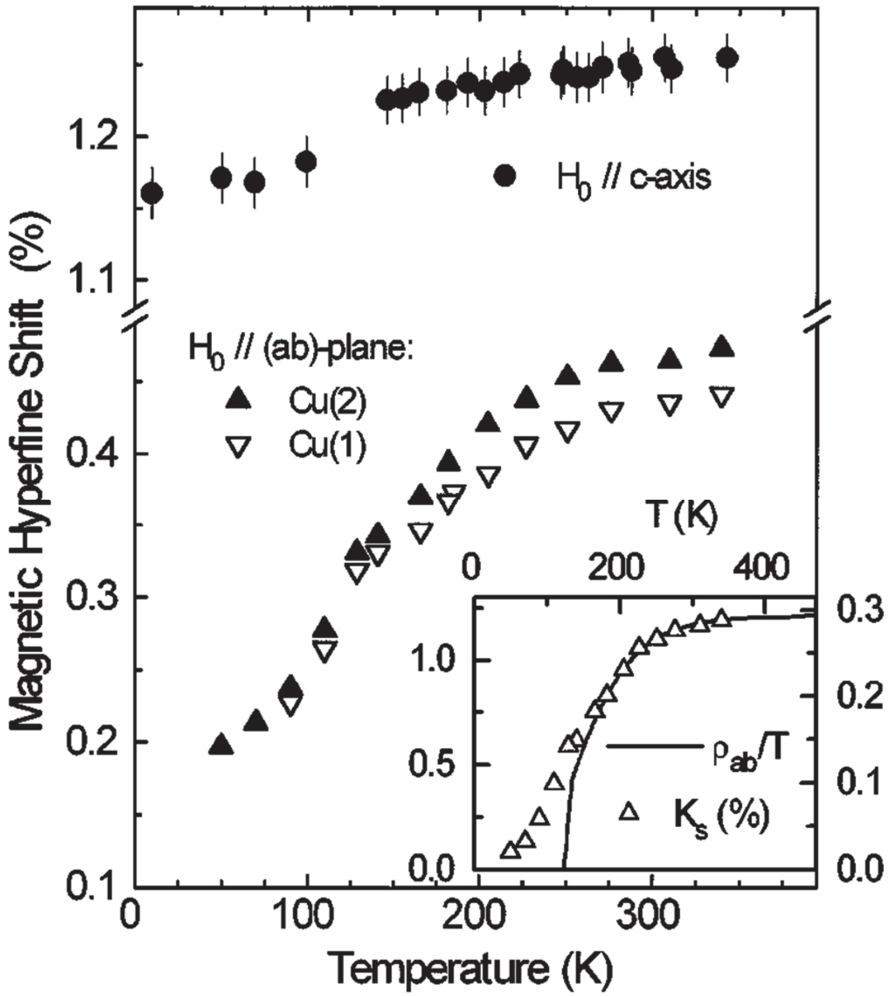
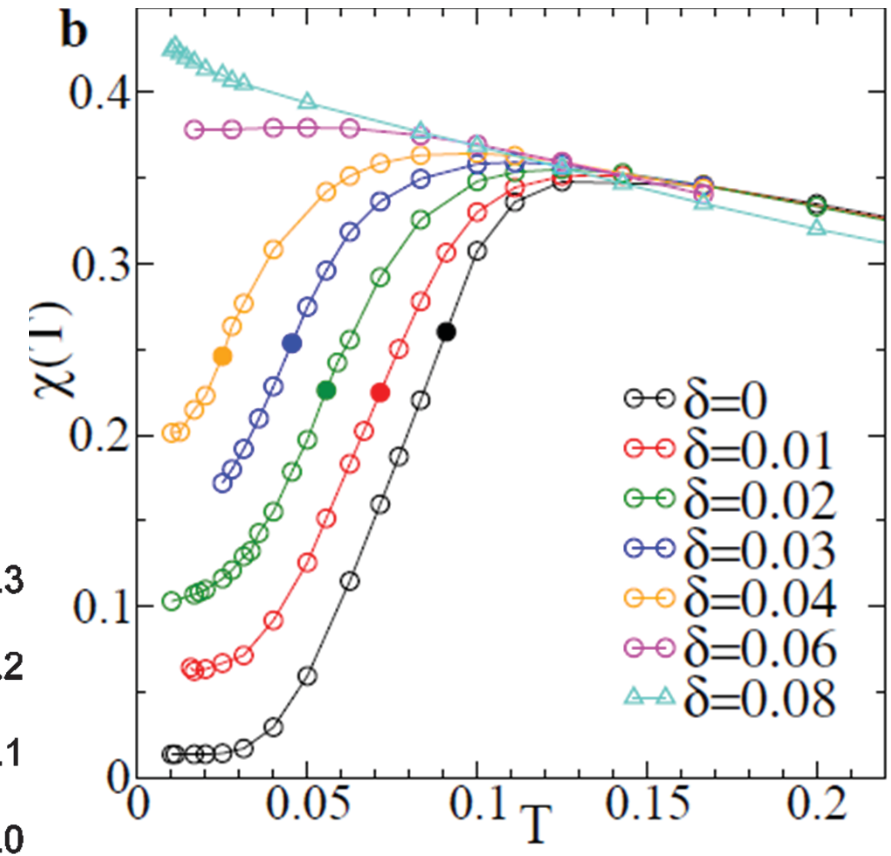
Spin susceptibility



Underdoped Hg1223

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



Sordi et al. Scientific Repts. 2012

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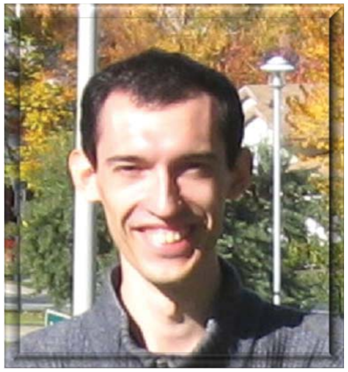

Giovanni Sordi

Patrick Sémon

Kristjan Haule

The Widom line

G. Sordi, *et al*. Scientific Reports 2, 547 (2012)

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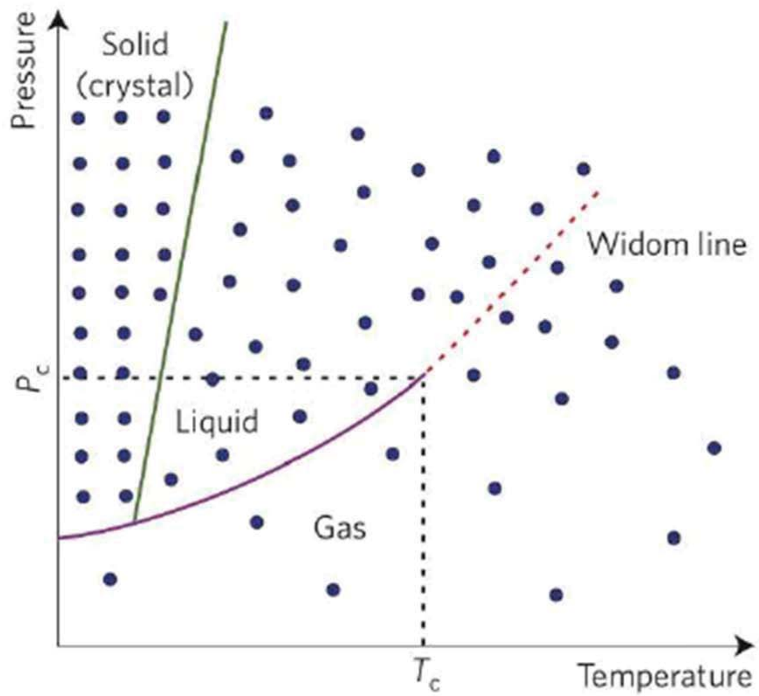
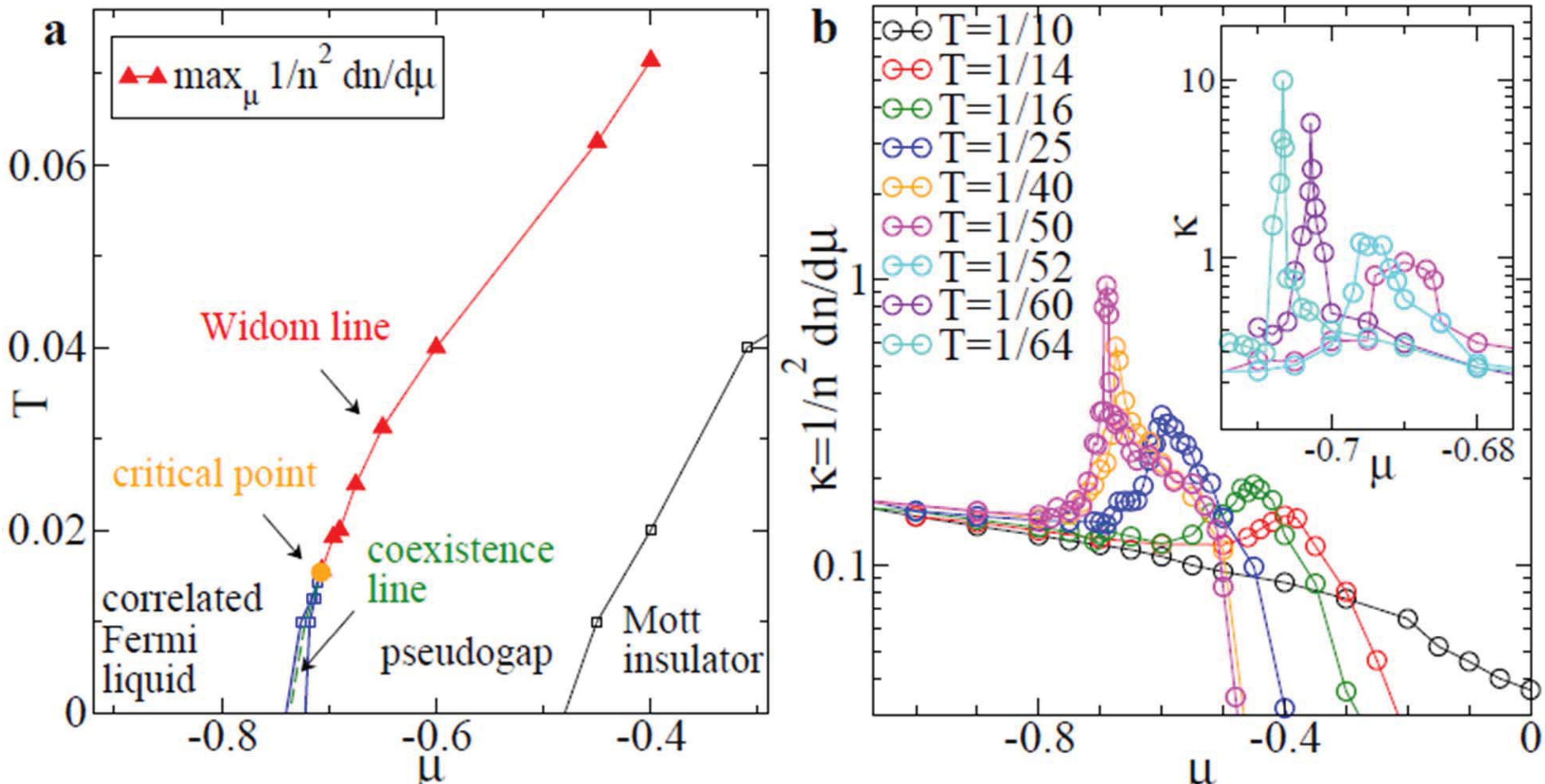
What is the Widom line?



McMillan and Stanley, Nat Phys 2010

- it is the continuation of the coexistence line in the supercritical region
- line where the maxima of different response functions touch each other asymptotically as $T \to T_p$
- liquid-gas transition in water: max in isobaric heat capacity C_p, isothermal compressibility, isobaric heat expansion, etc
- DYNAMIC crossover arises from crossing the Widom line!
  water: Xu et al, PNAS 2005, Simeoni et al Nat Phys 2010

Pseudogap along the Widom line

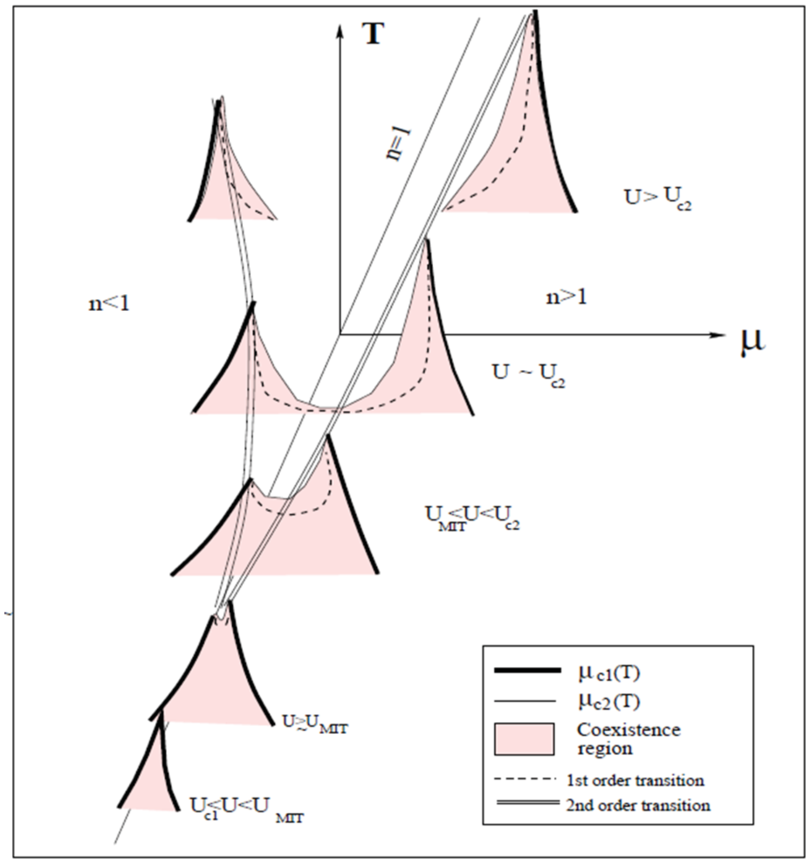


Widom line: defined from maxima of charge compressibility

$\kappa = 1/n^2(dn/d\mu)_T$

divergence of κ at the (classical) critical point!

Compressibility divergence at Mott and coexistence



G. Kotliar, S. Murthy, and M. J. Rozenberg, Phys. Rev. Lett. **89**, 046401 (2002).

S. Murthy, Rutgers thesis 2004

K. Frikach, M. Poirier, et al. PRB **61**, R6491 (2000).

S. R. Hassan, A. Georges, and H. R. Krishnamurthy PRL **94**, 036402 (2005)

Figure 2.19: Schematic phase diagram for the 2-band case. There is an asymmetry in the triangular peaks as compared to the 1-band case. The cross sections are on the $T-\mu$ plane for different values of U as before. μ_{c1} and U_{c1} are the chemical potential and

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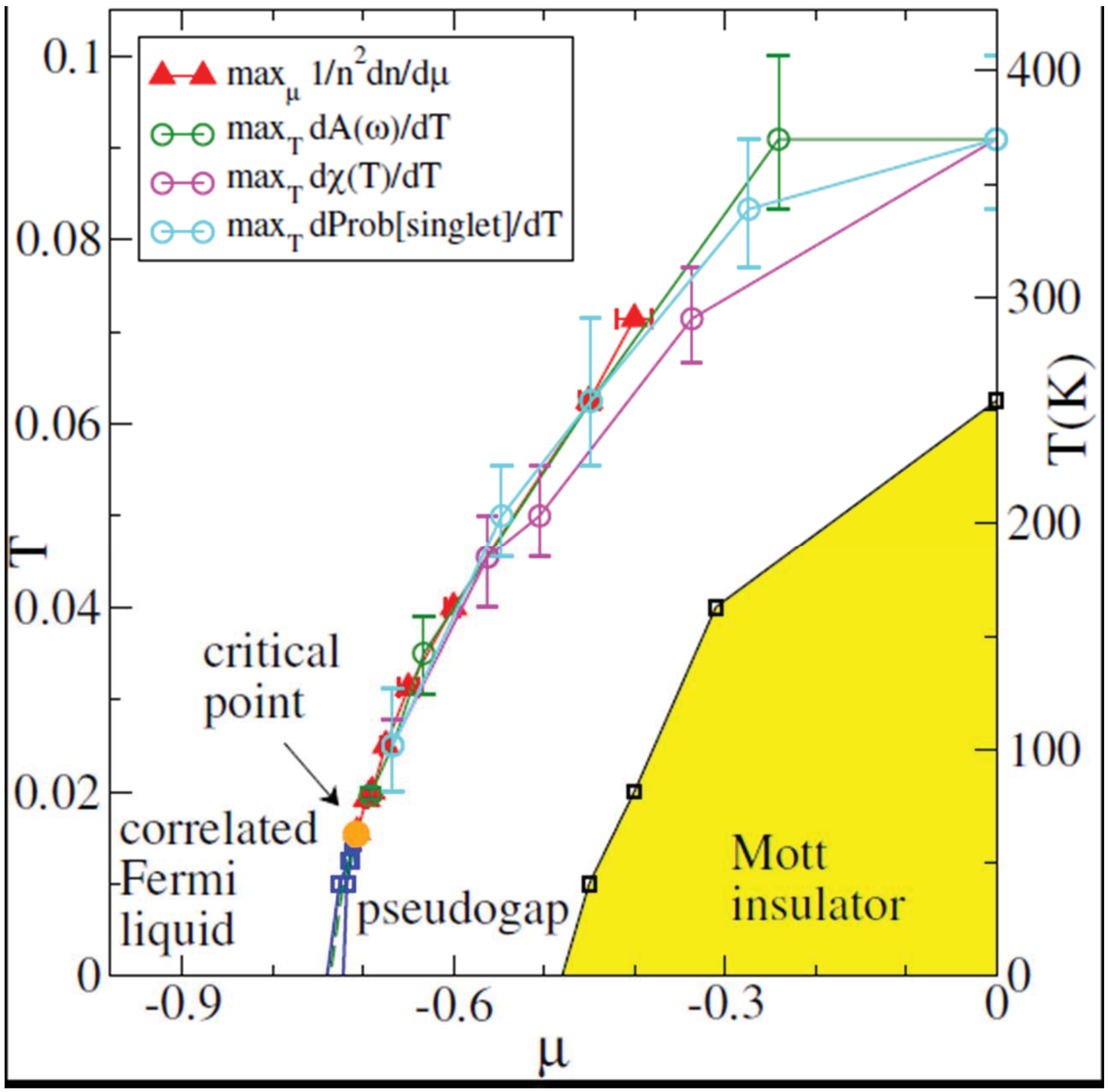
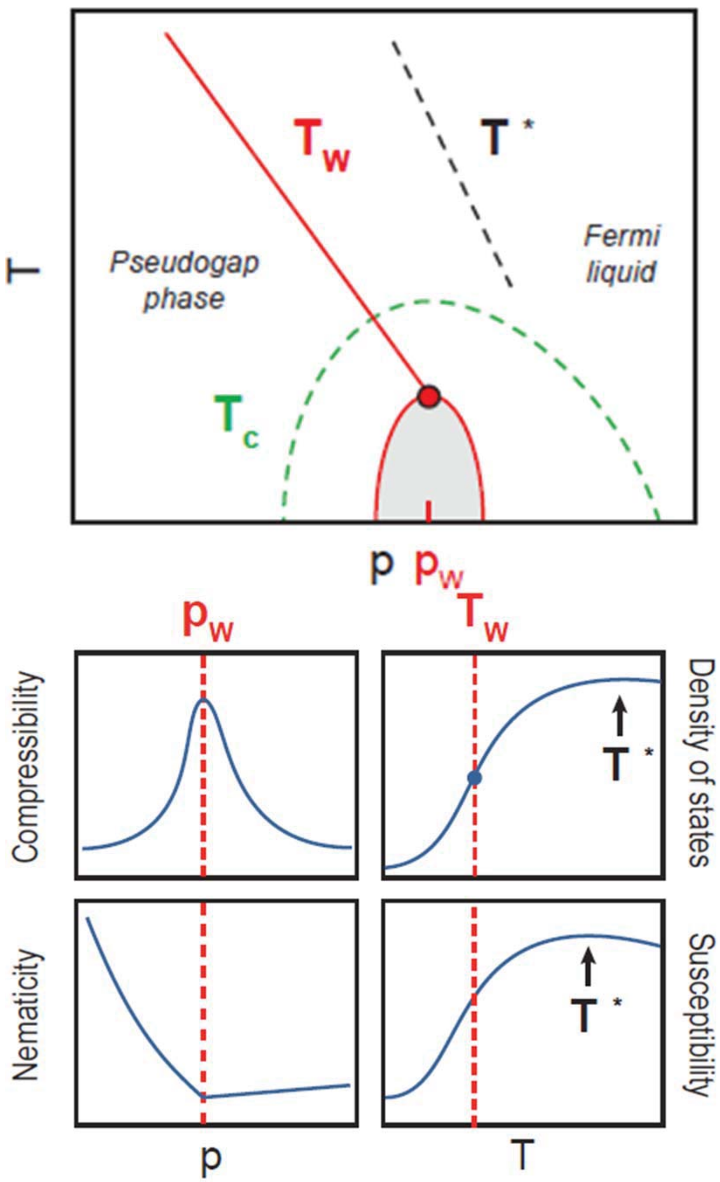
Rapid change also in dynamical quantities



An alternate point of view : next lecture



- - 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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3 measurements: Kerr, ARPES, TRR

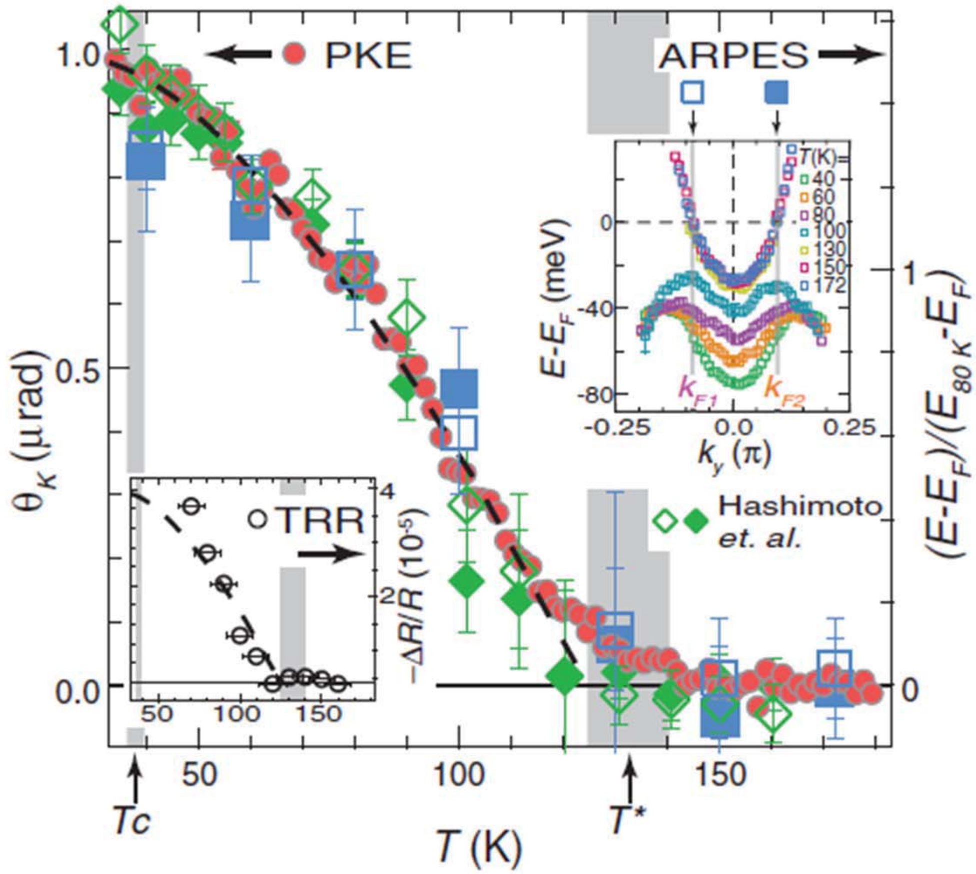
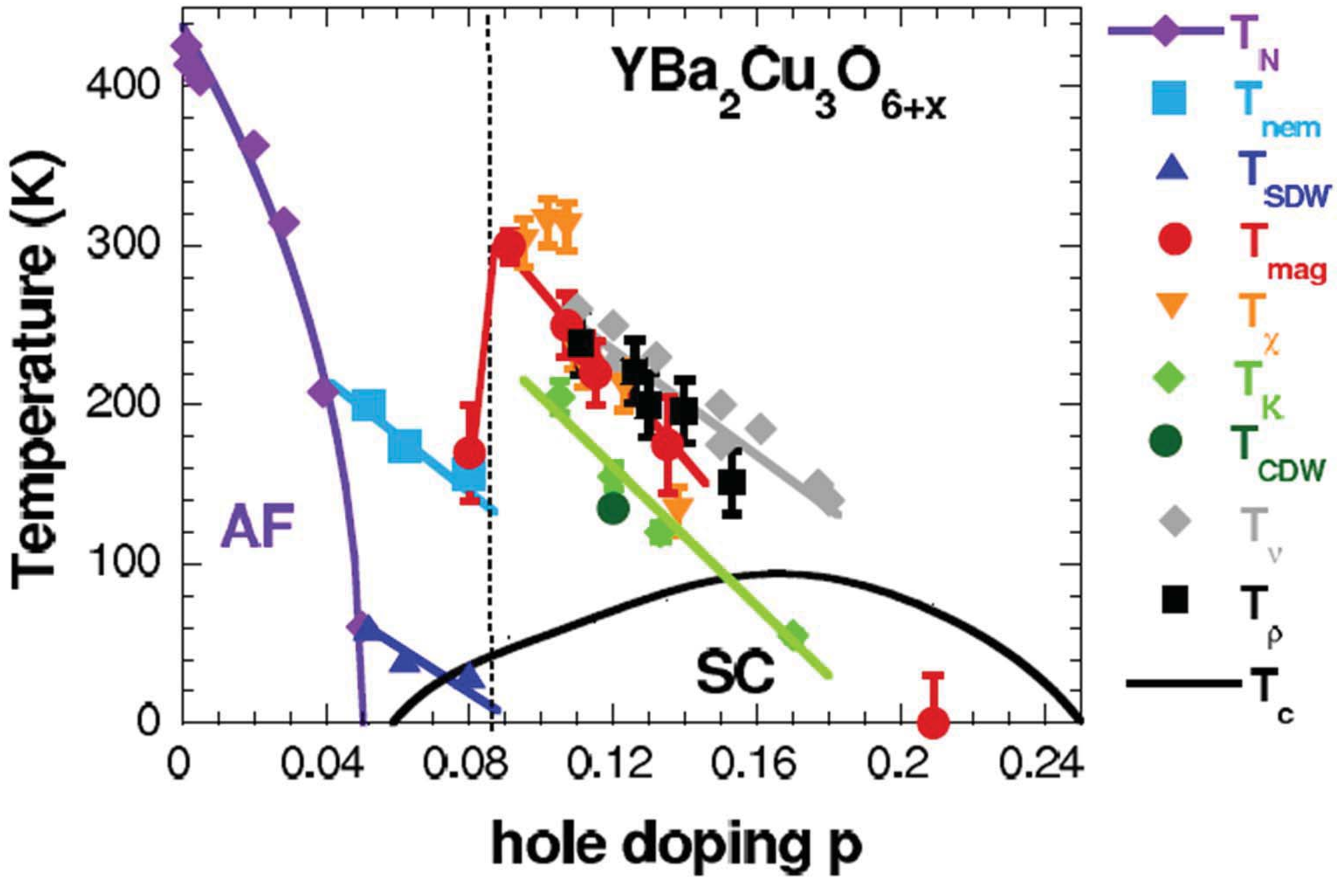


Fig. 3. Temperature dependence of Kerr rotation (θ_K) measured by PKE, in comparison with that of the binding energy position of the EDC maximum at k_F given by ARPES [reproduced from fig. S1F and (*29*)]. ARPES results are normalized to the 80 K values (free from the interference of fluctuating superconductivity). The dashed black curve is a guide to the eye for the PKE data, showing a mean-field–like critical behavior close to T^* [see additional discussion in (*27*)]. (**Left inset**) Temperature dependence of the transient reflectivity change measured by TRR (right axis). The dashed black curve (left axis) is reproduced from the main panel. Error bars (if not visible) are smaller than the symbol size. (**Right inset**) Dispersion of the EDC maximum at various temperatures above T_c, summarizing the results of Figs. 2A and 4A and fig. S1, A to E. All data were taken on samples from the same growth and annealing batch, except those reproduced from (*29*) on differently annealed samples.

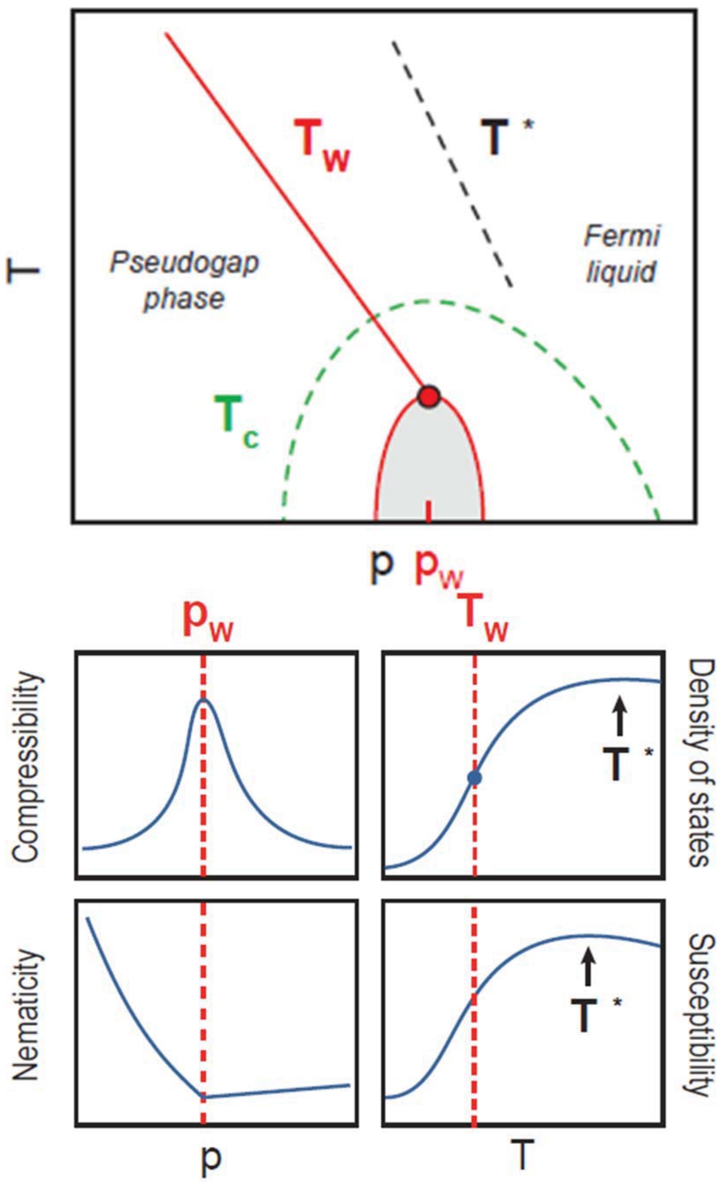
He et al, Science 2011, on Bi 2201

Intra-Unit-Cell loop order



Y Sidis and P Bourges 2013 *J. Phys.: Conf. Ser.* **449** 012012

An alternate point of view : next lecture



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Organics

Pseudogap

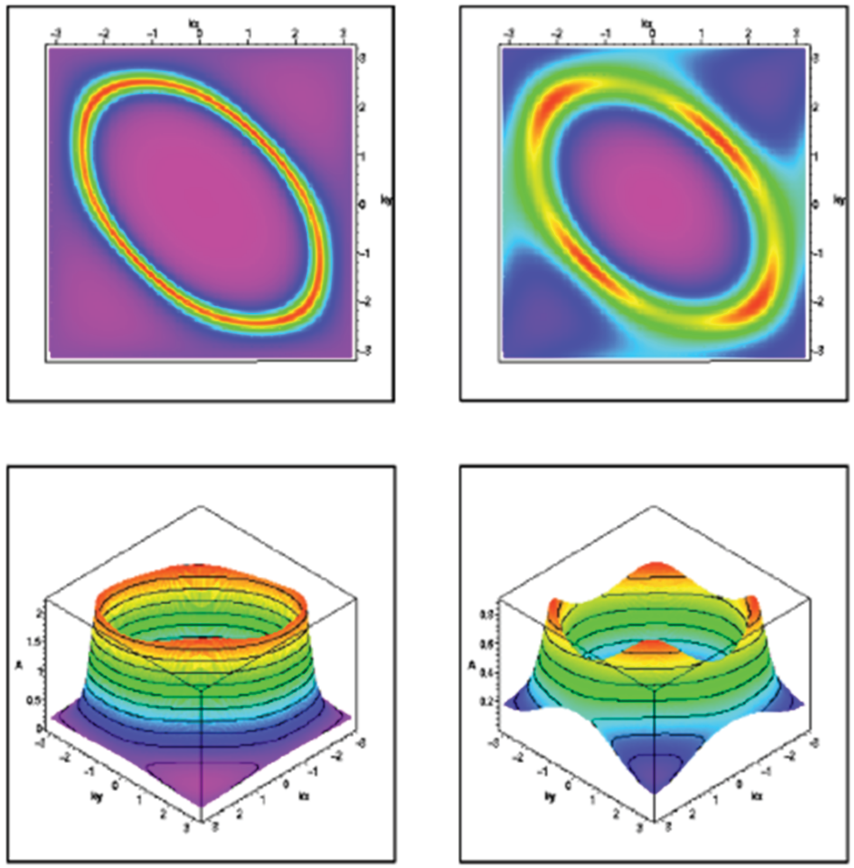
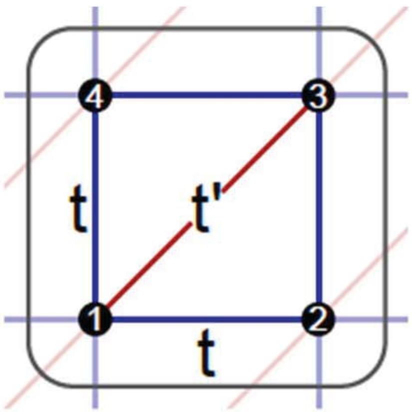
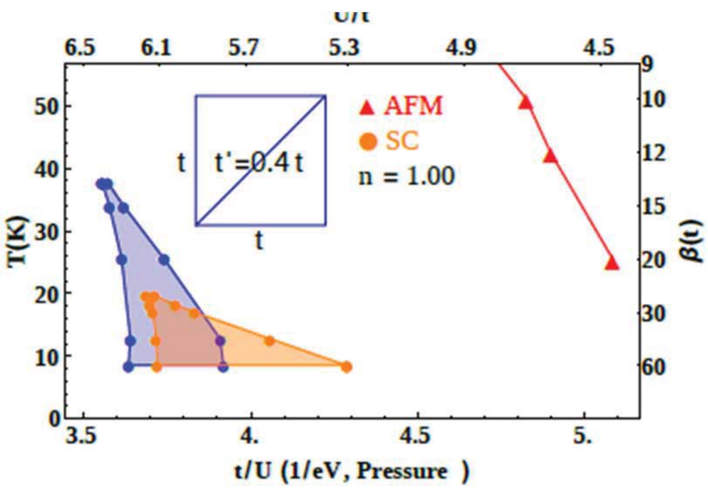


FIG. 4 (color online). Distribution of low energy spectral weight in k space $A(k, \omega = 0)$ for $T/D = 1/44$, $U/D = 2.0$ (left-hand panel) and $U/D = 2.25$ (right-hand panel). The top panels are color plots to see the Fermi surface and the bottom panels are 3D plots to see the variation of A. For intermediate U, cold and hot regions are visible around $(\frac{\pi}{2}, \frac{\pi}{2})$ and $(\pi, 0)$, respectively.

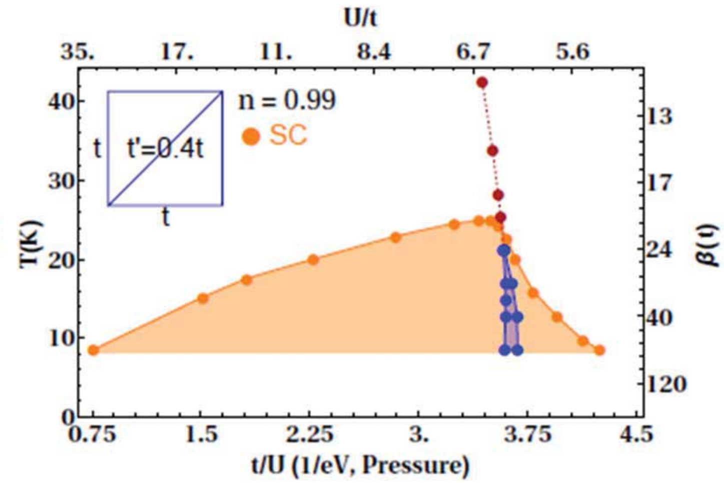
O. Parcollet, G. Biroli
G. Kotliar
PRL **92** (2004)

t’=0.4t

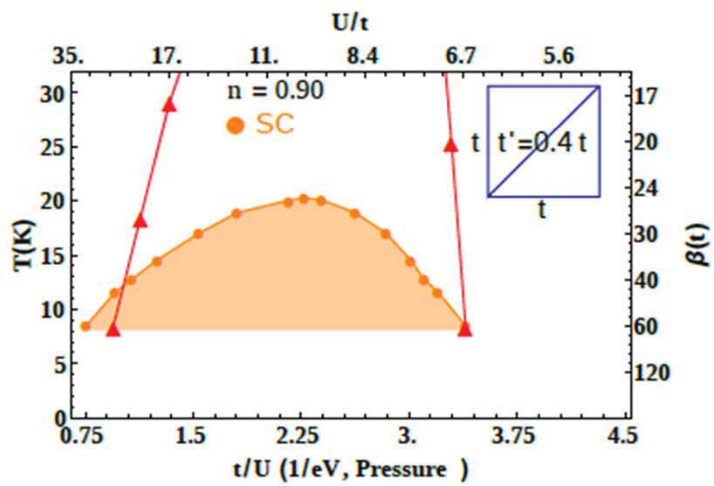


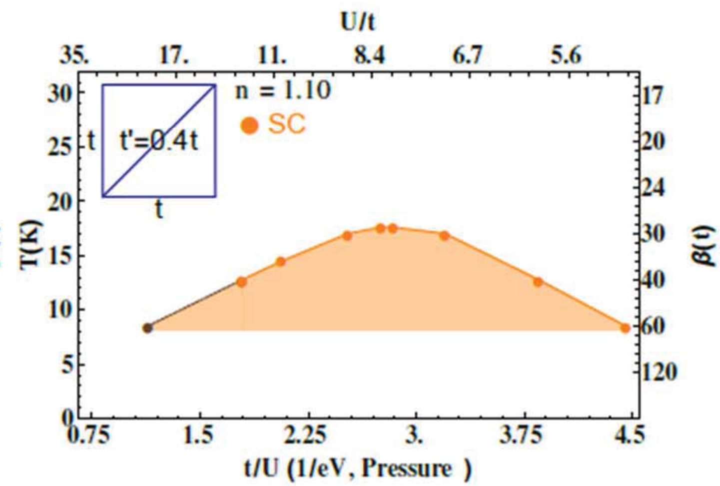


(a)



(b)





Charles-David Hébert, Patrick Sémon , AMT

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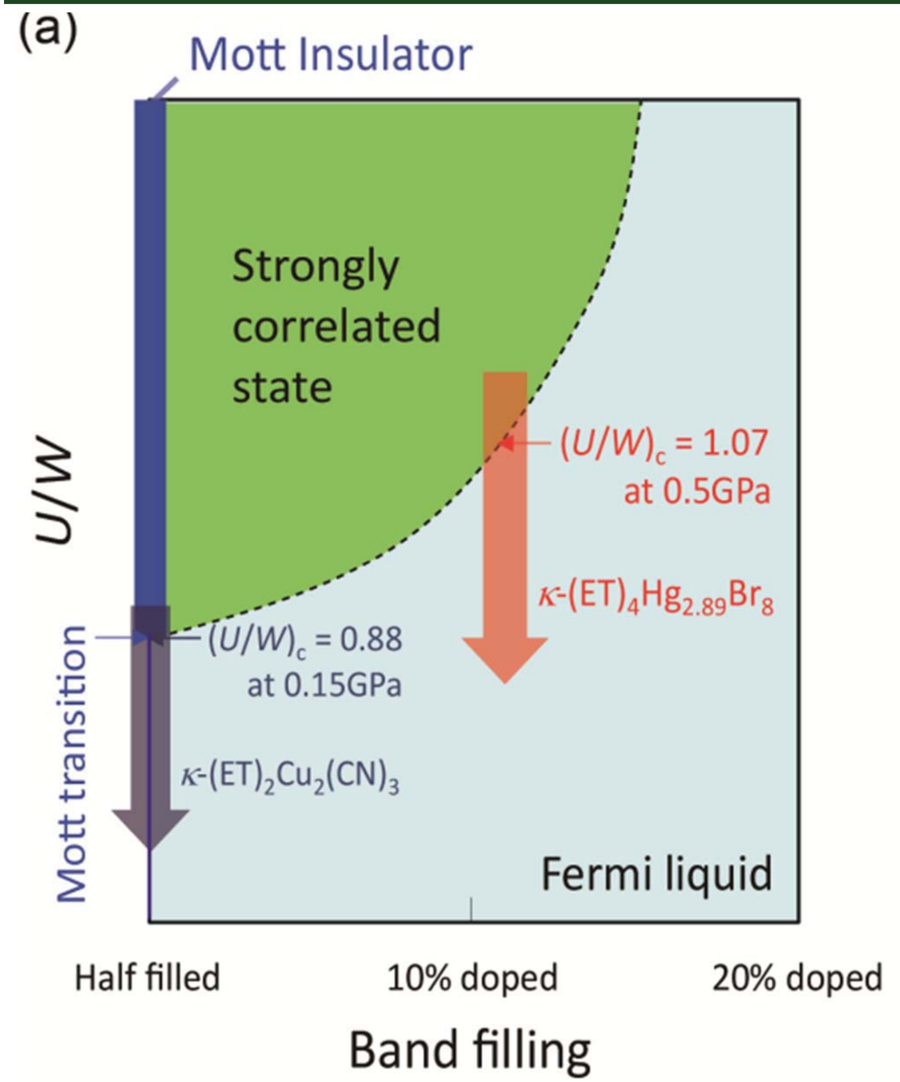
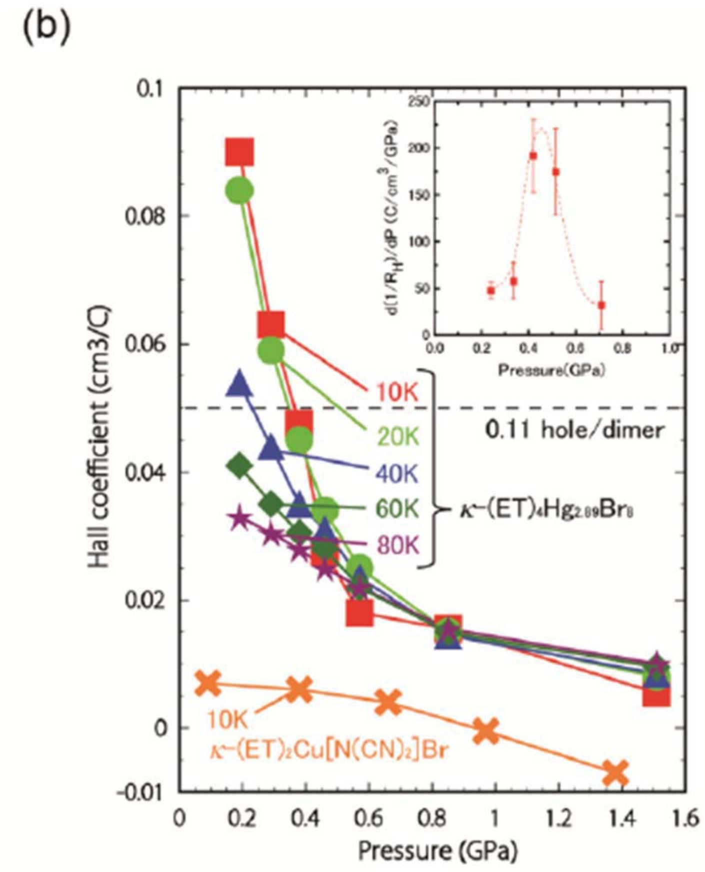
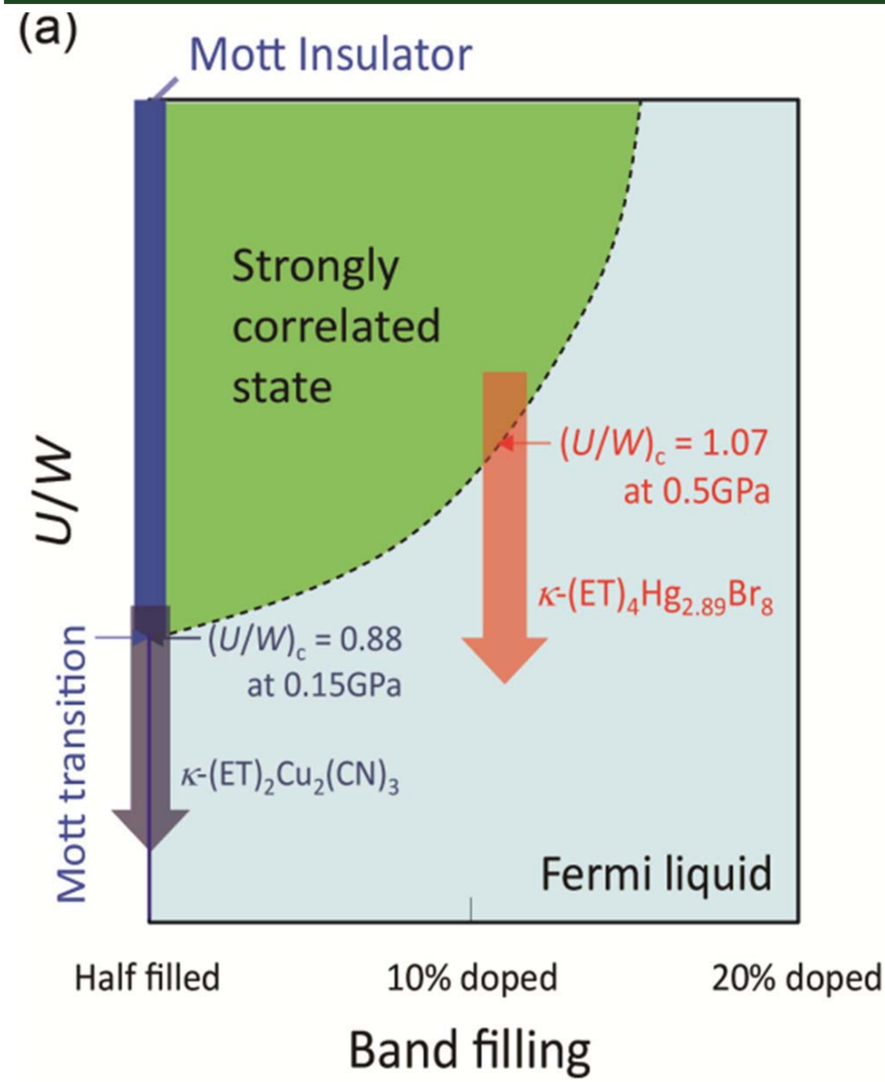
Doped BEDT

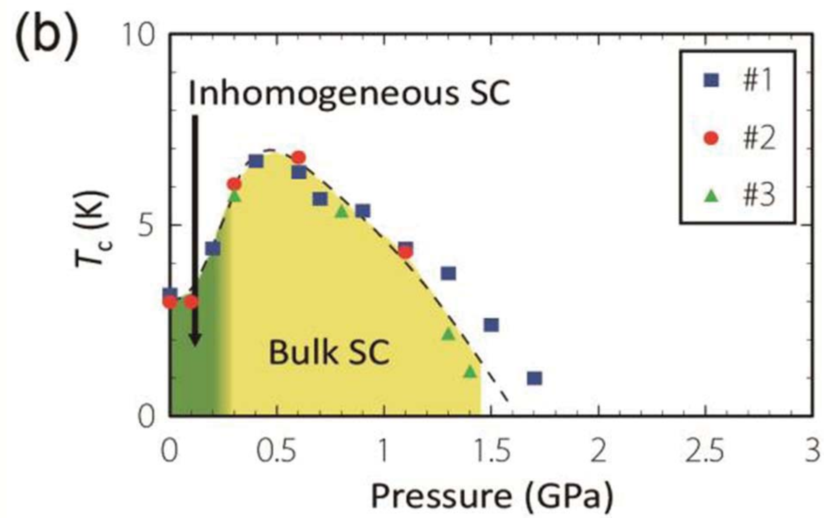


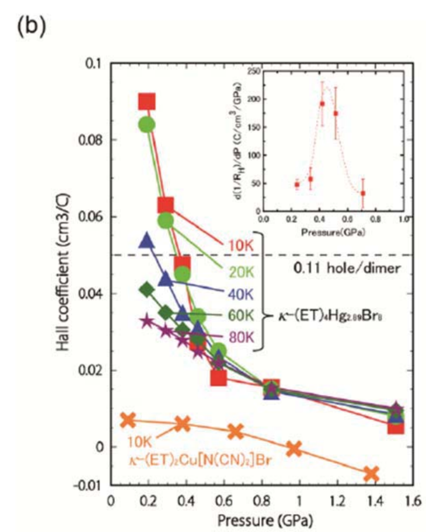


H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

Doped BEDT

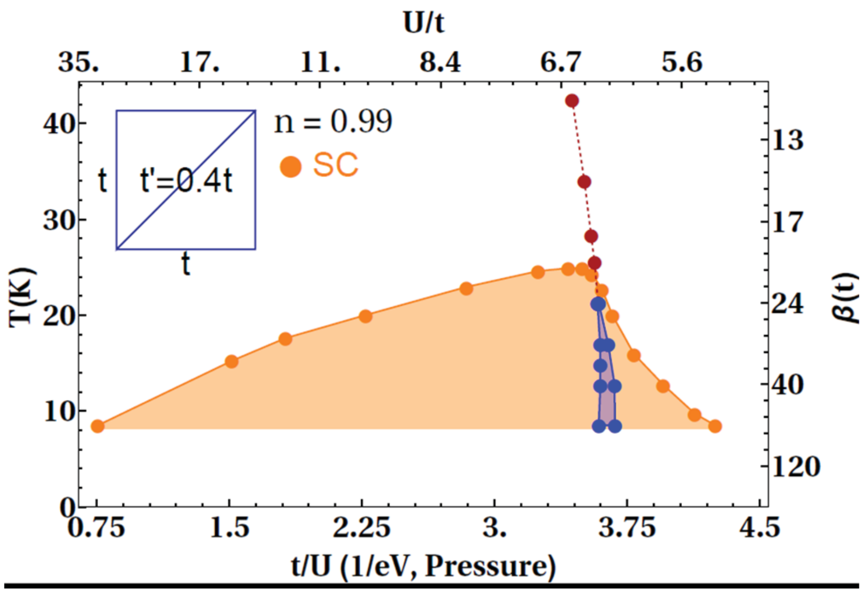


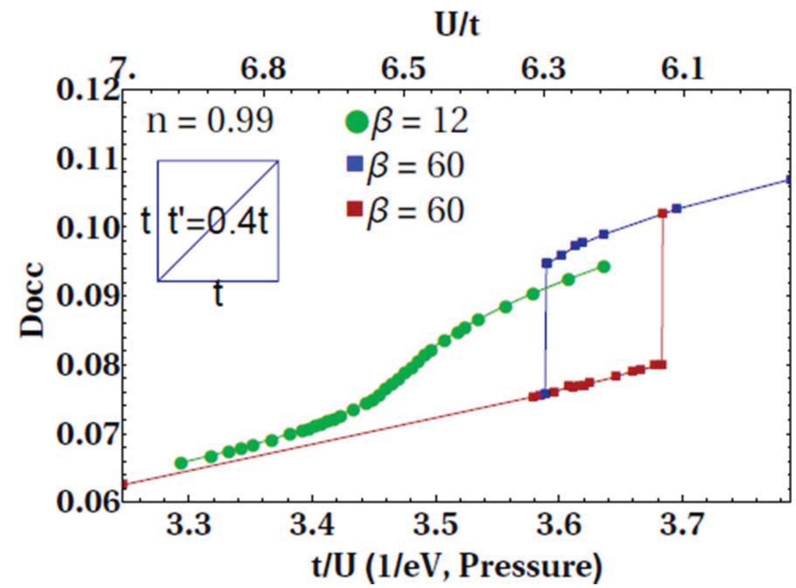


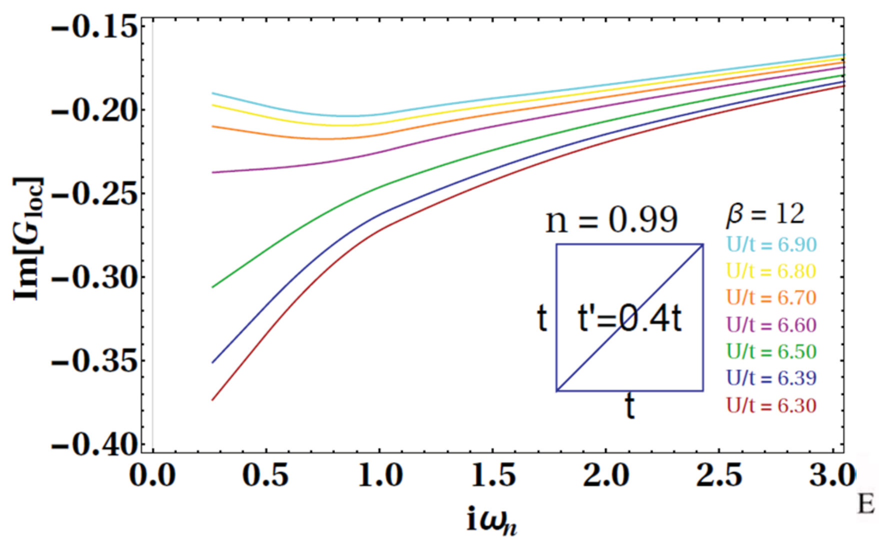


H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

Widom line in organics



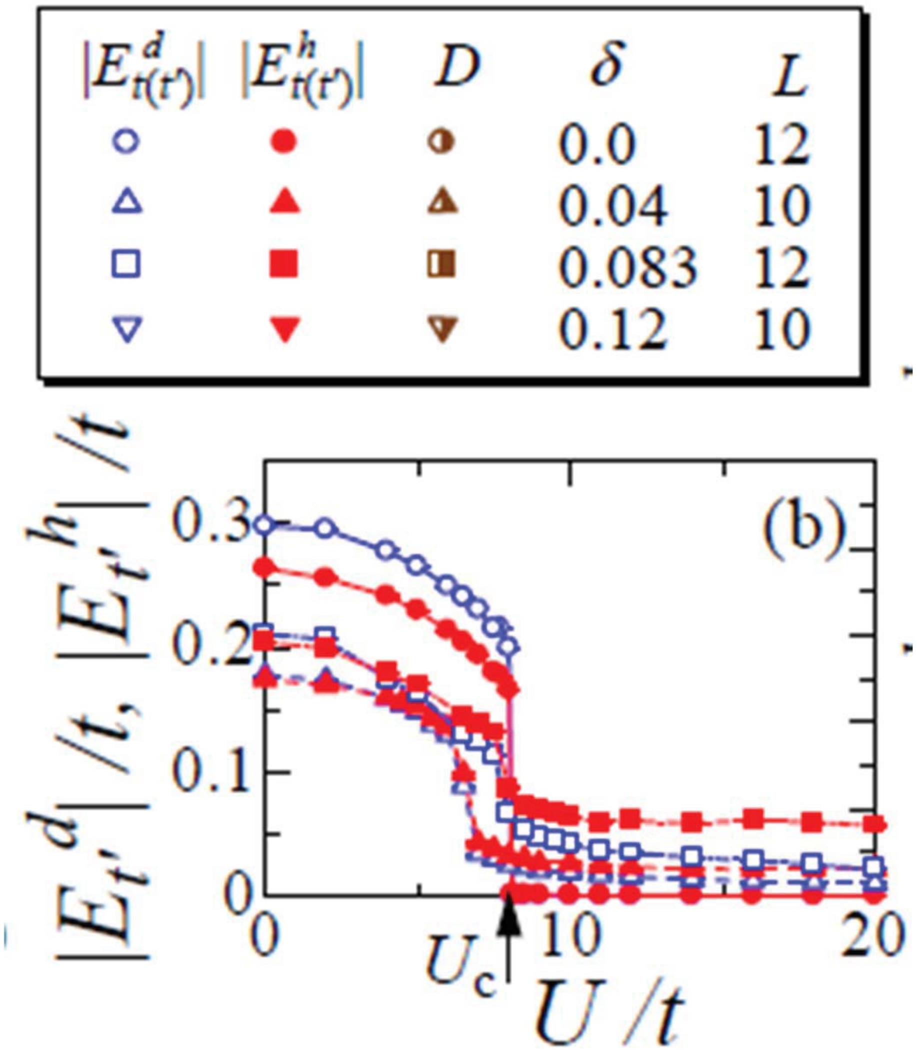




Charles-David Hébert, Patrick Sémon , AMT

E

Results from variational MC



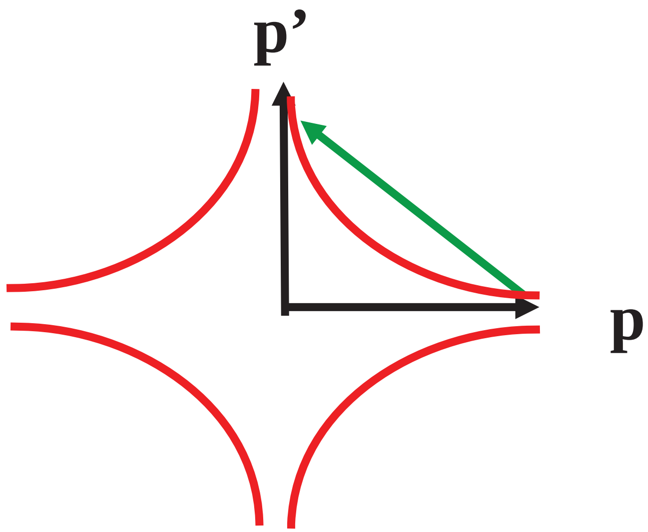
T. Watanabe, H. Yokoyama and M. Ogata
JPS Conf. Proc.
3, 013004 (2014)

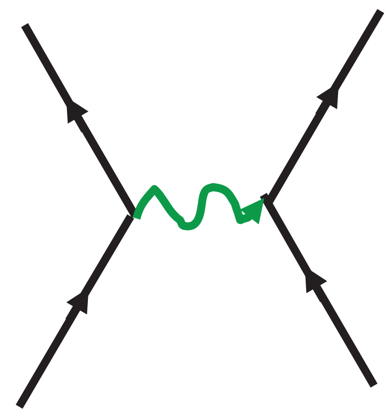
8. Superconductivity in general

Analog to weakly and strongly correlated antiferromagnets

Cartoon « BCS » weak-coupling picture

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





Exchange of spin waves?
Kohn-Luttinger
T_c with pressure

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

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

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

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

Pitaevskii Brückner:

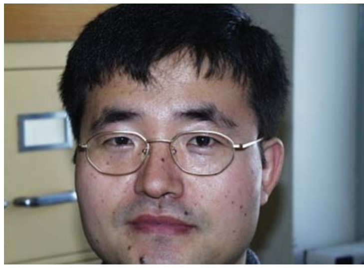
Pair state orthogonal to repulsive core of Coulomb interaction

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

Miyake, Schmitt–Rink, and Varma P.R. B **34**, 6554-6556 (1986)

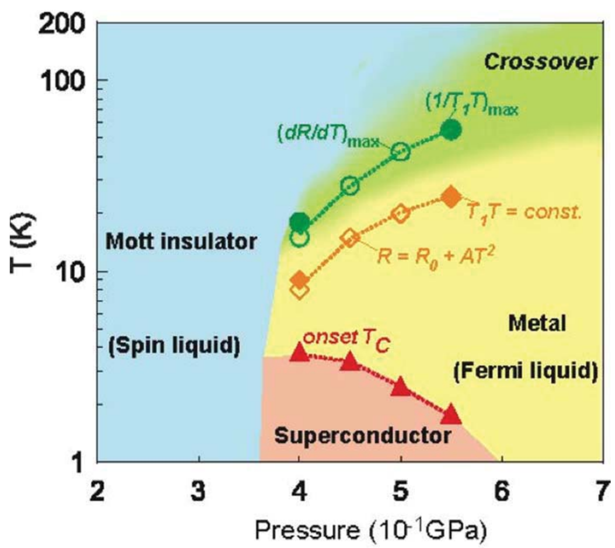
More sophisticated Slave Boson: Kotliar Liu PRB 1988

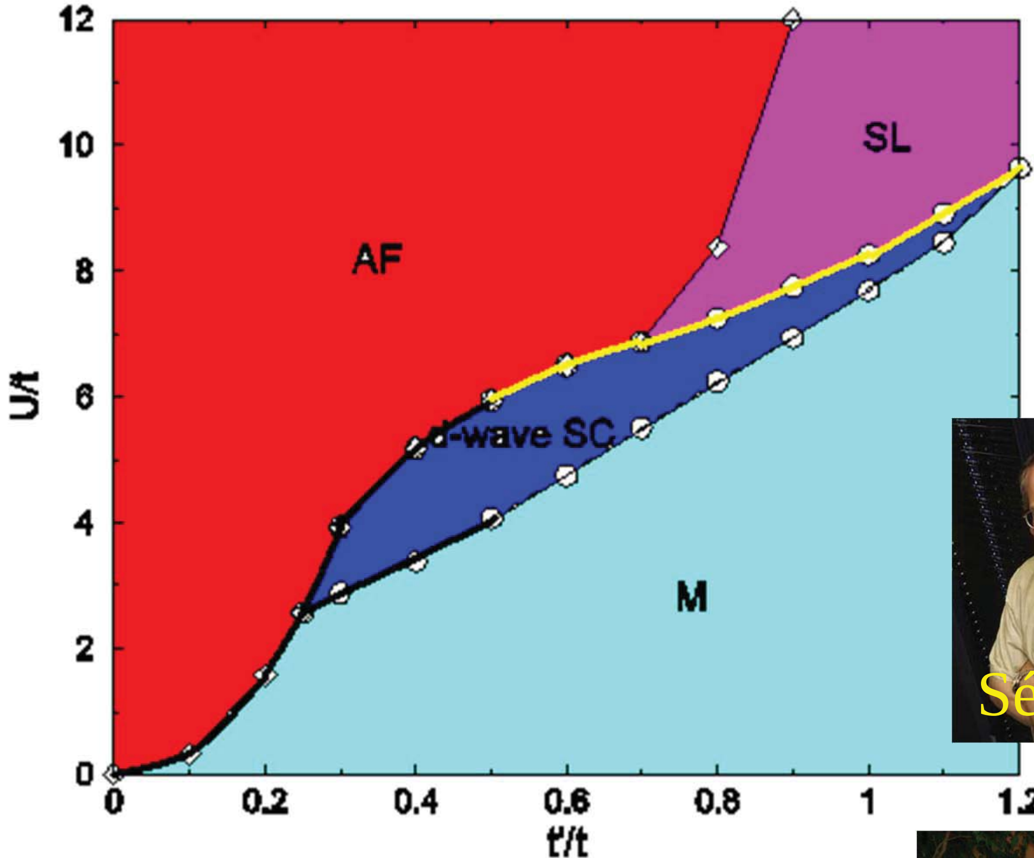
8. Superconductivity in the organics

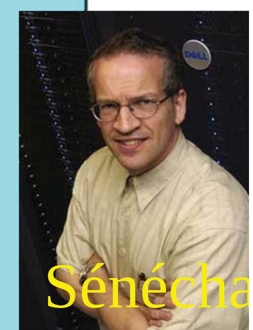


Theoretical phase diagram BEDT

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







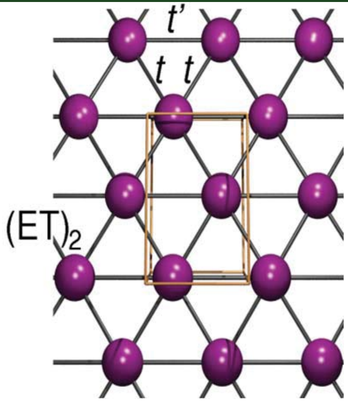
Kyung, A.-M.S.T. PRL 97, 046402 (2006)

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

Y. Kurisaki, et al.
Phys. Rev. Lett. **95**, 177001(2005) Y. Shimizu, et al. Phys. Rev. Lett. **91**, (2003)

Other compounds (R. Valenti et al.)

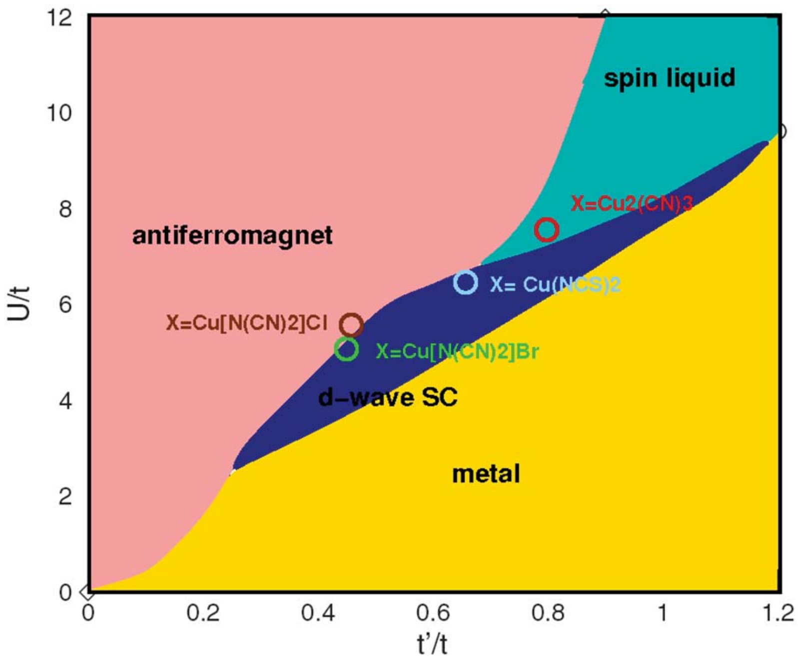
	Hueckel		DFT	
X	t'/t	U/t	t'/t	U/t
CN	1.06	8.2	0.83 (0.85)	7.3 (12)
SCN	0.84	6.8	0.58 (0.83)	6.0
Cl	0.75	7.5	0.44	7.5
Br	0.68	7.2	0.42	5.1



Kandpal et al. PRL (2009)

Nakamura et al. JPSJ (2009)

Komatsu et al. JPSJ (1996)



Kyung, Tremblay PRL (2006)

Tocchio, Parola, Gros, Becca PRB (2009)

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Analogous results with other methods

H. Morita et al., J. Phys. Soc. Jpn. 71, 2109 (2002).

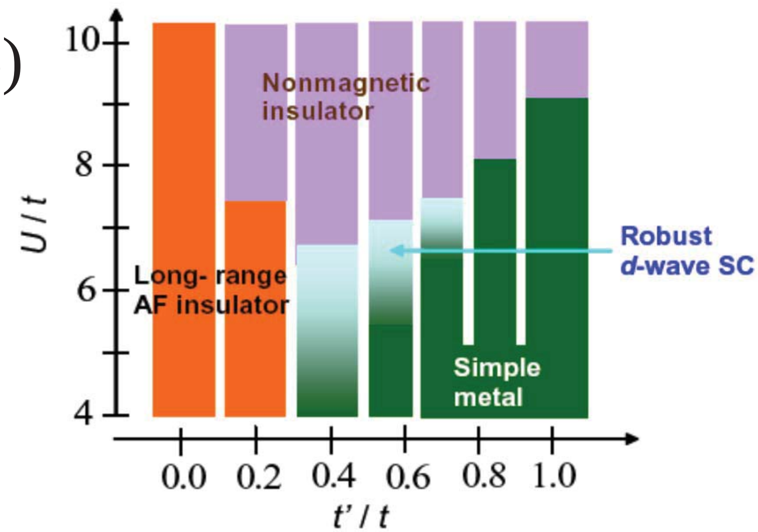
J. Liu et al., Phys. Rev. Lett. 94, 127003 (2005).

S.S. Lee et al., Phys. Rev. Lett. 95, 036403 (2005).

B. Powell et al., Phys. Rev. Lett. 94, 047004 (2005).

J.Y. Gan et al., Phys. Rev. Lett. 94, 067005 (2005).

T. Watanabe et J. Phys. Soc. Japan (2006)



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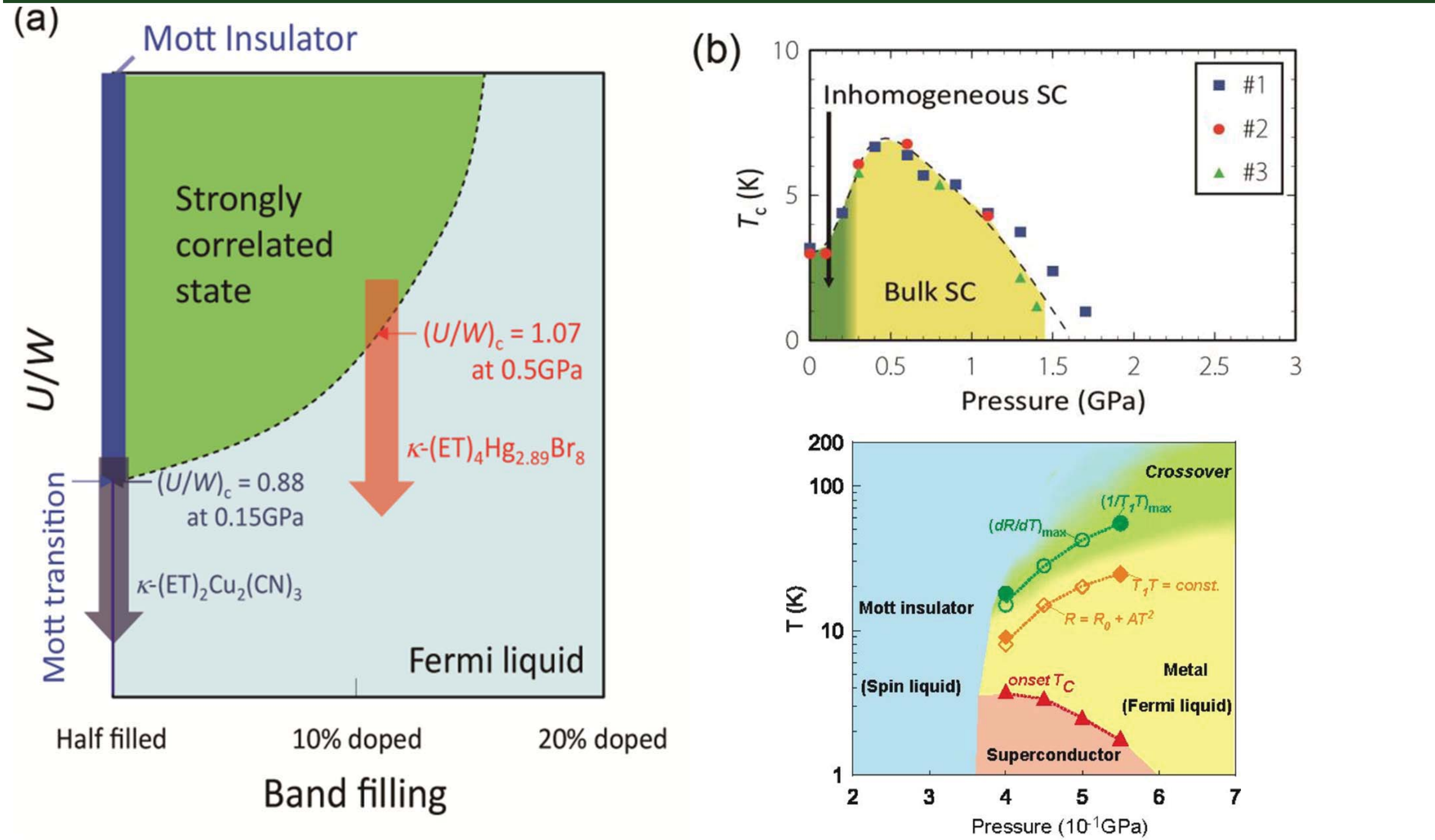

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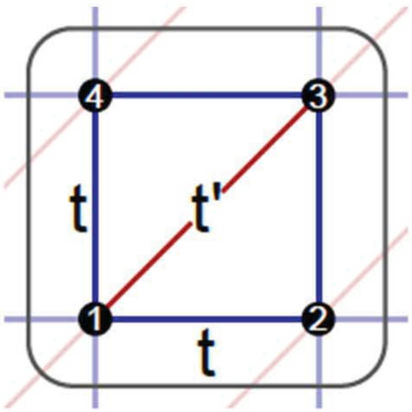
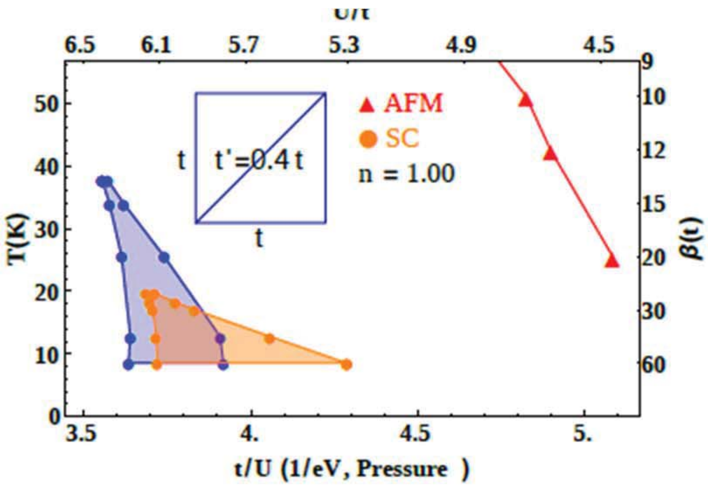
t’=0.4t

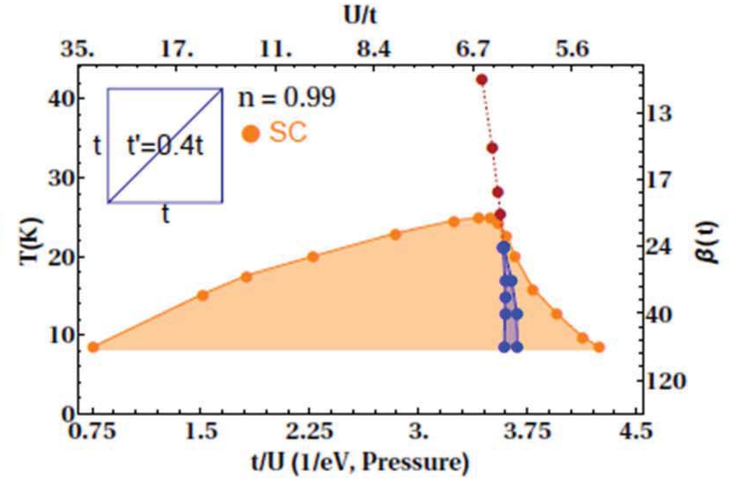


t
t'
t



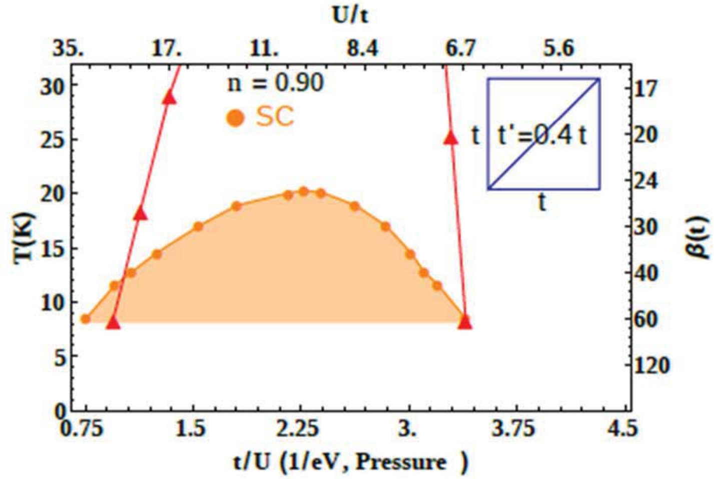
U/t
AFM
SC
n = 1.00
t'=0.4 t
T(K)
β(t)
t/U (1/eV, Pressure)

(a)

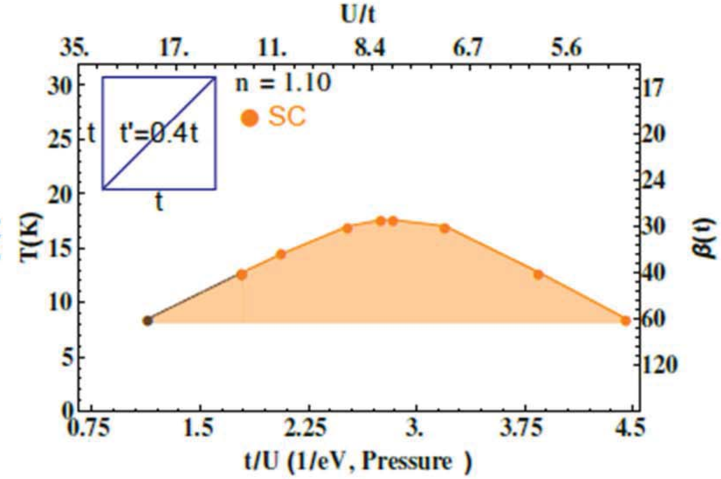


U/t
n = 0.99
SC
t'=0.4t
T(K)
β(t)
t/U (1/eV, Pressure)

(b)

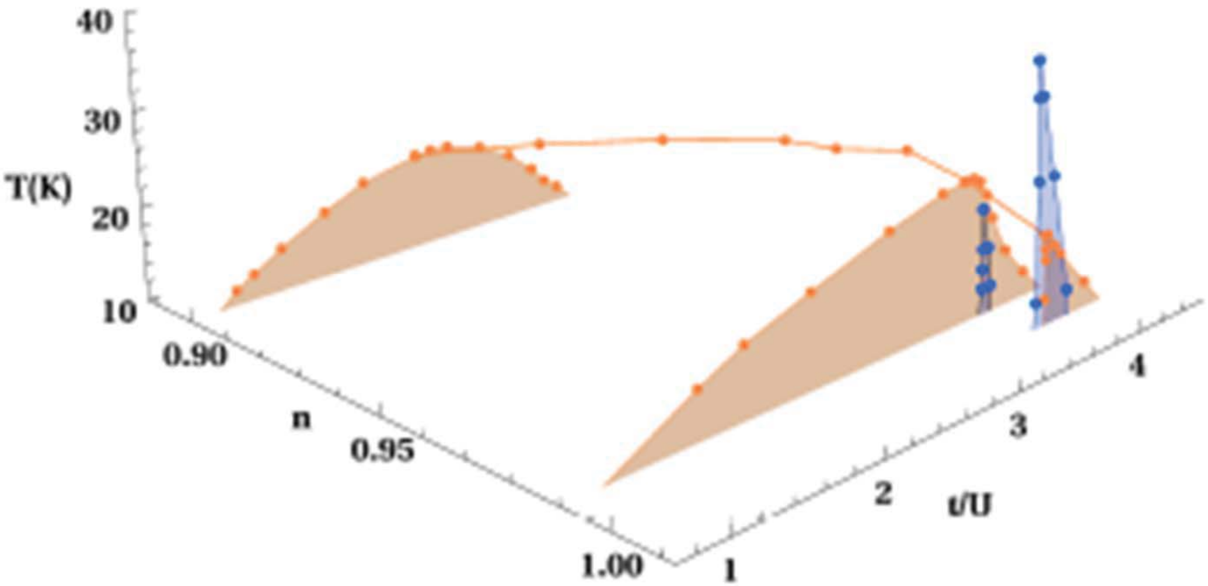


U/t
n = 0.90
SC
t'=0.4 t
T(K)
β(t)
t/U (1/eV, Pressure)



U/t
n = 1.10
SC
t'=0.4t
T(K)
β(t)
t/U (1/eV, Pressure)

t’ = 0.4t overview



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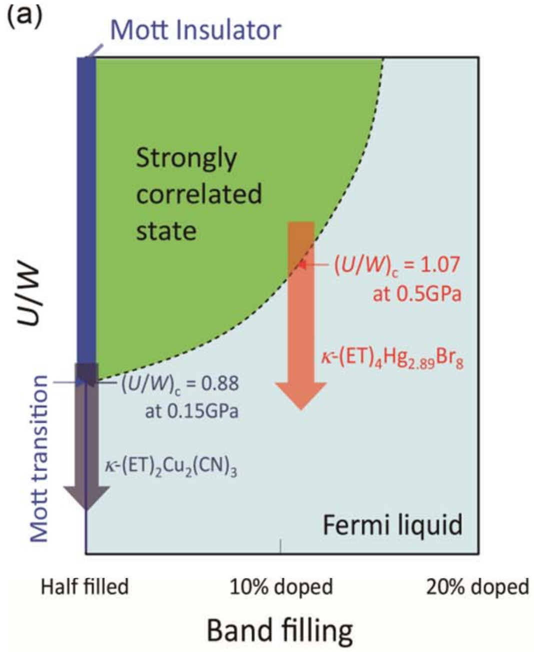
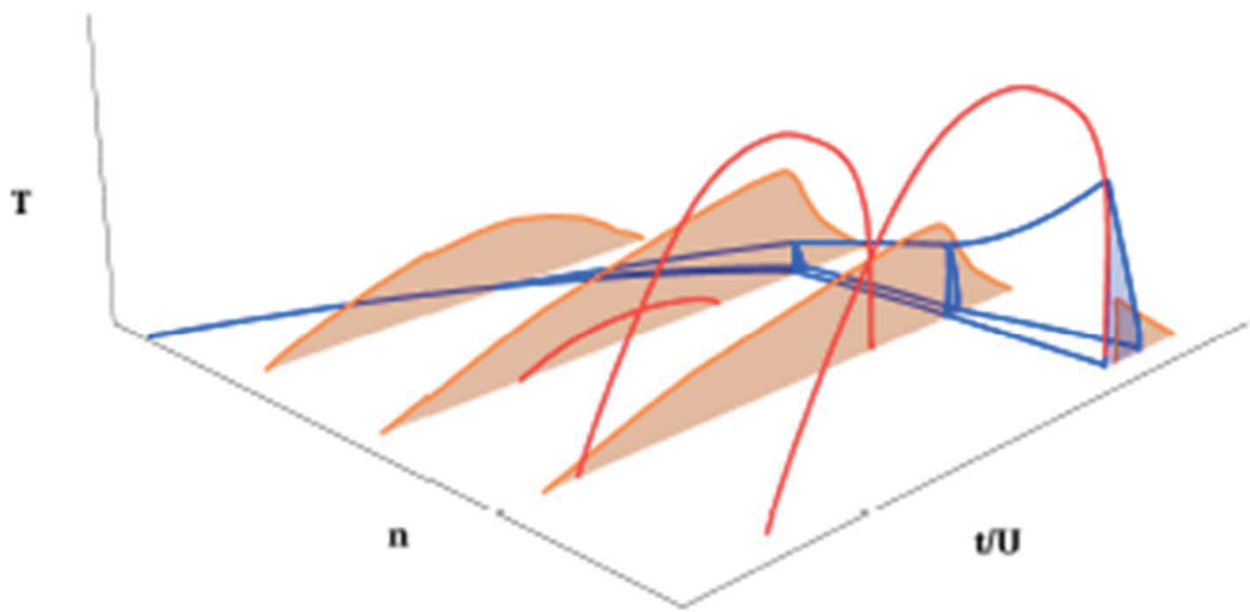
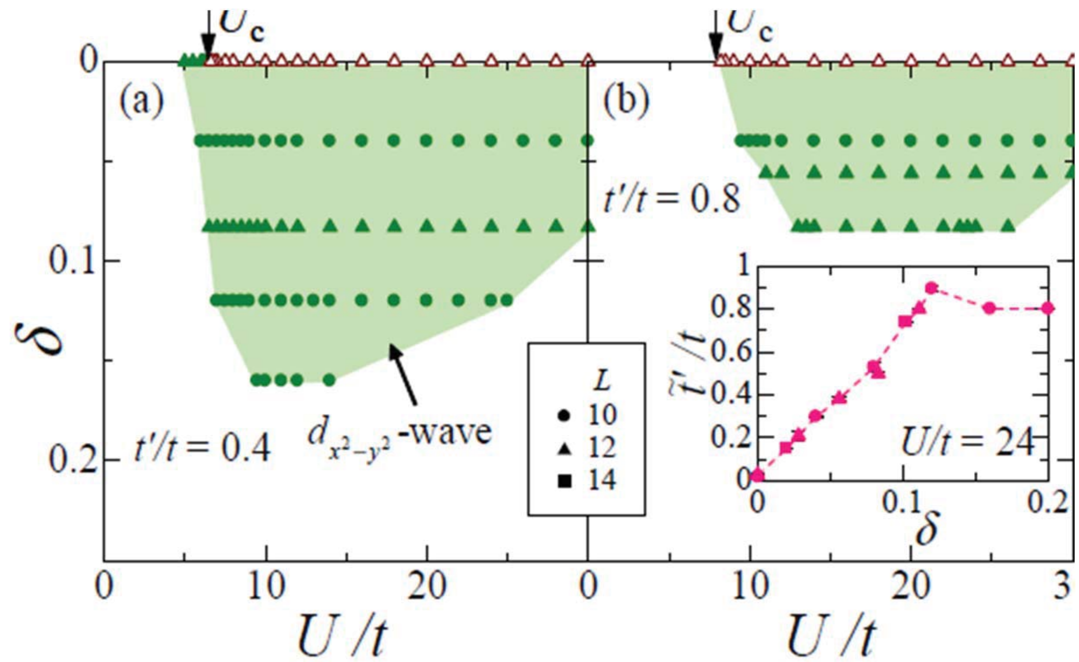
Generic case highly frustrated case





Results from variational MC



T. Watanabe, H. Yokoyama and M. Ogata
JPS Conf. Proc. **3**, 013004 (2014)

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 an AFM QCP. Extension of Mott
  - SC from short range J.
  - T_c decreases at Widom line

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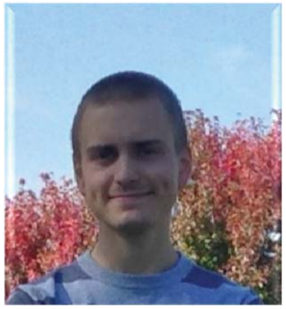
Main collaborators

Giovanni Sordi

Kristjan Haule

David Sénéchal

Bumsoo Kyung



Charles-David Hébert

Patrick Sémon

Dominic Bergeron

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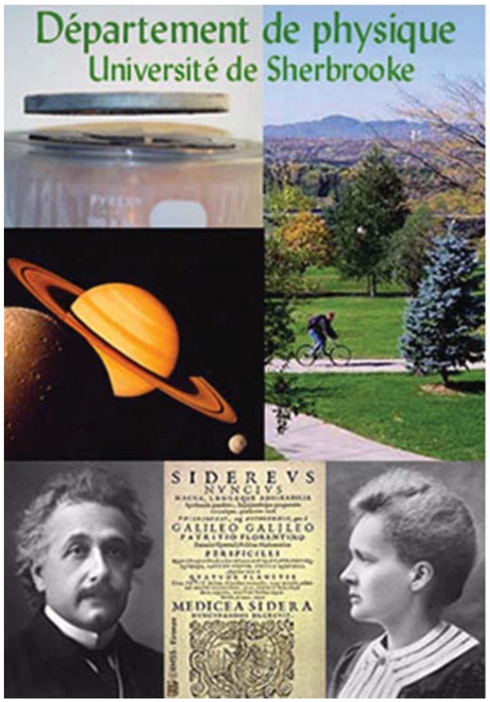

André-Marie Tremblay

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Next time

- Emergent finite doping first-order transition (Sordi transition) as an organizing principle
  - Pseudogap
  - Superconductivity
- Strongly correlated superconductivity and retardation.

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.)

Verlag des Forschungszentrum Jülich, 2013