Supraconductivité à haute température dans les cuprates et les organiques: Où en est-on?

André-Marie Tremblay

Université de Sherbrooke

Collège de France, 9, 16, 23 et 30 mars 2015
17h00 à 18h30

Two pillars of Condensed Matter Physics

- Band theory
  - DFT
  - Fermi liquid Theory
    - Metals
    - Semiconductors: transistor
- BCS theory of superconductivity
  - Broken symmetry
  - Emergent phenomenon
    - Also in particle physics, astrophysics…

Breakdown of band theory
Half-filled band is metallic?

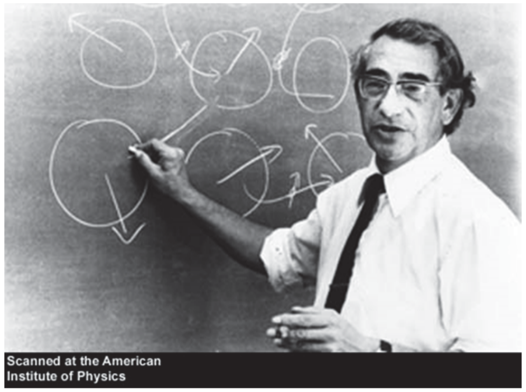
Half-filled band: Not always a metal

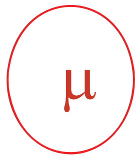
NiO, Boer and Verway

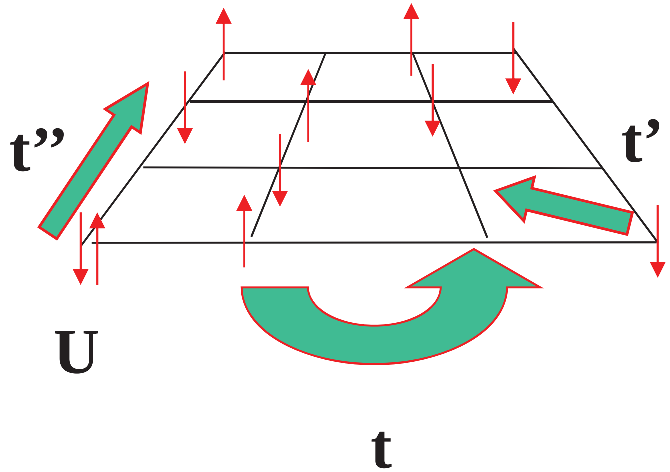
Peierls, 1937

Mott, 1949

Hubbard model

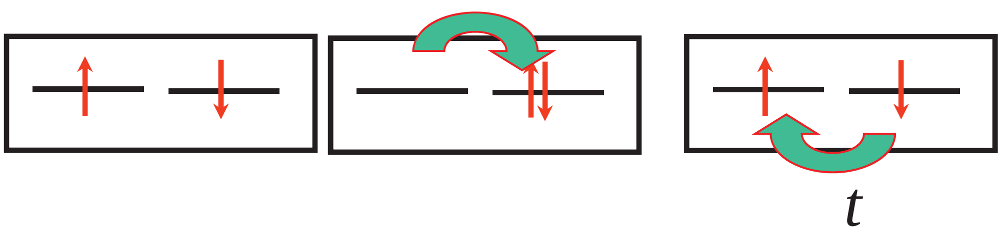






1931-1980

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



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

UNIVERSITÉ DE SHERBROOKE

High temperature superconductors and layered organic superconductors

Failure of

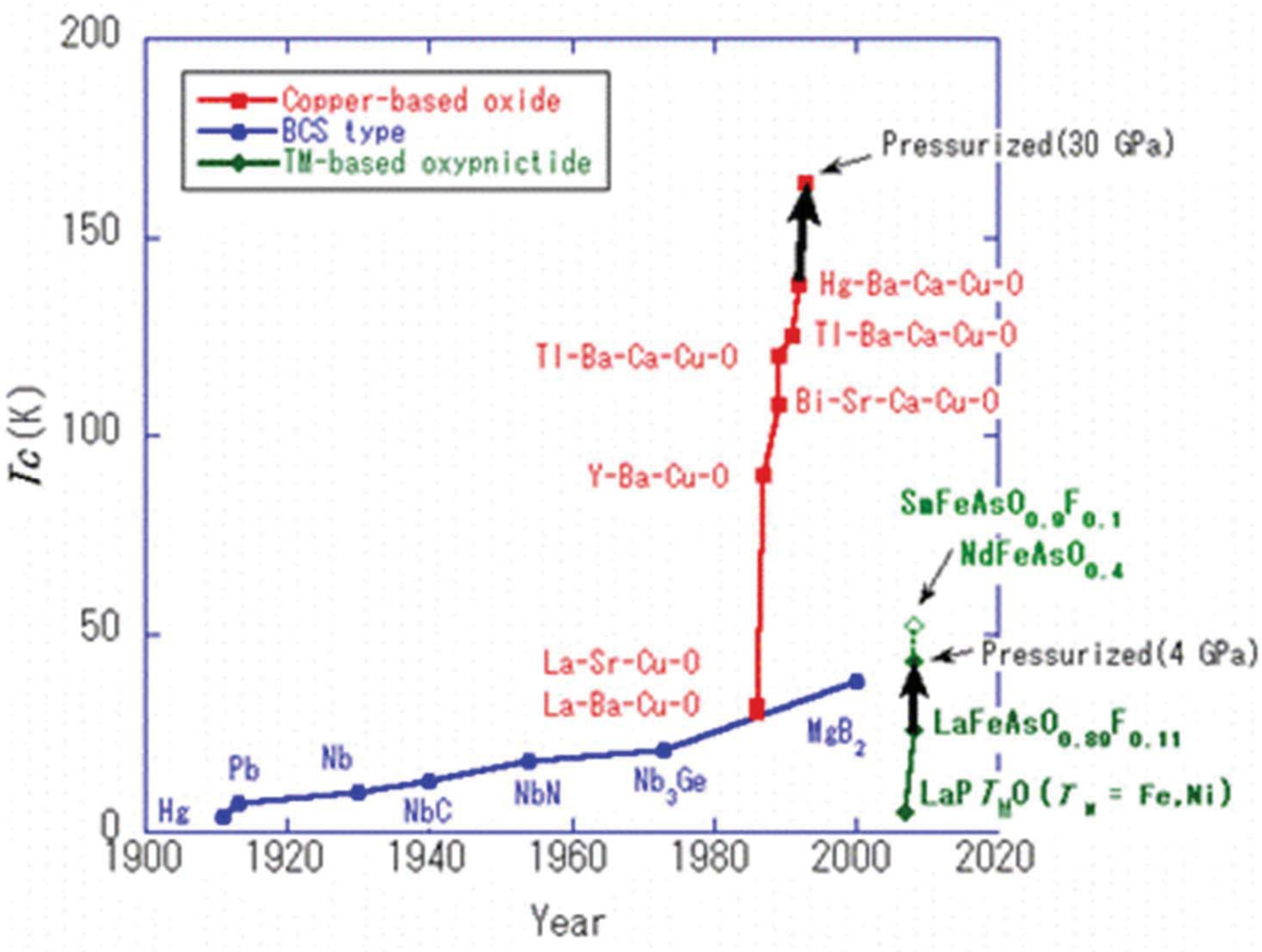
BCS theory

Band structure

and more

UNIVERSITÉ DE SHERBROOKE

New and old superconductors



H. Takahashi: JPSJ Online—News and Comments [June 10, 2008]

March meeting APS, 1987

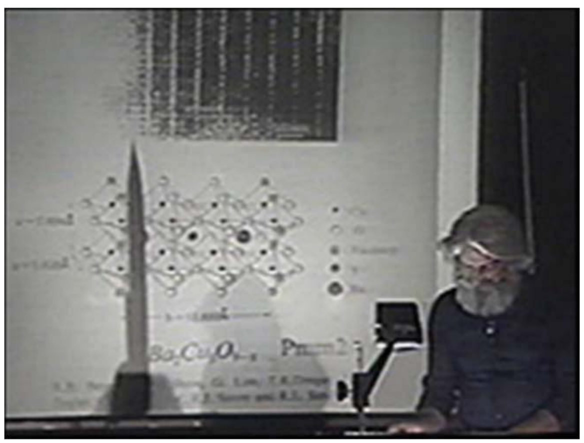
- New York Times headlines

"The Woodstock of Physics"

"They began lining up outside the New York Hilton Sutton Ballroom at 5:30PM for an evening session that would last until 3:00 AM"

15-18 Aug. 1969
500,000 participants

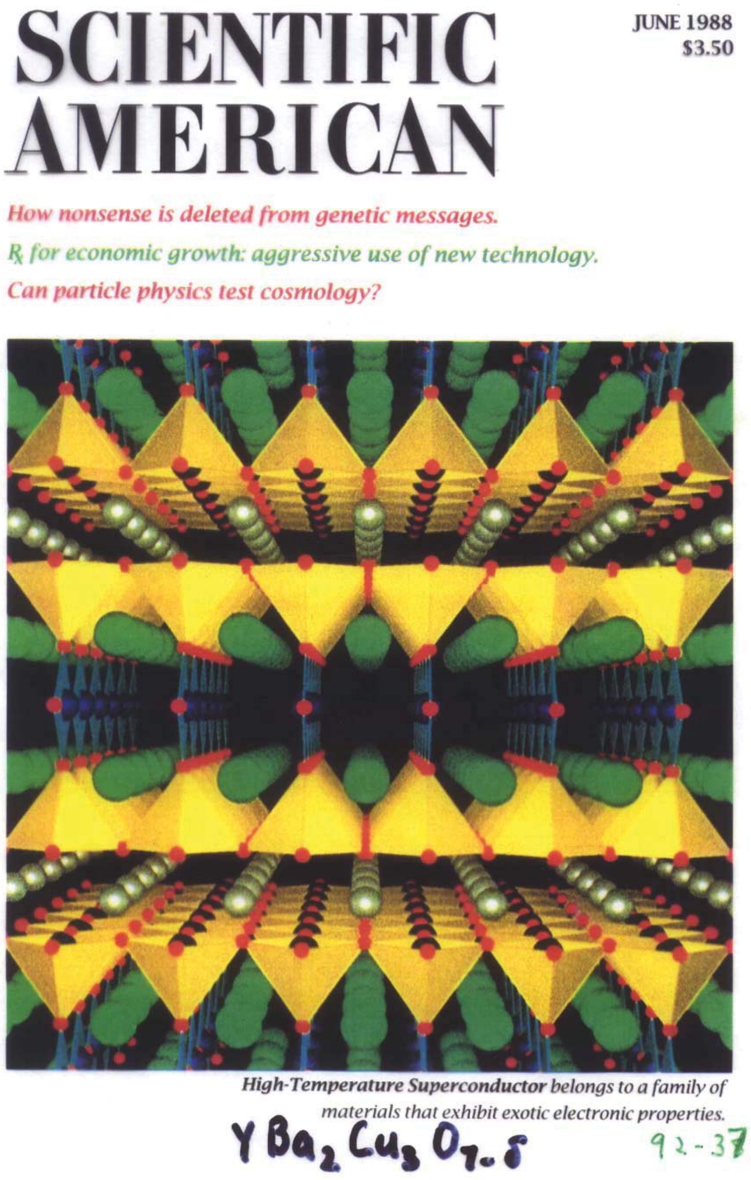
Université de Sherbrooke



UNIVERSITÉ DE SHERBROOKE

UNIVERSITÉ DE SHERBROOKE

Atomic structure


SCIENTIFIC AMERICAN

JUNE 1988
$3.50

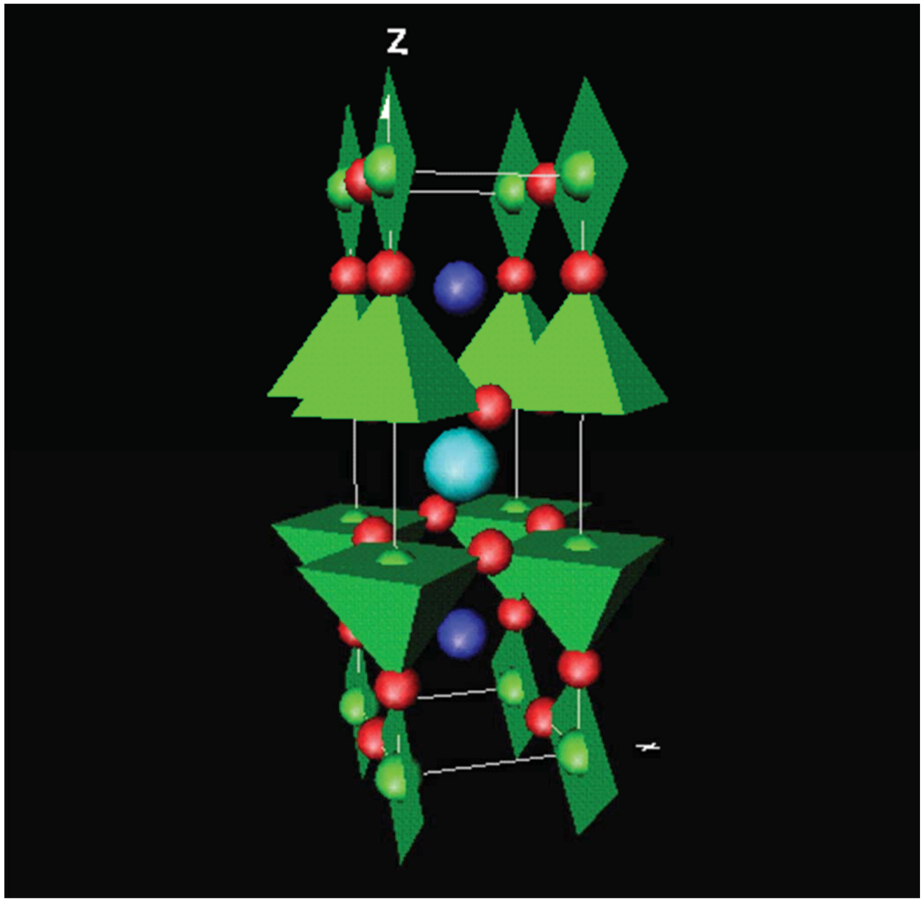
How nonsense is deleted from genetic messages.

℞ for economic growth: aggressive use of new technology.

Can particle physics test cosmology?

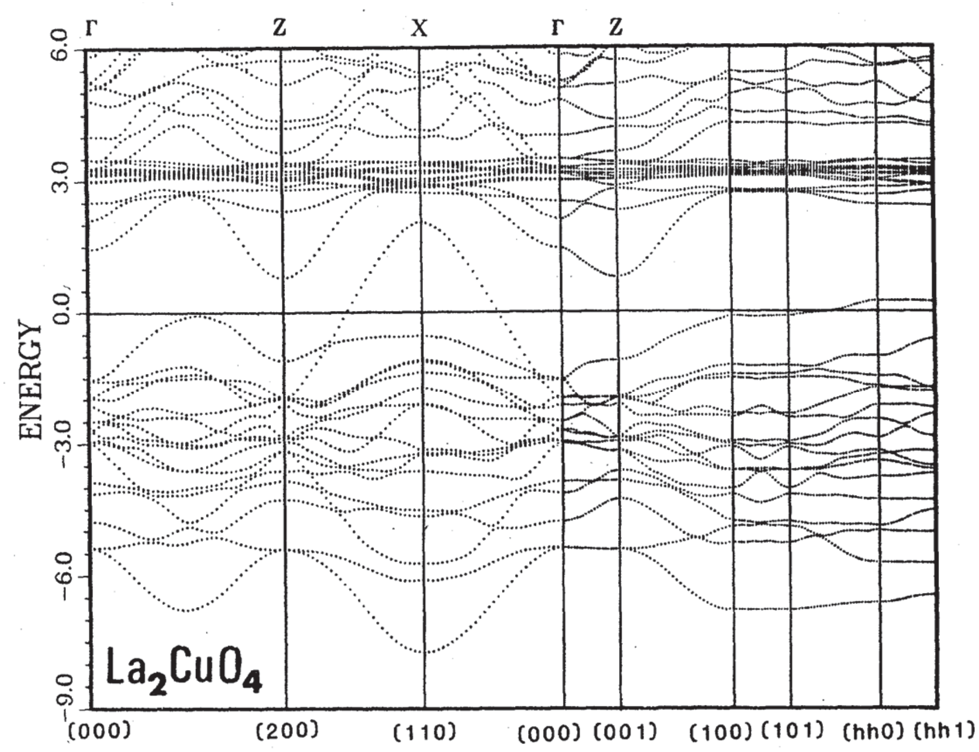
High-Temperature Superconductor belongs to a family of materials that exhibit exotic electronic properties.

$YBa_2Cu_3O_{7-\delta}$ 92-37



UNIVERSITÉ DE SHERBROOKE

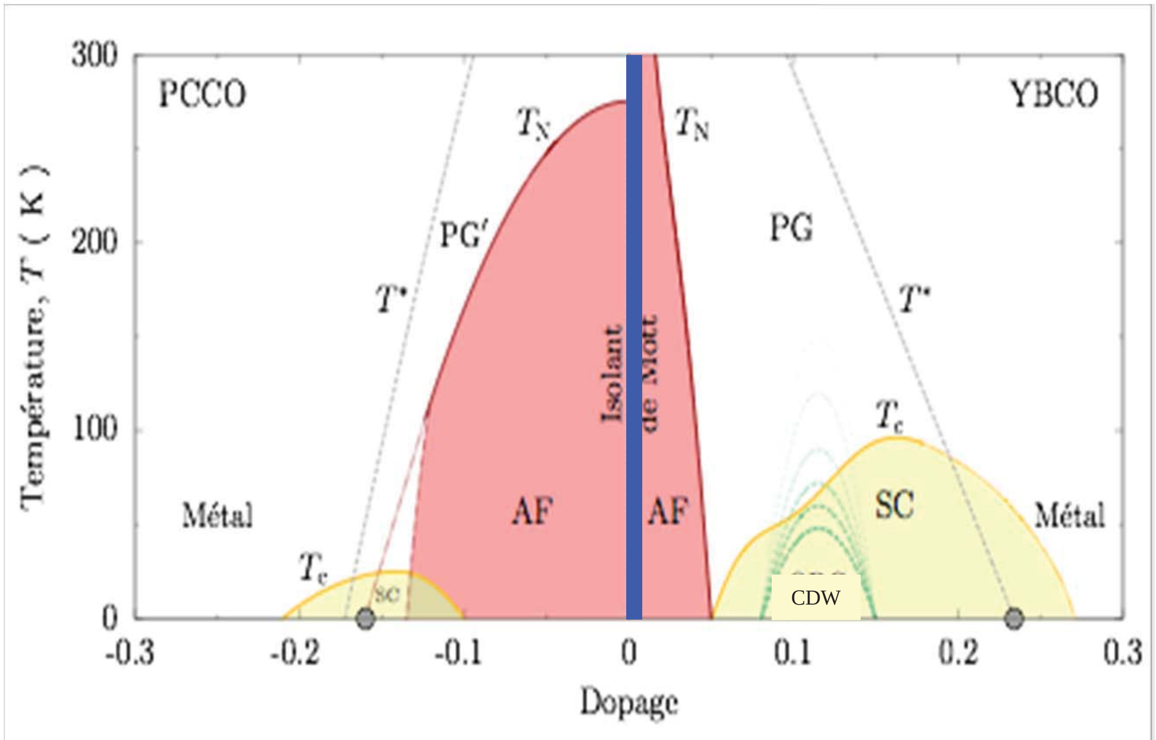
Band structure for high Tc

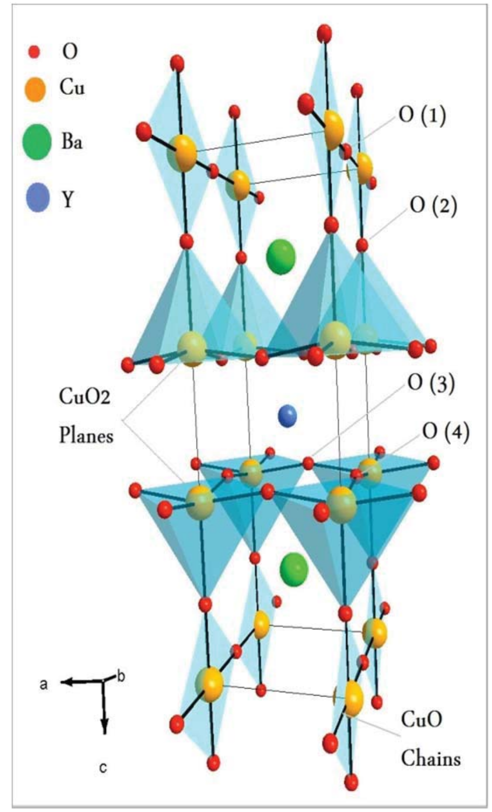


W. Pickett, Rev. Mod. Phys. 1989

Our road map

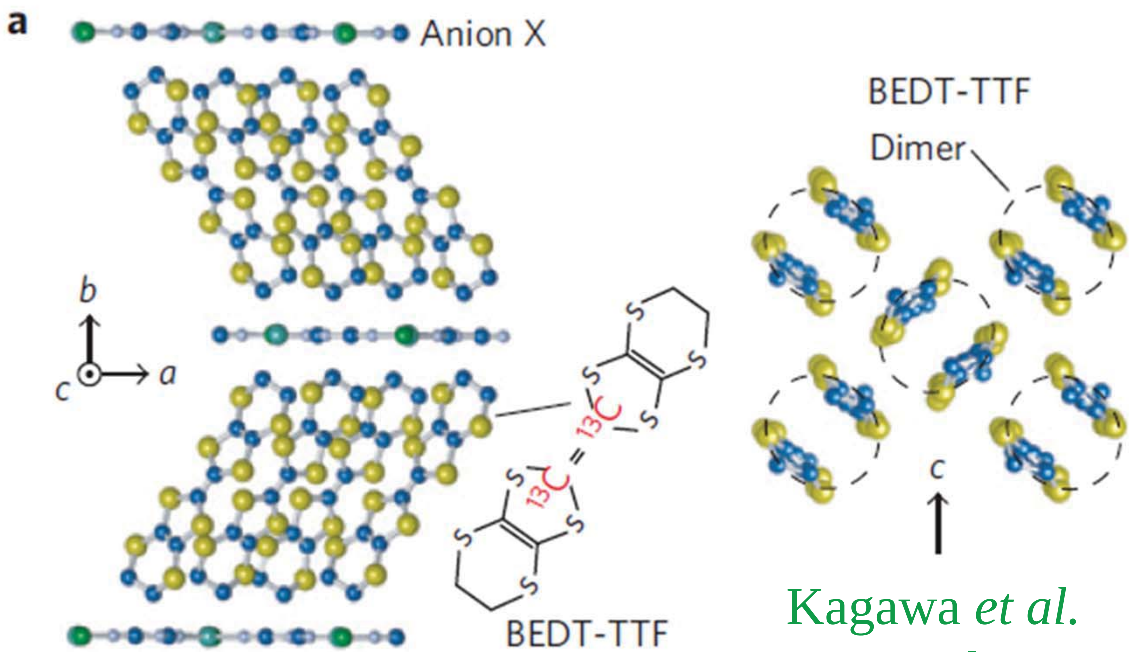
Thèse de Francis Laliberté,
Université de Sherbrooke



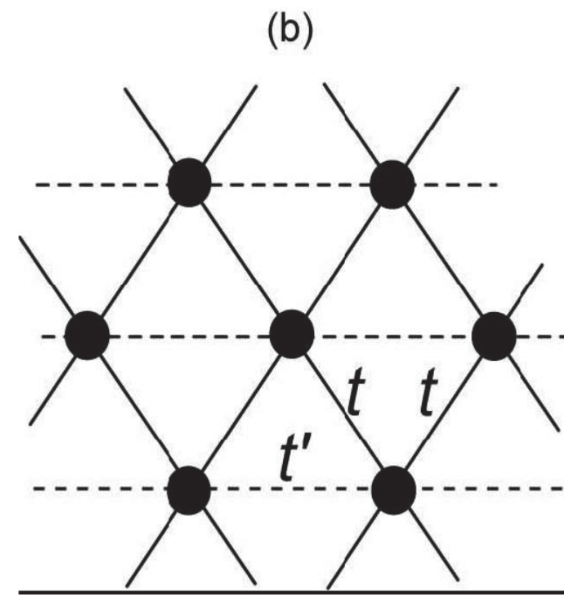


Hubbard on anisotropic triangular lattice

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*

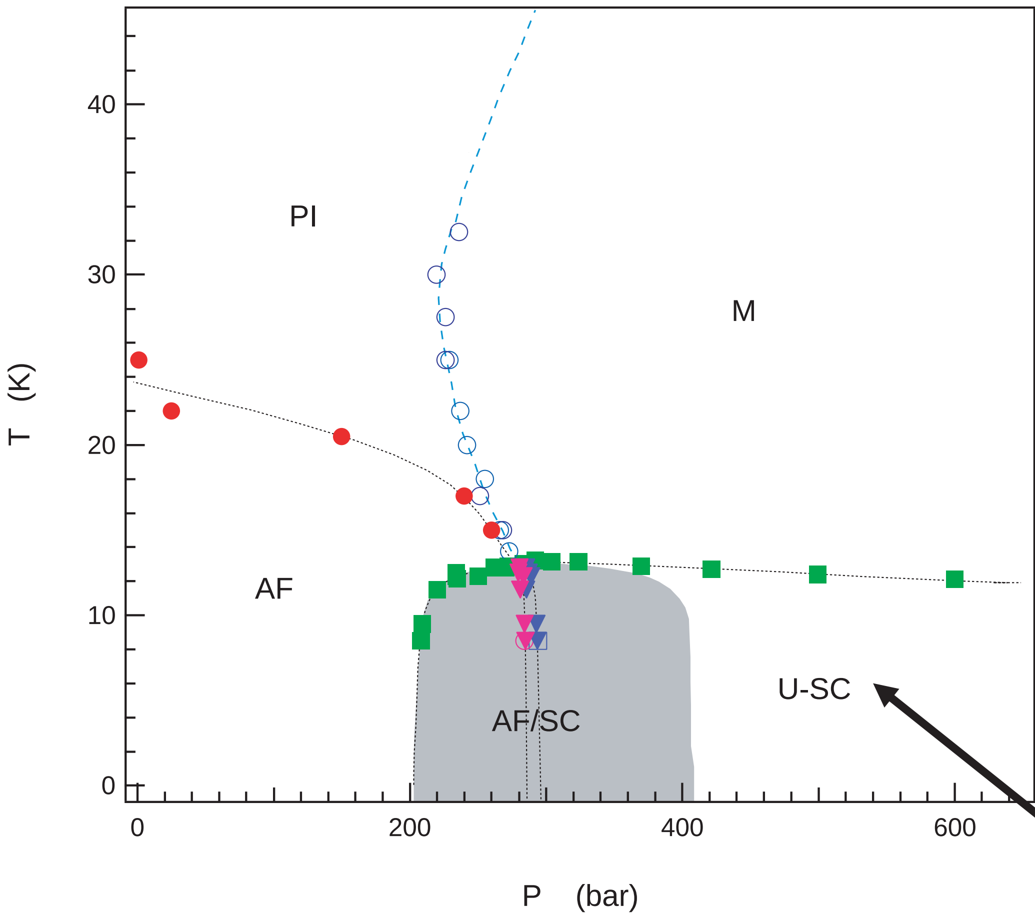
$$H = \sum_{ij\sigma}(t_{ij} - \delta_{ij}\mu)c^\dagger_{i\sigma}c_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}$$

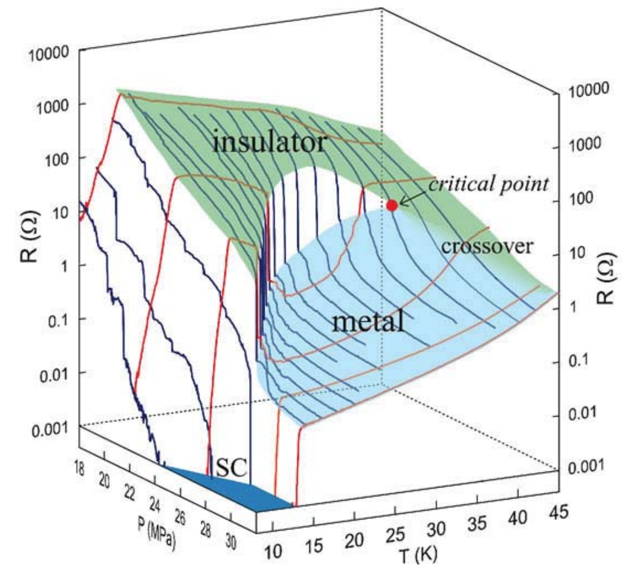
$t \approx 50\,\mathrm{meV}$

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

$t'/t \sim 0.6 - 1.1$

Phase diagram for organics





F. Kagawa, K. Miyagawa, + K. Kanoda

PRB **69** (2004) +Nature **436** (2005)

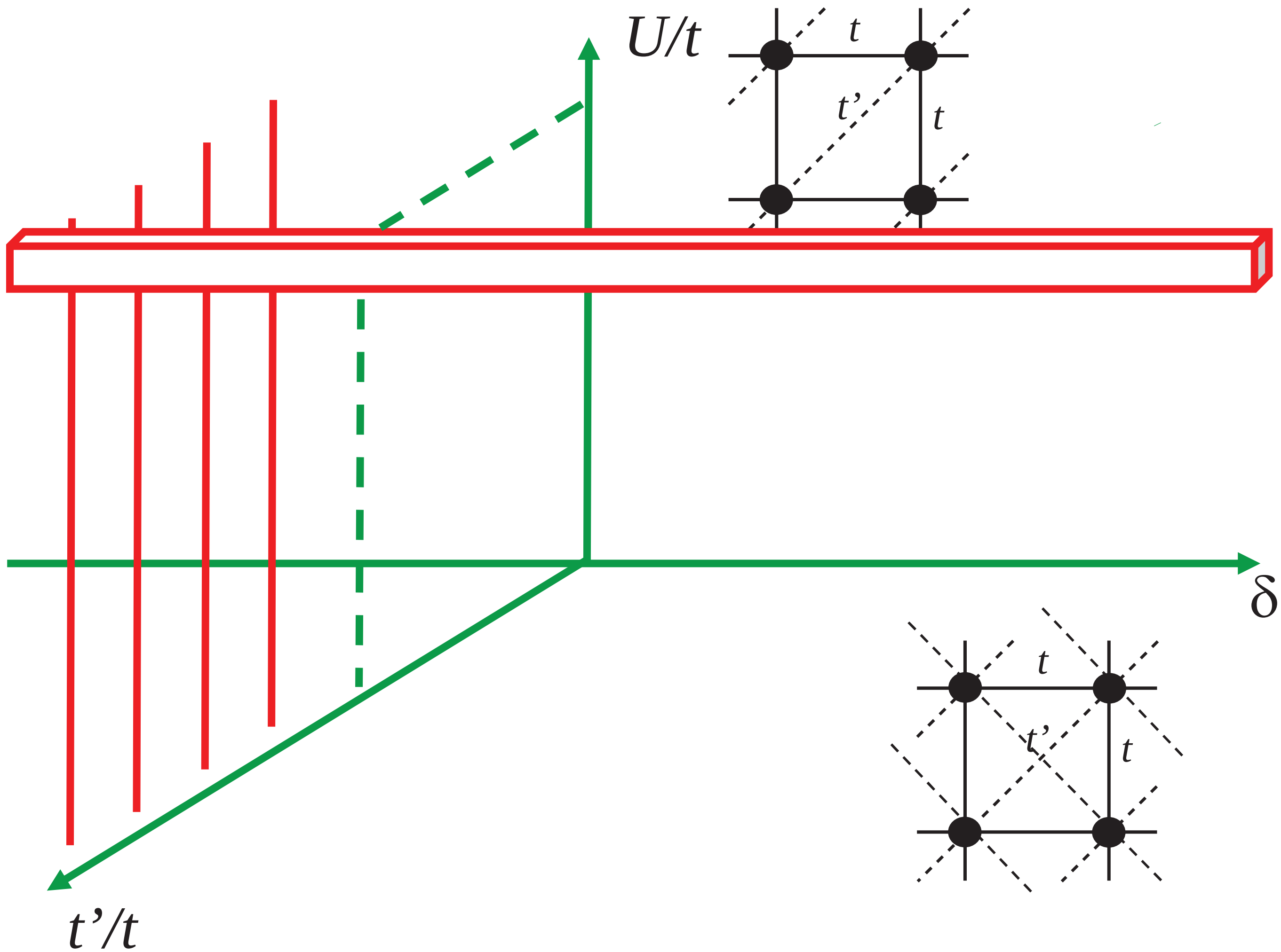
B_g for C_{2h} and B_{2g} for D_{2h}

Powell, McKenzie cond-mat/0607078

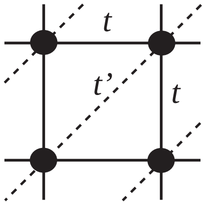
Phase diagram (X=$Cu[N(CN)_2]Cl$)

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

Perspective

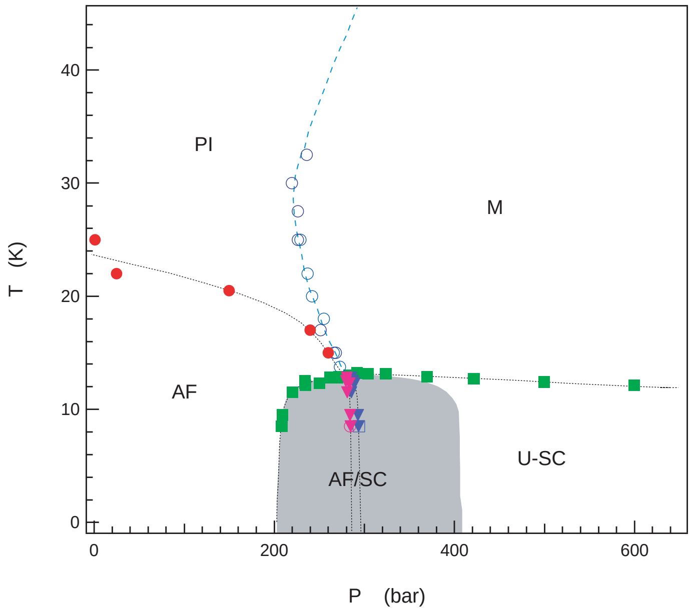


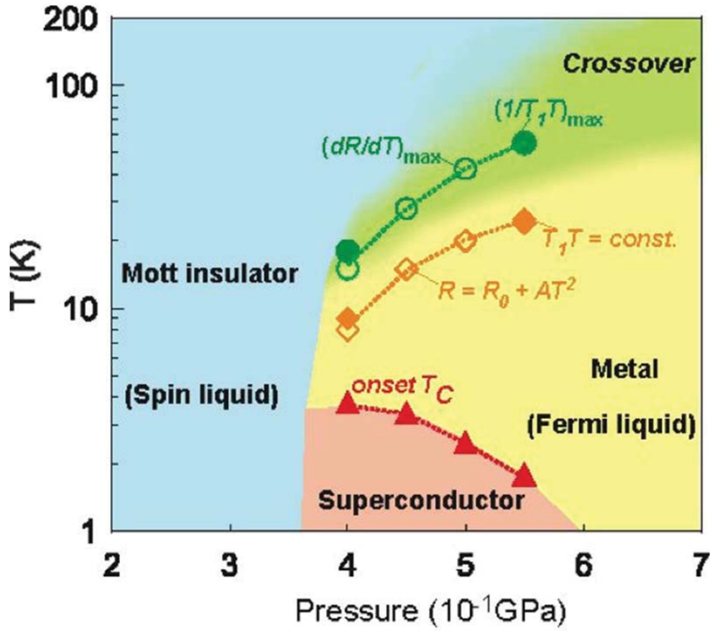
Phase diagram BEDT



$t' = 0.6t$

$X = Cu_2(CN)_3 \; (t' \sim t)$



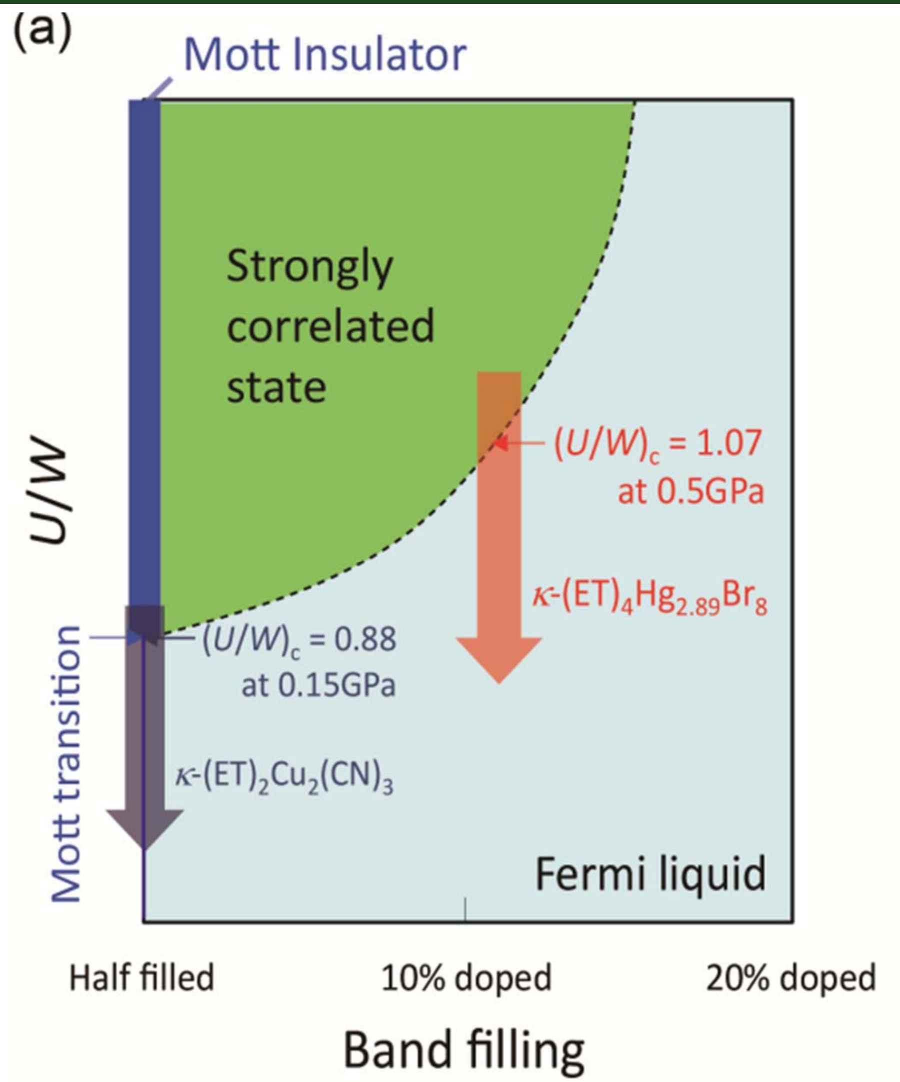


Y. Kurisaki, et al.
Phys. Rev. Lett. **95**, 177001(2005)

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

UNIVERSITÉ DE SHERBROOKE

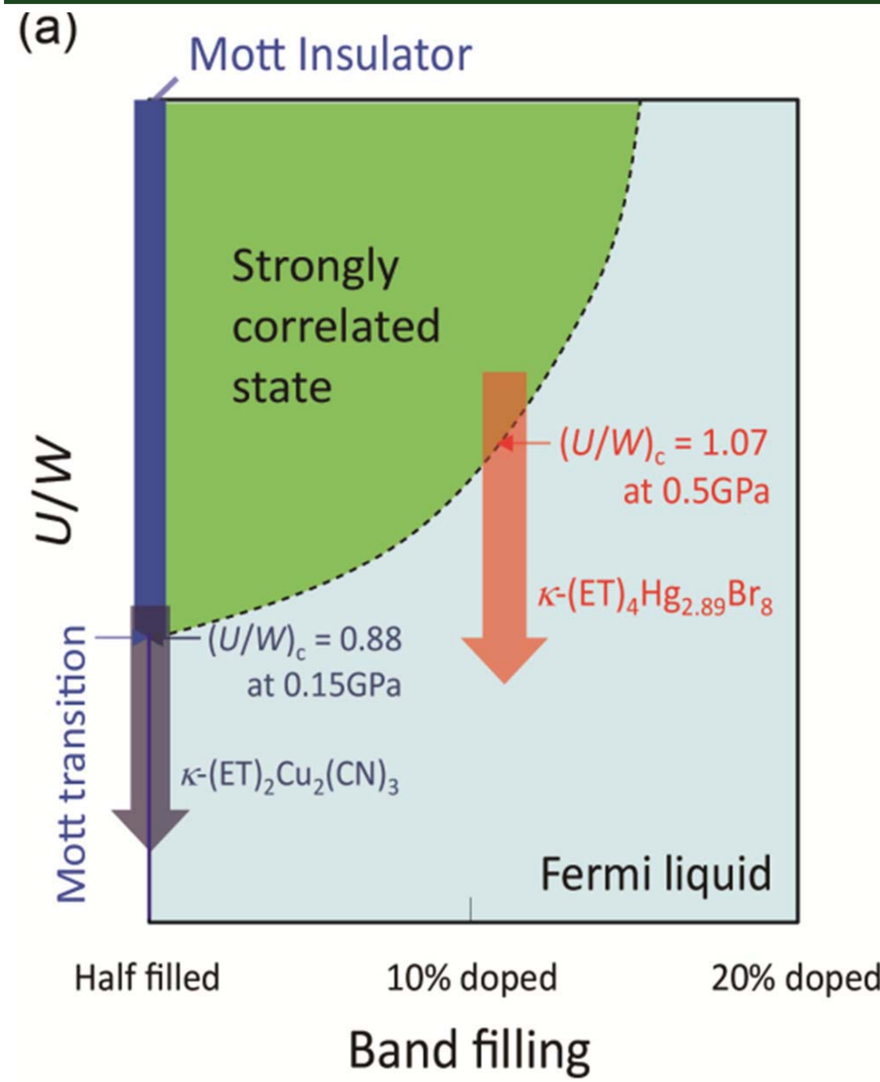
Doped organic

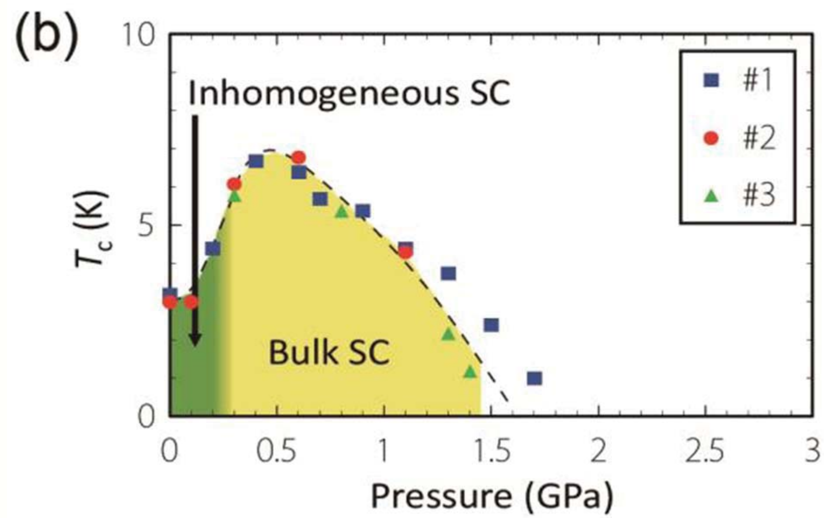


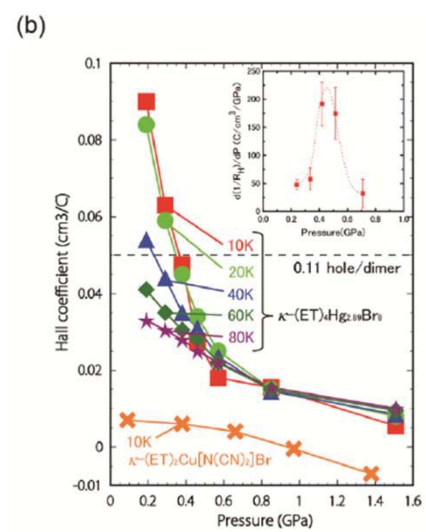
H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

Université de Sherbrooke

Doped BEDT

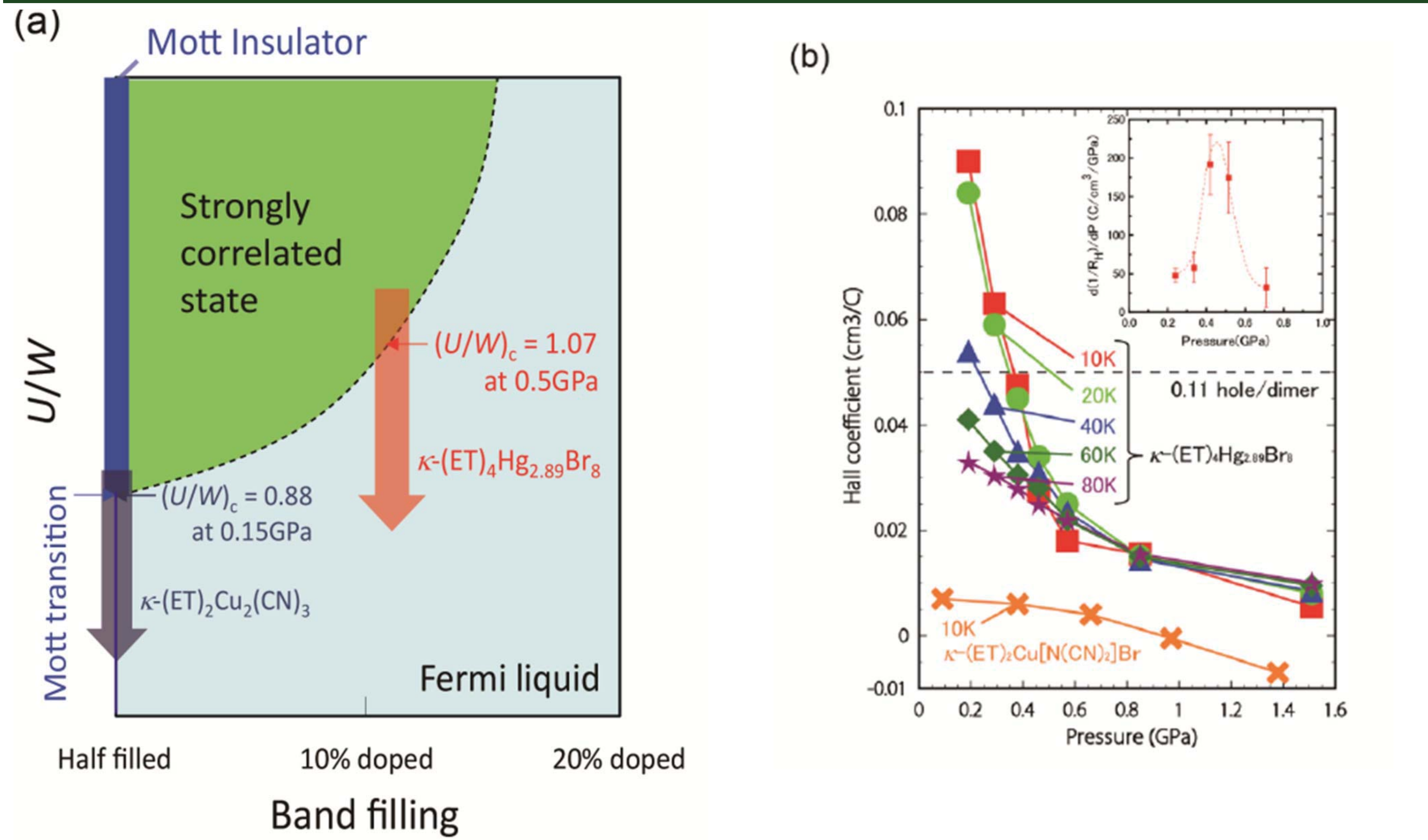






H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

Crossover to doped Mott insulator



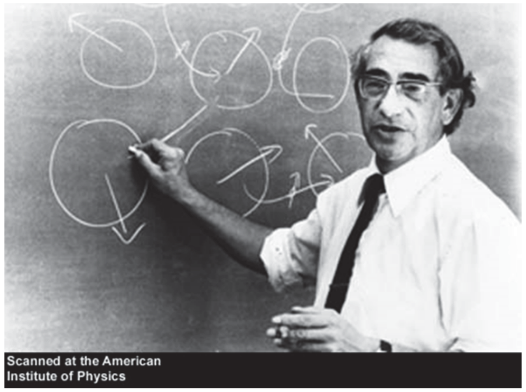
H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

2. The model

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

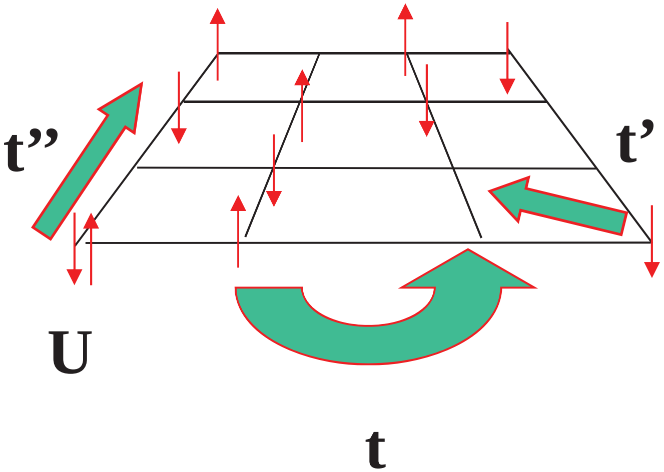
UNIVERSITÉ DE SHERBROOKE

Hubbard model



1931-1980

μ



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

Attn: Charge transfer insulator

P.W. Anderson

UNIVERSITÉ DE SHERBROOKE

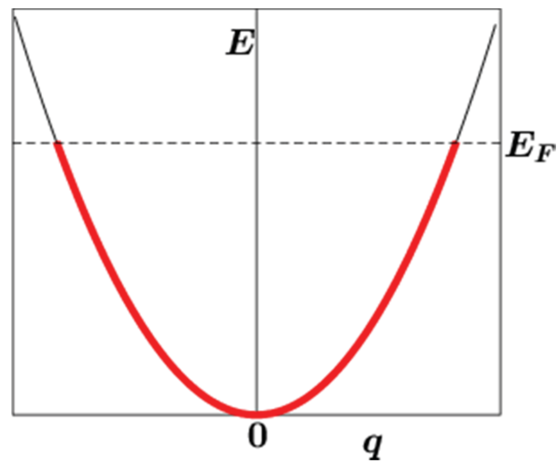
$U = 0$

$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}\right)$$

$$c_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_i} c_{\mathbf{k}\sigma}$$

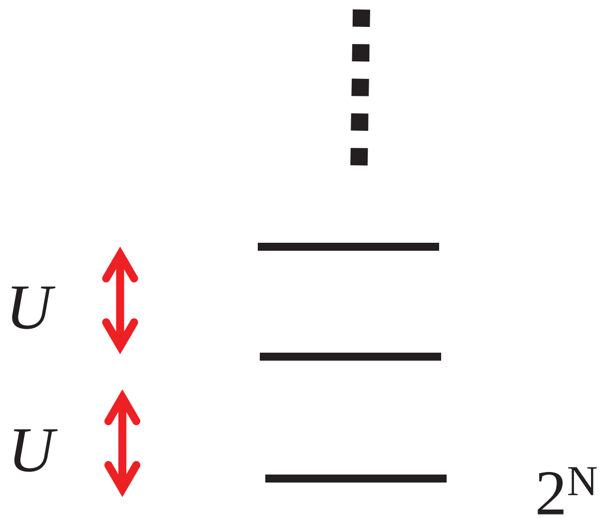
$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

$$|\Psi\rangle = \prod_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k}\sigma} |0\rangle$$



$t_{ij} = 0$

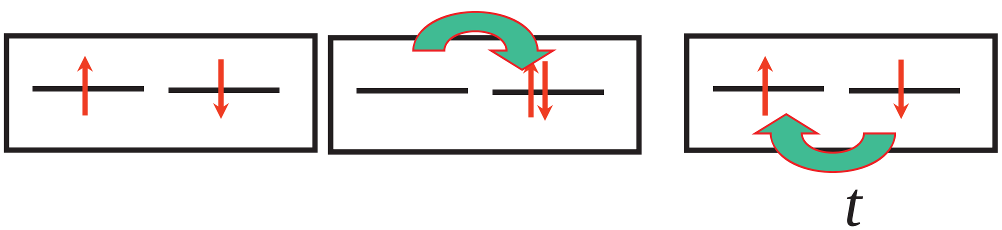
$$H = U \sum_i n_{i\uparrow} n_{i\downarrow}$$



$$|\Psi\rangle = \prod_{\mathbf{i}} c^\dagger_{\mathbf{i}\uparrow} \prod_{\mathbf{j}} c^\dagger_{\mathbf{j}\downarrow} |0\rangle$$

Interesting in the general case

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



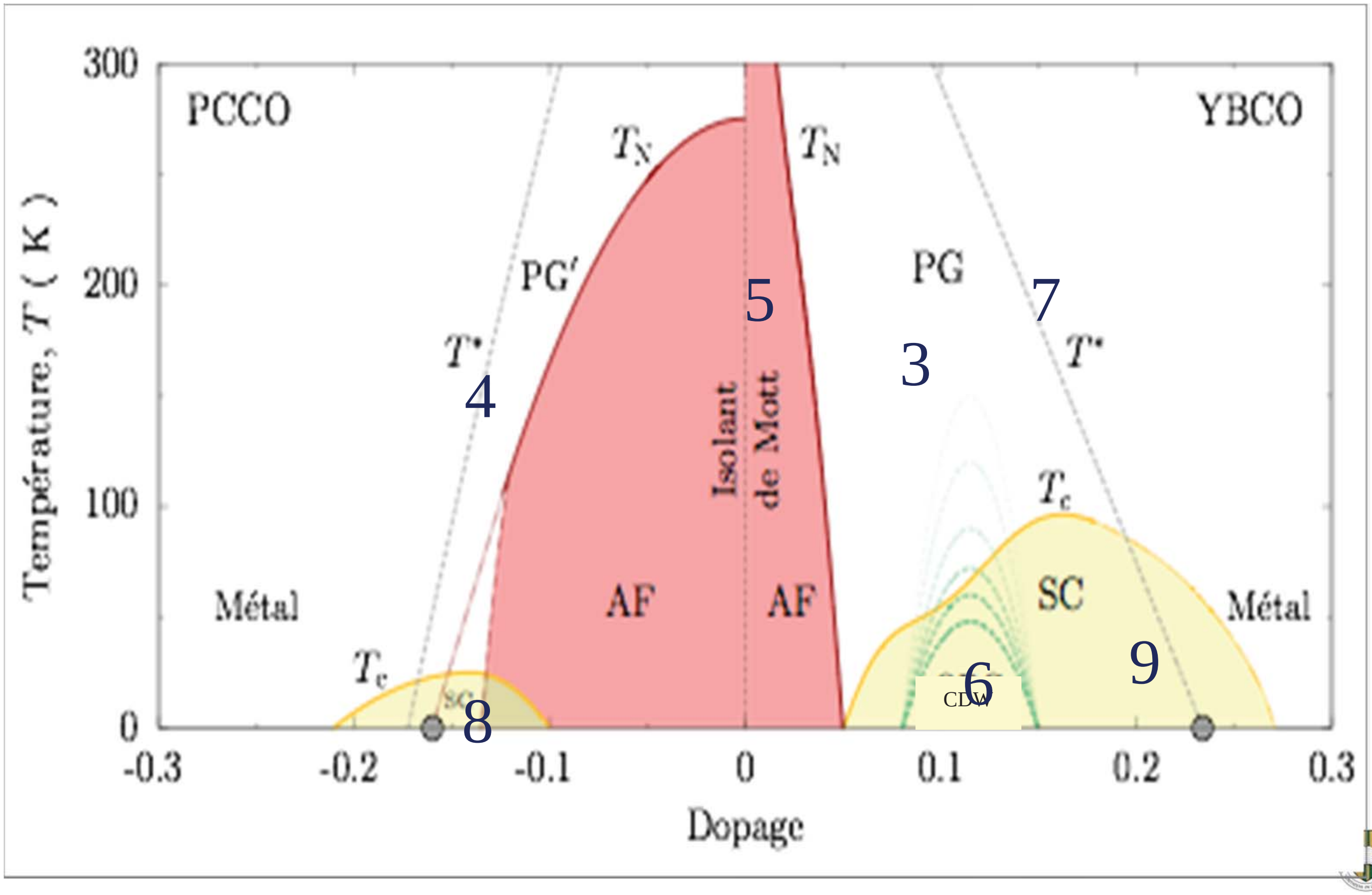
Effective model, Heisenberg: $J = 4t^2/U$

Outline

- Lecture 1: overview
  - What is the problem
  - Possible approaches and answers for organics
- Lecture 2 : h-doped
  - Strongly correlated superconductivity
  - Normal phase (pseudogap)
- Lecture 3: e-doped cuprates
  - Spin wave exchange (TPSC)
  - AFM quantum critical point
- Lecture 4
  - More on cluster generalizations of DMFT

Outline

For references, September 2013 Julich summer school
Strongly Correlated Superconductivity
http://www.cond-mat.de/events/correl13/manuscripts/tremblay.pdf

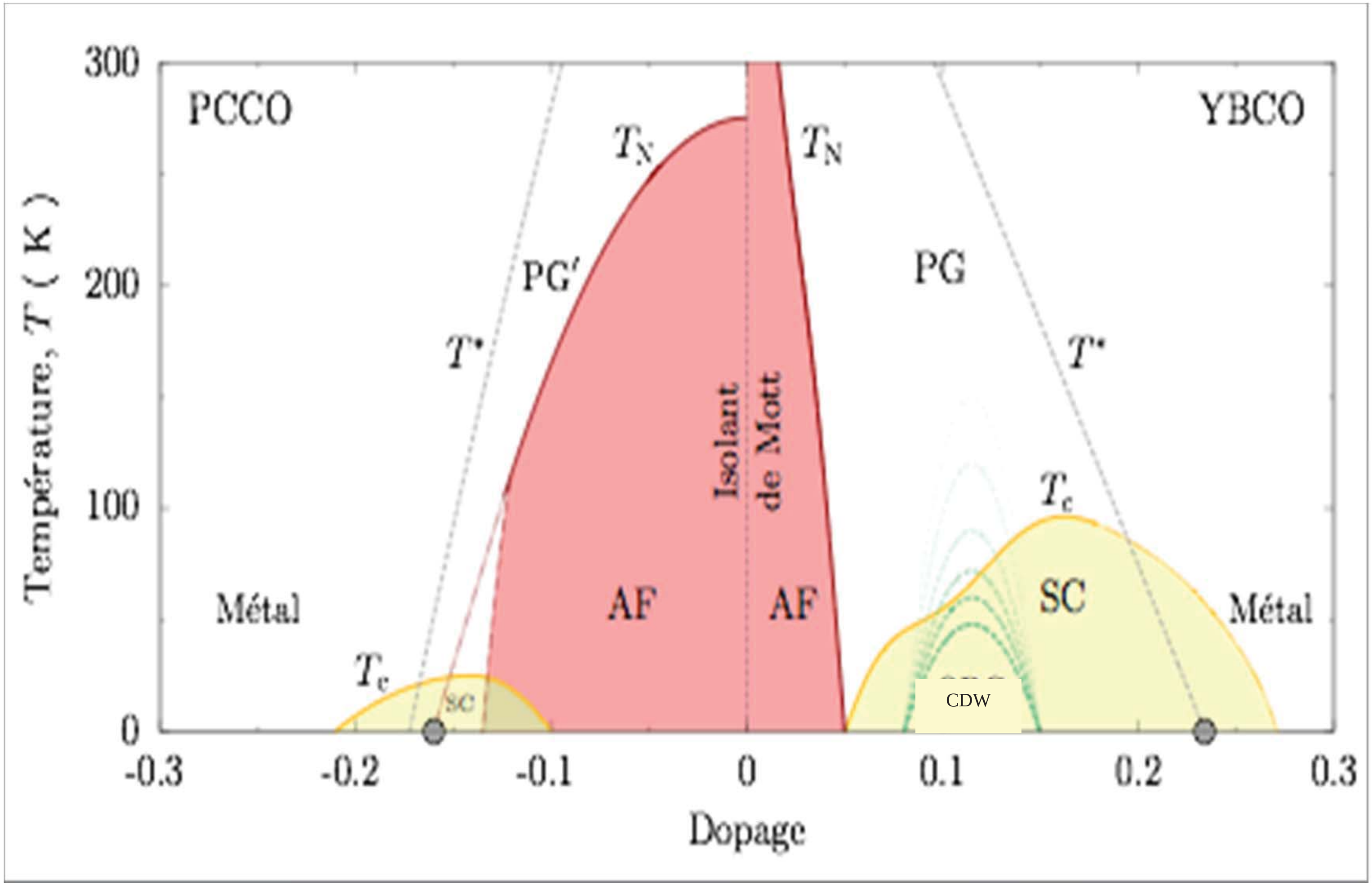


UNIVERSITÉ DE SHERBROOKE

3. A normal, normal state?

Our road map

Thèse de Francis Laliberté,
Université de Sherbrooke



h-doped are strongly correlated: evidence from the normal state

UNIVERSITÉ DE SHERBROOKE

Mott-Ioffe-Regel limit

$$\sigma = \frac{ne^2\tau}{m}$$

$$k_F\ell = \frac{2\pi}{\lambda_F}\ell \sim 2\pi$$

$$\sigma_{MIR} = \frac{e^2}{\hbar d}$$

Mott-Ioffe-Regel limit

$$\sigma = \frac{ne^2\tau}{m}$$

$$n = \frac{1}{2\pi d} k_F^2$$

$$\sigma = \left(\frac{1}{2\pi d} k_F^2\right) \frac{e^2\tau}{m}$$

$$\ell = \left(\frac{\hbar k_F}{m}\right) \tau$$

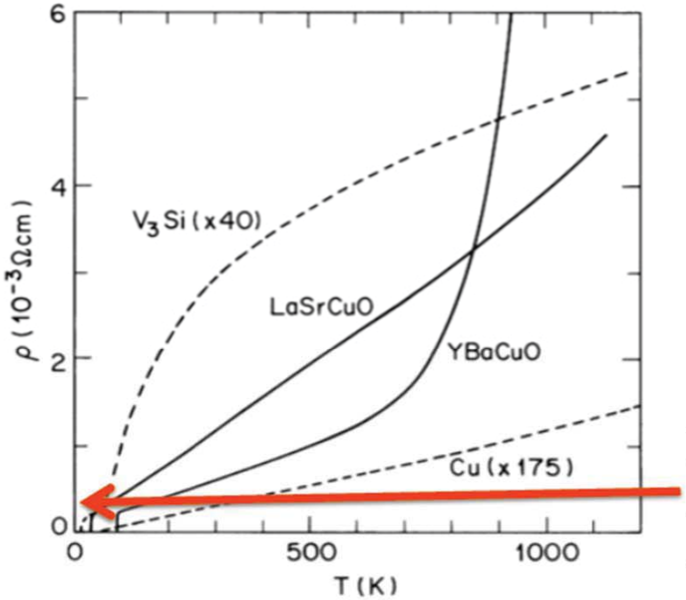
$$\sigma = \frac{1}{2\pi d} k_F e^2 \left(\frac{\ell}{\hbar}\right)$$

$$k_F \ell = \frac{2\pi}{\lambda_F} \ell \sim 2\pi$$

$$\sigma_{MIR} = \frac{e^2}{\hbar d}$$

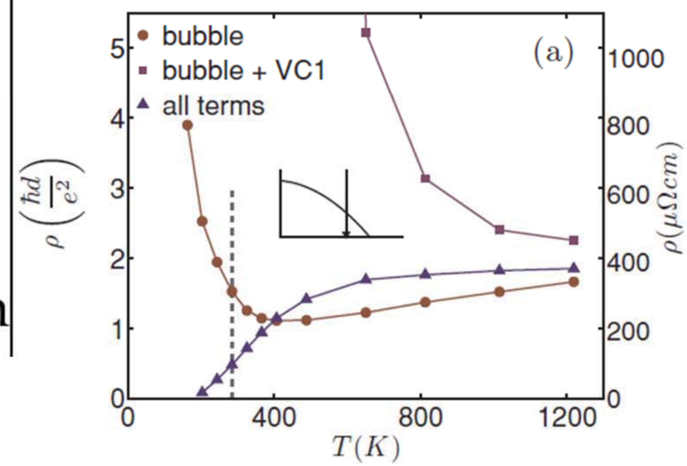
UNIVERSITÉ DE SHERBROOKE

Hole-doped cuprates and MIR limit



Gurvitch & Fiory
PRL 59, 1337
(1987)

MIR limit
Mean-free path
~ Fermi wavelength



LSCO 17%, YBCO optimal

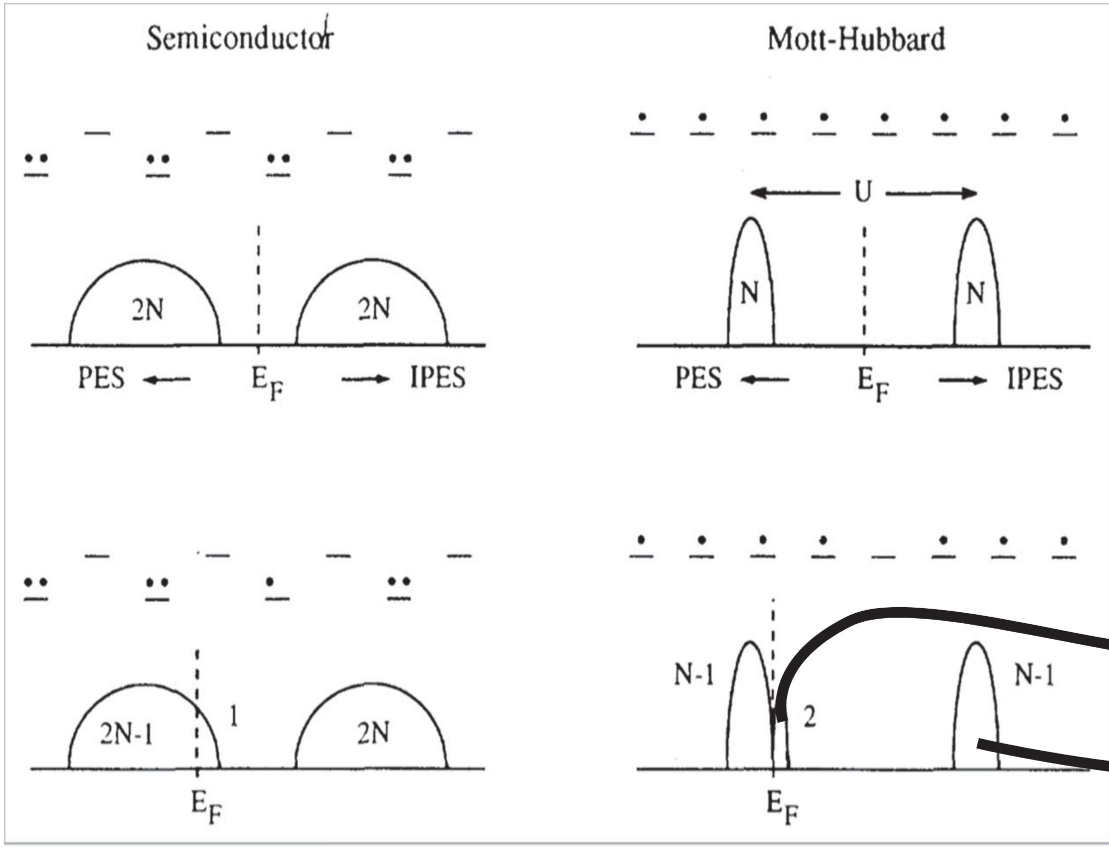
Dominic Bergeron & AMST
PRB 2011
TPSC

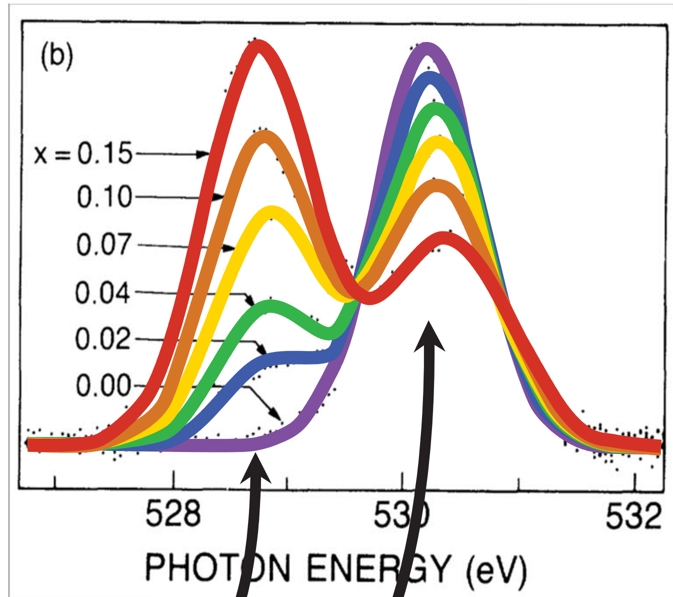
PHYSICAL REVIEW B **84**, 085128 (2011)

Optical and dc conductivity of the two-dimensional Hubbard model in the pseudogap regime and across the antiferromagnetic quantum critical point including vertex corrections

Experiment, X-Ray absorption

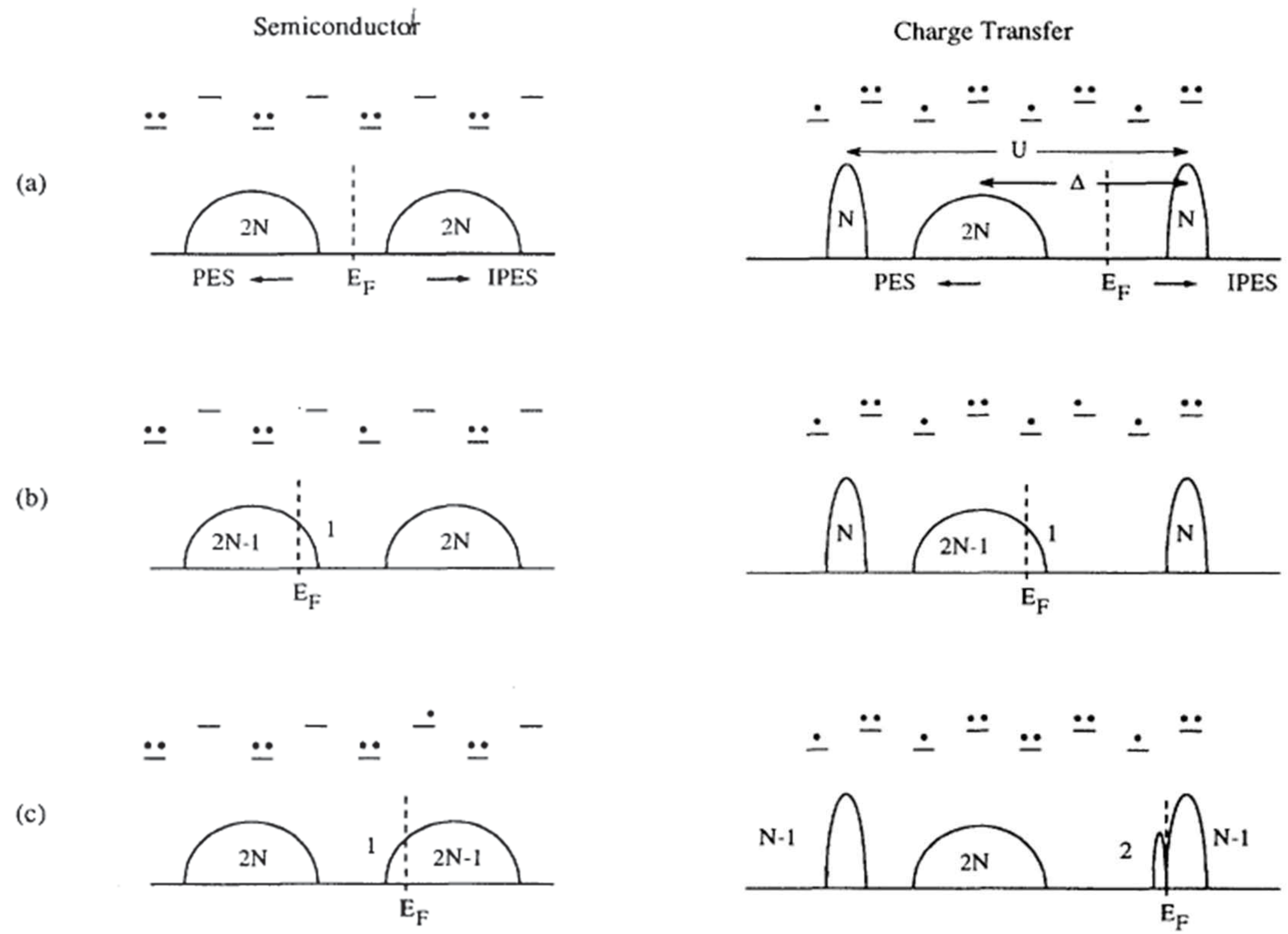
Meinders *et al.* PRB **48**, 3916 (1993)





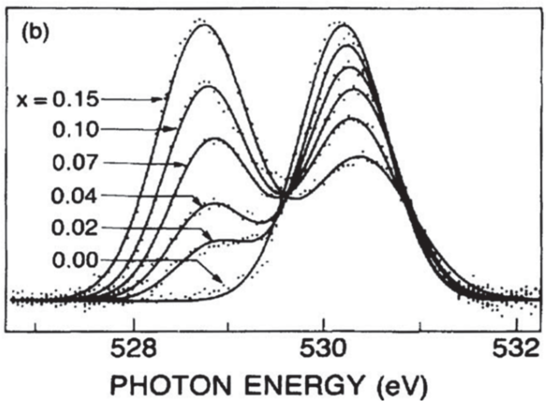
Chen et al. PRL **66**, 104 (1991)

Not obvious: Charge transfer insulator

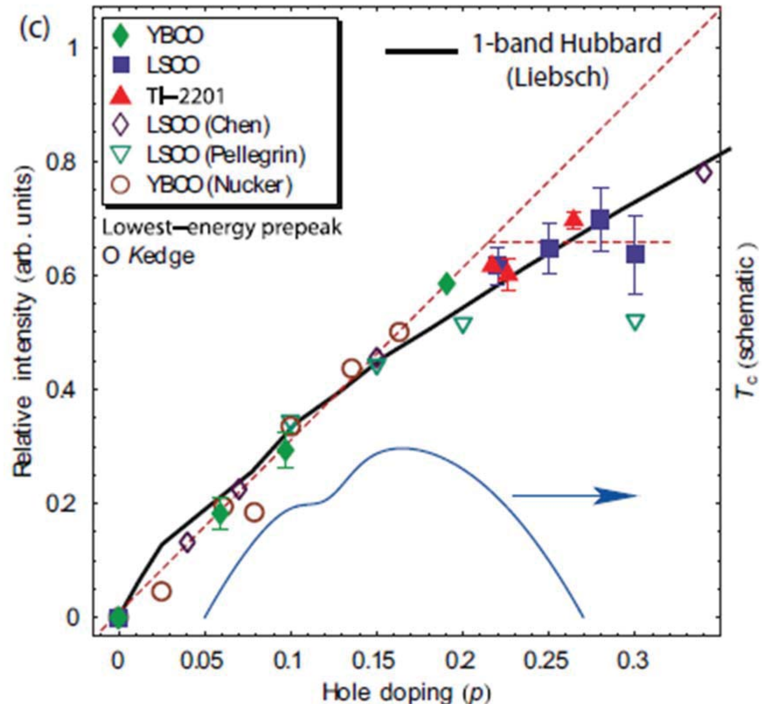


Meinders *et al.* PRB **48**, 3916 (1993)

Experiment: X-Ray absorption



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



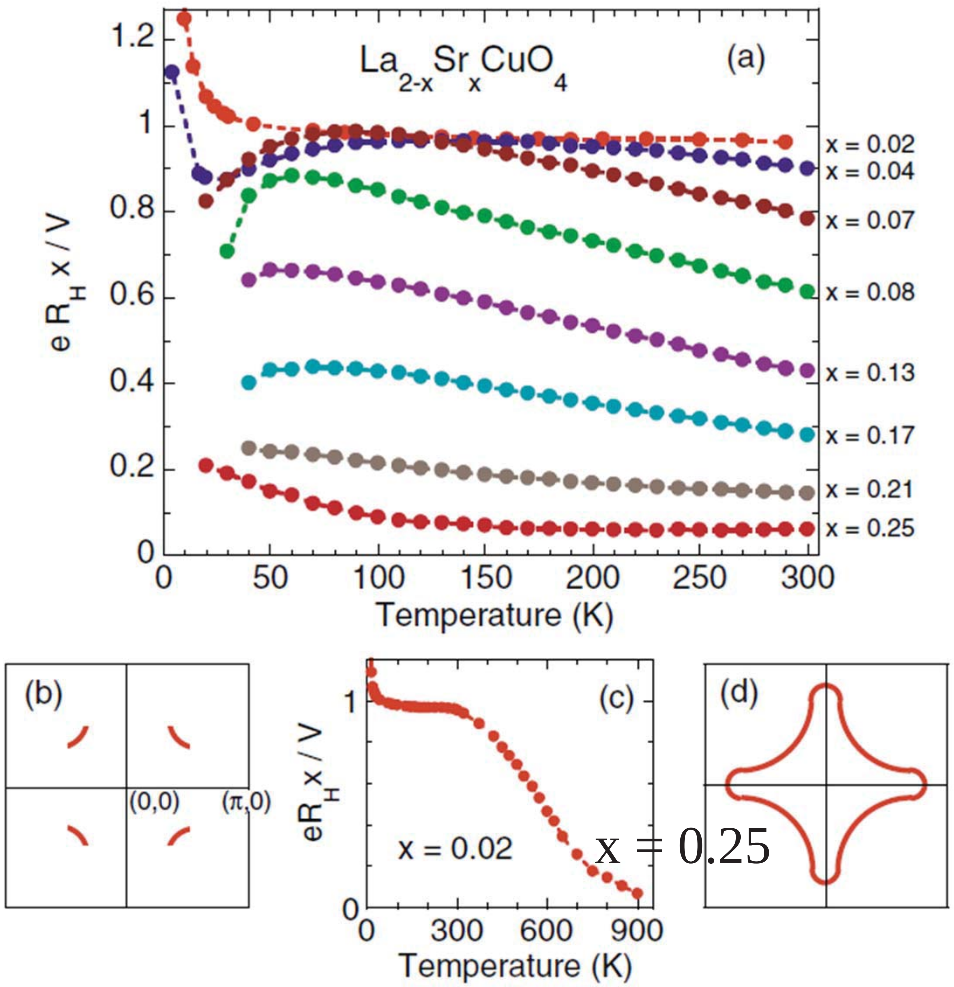
Peets et al. PRL **103**, (2009),
Phillips, Jarrell PRL , vol. **105**, 199701 (2010)

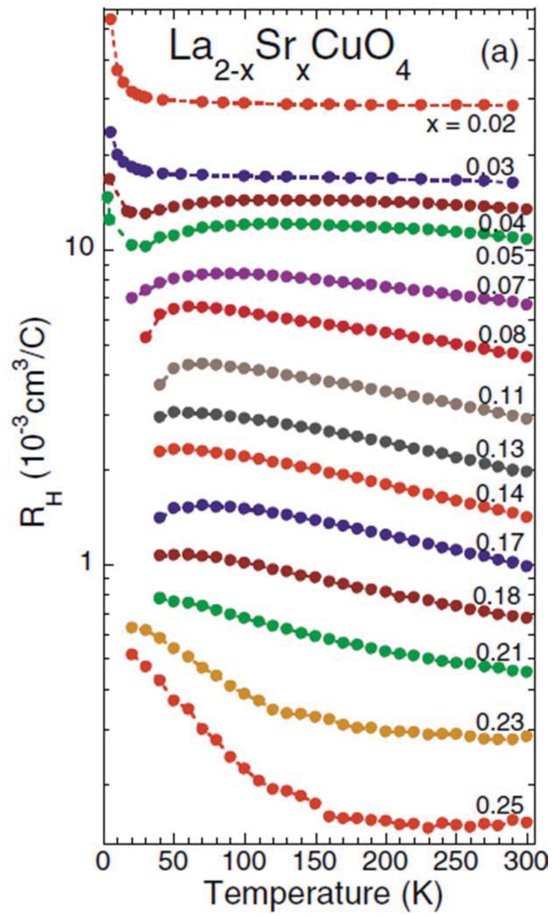
Number of low energy states above ω = 0 scales as *2x* +
Not as 1+x as in Fermi liquid

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

Université de Sherbrooke

Hall coefficient

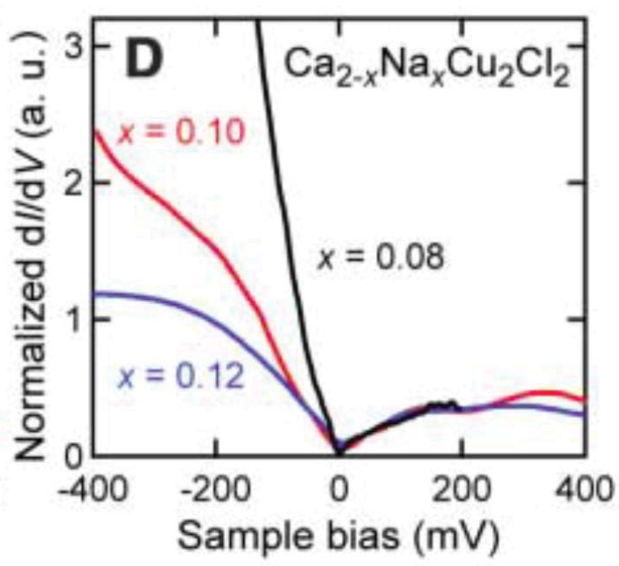




Ando et al. PRL **92**, 197001 (2004)

UNIVERSITÉ DE SHERBROOKE

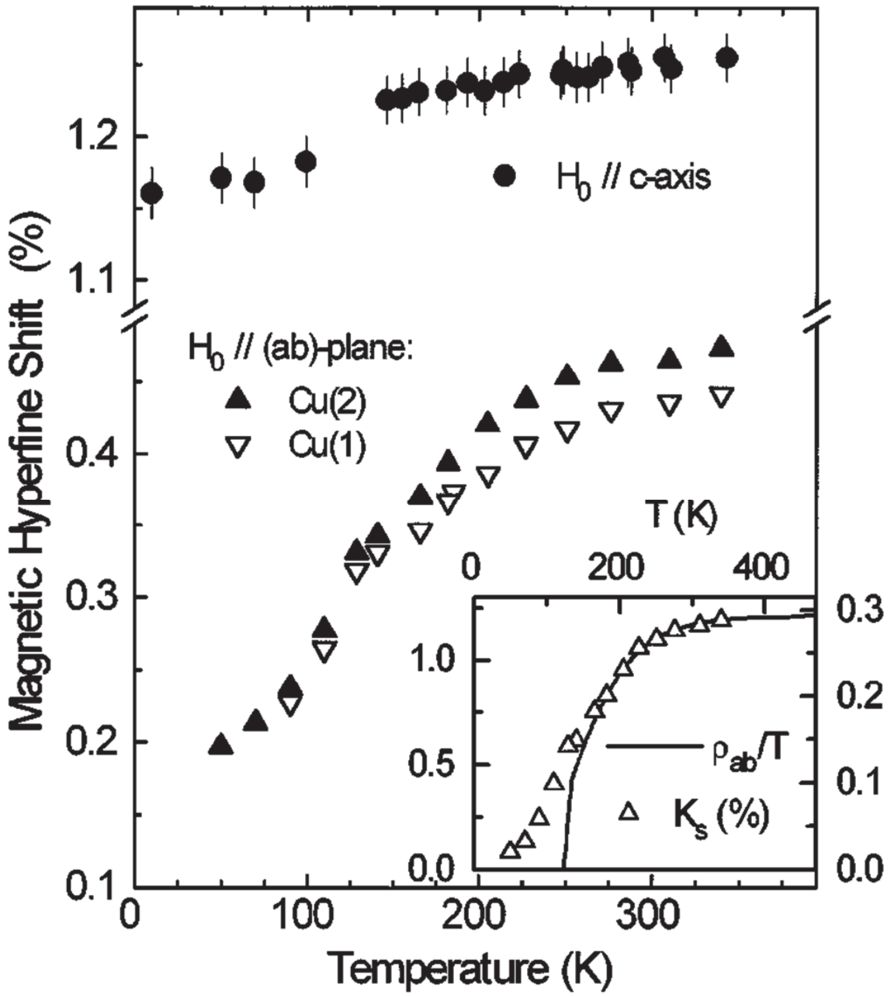
Density of states (STM)



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

UNIVERSITÉ DE SHERBROOKE

Spin susceptibility (Knight shift): Pseudogap

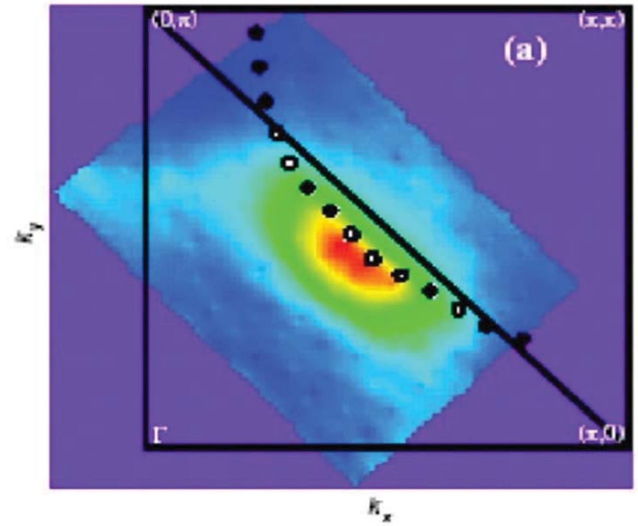


Underdoped Hg1223

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

ARPES: (Pseudogap)

Hole-doped, 10%



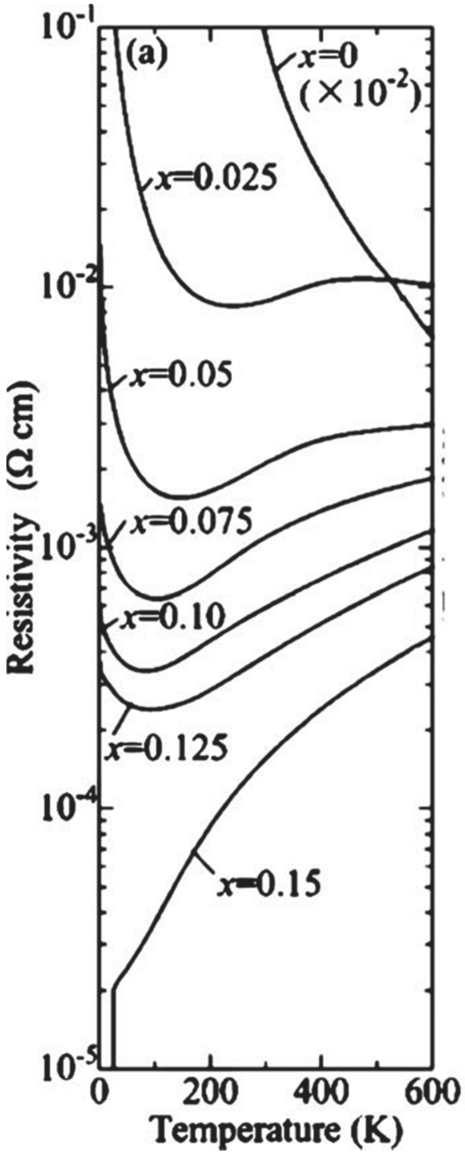
F. Ronning et al. Jan. 2002, $Ca_{2-x}Na_xCuO_2Cl_2$

Ronning *et al.* (PRB 2003)

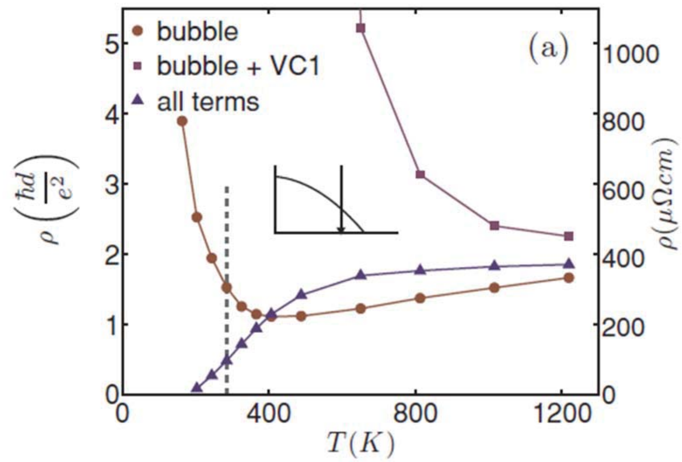
4. e-doped cuprates

Less strongly coupled: evidence from the normal state

Electron-doped and MIR limit



NCCO



Dominic Bergeron et al. TPSC
PRB **84**, 085128 (2011)

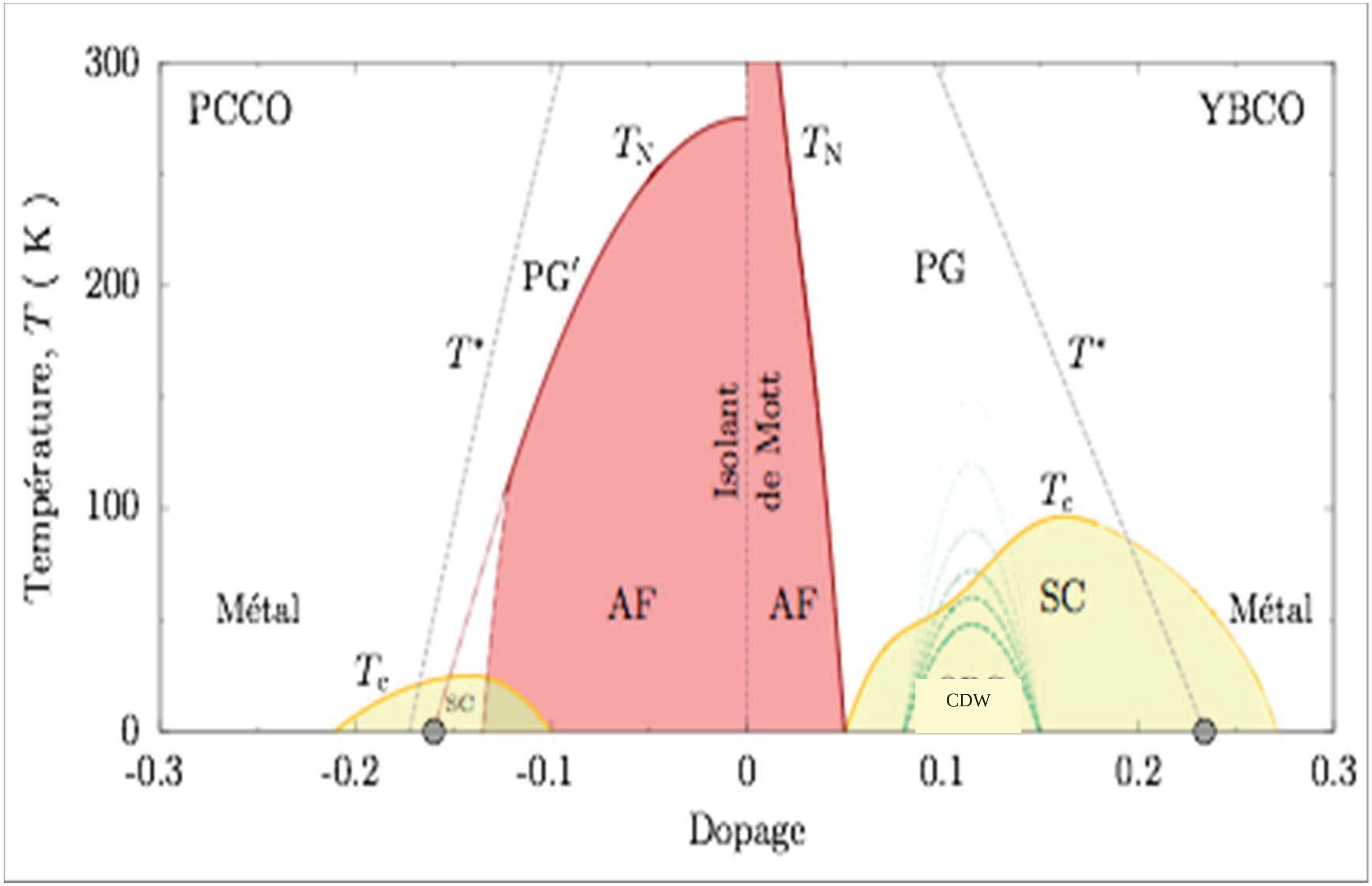
Onose et al. 2004

5. Weakly and strongly correlated antiferromagnets

What is a phase?

Our road map

Thèse de Francis Laliberté,
Université de Sherbrooke



UNIVERSITÉ DE SHERBROOKE

Antiferromagnetic phase: emergent properties

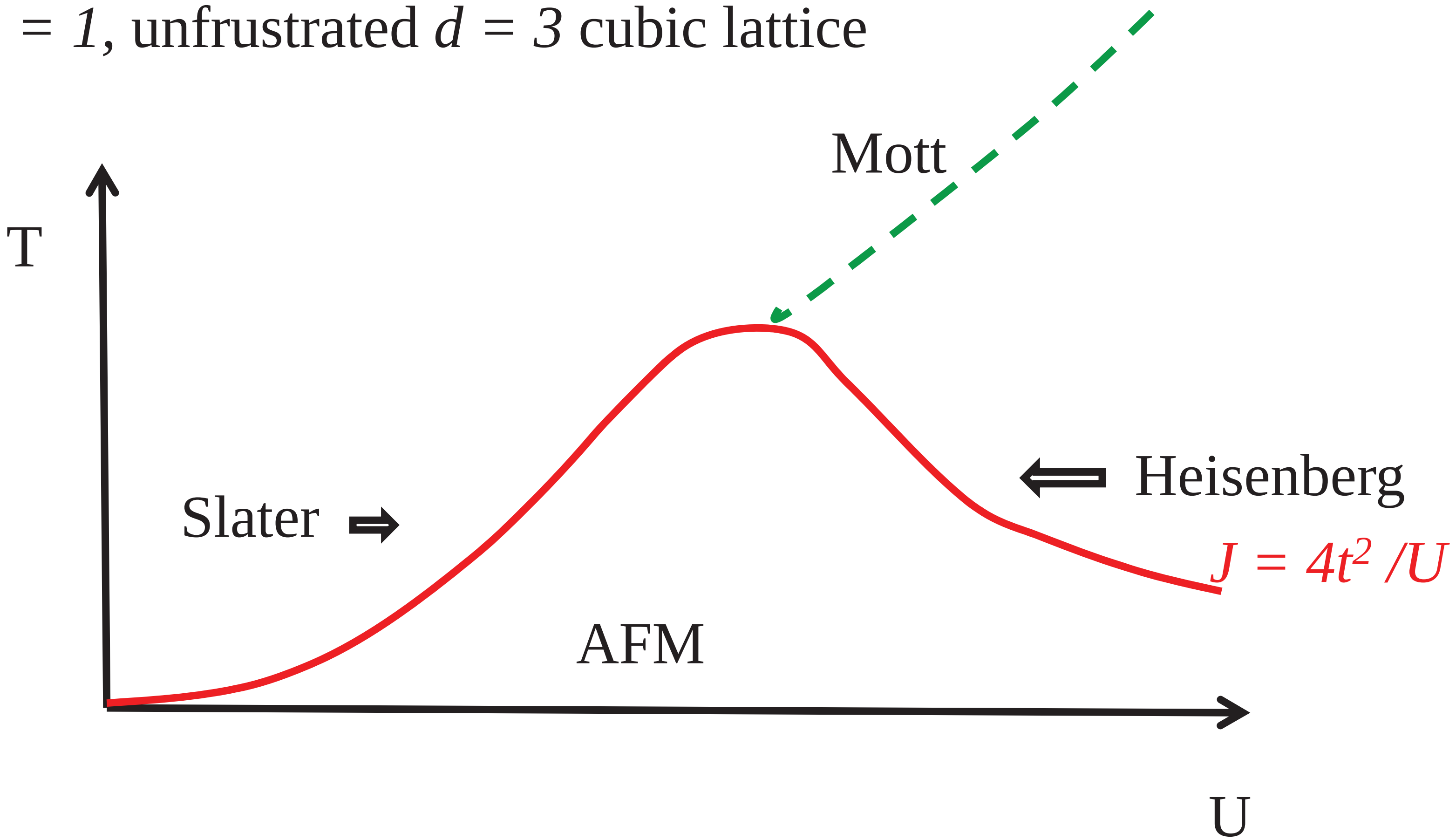
- Some broken symmetries
  - Time reversal symmetry
  - Translation by one lattice spacing
  - Unbroken Time-reversal times translation by lattice vector **a**
  - Spin waves
  - Single-particle gap

Differences between weakly and strongly correlated

- Different in ordered phase (finite frequency)
  - Ordered moment
  - Landau damping
    - Spin waves all the way or not to J
- Different, even more, in the normal state:
  - metallic in $d = 3$ if weakly correlated
  - Insulating if strongly correlated
  - Pressure dependence of T_N

Local moment and Mott transition

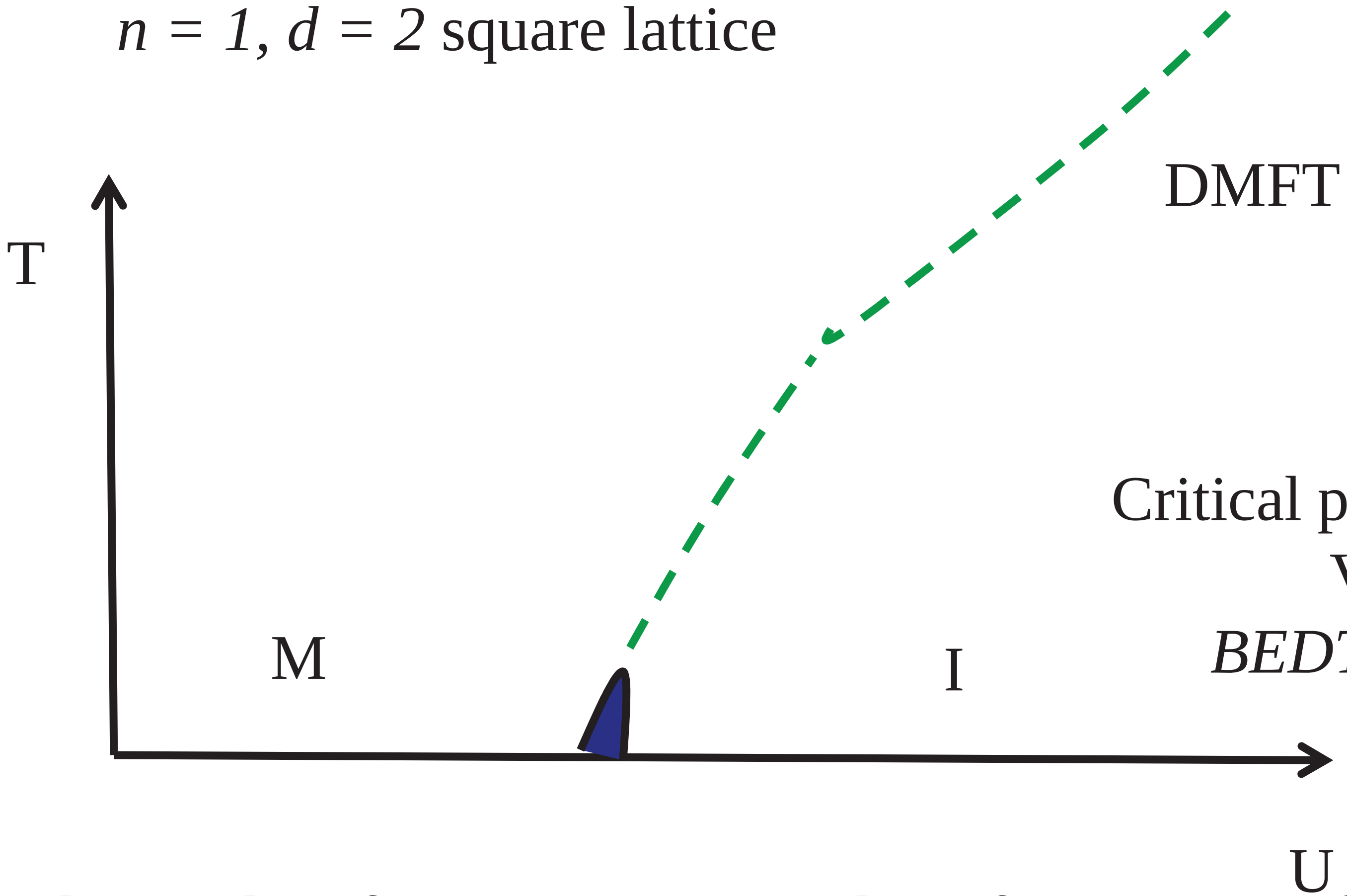
$n = 1$, unfrustrated $d = 3$ cubic lattice



UNIVERSITÉ DE SHERBROOKE

Local moment and Mott transition

n = 1, d = 2 square lattice



Critical point visible in V_2O_3,
BEDT organics

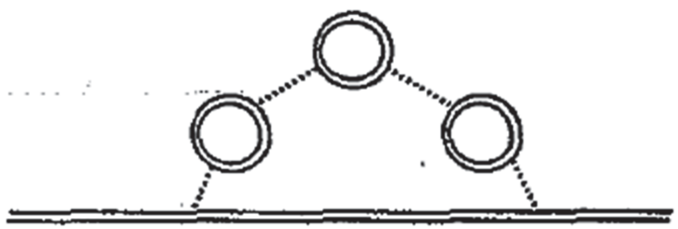
Understanding finite temperature phase from a *mean-field theory* down to $T = 0$

Strong vs weak correlations

Contrasting methods

Ordered state

- Mean-field (Hartree-Fock) for AFM



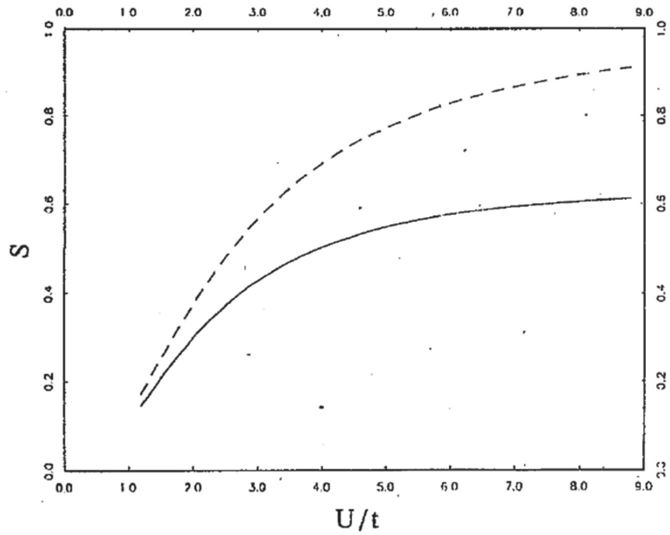


FIG. 7. The solid line represents the sublattice magnetization including the fluctuation effects. The dashed line is the mean-field result.

Schrieffer, Wen, Zhang, PRB 1989

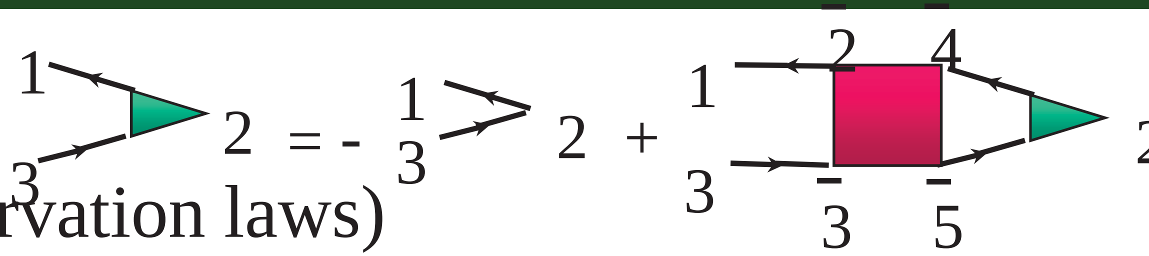
More methods for ordered states, n=1

- Numerically, stochastic series expansion,
- High-temperature series expansion,
- Quantum Monte Carlo
- World-line
- Worm algorithms
- Variational methods

• Ground state of S=1/2 in *d=2* is AFM, not spin liquid

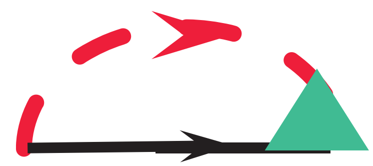
In paramagnetic state

Theory difficult even at weak to intermediate correlation!



- RPA (OK with conservation laws)
  - Mermin-Wagner
  - Pauli
- Moryia (Conjugate variables HS $\phi^4 = \langle\phi^2\rangle\, \phi^2$)
  - Adjustable parameters: c and U_{eff}
  - Pauli
- FLEX
  - No pseudogap
  - Pauli
- Renormalization Group
  - 2 loops

Σ =



Zanchi Schultz, (2000)
Rohe and Metzner (2004)
Katanin and Kampf (2004)

UNIVERSITÉ DE SHERBROOKE

Two-Particle Self-Consistent (idea)

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

Vilk, AMT J. Phys. I France, **7**, 1309 (1997); Allen et al.in *Theoretical methods for strongly correlated electrons* also cond-mat/0110130

(Mahan, third edition)

UNIVERSITÉ DE SHERBROOKE

Doped Mott insulator : strong correlations

Normal state

At strong coupling

- Gutzwiller
- Variational approaches
- Slave particles (Review: Lee Nagaosa RMP)
- Extremely Correlated Fermi liquids (Shastry)

YRZ

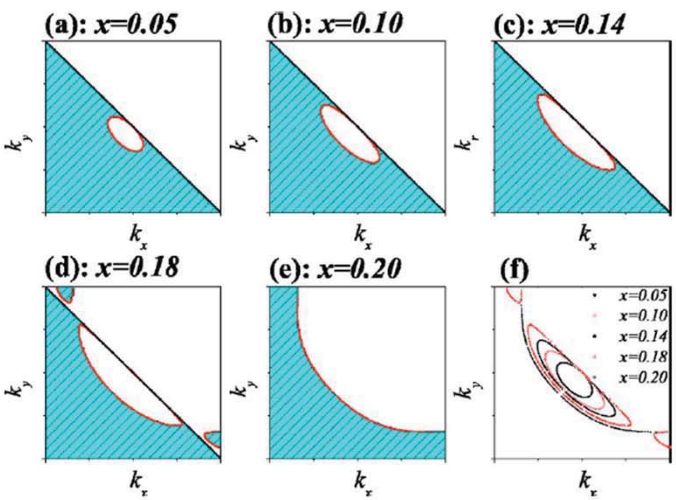
$$G^{RVB}(\boldsymbol{k},\omega) = \frac{g_t}{\omega - \xi(\boldsymbol{k}) - \Delta_R^2/[\omega + \xi_0(\boldsymbol{k})]} + G_{inc},$$

where $\boldsymbol{k} = (k_x, k_y)$,

$$\xi_0(\boldsymbol{k}) = -2t(x)(\cos k_x + \cos k_y),$$

$$\Delta_R(\boldsymbol{k}) = \Delta_0(x)(\cos k_x - \cos k_y),$$

$$\xi(\boldsymbol{k}) = \xi_0(\boldsymbol{k}) - 4t'(x)\cos k_x \cos k_y - 2t''(x)(\cos 2k_x + \cos 2k_y) - \mu_p.$$



K.-Y. Yang, T.M. Rice, and F.-C. Zhang, Phys. Rev. B 73, 174501 (2006)
See numerous papers of Carbotte and Nicol and detailed discussions in
K. Le Hur and T.M. Rice, Annals of Physics **324**, 1452 (2009)

UNIVERSITÉ DE SHERBROOKE

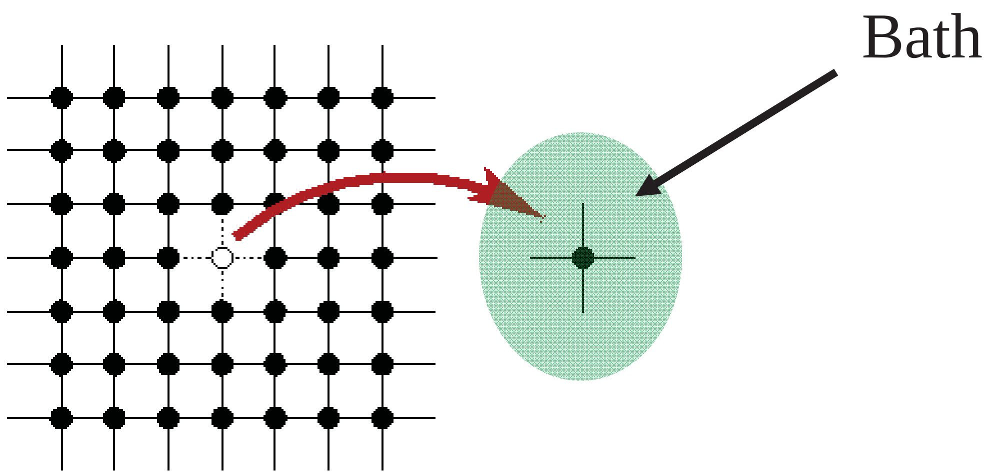
Method

"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.

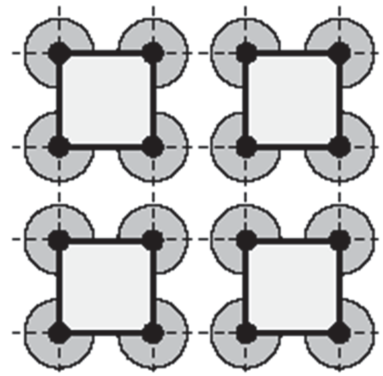


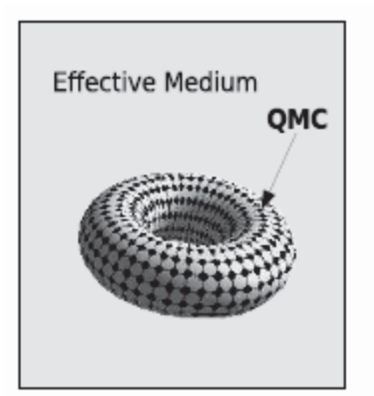
W. Metzner and D. Vollhardt, PRL (1989)
A. Georges and G. Kotliar, PRB (1992)
M. Jarrell PRB (1992)
A. Georges et al. RMP (1996)

DMFT, (d = 3)

2d Hubbard: Quantum cluster method

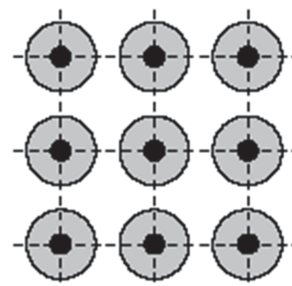
C-DMFT





DCA

DMFT



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

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

+ 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

Details on method in Lecture 4

Many active groups

- Paris: A. Georges, M. Ferrero, O. Parcollet
- Rutgers: K. Haule, G. Kotliar,
- Bâton Rouge: M. Jarrell
- Columbia: A. Millis
- Michigan: E. Gull
- Oakridge: Th. Maier, S.Okamoto
- Tokyo: M. Imada, Motome, Sakai
- Julich: A. Liebsch
- Graz: M. Aichhorn
- Hamburg: Potthoff
- LPS: M. Civelli
- ESRF: L. de Medici
- Trieste: M. Capone
- Vienna: Held
- Royal Holloway: G. Sordi
- Sherbrooke: D. Sénéchal, B. Kyung, P. Sémon, A.-M.S. Tremblay

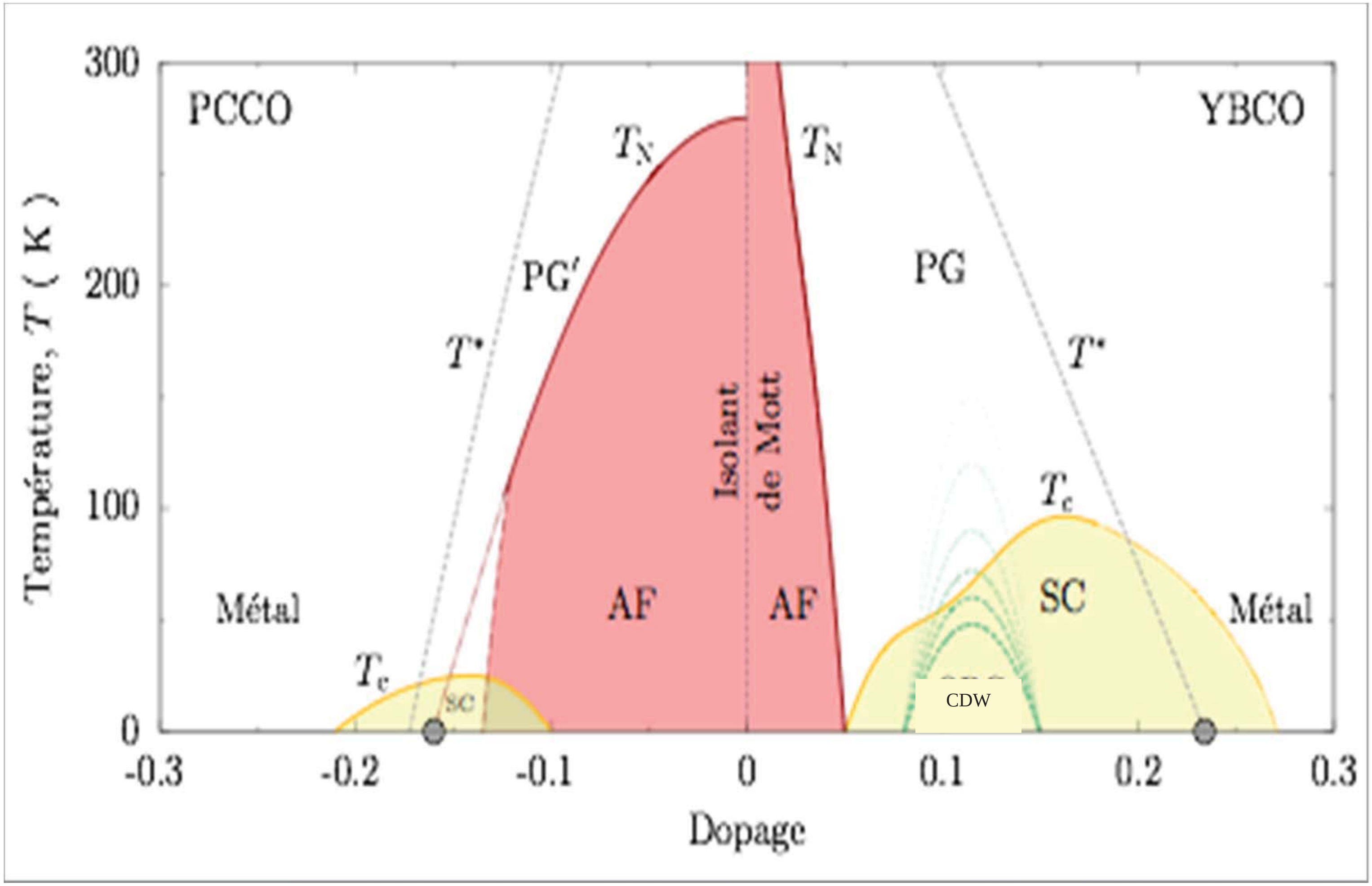
Bio break

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

6. Charge Density Wave

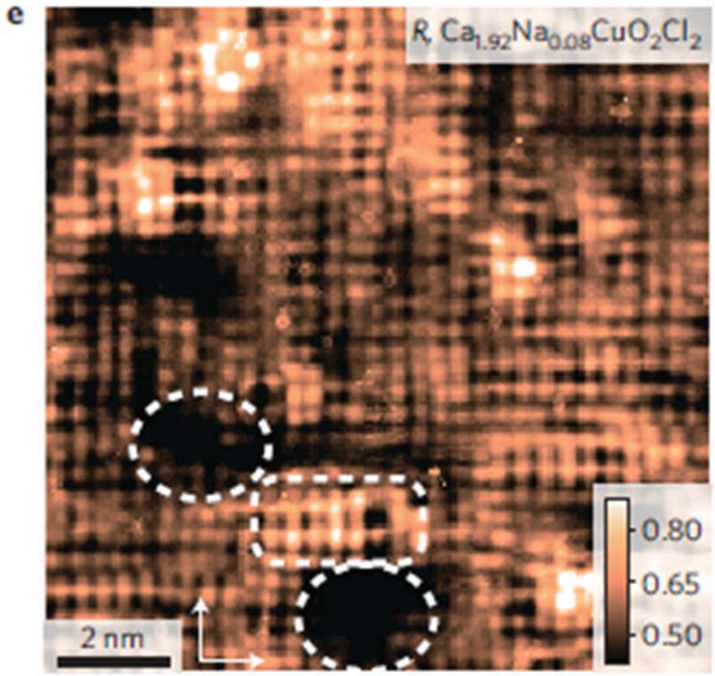
h-doped

Our road map



Thèse de Francis Laliberté, Université de Sherbrooke

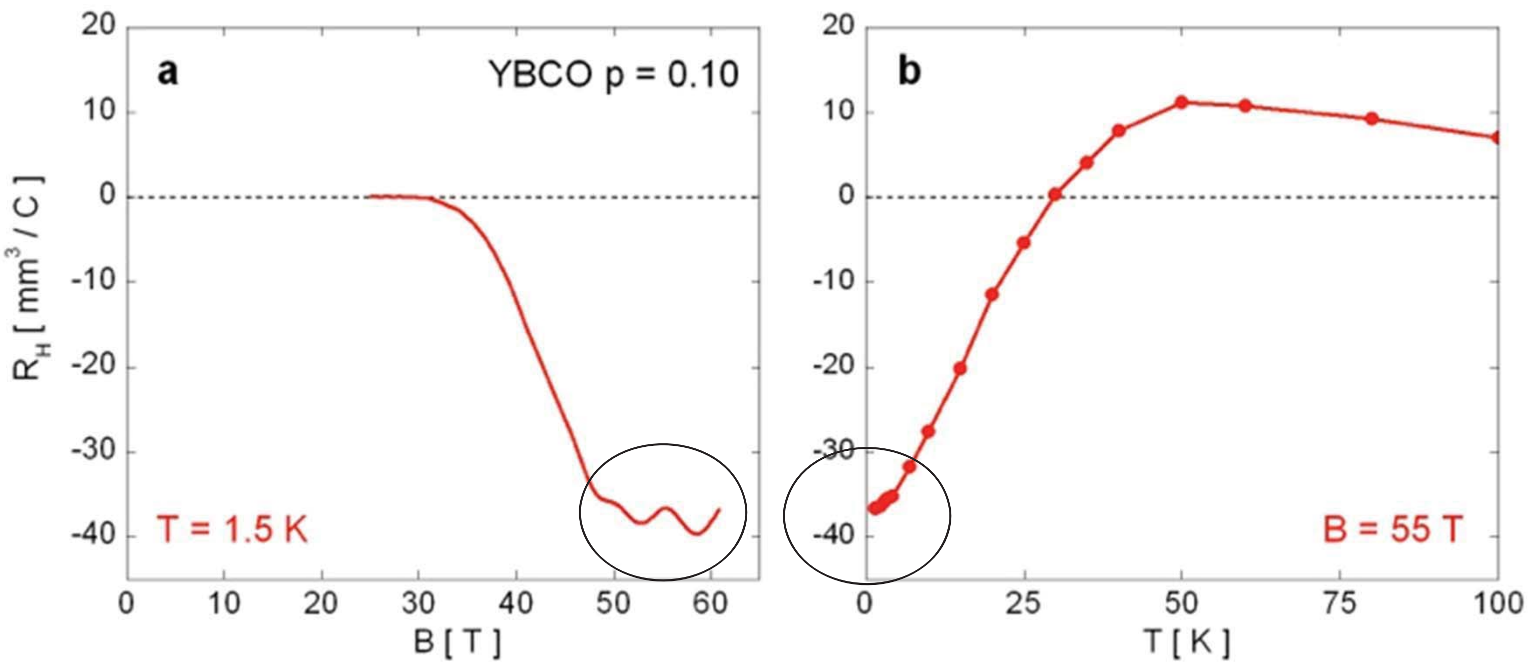
Intra-unit cell nematic order: STM

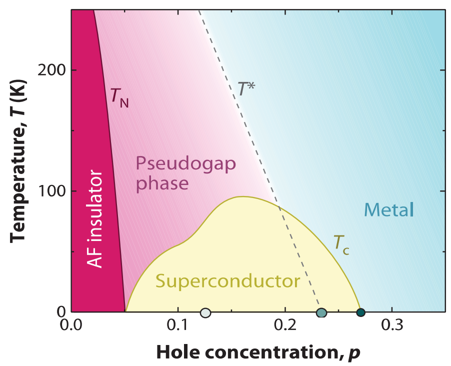


Kohsaka et al. Nature Physics 2012

Quantum oscillations in cuprates: 2007

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



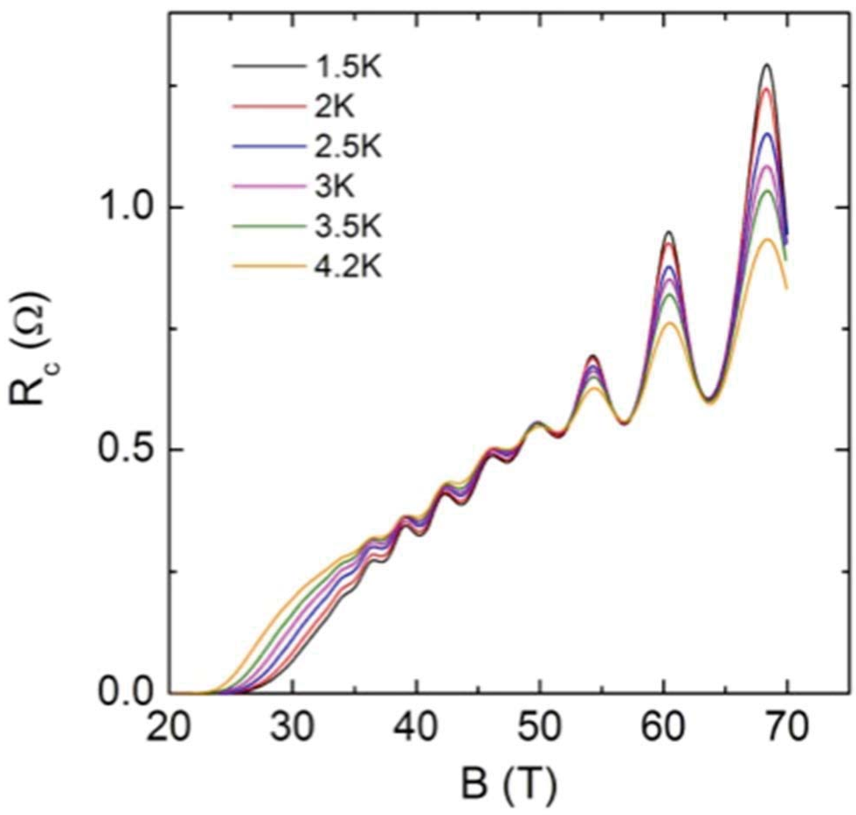


Quantum oscillations $R_H < 0$

Fermi surface includes a small *electron* pocket !

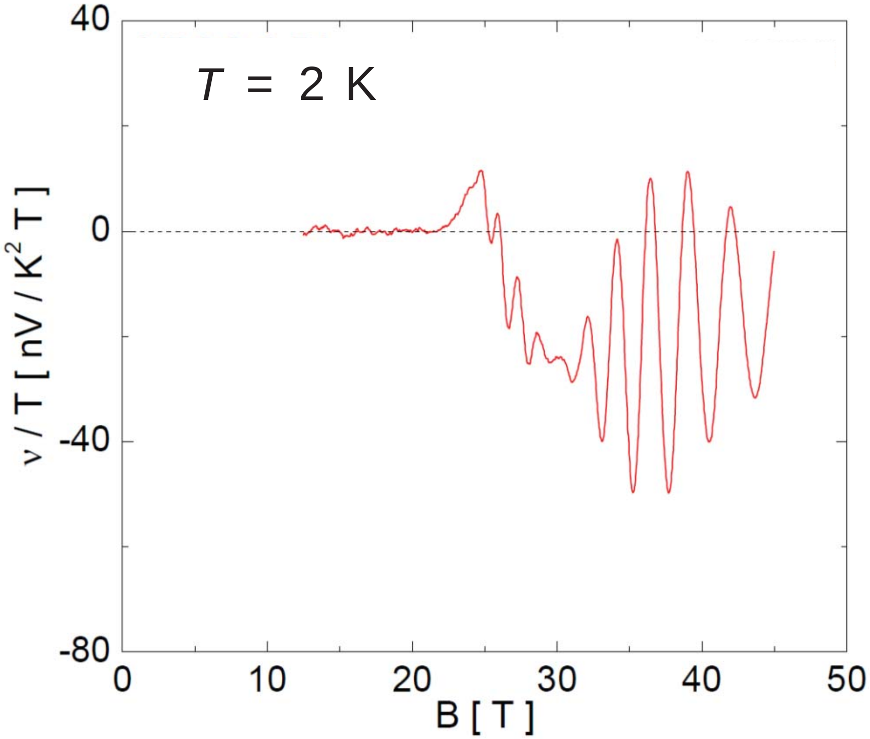
Quantum oscillations in cuprates: 2013

Resistance



LNCMI, Toulouse

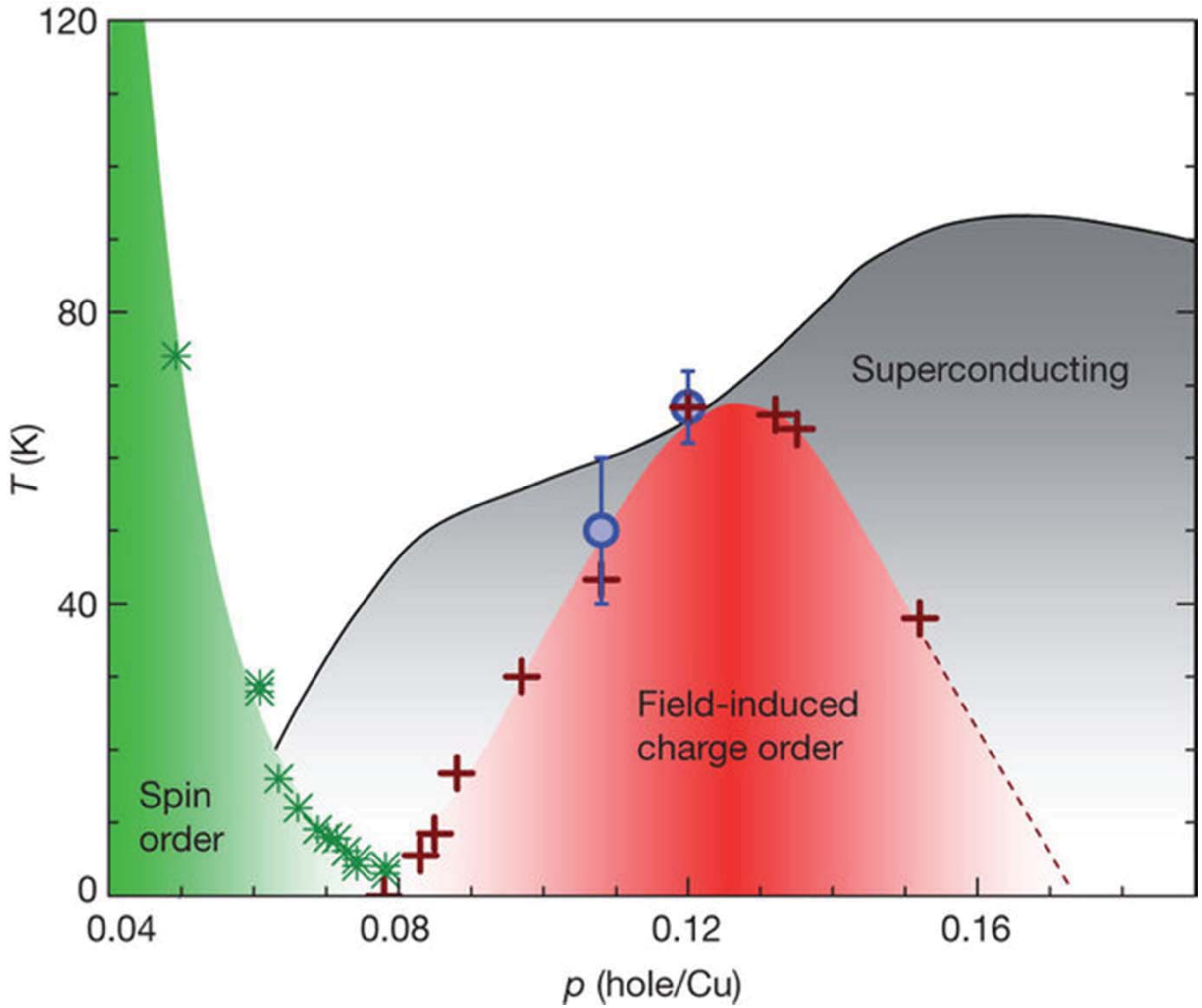
Nernst



NHMFL, Tallahassee

UNIVERSITÉ DE SHERBROOKE

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).

UNIVERSITÉ DE SHERBROOKE

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]

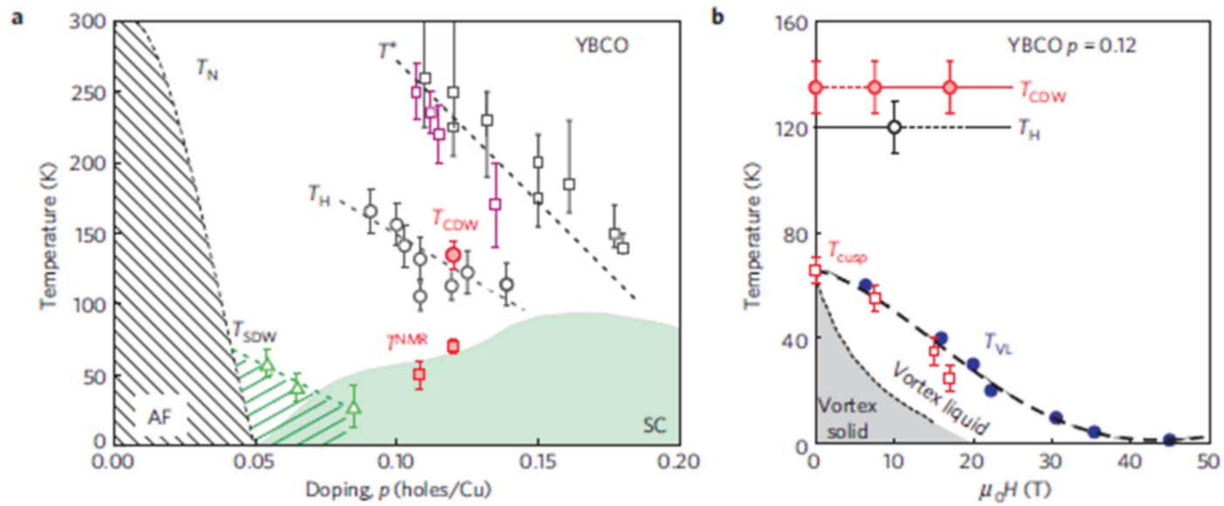
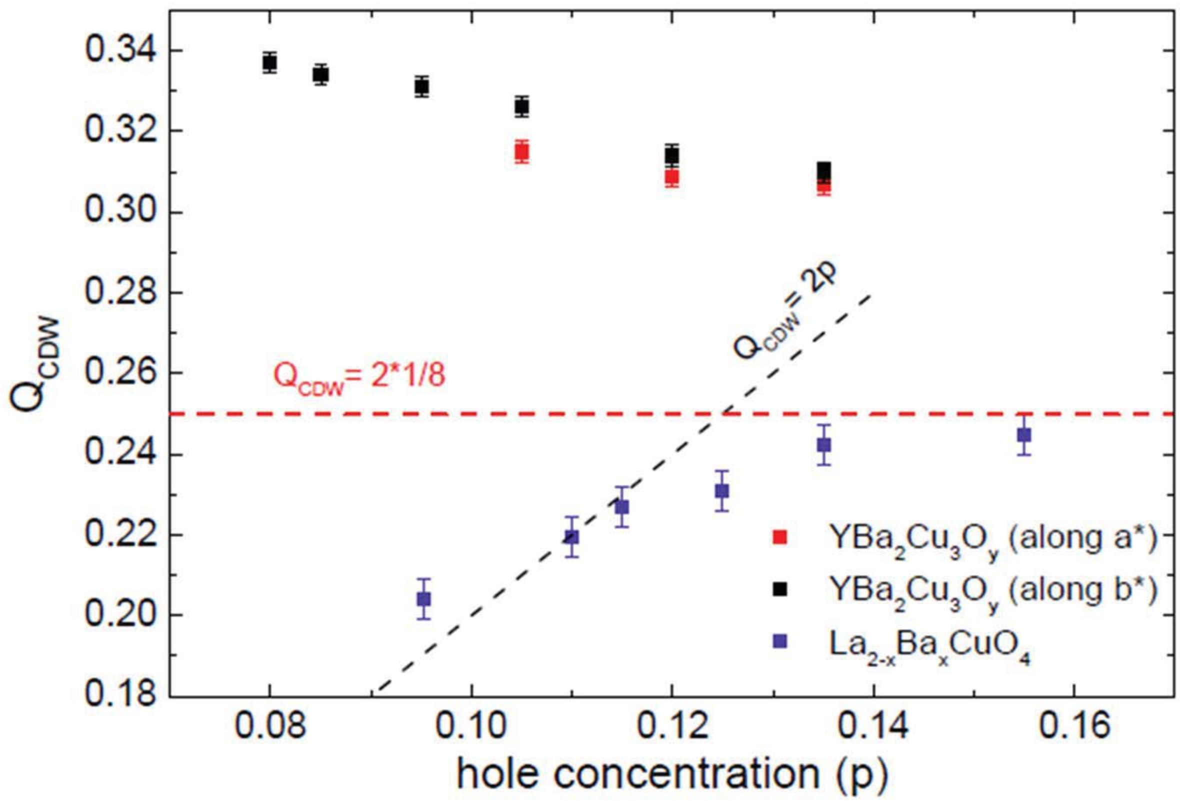


Figure 4 | Phase diagram of $YBa_2Cu_3O_{7-x}$. a, Doping dependence of the antiferromagnetic ordering temperature T_N, the incommensurate spin-density wave order T_{SDW} (green triangles; ref. 21), the superconducting temperature T_c and the pseudogap temperature T^* as determined from the Nernst effect[30]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

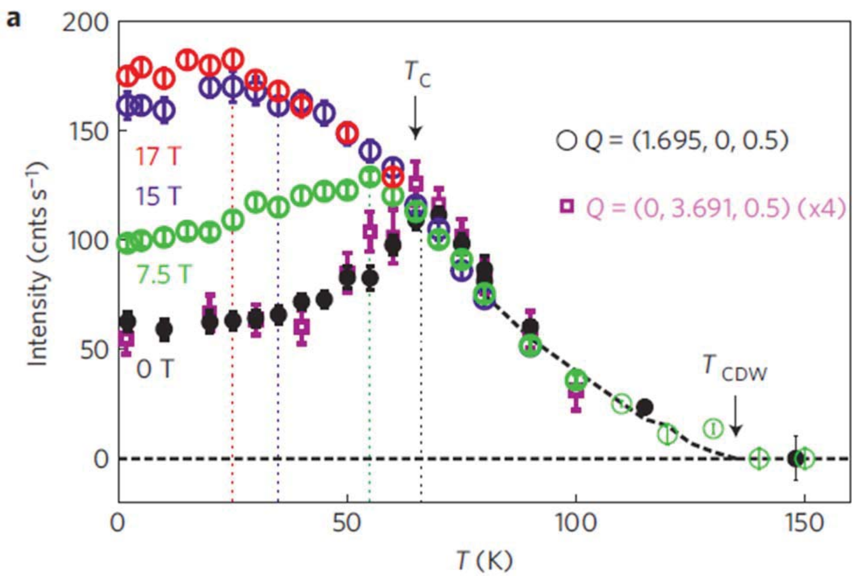
S. Sachdev and R. La Placa Phys. Rev. Lett. **111**, 027202 (2013)
D. Chowdhury, S. Sachdev arxiv. 1501.00002

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

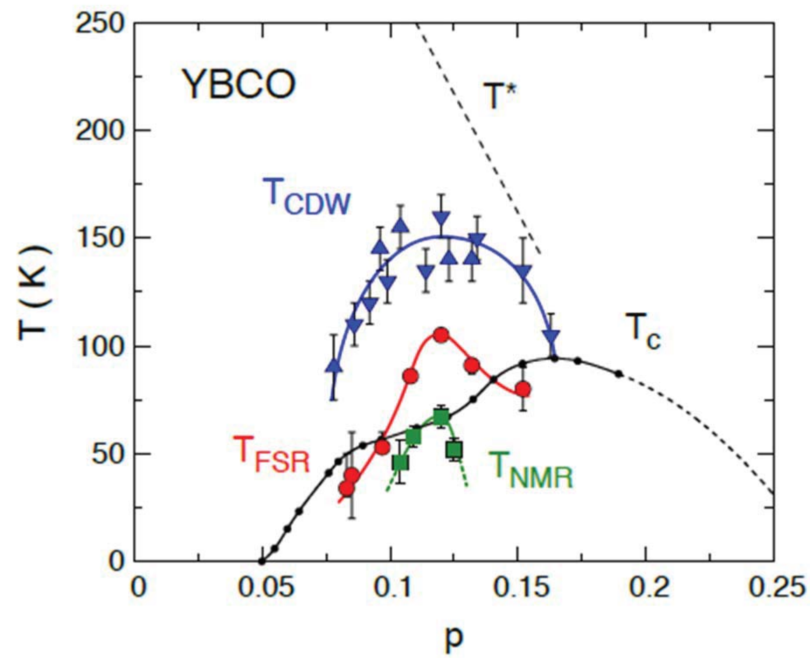
Y. Wang and A. Chubukov, Phys. Rev. B 90, 035149 (2014).

…

Competition between CDW and SC

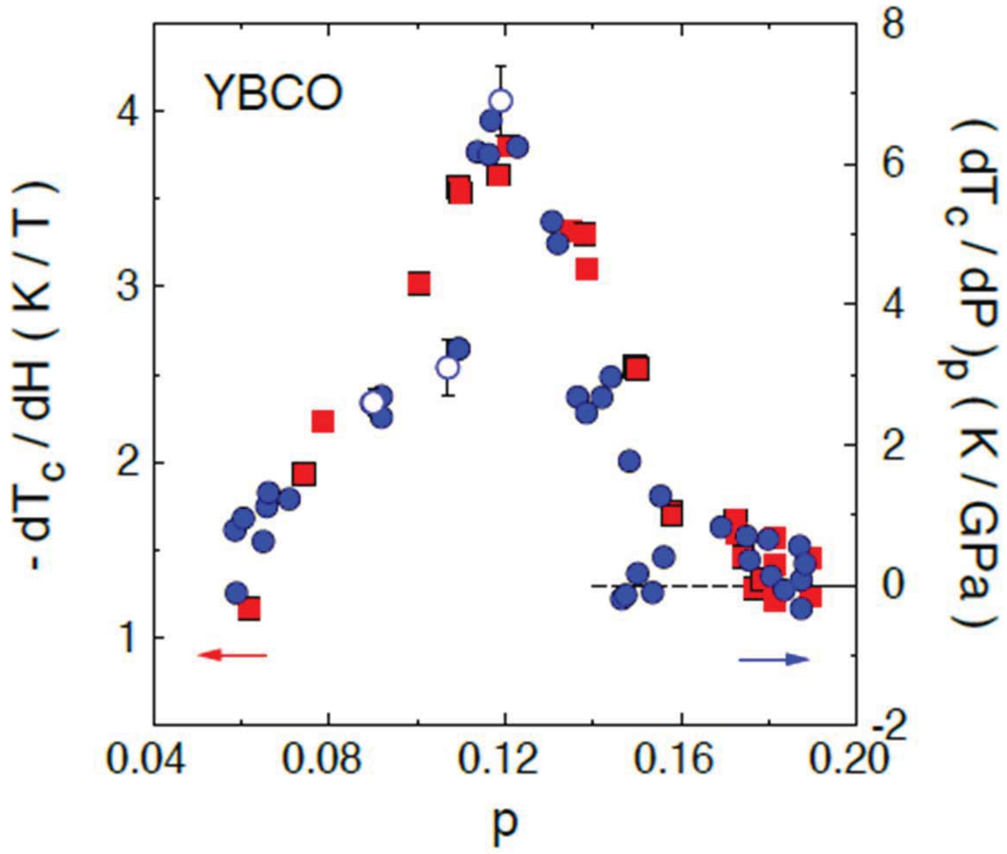


J. Chang *et al.*, *Nat. Phys.* **8**, 871-876 (2012).



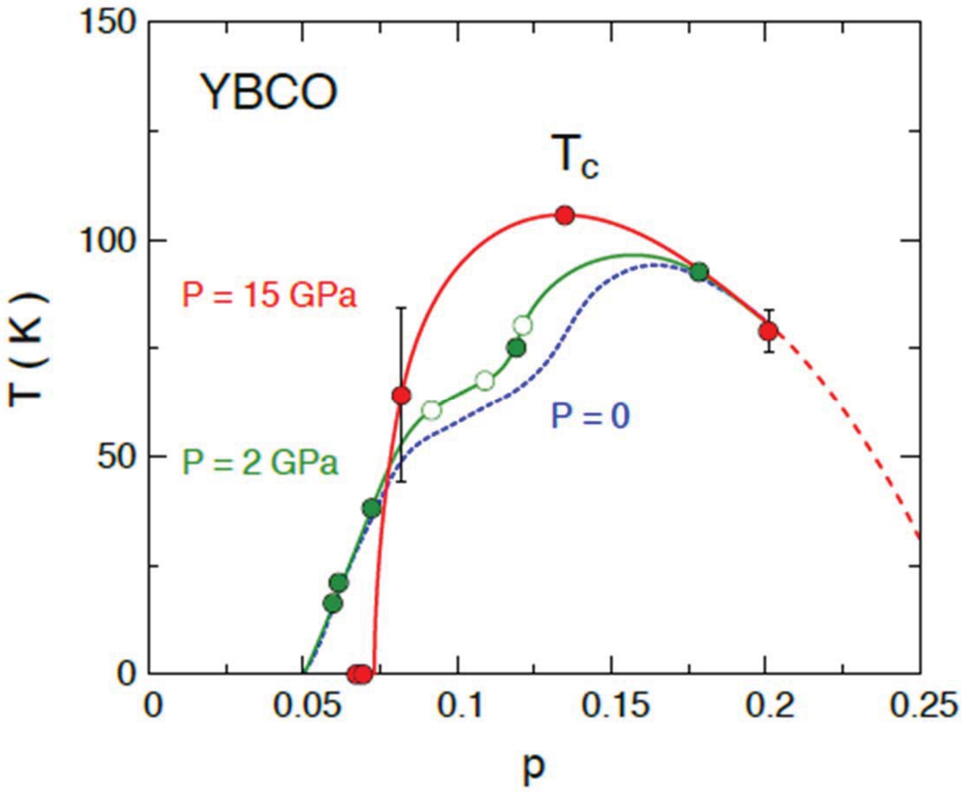
Cyr-Choinière et al, arxiv1503.02033

Tuning SC and CDW



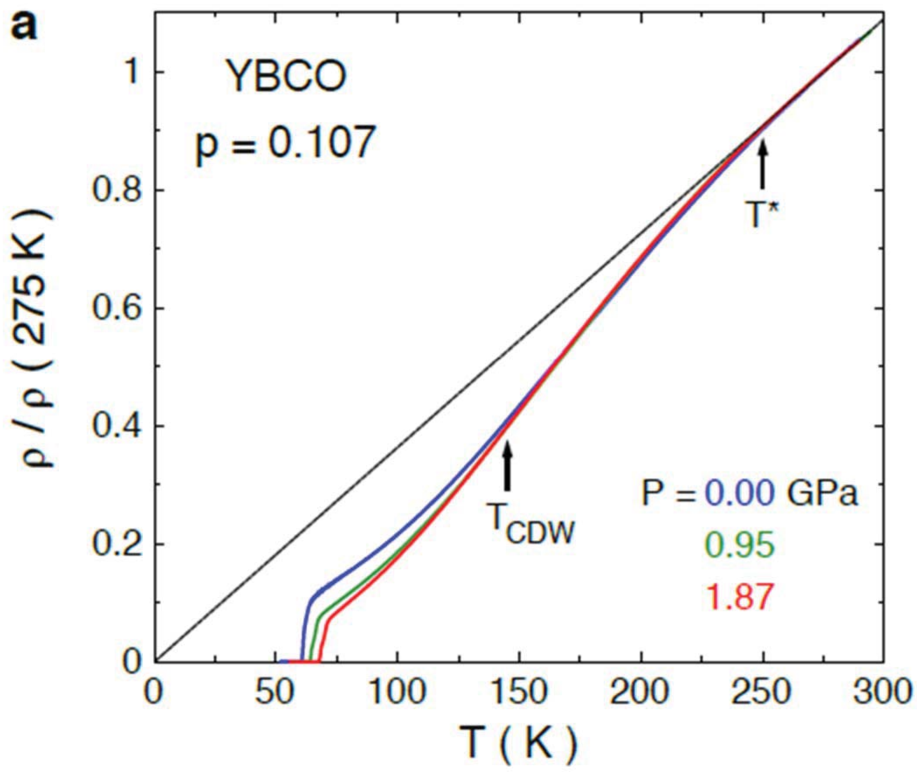
Cyr-Choinière et al, arxiv1503.02033

Getting rid of the CDW



Cyr-Choinière et al, arxiv1503.02033

T* not affected



Cyr-Choinière et al, arxiv1503.02033

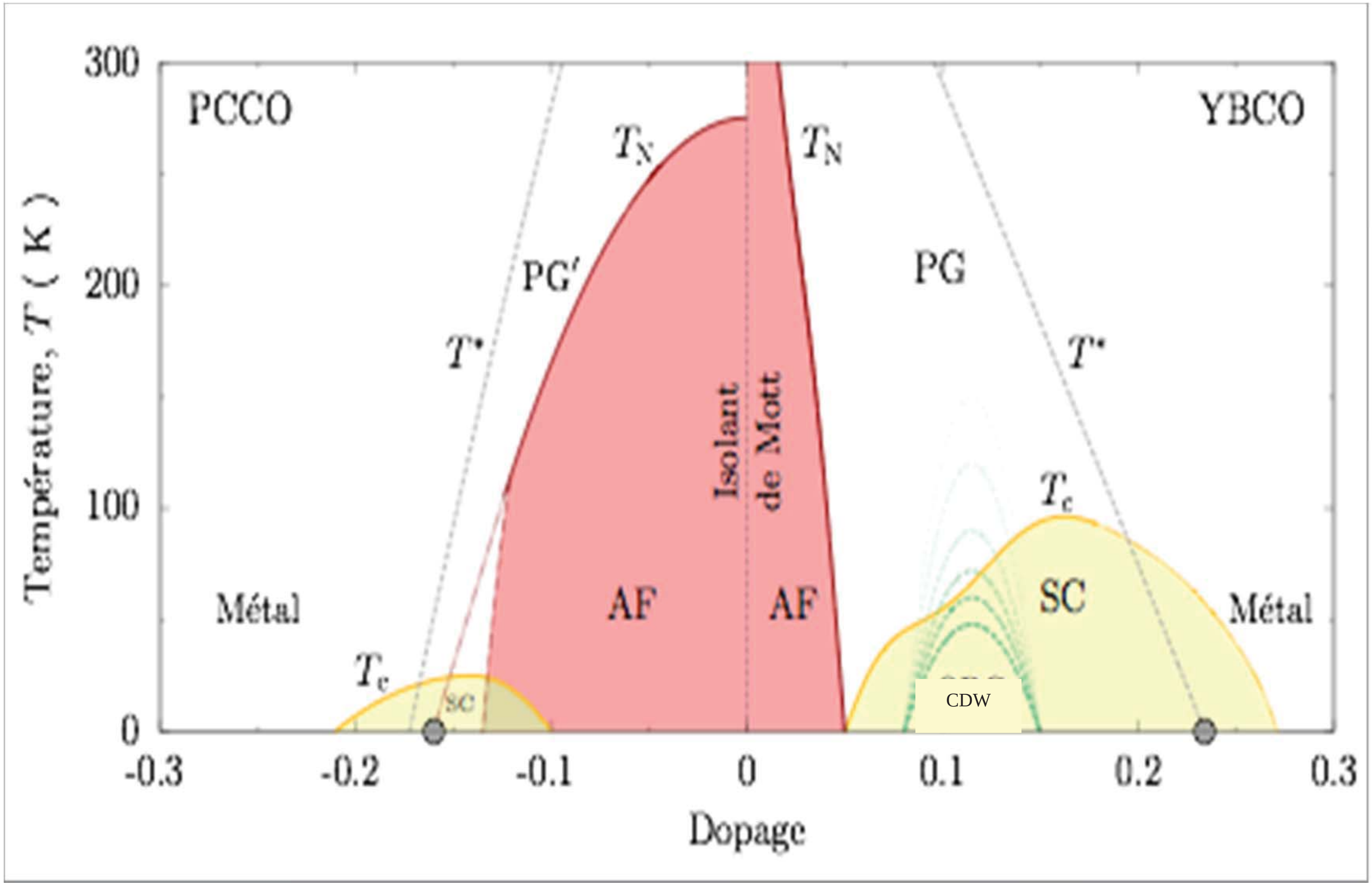
7. Pseudogap

h-doped

UNIVERSITÉ DE SHERBROOKE

Our road map

Thèse de Francis Laliberté,
Université de Sherbrooke



UNIVERSITÉ DE SHERBROOKE

Three classes of mechanisms

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

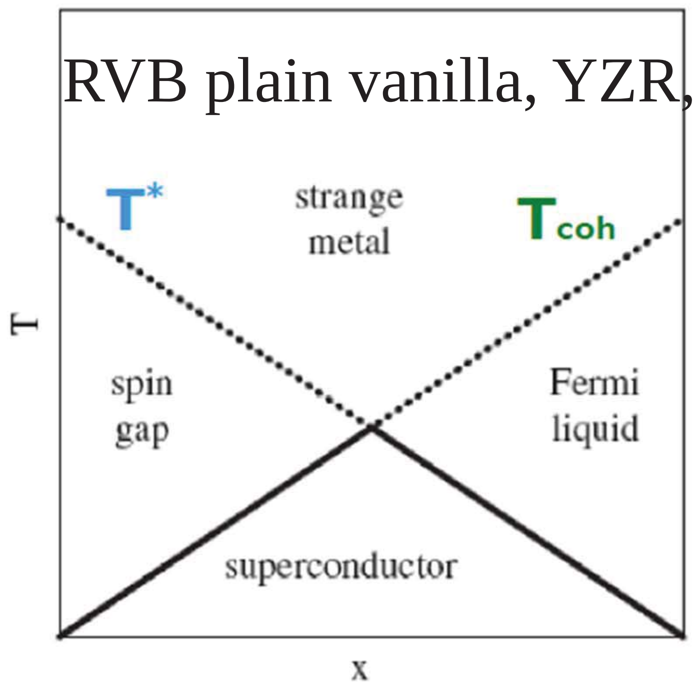
Consider first this Mott hypothesis (Cannot be CDW)

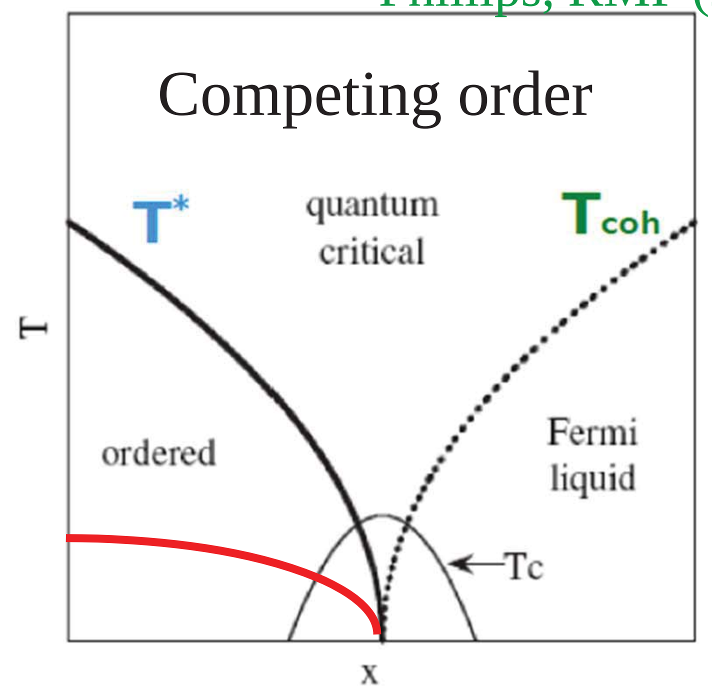
- Competing order
  - Current loops: Varma, PRB **81,** 064515 (2010)
  - Stripes or nematic: Kivelson et al. RMP 75 1201(2003); J.C.Davis
  - d-density wave : Chakravarty, Nayak, Phys. Rev. B **63**, 094503 (2001); Affleck et al. flux phase
  - SDW: Sachdev PRB **80**, 155129 (2009) ...
- Or Mott Physics?
  - RVB: P.A. Lee Rep. Prog. Phys. **71,** 012501 (2008)

UNIVERSITÉ DE SHERBROOKE

Three views (caricature)

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



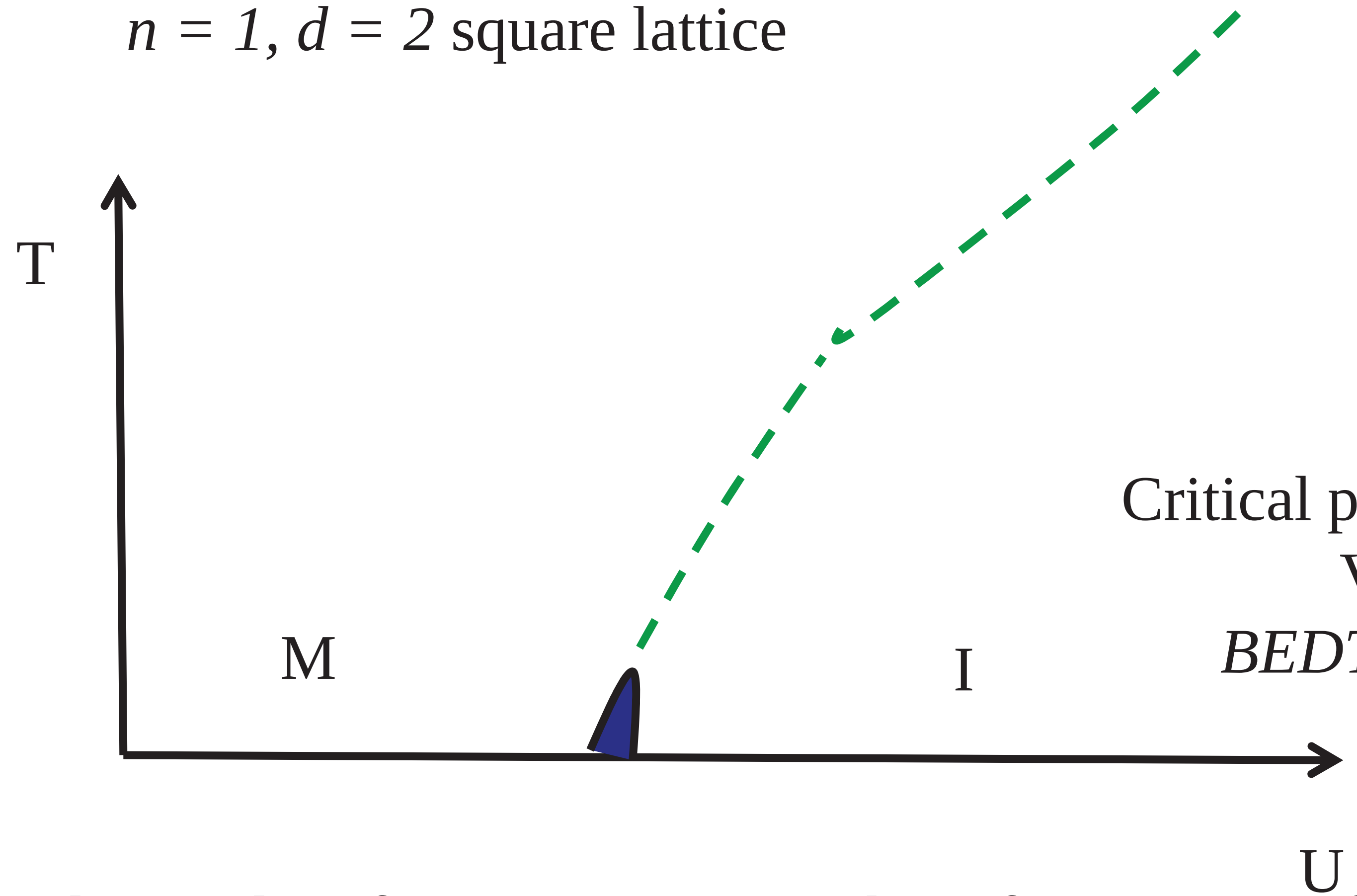


Why T_c decreases?
What is the origin of T^*?
What is the strange metal?

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

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 $T = 0$

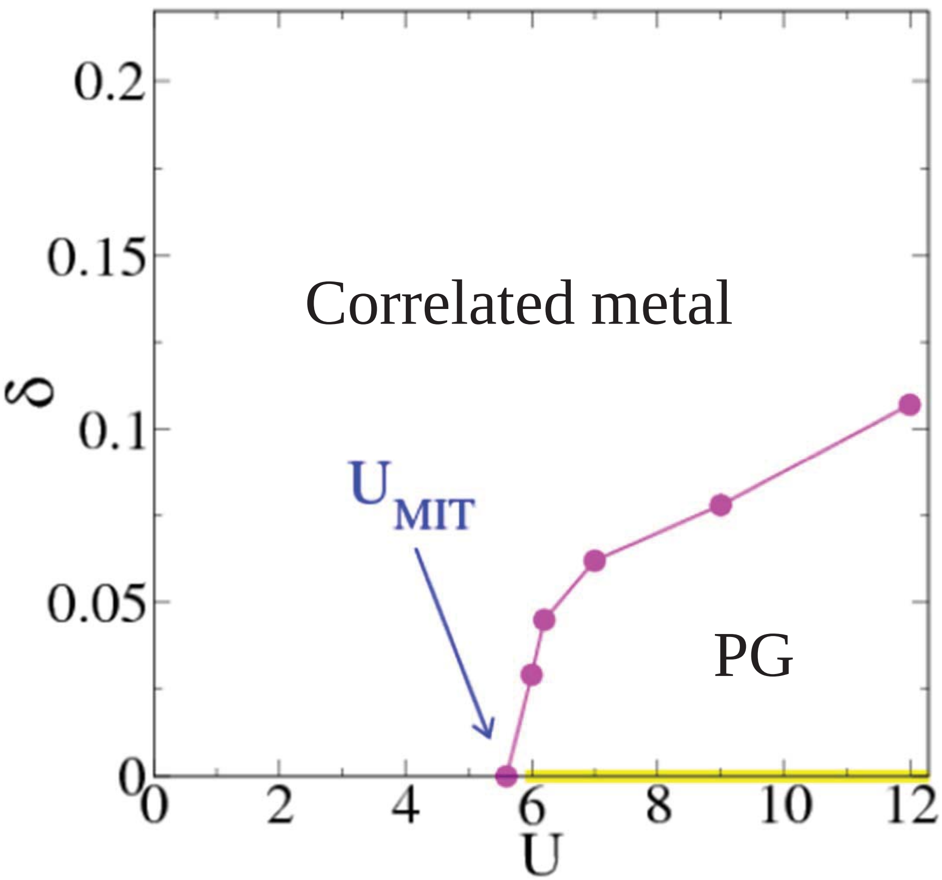
Interaction-induced Mott transition, *n = 1*

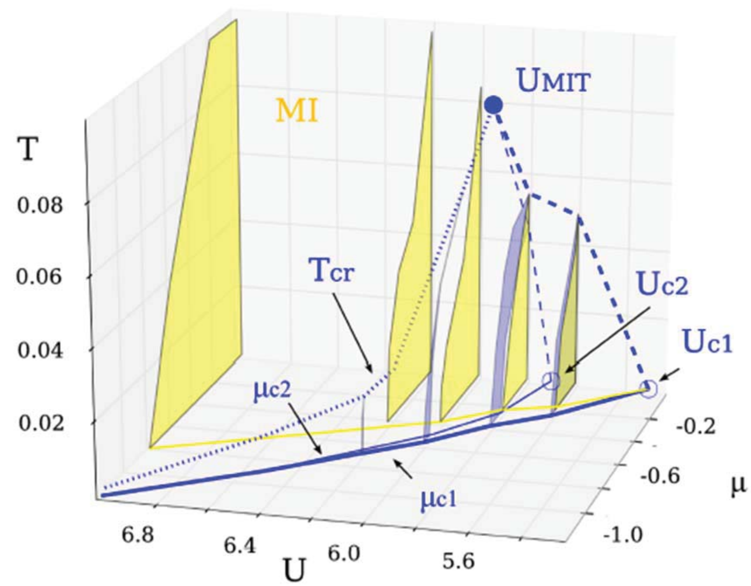
Method	U_{c1}	U_c	U_{c2}	Ref.
VCA+ED 2 x 2 + 8b	5.25	5.5	6.37	Balzer et al. EPL (2009)
CDMFT+CTQMC+H 2 x 2	5.3		5.7	Park et al. PRL (2008)
DCA+CTQMC+H 8	5.7		6.4	Gull et al. cond-mat (2009)
DCA+CTQMC+H 4	!	~4.2	!	Gull et al. EPL (2008)
Dual fermions	!	~6.5	!	Hafermann et al. (2008)
CDMFT+ED 2 x 2 + 8b 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)

UNIVERSITÉ DE SHERBROOKE

Link to Mott transition up to optimal doping

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

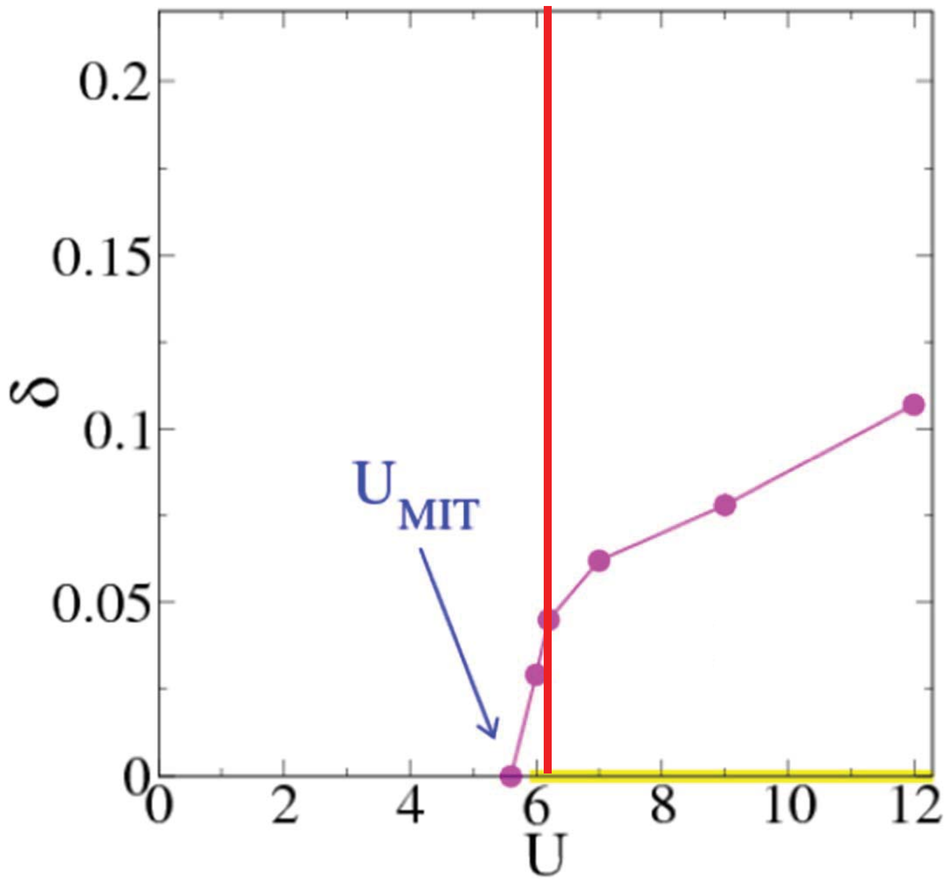


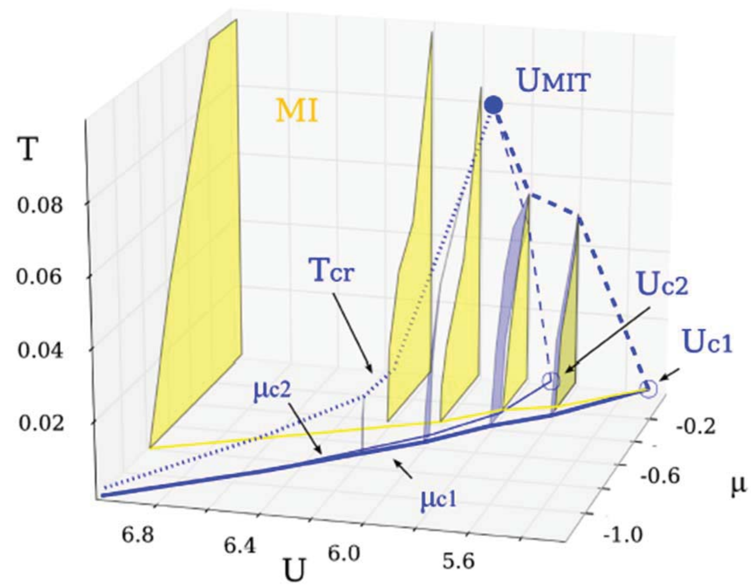


Sordi et al. PRL 2010, PRB 2011

Link to Mott transition up to optimal doping
Another emergent transition

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

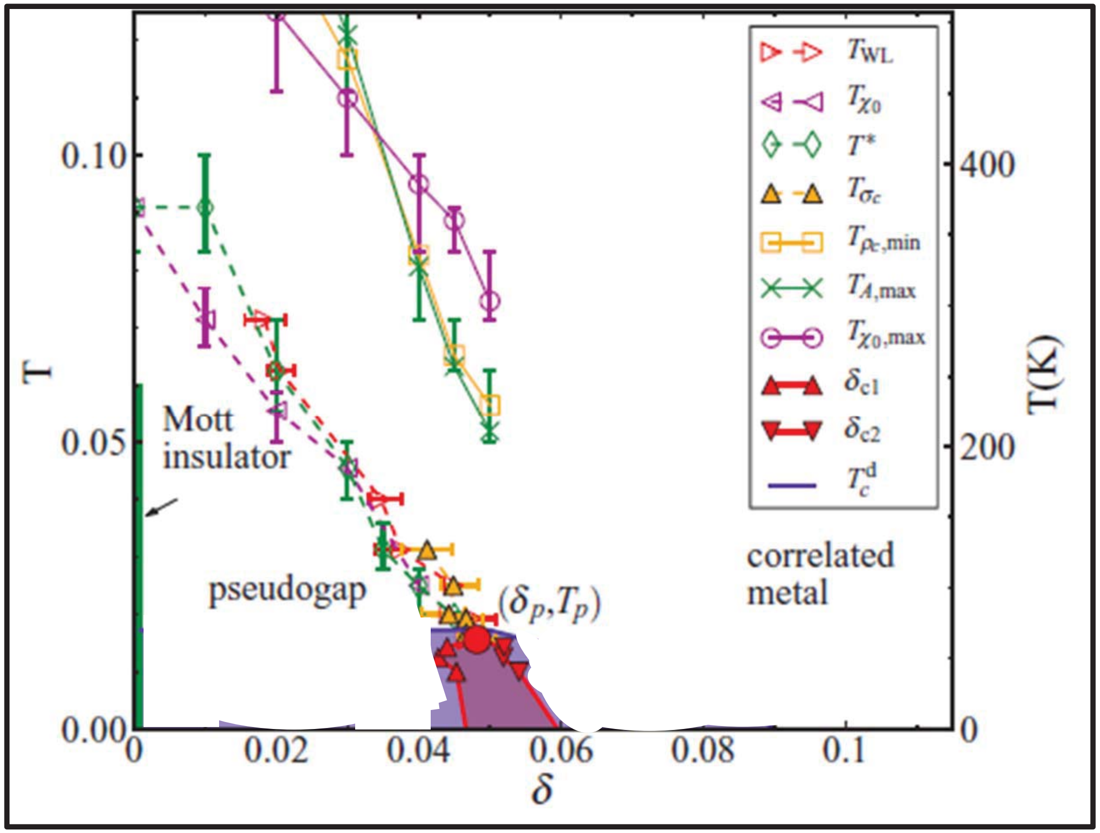




Smaller *D* and *S*

UNIVERSITÉ DE SHERBROOKE

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)

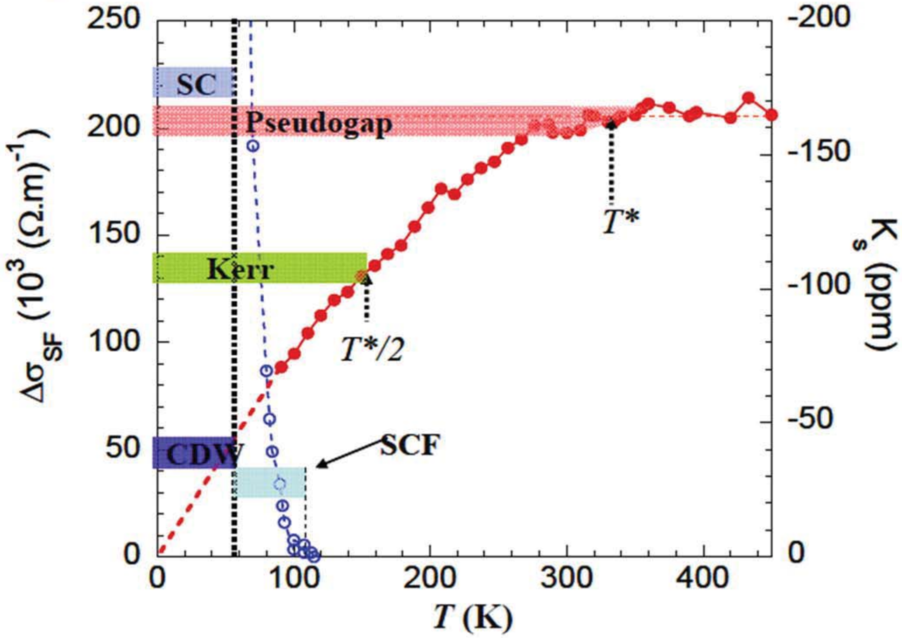
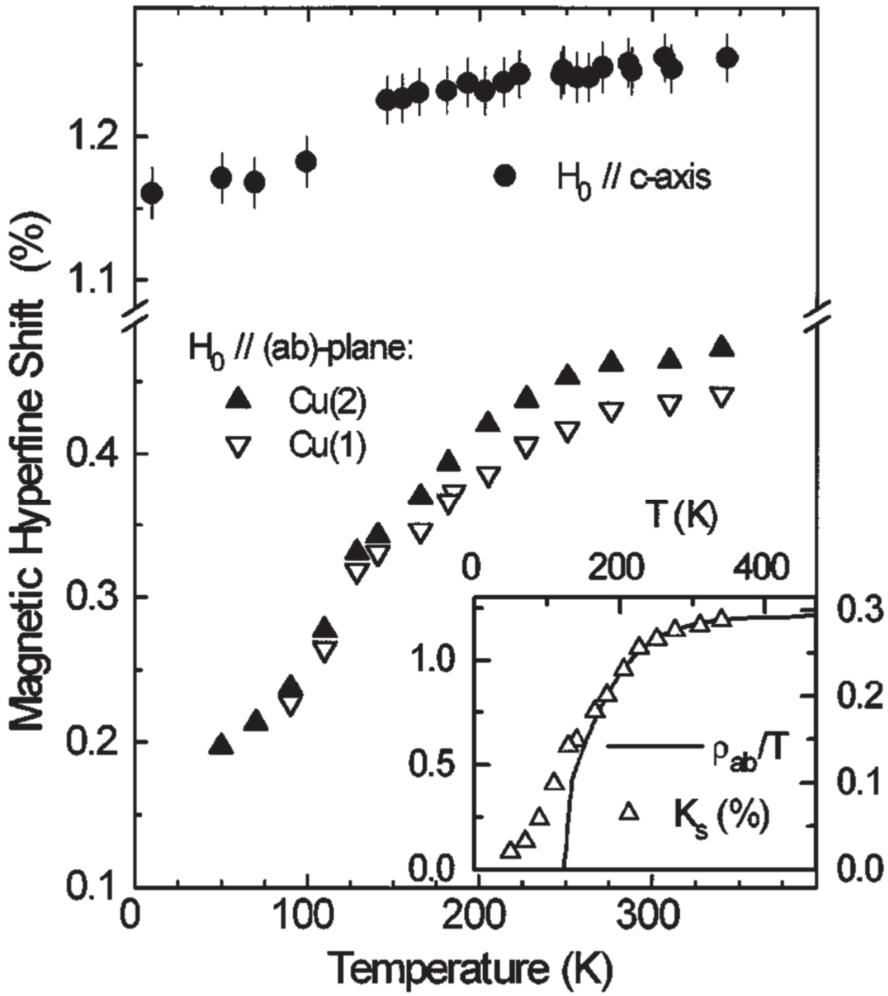


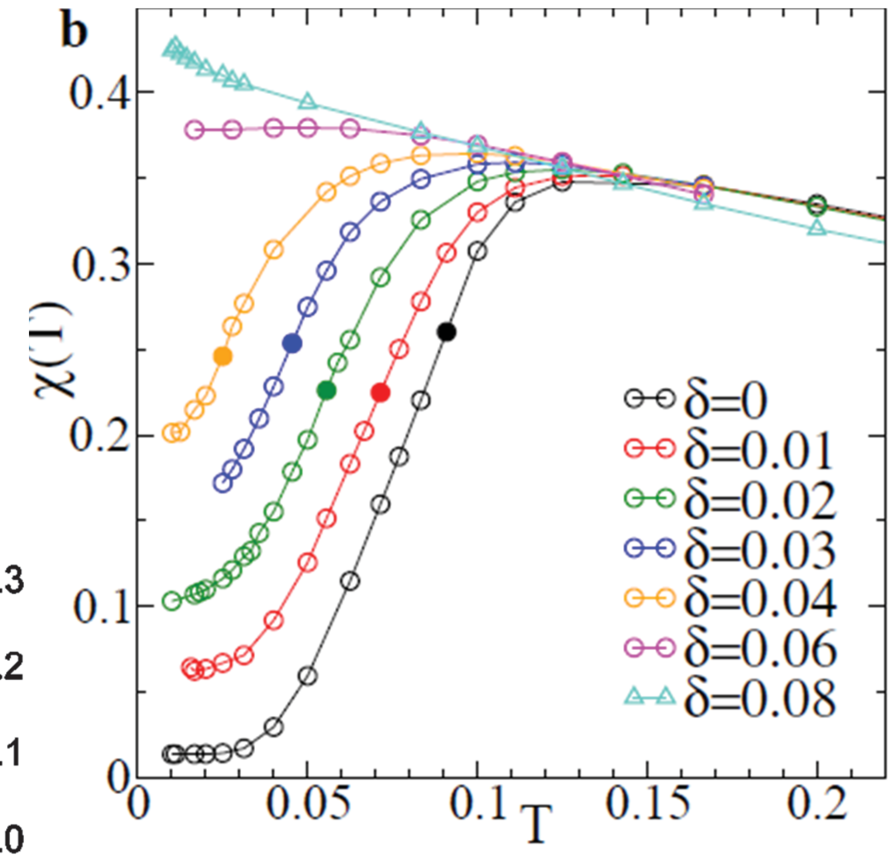
Fig 1 Spin contribution K_s to the ^{89}Y NMR Knight shift [11] for $YBCO_{6.6}$ permit to define the PG onset T^*. Here K_s is reduced by a factor two at $T\sim T^*/2$. The sharp drop of the SC fluctuation conductivity (SCF) is illustrated (left scale) [23]. We report as well the range over which a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

Spin susceptibility



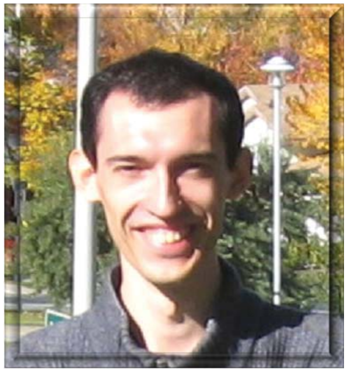
Underdoped Hg1223

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



Sordi et al. Scientific Repts. 2012

UNIVERSITÉ DE SHERBROOKE



Giovanni Sordi

Patrick Sémon

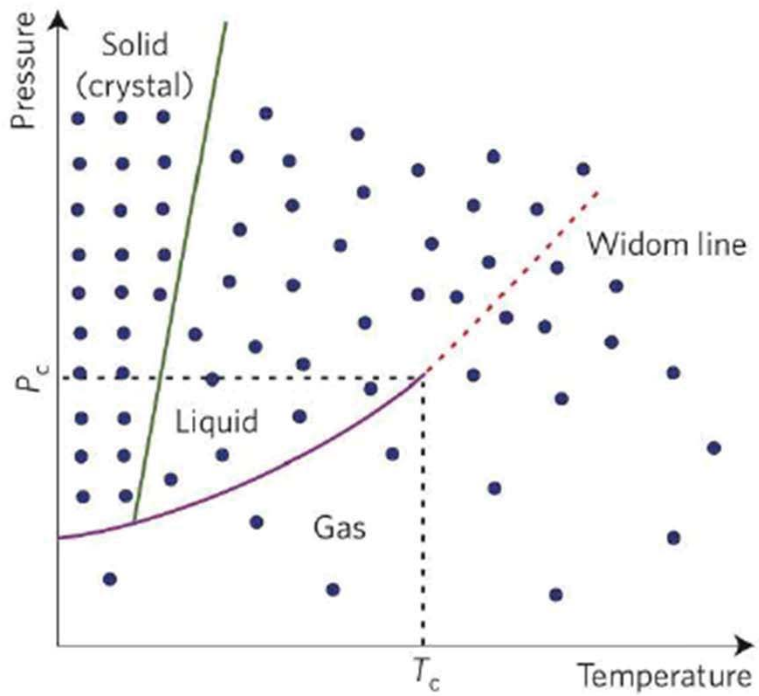
Kristjan Haule

The Widom line

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

UNIVERSITÉ DE SHERBROOKE

What is the Widom line?



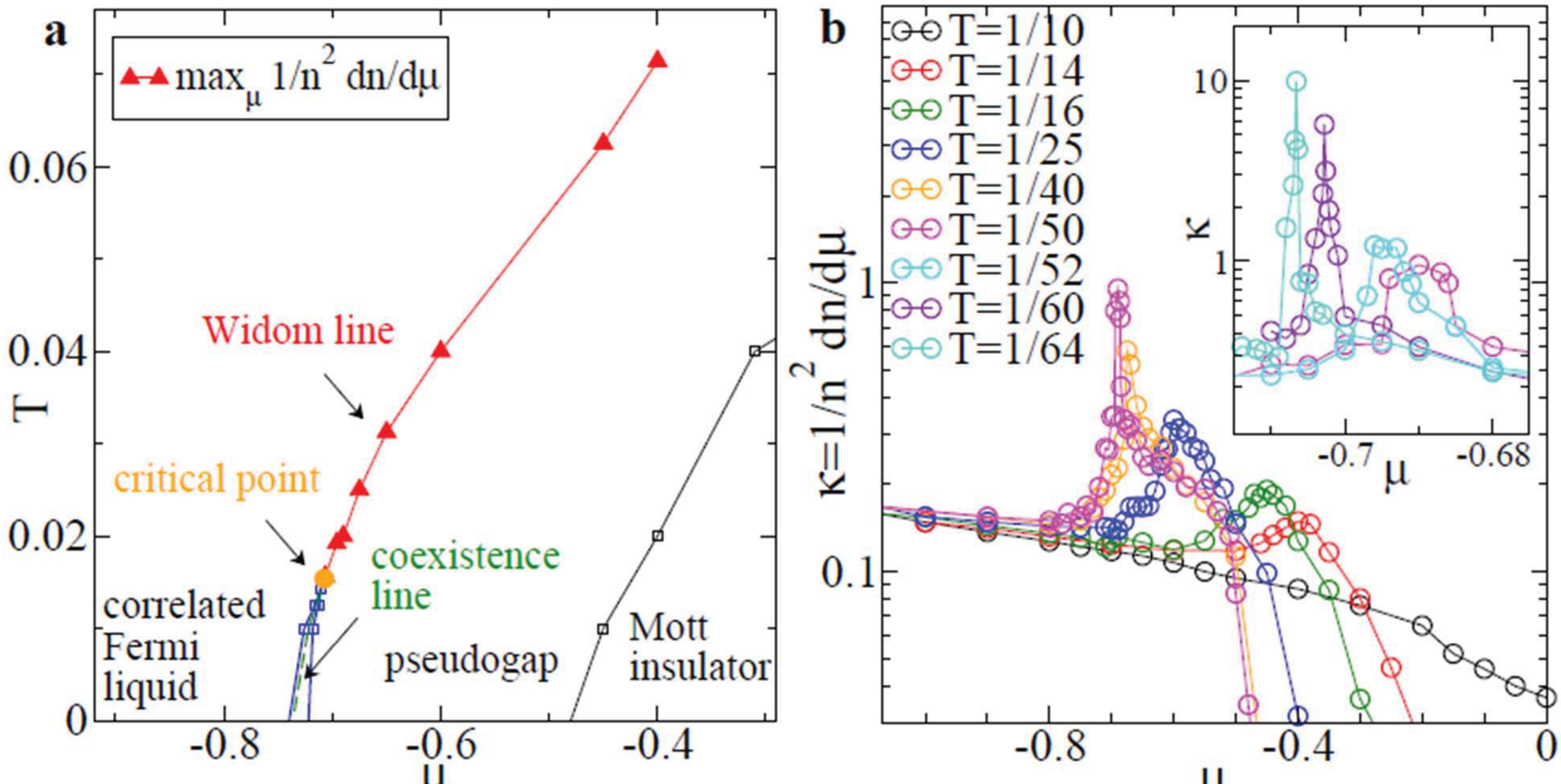
McMillan and Stanley, Nat Phys 2010

- 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

UNIVERSITÉ DE SHERBROOKE

Pseudogap along the Widom line



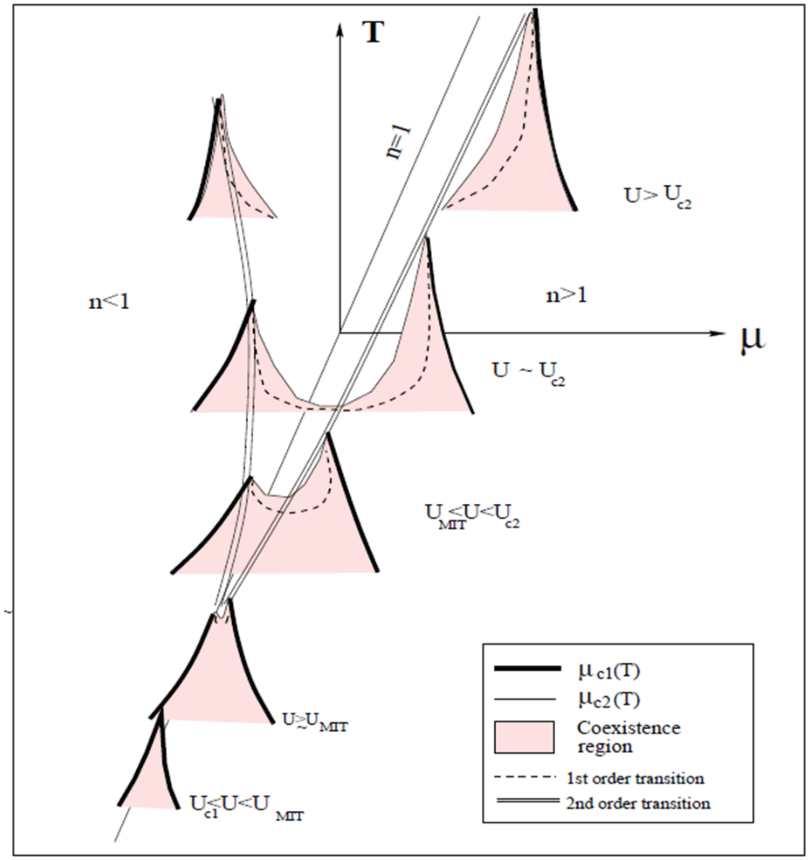
Widom line: defined from maxima of charge compressibility

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

divergence of κ at the (classical) critical point!

UNIVERSITÉ DE SHERBROOKE

Compressibility divergence at Mott and coexistence



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

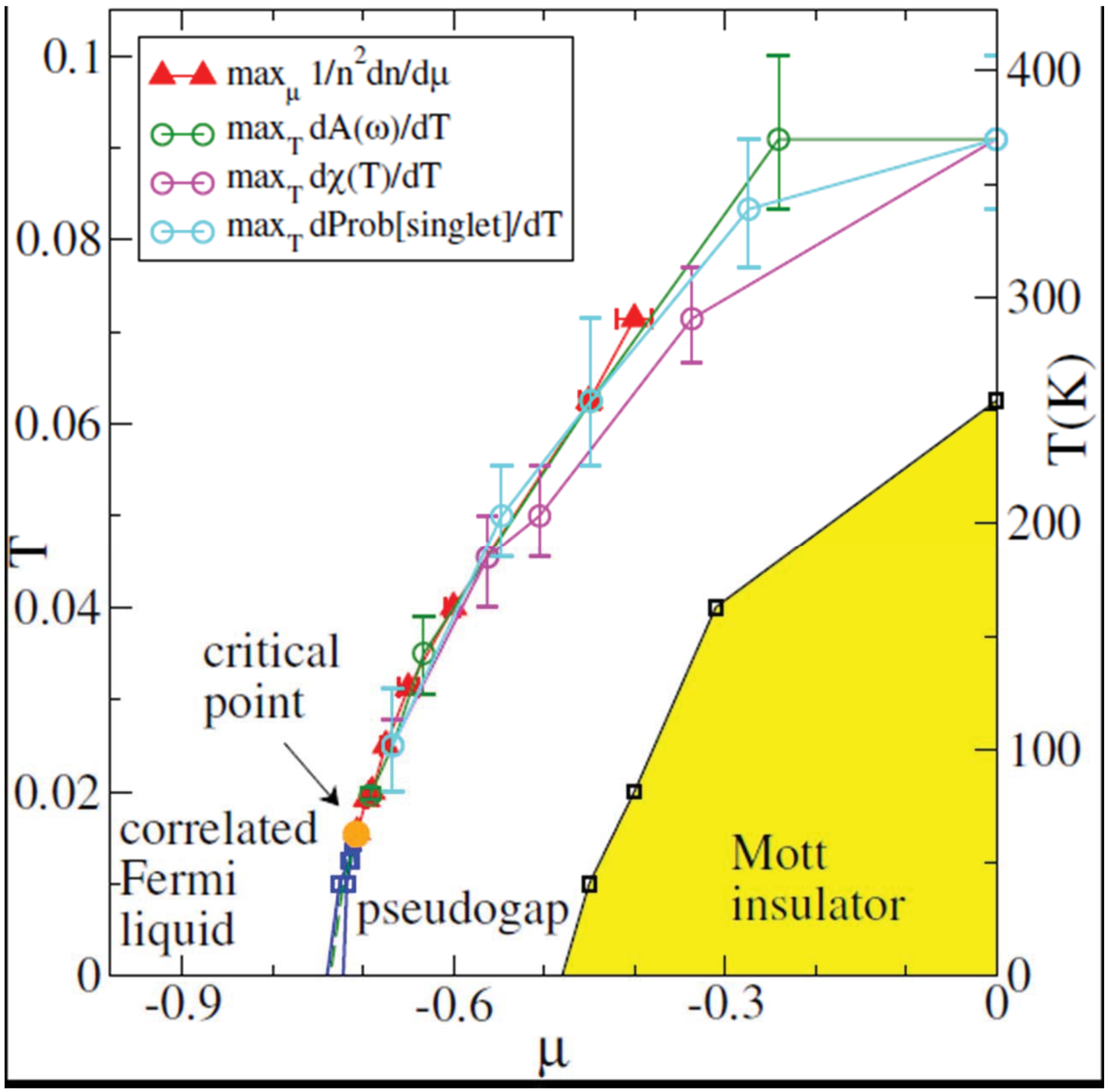
S. Murthy, Rutgers thesis 2004

K. Frikach, M. Poirier, et al. PRB **61**, R6491 (2000).
S. R. Hassan, A. Georges, and H. R. Krishnamurthy PRL **94**, 036402 (2005)

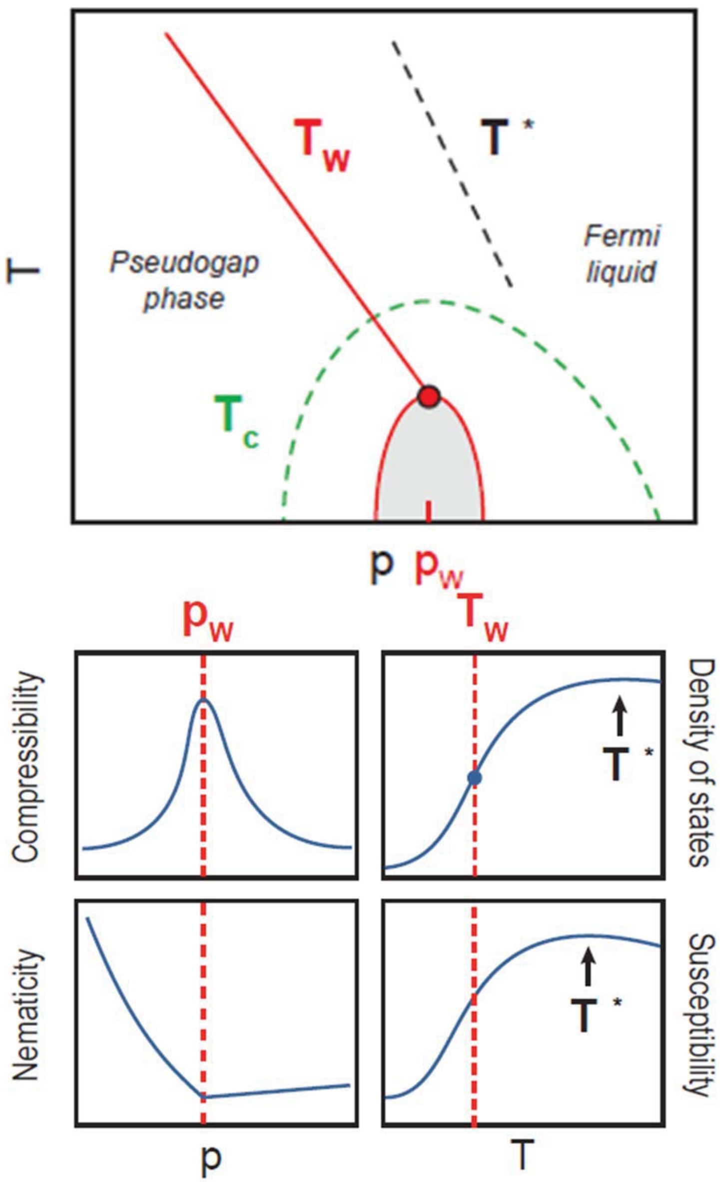
Figure 2.19: Schematic phase diagram for the 2-band case. There is an asymmetry in the triangular peaks as compared to the 1-band case. The cross sections are on the $T-\mu$ plane for different values of U as before. μ_{c1} and U_{c1} are the chemical potential and

UNIVERSITÉ DE SHERBROOKE

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?

3 measurements: Kerr, ARPES, TRR

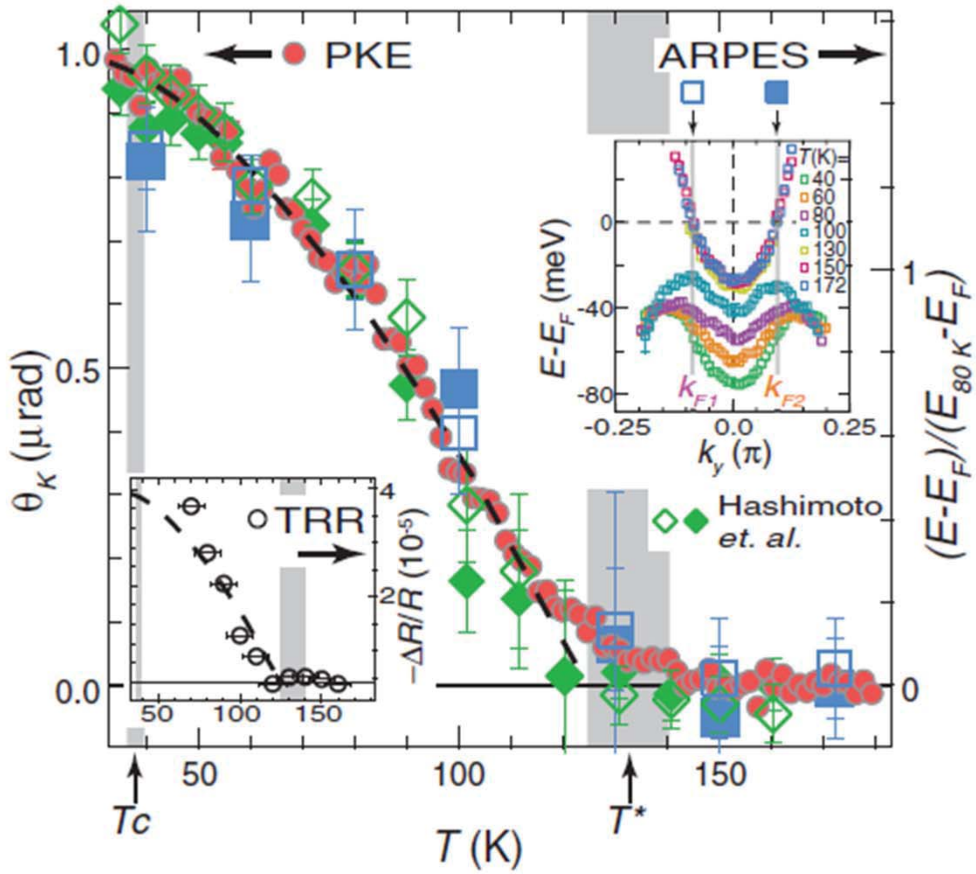
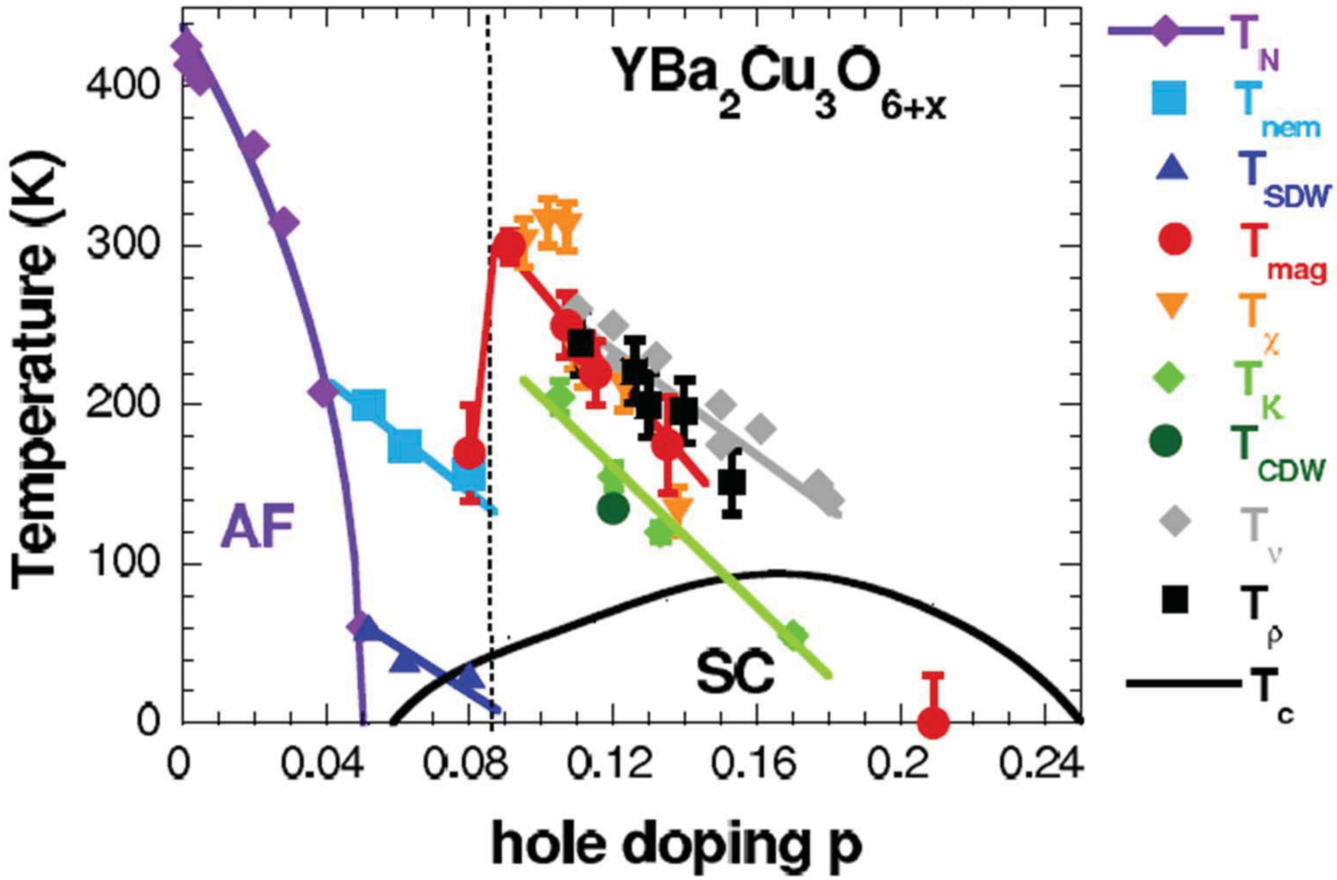


Fig. 3. Temperature dependence of Kerr rotation (θ_K) measured by PKE, in comparison with that of the binding energy position of the EDC maximum at k_F given by ARPES [reproduced from fig. S1F and (*29*)]. ARPES results are normalized to the 80 K values (free from the interference of fluctuating superconductivity). 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.

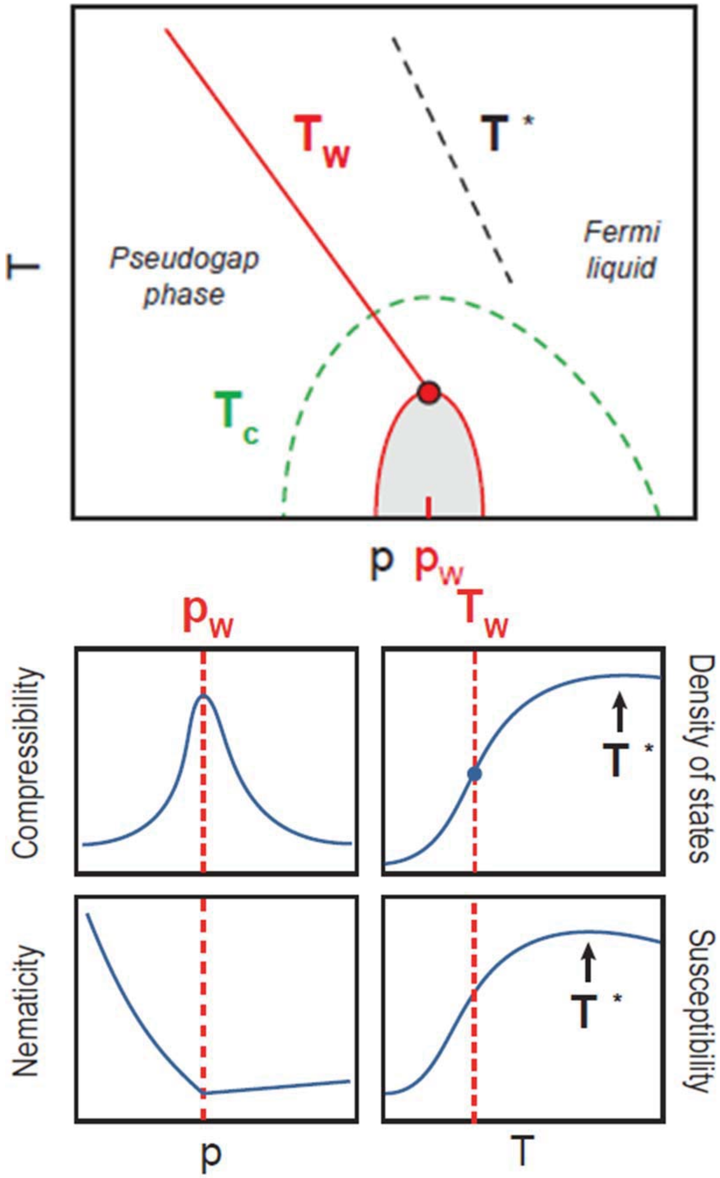
He et al, Science 2011, on Bi 2201

Intra-Unit-Cell loop order



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

An alternate point of view : next lecture



- - 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?

UNIVERSITÉ DE SHERBROOKE

Organics

Pseudogap

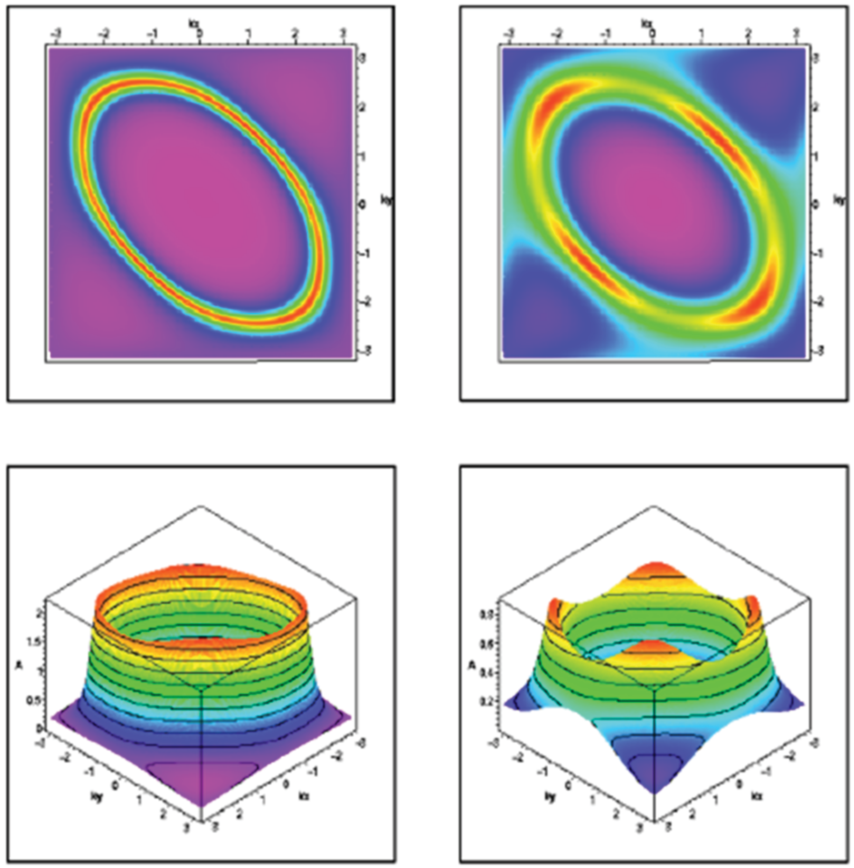
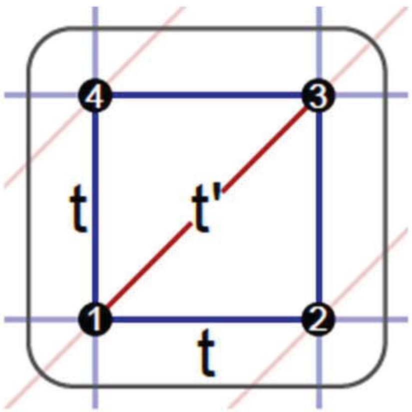


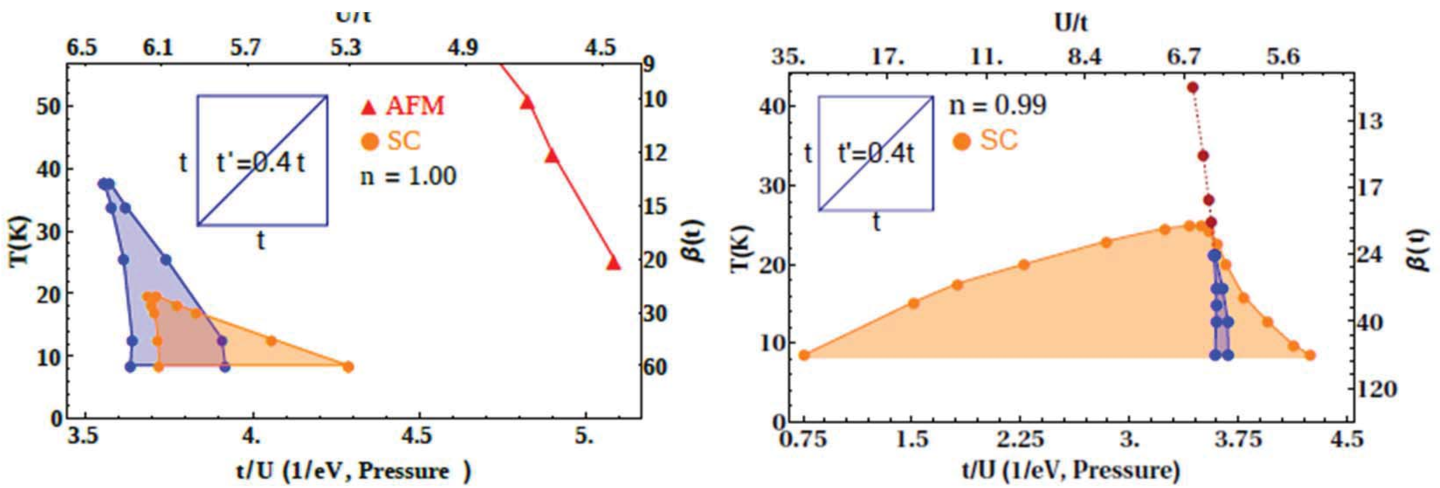
FIG. 4 (color online). Distribution of low energy spectral weight in k space $A(k, \omega = 0)$ for $T/D = 1/44$, $U/D = 2.0$ (left-hand panel) and $U/D = 2.25$ (right-hand panel). The top panels are color plots to see the Fermi surface and the bottom panels are 3D plots to see the variation of A. For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

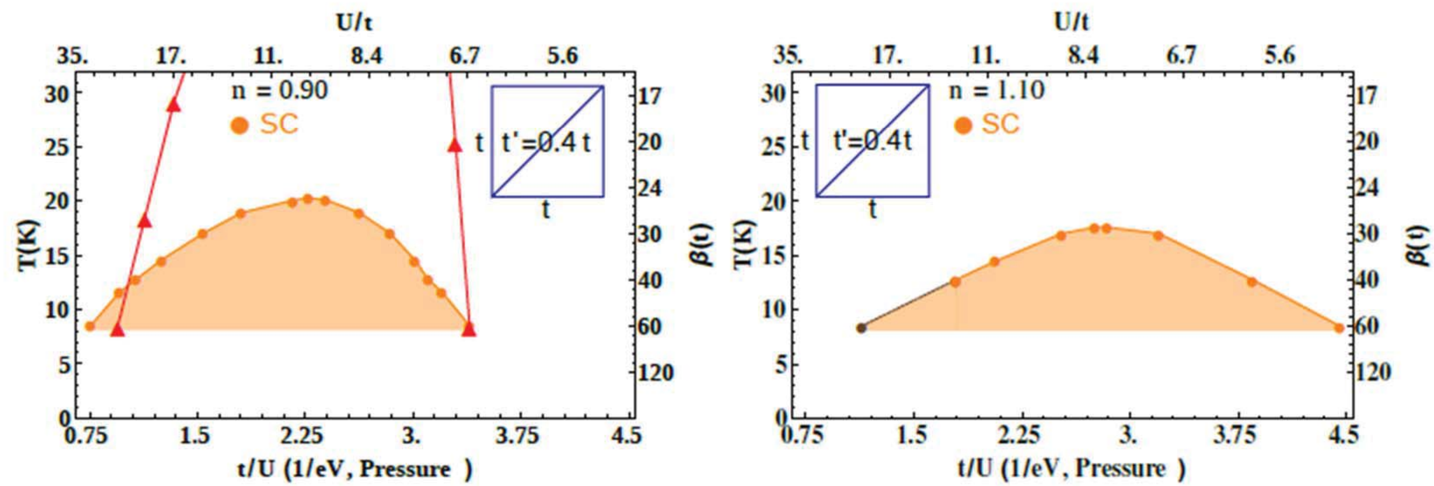
UNIVERSITÉ DE SHERBROOKE

t'=0.4t





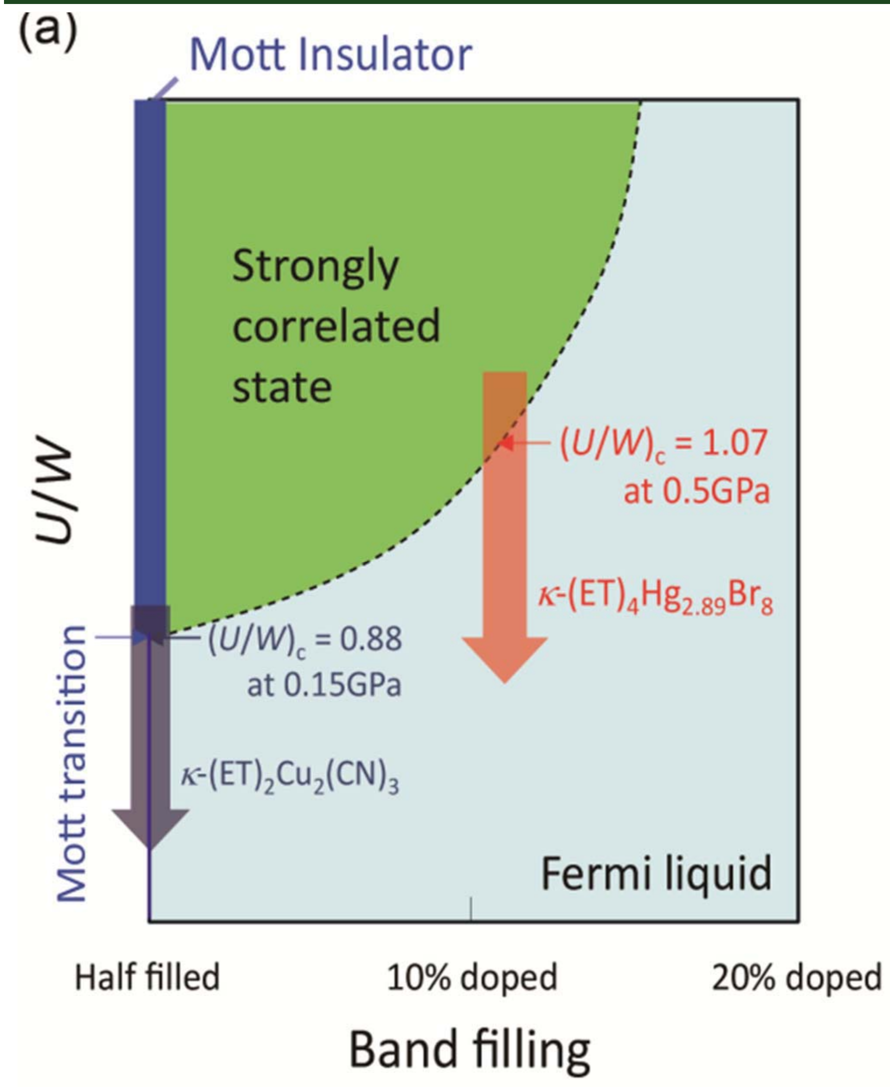
(a) (b)

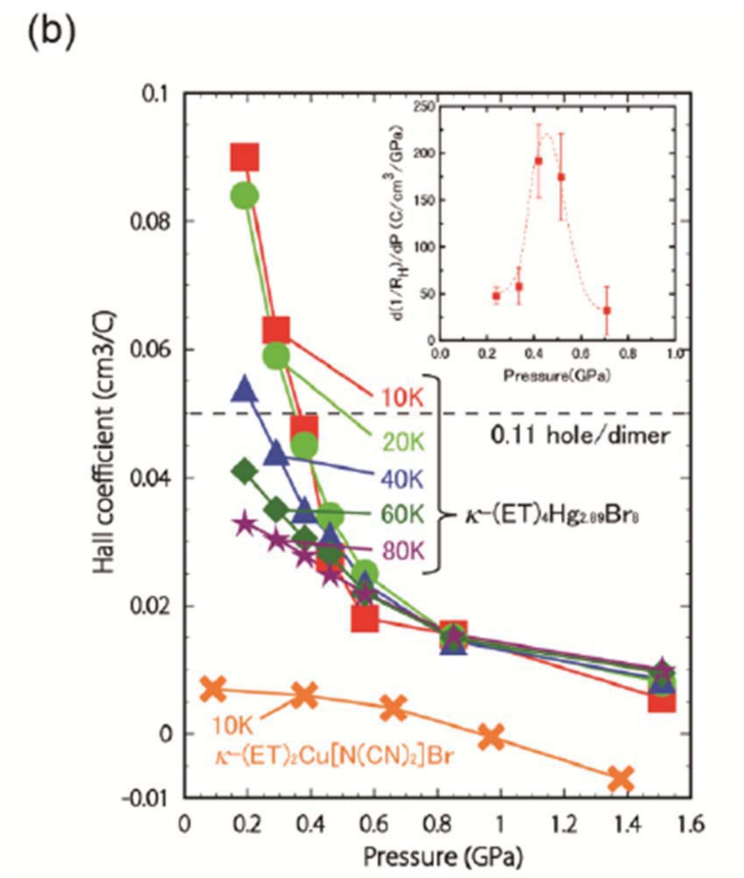


Charles-David Hébert, Patrick Sémon , AMT

UNIVERSITÉ DE SHERBROOKE

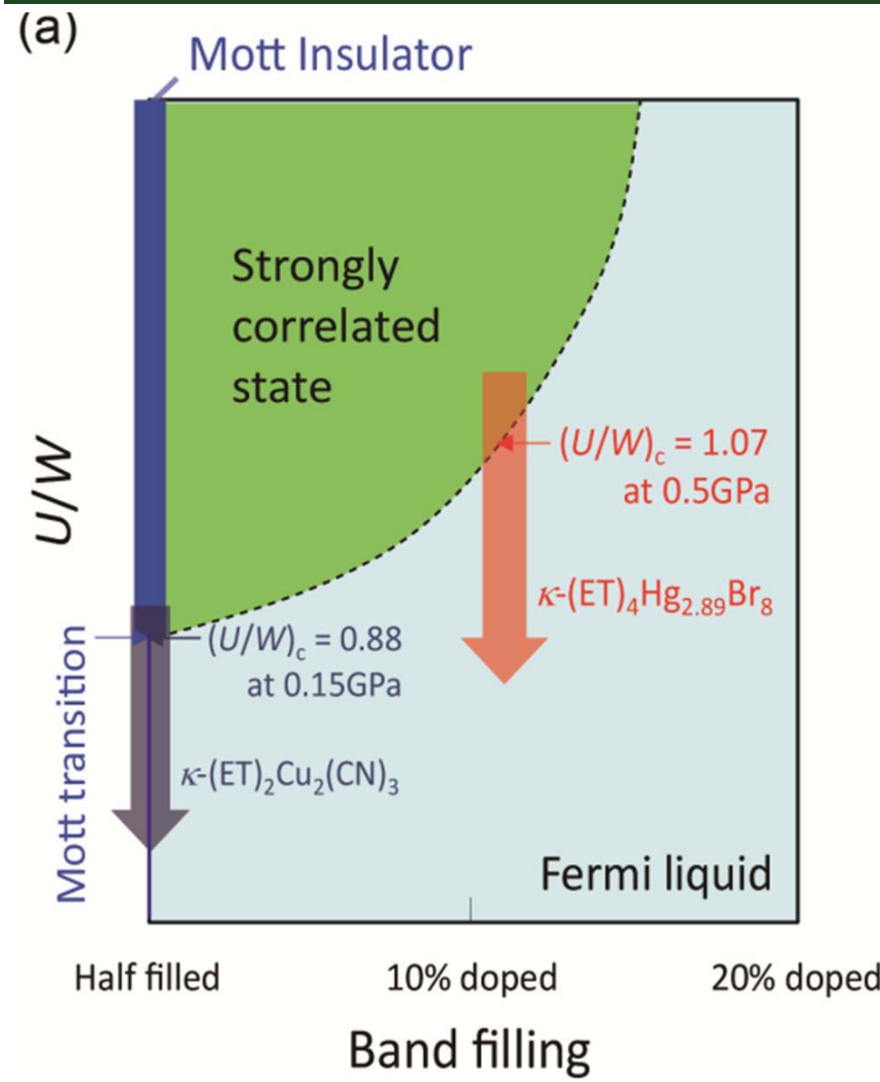
Doped BEDT

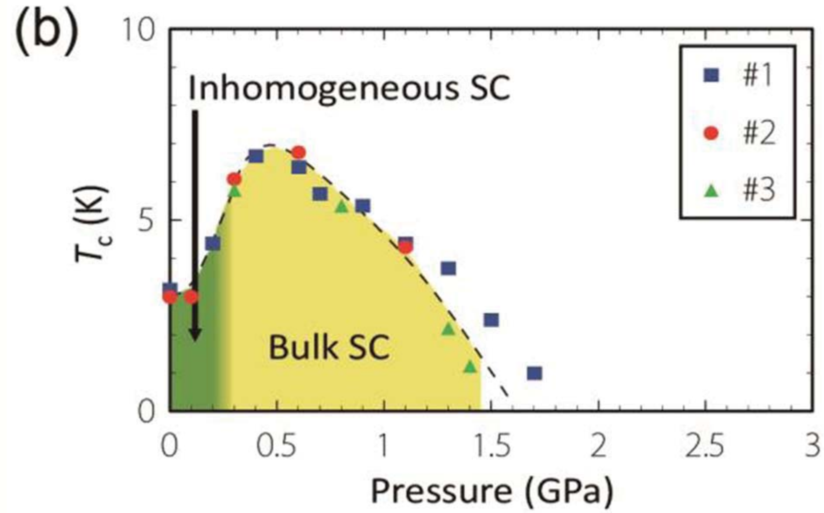


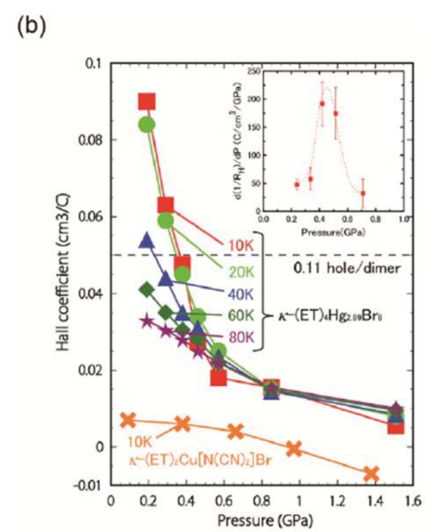


H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

Doped BEDT

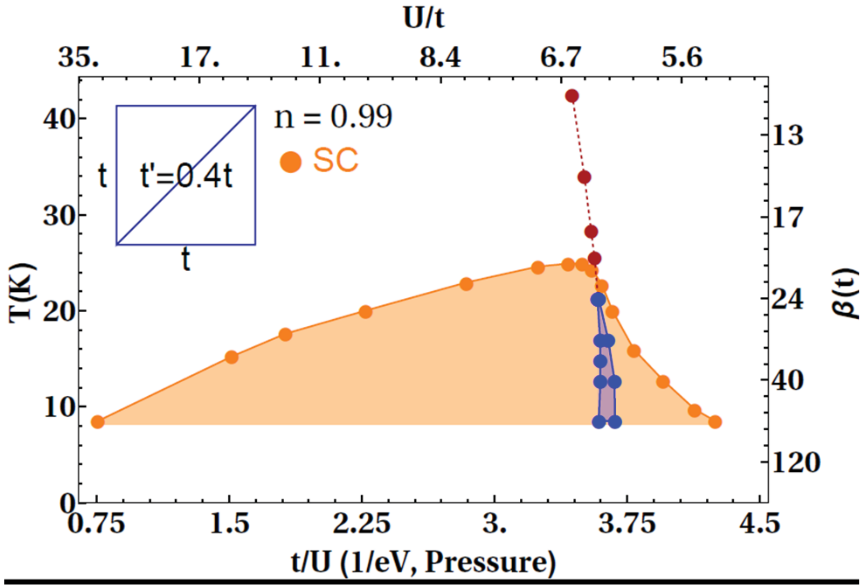


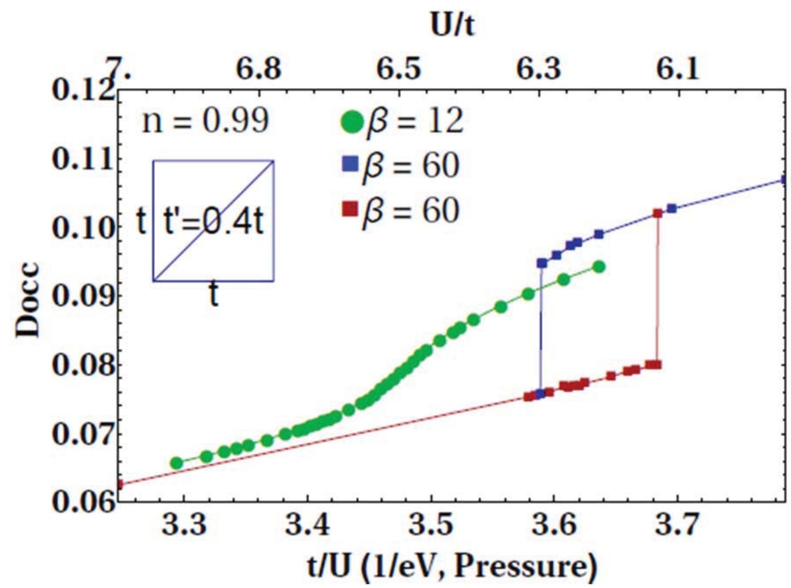


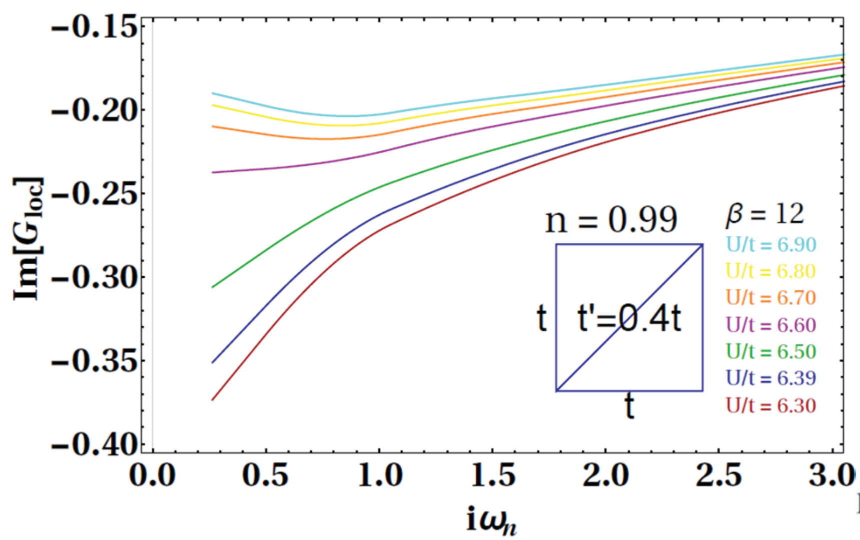


H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

Widom line in organics



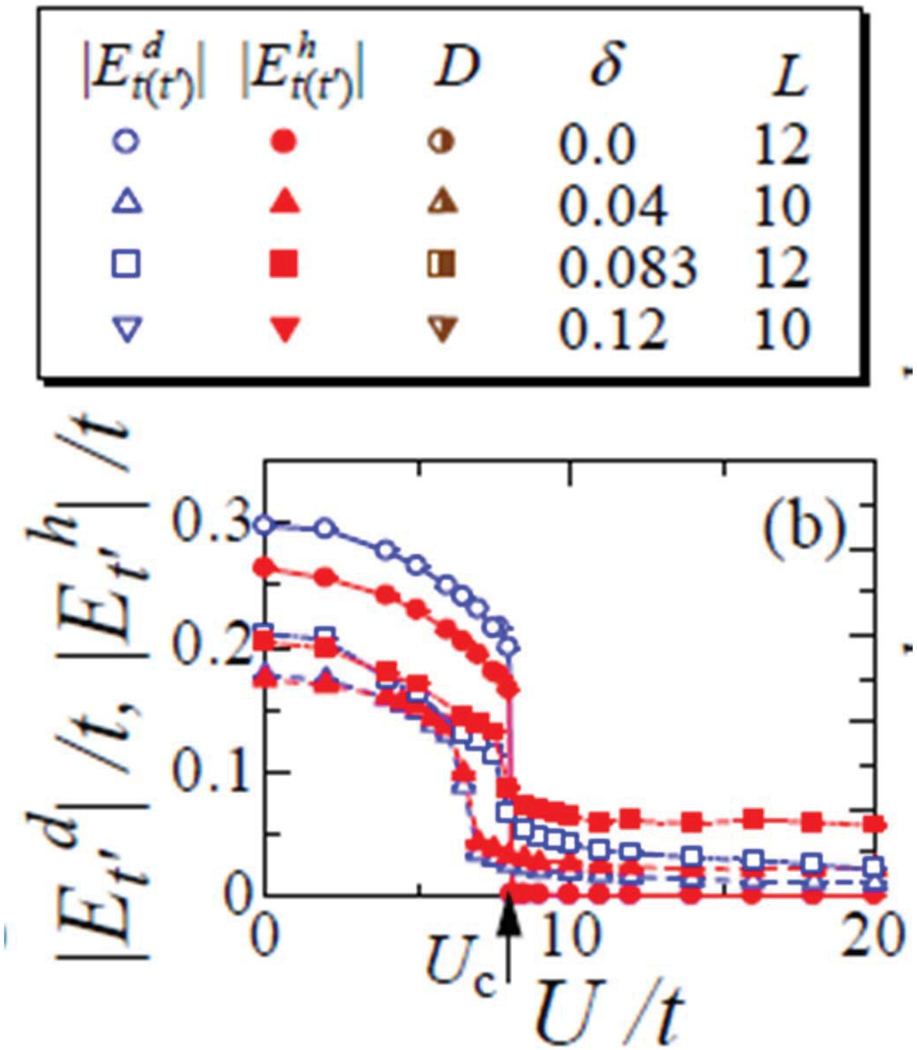




Charles-David Hébert, Patrick Sémon , AMT

E

Results from variational MC



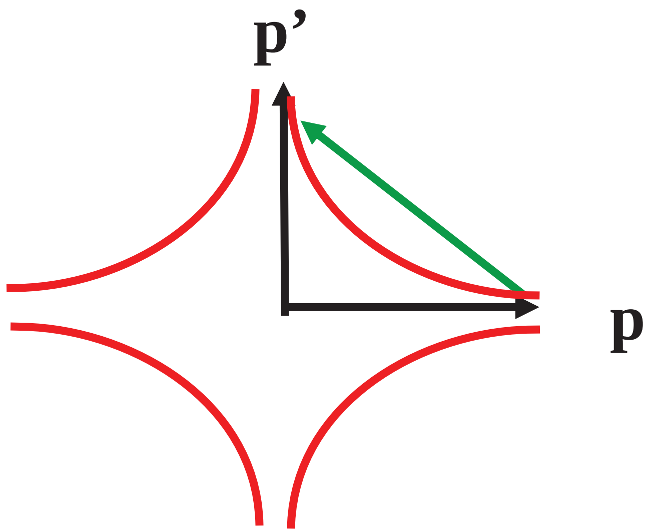
T. Watanabe, H. Yokoyama and M. Ogata
JPS Conf. Proc.
3, 013004 (2014)

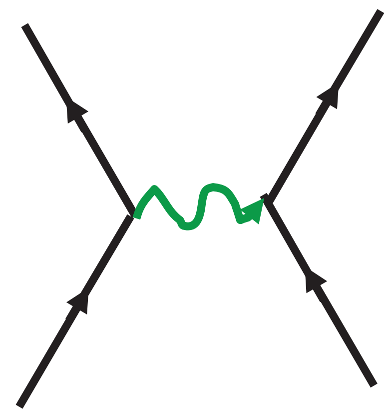
8. Superconductivity in general

Analog to weakly and strongly correlated antiferromagnets

Cartoon « BCS » weak-coupling picture

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





Béal–Monod, Bourbonnais, Emery
P.R. B. **34**, 7716 (1986).

Exchange of spin waves?
Kohn-Luttinger
T_c with pressure

D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch
P.R. B **34**, 8190-8192 (1986).

Kohn, Luttinger, P.R.L. **15**, 524 (1965).

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

UNIVERSITÉ DE SHERBROOKE

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

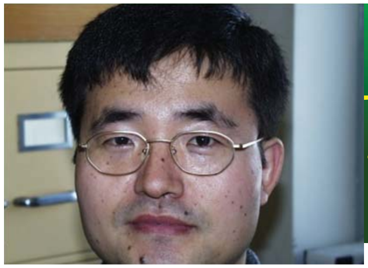
P.W. Anderson Science 317, 1705 (2007)

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

More sophisticated Slave Boson: Kotliar Liu PRB 1988

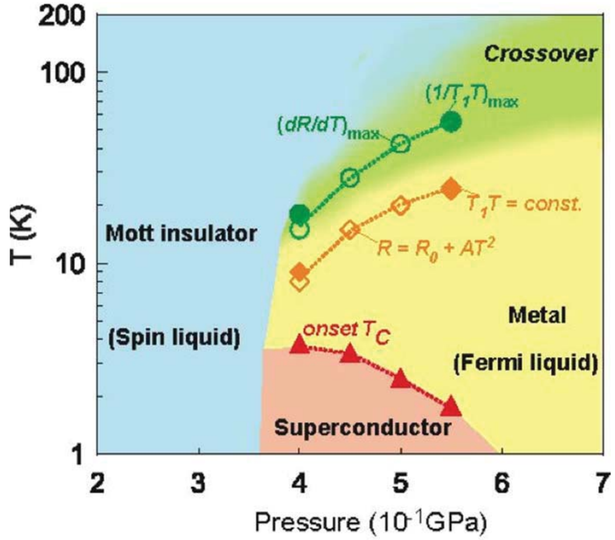
UNIVERSITÉ DE SHERBROOKE

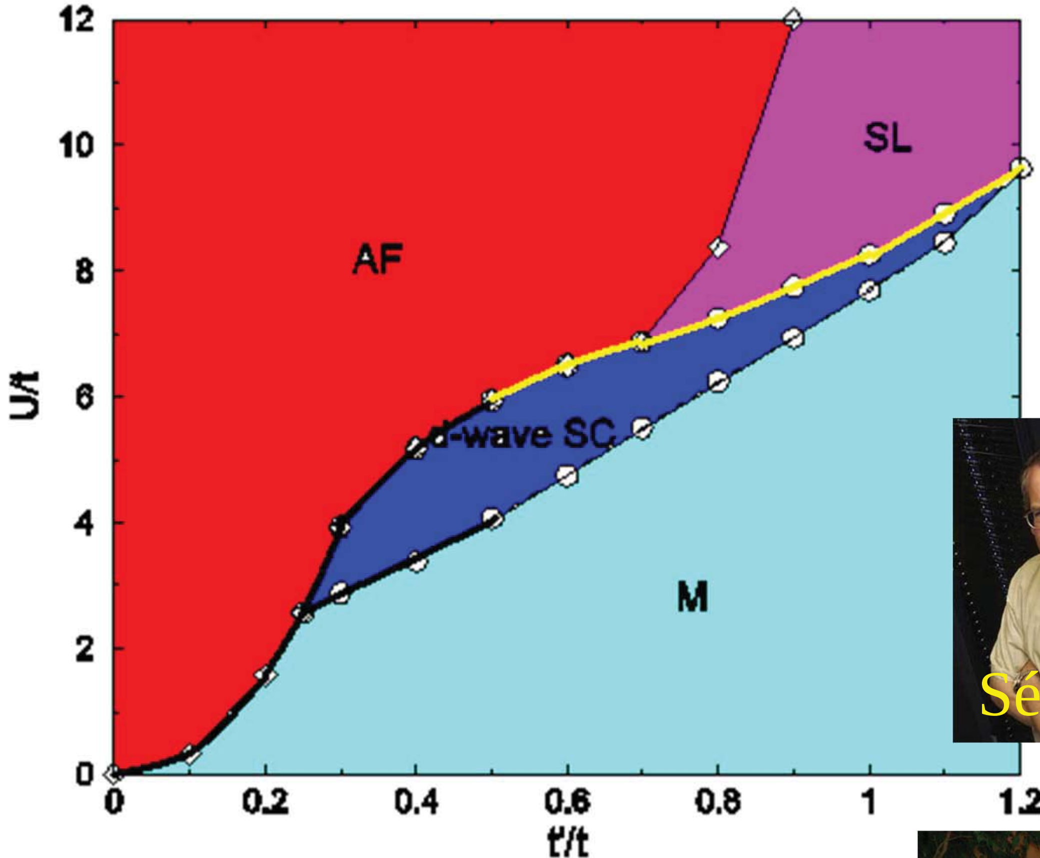
8. Superconductivity in the organics

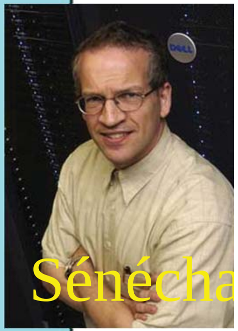


Theoretical phase diagram BEDT

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

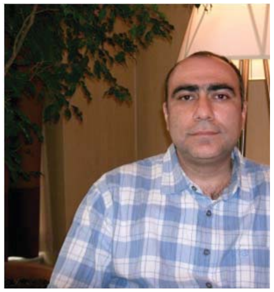






Kyung, A.-M.S.T. PRL 97, 046402 (2006)

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

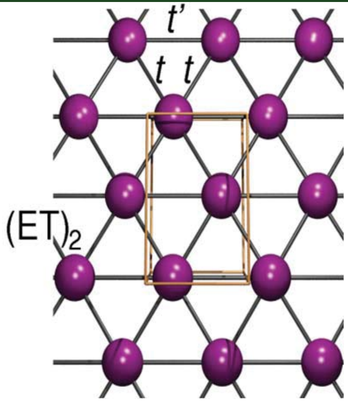


Y. Kurisaki, et al.

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

Other compounds (R. Valenti et al.)

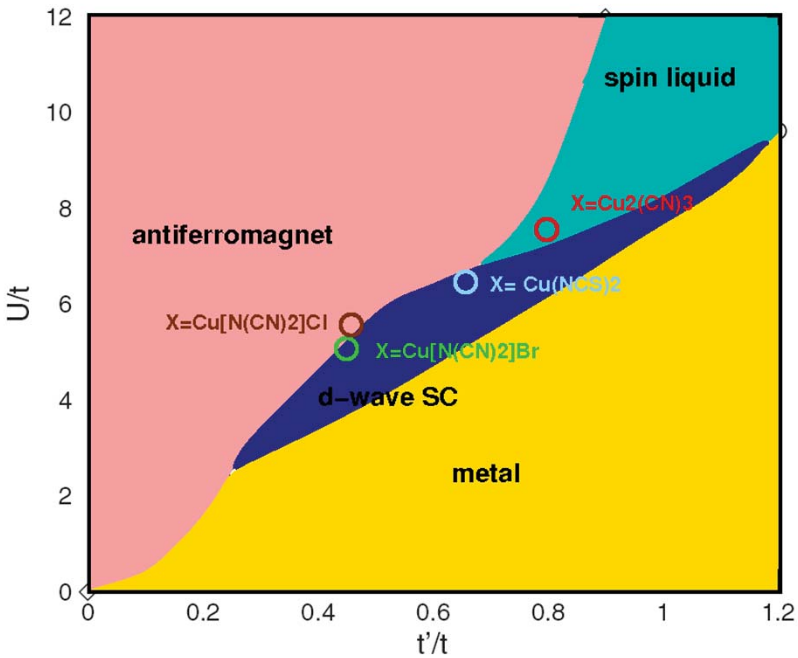
X	Hueckel t'/t	Hueckel U/t	DFT t'/t	DFT U/t
CN	1.06	8.2	0.83 (0.85)	7.3 (12)
SCN	0.84	6.8	0.58 (0.83)	6.0
Cl	0.75	7.5	0.44	7.5
Br	0.68	7.2	0.42	5.1



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)

UNIVERSITÉ DE SHERBROOKE

Analogous results with other methods

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

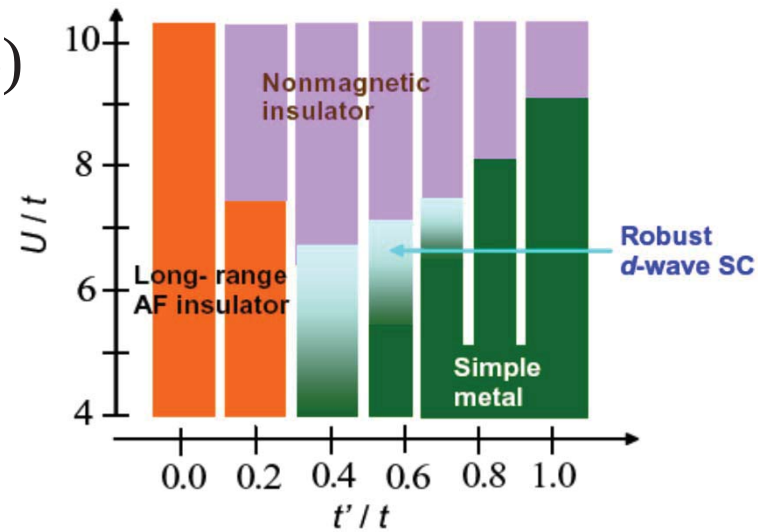
J. Liu et al., Phys. Rev. Lett. 94, 127003 (2005).

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

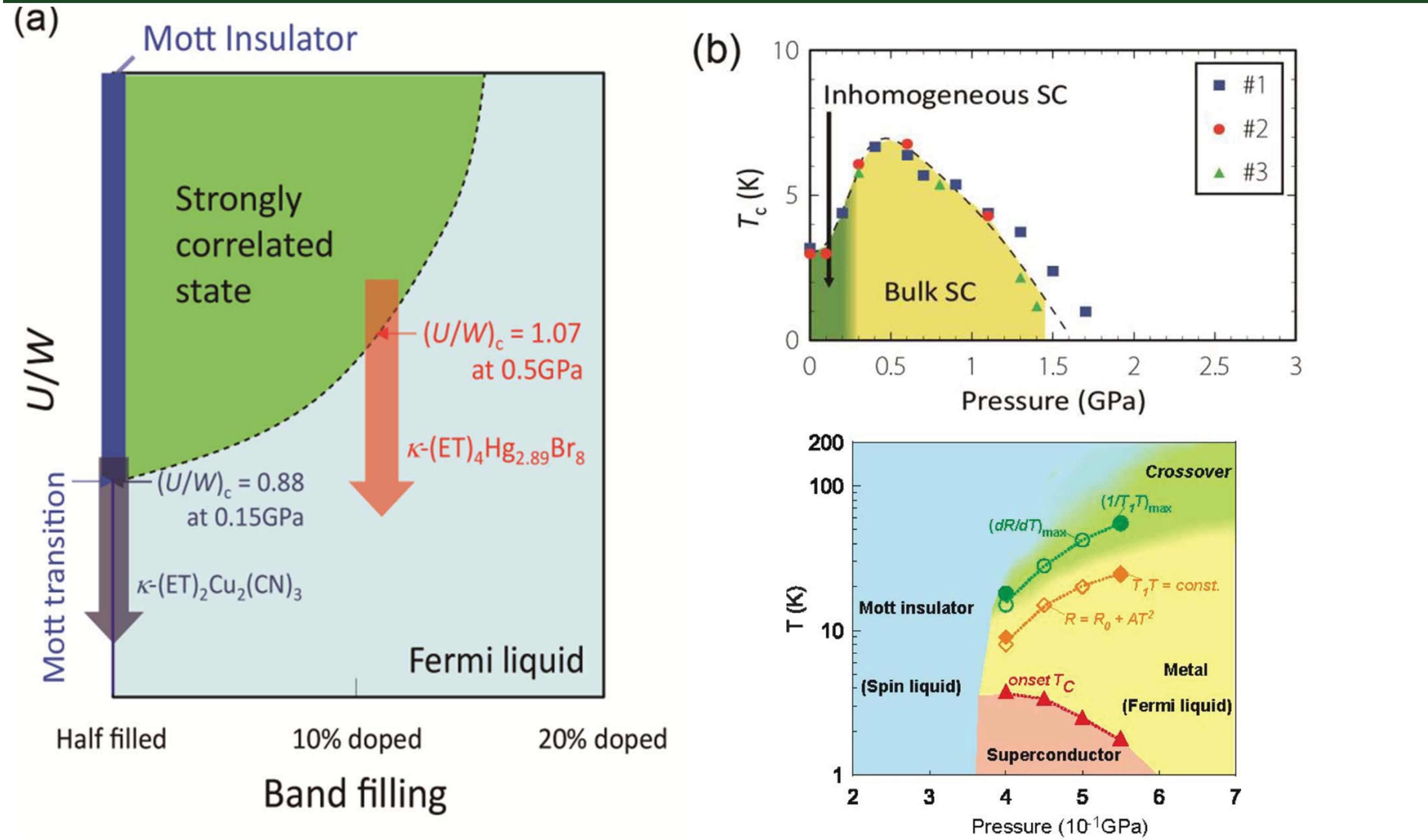
B. Powell et al., Phys. Rev. Lett. 94, 047004 (2005).

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

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



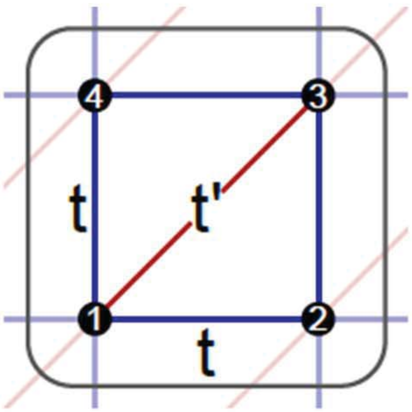
Doped BEDT



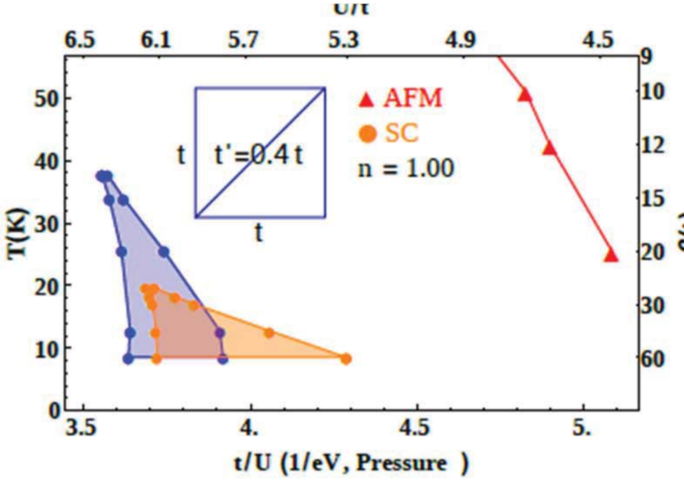
H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

UNIVERSITÉ DE SHERBROOKE

t'=0.4t

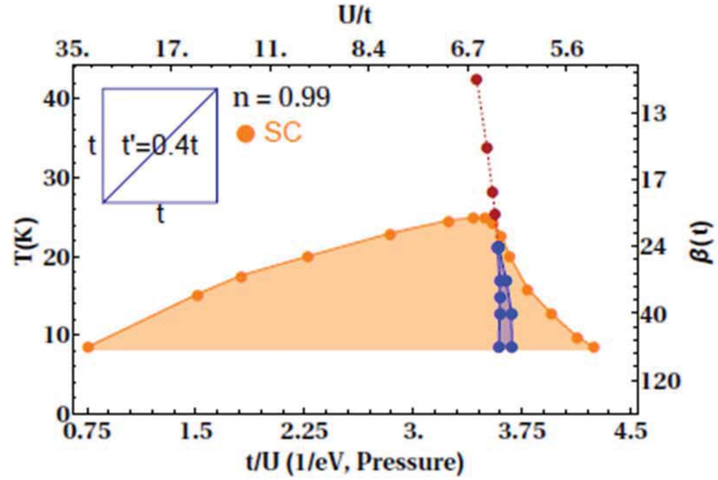


t
t'
t
1
2
3
4



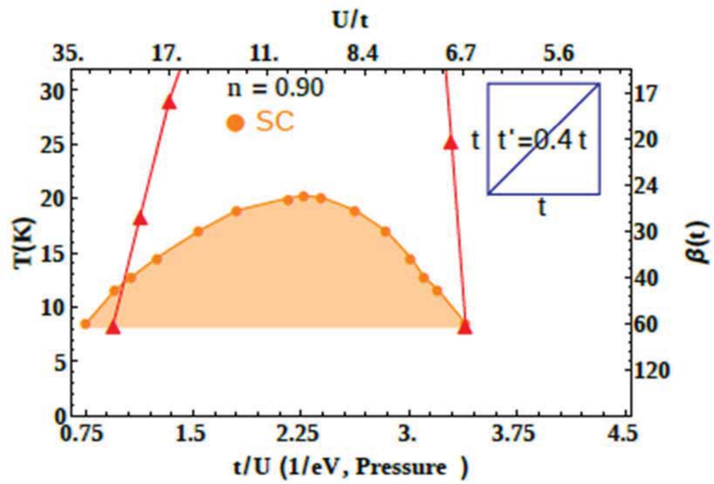
U/t
AFM
SC
n = 1.00
t'=0.4 t
T(K)
β(t)
t/U (1/eV, Pressure)

(a)

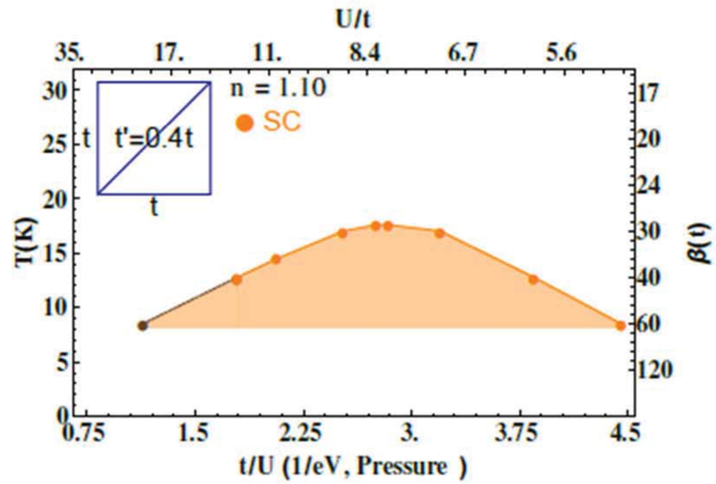


U/t
n = 0.99
SC
t'=0.4t
T(K)
β(t)
t/U (1/eV, Pressure)

(b)

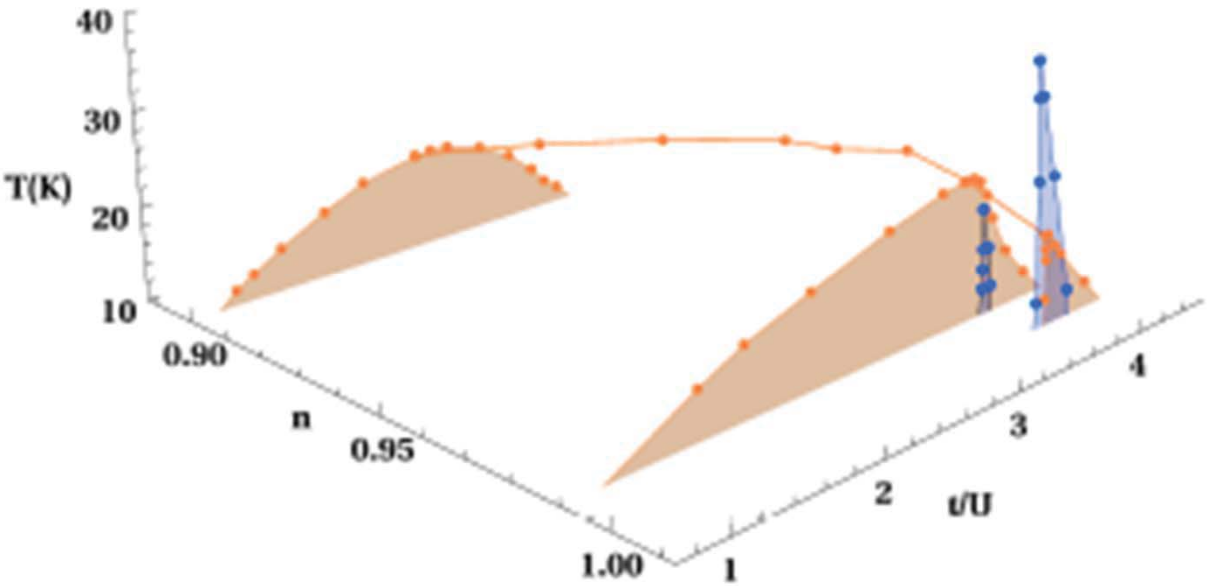


U/t
n = 0.90
SC
t'=0.4 t
T(K)
β(t)
t/U (1/eV, Pressure)

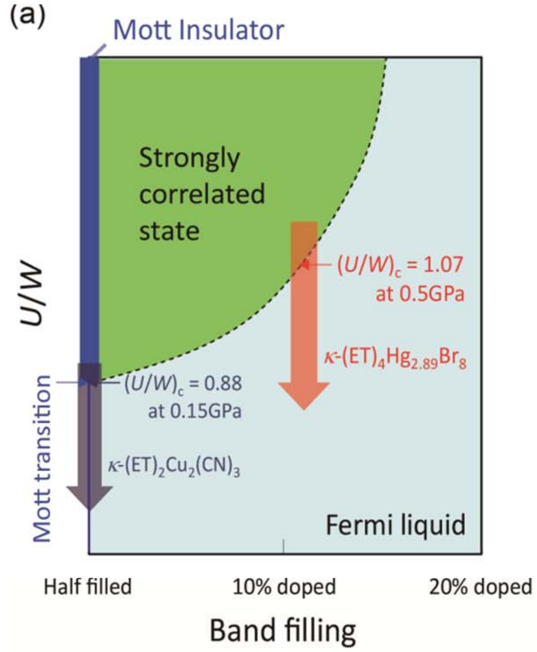


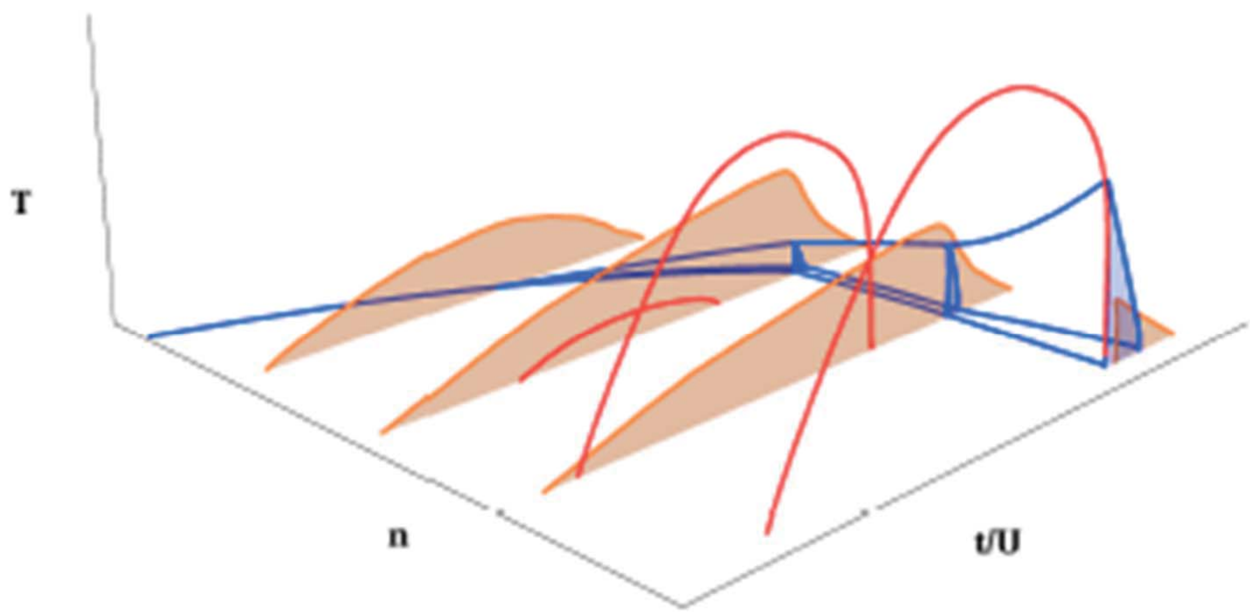
U/t
n = 1.10
SC
t'=0.4t
T(K)
β(t)
t/U (1/eV, Pressure)

t' = 0.4t overview

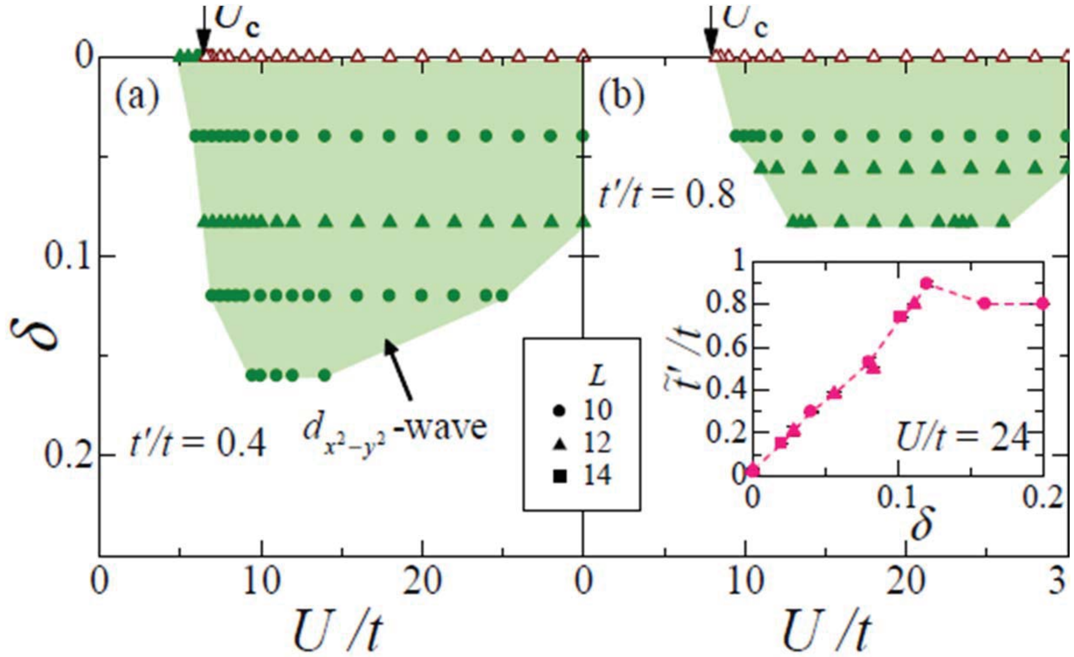


Generic case highly frustrated case





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

UNIVERSITÉ DE SHERBROOKE

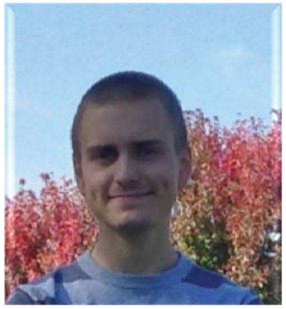
Main collaborators


Giovanni Sordi


Kristjan Haule


David Sénéchal

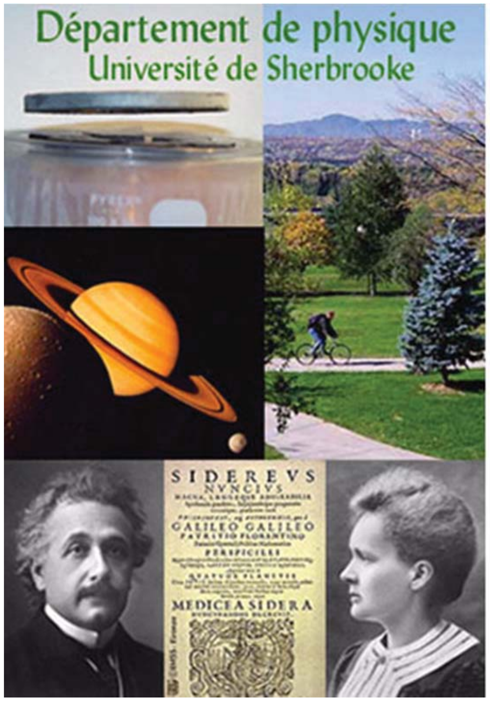

Bumsoo Kyung


Charles-David Hébert


Patrick Sémon


Dominic Bergeron

UNIVERSITÉ DE SHERBROOKE



André-Marie Tremblay

CANADA RESEARCH CHAIRS
CHAIRES DE RECHERCHE DU CANADA

RQMP
Le regroupement québécois sur les matériaux de pointe

UNIVERSITÉ DE SHERBROOKE

CIAR The Canadian Institute for Advanced Research

Sponsors:

CRSNG NSERC | Fonds FCAR | RQCHP | Fondation canadienne pour l'innovation

UNIVERSITÉ DE SHERBROOKE

Mammouth

Éducation, Loisir et Sport
Québec

Canada Foundation for Innovation
Fondation canadienne pour l'innovation

compute • calcul
CANADA

High Performance Computing
CREATING KNOWLEDGE
DRIVING INNOVATION
BUILDING THE DIGITAL ECONOMY

Le calcul de haute performance
CRÉER LE SAVOIR
ALIMENTER L'INNOVATION
BÂTIR L'ÉCONOMIE NUMÉRIQUE

Calcul Québec

UNIVERSITÉ DE SHERBROOKE

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