Pseudogaps and strongly correlated superconductivity

A.-M. Tremblay

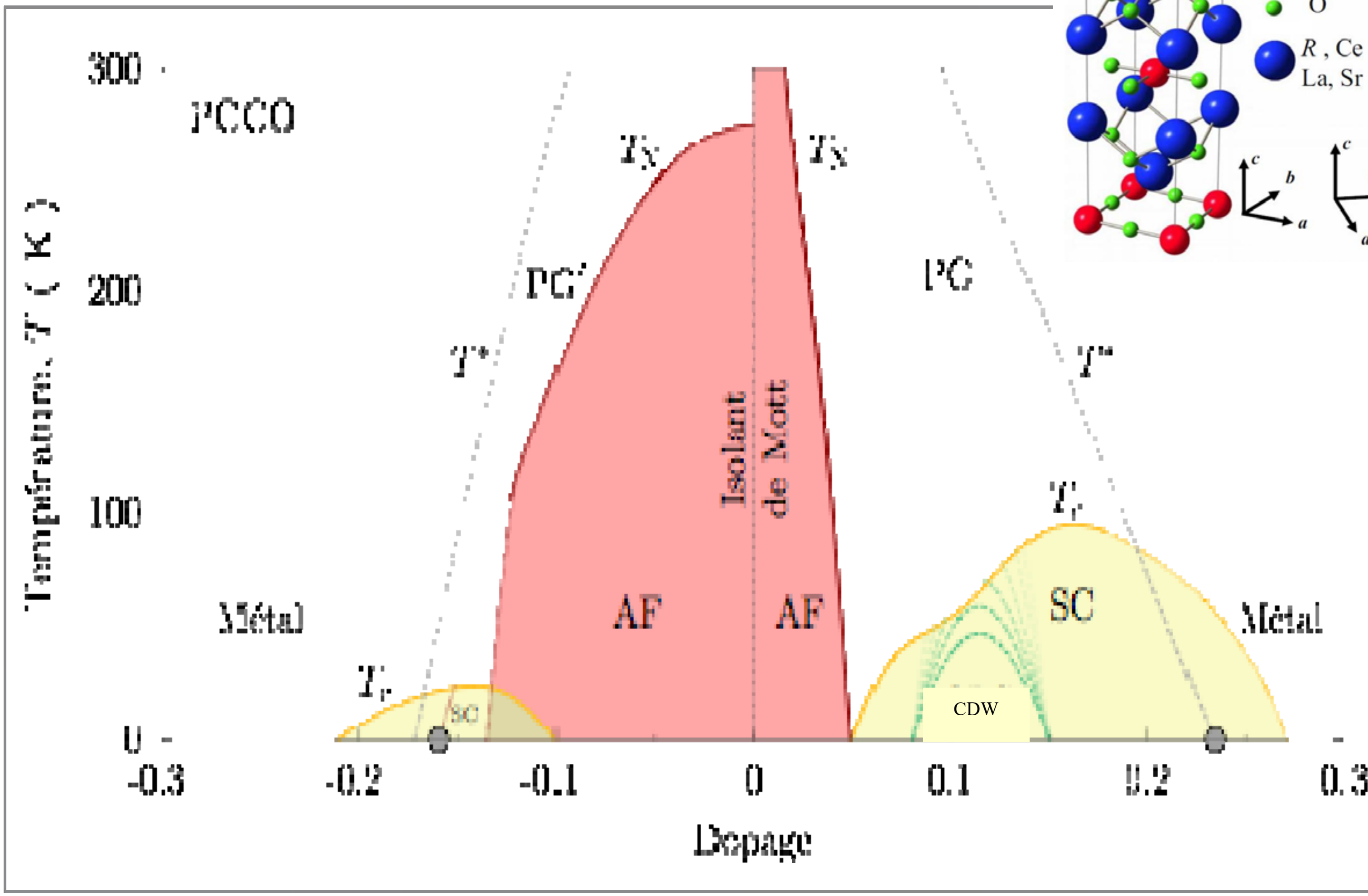
Institut quantique

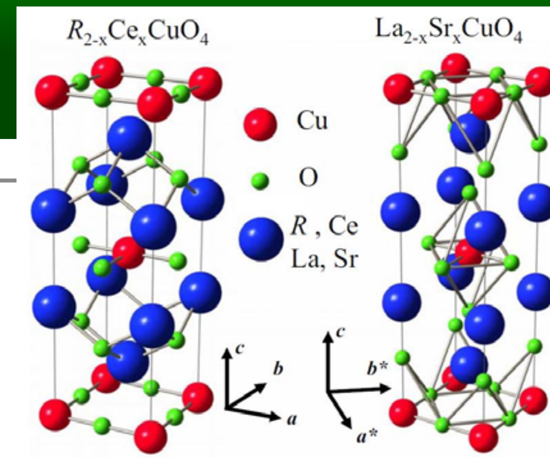
Brookhaven National Laboratory
Wednesday January 18, 2017

CIFAR
CANADIAN INSTITUTE for ADVANCED RESEARCH

UNIVERSITÉ DE SHERBROOKE

Our road map





Thèse de Francis Laliberté,
Université de Sherbrooke

UNIVERSITÉ DE SHERBROOKE

Outline

- Part I
  - Pseudogap
    - Mott physics
    - Precursor to LRO
- Part II
  - Strongly correlated superconductivity (BEDT)
  - Retardation

Part I

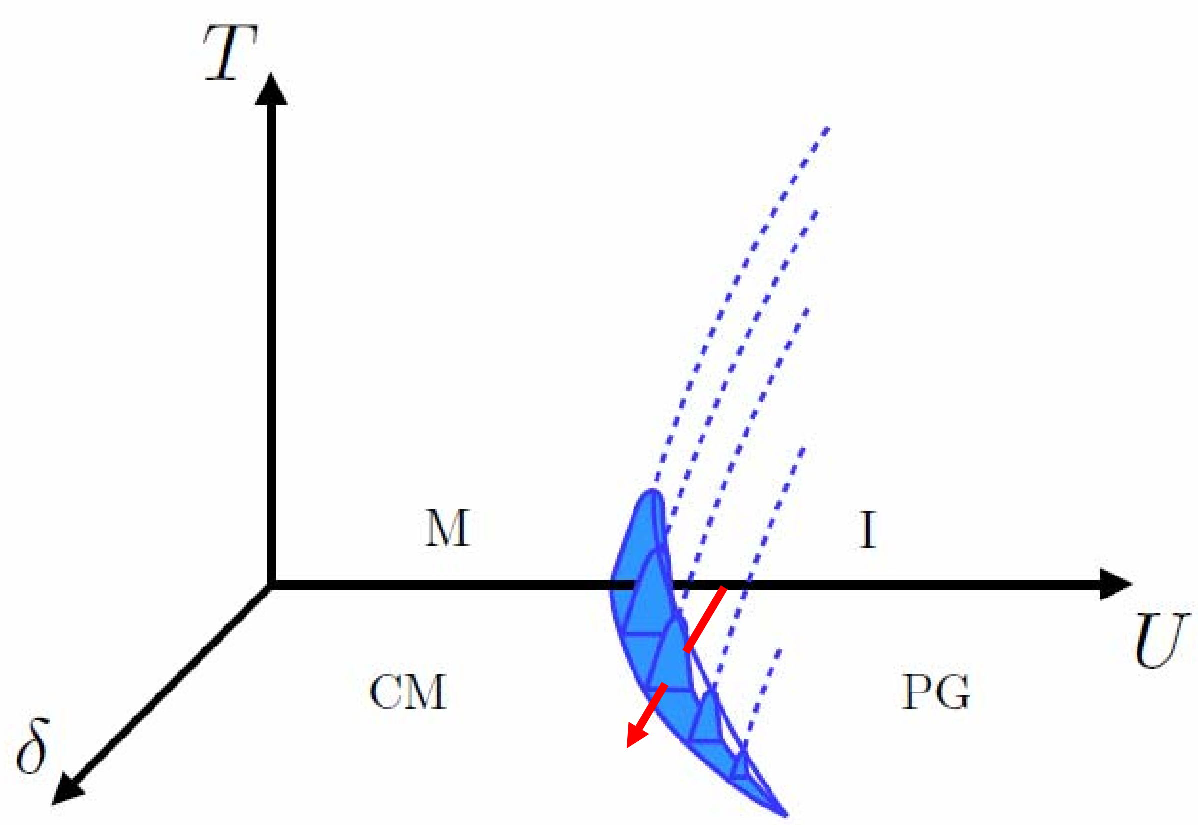
Pseudogap

Three broad classes of mechanisms for pseudogap

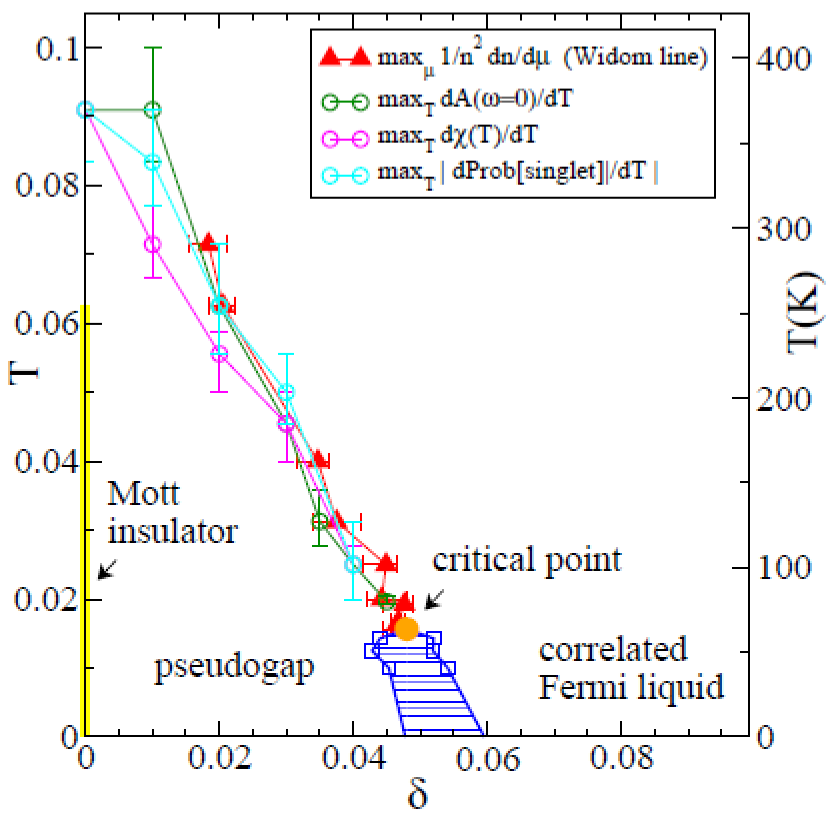
- Phase with a broken symmetry (discrete)
- Mott Physics + J
- Precursor of LRO ($d = 2$)
  - Mermin-Wagner allows a large fluctuation regime
  - Even with weak correlations

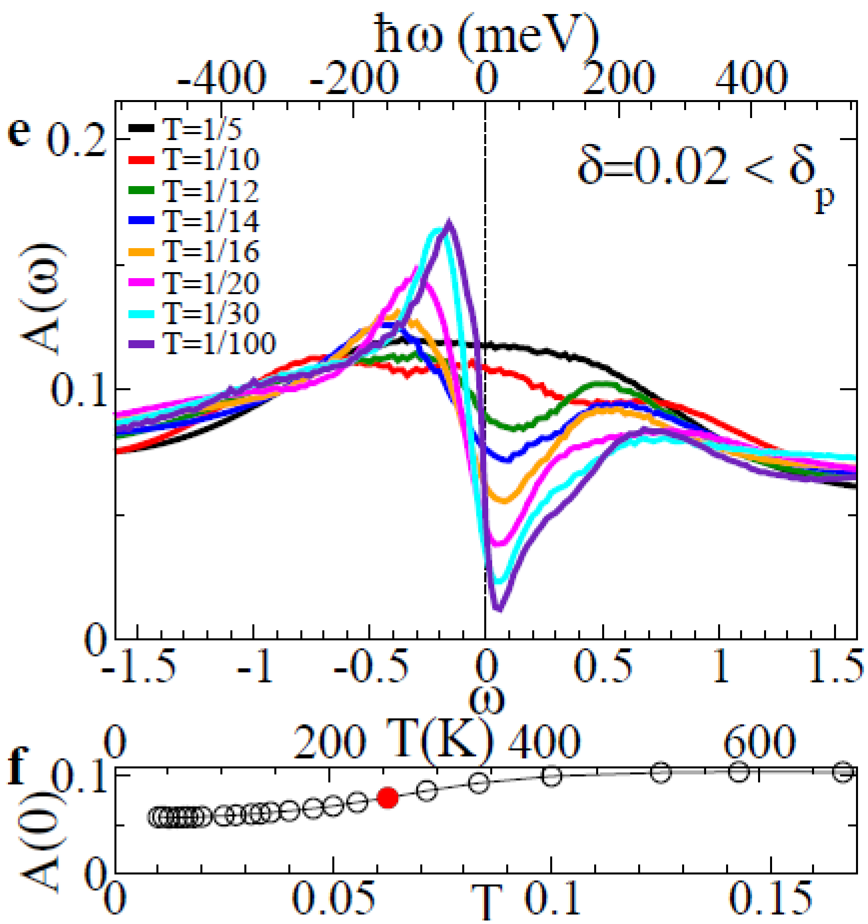
Influence of Mott transition away from half-filling

n = 1, d = 2 square lattice

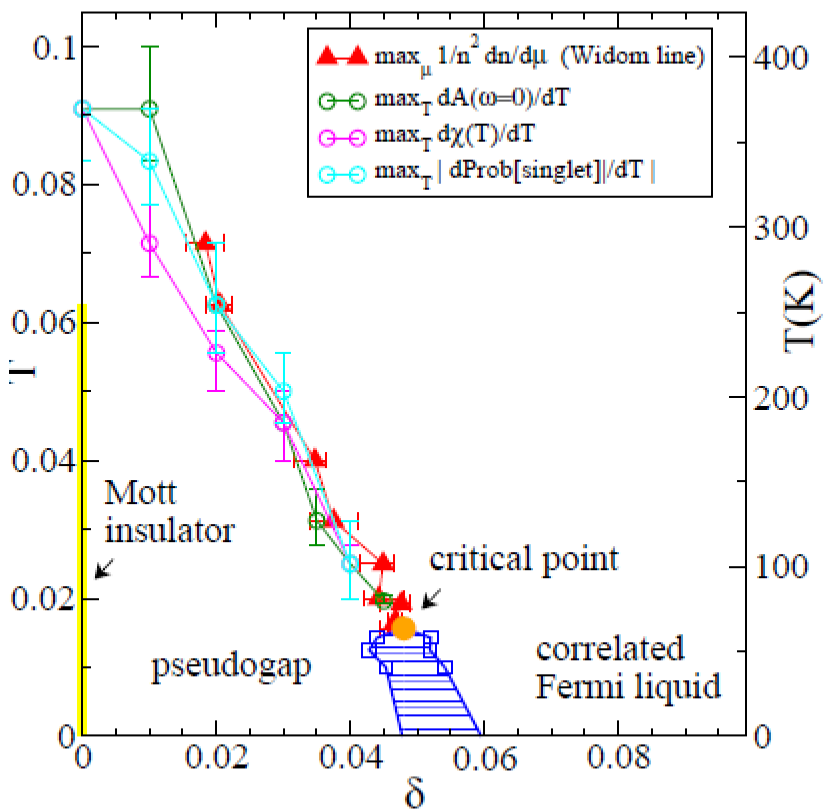


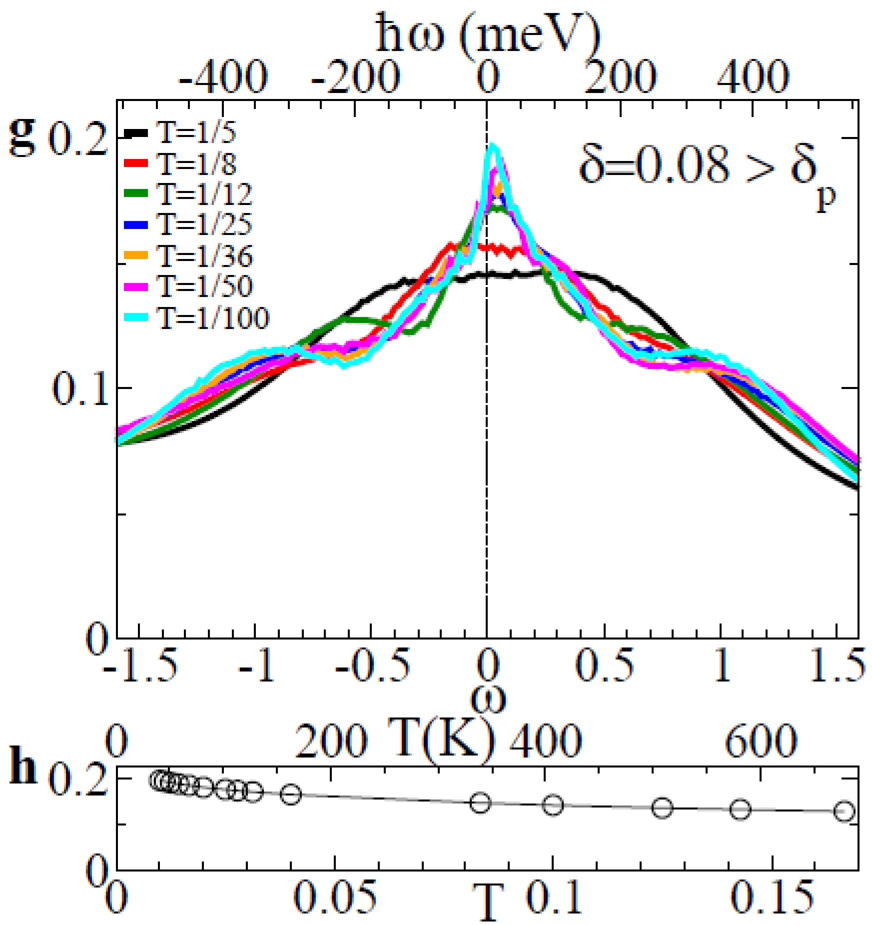
Density of states



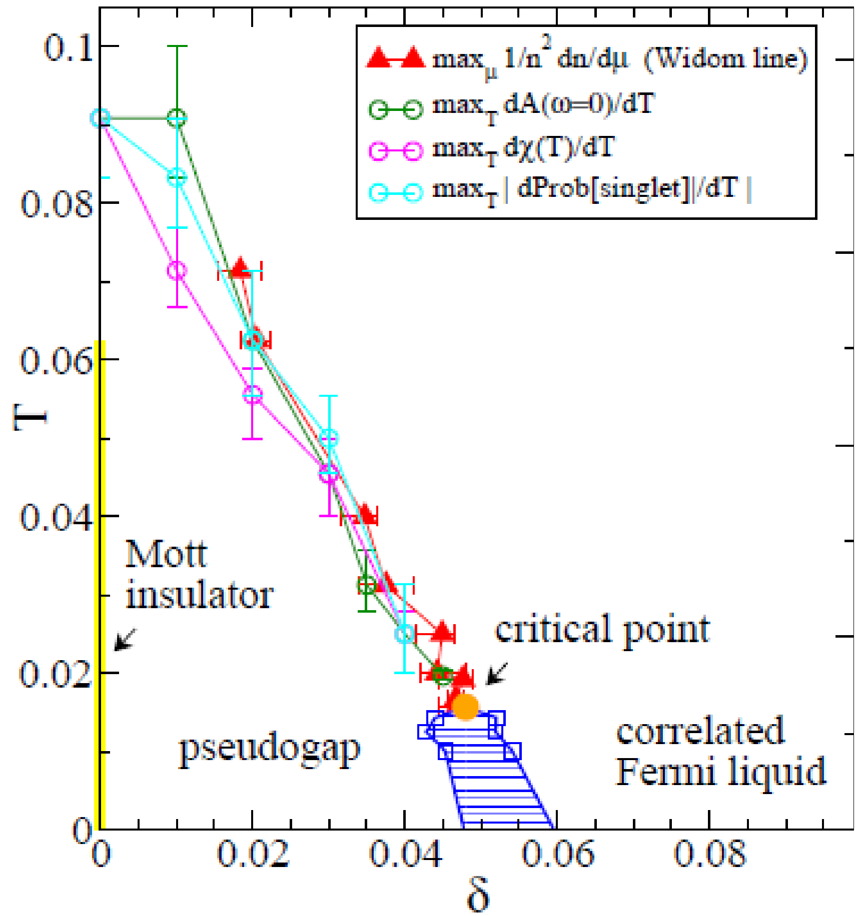


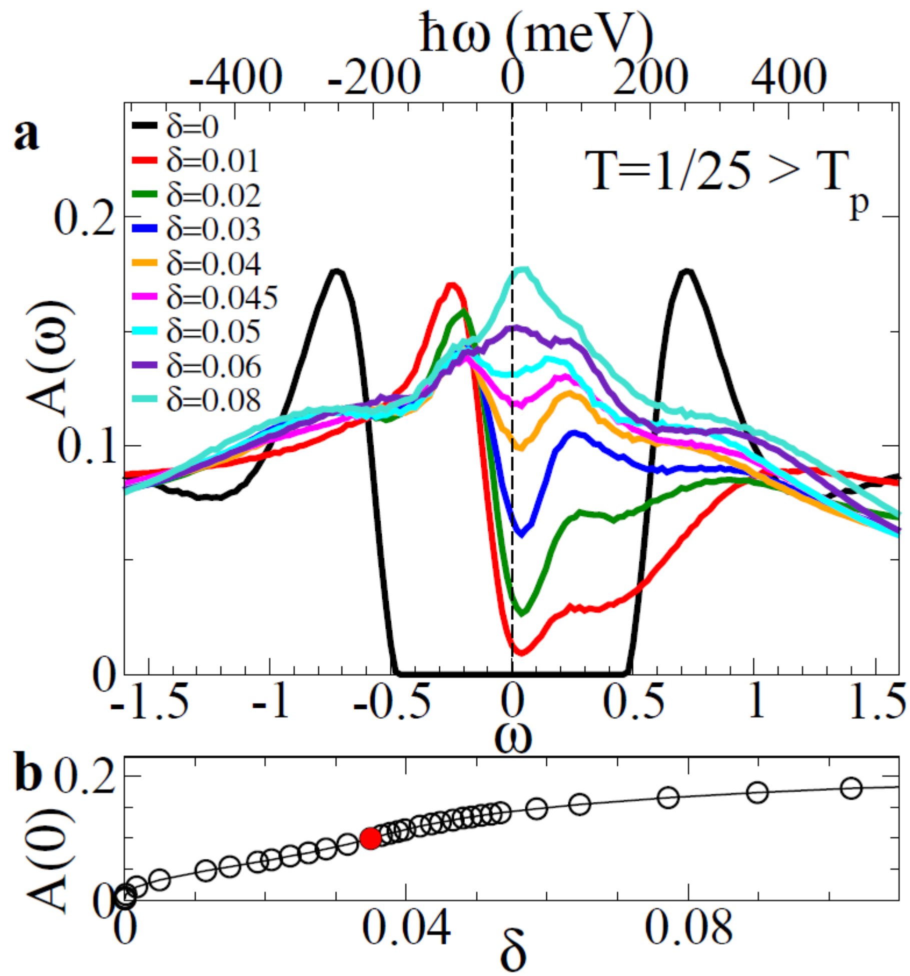
Density of states



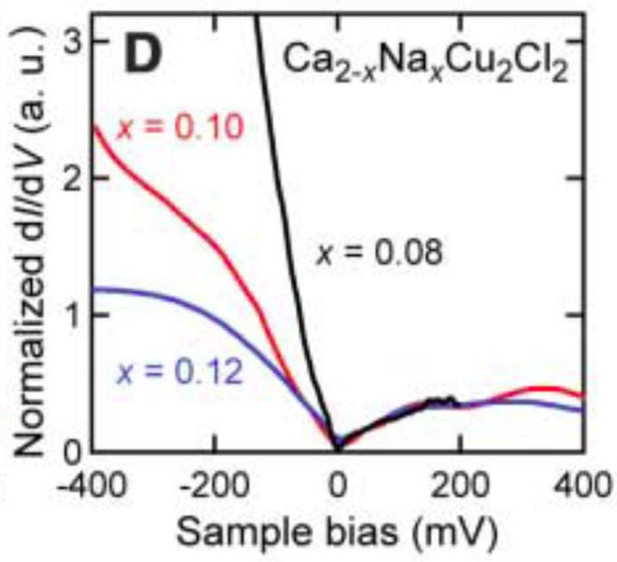


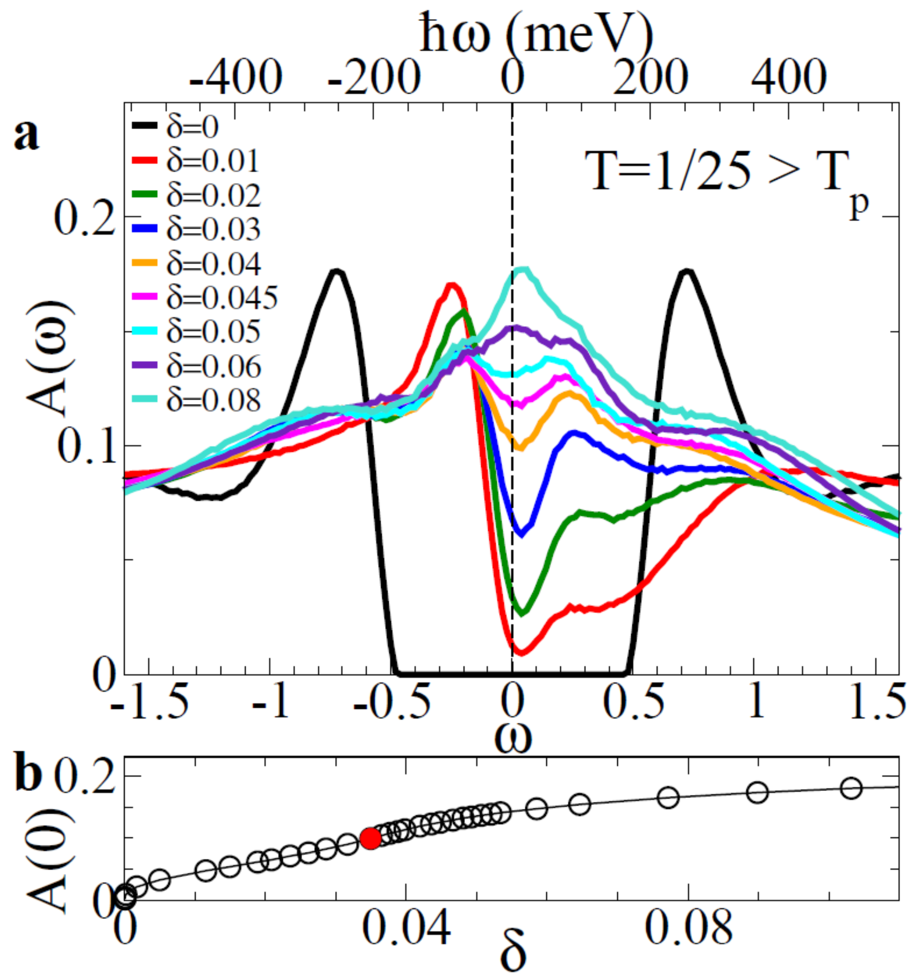
$U = 6.2\ t$ Normal state. Density of states





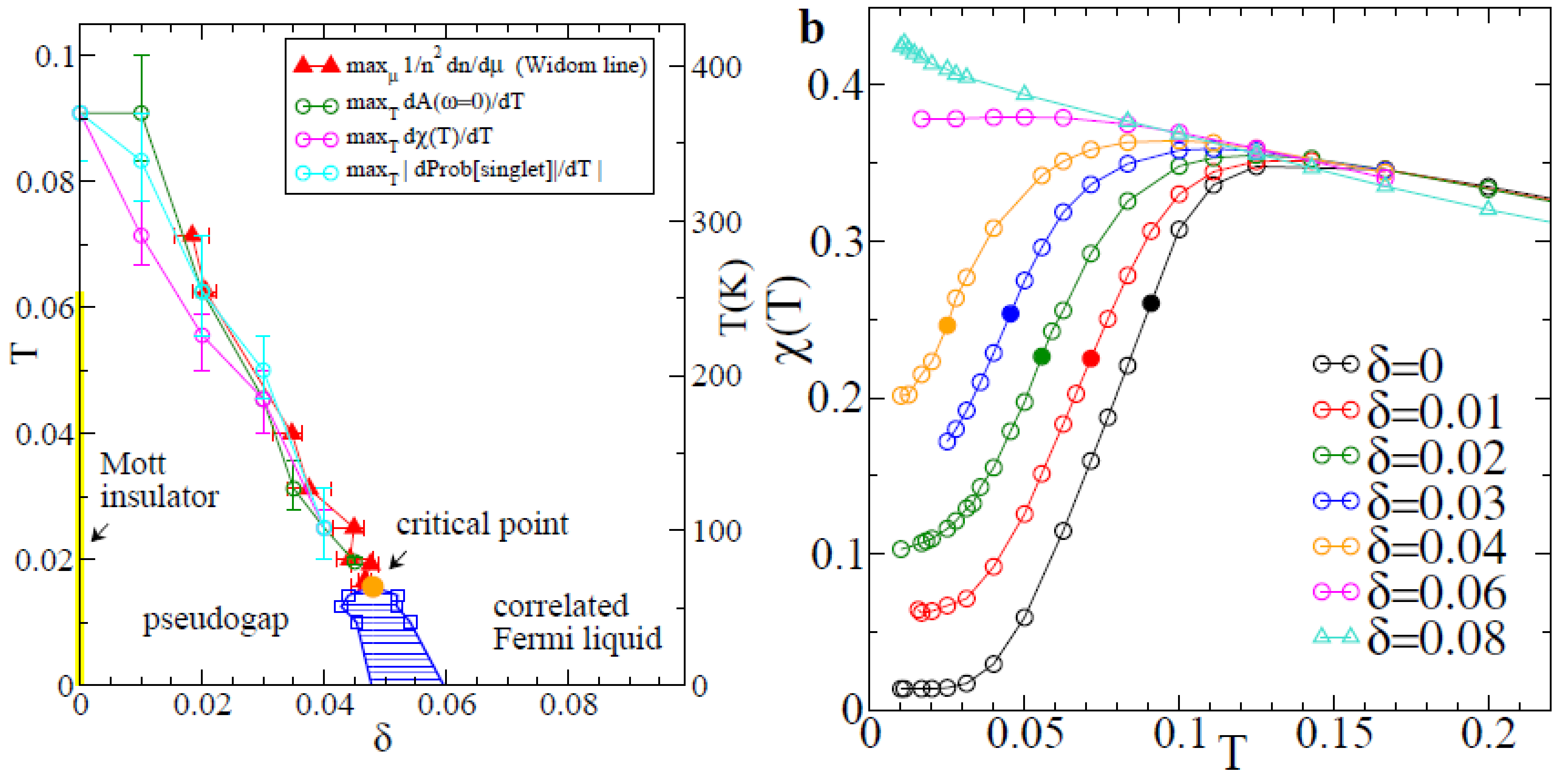
Density of states



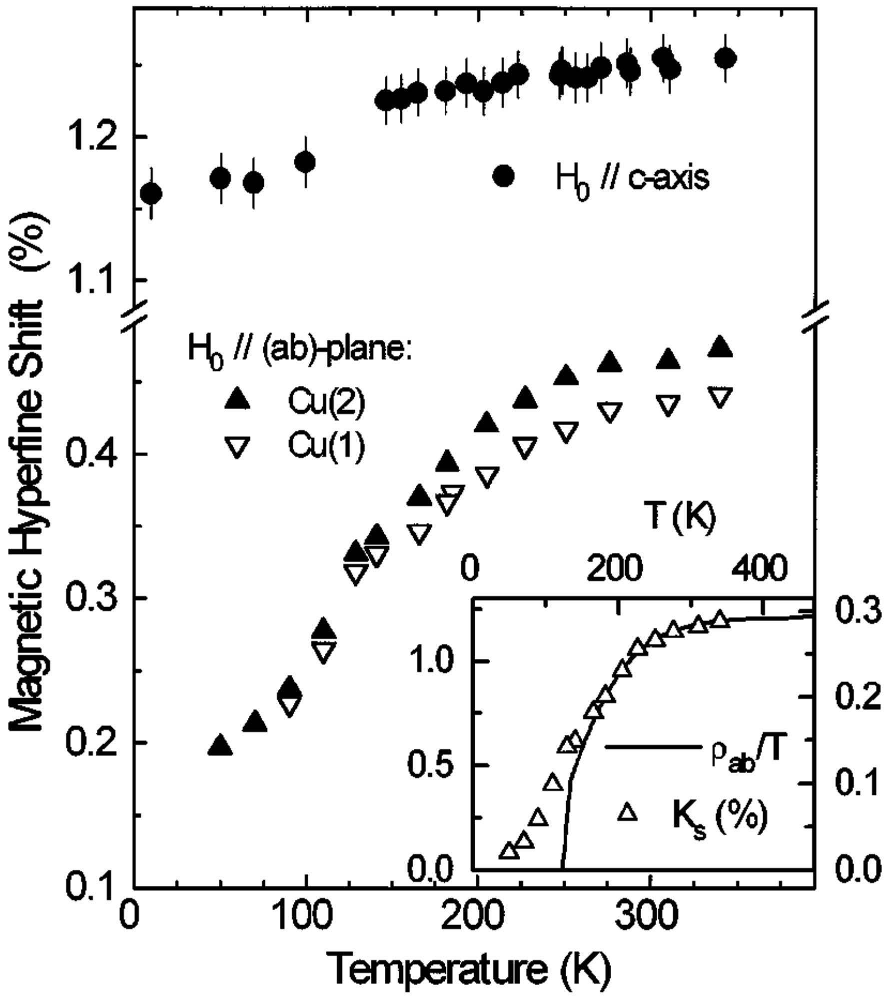


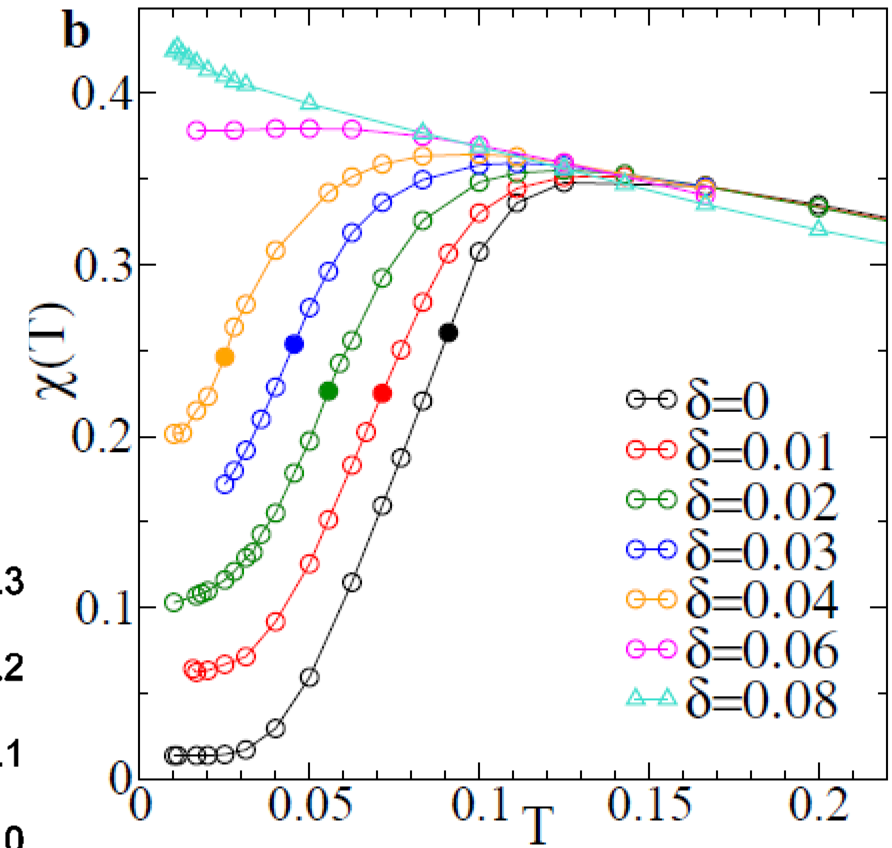
Khosaka et al. *Science* **315**, 1380 (2007);

Spin susceptibility



Spin susceptibility





Underdoped Hg1223

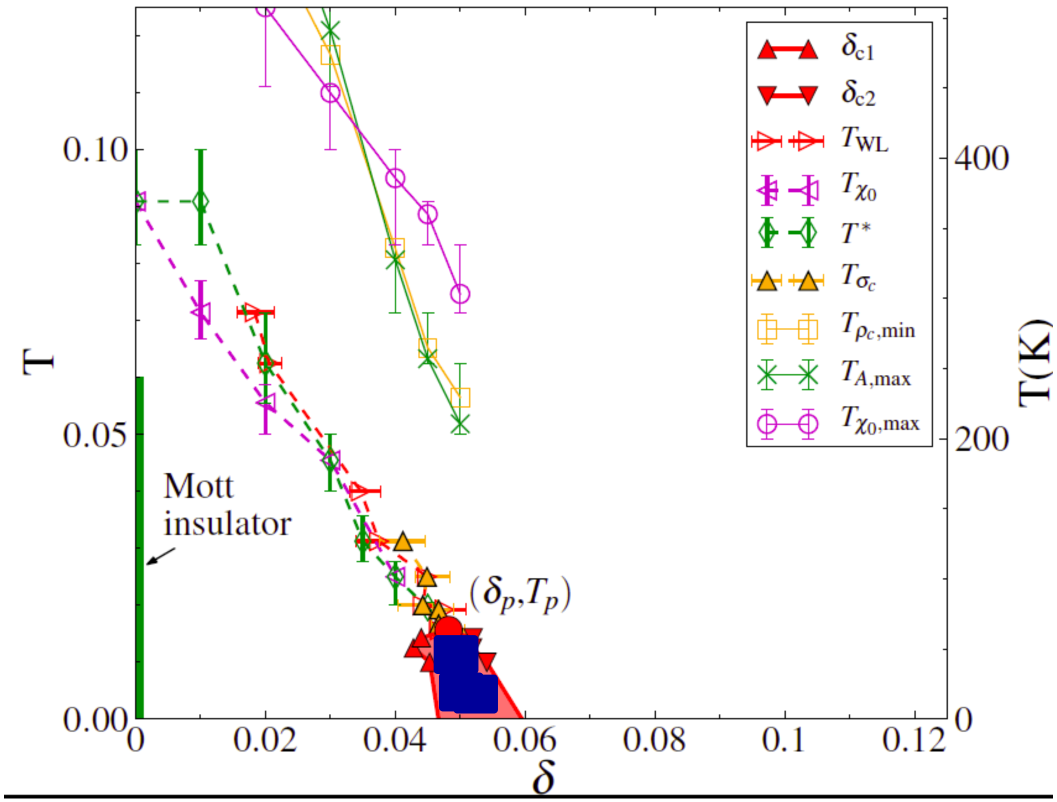
Julien et al. PRL **76,** 4238 (1996)

UNIVERSITÉ DE SHERBROOKE

Two crossover lines

Giovanni Sordi

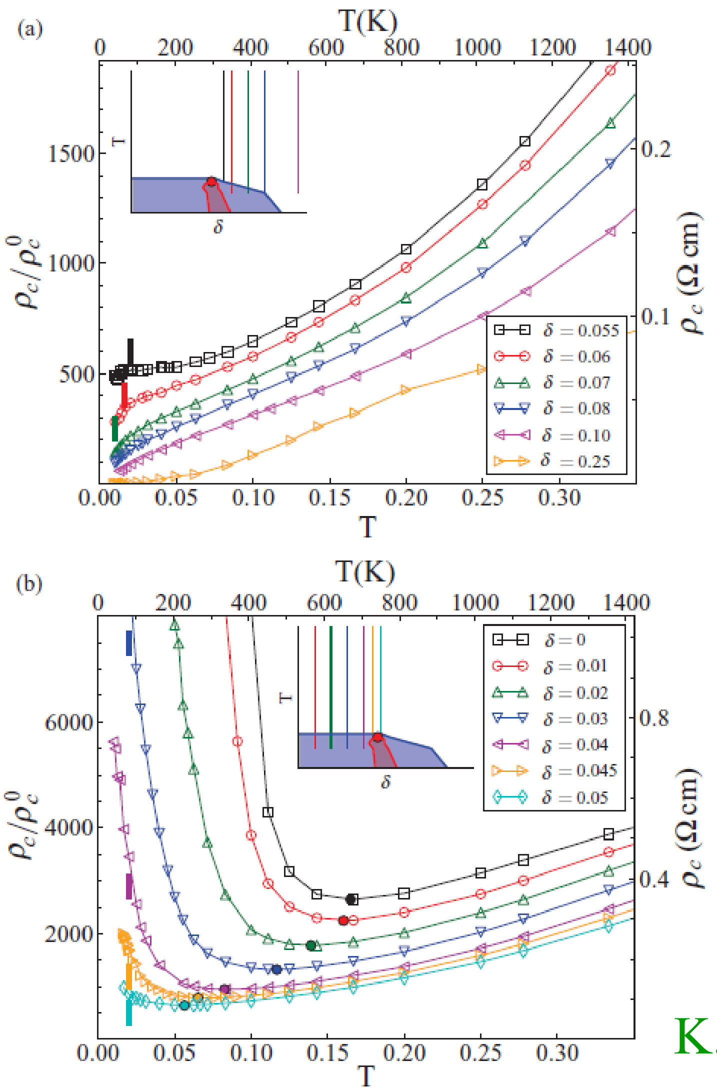
Patrick Sémon

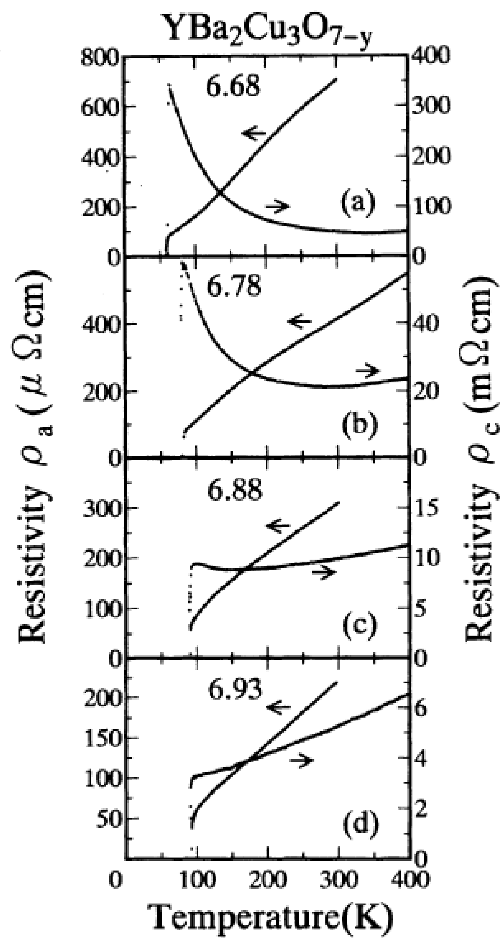


G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)
P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B **89**, 165113/1-6 (2014)

UNIVERSITÉ DE SHERBROOKE

c-axis resistivity



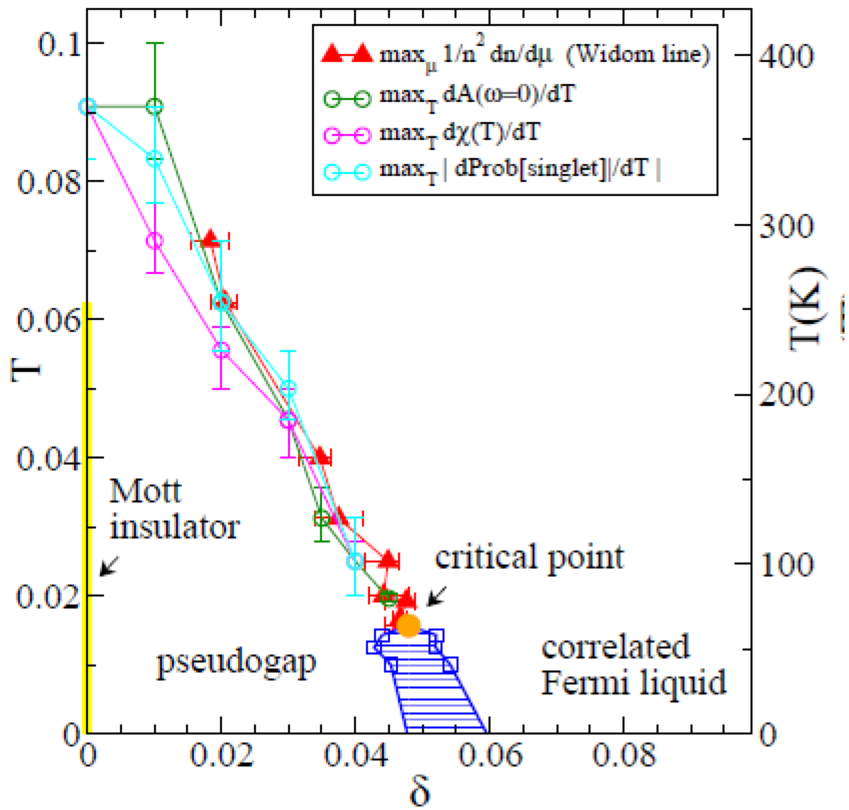


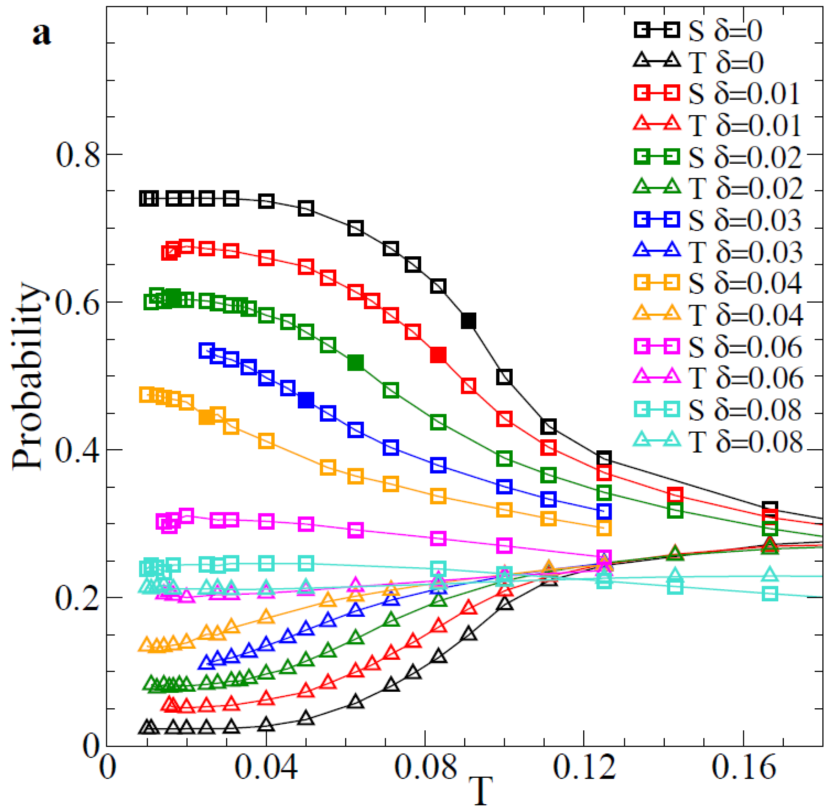
K. Takenaka, K. Mizuhashi, H. Takagi, and S. Uchida, Phys. Rev.B 50, 6534 (1994).

UNIVERSITÉ DE SHERBROOKE

Physics

Plaquette eigenstates





See also:

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

UNIVERSITÉ DE SHERBROOKE

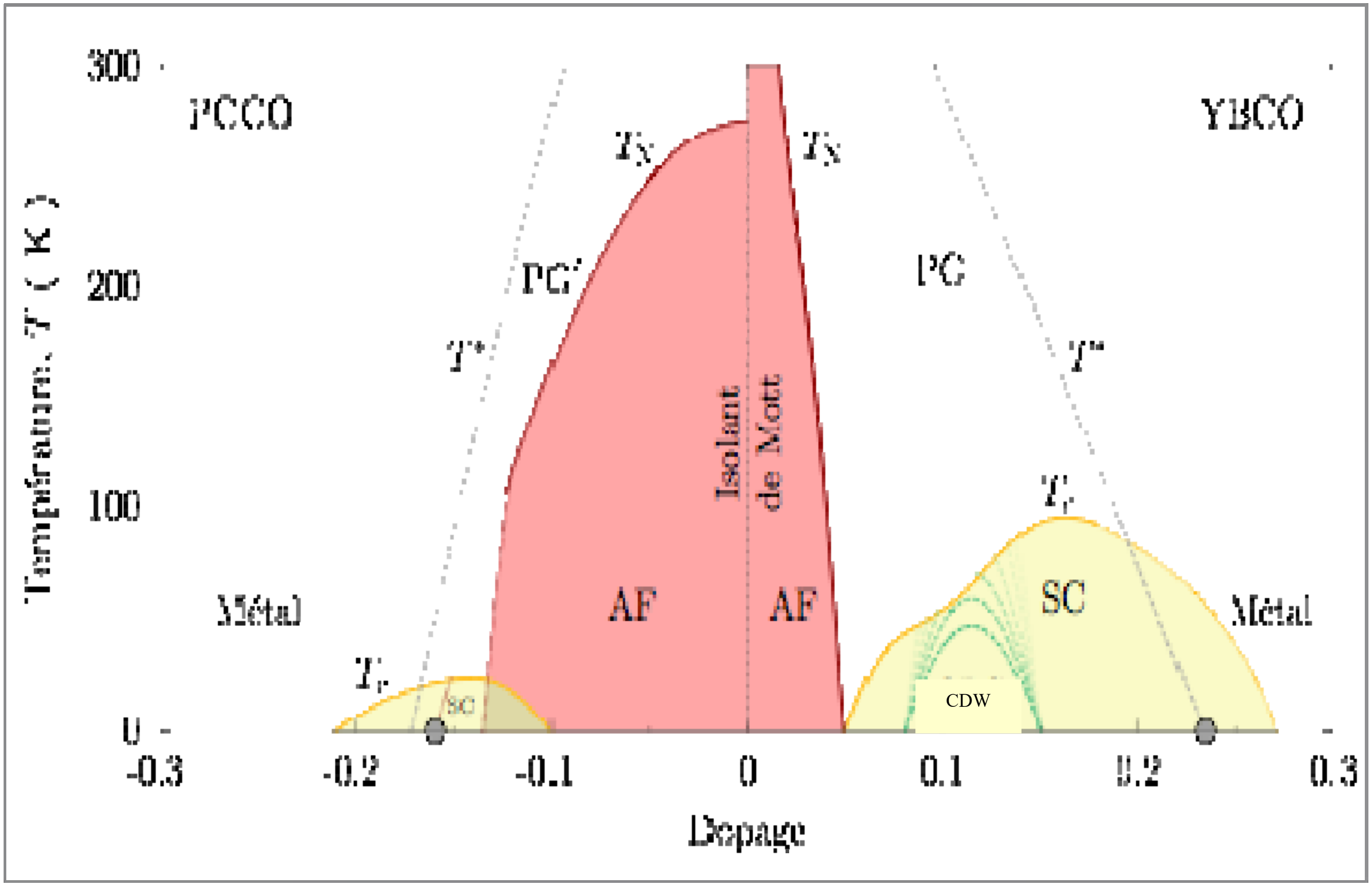
The pseudogap in electron-doped cuprates

UNIVERSITÉ DE SHERBROOKE

TPSC: Theory vs experiment

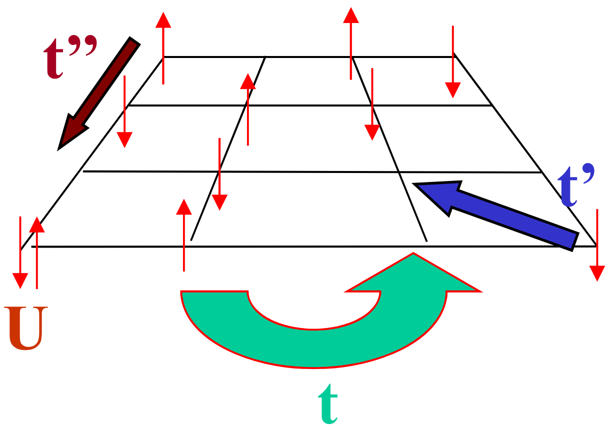
Our road map

Thèse de Francis Laliberté, Université de Sherbrooke



Model parameters

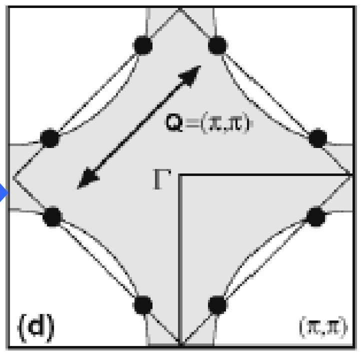
$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$



fixed

$t' = -0.175t$, $t'' = 0.05t$

$t = 350$ meV, $T = 200$ K



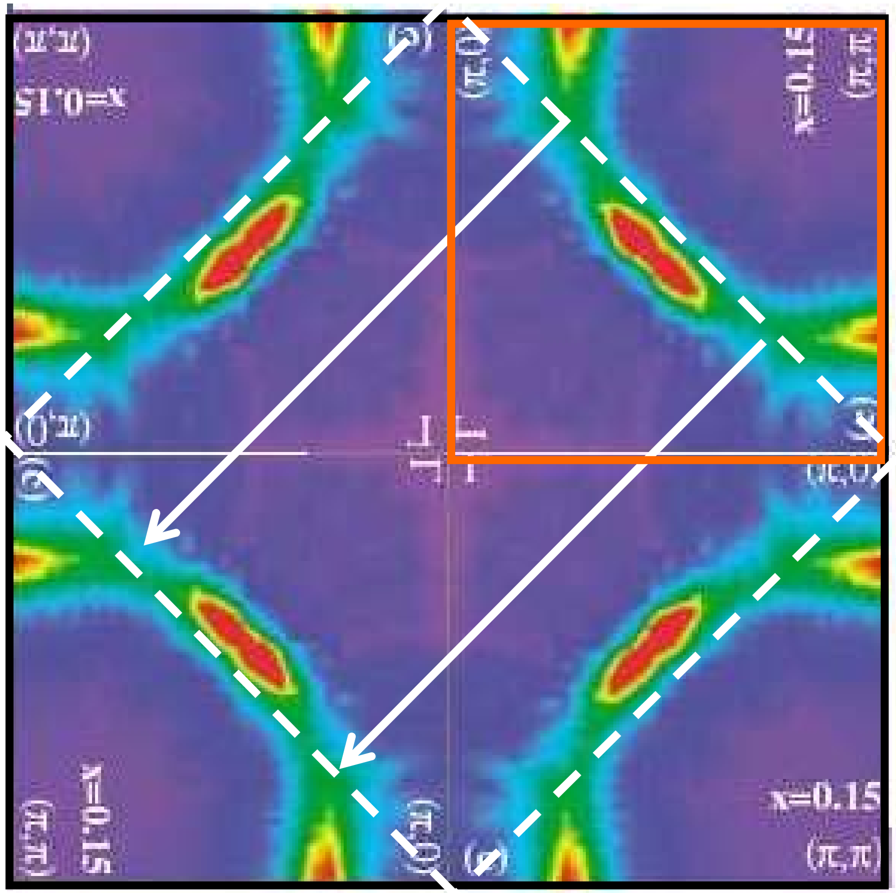
Weak coupling $U<8t$

$n=1+x$ – electron filling

Hot spots from AFM quasi-static scattering

Mermin-Wagner

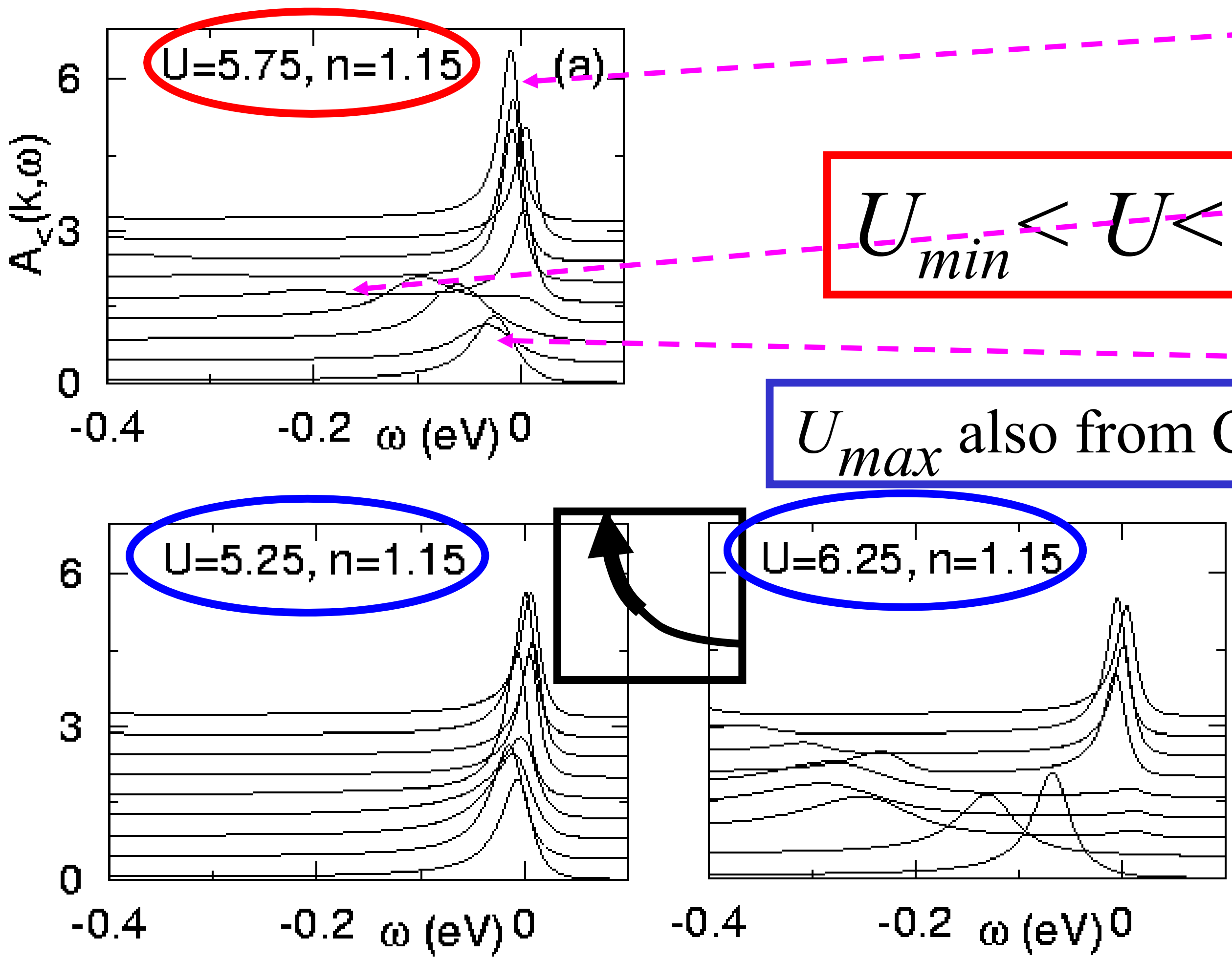
$d = 2$



Vilk, A.-M.S.T (1997)
Kyung, Hankevych, A.-M.S.T., PRL, 2004

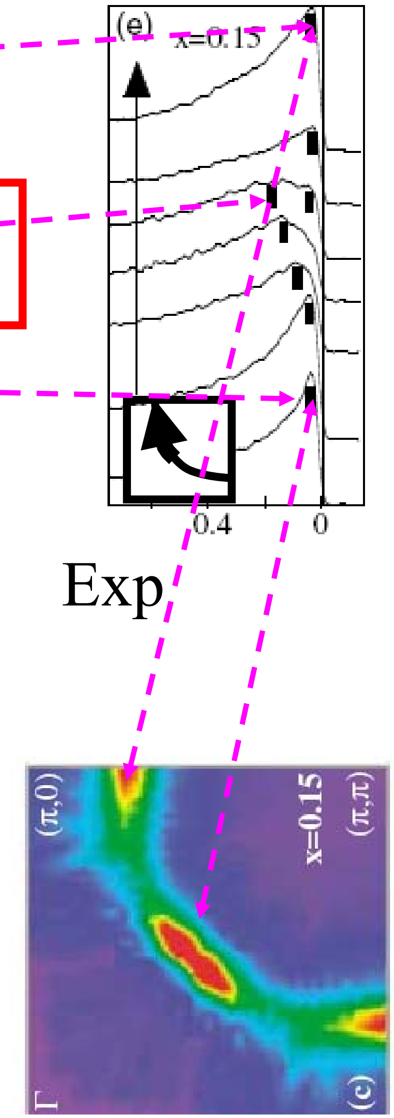
Armitage et al. PRL 2001

15% doping: EDCs along the Fermi surface TPSC



$U_{min} < U < U_{max}$

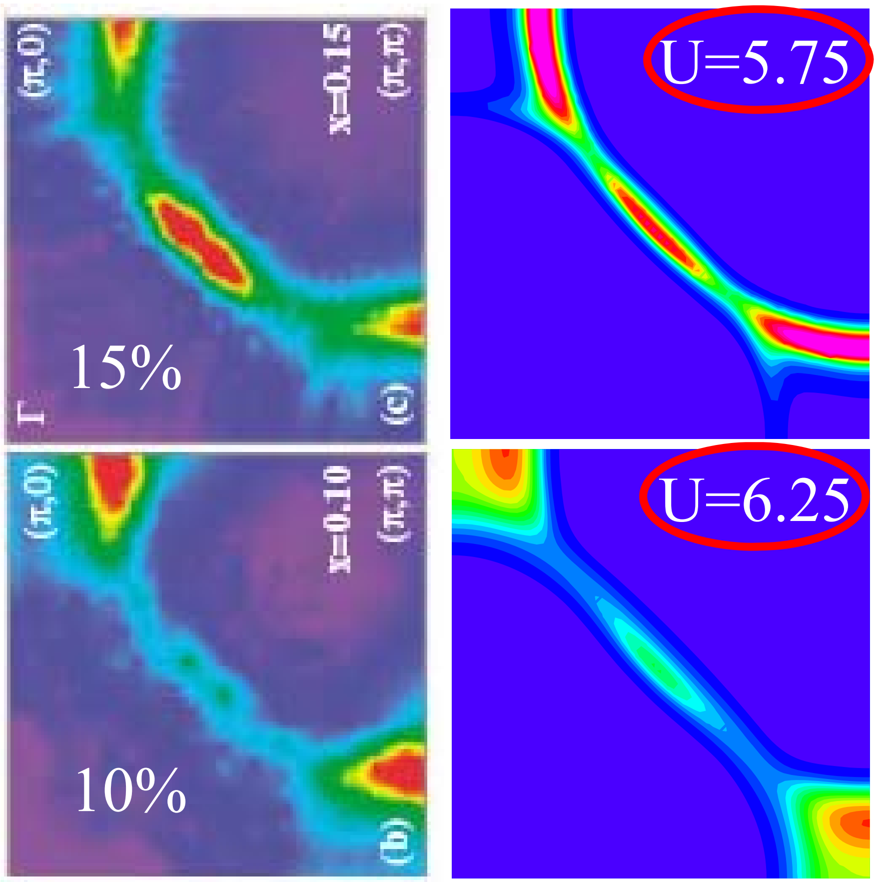
U_{max} also from CPT



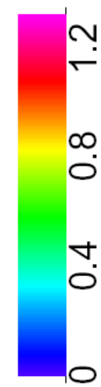
Hankevych, Kyung, A.-M.S.T., PRL, sept. 2004

Fermi surface plots

Hubbard repulsion *U* has to…



be not too large

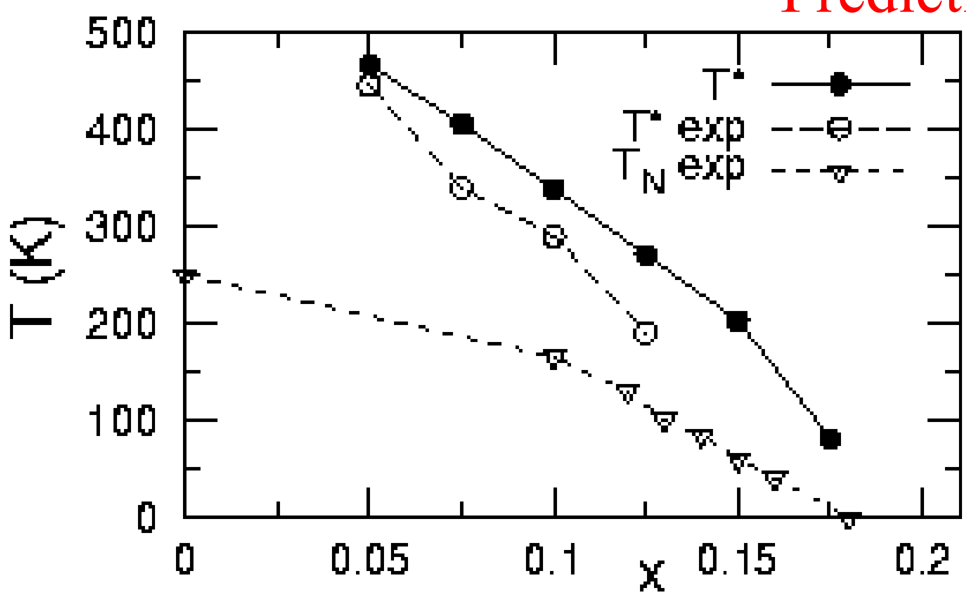


increase for
smaller doping

B.Kyung *et al.*,PRB **68**, 174502 (2003)

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

Pseudogap temperature and QCP



Prediction ➢ $\xi \approx \xi_{th}$ at PG temperature T^*, and $\xi > \xi_{th}$ for $T < T^*$

supports further AFM fluctuations origin of PG

➢ $\Delta_{PG} \approx 10 k_B T^*$ comparable with optical measurements

Hankevych, Kyung, A.-M.S.T., PRL 2004 : Expt: Y. Onose et al., PRL (2001).

Thermal de Broglie wavelength

$$\Delta\varepsilon \sim k_B T$$

$$\nabla_{\mathbf{k}}\varepsilon \; \Delta k \sim k_B T$$

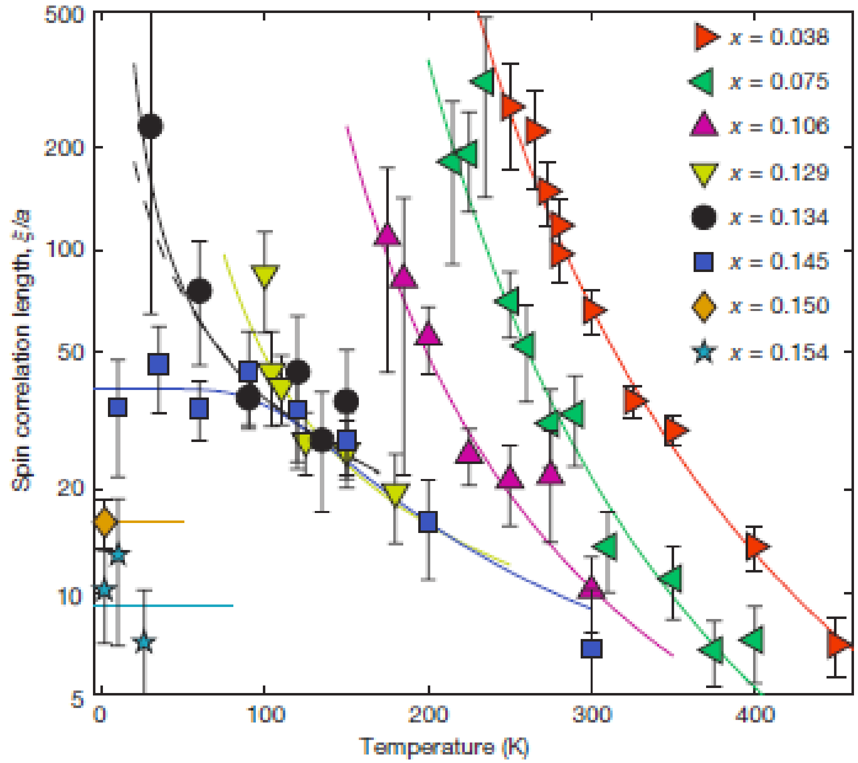
$$\xi_{th} \sim \frac{v_F}{T}$$

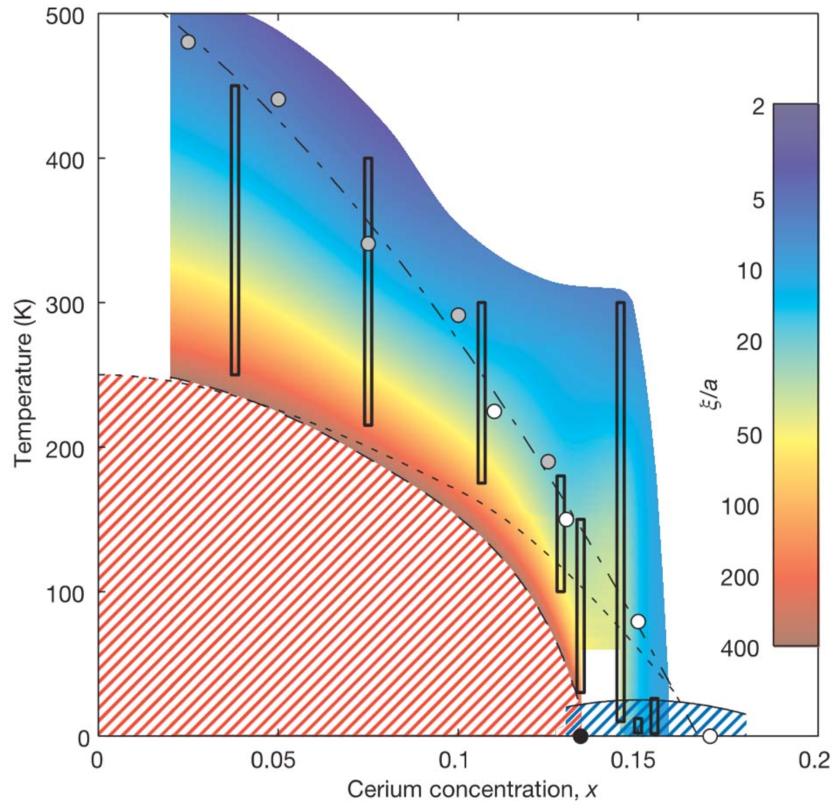
$$\Delta k \sim \frac{k_B T}{\hbar v_F}$$

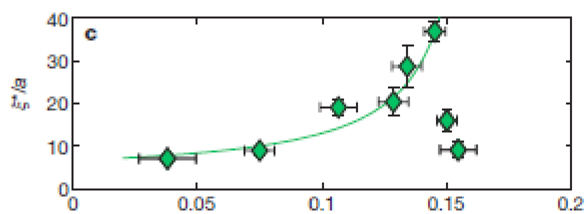
$$\frac{2\pi}{\xi_{th}} \sim \frac{k_B T}{\hbar v_F}$$

e-doped pseudogap

E. M. Motoyama et al.. Nature 445, 186–189 (2007).







Vilk criterion $\xi^* = 2.6(2)\xi_{th}$.

UNIVERSITÉ DE SHERBROOKE

Precursor of SDW state (dynamic symmetry breaking)

- Y.M. Vilk and A.-M.S. Tremblay, J. Phys. Chem. Solids **56**, 1769-1771 (1995).
- Y. M. Vilk, Phys. Rev. B 55, 3870 (1997).
- J. Schmalian, *et al.* Phys. Rev. B **60**, 667 (1999).
- B.Kyung *et al.*,PRB **68**, 174502 (2003).
- Hankevych, Kyung, A.-M.S.T., PRL, sept 2004
- Kusko *et al.* PRB **66**, 140513 (2002).

UNIVERSITÉ DE SHERBROOKE

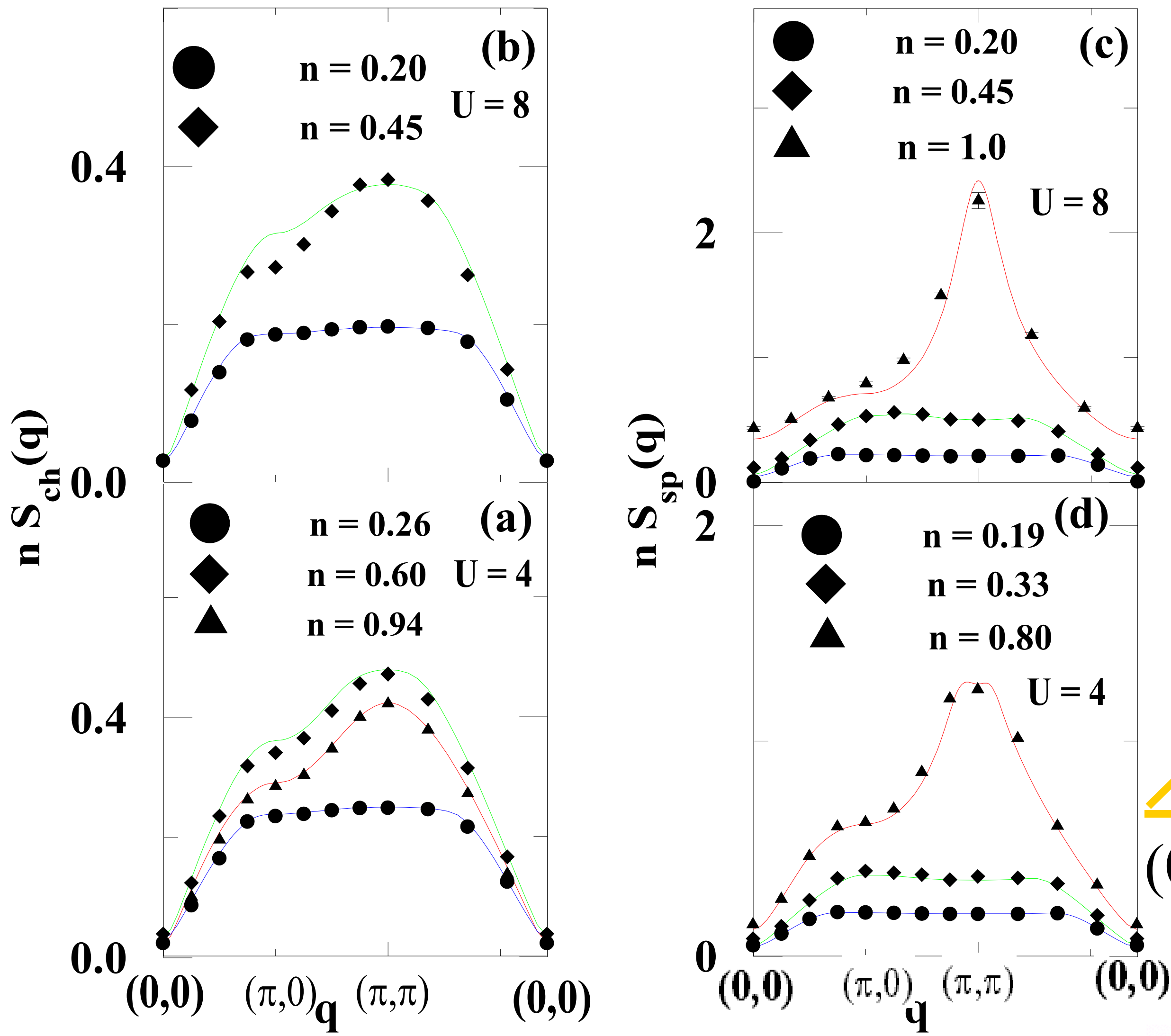
Benchmarks for TPSC

Normal state

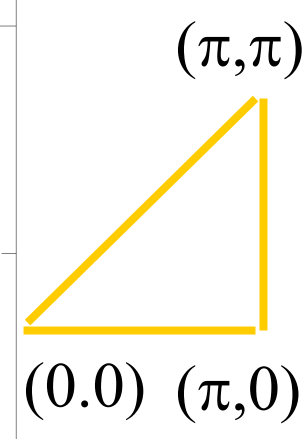
Benchmark comparison with QMC

Notes:
-F.L. parameters

-Self also Fermi-liquid



U > 0
β = 5
8 X 8

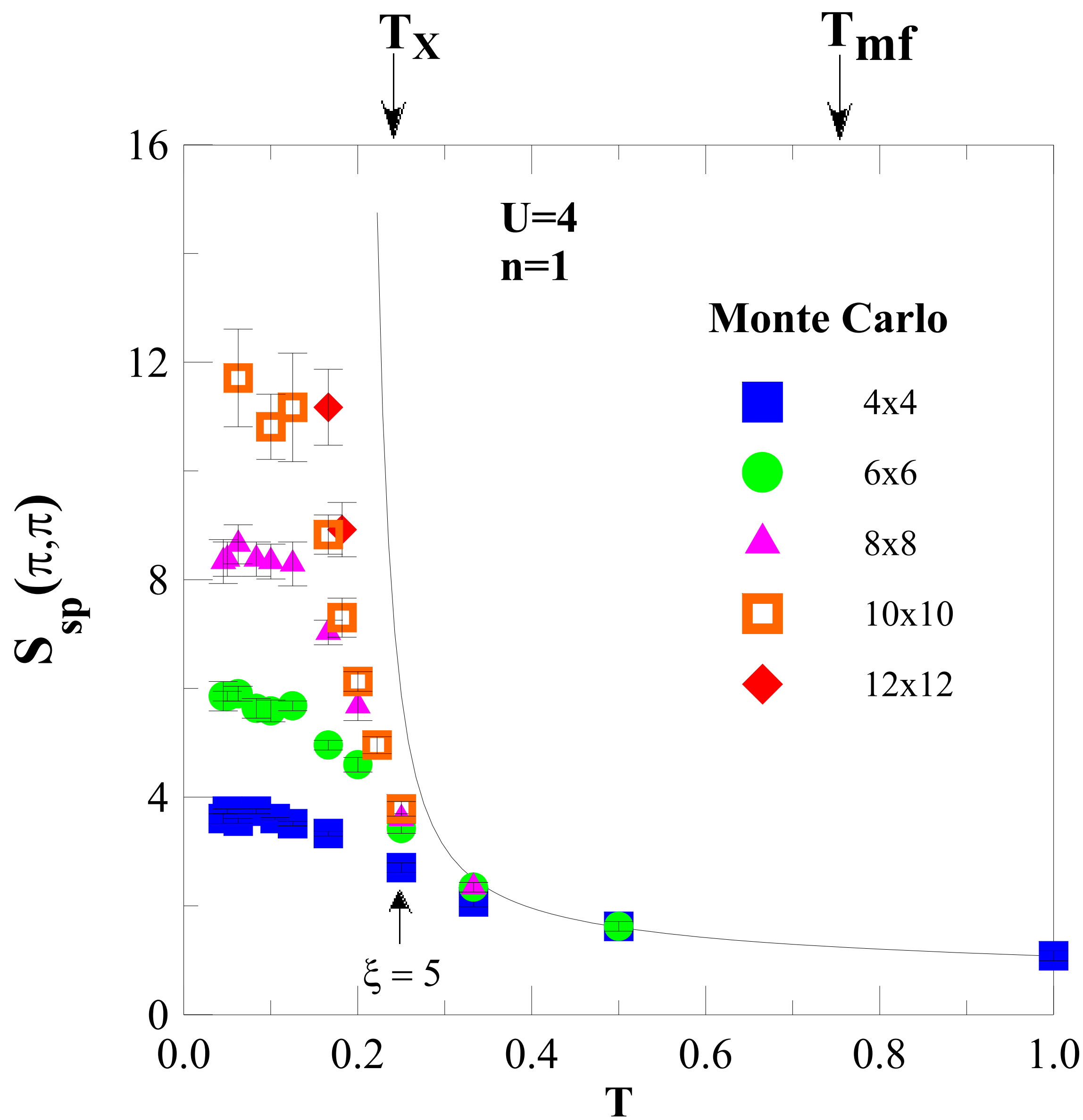


QMC + cal.: Vilk et al. P.R. B **49,** 13267 (1994)

UNIVERSITÉ DE SHERBROOKE

n=1

$\xi \sim \exp(C(T)/T)$



Calc.: Vilk et al. P.R. B **49,** 13267 (1994)

QMC: S. R. White, et al. Phys. Rev. **40**, 506 (1989).

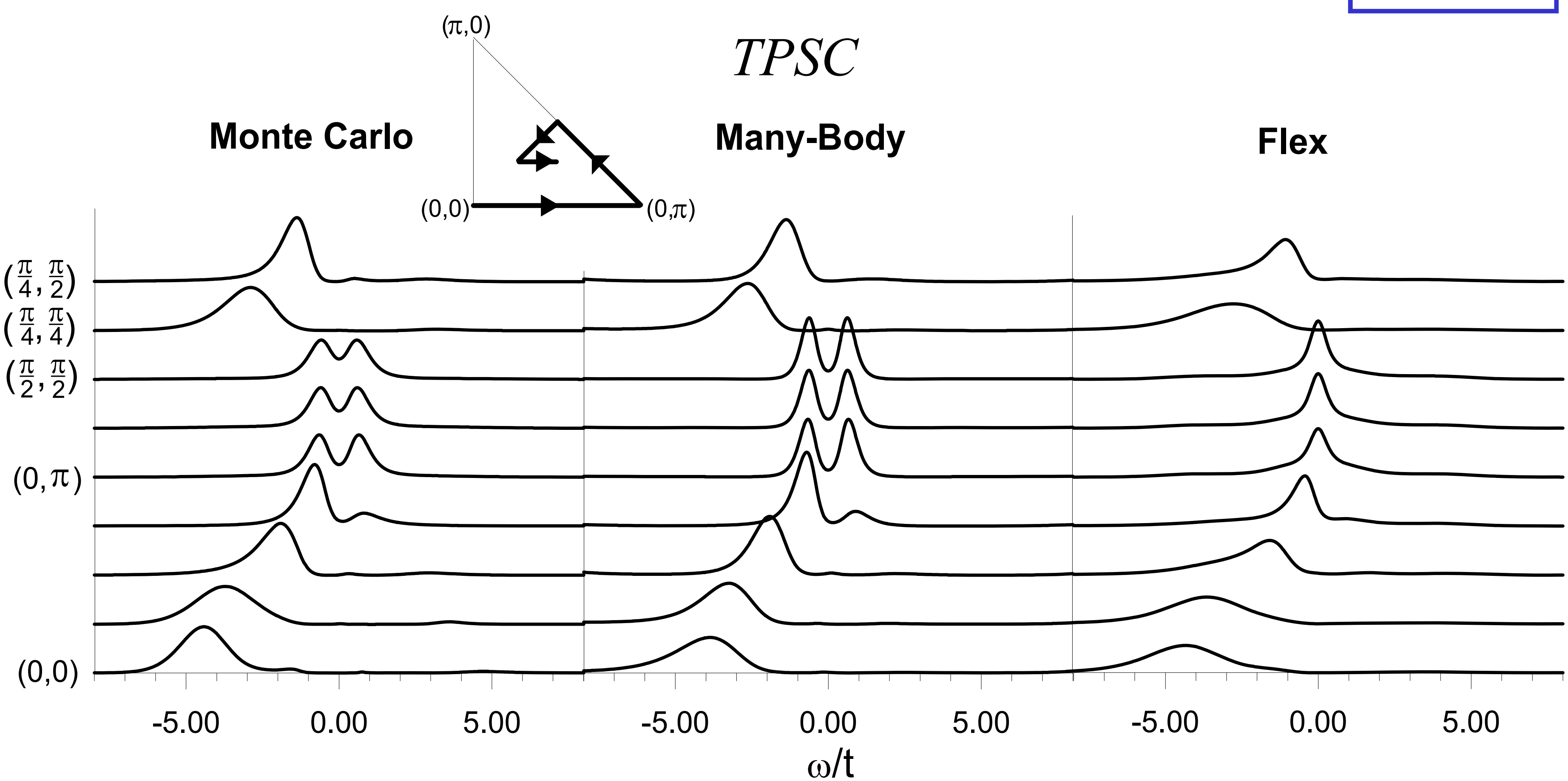
$O(N=\infty)$ A.-M. Daré, Y.M. Vilk and A.-M.S.T Phys. Rev. B **53**, 14236 (1996)

UNIVERSITÉ DE SHERBROOKE

Proofs...

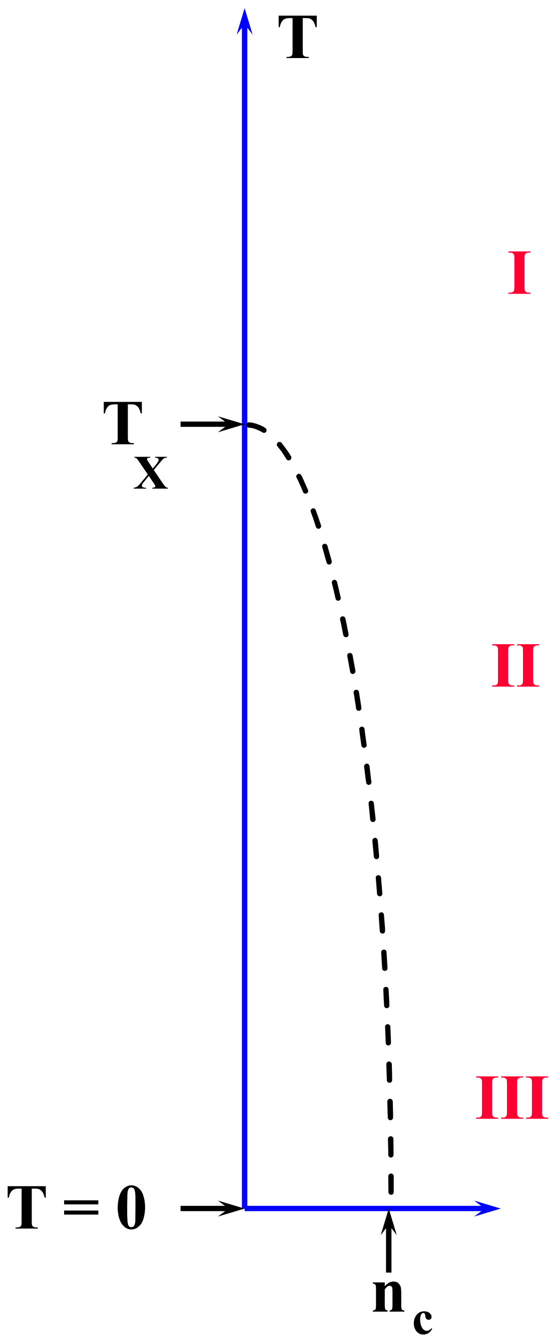
$U = +4$
$\beta = 5$

TPSC



Calc. + QMC: Moukouri et al. P.R. B 61, 7887 (2000).

UNIVERSITÉ DE SHERBROOKE


T
I
T_X
II
III
T = 0
n_c

Theoretical difficulties

Theory without small parameter: How should we proceed?

- Identify important physical principles and laws to constrain non-perturbative approximation schemes
  - From weak coupling (kinetic)
  - From strong coupling (potential)
- Benchmark against “exact” (numerical) results.
- Check that weak and strong correlation approaches agree in intermediate range.
- Compare with experiment

UNIVERSITÉ DE SHERBROOKE

TPSC: How it works

e-doped

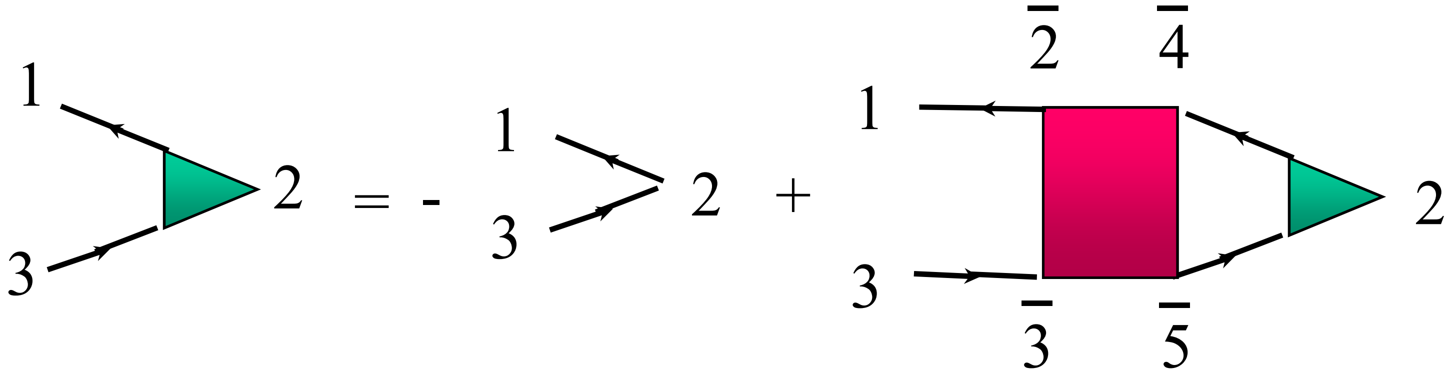
TPSC: general ideas

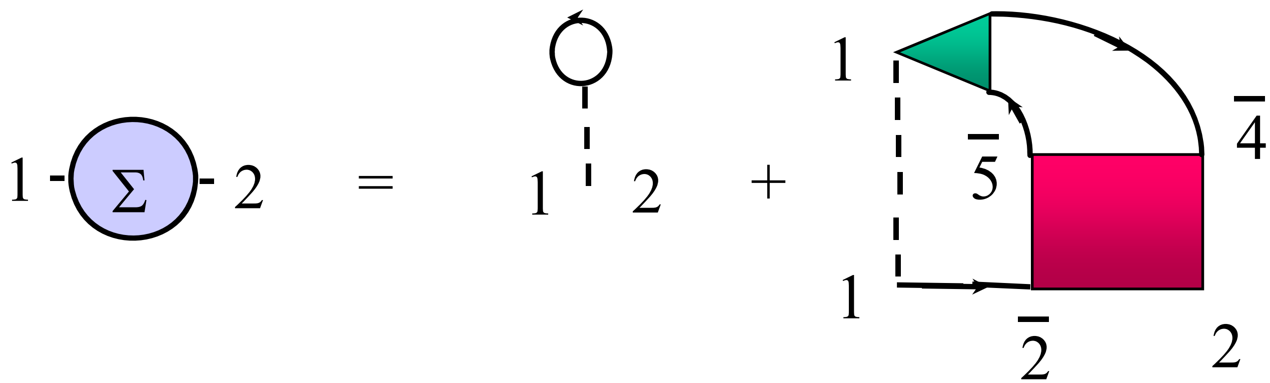
- General philosophy
  - Drop diagrams
  - Impose constraints and sum rules
    - Conservation laws
    - Pauli principle ($\langle n_\sigma^2 \rangle = \langle n_\sigma \rangle$)
    - Local moment and local density sum-rules
- Get for free:
    - Mermin-Wagner theorem
    - Kanamori-Brückner screening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

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

TPSC: Single-particle properties

A better approximation for single-particle properties (Ruckenstein)

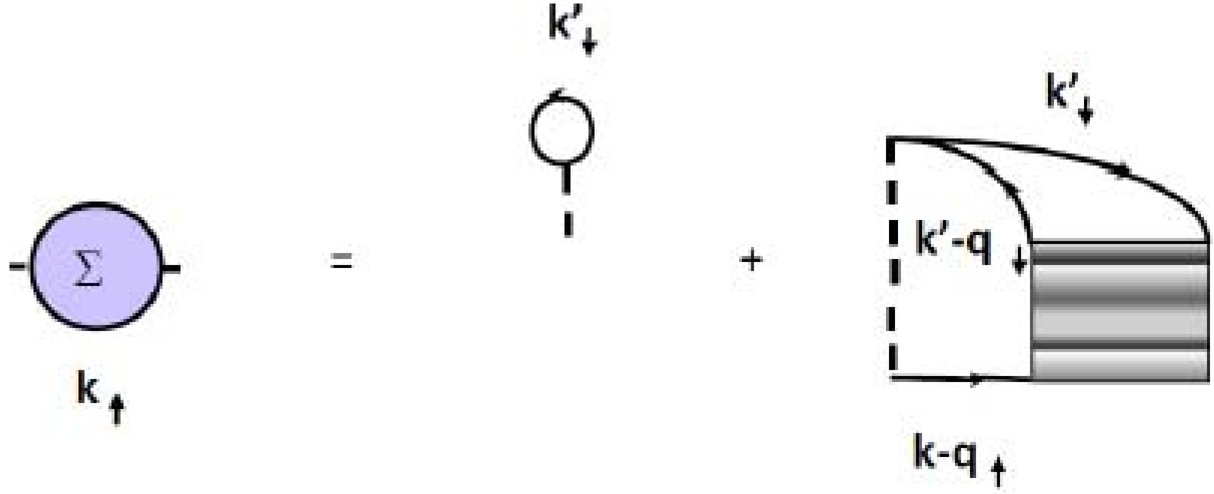




Y.M. Vilk and A.-M.S. Tremblay, J. Phys. Chem. Solids **56**, 1769 (1995).
Y.M. Vilk and A.-M.S. Tremblay, Europhys. Lett. **33**, 159 (1996);

N.B.: No Migdal theorem

Crossing symmetry



TPSC approach: two steps

I: Two-particle self consistency

1. Functional derivative formalism (conservation laws)

   (a) spin vertex: $$U_{sp} = \frac{\delta \Sigma_\uparrow}{\delta G_\downarrow} - \frac{\delta \Sigma_\uparrow}{\delta G_\uparrow}$$

   (b) analog of the Bethe-Salpeter equation:

$$\chi_{sp} = \frac{\delta G}{\delta \phi} = GG + GU_{sp}\chi_{sp}G$$

   (c) self-energy:

$$\Sigma_\sigma\left(1,\overline{1};\{\phi\}\right)G_\sigma\left(\overline{1},2;\{\phi\}\right) = -U\left\langle c^\dagger_{-\sigma}\left(1^+\right)c_{-\sigma}\left(1\right)c_\sigma\left(1\right)c^\dagger_\sigma\left(2\right)\right\rangle_\phi$$
$$\approx A_{\{\phi\}}G^{(1)}_{-\sigma}\left(1,1^+;\{\phi\}\right)G^{(1)}_\sigma\left(1,2;\{\phi\}\right)$$

2. Factorization

TPSC…

$$U_{sp} = U \frac{\langle n_\uparrow n_\downarrow \rangle}{\langle n_\uparrow \rangle \langle n_\downarrow \rangle}$$

Kanamori-Brückner screening

$$\chi_{sp}^{(1)}(q) = \frac{\chi_0(q)}{1 - \frac{1}{2} U_{sp} \chi_0(q)}$$

3. The F.D. theorem and Pauli principle

$$\left\langle (n_\uparrow - n_\downarrow)^2 \right\rangle = \langle n_\uparrow \rangle + \langle n_\downarrow \rangle - 2 \langle n_\uparrow n_\downarrow \rangle$$

$$\frac{T}{N} \sum_q \chi_{sp}^{(1)}(q) = n - 2 \langle n_\uparrow n_\downarrow \rangle$$

II: Improved self-energy

Insert the first step results

into exact equation: $\Sigma_\sigma(1, \bar{1}; \{\phi\}) G_\sigma(\bar{1}, 2; \{\phi\}) = -U \left\langle c_{-\sigma}^\dagger(1^+) c_{-\sigma}(1) c_\sigma(1) c_\sigma^\dagger(2) \right\rangle_\phi$

$$\Sigma_\sigma^{(2)}(k) = U n_{\bar{\sigma}} + \frac{U}{8} \frac{T}{N} \sum_q \left[3 U_{sp} \chi_{sp}^{(1)}(q) + U_{ch} \chi_{ch}^{(1)}(q) \right] G_\sigma^{(1)}(k+q)$$

SHERBROOKE

Internal accuracy check

Internal accuracy check

$$\frac{1}{2}\mathrm{Tr}\left(\Sigma^{(2)}G^{(1)}\right)=U\left\langle n_{\uparrow}n_{\downarrow}\right\rangle \qquad \frac{1}{2}\mathrm{Tr}\left(\Sigma^{(2)}G^{(2)}\right)$$

f- sum rule (conservation law)

$$\int\frac{d\omega}{\pi}\omega\chi''_{ch,sp}\left(\mathbf{q},\omega\right)=\lim_{\eta\to0}T\sum_{i\omega_n}\left(e^{-i\omega_n\eta}-e^{i\omega_n\eta}\right)i\omega_n\chi_{ch,sp}\left(\mathbf{q},i\omega_n\right)$$

$$=\frac{1}{N}\sum_{\mathbf{k}\sigma}\left(\epsilon_{\mathbf{k}+\mathbf{q}}+\epsilon_{\mathbf{k}-\mathbf{q}}-2\epsilon_{\mathbf{k}}\right)n_{\mathbf{k}\sigma}$$

Main collaborators on TPSC


Liang Chen


Yury Vilk

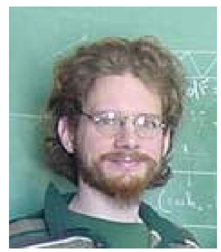

Bumsoo Kyung

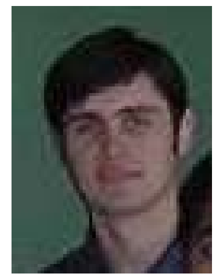

D. Poulin


S. Moukouri


F. Lemay


H. Touchette


J.S. Landry


V. Hankevych


A.-M. Daré


Dominic Bergeron


Bahman Davoudi

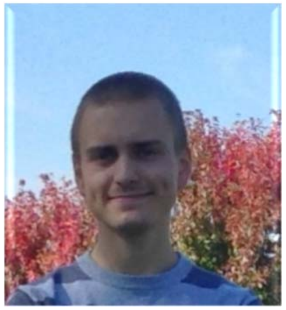

Syed Hassan


Steve Allen

UNIVERSITÉ DE SHERBROOKE

Part II

Strongly correlated superconductivity



Charles-David Hébert

Patrick Sémon

Organics : Phase diagram, finite T

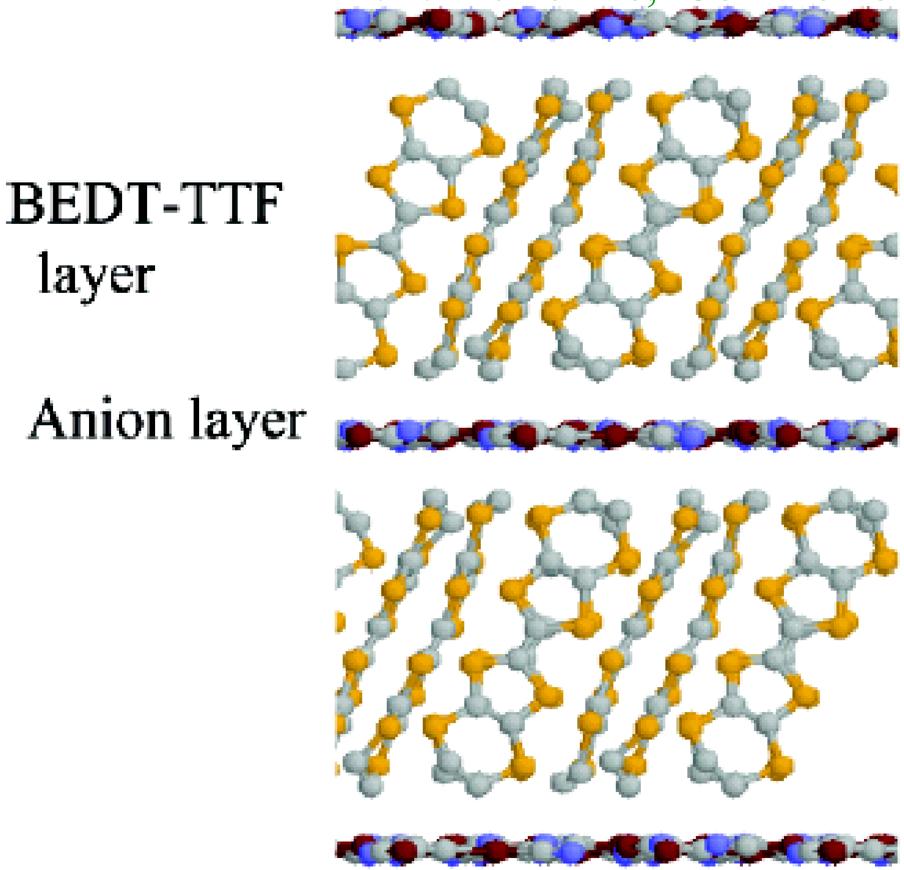
Made possible by algorithmic improvements

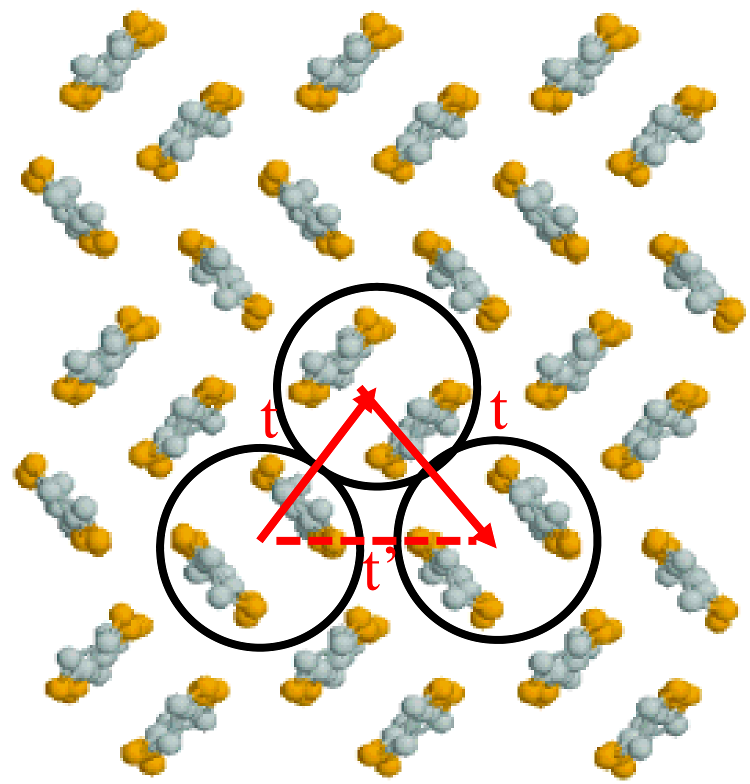
P. Sémon *et al.*
PRB **85**, 201101(R) (2012)
PRB **90** 075149 (2014);
and PRB **89**, 165113 (2014)

UNIVERSITÉ DE SHERBROOKE

Layered organics (κ–BEDT-X family)

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





Y. Shimizu, et al. Phys. Rev. Lett. **91**, 107001(2003)

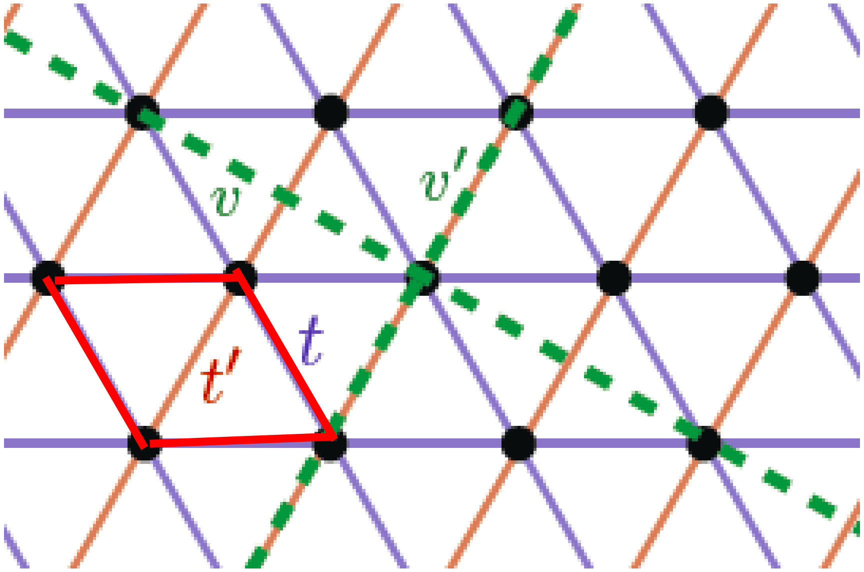
$$t \approx 50\,\mathrm{meV}$$

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

$$t'/t \sim 0.6 - 1.1$$

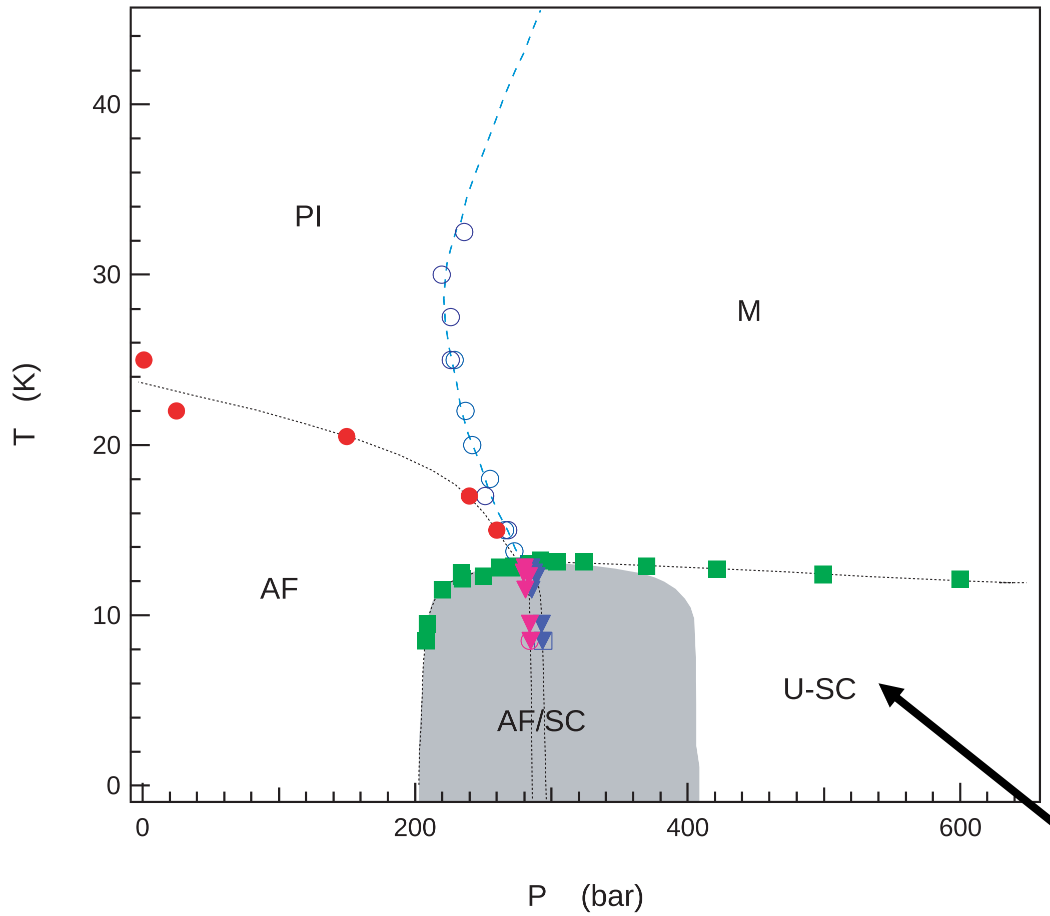
UNIVERSITÉ DE SHERBROOKE

Anisotropic triangular lattice



See: Poster Shaheen Acheche

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}

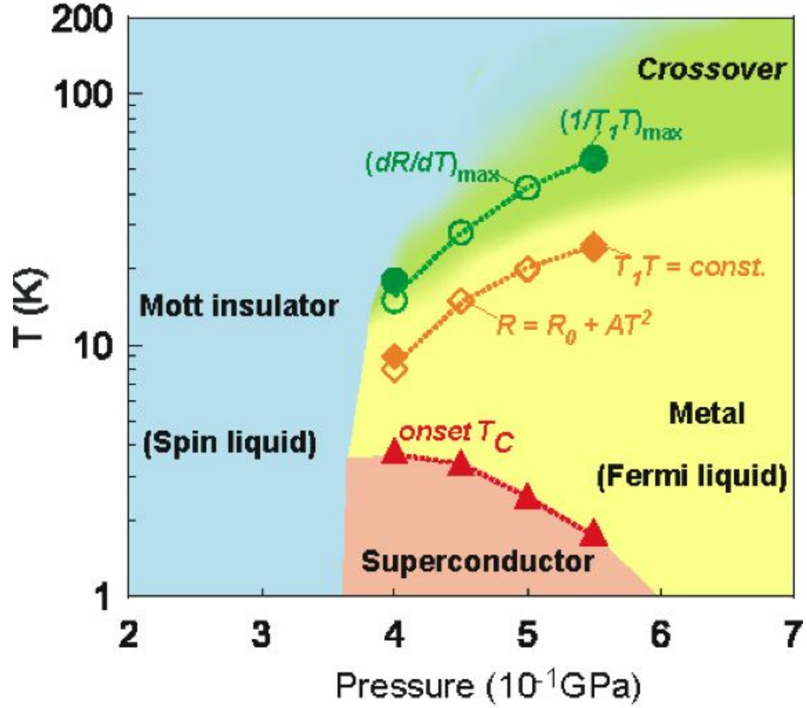
Powell, McKenzie cond-mat/0607078

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

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

Phase diagram at *n = 1*

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

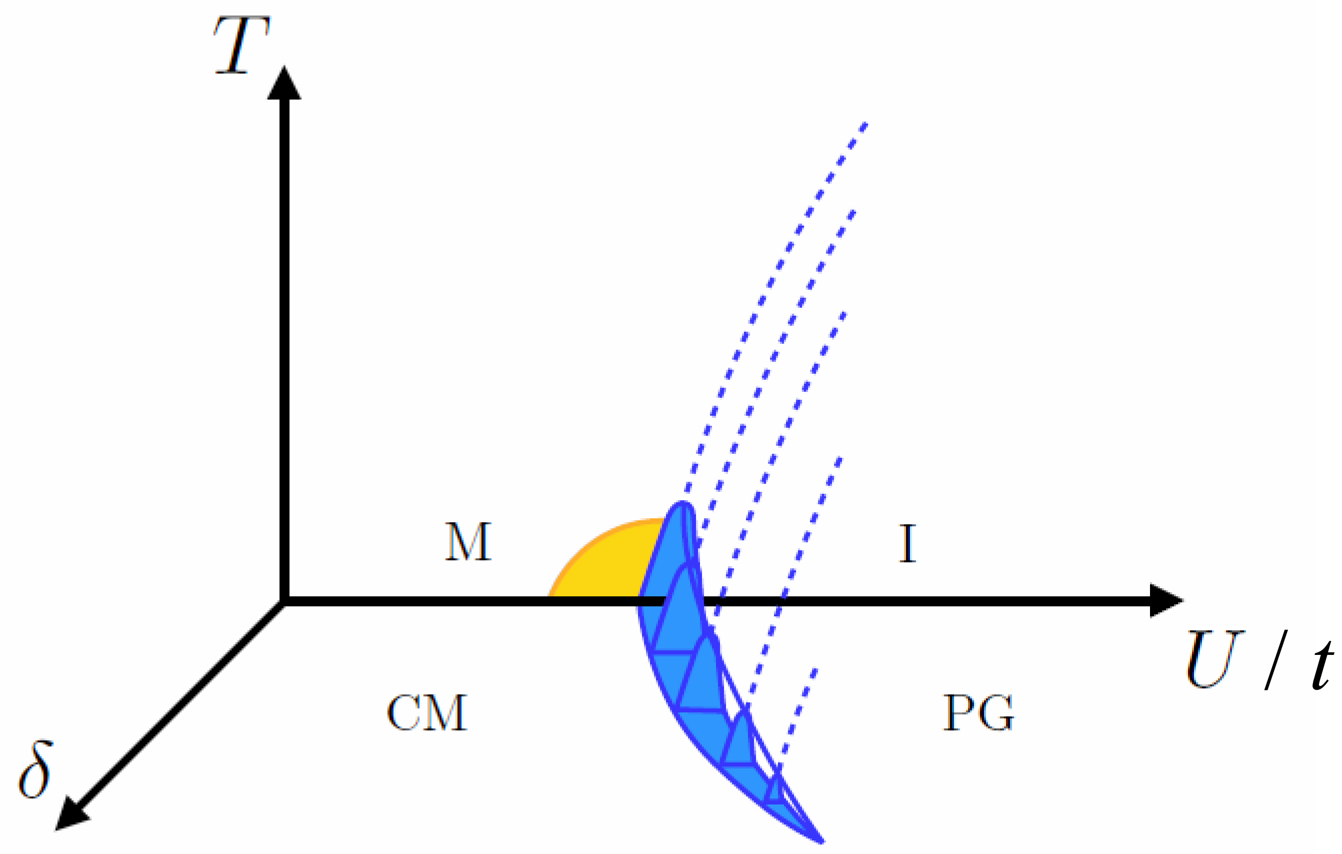


Y. Kurisaki, et al.
Phys. Rev. Lett. **95**, 177001(2005)

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

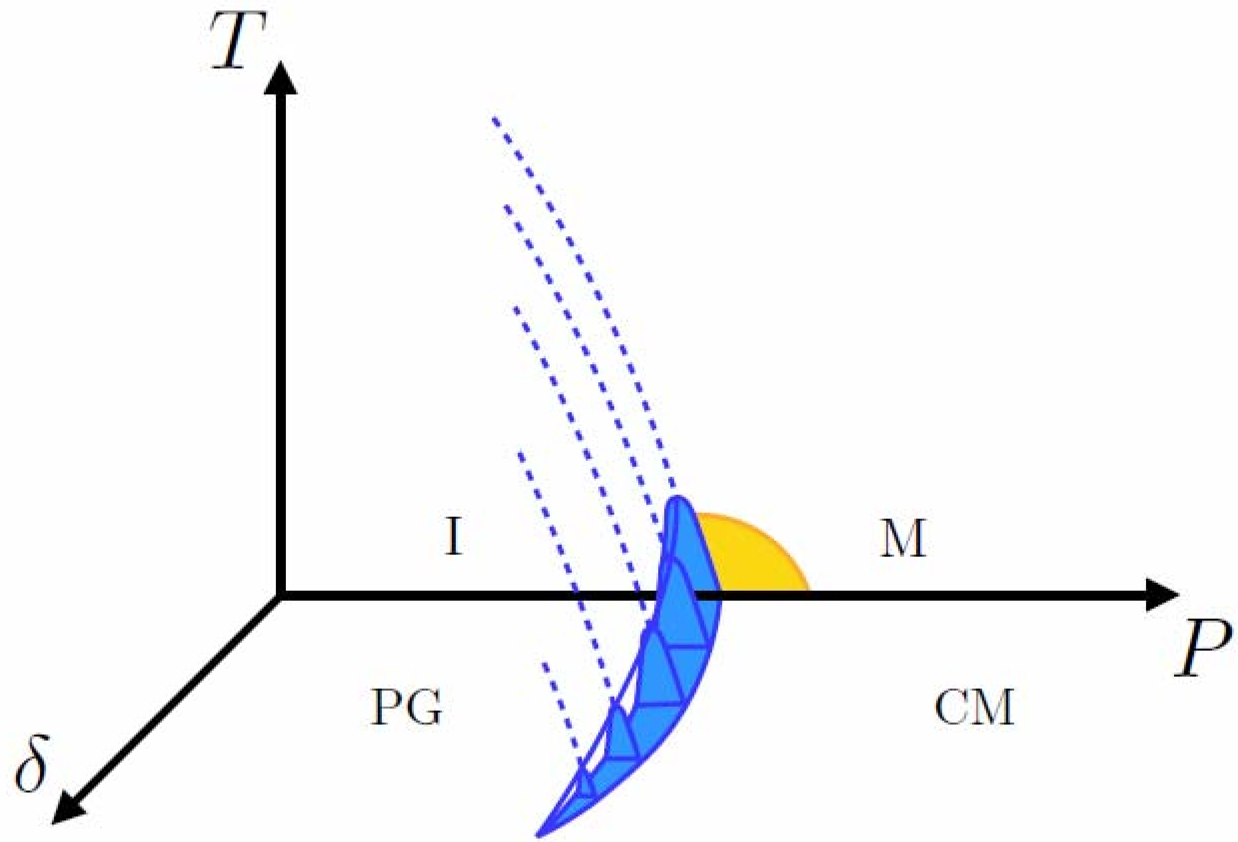
Superconductivity near the Mott transition

$n = 1$, $d = 2$ square lattice

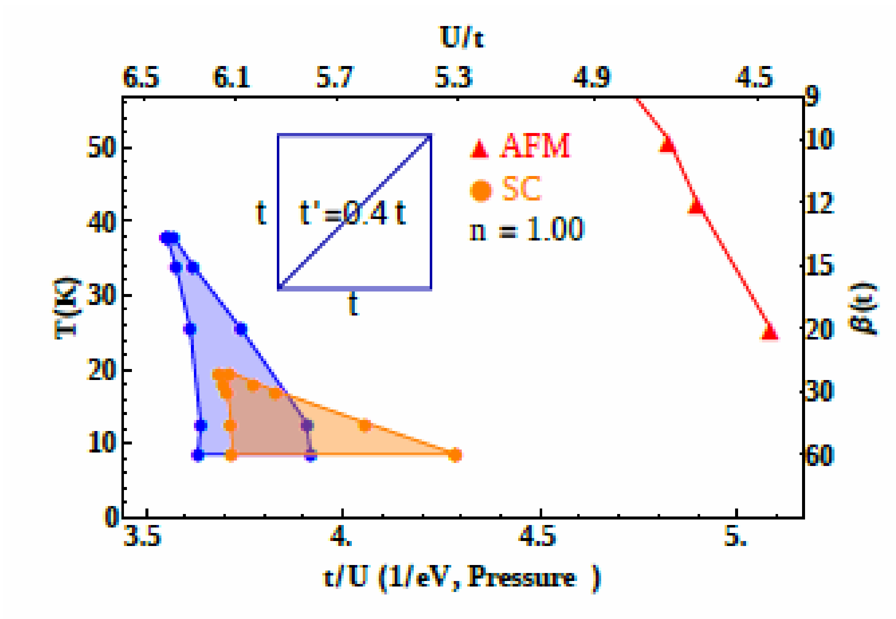


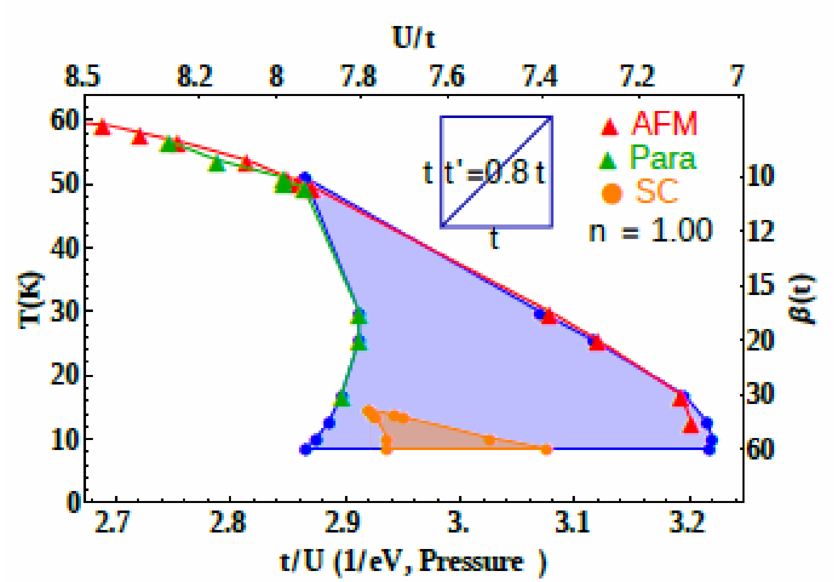
Superconductivity near the Mott transition

$n = 1, d = 2$ square lattice



Superconductivity near Mott transition ($n = 1$)



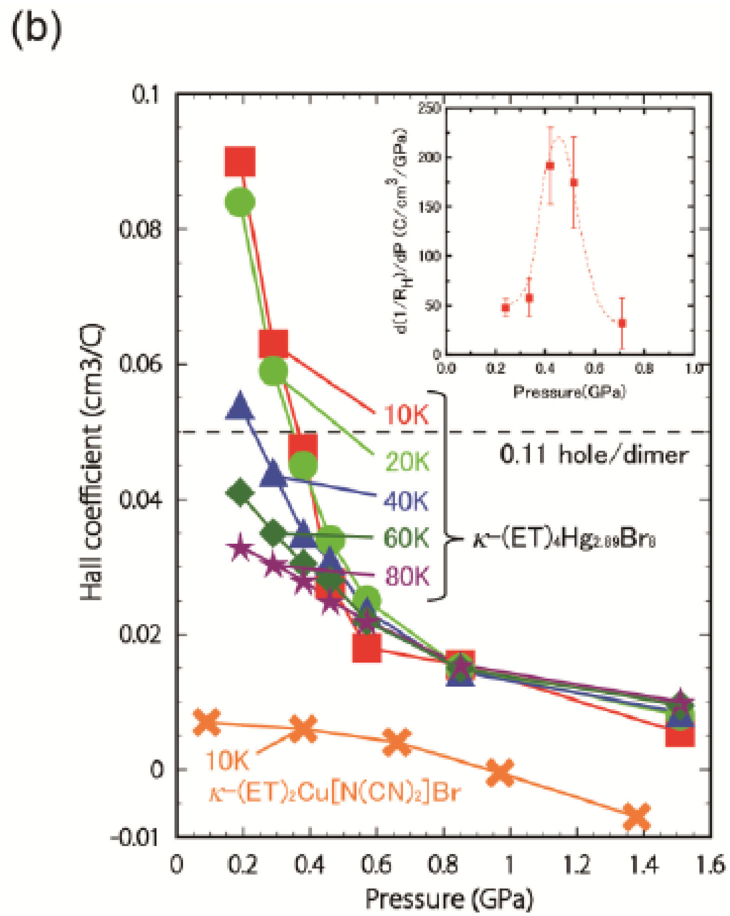


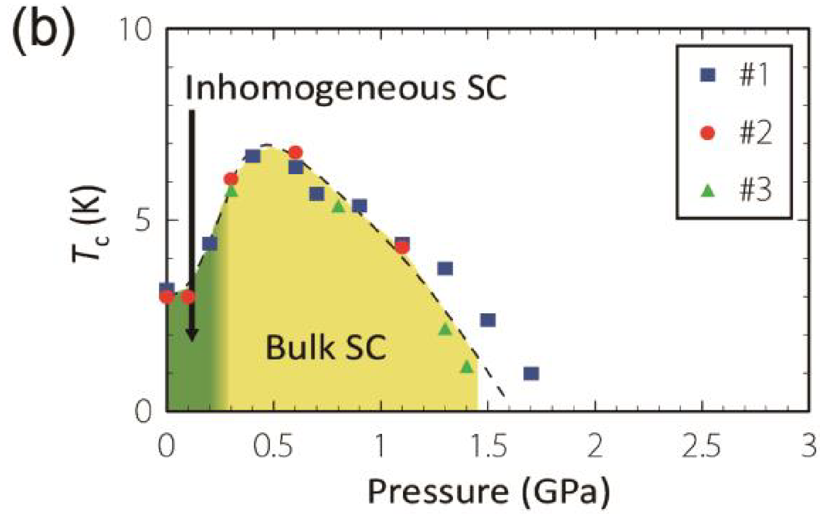
C.-D. Hébert, P. Sémon, A.-M.S. T PRB **92**, 195112 (2015)

UNIVERSITÉ DE SHERBROOKE

Doped Organics

Doped BEDT

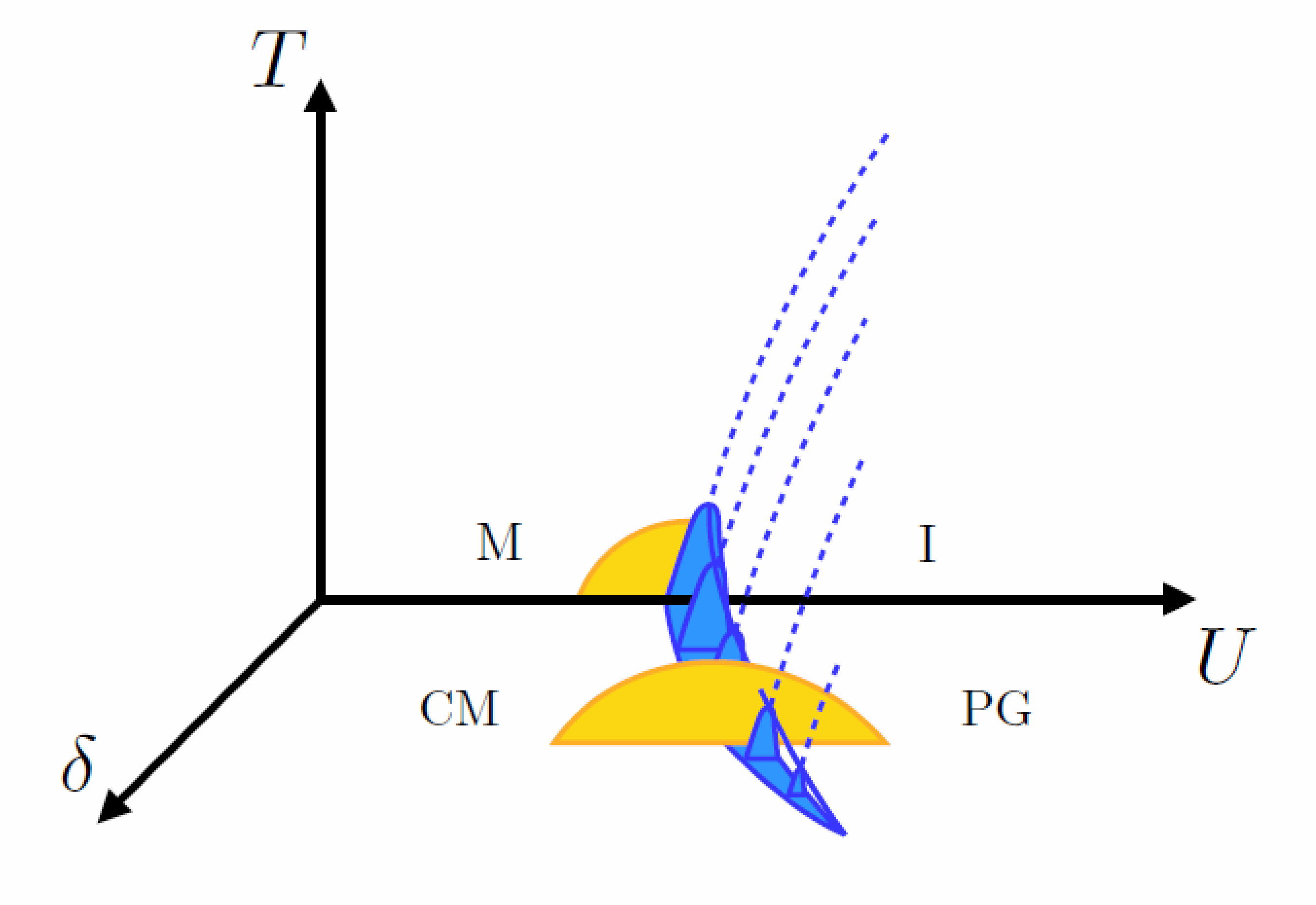




H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

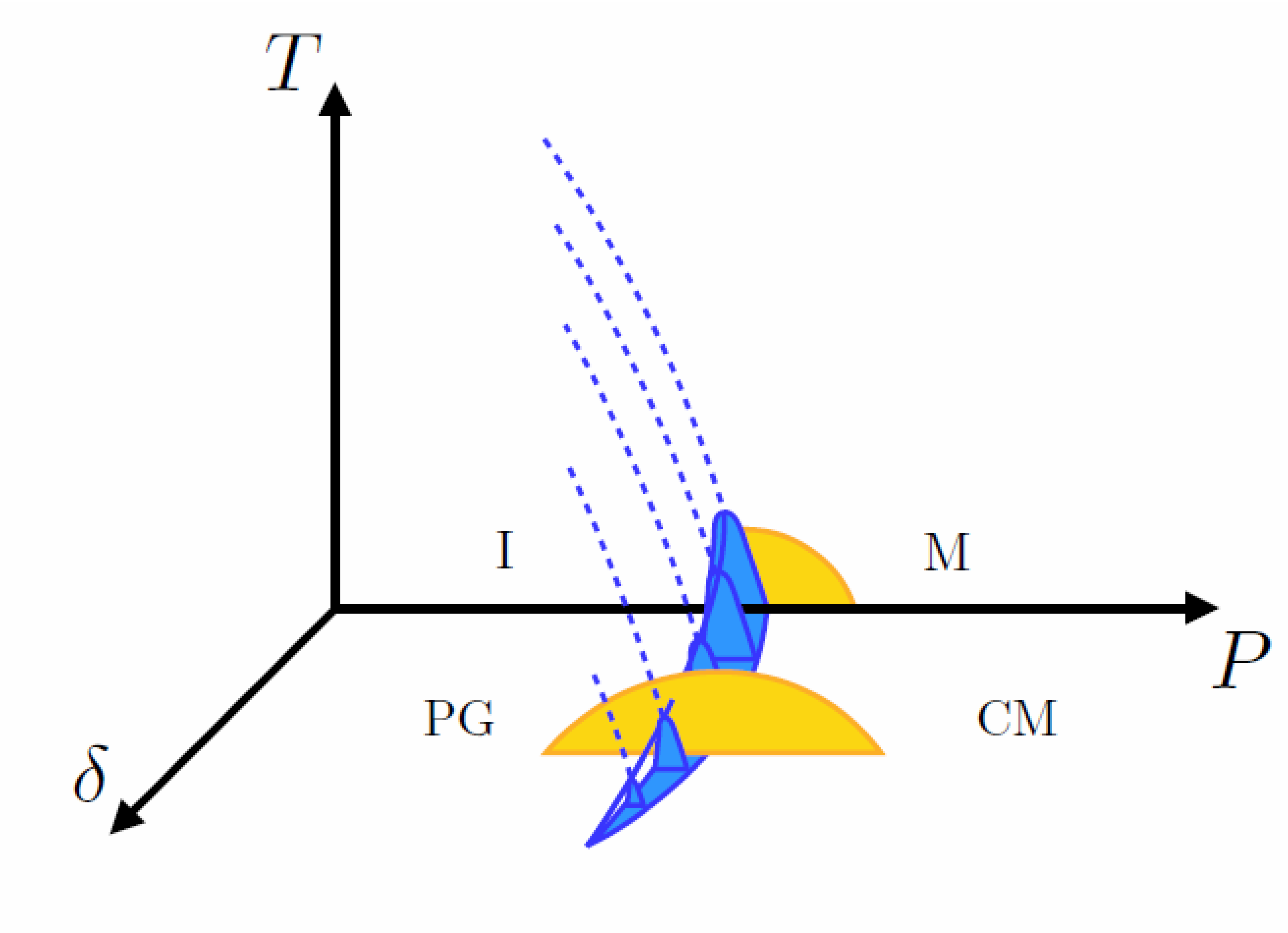
Doped organics

$n = 1$, $d = 2$ square lattice

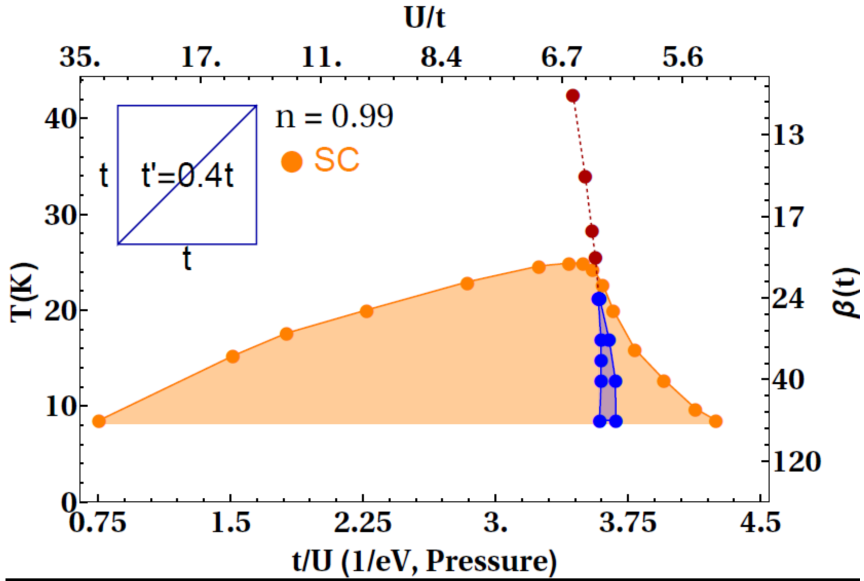


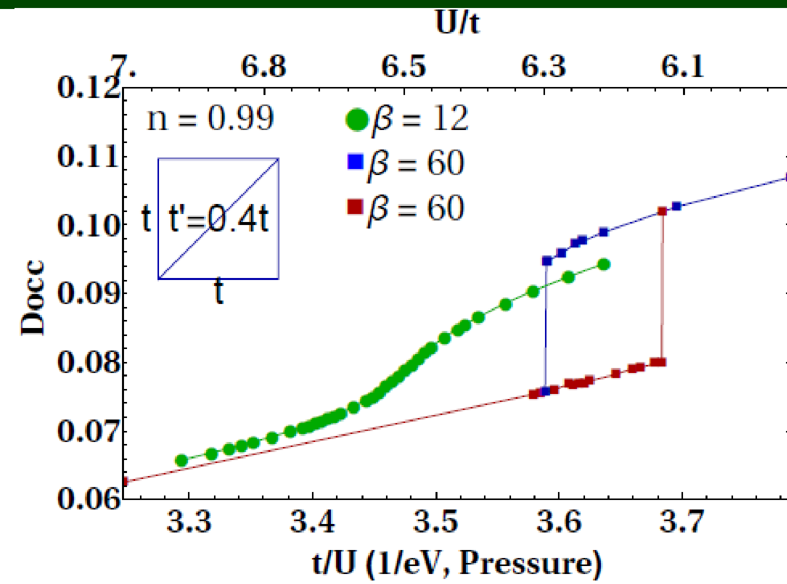
Doped organics

$n = 1, d = 2$ square lattice



First order and Widom line in organics



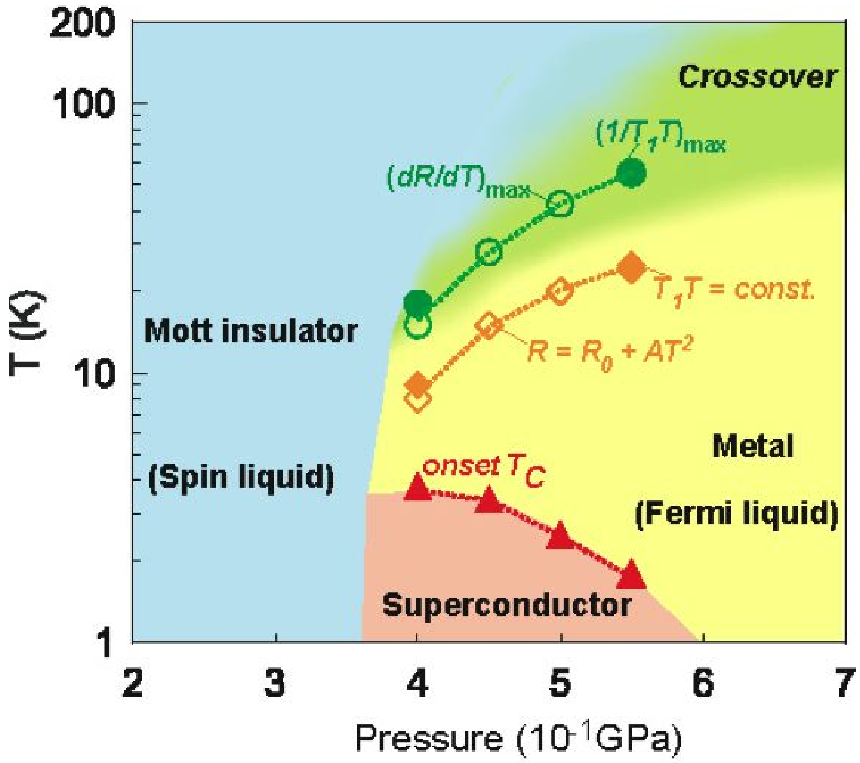


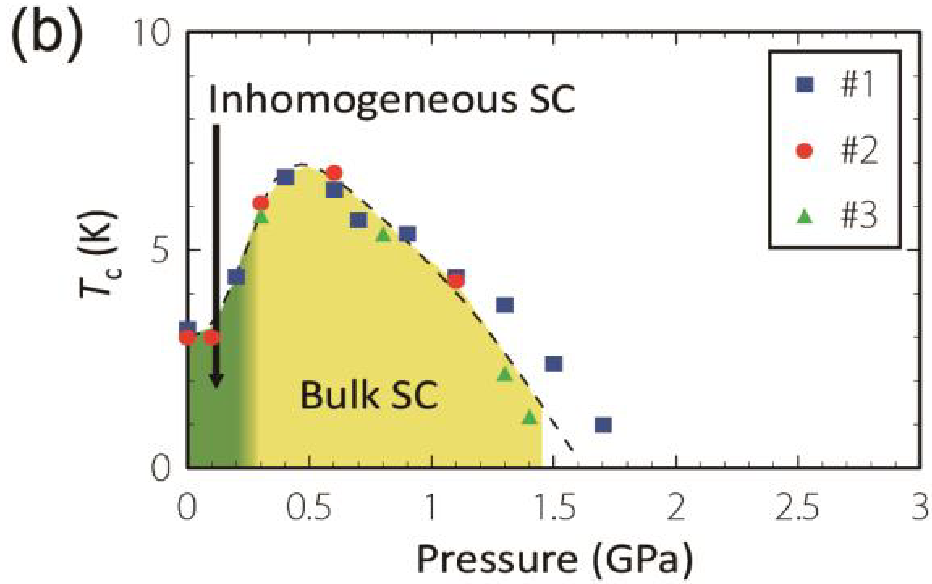
Compare: T. Watanabe, H. Yokoyama and M. Ogata JPS Conf. Proc. **3**, 013004 (2014)

C.-D. Hébert, P. Sémon, A.-M.S. T PRB **92**, 195112 (2015)

UNIVERSITÉ DE SHERBROOKE

Doped BEDT



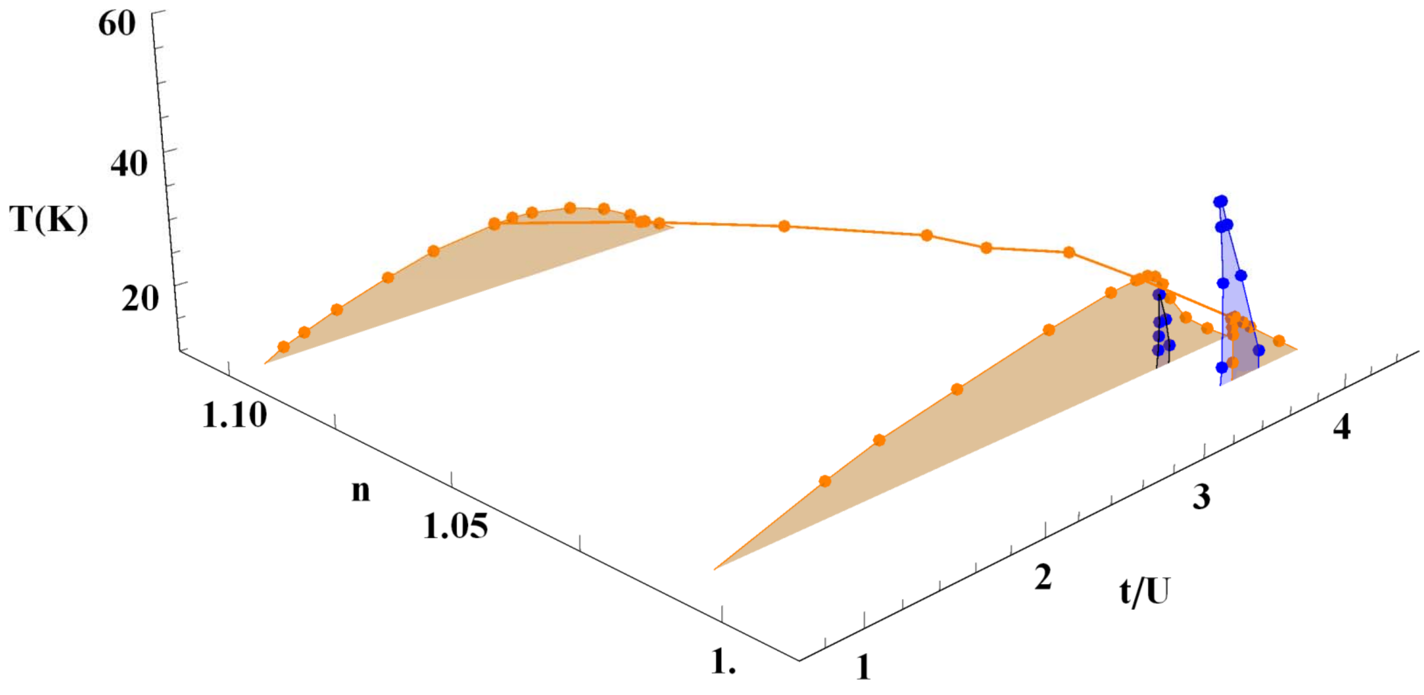


$n = 1$

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

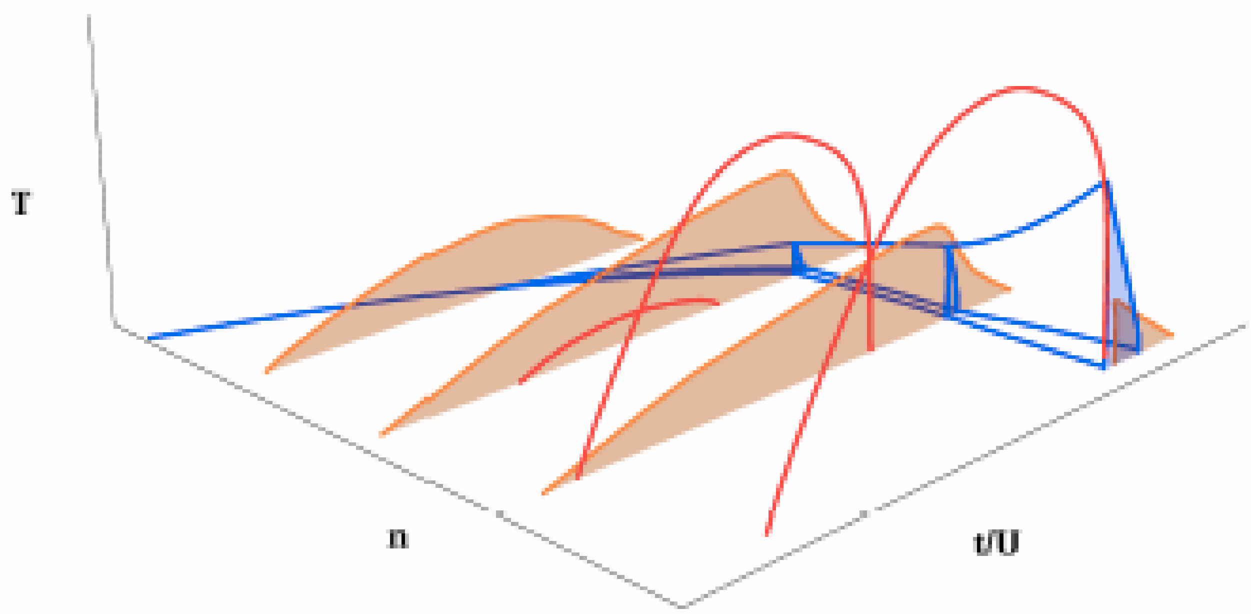
UNIVERSITÉ DE SHERBROOKE

t' = 0.4t overview



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

Generic case highly frustrated case



Summary : organics

- Agreement with experiment
  - SC: larger T_c and broader P range if doped
  - Larger frustration: Decrease T_N *much more* than T_c
  - Normal state metal to pseudogap crossover
- Predictions
  - First order transition at low T in normal state (B induced)
  - Crossovers in SC state associated with normal state.
- Physics
  - SC dome without an AFM QCP. Extension of Mott
  - SC from short range J.
  - T_c dome maximum near normal state 1st order

UNIVERSITÉ DE SHERBROOKE

Pairing mechanism

Back to high T_c

The glue

A cartoon strong correlation picture

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

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

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

Pitaevskii Brückner:

Pair state orthogonal to repulsive core of Coulomb interaction

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

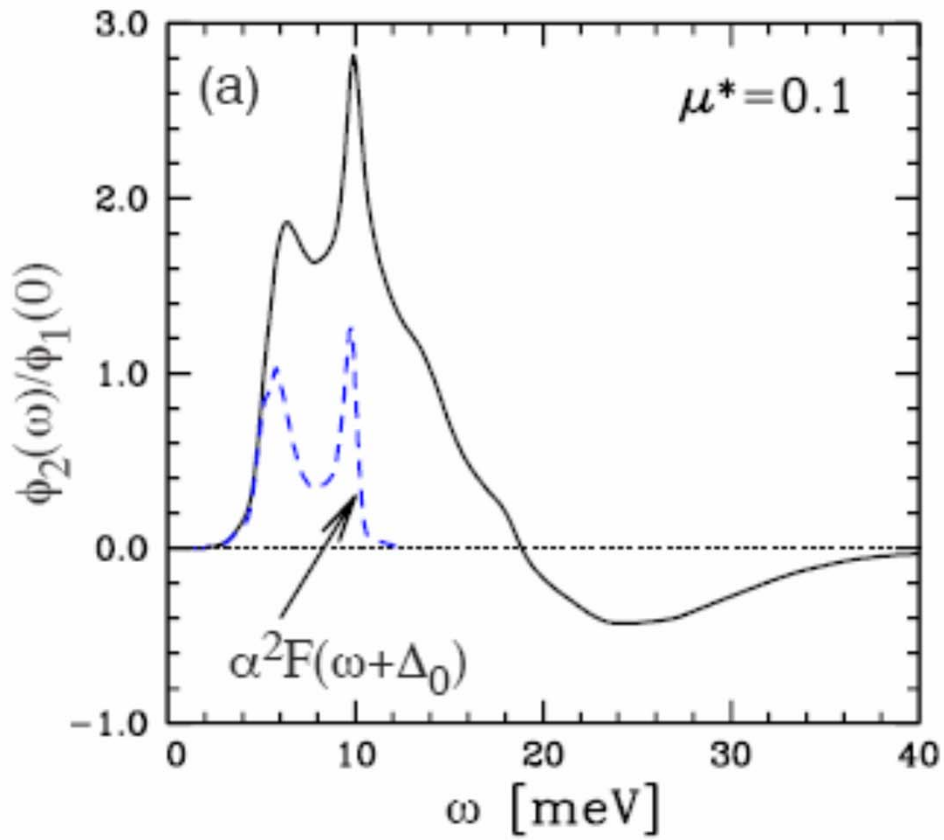
Miyake, Schmitt–Rink, and Varma P.R. B **34**, 6554-6556 (1986)

More sophisticated Slave Boson: Kotliar Liu PRB 1988

UNIVERSITÉ DE SHERBROOKE

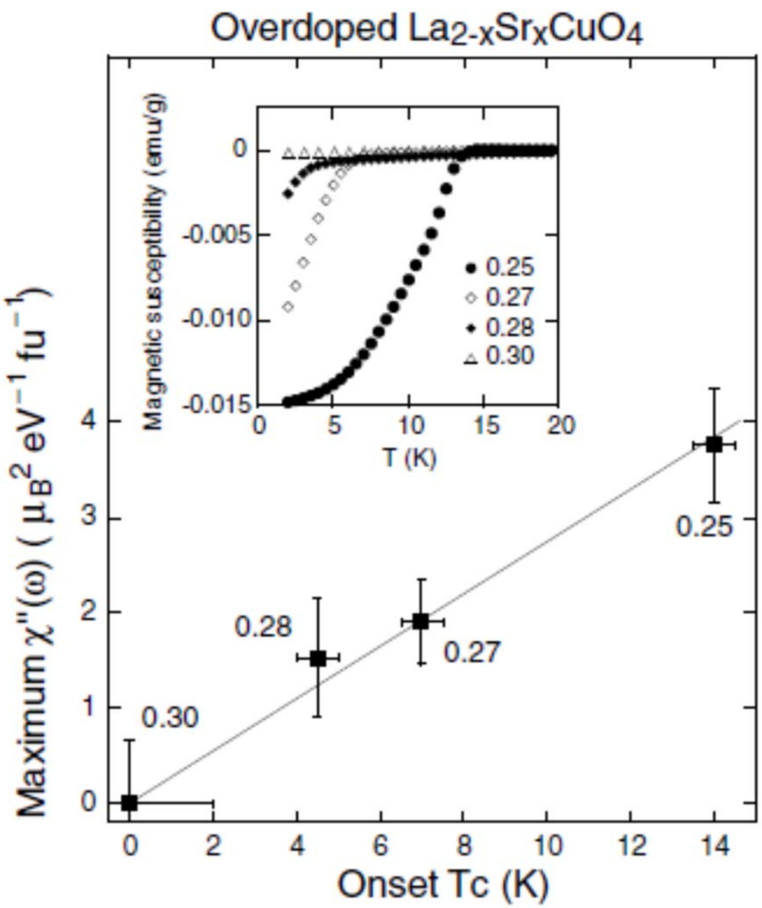
Im Σ_{an} and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

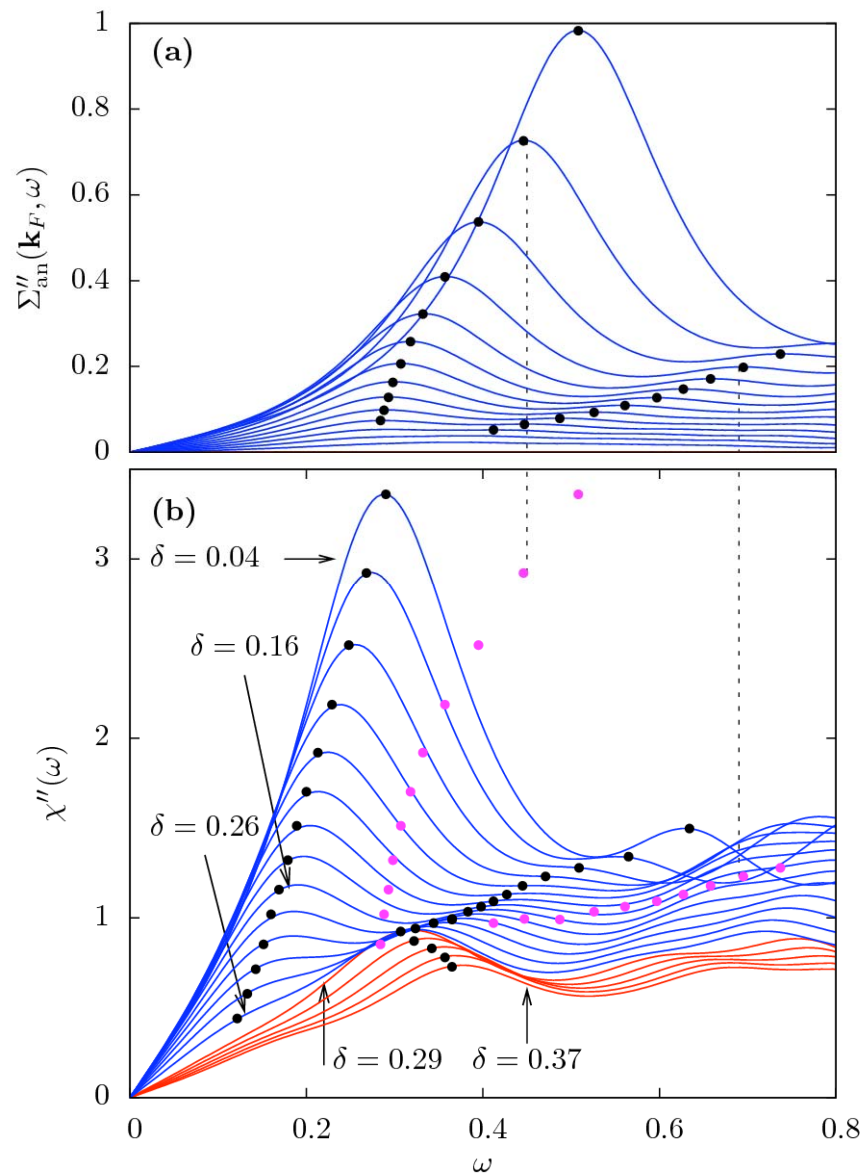


The glue

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



Wakimoto … Birgeneau PRL (2004)



The glue and neutrons

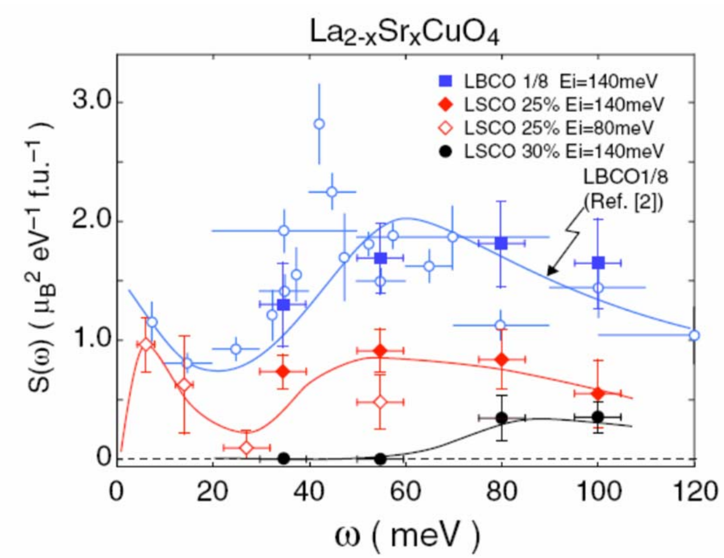
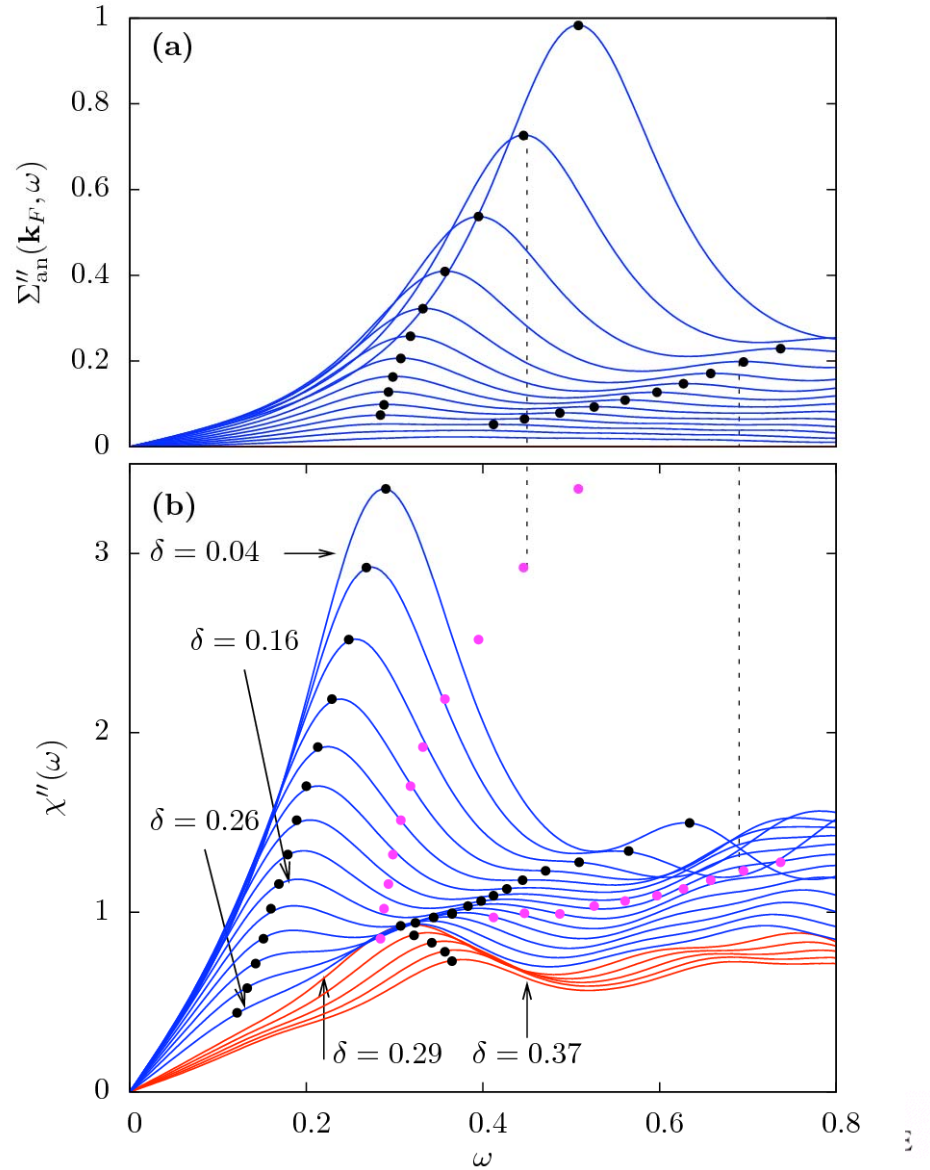


FIG. 3 (color online). **Q**-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i = 140$ meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO 1/8 (open circles) from [2]. The solid lines following data of LSCO $x = 0.25$ and 0.30 are guides to the eyes.

Wakimoto … Birgeneau PRL (2007);
PRL (2004)



The glue in CDMFT and DCA

Th. Maier, D. Poilblanc, D.J. Scalapino, PRL (2008)

M. Civelli, PRL **103**, 136402 (2009)

M. Civelli PRB **79**, 195113 (2009)

E. Gull, A. J. Millis PRB 90, 041110(R) (2014)

S. Sakai, M. Civelli, M. Imada arXiv:1411.4365

Frequencies important for pairing

Bumsoo Kyung

David Sénéchal

Anomalous Green function

$$[\mathcal{F}_{an}(t)]_{lm} = -i\theta(t)\,\langle\{\hat{c}_{l\uparrow}(t), \hat{c}_{m\downarrow}(0)\}\rangle_{\mathcal{H}_{AIM}}$$

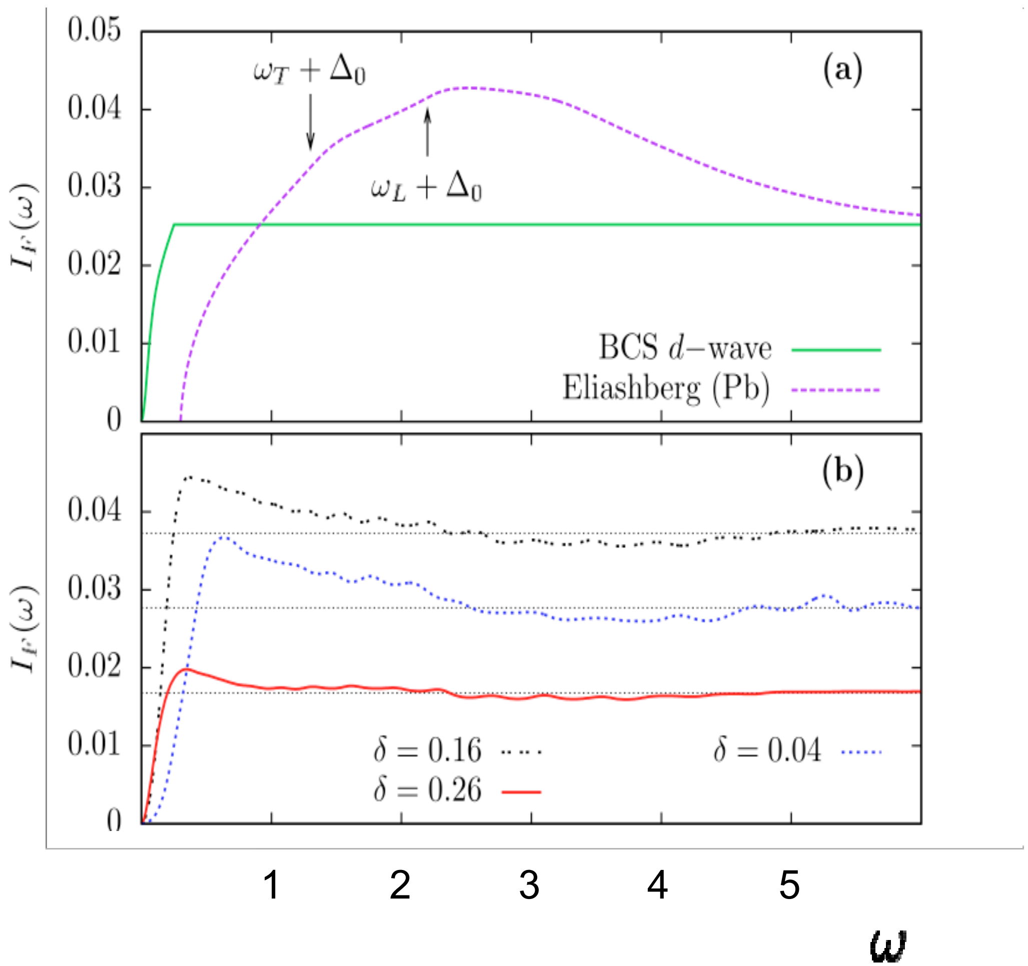
Anomalous spectral function

$$[A_{an}(\omega)]_{lm} = -\frac{1}{\pi}\,\mathrm{Im}\,[\mathcal{F}_{an}(\omega)]_{lm}$$

Cumulative order parameter:

$$I_{\mathcal{F}}(\omega) = -\int_0^{\omega}\frac{d\omega'}{\pi}\,\mathrm{Im}\,[\mathcal{F}_{an}(\omega')]_{lm}$$

$$I_{\mathcal{F}}(\omega)\xrightarrow[\omega\to+\infty]{}\langle\hat{c}_{l\uparrow}\hat{c}_{m\downarrow}\rangle_{\mathcal{H}_{AIM}}$$



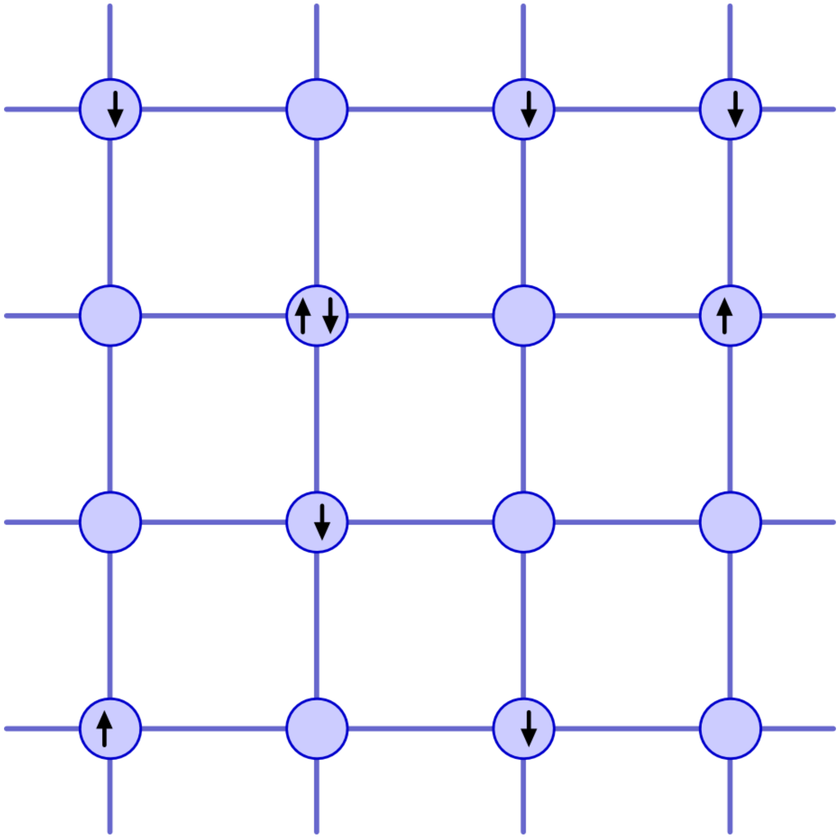
Scalapino, Schrieffer, Wilkins, Phys. Rev. **148** (1966)

UNIVERSITÉ DE SHERBROOKE

Nearest-neighbor repulsion should destroy Tc?

UNIVERSITÉ DE SHERBROOKE

Extended Hubbard model



$$\hat{\mathcal{H}} = -t \sum_{\langle i,j \rangle\ \sigma} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + c.h \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + V \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j - \mu \sum_{i} \hat{n}_i$$

UNIVERSITÉ DE SHERBROOKE

Resilience to near-neighbor repulsion V (Scalapino)

$$\hat{\mathcal{H}}_{Hubbard} = -\sum_{\langle i,j\rangle_{1,2,3}\,\sigma} \left(t_{ij}\,\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + c.h\right) + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + V\sum_{\langle i,j\rangle}\hat{n}_i\hat{n}_j - \mu\sum_{i\,\sigma}\hat{n}_{i\sigma}$$

$YBa_2Cu_3O_7$: $t = 1$ $t' = -0.3$ $t'' = 0.2$

We expect superconductivity to disappear when:

$V > \frac{U^2}{W}$ **In weakly correlated case U/W < 1**

$V > J$ **In mean-field strongly correlated case**

In cuprates:

$V = 400\,\mathrm{meV}$

$J = 130\,\mathrm{meV}$

$U_c = V_c/[1 + N(0)V_c \ln(E_F/\omega_c)]$ Anderson-Morel

S. Onari, R. Arita, K. Kuroki et H. Aoki, PRB **70**, 094523 (2004)

S. Raghu, E. Berg, A. V. Chubukov et S. A. Kivelson, PRB **85**, 024516 (2012)

S. Sorella, et al. Phys. Rev. Lett. 88, 117002 (2002)

d-wave in mean-field

$$\hat{\mathcal{H}}_{\text{modèle } t-J} = -t \sum_{\langle i,j \rangle\, \sigma} \hat{P}\left(\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + c.h\right)\hat{P} + J \sum_{\langle i,j \rangle} \left(\hat{\vec{S}}_i . \hat{\vec{S}}_j - \frac{1}{4}\hat{n}_i \hat{n}_j\right)$$

$$\begin{aligned}
J\hat{S}^z_i \hat{S}^z_j &= J(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})(\hat{n}_{j\uparrow} - \hat{n}_{j\downarrow}) \\
&= J(\hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow} - \hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow})(\hat{c}^\dagger_{j\uparrow}\hat{c}_{j\uparrow} - \hat{c}^\dagger_{j\downarrow}\hat{c}_{j\downarrow}) \\
&= -J(\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}\hat{c}^\dagger_{j\uparrow}\hat{c}_{j\uparrow} + \hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow}\hat{c}^\dagger_{j\downarrow}\hat{c}_{j\downarrow}) + \ldots \\
&= -J(\hat{c}^\dagger_{j\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}\hat{c}_{j\uparrow} + \hat{c}^\dagger_{i\uparrow}\hat{c}^\dagger_{j\downarrow}\hat{c}_{j\downarrow}\hat{c}_{i\uparrow}) + \ldots
\end{aligned}$$

Hartree-Fock :

$$d^* = \langle \hat{c}^\dagger_{j\uparrow}\hat{c}^\dagger_{i\downarrow}\rangle_{\mathcal{H}_{\text{modèle } t-J}}$$

$$\langle J\hat{S}^z_i \hat{S}^z_j \rangle = -2J\, d^* d + \ldots$$

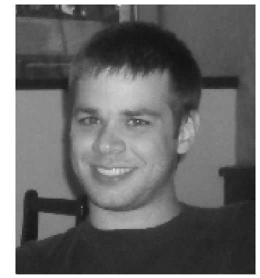
Miyake, Schmitt–Rink et Varma, PRB **34**, 6554-6556 (1986)

Anderson, Baskaran, Zou et Hsu, PRL **58**, 26 (1987)

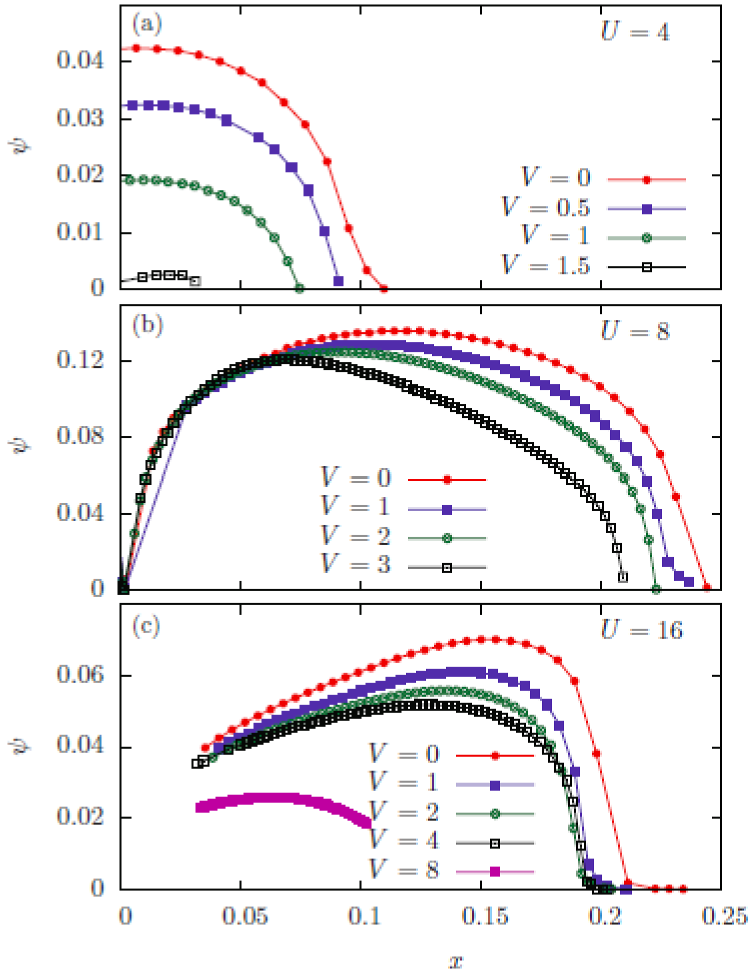
Resilience to near-neighbor repulsion

David Sénéchal

Alexandre Day



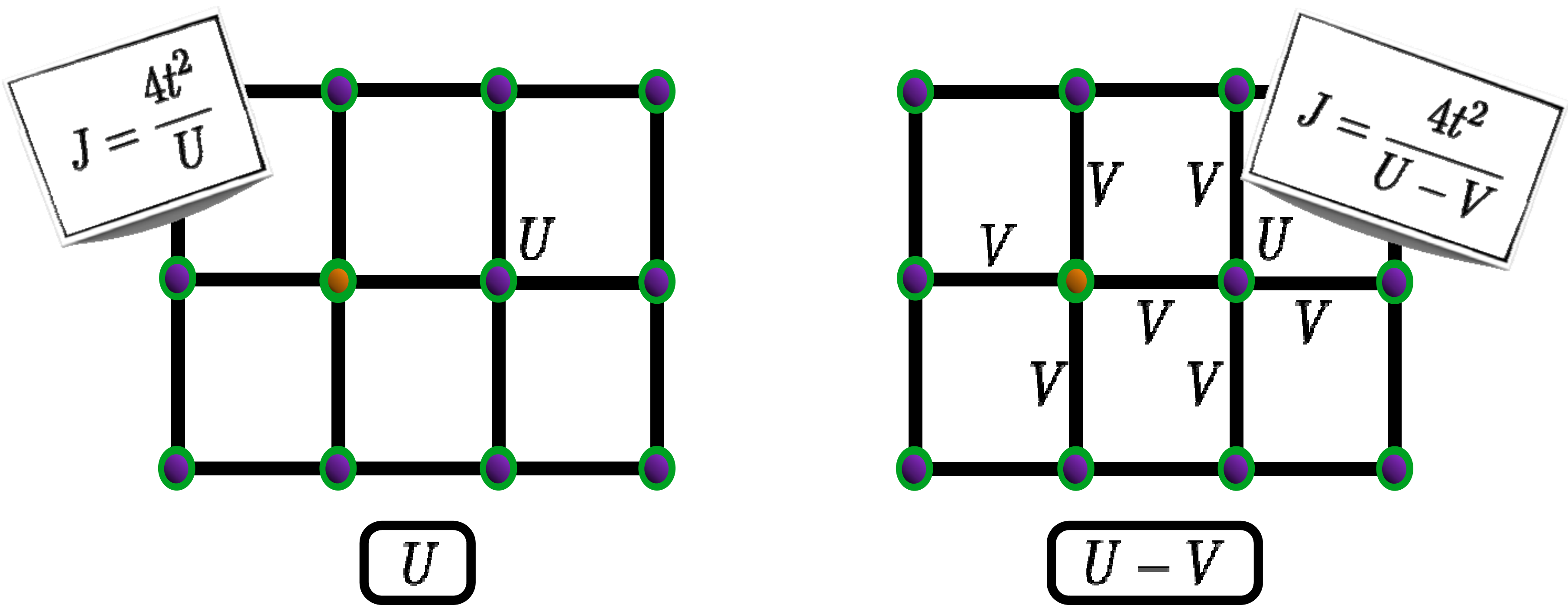
Vincent Bouliane



Sénéchal, Day, Bouliane, AMST PRB **87**, 075123 (2013)

UNIVERSITÉ DE SHERBROOKE

V also increases J

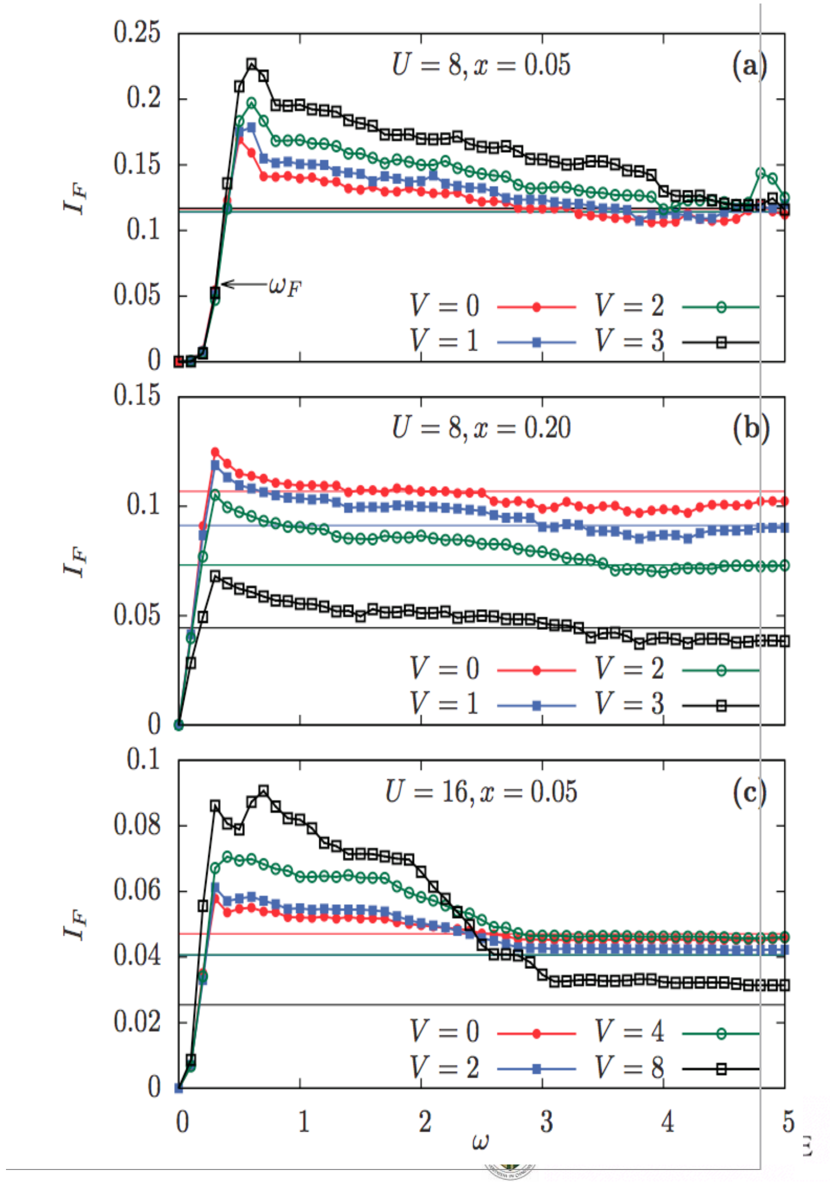


Binding aspects of V

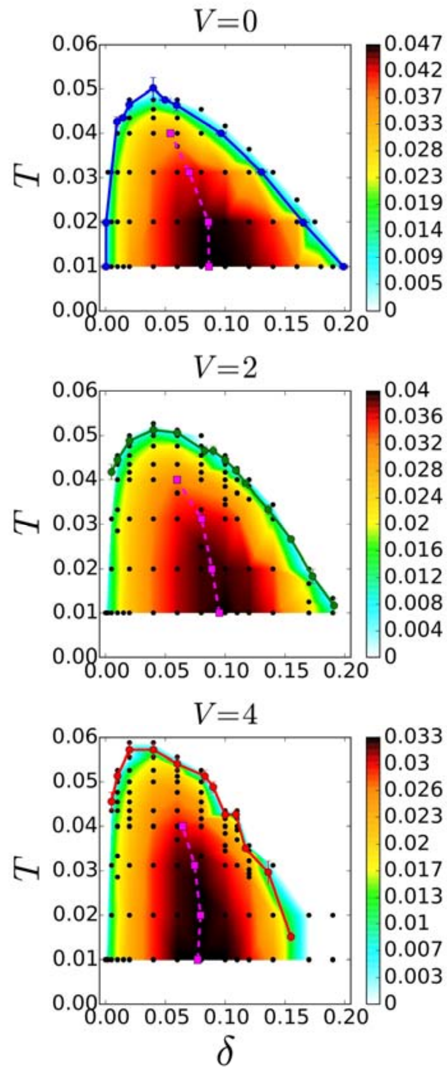
$$J = \frac{4t^2}{U - V}$$

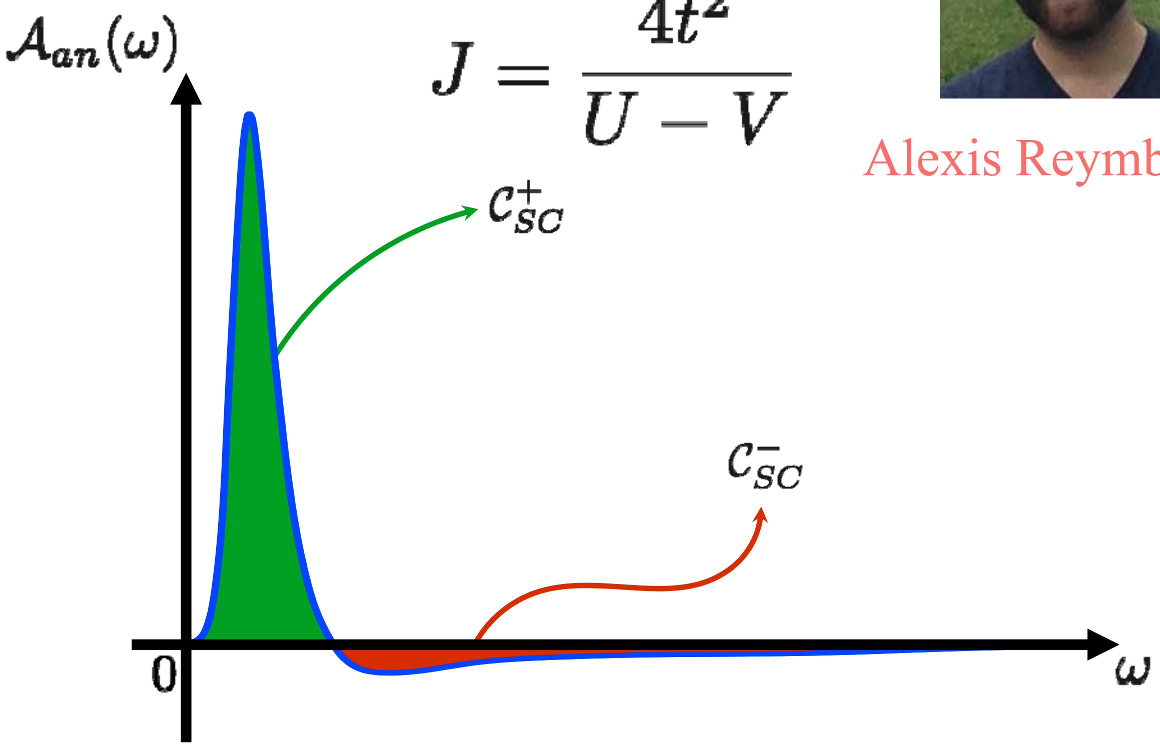
***J* increases with *V* explaining better pairing at low frequency**

But V also induces more repulsion at high frequency, explaining the negative impact at high frequency on binding



Antagonistic effects of *V* at finite T





$$J = \frac{4t^2}{U - V}$$

Alexis Reymbaut

A. Reymbaut *et al.* PRB **94** 155146 (2016)

UNIVERSITÉ DE SHERBROOKE

Summary

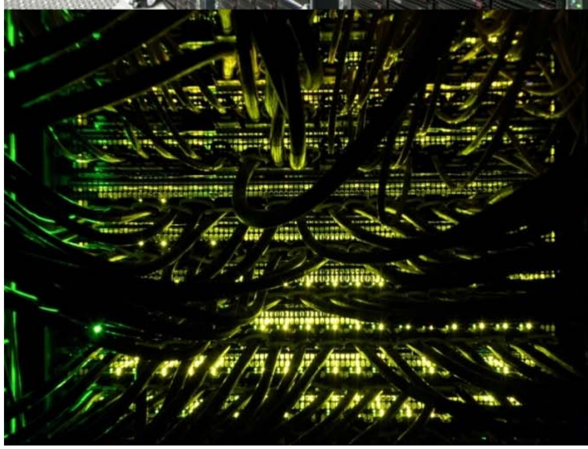
- Pseudogap in e-doped is a *d=2* precursor of AFM
- Normal state first-order transition from Mott & J is an organizing principle for
  - The normal and superconducting states
  - Cuprates and organics are examples
  - Predictions for organics
- Mechanism: *J* short-range is retarded and resilient to *V*

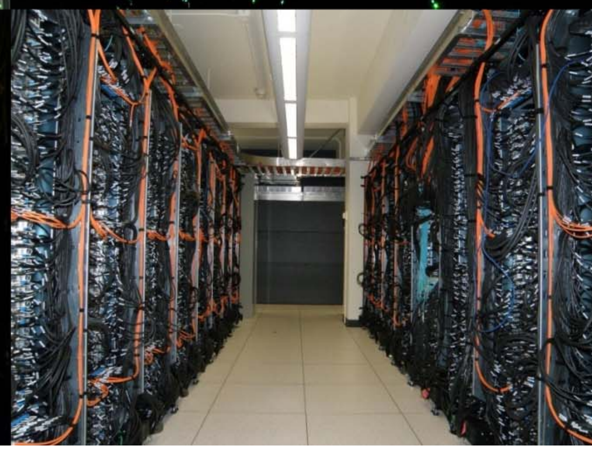
Open questions

- Why does T_c start to go down at such large filling?
- Effect of competition with other order.

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

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

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