

Superconductivity in doped or pressurized insulators : cuprates and organics

A.-M. Tremblay

G. Sordi, K. Haule, D. Sénéchal, C.-D. Hébert
P. Sémon, B. Kyung, G. Kotliar,
M. Civelli, S. Kancharla,



Caen, 20 March, 2015



Half-filled band is metallic?



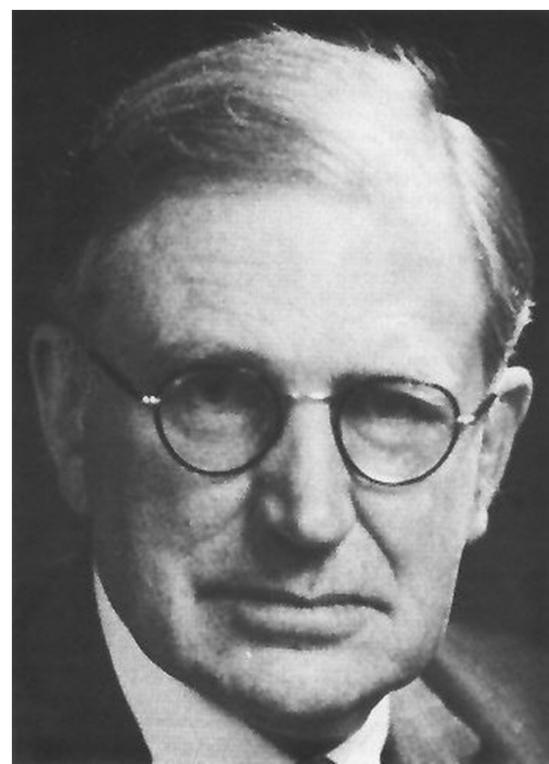
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Half-filled band: Not always a metal

NiO, Boer and Verway



Peierls, 1937

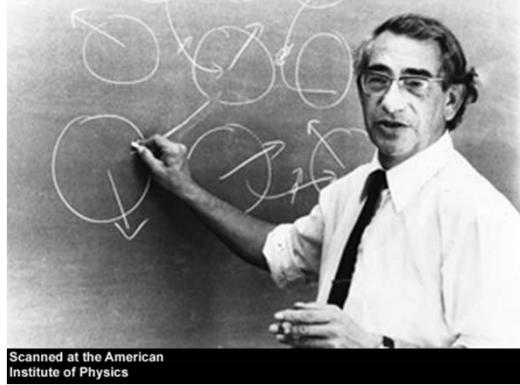


Mott, 1949



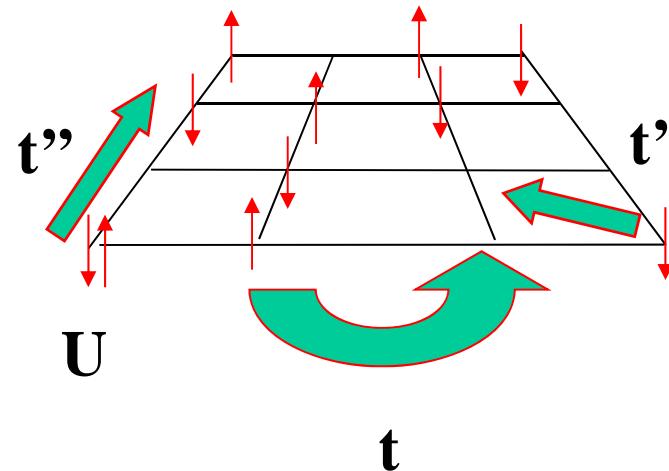
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Hubbard model

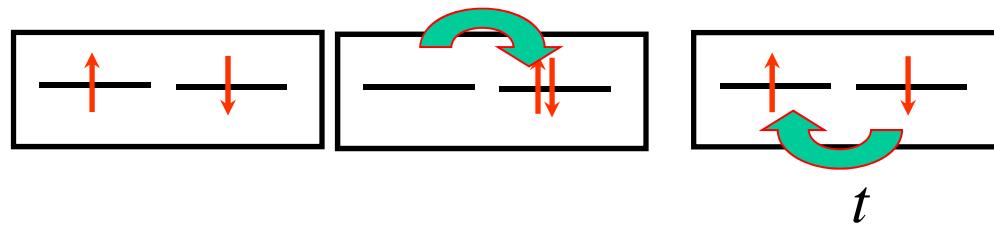


Scanned at the American
Institute of Physics

1931-1980



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



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



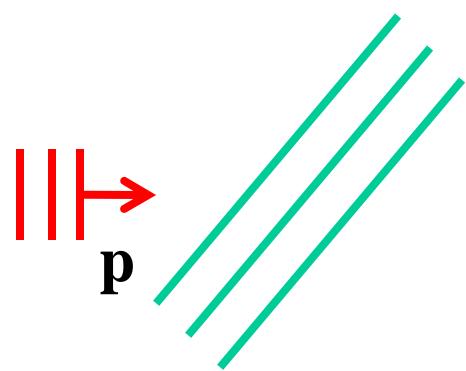
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Superconductivity and attraction?



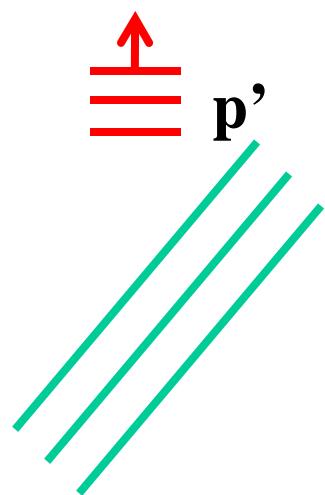
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Attraction mechanism in the metallic state



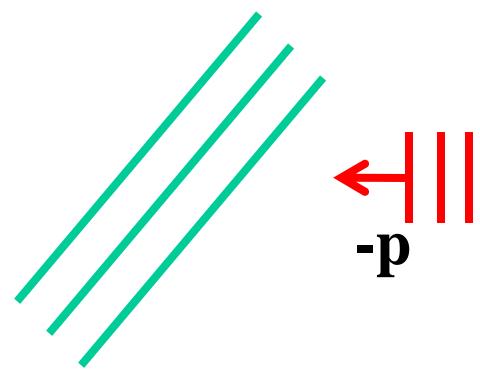
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Attraction mechanism in the metallic state



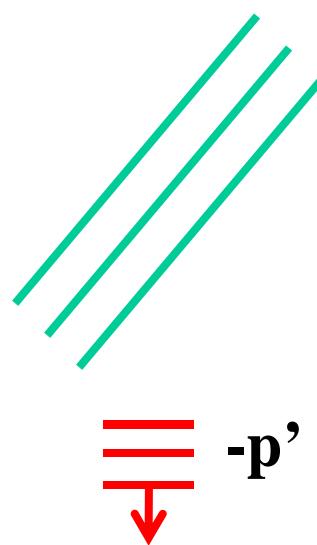
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Attraction mechanism in the metallic state



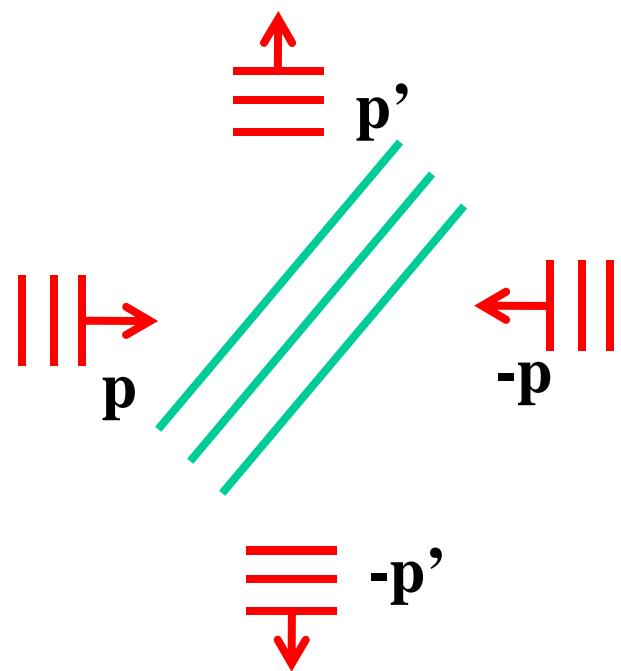
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Attraction mechanism in the metallic state



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Attraction mechanism in the metallic state



#1 Cooper pair, #2 Phase coherence

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

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

$$|\text{BCS}(\theta)\rangle = \dots + e^{iN\theta} |N\rangle + e^{i(N+2)\theta} |N+2\rangle + \dots$$

Cuprates

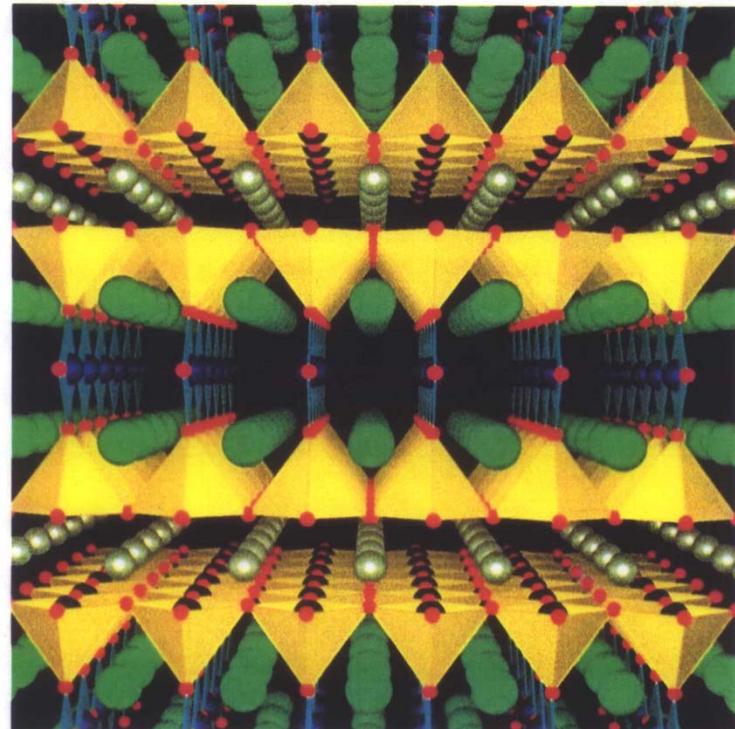
SCIENTIFIC AMERICAN

How nonsense is deleted from genetic messages.

Rx for economic growth: aggressive use of new technology.

Can particle physics test cosmology?

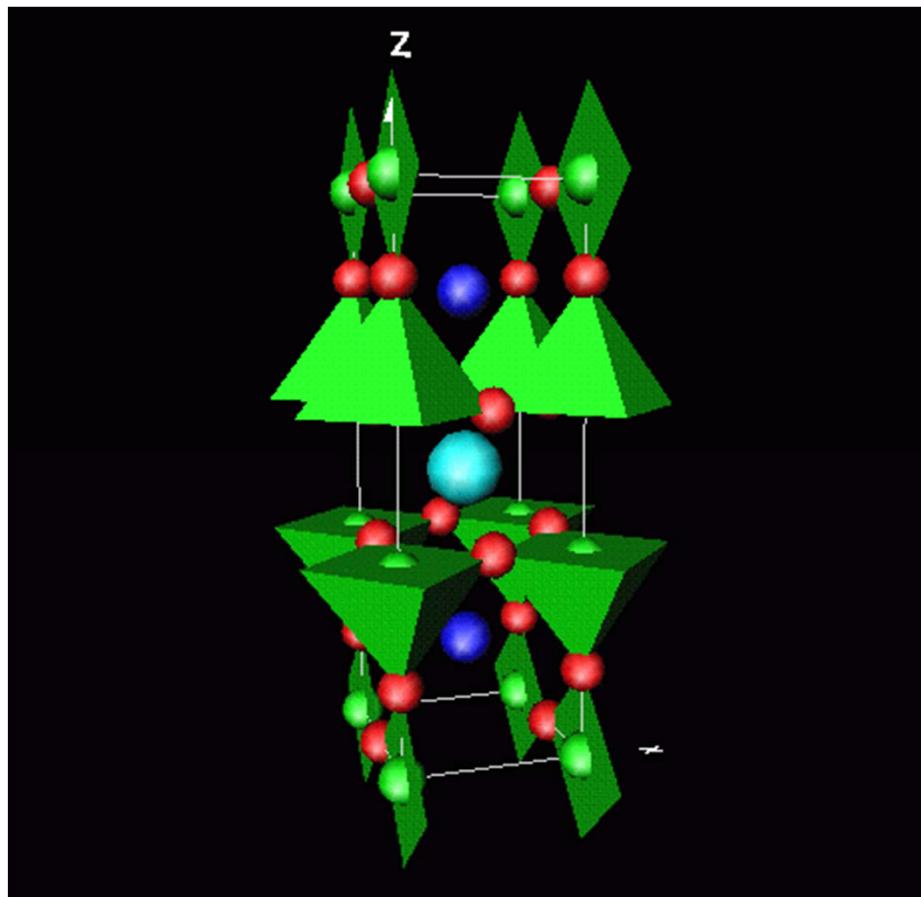
JUNE 1988
\$3.50



High-Temperature Superconductor belongs to a family of materials that exhibit exotic electronic properties.

$\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$

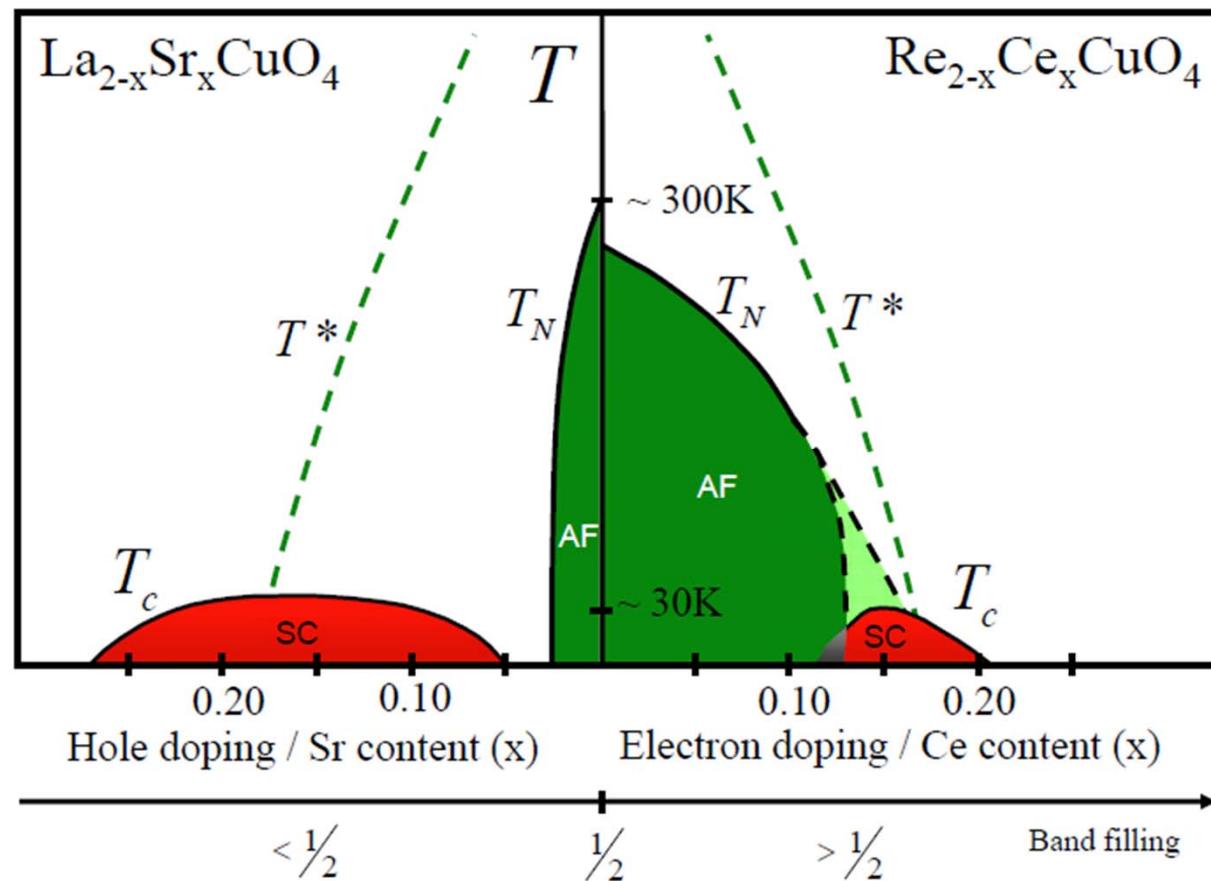
92-37



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High-temperature superconductors

Armitage, Fournier, Greene, RMP (2009)



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Superconductivity



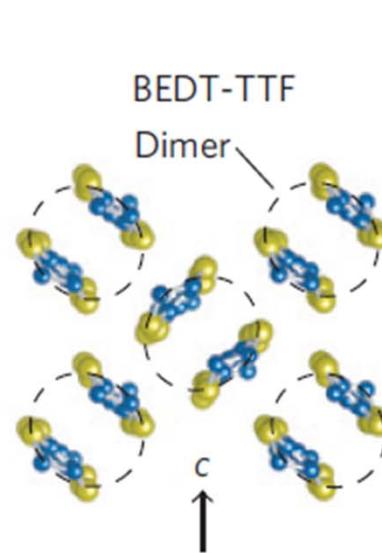
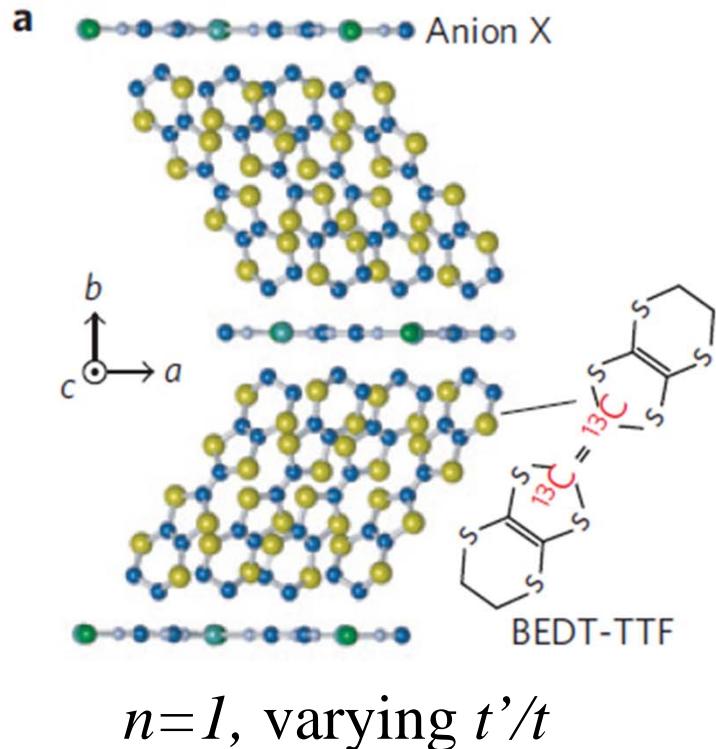
© Alexis Reymbaut



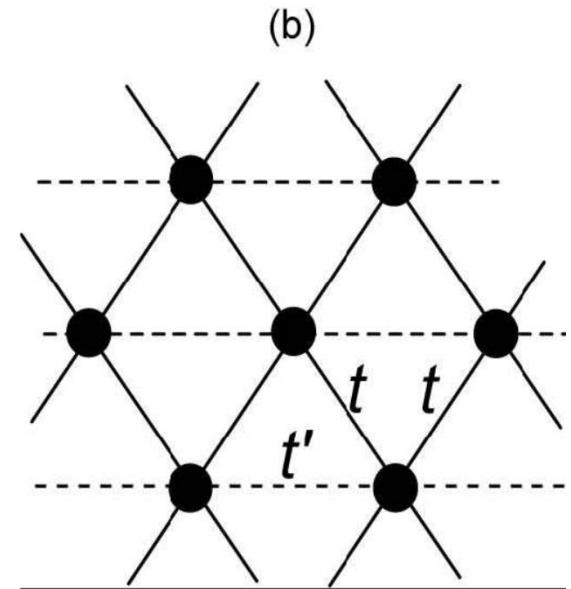
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Hubbard on anisotropic triangular lattice

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)



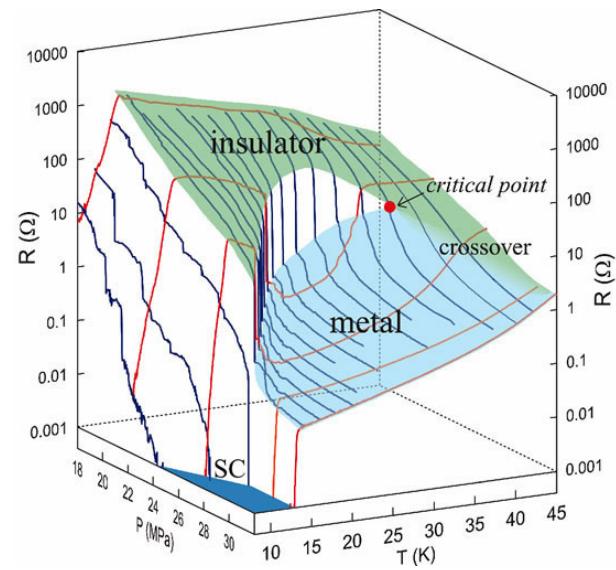
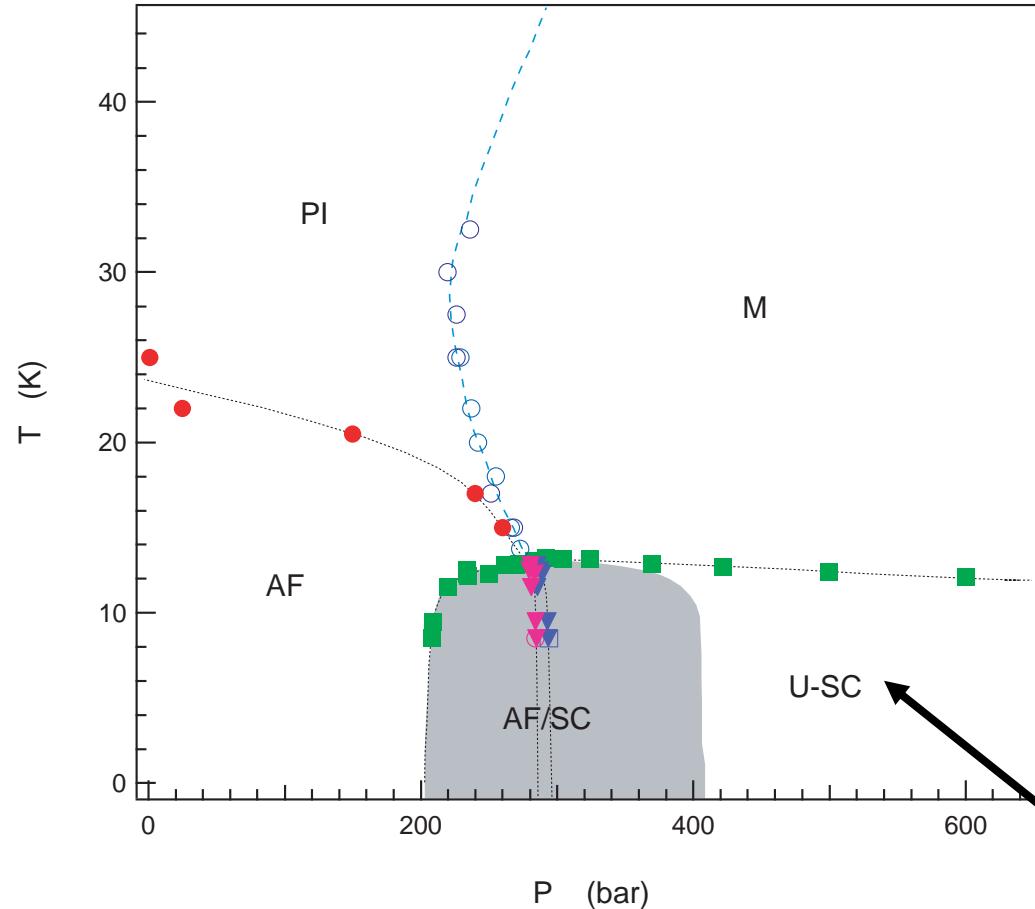
$$t \approx 50 \text{ meV}$$

$$\Rightarrow U \approx 400 \text{ meV}$$
$$t'/t \sim 0.6 - 1.1$$

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



Phase diagram for organics



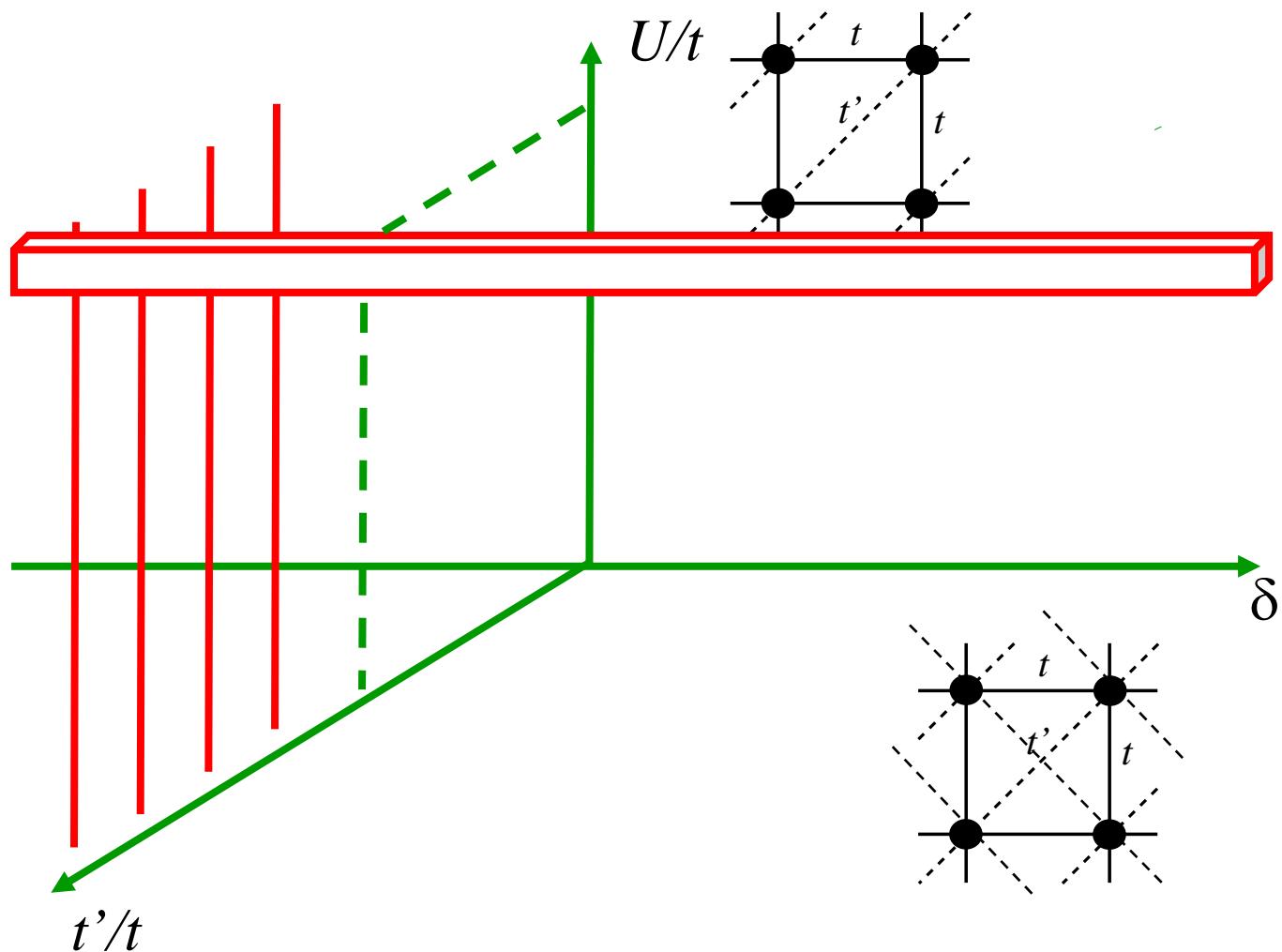
F. Kagawa, K. Miyagawa, + K. Kanoda
PRB **69** (2004) +Nature **436** (2005)

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

Phase diagram ($X=\text{Cu}[\text{N}(\text{CN})_2]\text{Cl}$)^{Powell, McKenzie cond-mat/0607078}
S. Lefebvre et al. PRL **85**, 5420 (2000), P. Limelette, et al. PRL **91** (2003)



Perspective



Outline

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



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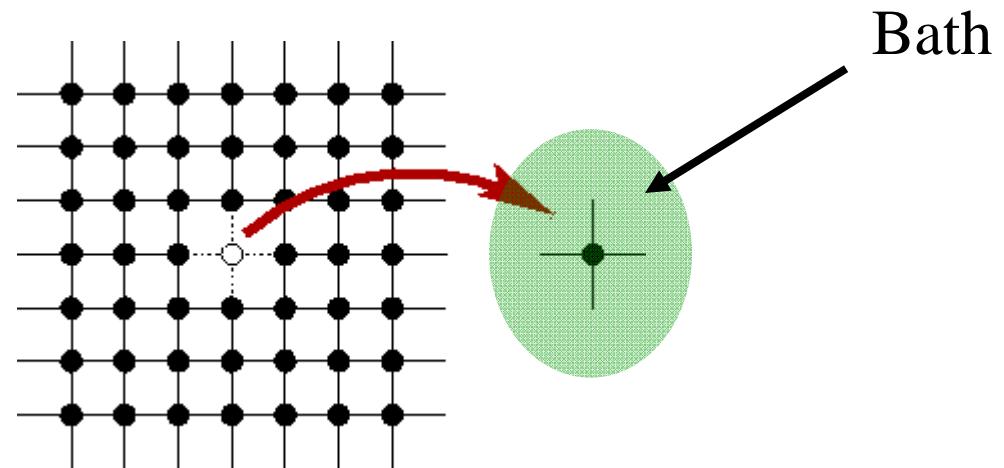
Method

“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 $d = \text{infinity}$

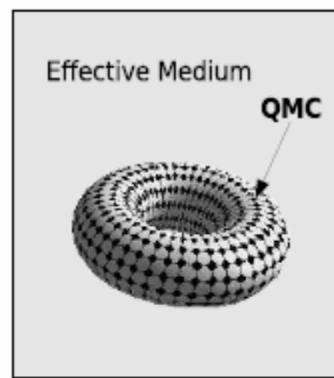
- Compute scattering rate (self-energy) of impurity problem.
- Use that self-energy (ω dependent) for lattice.
- Project lattice on single-site and adjust bath so that single-site DOS obtained both ways be equal.



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

DMFT, ($d = 3$)

2d Hubbard: Quantum cluster method

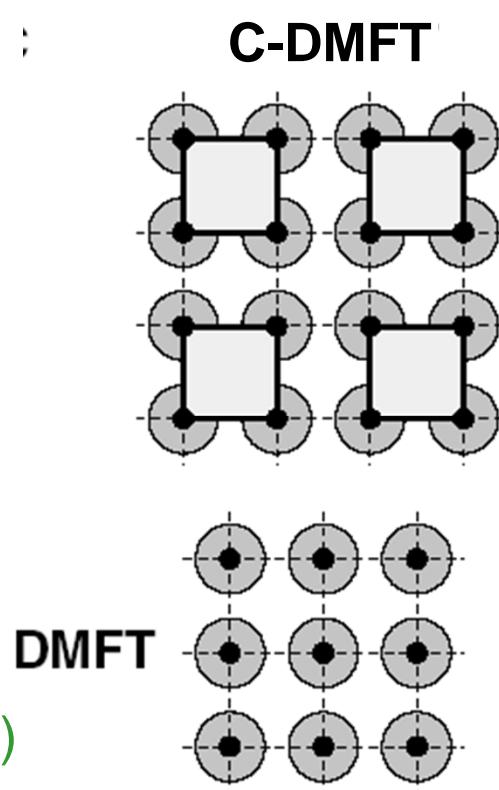


DCA

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)

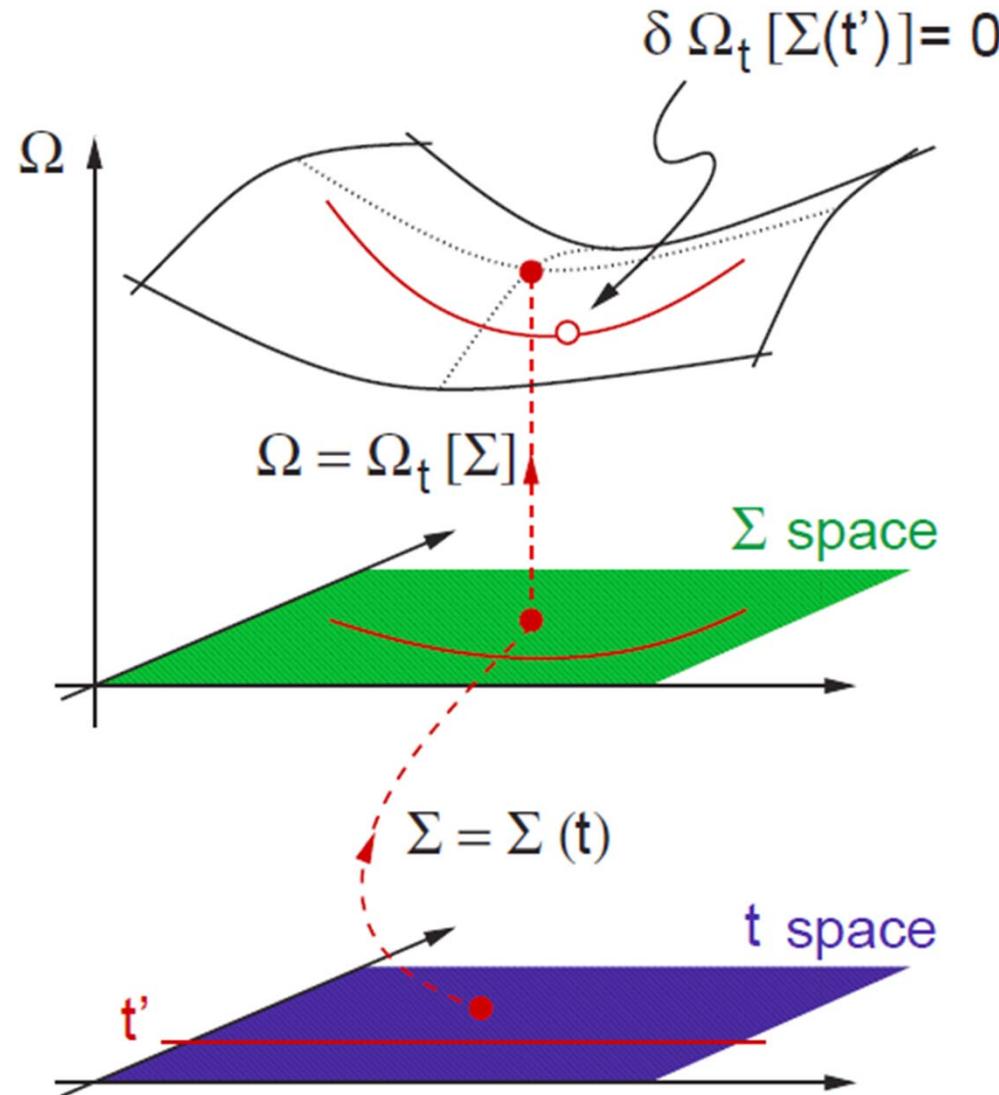
Kotliar et al. RMP (2006)

AMST et al. LTP (2006)



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DMFT as a stationnary point



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

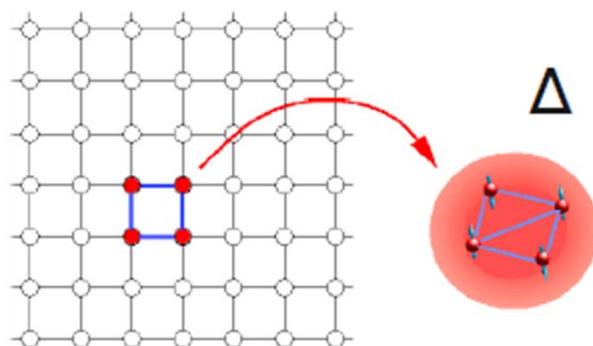
+ and -

- 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

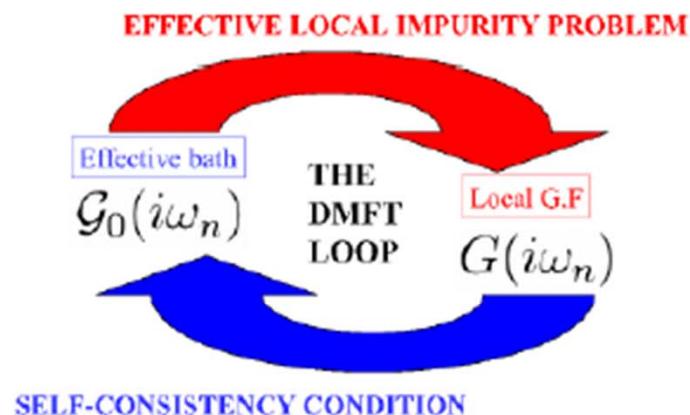


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C-DMFT



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



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

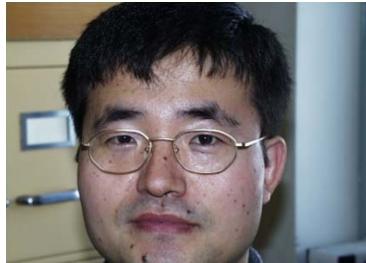
Why important

$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n)$$

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

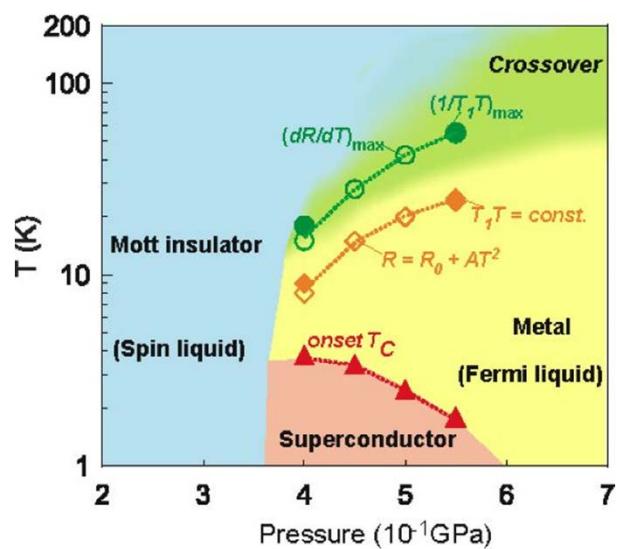
$T = 0$ phase diagram $n = 1$

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



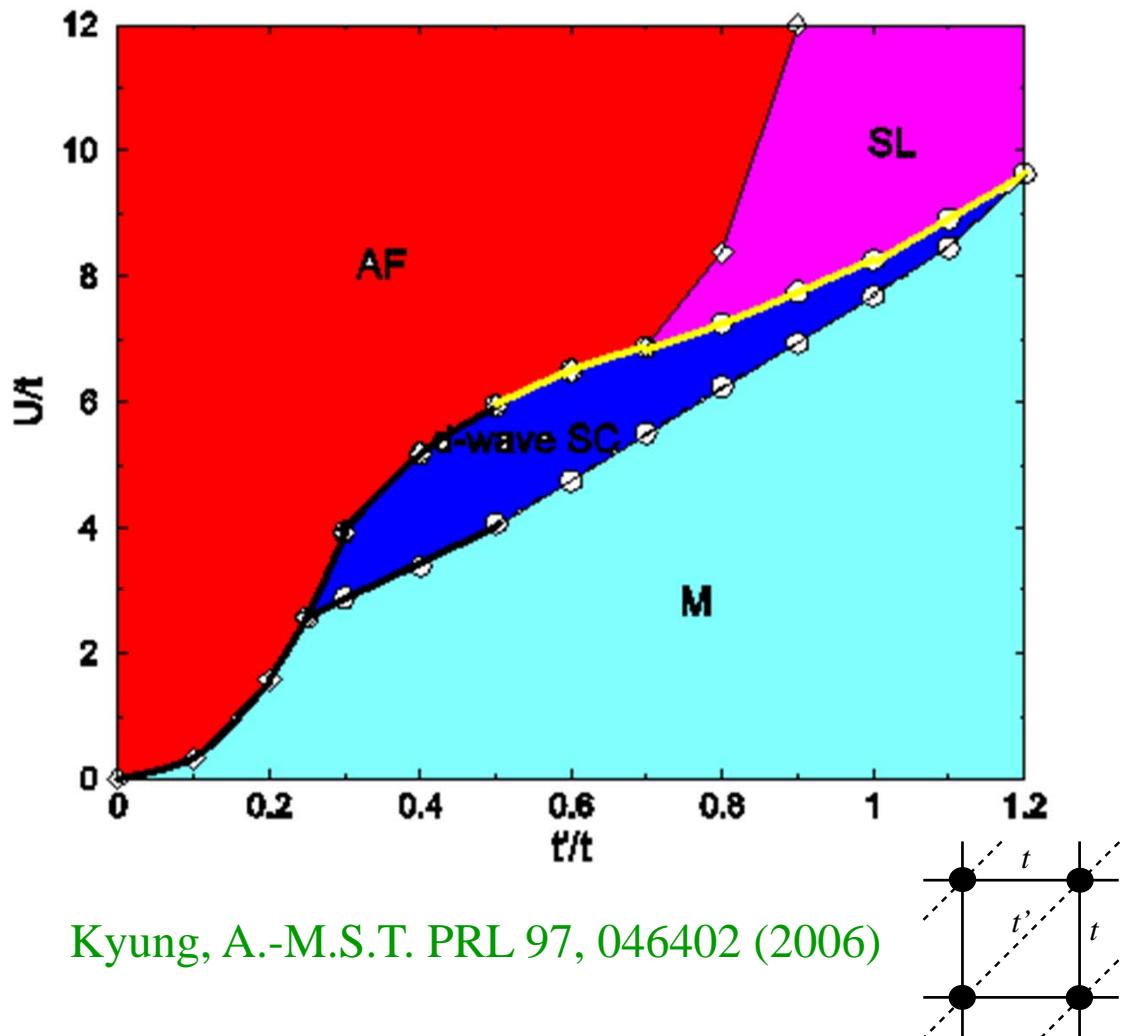
Theoretical phase diagram BEDT

$X = \text{Cu}_2(\text{CN})_3$ ($t' \sim t$)



Y. Kurisaki, et al.

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

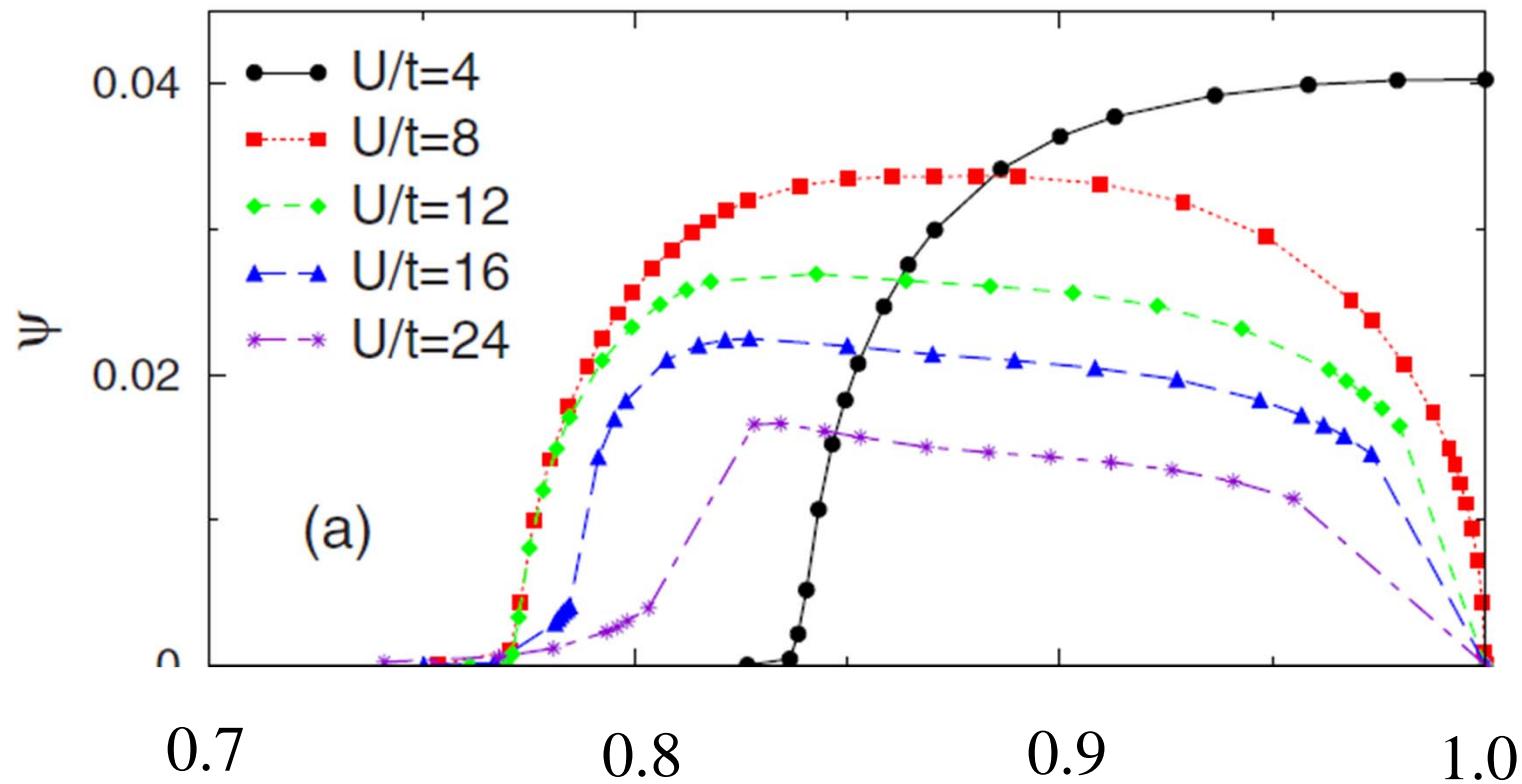


Kyung, A.-M.S.T. PRL 97, 046402 (2006)

$T = 0$ phase diagram: cuprates

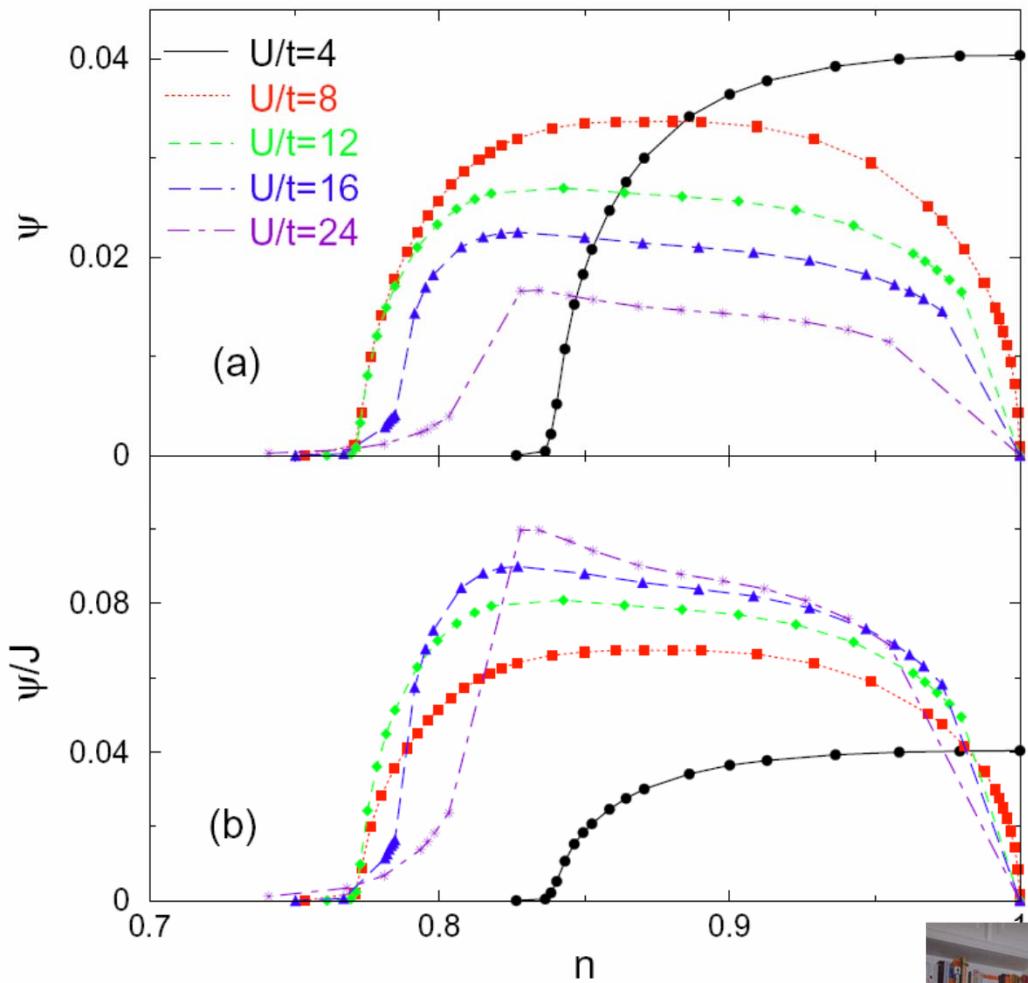
Phase diagram
Exact diagonalization as impurity
solver ($T=0$).

Theory: effect of Mott on order parameter



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

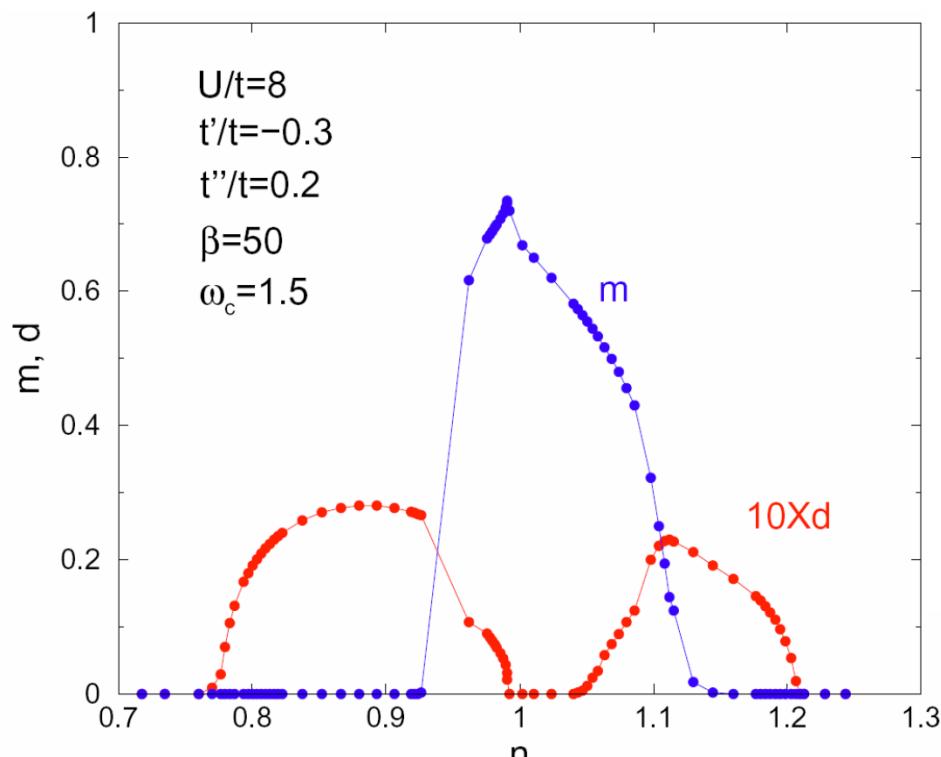
Dome vs Mott (CDMFT)



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

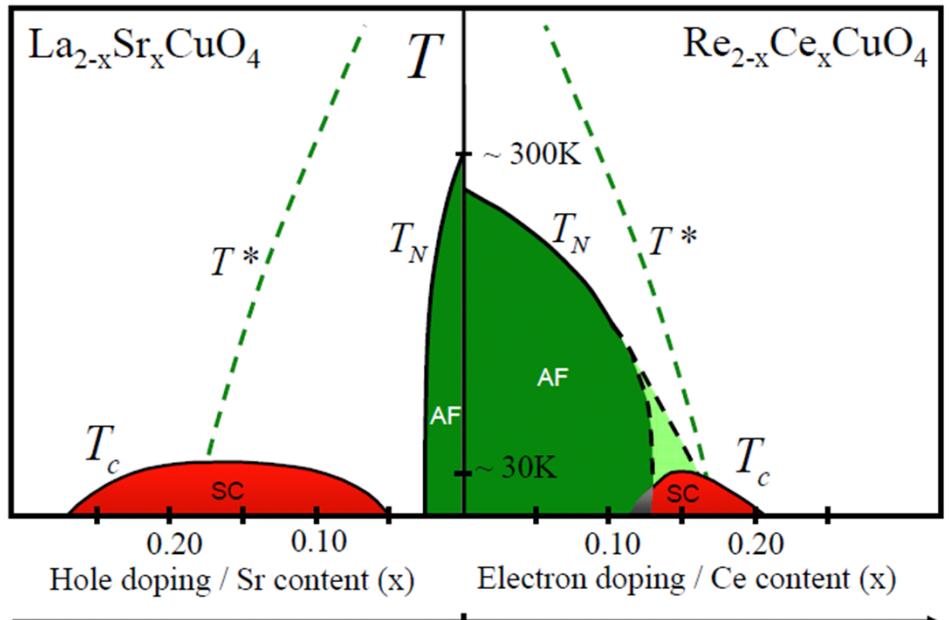


CDMFT global phase diagram



Kancharla, Kyung, Civelli,
Sénéchal, Kotliar AMST

Phys. Rev. B (2008)
AND Capone, Kotliar PRL (2006)



Armitage, Fournier, Greene, RMP (2009)



Outline

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

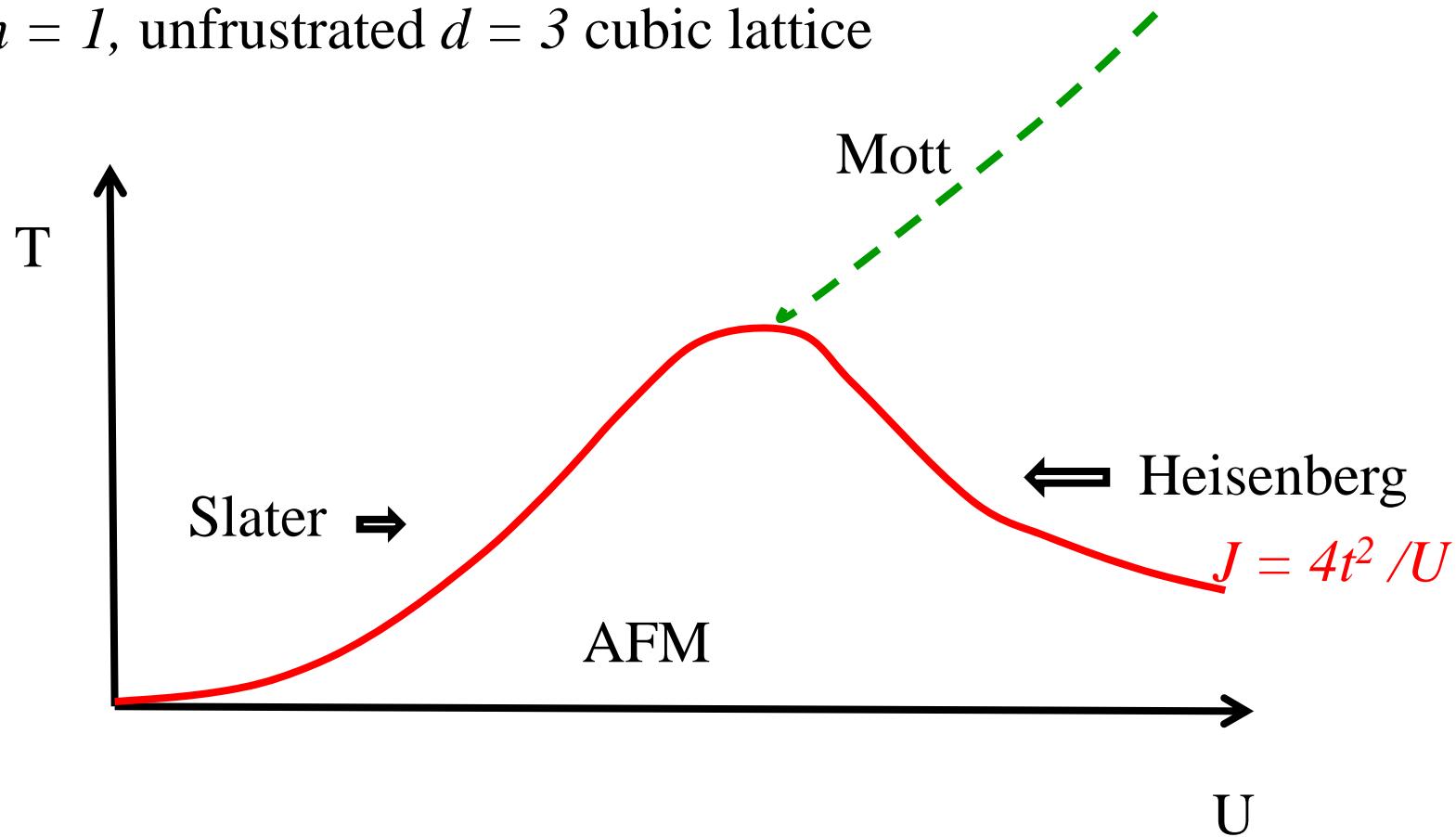
Normal state of the cuprates



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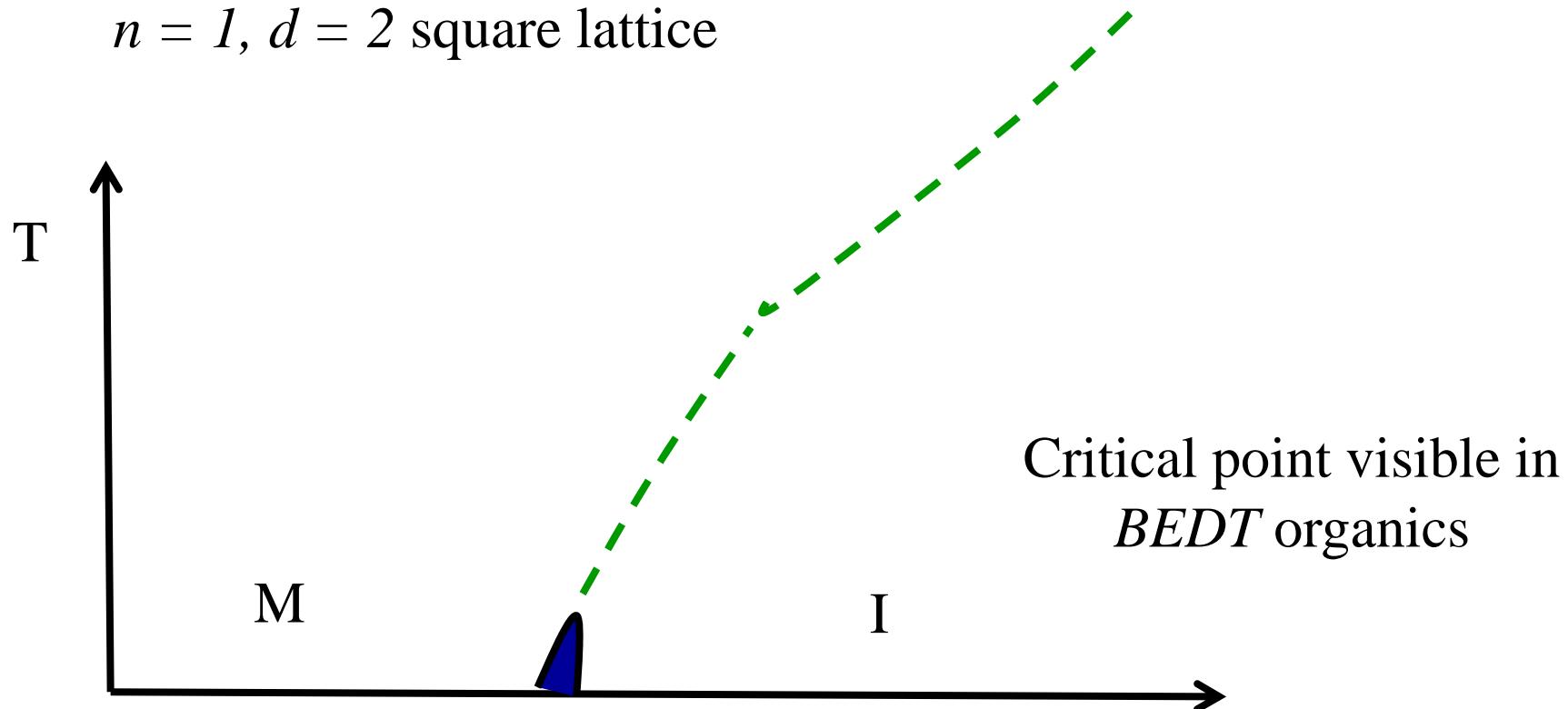
Preliminary: Weak vs Strong correlations

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



Local moment and Mott transition

$n = 1, d = 2$ square lattice



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

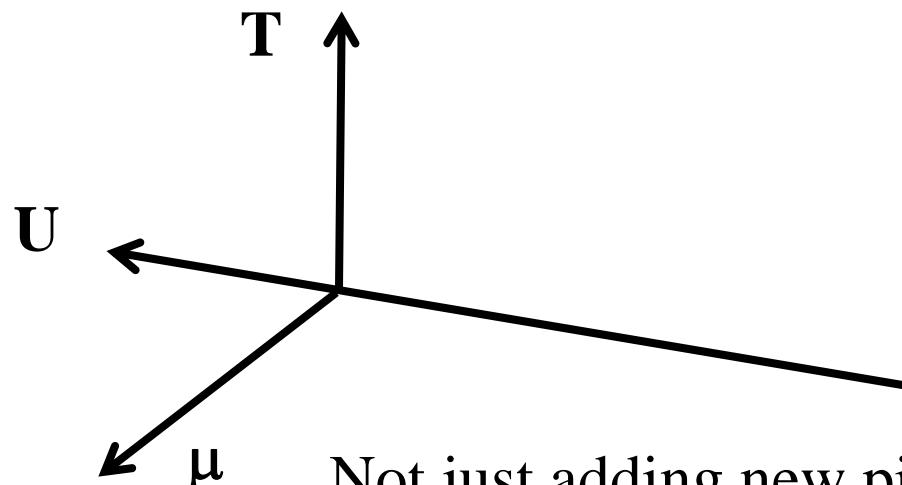


Giovanni Sordi

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

Phys. Rev. B, **84**, 075161 (2011)

Doping-induced Mott transition ($t'=0$)



Not just adding new piece:

Lesson from DMFT, first order transition + critical
point governs phase diagram

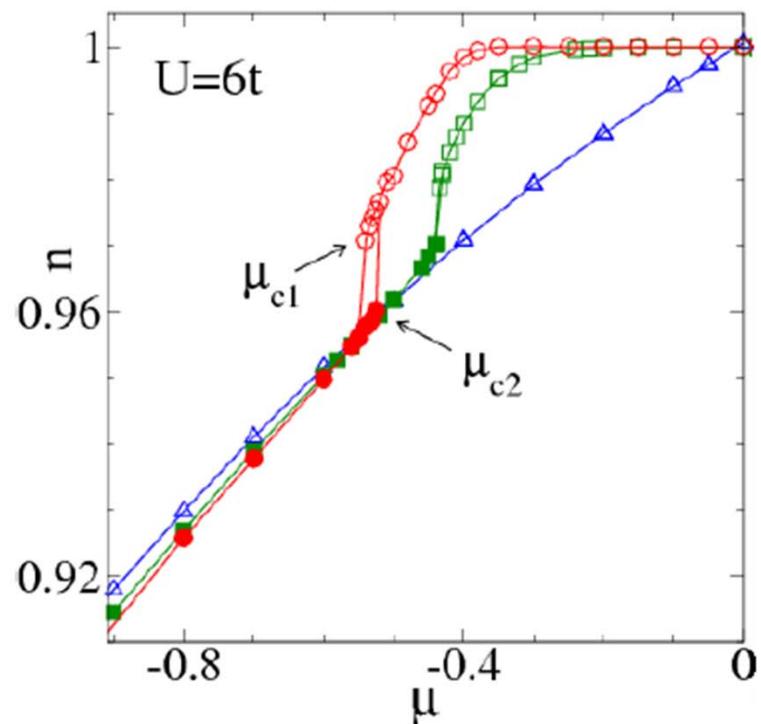


Kristjan Haule



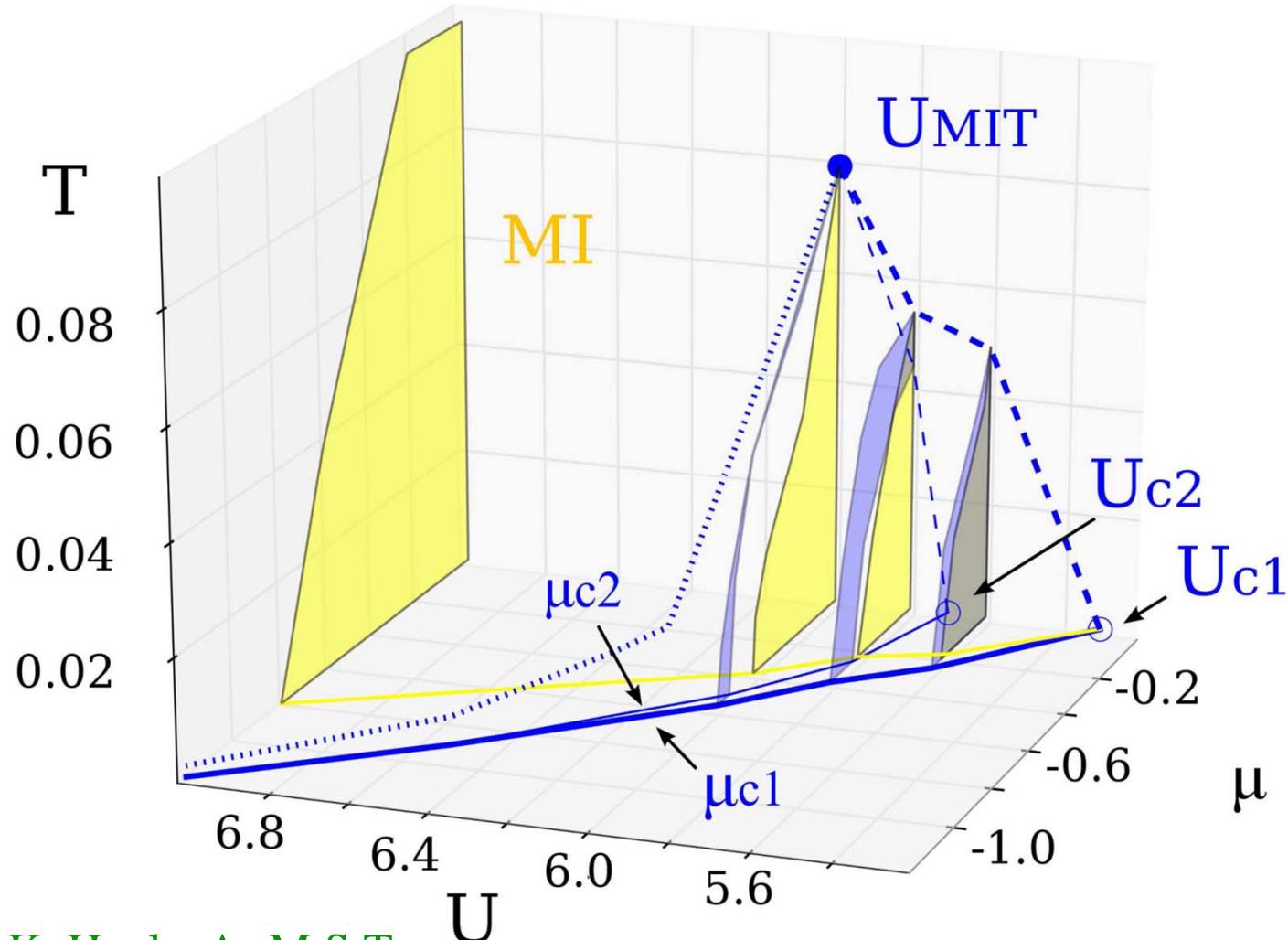
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First order transition at finite doping



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

Normal state phase diagram



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

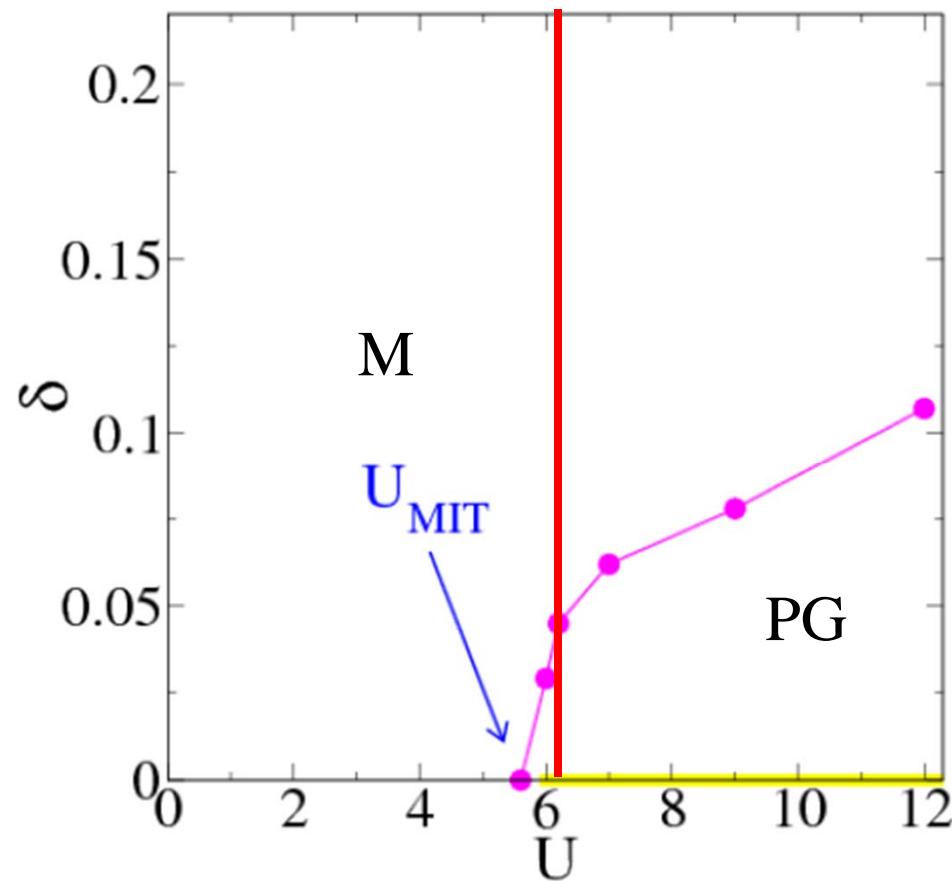
$\mu = 0$, H. Park, K. Haule, and G. Kotliar,
Phys. Rev. Lett. 101, 186403 (2008).



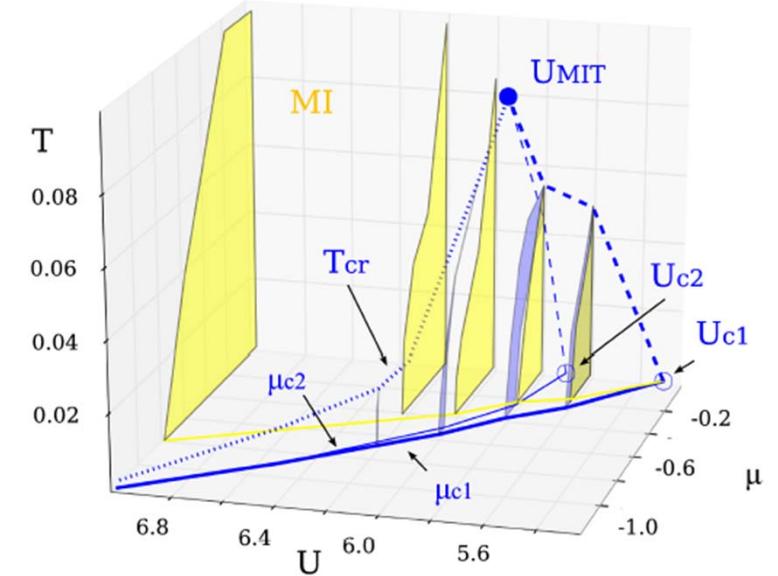
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Link to Mott transition up to optimal doping

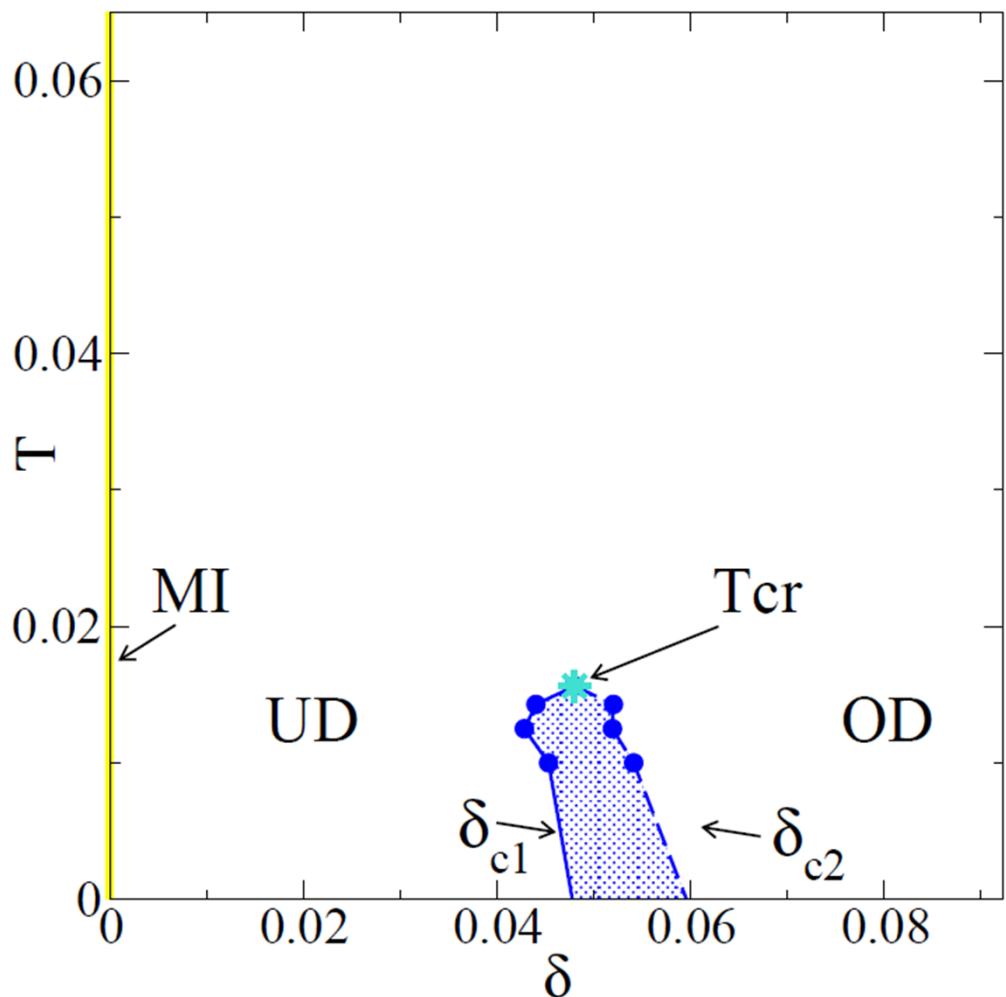
Doping dependence of critical point as a function of U



Smaller D and S



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



$U > U_{MIT}$:

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?





Giovanni Sordi



Patrick Sémon



Kristjan Haul

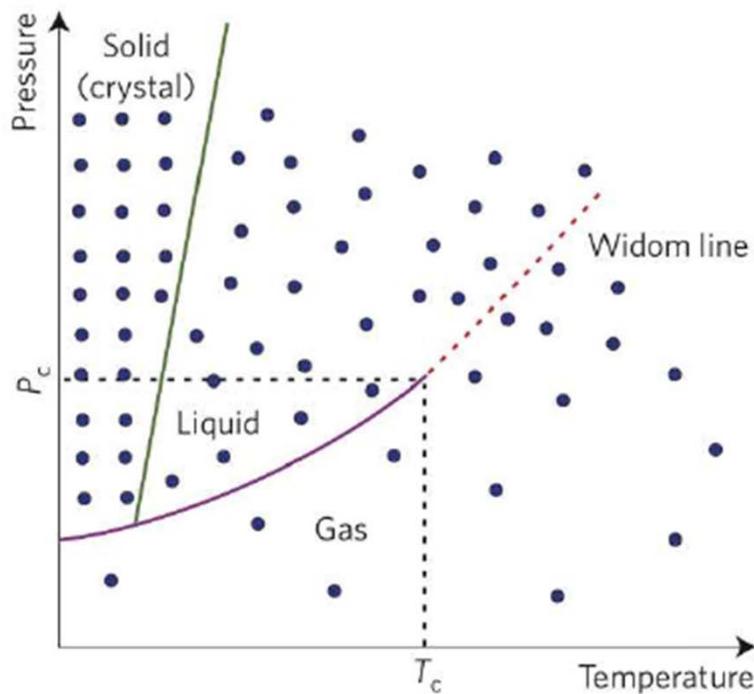
Widom line ($t' = 0$)

Pseudogap in the normal state and the
Widom line



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What is the Widom line?

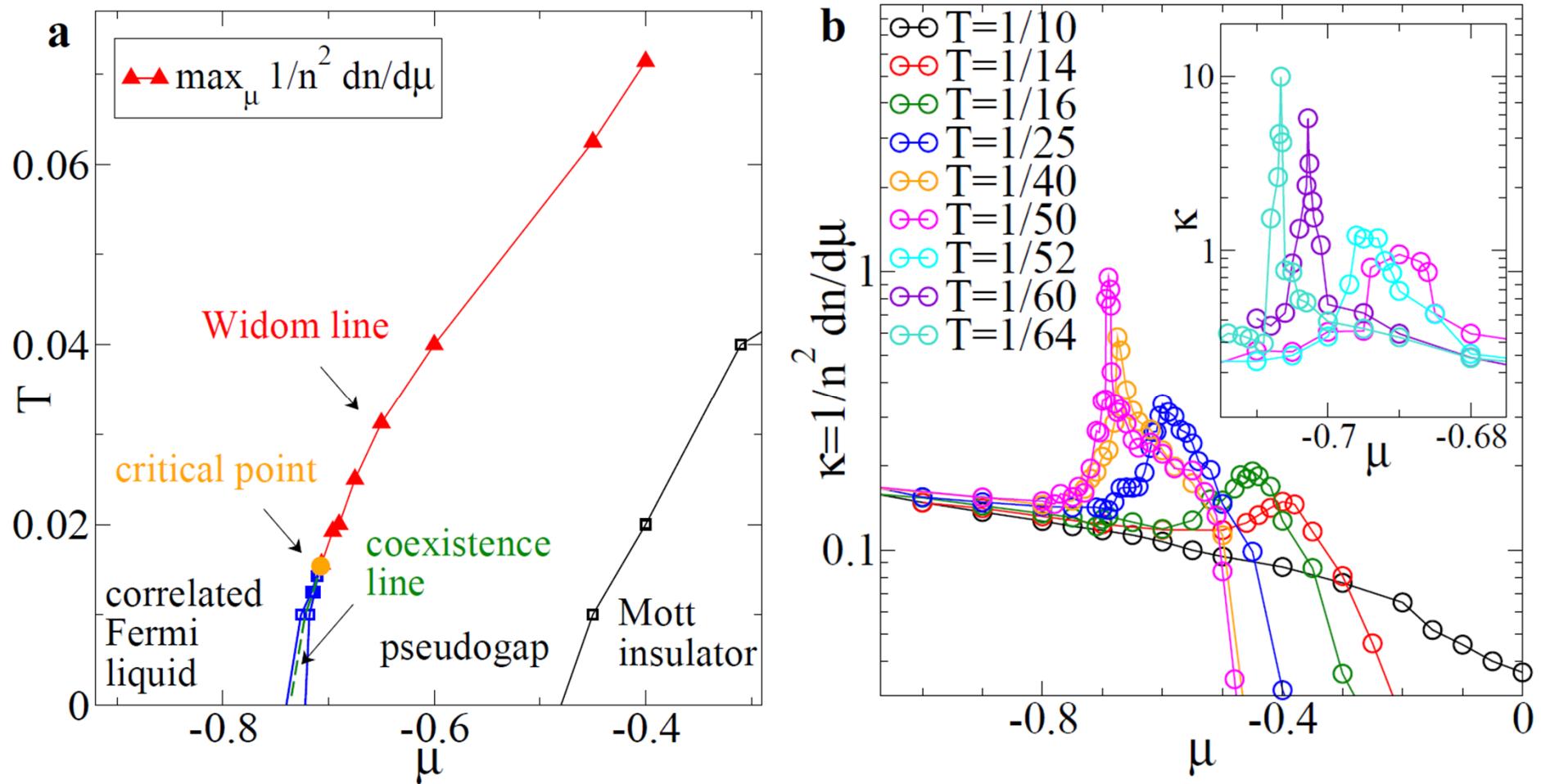


McMillan and Stanley, Nat Phys 2010

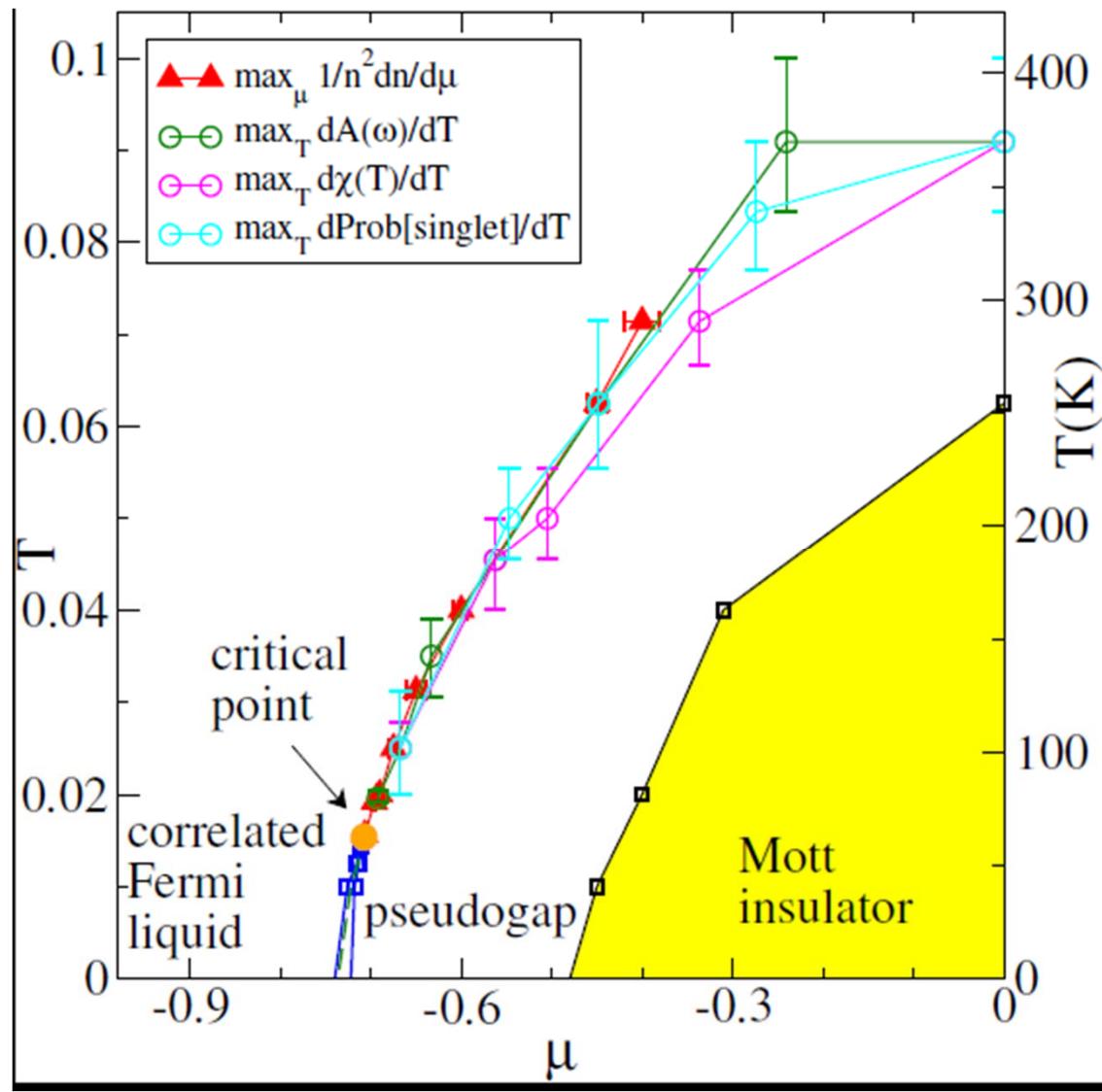
- ▶ it is the continuation of the coexistence line in the supercritical region
- ▶ line where the **maxima of different response functions** touch each other asymptotically as $T \rightarrow T_p$
- ▶ liquid-gas transition in water: max in isobaric heat capacity C_p , isothermal compressibility, isobaric heat expansion, etc

- ▶ **DYNAMIC crossover arises from crossing the Widom line!**
water: Xu et al, PNAS 2005,
Simeoni et al Nat Phys 2010

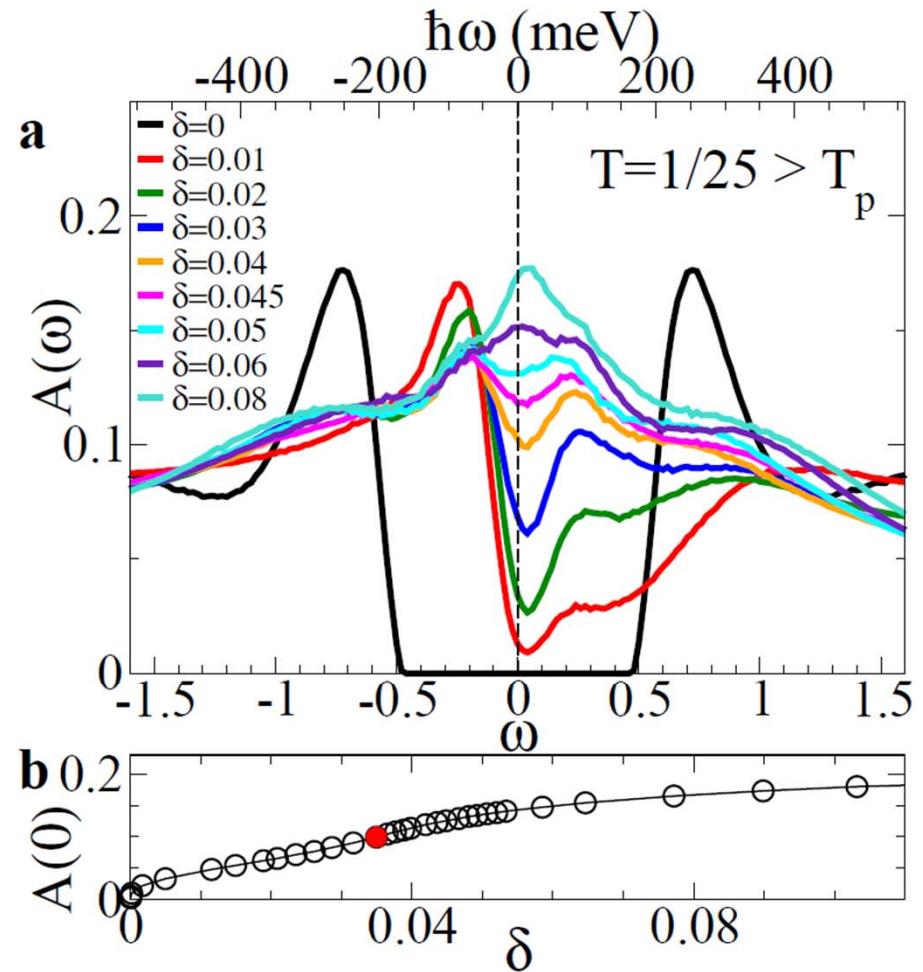
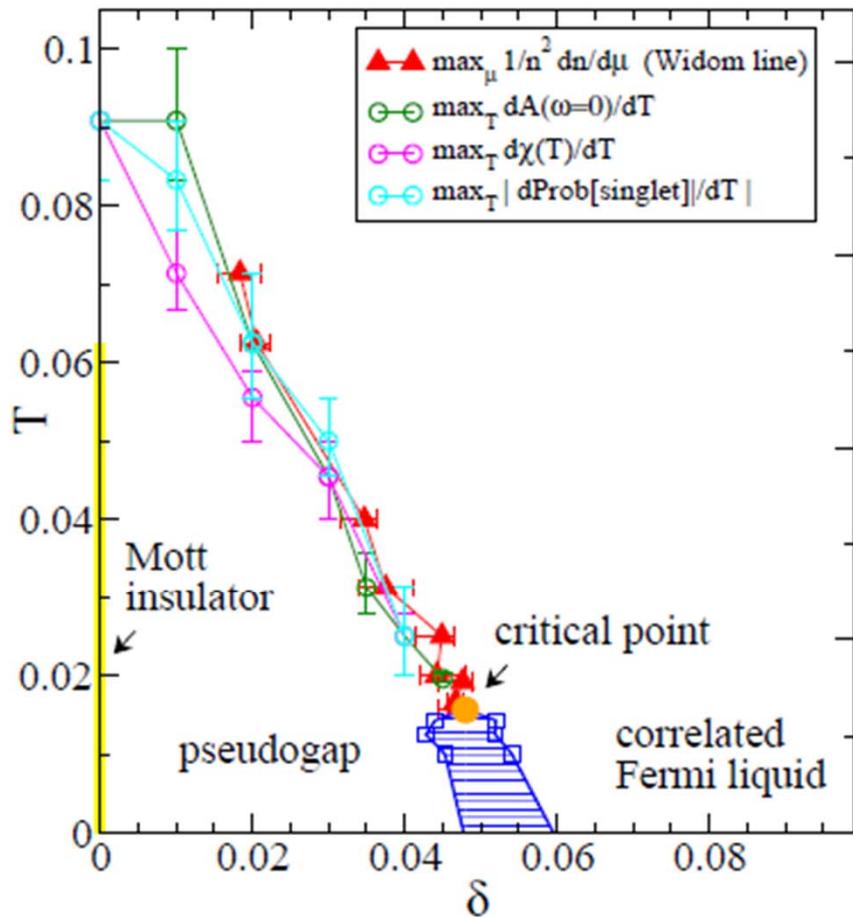
The Widom line



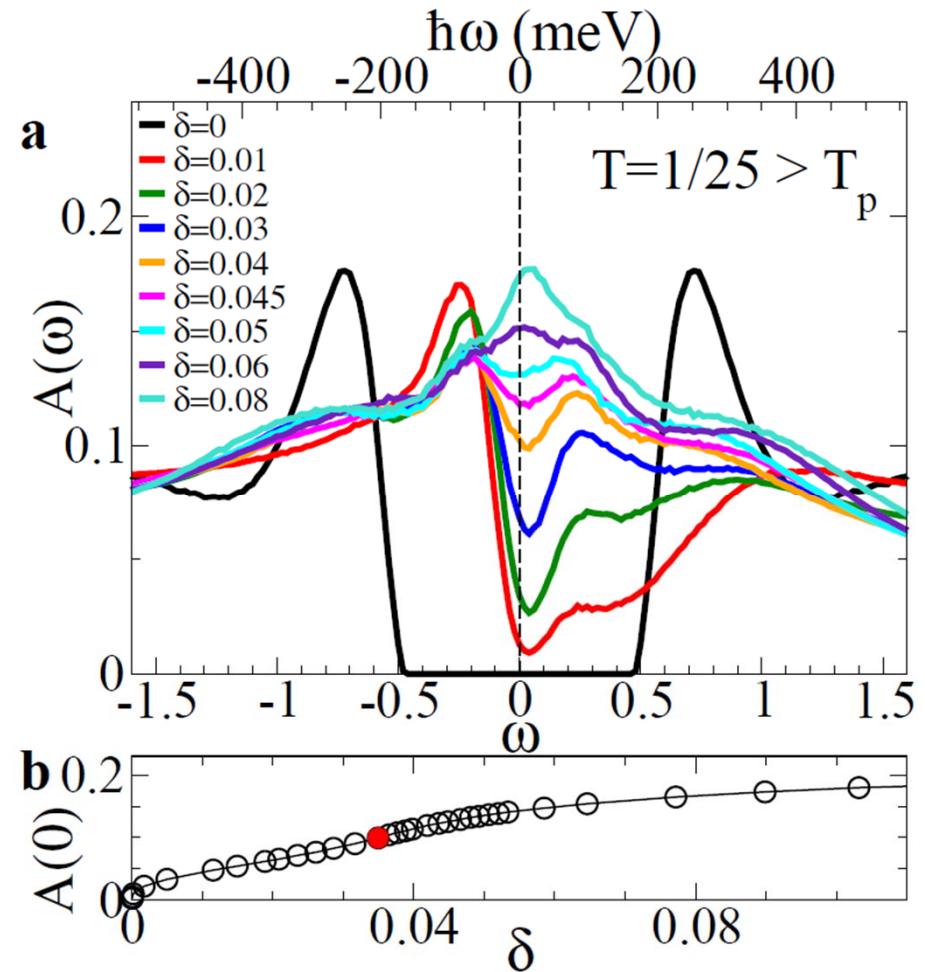
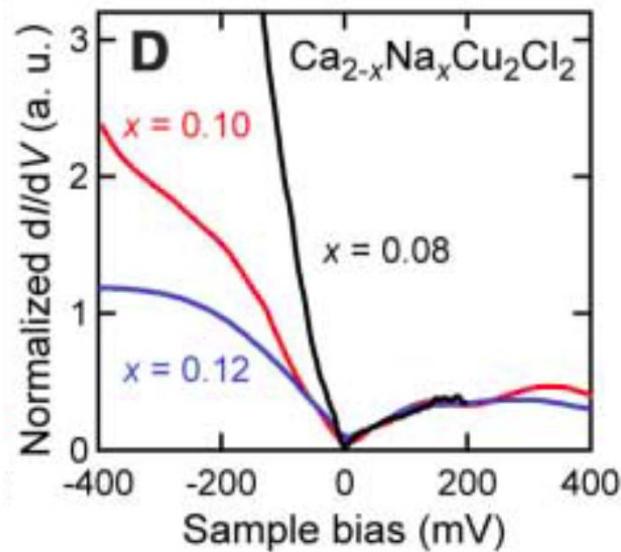
Rapid change also in dynamical quantities



Density of states



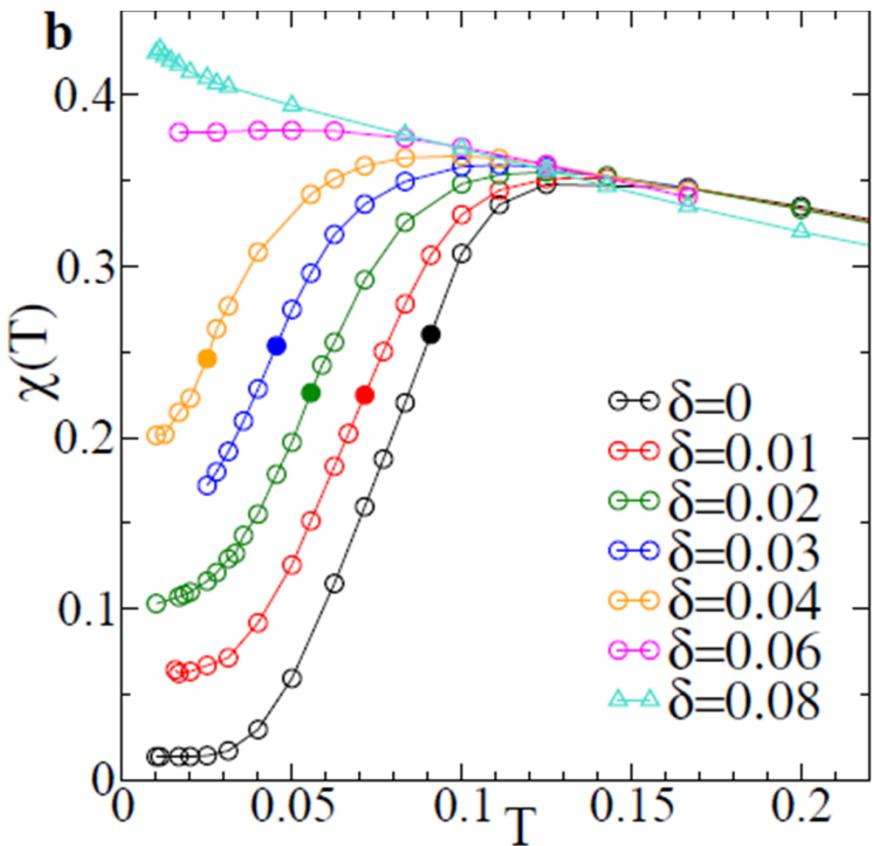
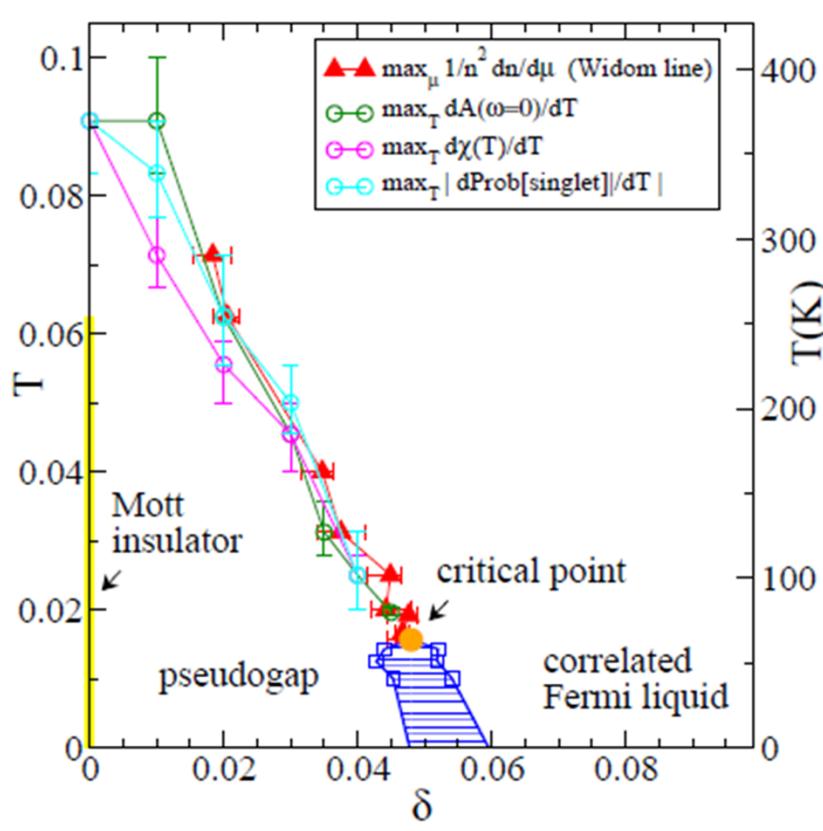
Density of states



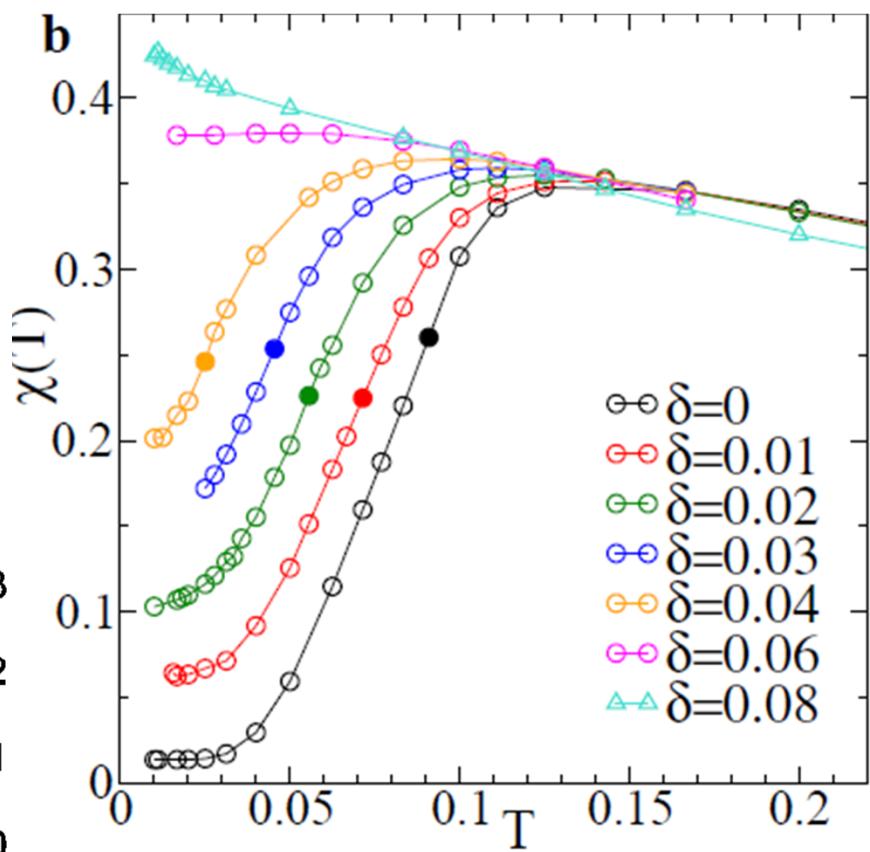
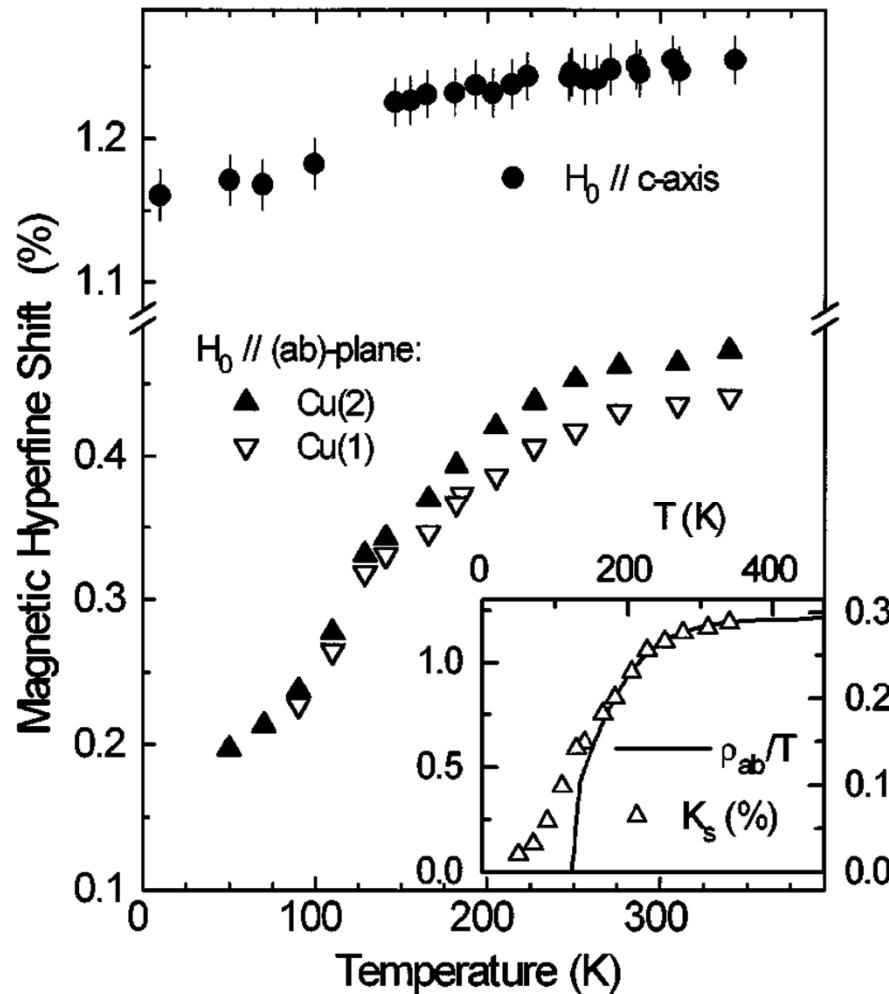
Khosaka et al. *Science* **315**, 1380 (2007);



Spin susceptibility



Spin susceptibility



Underdoped Hg1223

Julien et al. PRL 76, 4238 (1996)



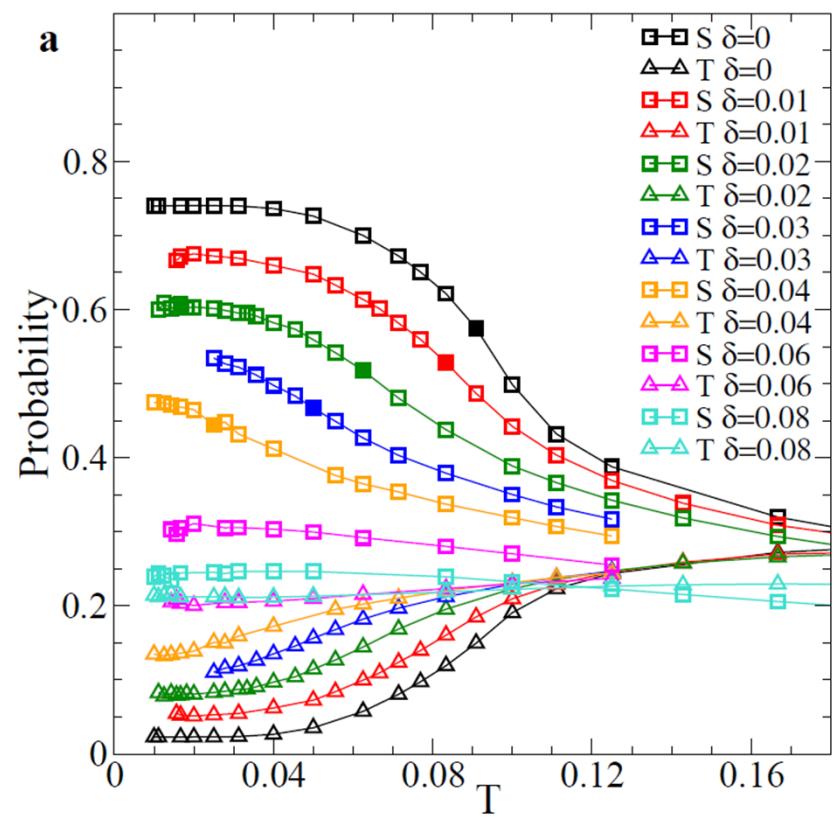
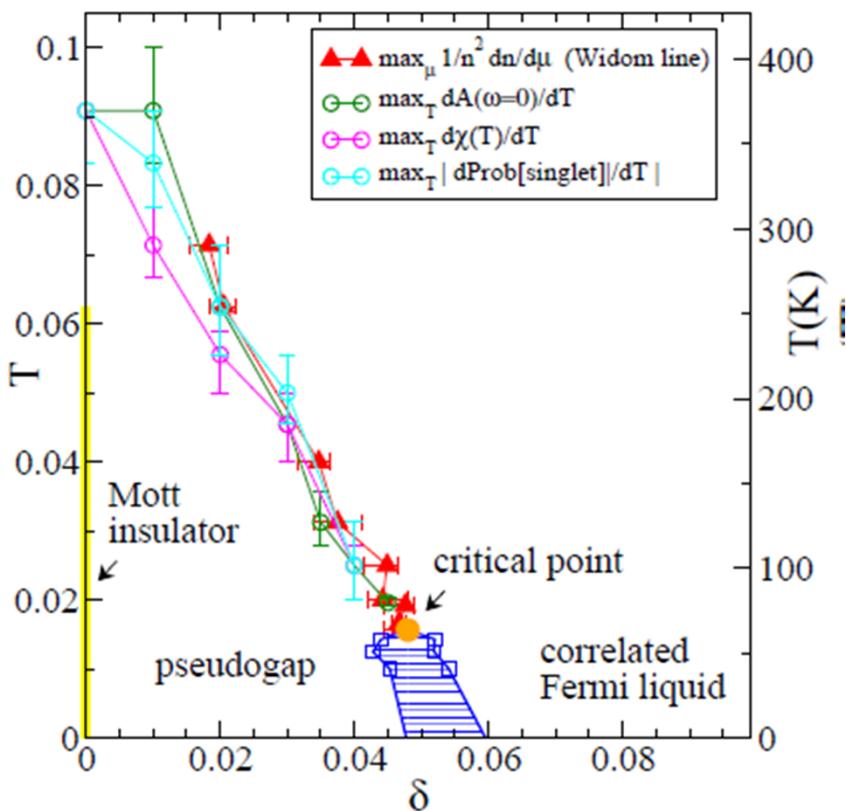
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Physics



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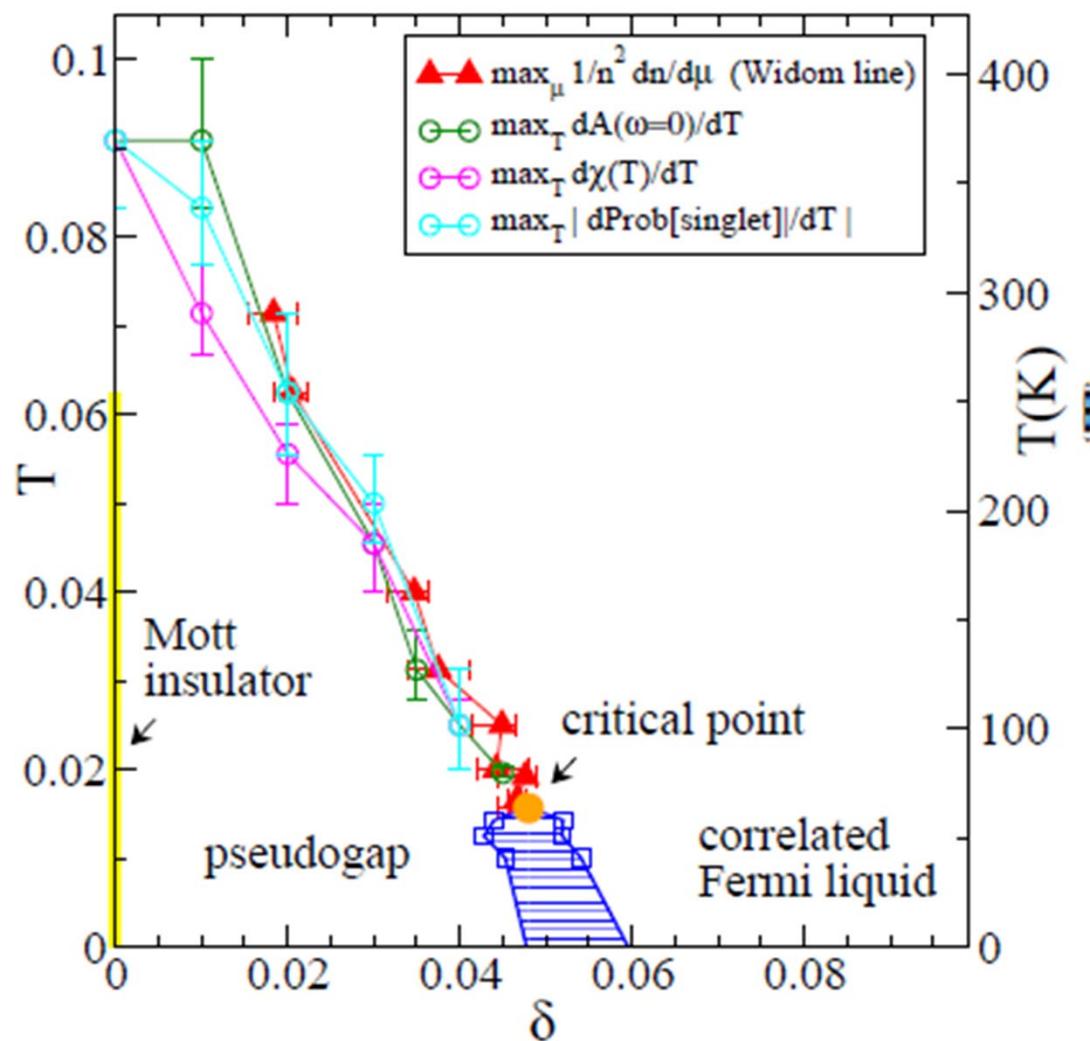
Plaquette eigenstates



See also:

Michel Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, A. Georges
 PRB 80, 064501 (2009)

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)

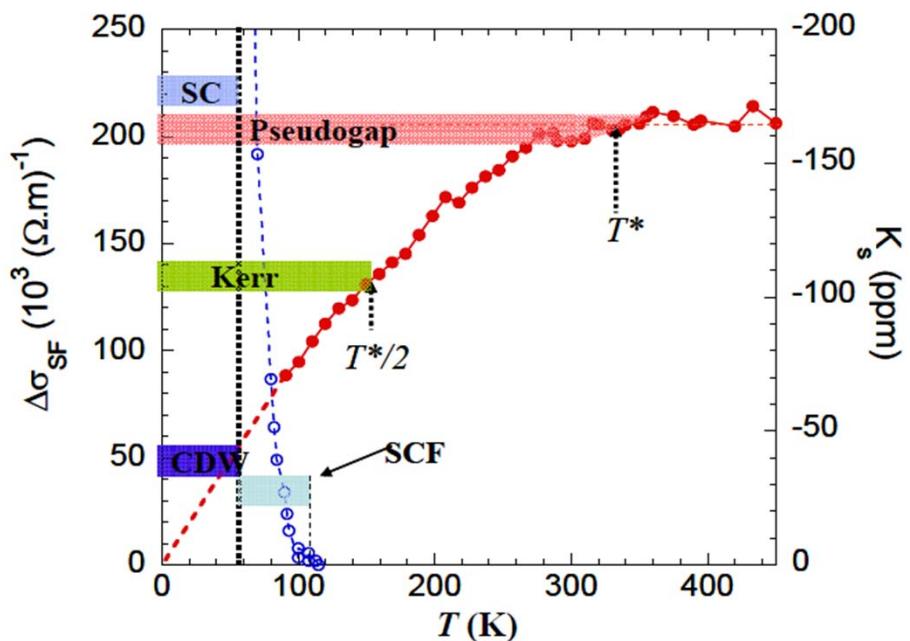


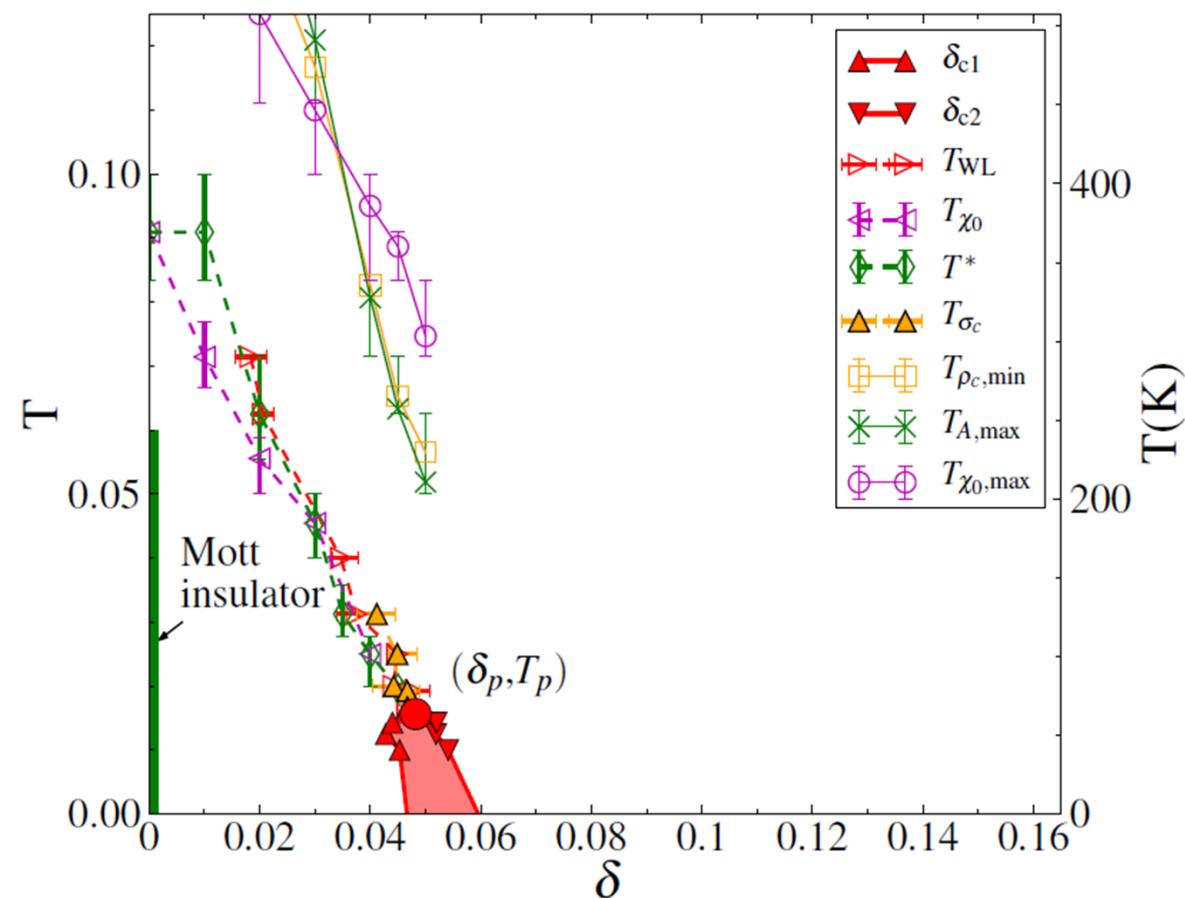
Fig 1 Spin contribution K_s to the ^{89}Y NMR Knight shift [11] for $\text{YBCO}_{6.6}$ permit to define the PG onset T^* . Here K_s is reduced by a factor two at $T \sim T^*/2$. The sharp drop of the SC fluctuation conductivity (SCF) is illustrated (left scale) [23]. We report as well the range over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



Giovanni Sordi



Patrick Sémon



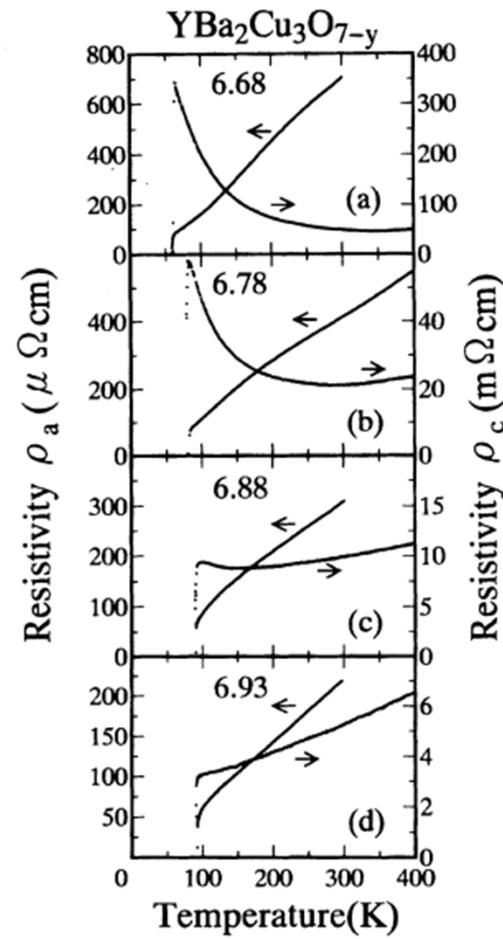
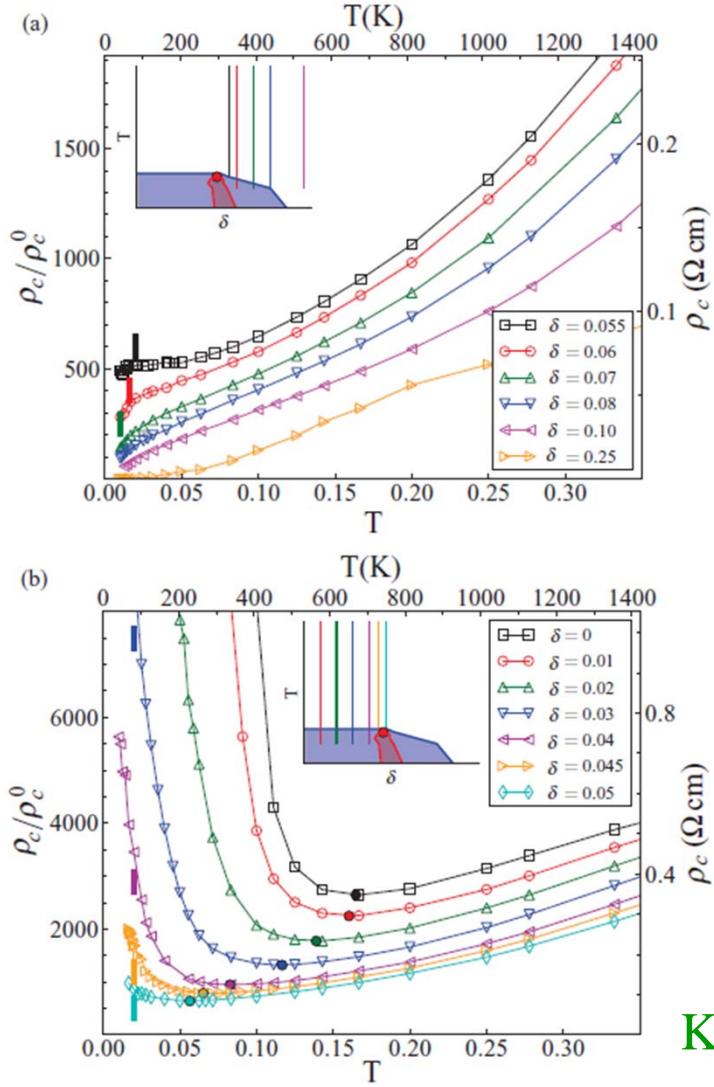
G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)

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



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C-axis resistivity

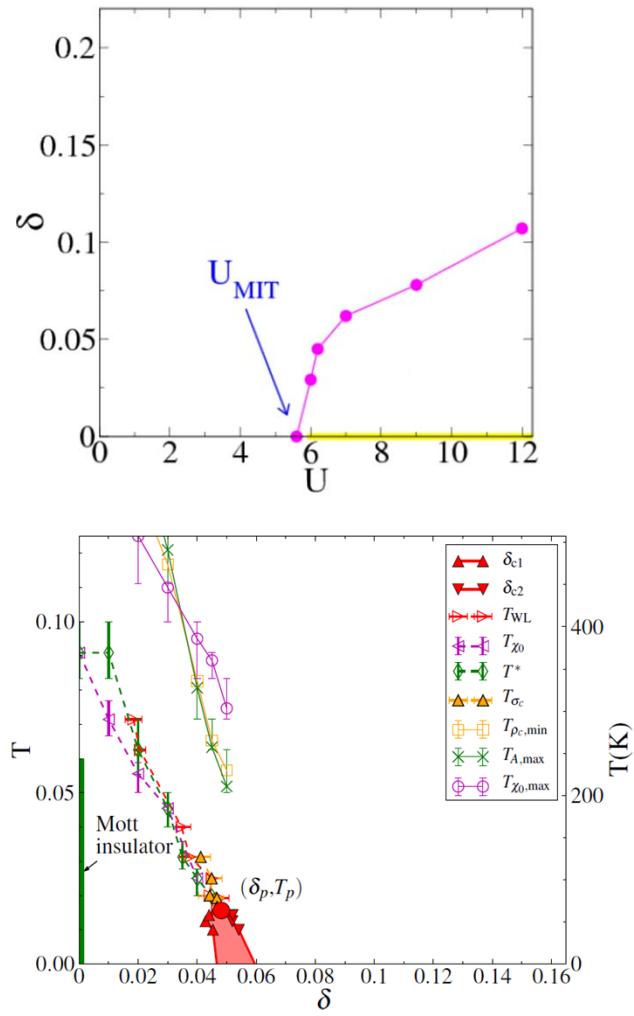


K. Takenaka, K. Mizuhashi, H. Takagi, and S. Uchida,
Phys. Rev.B 50, 6534 (1994).



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Summary: normal state



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

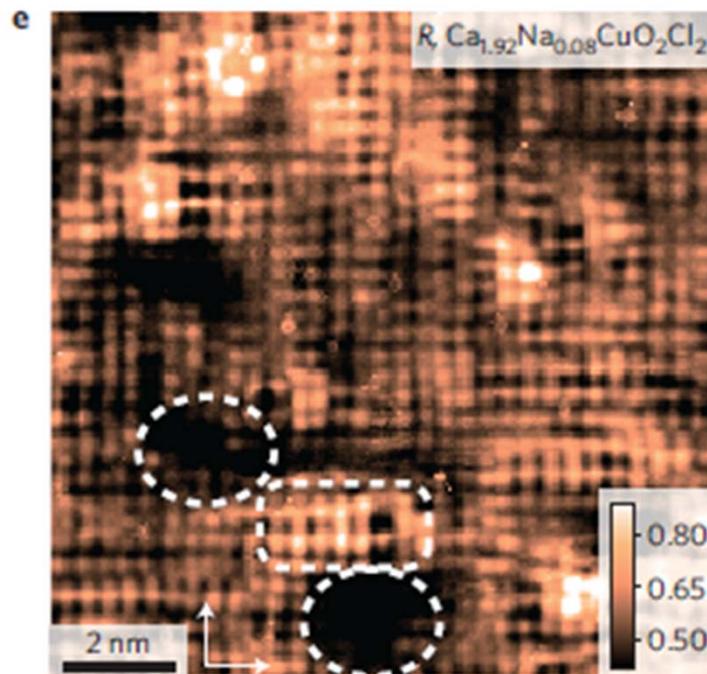
Charge Density Wave Back to experiment

h-doped



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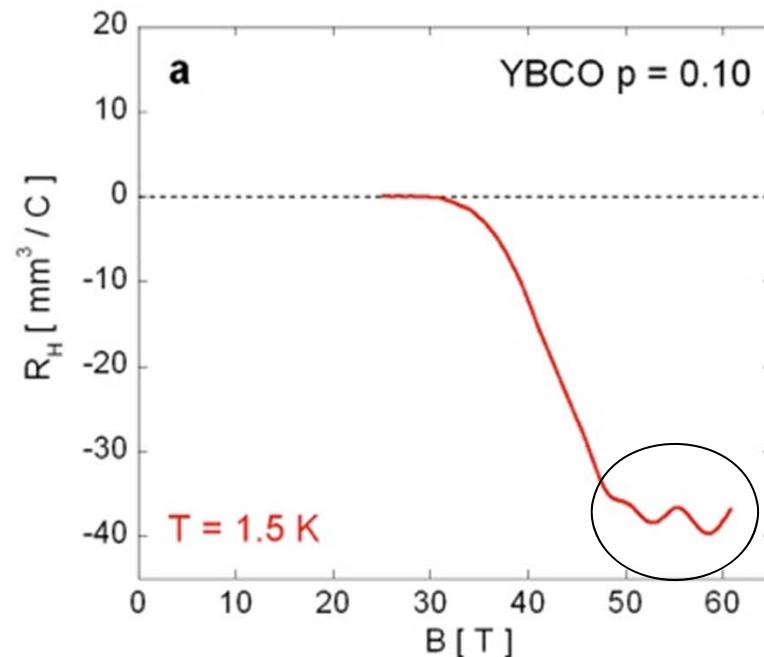
Intra-unit cell nematic order: STM



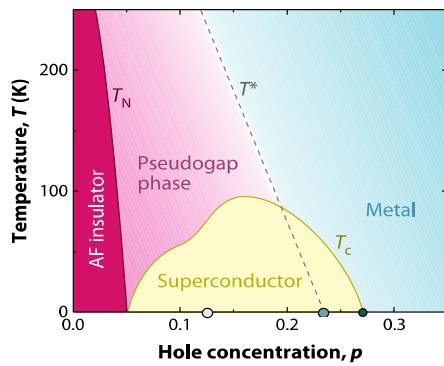
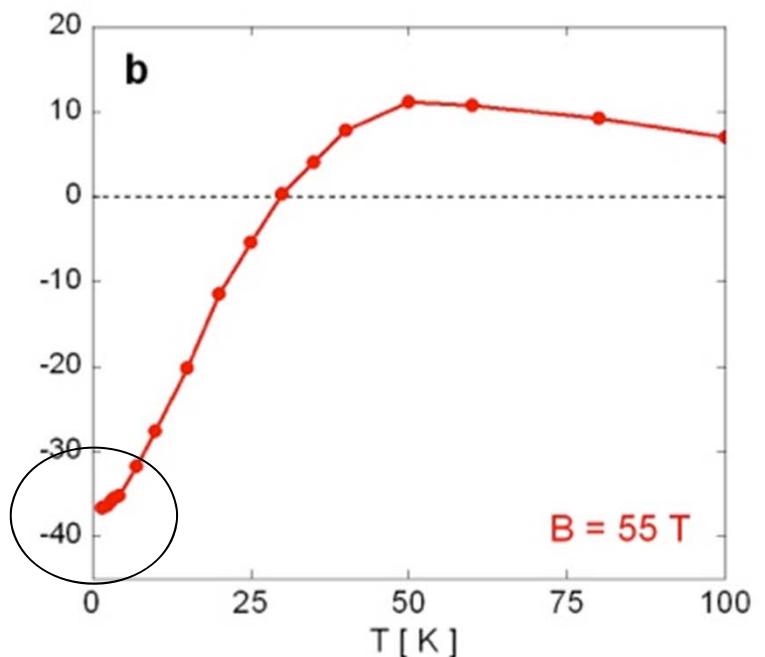
Kohsaka et al. Nature Physics 2012

Quantum oscillations in cuprates: 2007

N. Doiron-Leyraud et al., Nature 2007



D. LeBoeuf et al., Nature 2007



Quantum oscillations

$R_H < 0$

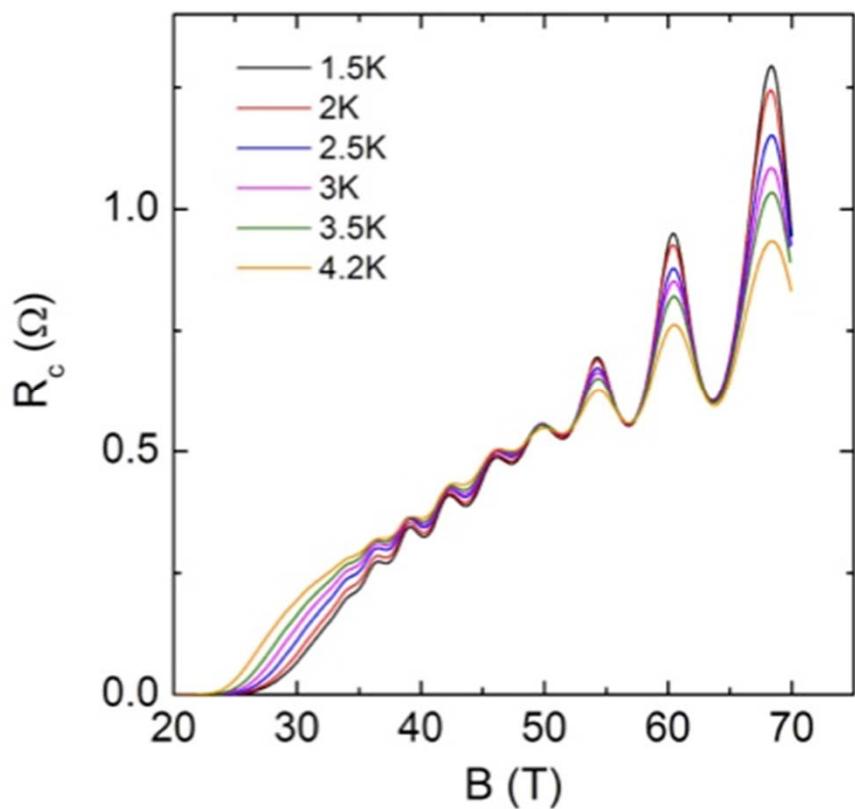
Fermi surface includes a small **electron pocket** !



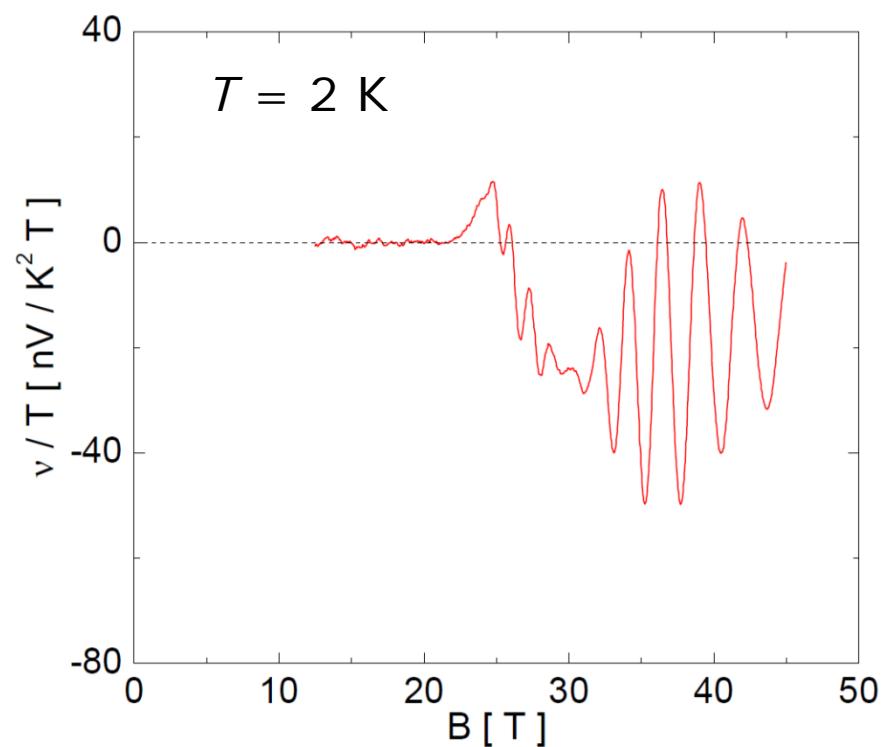
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Quantum oscillations in cuprates: 2013

Resistance



Nernst



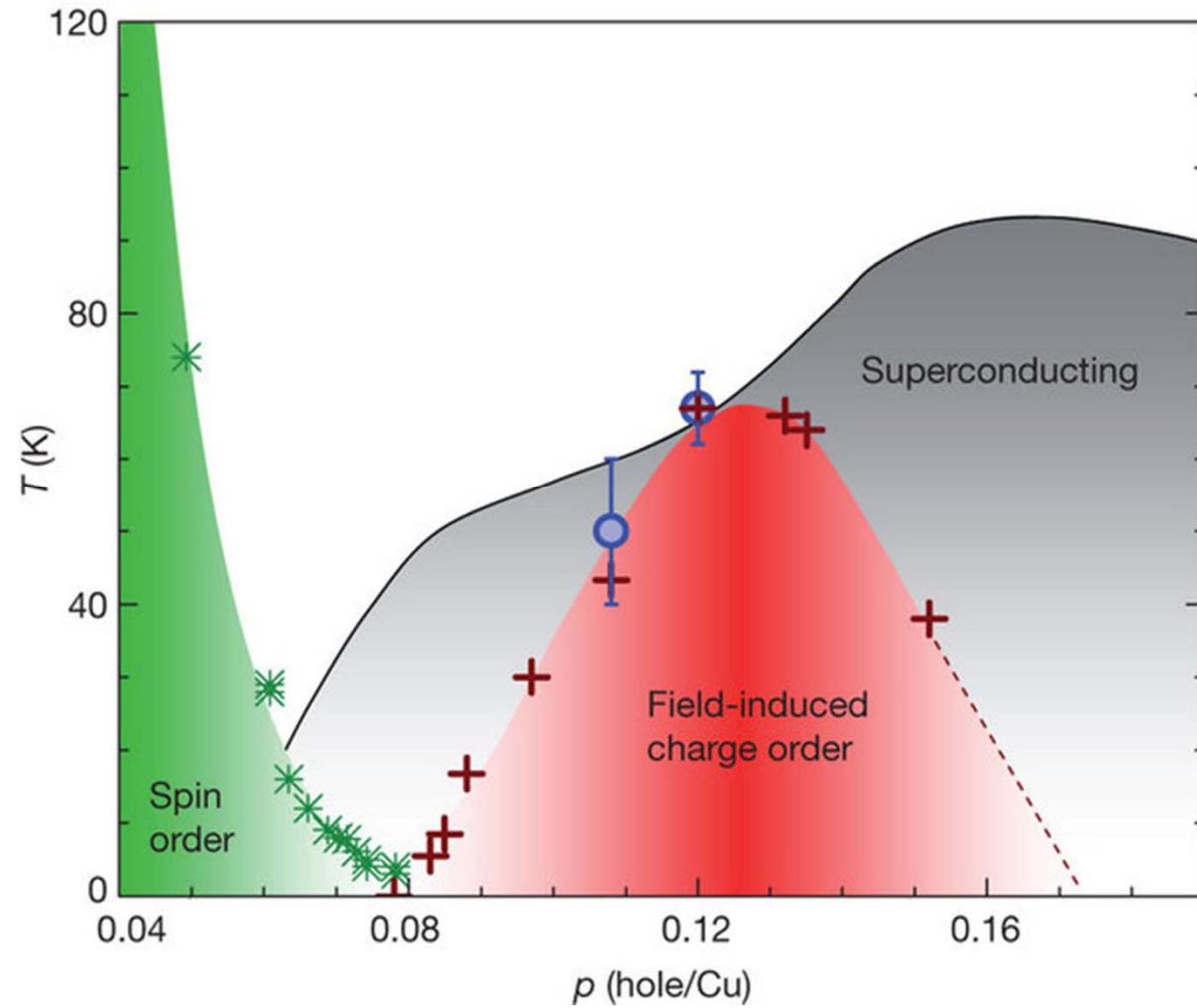
LNCMI, Toulouse

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-T_c copper-oxide pseudogap states. *Nature* 466, 347351 (2010).
- Parker, C. V. et al. Fluctuating stripes at the onset of the pseudogap in the high-T_c superconductor B₂Sr₂CaCu₂O₈C_x. *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)Ba₂Cu₃O₆C_x. *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 YBa₂Cu₃O_y. *Nature* 477, 192194 (2011).
- LeBoeuf, D. et al. Thermodynamic phase diagram of static charge order in underdoped YBa₂Cu₃O_y. *Nature Phys.* 9, 7983 (2013).

Direct observation of competition between superconductivity and charge density wave order in $\text{YBa}_2\text{Cu}_3\text{O}_{6.67}$

J. Chang^{1,2*}, E. Blackburn³, A. T. Holmes³, N. B. Christensen⁴, J. Larsen^{4,5}, J. Mesot^{1,2},
Ruixing Liang^{6,7}, D. A. Bonn^{6,7}, W. N. Hardy^{6,7}, A. Watenphul⁸, M. v. Zimmermann⁸, E. M. Forgan³
and S. M. Hayden⁹

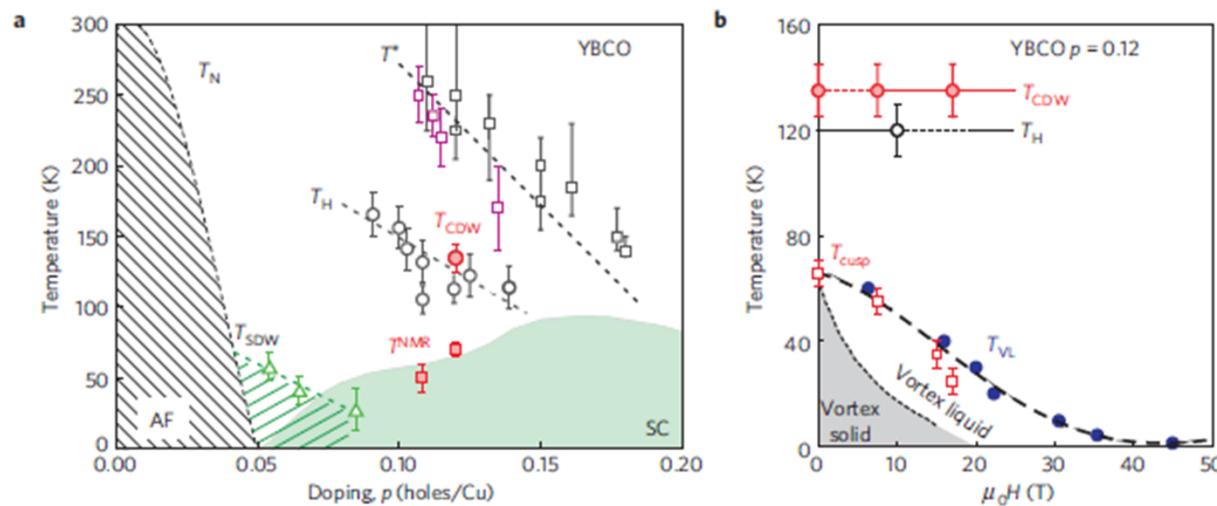
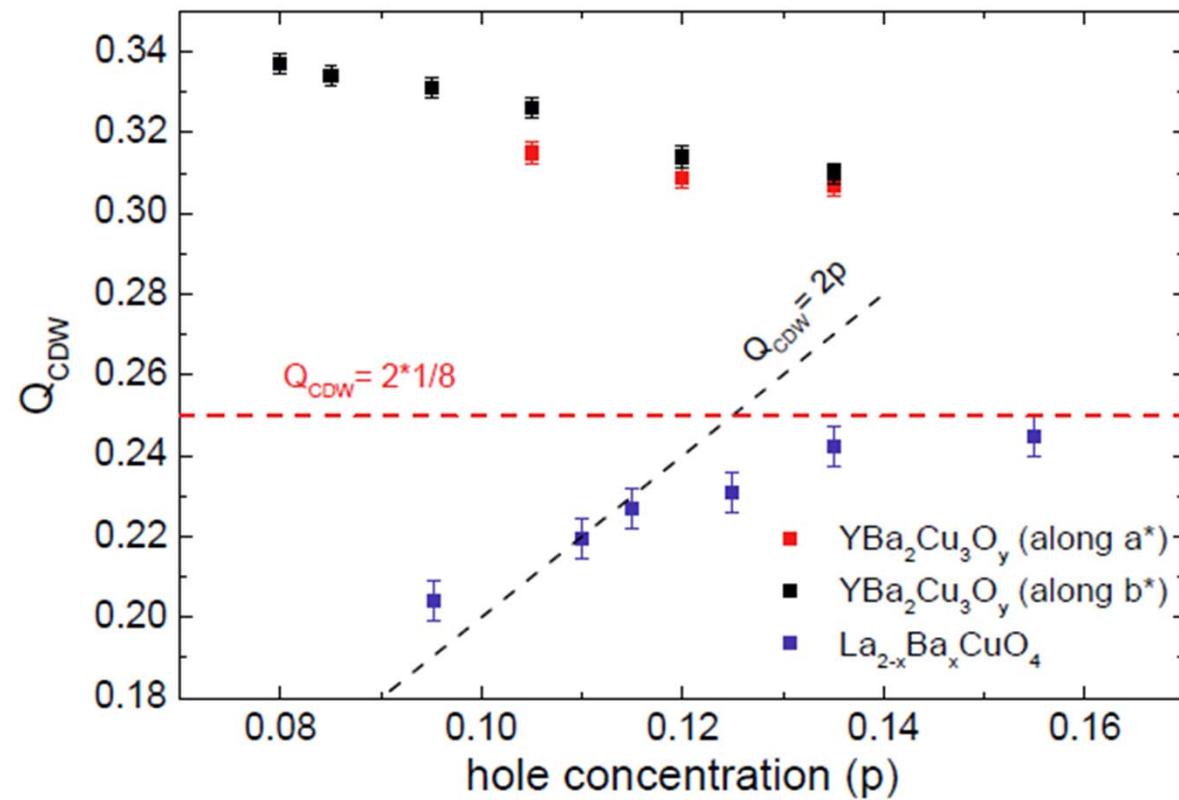


Figure 4 | Phase diagram of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$. a, Doping dependence of the antiferromagnetic ordering temperature T_N , the incommensurate spin-density wave order T_{SDW} (green triangles; ref. 21), the superconducting temperature T_c and the pseudogap temperature T^* as determined from the Nernst effect³⁰ (black squares) and neutron diffraction²⁹ (purple squares). Notice that the Nernst effect³⁰ indicates a broken rotational symmetry inside the pseudogap region, whereas a translational symmetry preserving magnetic order is found by neutron scattering²⁹. Below temperature scale T_H (black circles), a larger and negative Hall coefficient was observed²⁶ and interpreted in terms of a Fermi surface reconstruction. Our X-ray diffraction experiments show that in $\text{YBCO } p = 0.12$ 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 order¹³. 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 forms²⁶. 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



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Theories

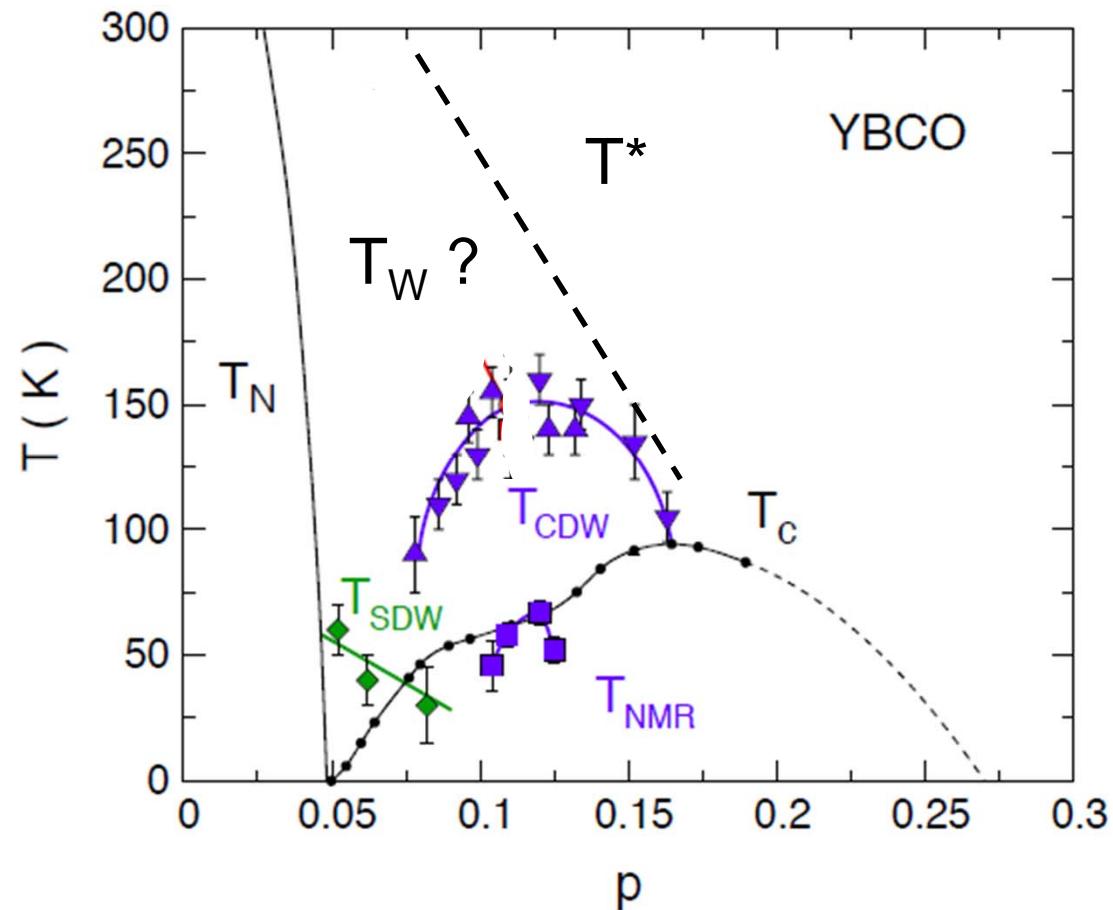
S. Sachdev and R. La Placa Phys. Rev. Lett. **111**, 027202 (2013)
D. Chowdhury, S. Sachdev arxiv. 1501.00002

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

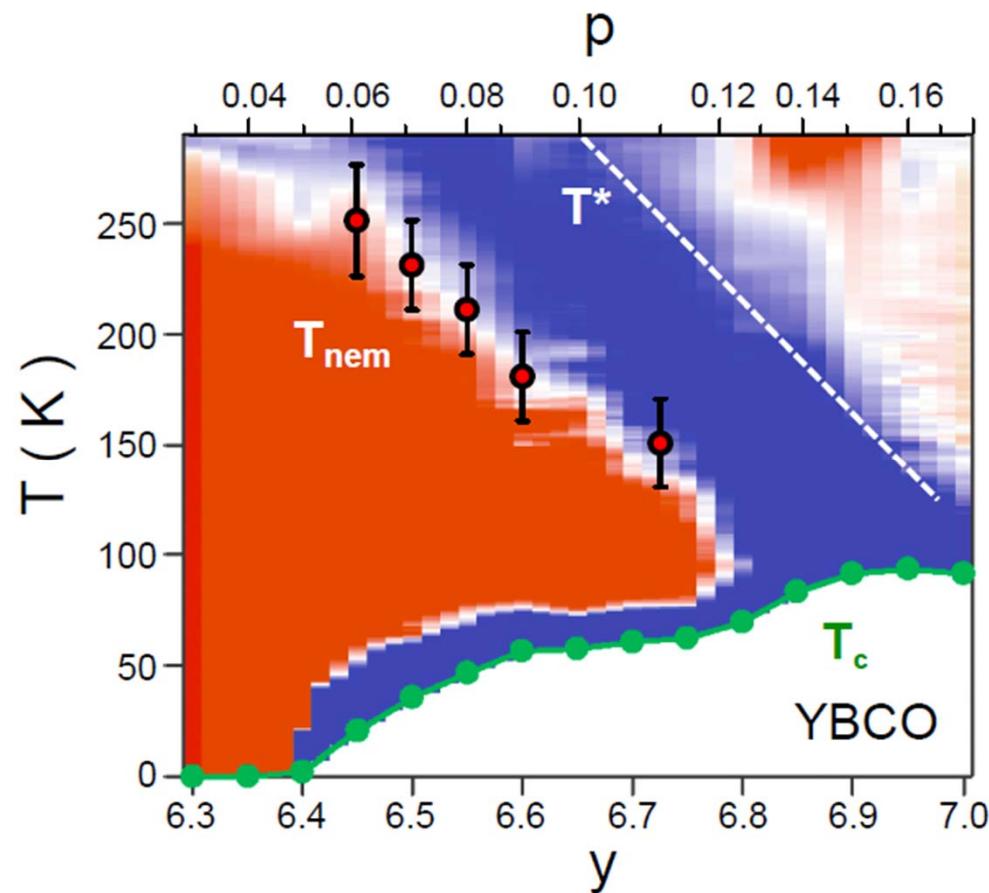
Y. Wang and A. Chubukov, Phys. Rev. B **90**, 035149 (2014).

...

Phase diagram for hole-doped cuprates



Resistivity anisotropy and curvature map



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

$T = 0$ phase diagram

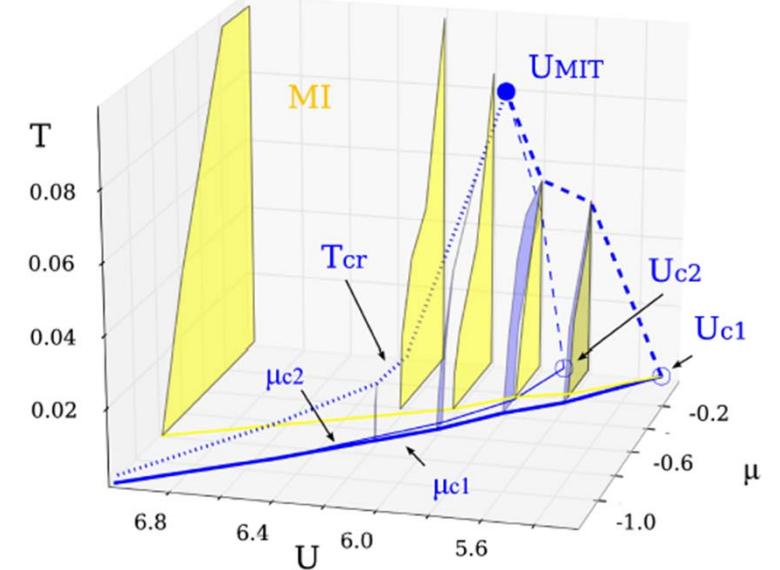
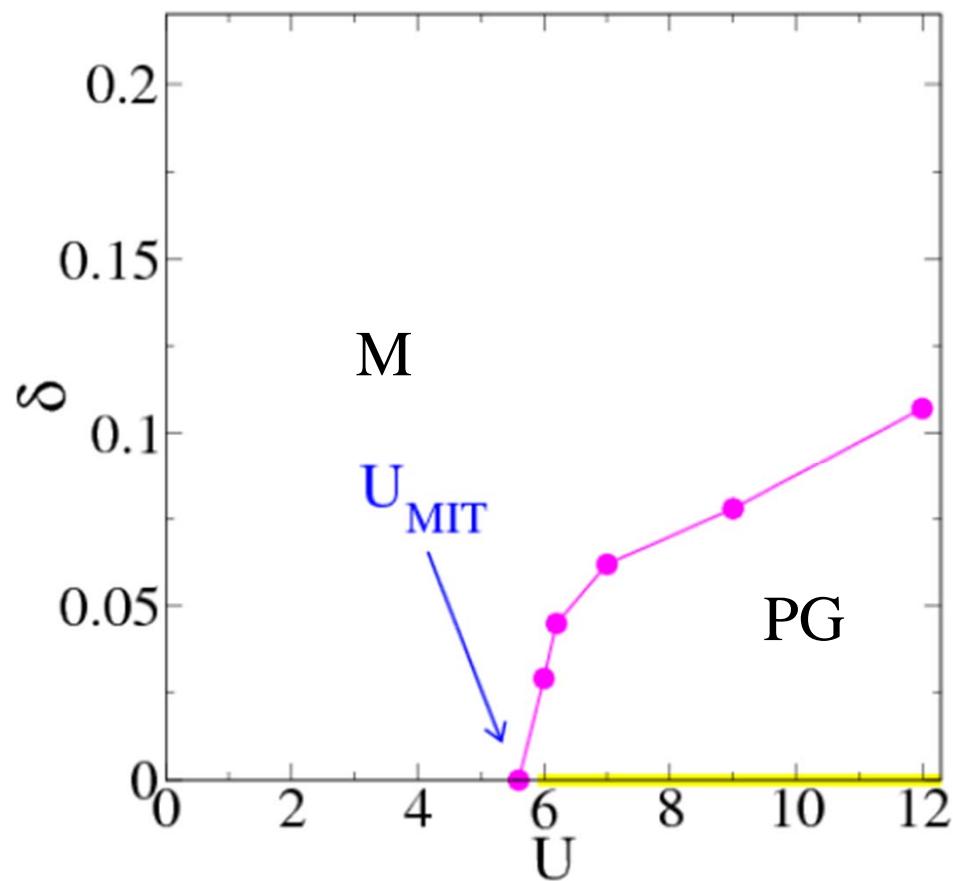
Normal state and large anisotropy



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Recall phase diagram

Doping dependence of critical point as a function of U



Underdoped metal very sensitive to anisotropy

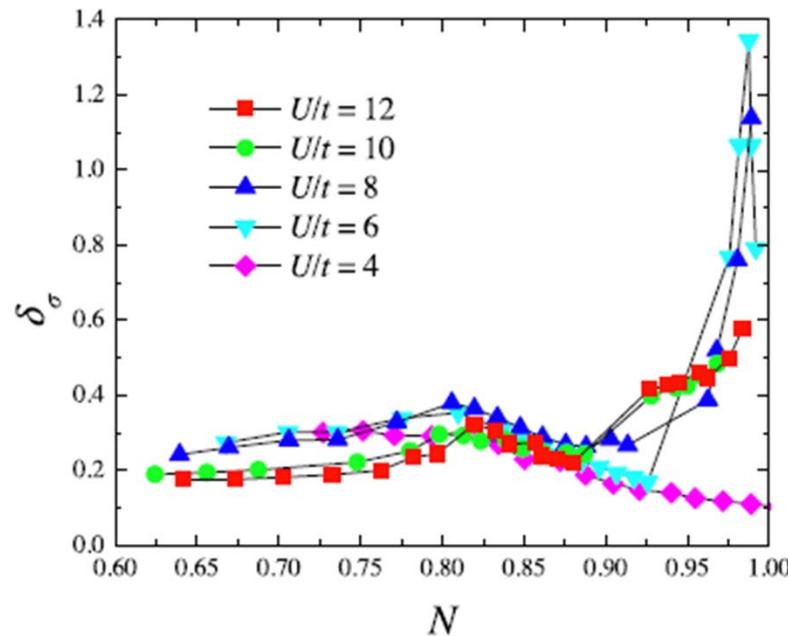
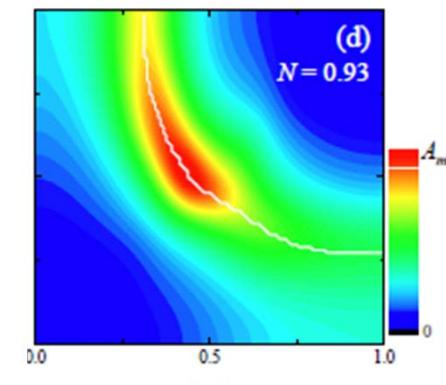
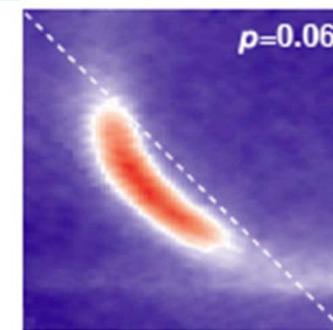


FIG. 3: (Color online) Anisotropy in the CDMFT conductivity $\delta_\sigma = 2 [\sigma_x(0) - \sigma_y(0)] / [\sigma_x(0) + \sigma_y(0)]$ as a function of filling N for various values of U and $\eta = 0.1$, $\delta_0 = 0.04$.



(d)



(g)



Satoshi Okamoto



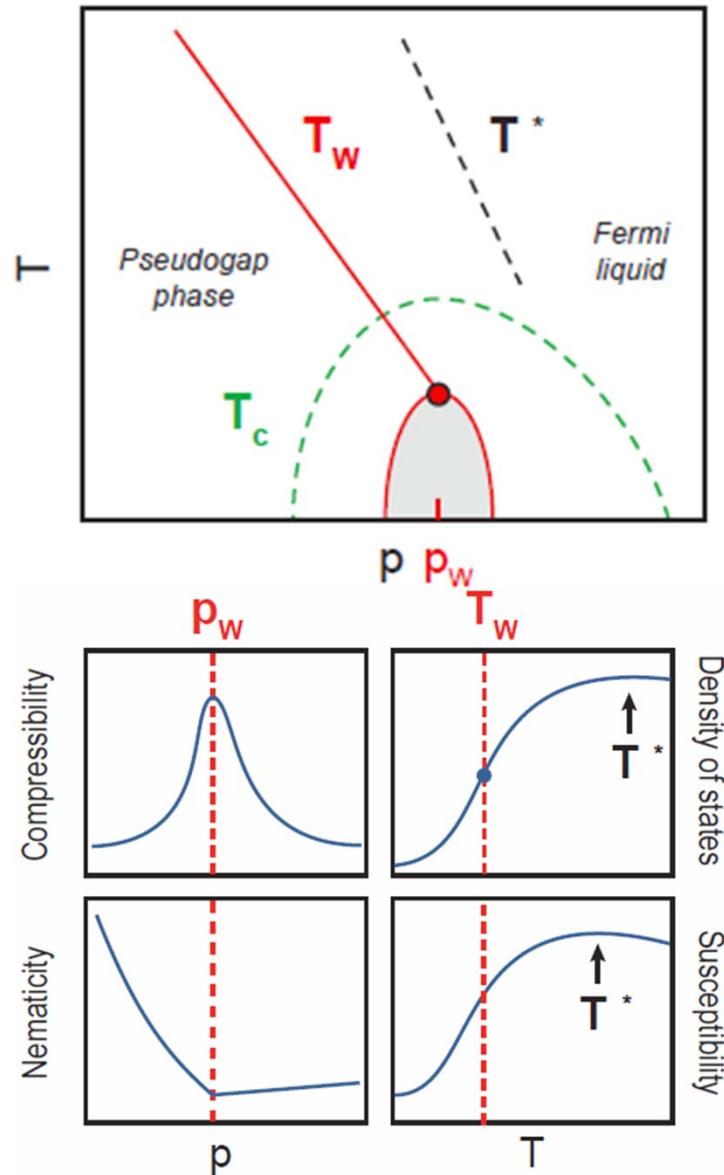
David Sénéchal



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

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

Summary



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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)



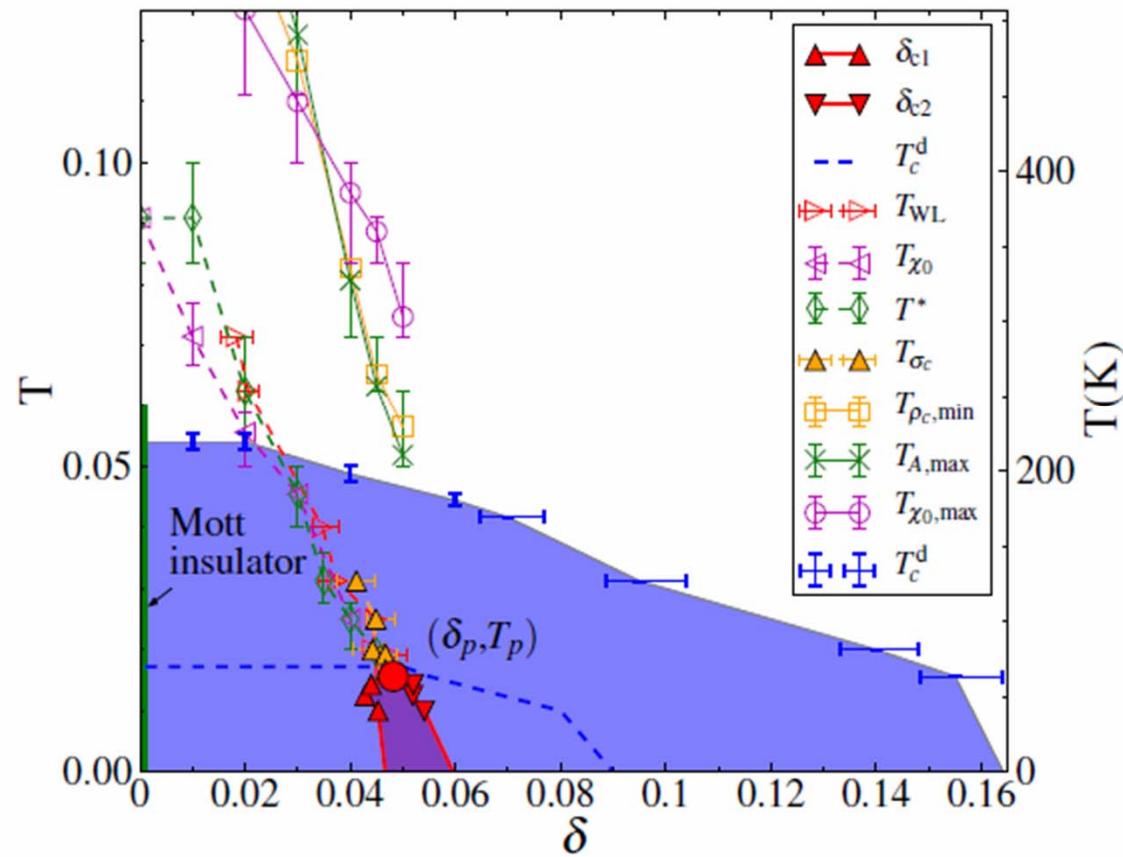
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Giovanni Sordi



Patrick Sémon



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

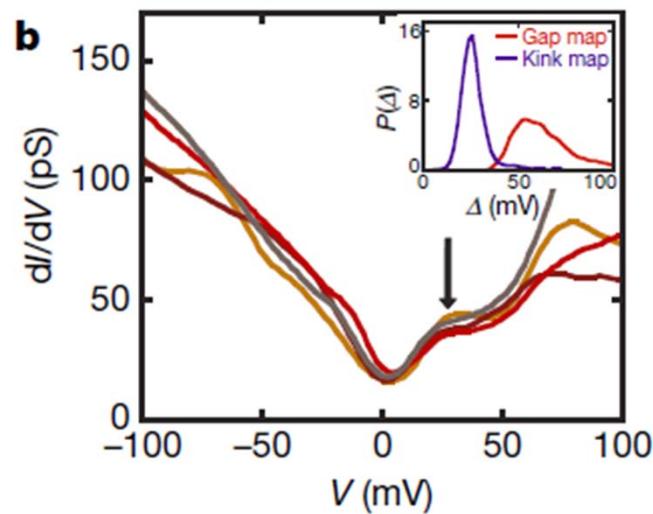
P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B **89**, 165113/1-6 (2014)



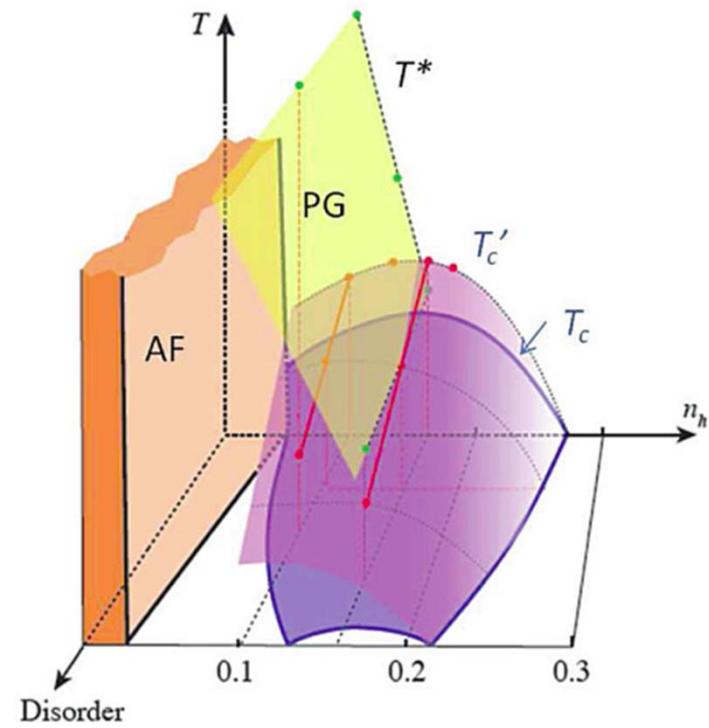
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Meaning of T_c^d

- Local pair formation

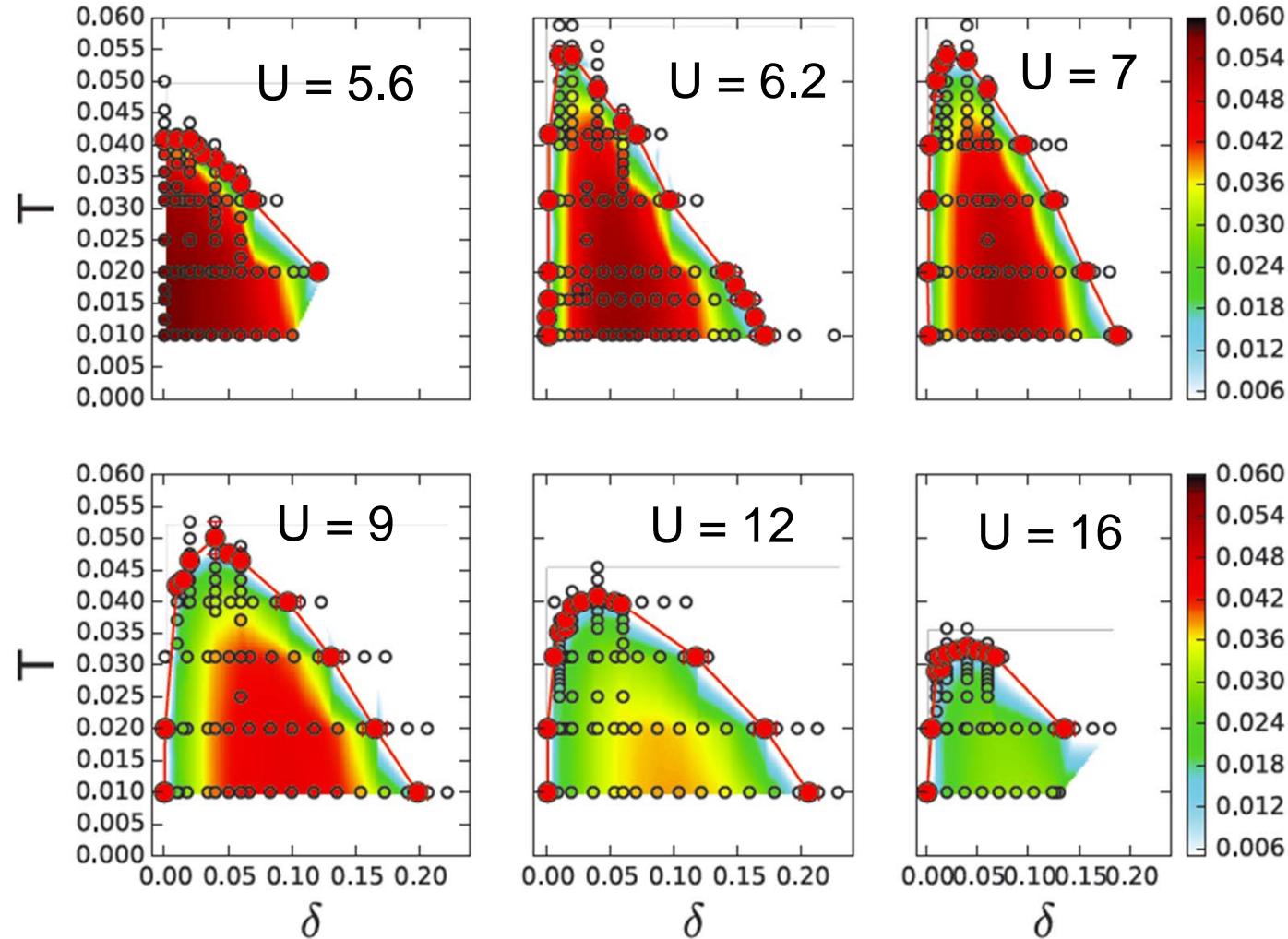


K. K. Gomes, A. N. Pasupathy, A. Pushp,
S. Ono, Y. Ando, and A. Yazdani,
Nature **447**, 569 (2007)



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

Order parameter (color) and T_c

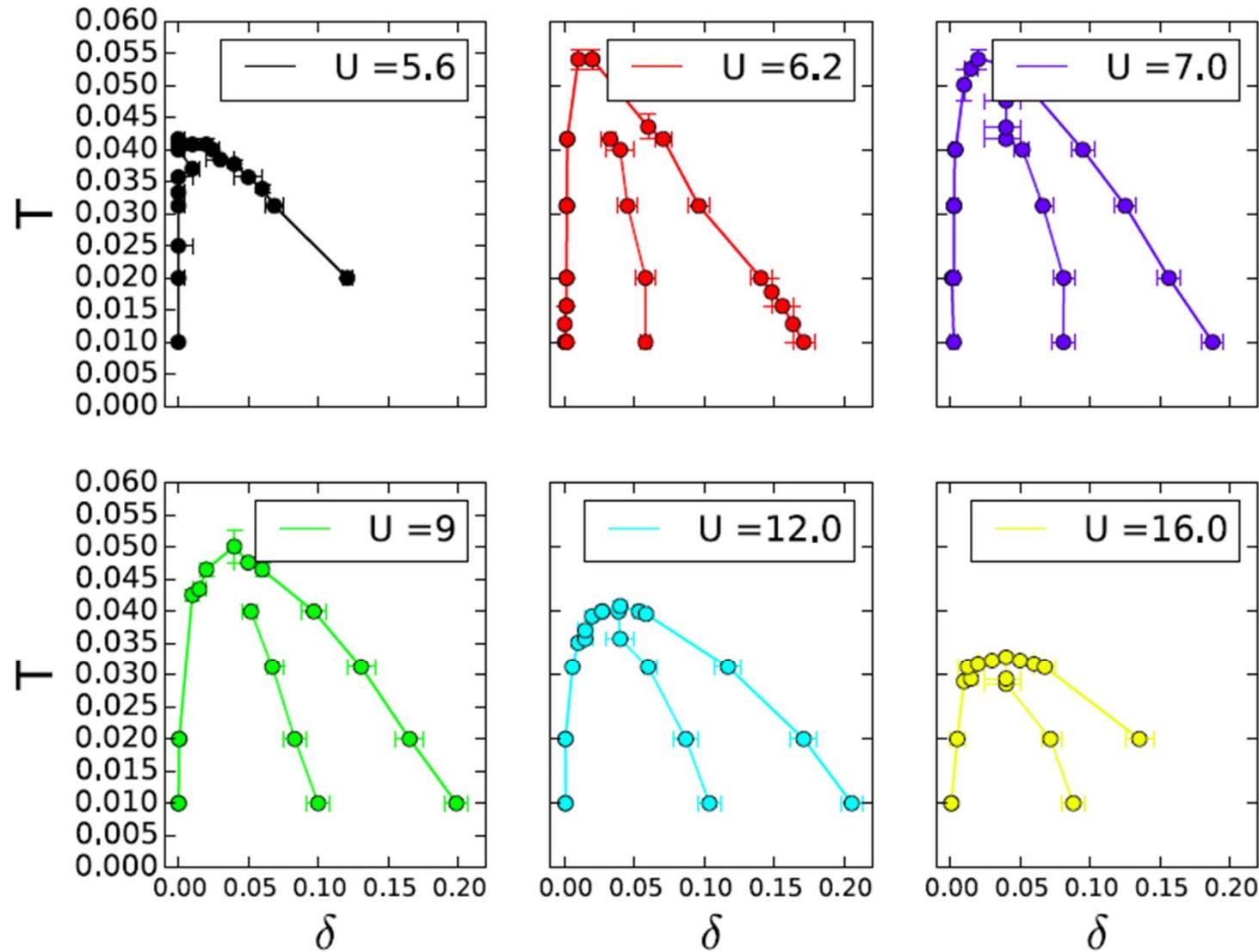


L. Fratini, G. Sordi (unpublished)



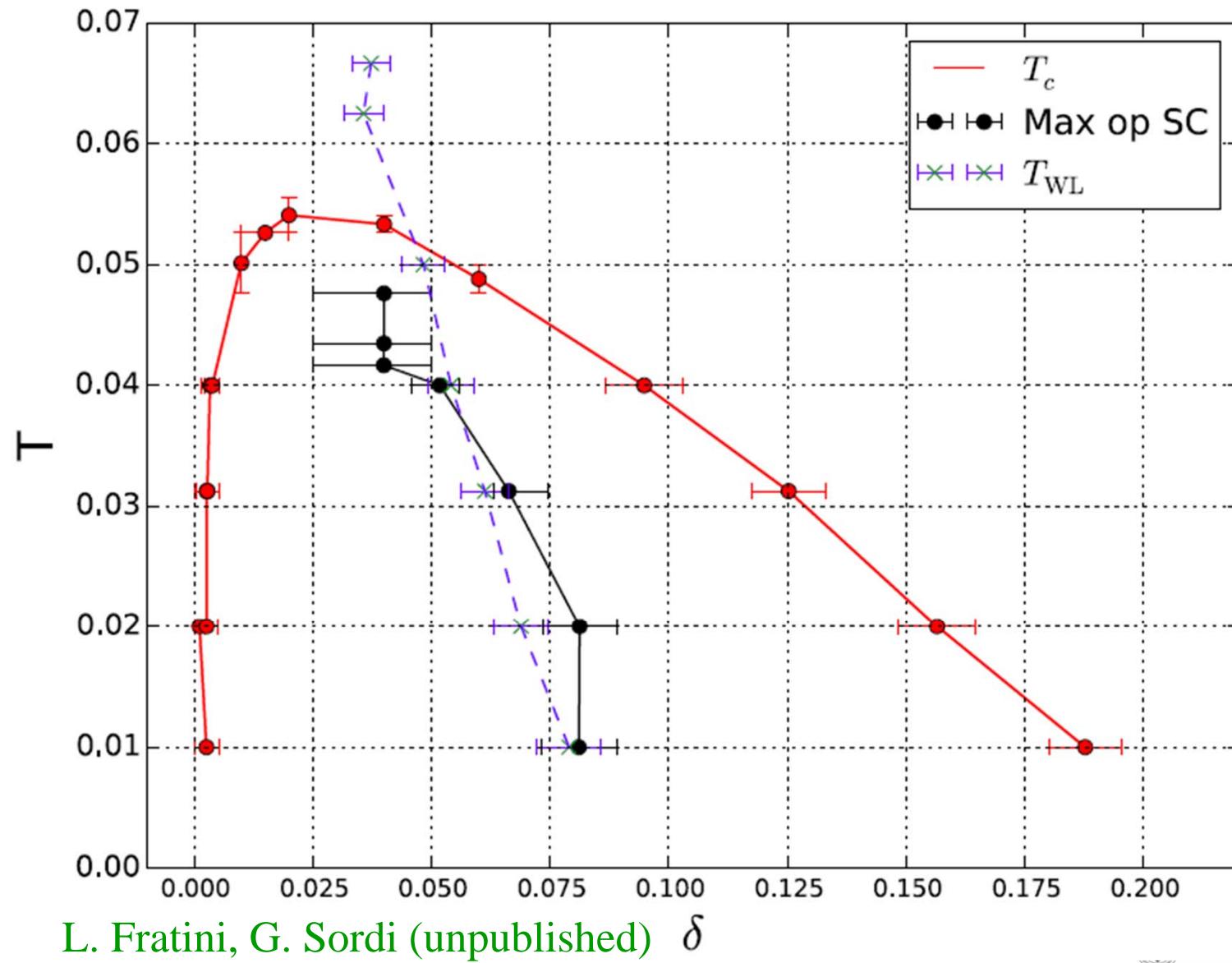
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T_c vs T_{\max} order parameter



L. Fratini, G. Sordi (unpublished)

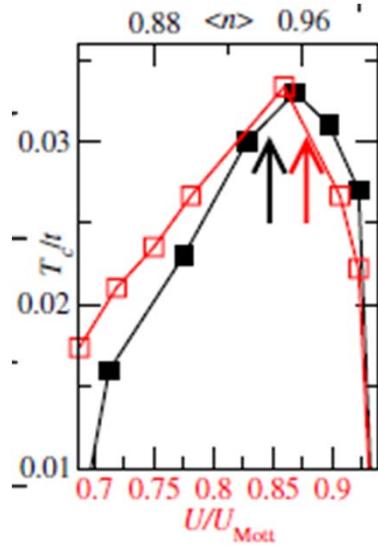
$U=7$, T_W vs T_c vs T_{\max} order parameter



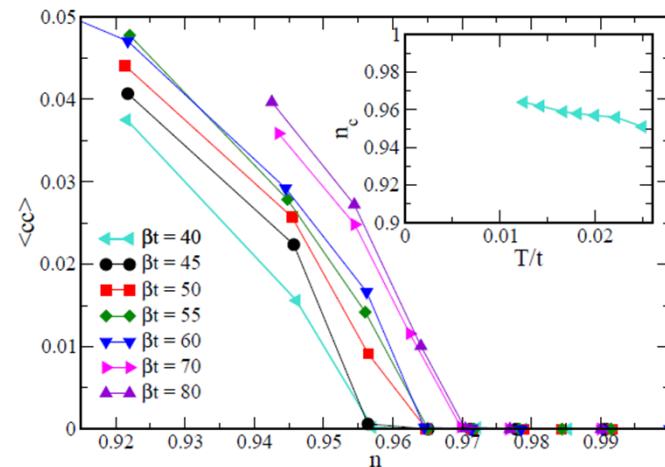
L. Fratini, G. Sordi (unpublished)

Larger clusters

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



8 site DCA, $U=6t$

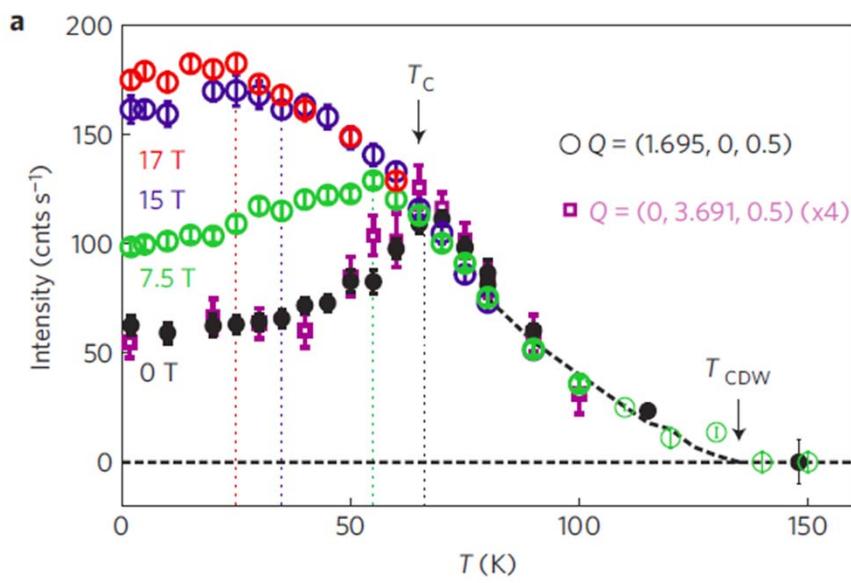


8 site DCA, $U=6.5t$

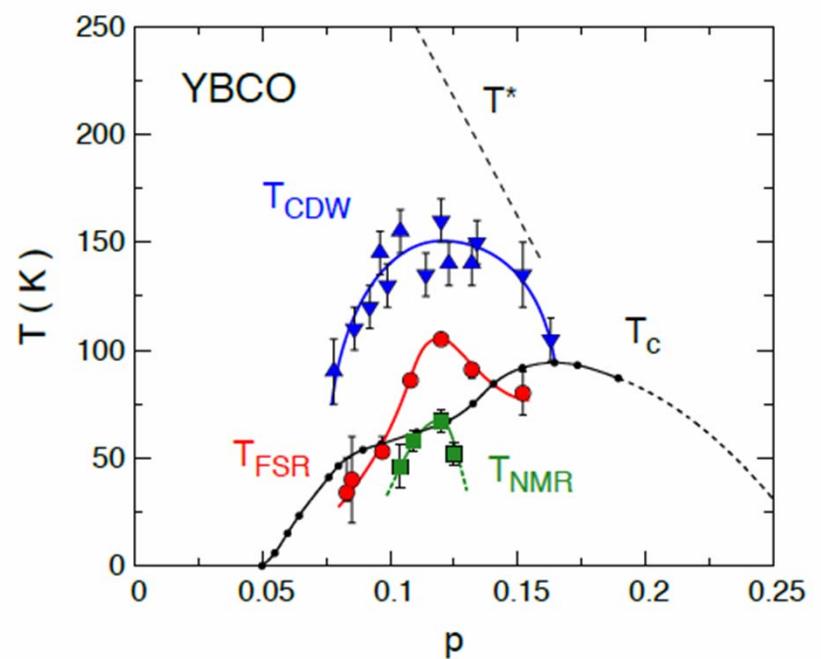
Gull Parcollet Millis,
PRL 110, 216405 (2013)

Back to experiment: CDW vs SC

Competition between CDW and SC

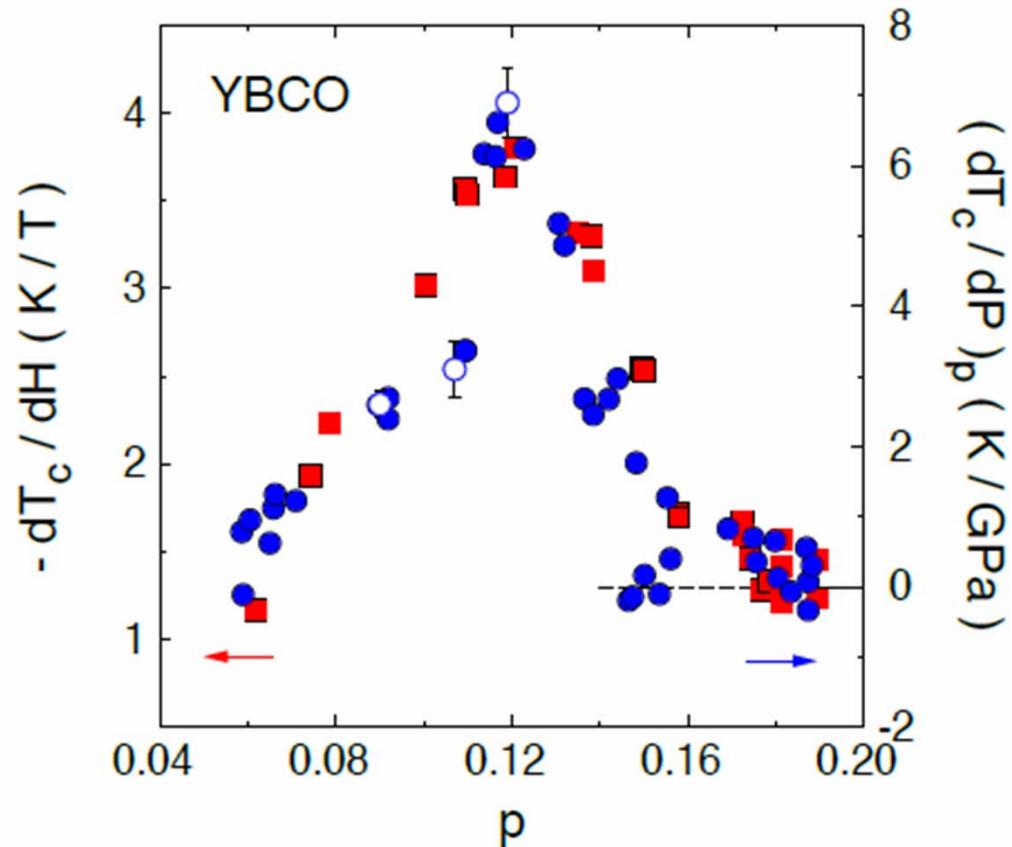


J. Chang *et al.*, *Nat. Phys.* **8**, 871-876 (2012).



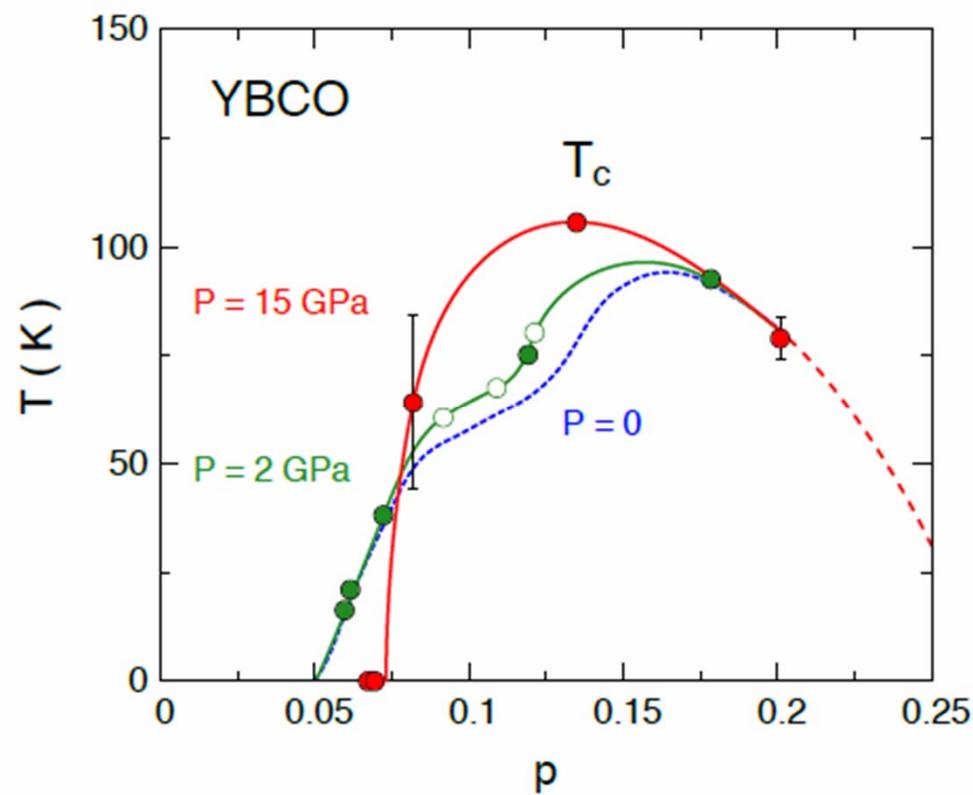
Cyr-Choinière et al, arxiv1503.02033

Tuning SC and CDW



Cyr-Choinière et al, arxiv1503.02033

Getting rid of the CDW

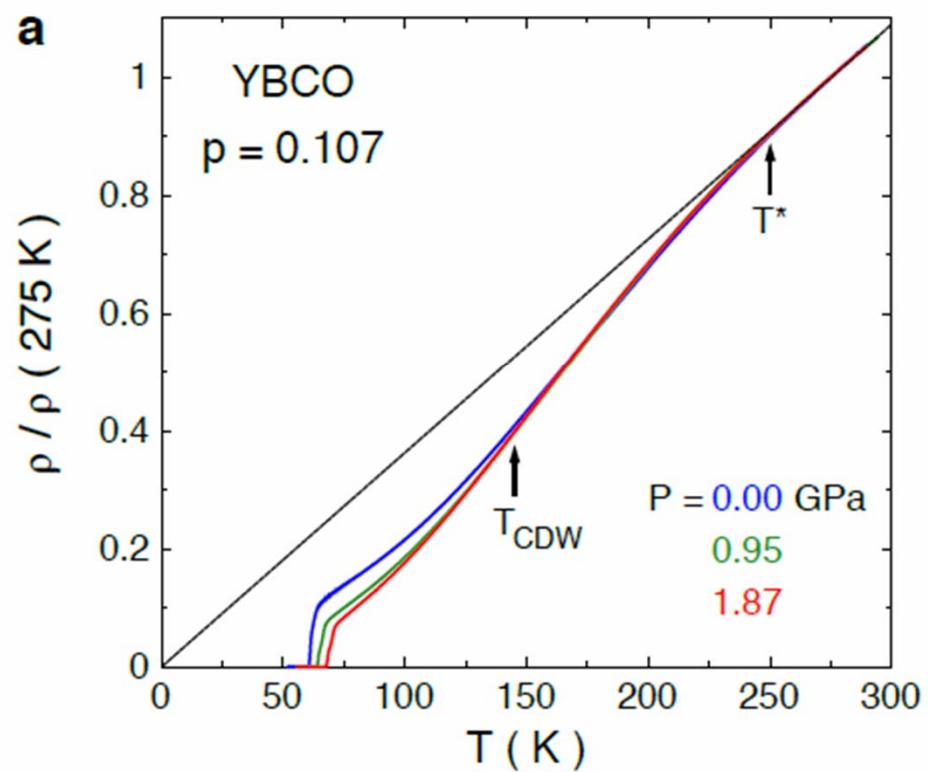


Cyr-Choinière et al, arxiv1503.02033



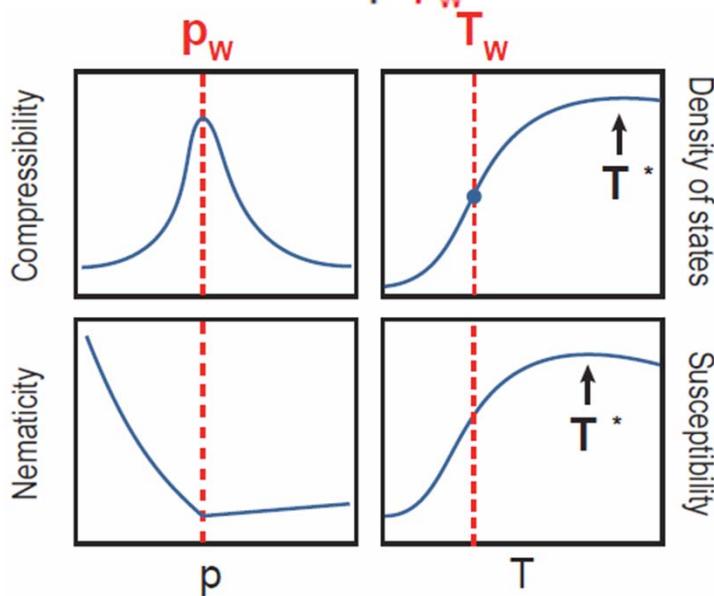
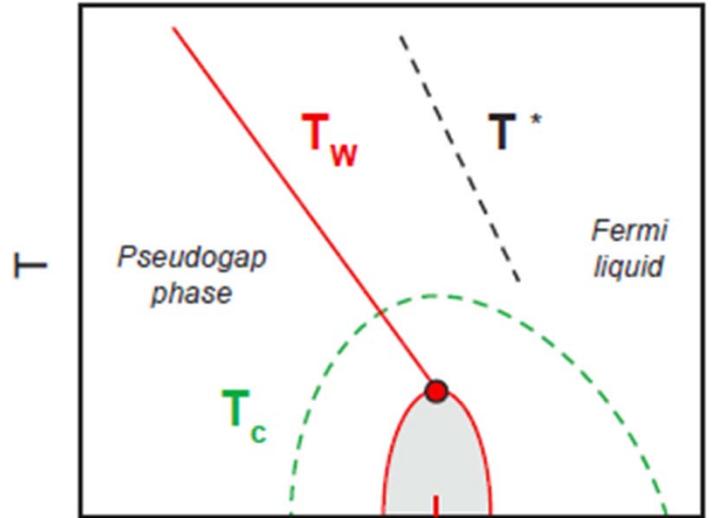
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T* not affected



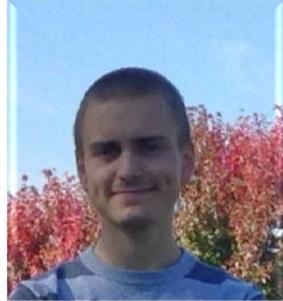
Cyr-Choinière et al, arxiv1503.02033

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?





Charles-David Hébert

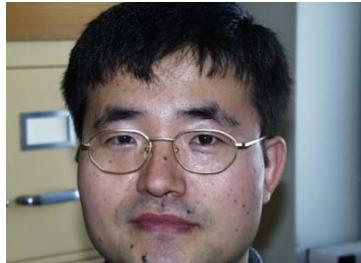


Patrick Sémon

Bandwidth control and doping control of the Mott transition in organics

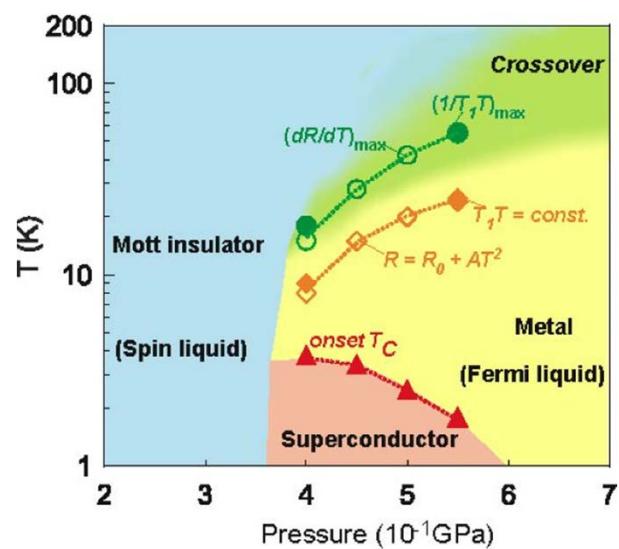


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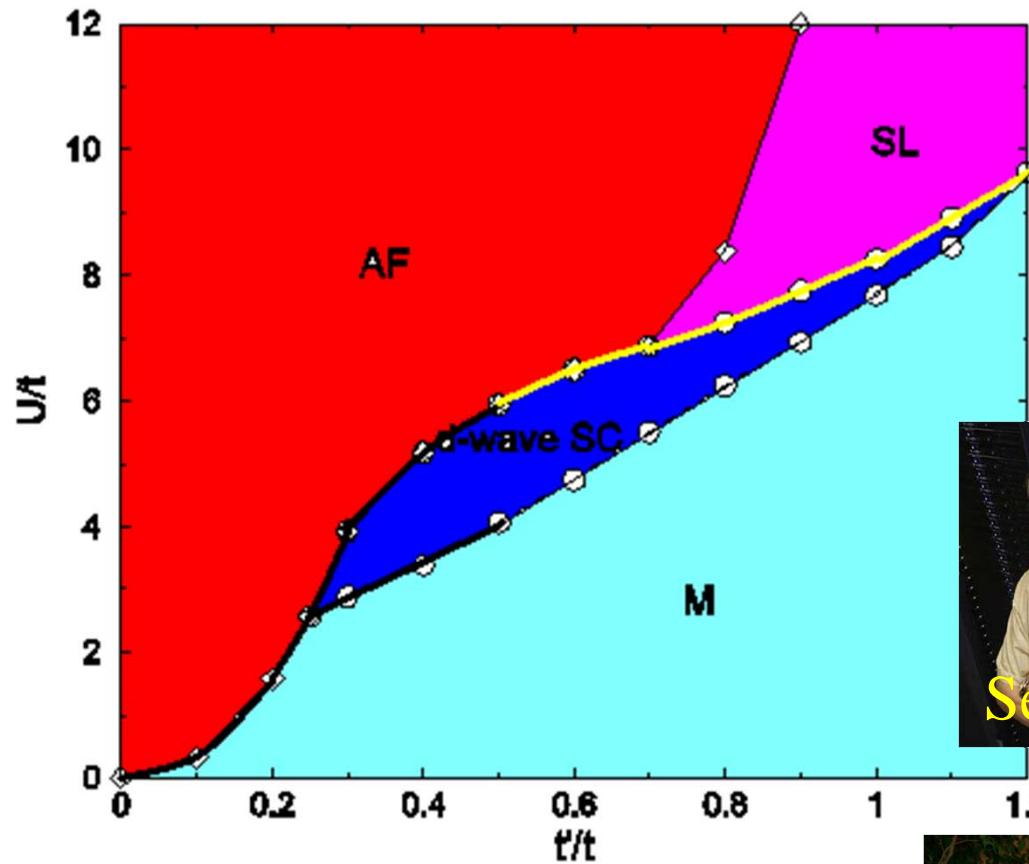
Theoretical phase diagram BEDT

$X = \text{Cu}_2(\text{CN})_3$ ($t' \sim t$)



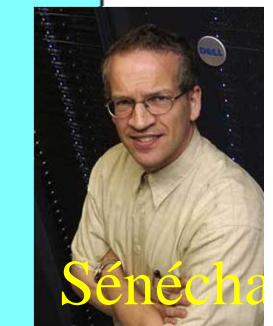
Y. Kurisaki, et al.

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



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

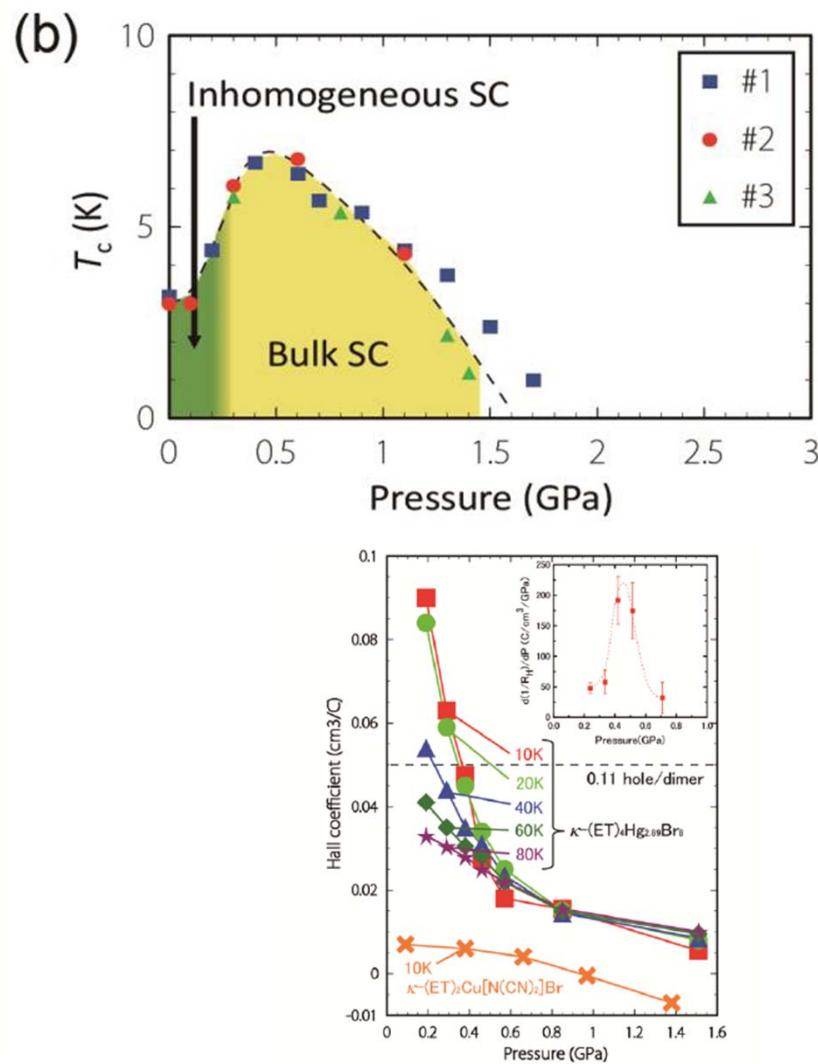
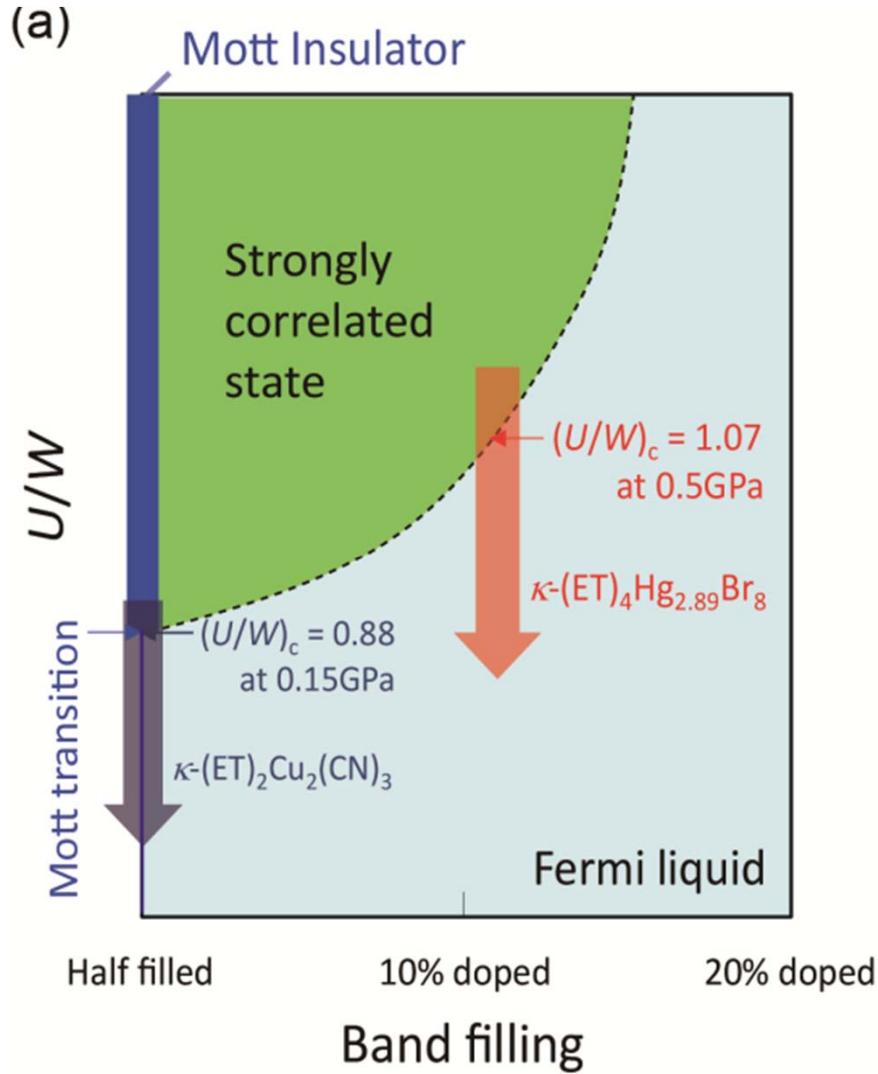
Sénéchal, Sahebsara, Phys. Rev. Lett. **97**, 257004



Sénéchal



Doped BEDT

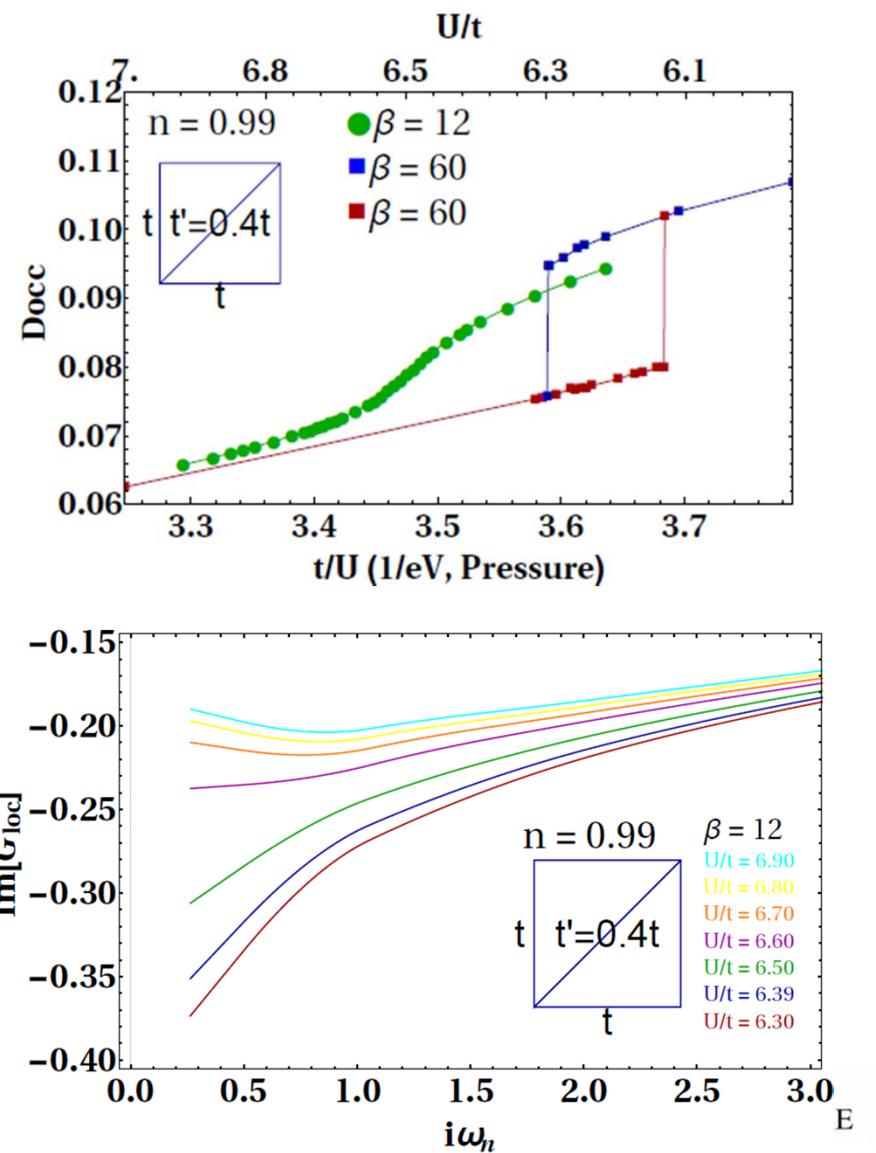
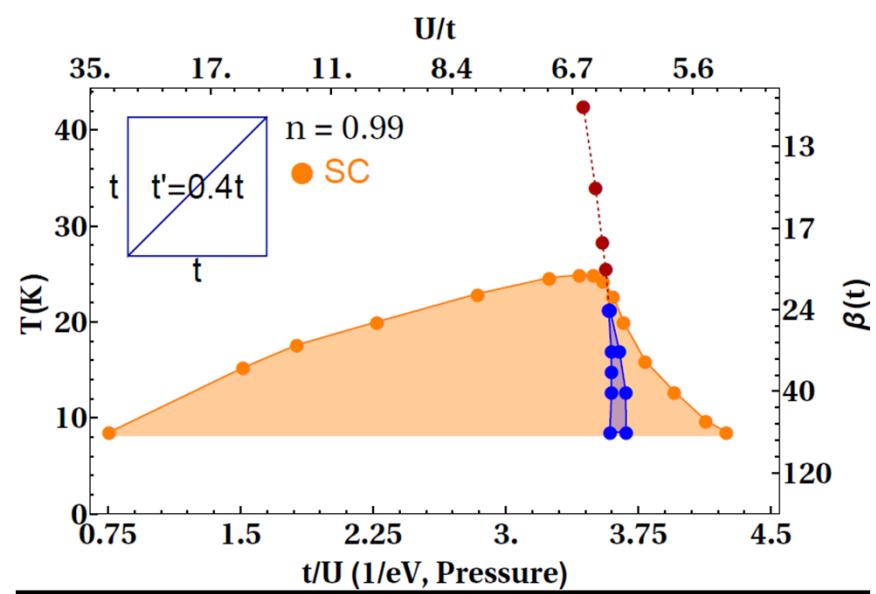


H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)



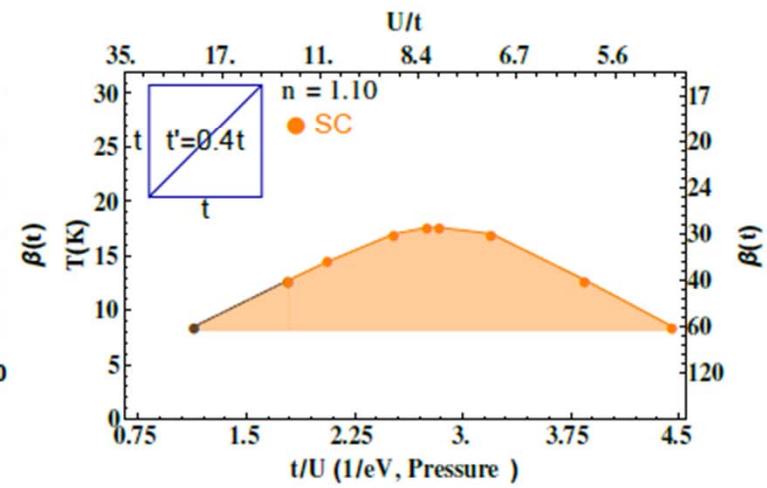
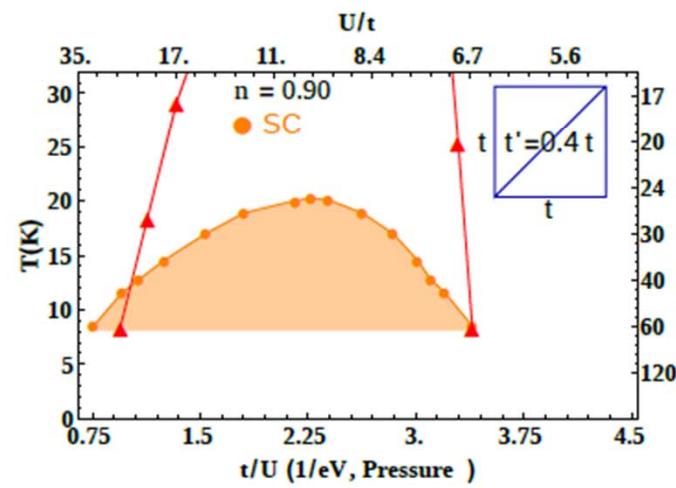
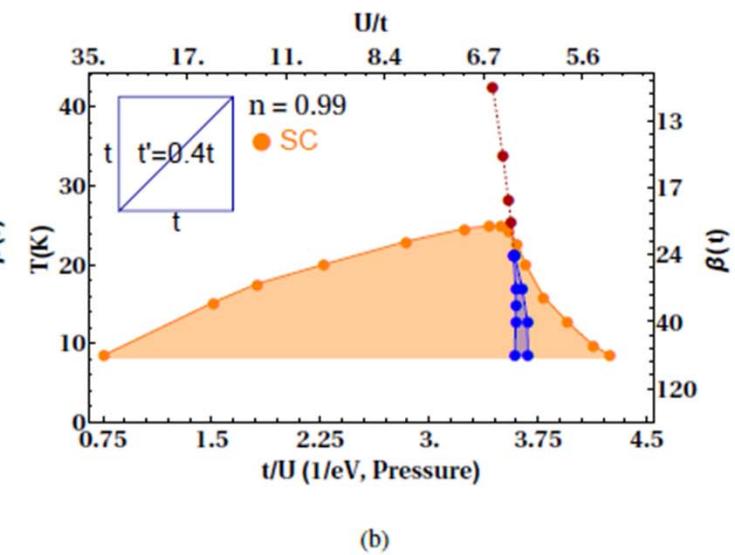
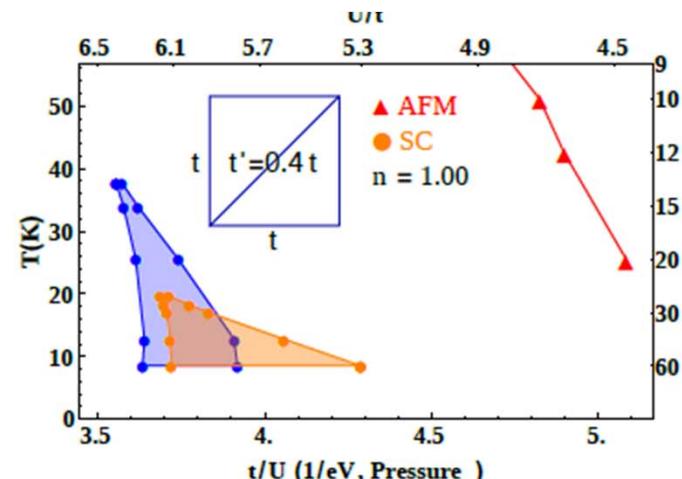
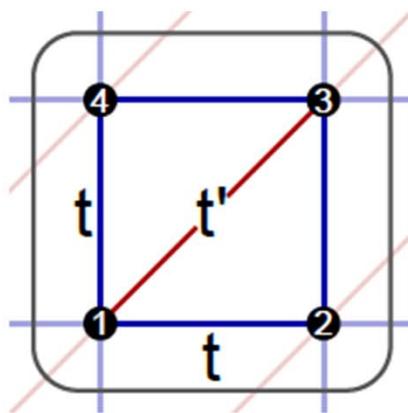
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Widom line in organics



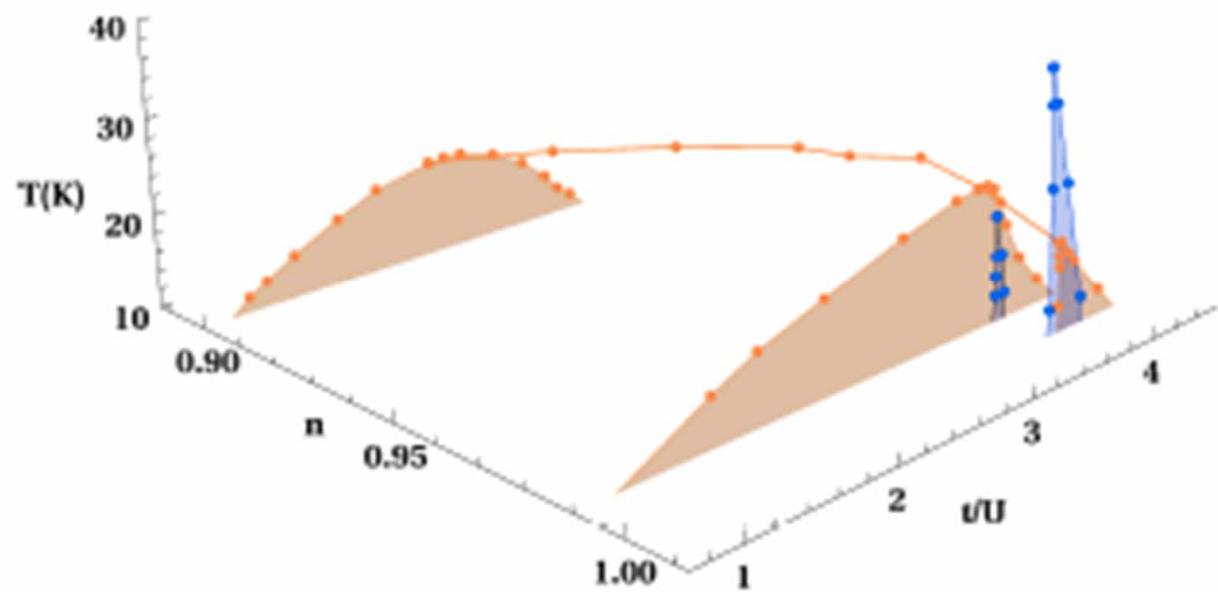
Charles-David Hébert, Patrick Sémond , AMT

$$t' = 0.4t$$



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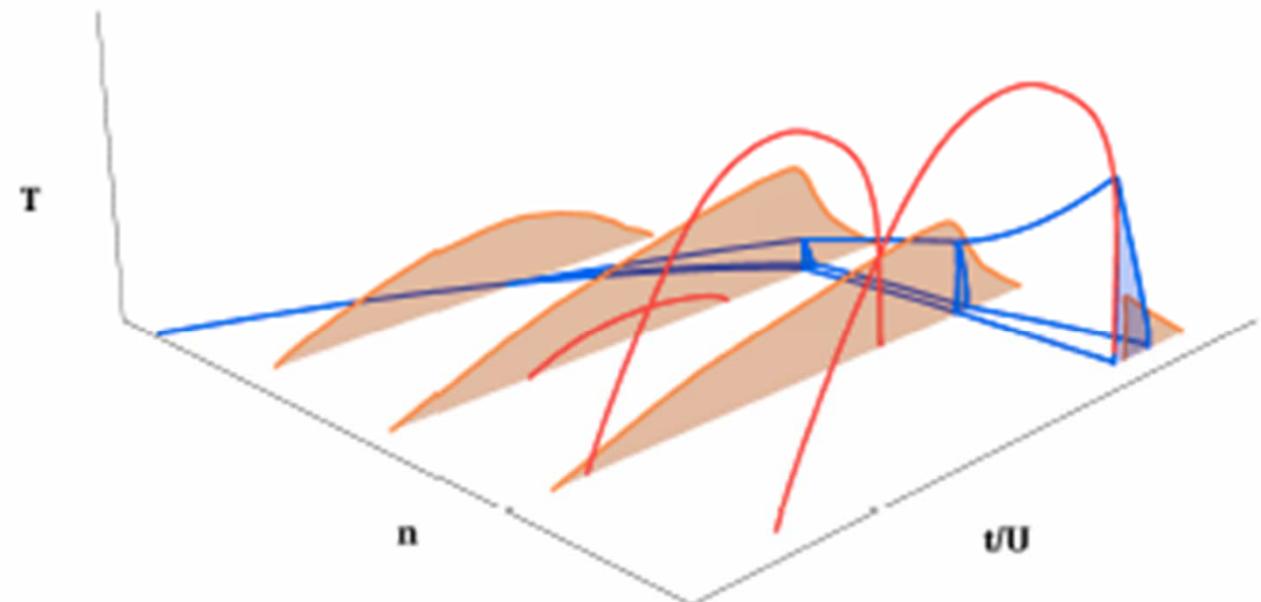
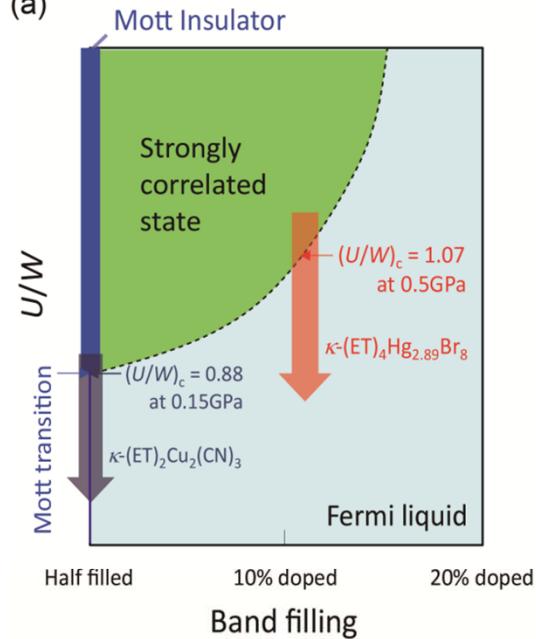
$t' = 0.4t$ overview



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Generic case

(a)



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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

Main collaborators



Giovanni Sordi



Kristjan Haule



David Sénéchal



Bumsoo Kyung



Patrick Sémon



Charles-David Hébert



Sarma Kancharla



Marcello Civelli



Massimo Capone

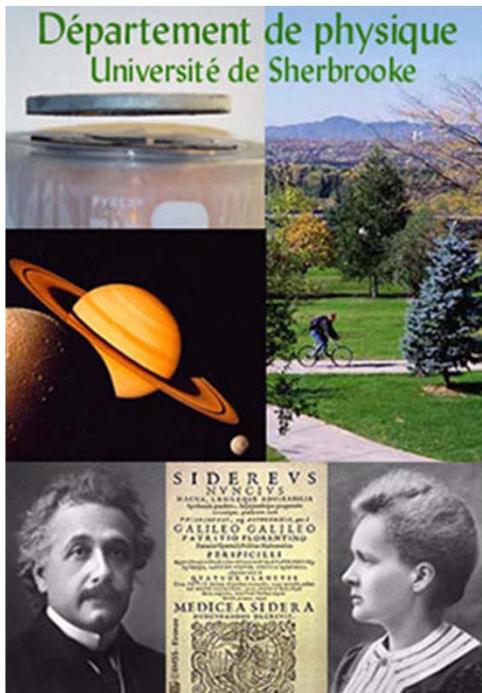


Gabriel Kotliar



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André-Marie Tremblay



Le regroupement québécois sur les matériaux de pointe



Sponsors:



Mammouth



Review: A.-M.S.T. arXiv: 1310.1481



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