Mott Physics in Superconductors

A.-M. Tremblay

G. Sordi, D. Sénéchal, K. Haule,

S. Okamoto, B. Kyung, M. Civelli

CIFAR
CANADIAN INSTITUTE
for ADVANCED RESEARCH

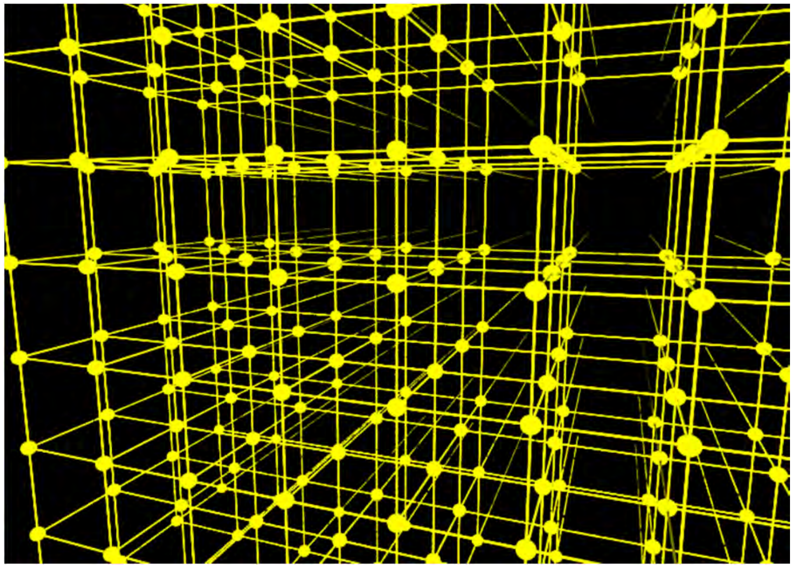
UNIVERSITÉ DE
SHERBROOKE

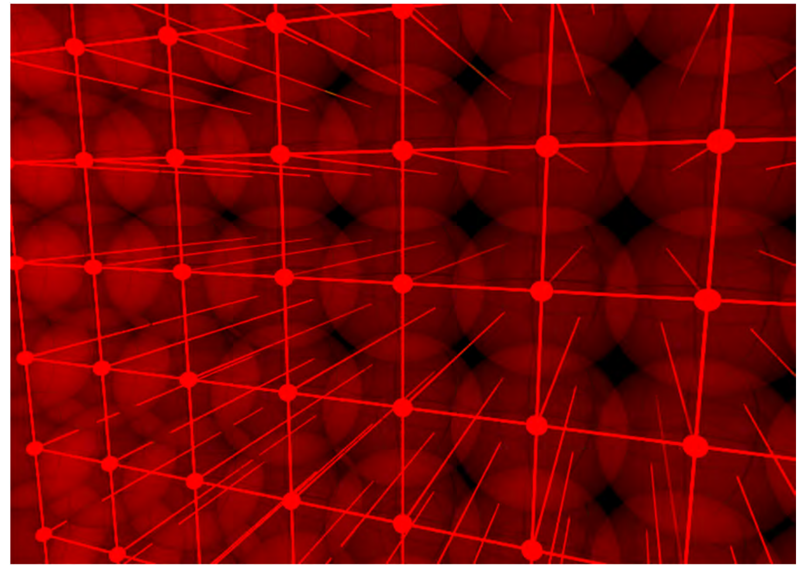
VERITATEM IN CHARITATE

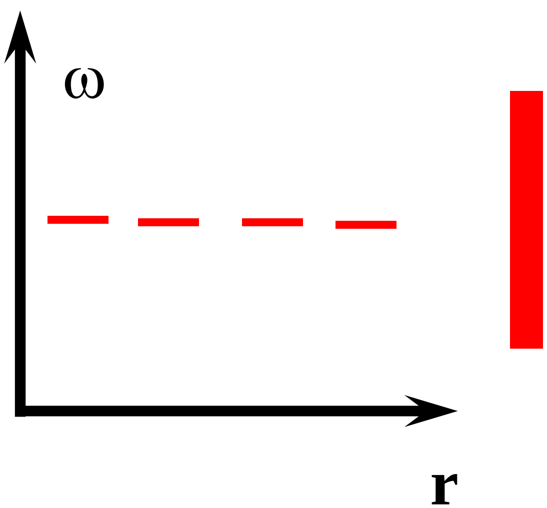
UNIVERSITÉ DE
SHERBROOKE

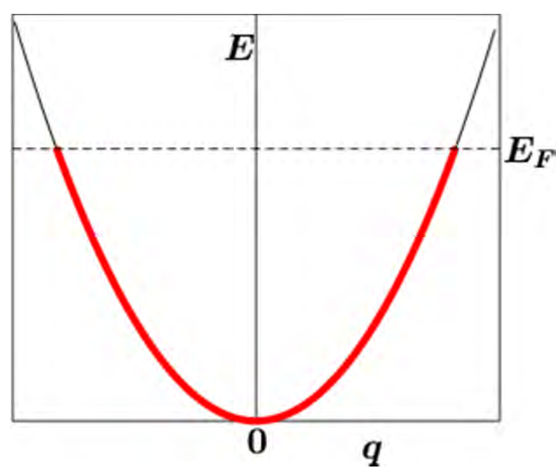
MIT, 3 October, 2011

How to make a metal









Courtesy, S. Julian

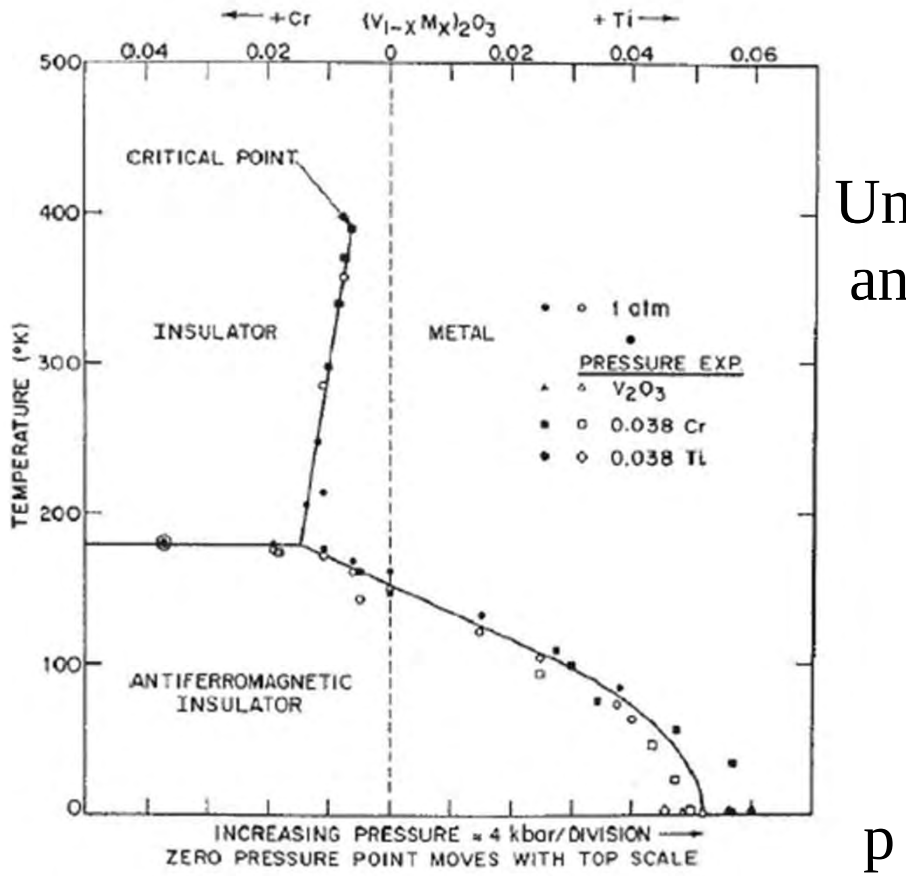
Not always

NiO, Boer and Verway

Peierls, 1937

Mott, 1949

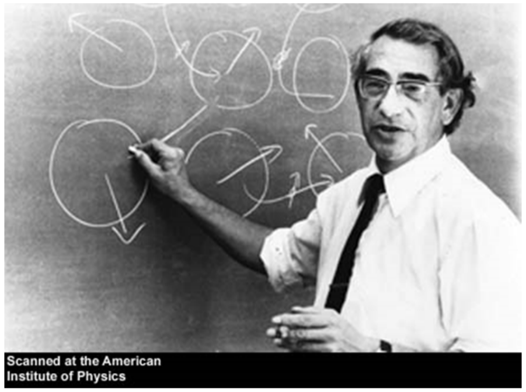
« Conventional » Mott transition



Understood from Hubbard model and dynamical mean field theory

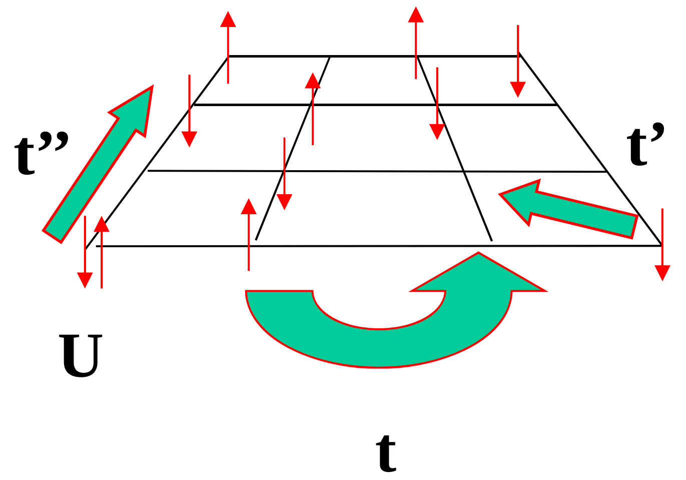
Figure: McWhan, PRB 1970; Limelette, Science 2003

Hubbard model

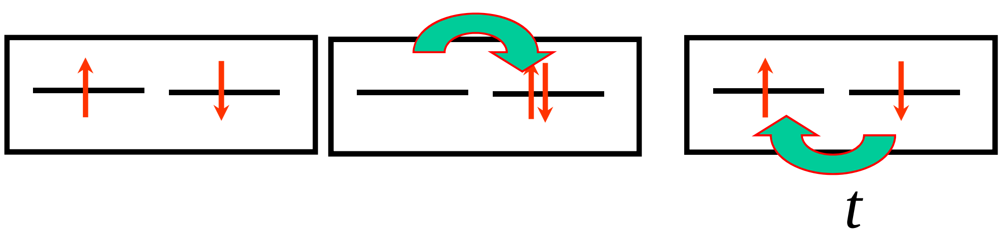


1931-1980

μ

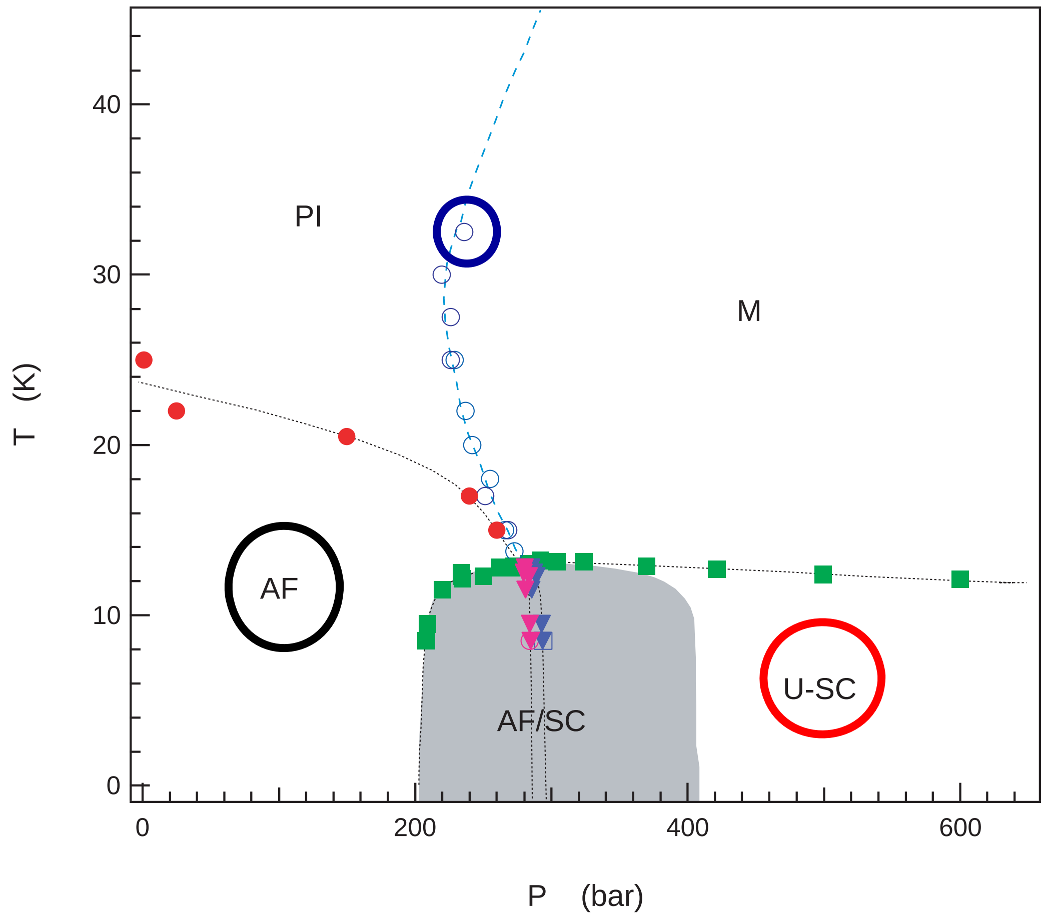


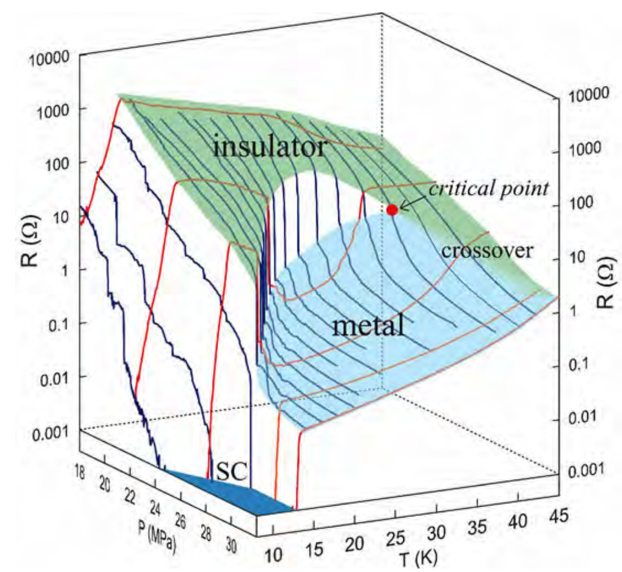
$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$



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

Bare Mott critical point in organics





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

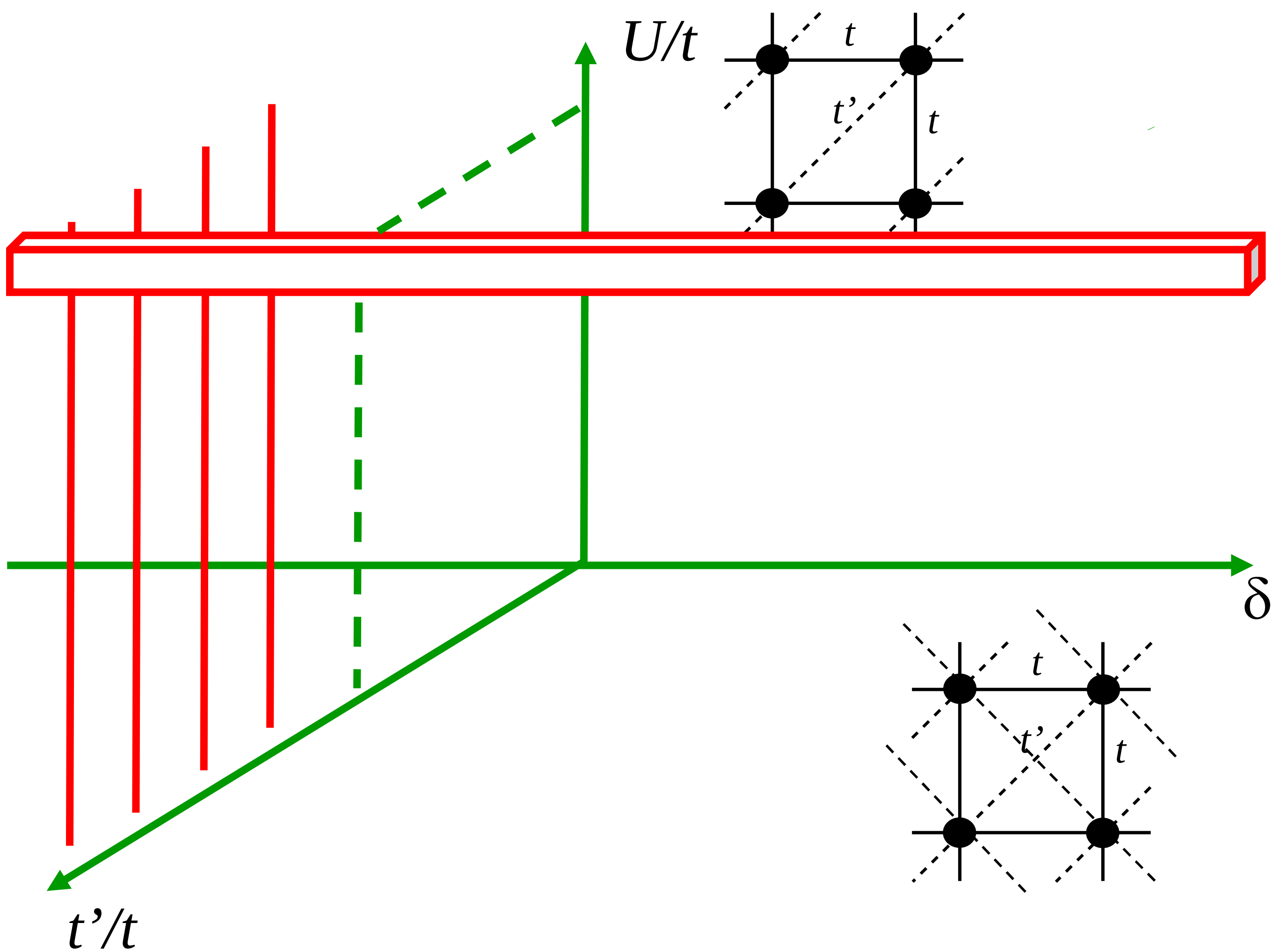
Phase diagram (X=Cu[N(CN)$_2$]Cl)

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

CIAR The Canadian Institute for Advanced Research

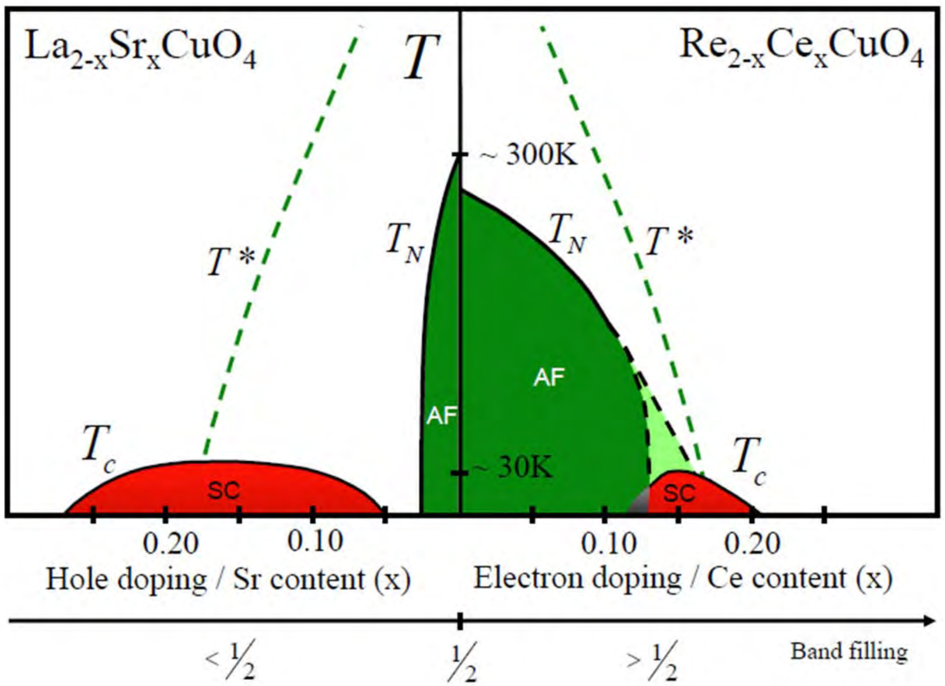
UNIVERSITÉ DE SHERBROOKE

Perspective



Normal state of high-temperature superconductors

Armitage, Fournier, Greene, RMP (2009)



What is under the dome?
Mott Physics away from *n = 1*

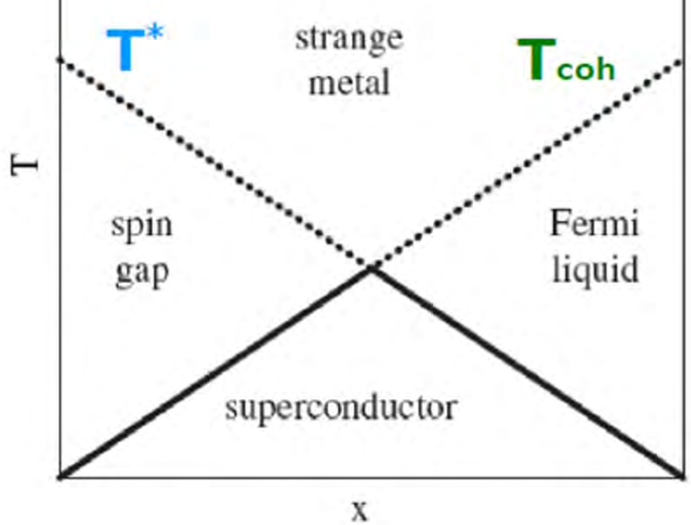
- Competing order
  - Current loops: Varma, PRB **81,** 064515 (2010)
  - Stripes or nematic: Kivelson et al. RMP 75 1201(2003); J.C.Davis
  - d-density wave : Chakravarty, Nayak, Phys. Rev. B **63**, 094503 (2001); Affleck et al. flux phase
  - SDW: Sachdev PRB **80**, 155129 (2009) ...
- Or Mott Physics?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

UNIVERSITÉ DE SHERBROOKE

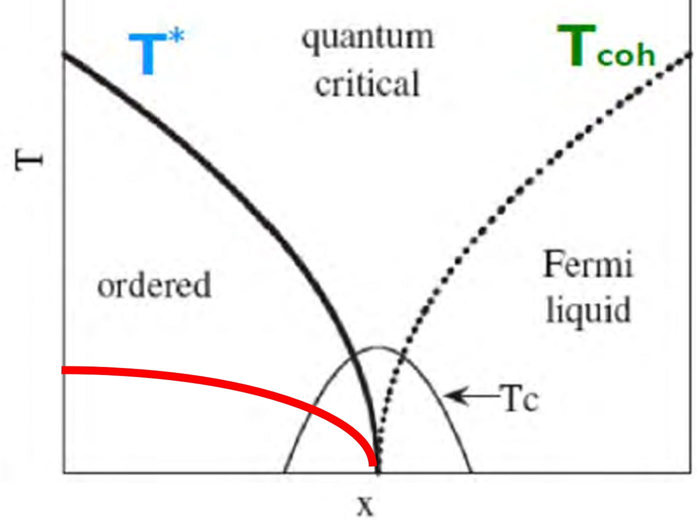
Two views (caricature)

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

RVB plain vanilla, YZR,



Competing order

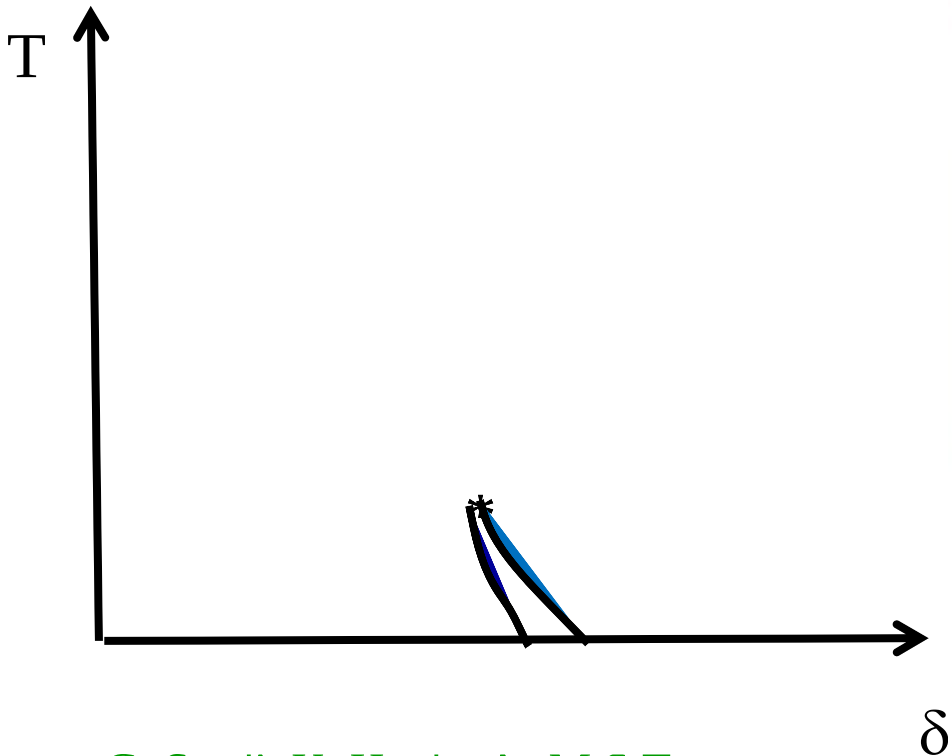


Why T_c decreases?
What is the origin of T^*?
What is the strange metal?

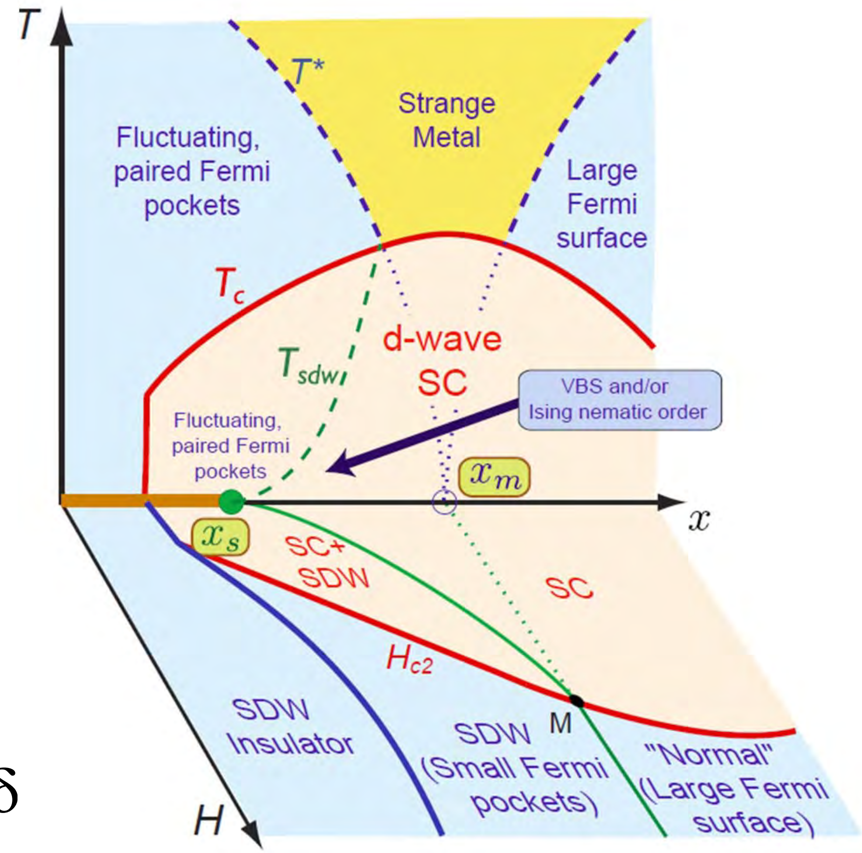
Broken symmetry or not.
What lies beneath the dome.
Mott Physics away from $n = 1$

UNIVERSITÉ DE SHERBROOKE

An alternate view (a bit of both)



G. Sordi, K. Haule, A.-M.S.T
PRL, **104**, 226402 (2010)
and
Phys. Rev. B. **84**, 075161 (2011)



S. Sachdev, Physica C **470**, S4 (2010)
Matthias Punk + Subir Sachdev (unpublished)
T. C. Ribeiro and X.-G. Wen,
PRL (2005) and Phys. Rev. B 74, 155113 (2006)

UNIVERSITÉ DE SHERBROOKE

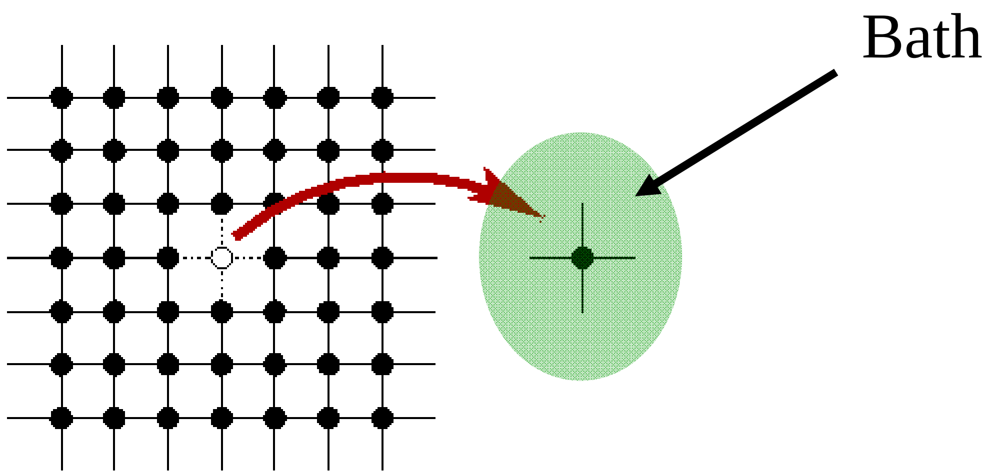
Outline

- Method
- Normal state
  - First order transition
  - Widom line and pseudogap
- Superconducting state
  - Glue

Method

Mott transition and Dynamical Mean-Field Theory. The beginnings in d = *infinity*

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

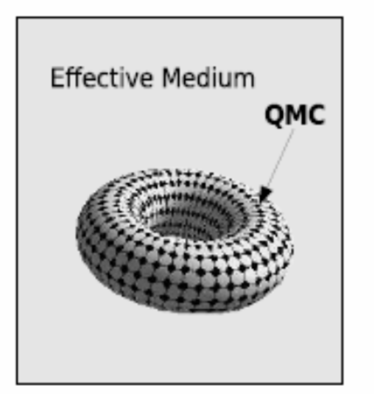


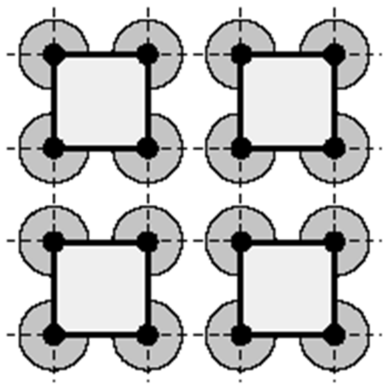
W. Metzner and D. Vollhardt, PRL (1989)
A. Georges and G. Kotliar, PRB (1992)
M. Jarrell PRB (1992)

DMFT, (d = *3*)

2d Hubbard: Quantum cluster method

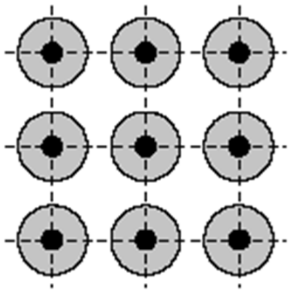
C-DMFT





DCA

DMFT



Hettler …Jarrell…Krishnamurty PRB **58** (1998)
Kotliar et al. PRL **87** (2001)
M. Potthoff *et al.* PRL **91,** 206402 (2003).
Maier, Jarrell et al., Rev. Mod. Phys. **77**, 1027 (2005)

Another way to look at this (Potthoff)

$$\Omega_{\mathbf{t}}[G] = \Phi[G] - Tr[(G_{0\mathbf{t}}^{-1} - G^{-1})G] + Tr\ln(-G)$$

$$\boxed{\frac{\delta\Phi[G]}{\delta G} = \Sigma}$$

$$\Omega_{\mathbf{t}}[\Sigma] = \boxed{\Phi[G] - Tr[\Sigma G]} - Tr\ln(-G_{0\mathbf{t}}^{-1} + \Sigma)$$

Still stationary (chain rule)

$$\Omega_{\mathbf{t}}[\Sigma] = \boxed{F[\Sigma]} - Tr\ln(-G_{0\mathbf{t}}^{-1} + \Sigma)$$

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

SFT : Self-energy Functional Theory

With $F[\Sigma]$ Legendre transform of Luttinger-Ward funct.

$$\Omega_{\mathbf{t}}[\Sigma] = \boxed{F[\Sigma]} + \mathrm{Tr}\ln(-(G_0^{-1} - \Sigma)^{-1})$$

is stationary with respect to Σ and equal to grand potential there.

$$\Omega_{\mathbf{t}}[\Sigma] = \boxed{\Omega_{\mathbf{t}'}[\Sigma] - \mathrm{Tr}\ln(-(G_0'^{-1} - \Sigma)^{-1})} + \mathrm{Tr}\ln(-(G_0^{-1} - \Sigma)^{-1}).$$

Vary with respect to parameters of the cluster (including Weiss fields)

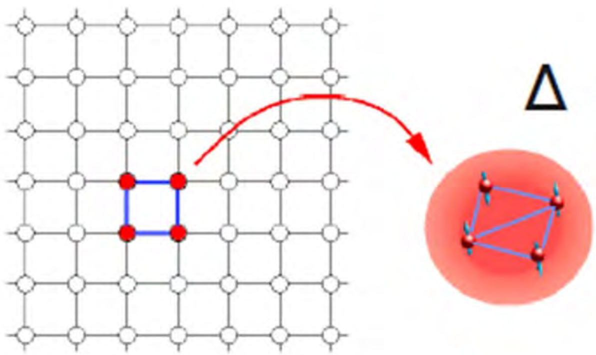
Variation of the self-energy, through parameters in $H_0(\mathbf{t'})$

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

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

- Fermi liquid
  - Start from Fermi sea
  - Self-energy analytical
  - One to one correspondence of elementary excitations
  - Landau parameters
- Mott insulator
  - Hubbard model
  - Atomic limit
  - Self-energy singular
  - DMFT
  - How many sites in the cluster determines how low in temperature your description of the normal state is valid.

C-DMFT

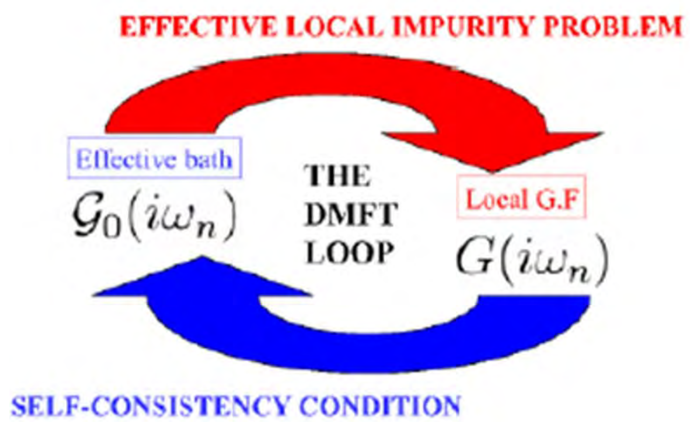


Mean-field is not a trivial problem! Many impurity solvers.

Here: continuous time QMC

P. Werner, PRL 2006
P. Werner, PRB 2007
K. Haule, PRB 2007

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

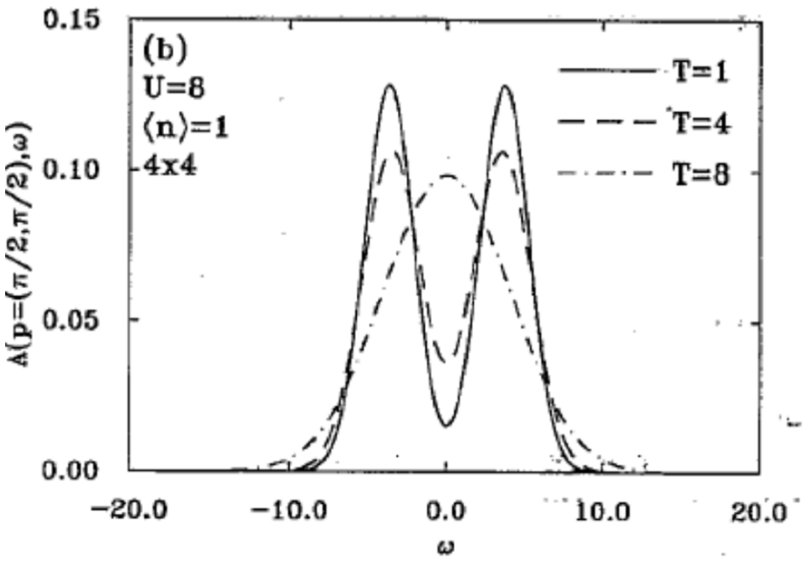


$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n) - \left[\sum_{\tilde{k}} \frac{1}{i\omega_n + \mu - t_c(\tilde{k}) - \Sigma_c(i\omega_n)} \right]^{-1}$$

Solving cluster in a bath problem

- Continuous-time Quantum Monte Carlo calculations to sum all diagrams generated from expansion in powers of hybridization.
  - P. Werner, A. Comanac, L. de' Medici, M. Troyer, and A. J. Millis, Phys. Rev. Lett. **97**, 076405 (2006).
  - K. Haule, Phys. Rev. B **75**, 155113 (2007).

Mott insulator at finite T



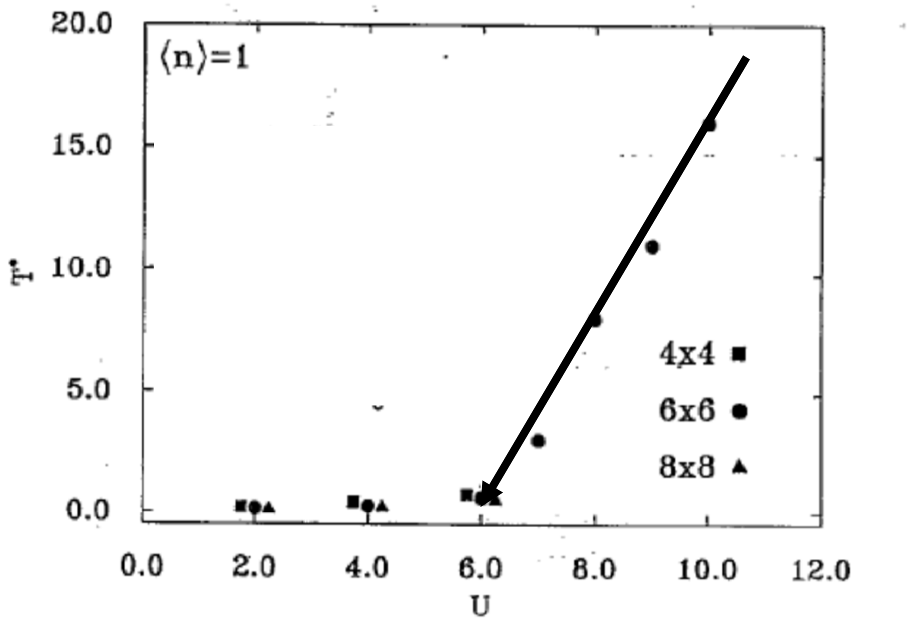


FIG. 5. The temperature T^* at which the gap develops vs U for 4×4, 6×6, and 8×8 lattices.

M. Vekic and S.R. White, PRB 47, 1160 (1993)

Interaction-induced Mott transition, *n = 1*

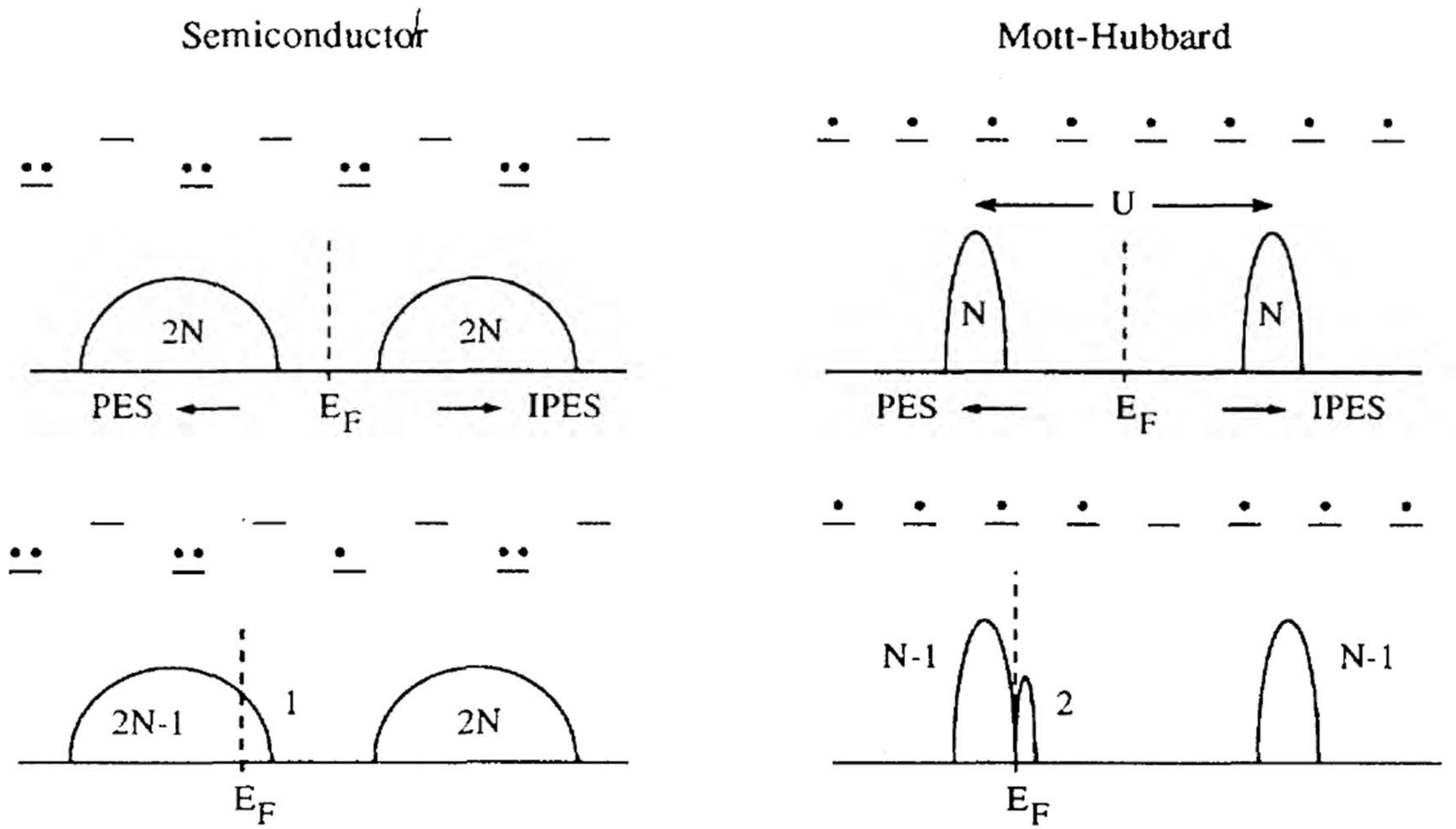
Method	U_{c1}	U_c	U_{c2}	Ref.
VCA+ED 2 x 2 + 8b	5.25	5.5	6.37	Balzer et al. EPL (2009)
CDMFT+CTQMC+H 2 x 2	5.3		5.7	Park et al. PRL (2008)
DCA+CTQMC+H 8	5.7		6.4	Gull et al. cond-mat (2009)
DCA+CTQMC+H 4	!	~4.2	!	Gull et al. EPL (2008)
Dual fermions	!	~6.5	!	Hafermann et al. (2008)
CDMFT+ED 2 x 2 + 8b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

Cuprates as doped Mott insulators

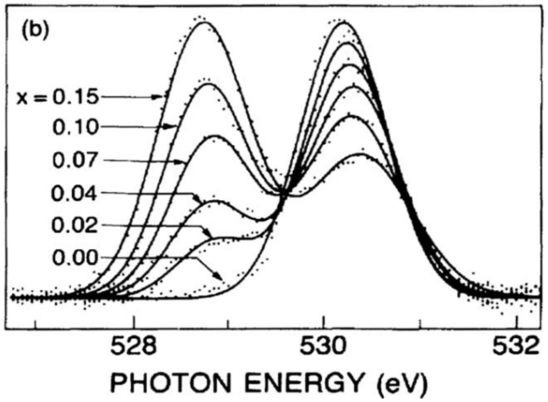
UNIVERSITÉ DE SHERBROOKE

Spectral weight transfer

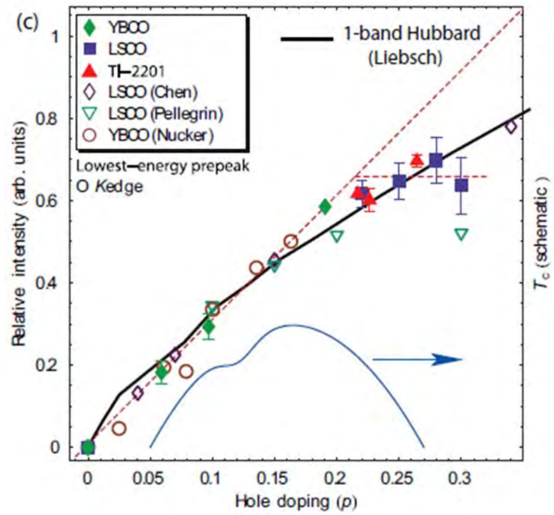


Meinders *et al.* PRB **48**, 3916 (1993)

Experiment: X-Ray absorption



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



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

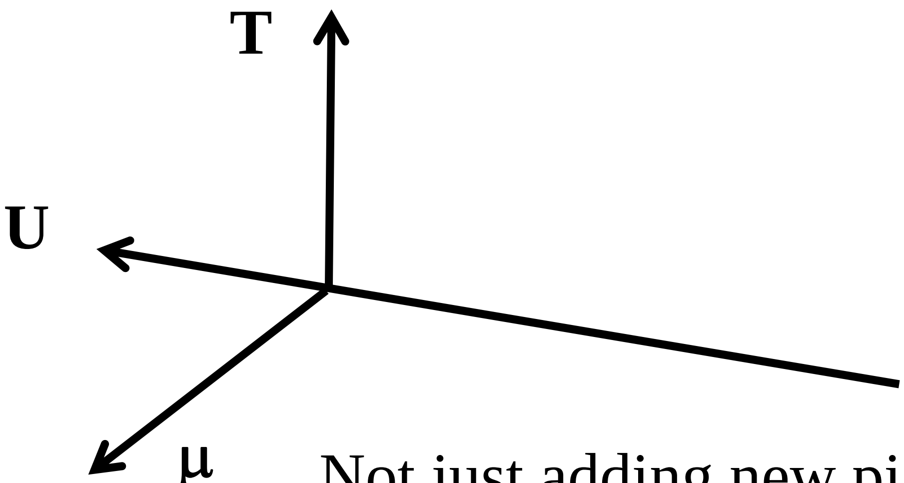
Number of low energy states above $\omega = 0$ scales as $2x$ +
Not as 1+x as in Fermi liquid

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

Giovanni Sordi

G. Sordi, K. Haule, A.-M.S.T
PRL, **104**, 226402 (2010)
and
Phys. Rev. B. **84**, 075161 (2011)

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



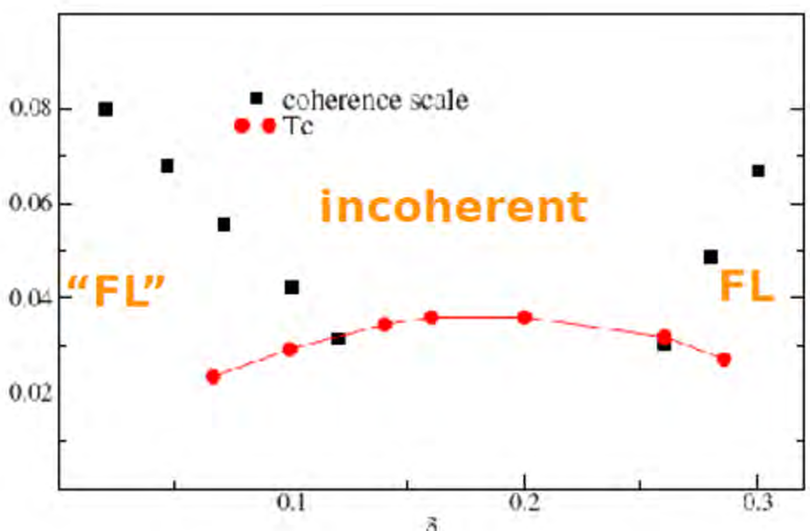
Kristjan Haule

Not just adding new piece:
Lesson from DMFT, first order transition + critical point governs phase diagram

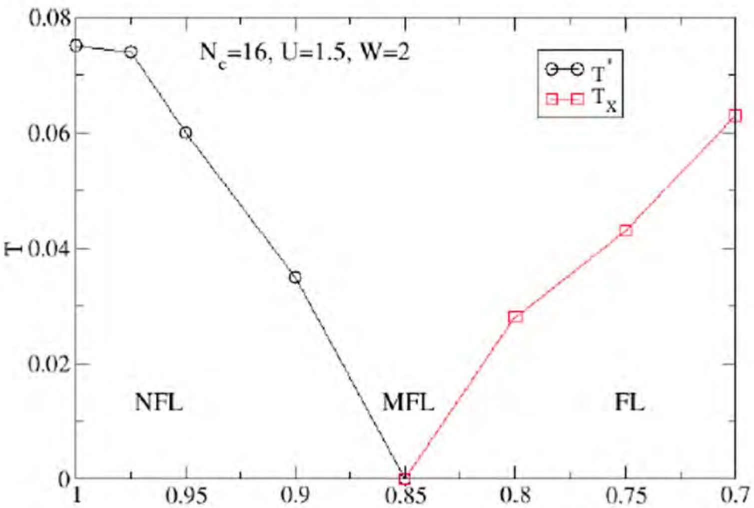
UNIVERSITÉ DE SHERBROOKE

Doping driven Mott transition, *t’ = 0*

Method	t’	Orbital selective	U	Critical point	Ref.
D+C+H 8			7		Werner et al. cond-mat (2009)
D+C+H 4					Gull et al. EPL (2008)
	-0.3		10,6		Liebsch, Merino… (2008)
					Ferrero et al. PRB (2009)
D+C+H 8			7		Gull, et al. PRB (2009)

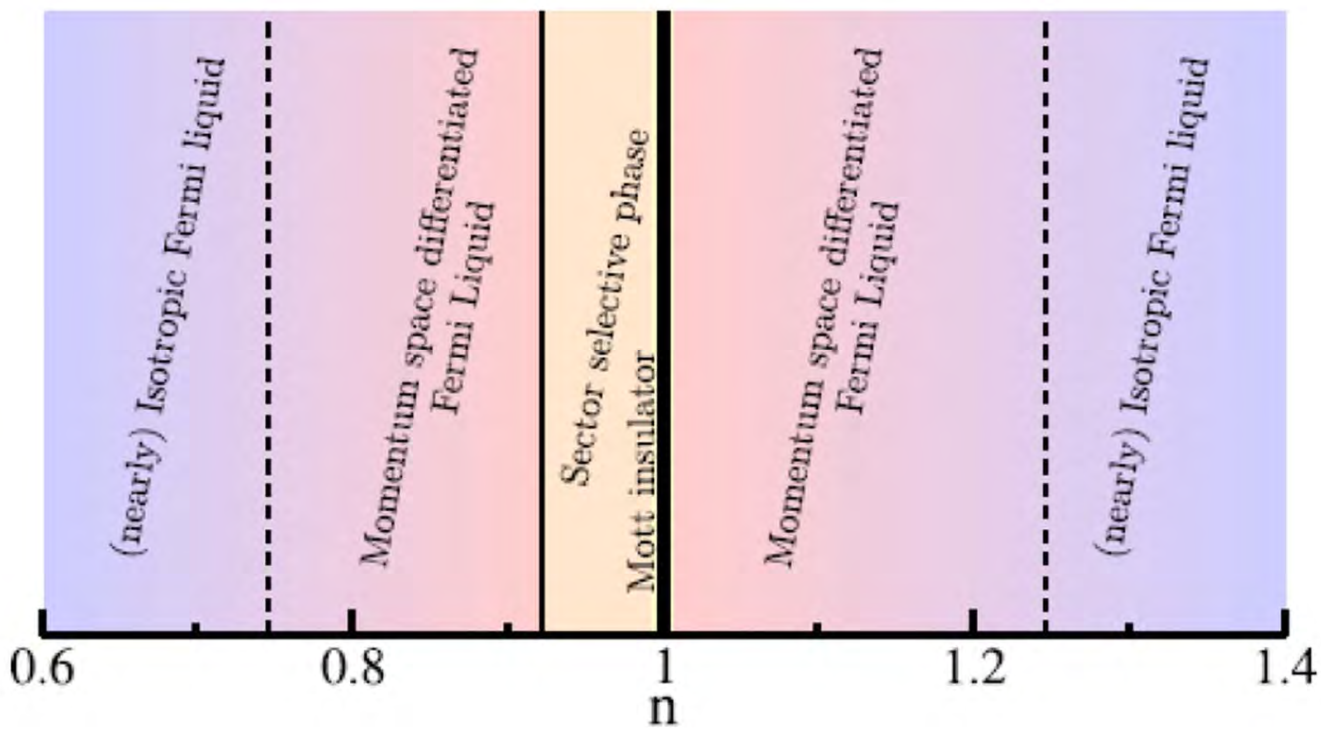


K. Haule, G. Kotliar, PRB (2008)



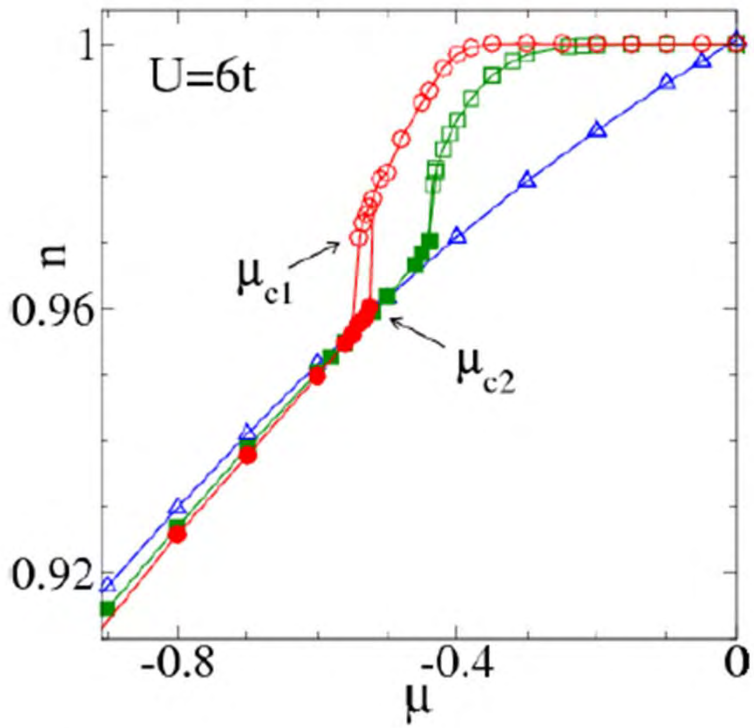
Vildhyadhiraja, PRL (2009)

Doping driven Mott transition



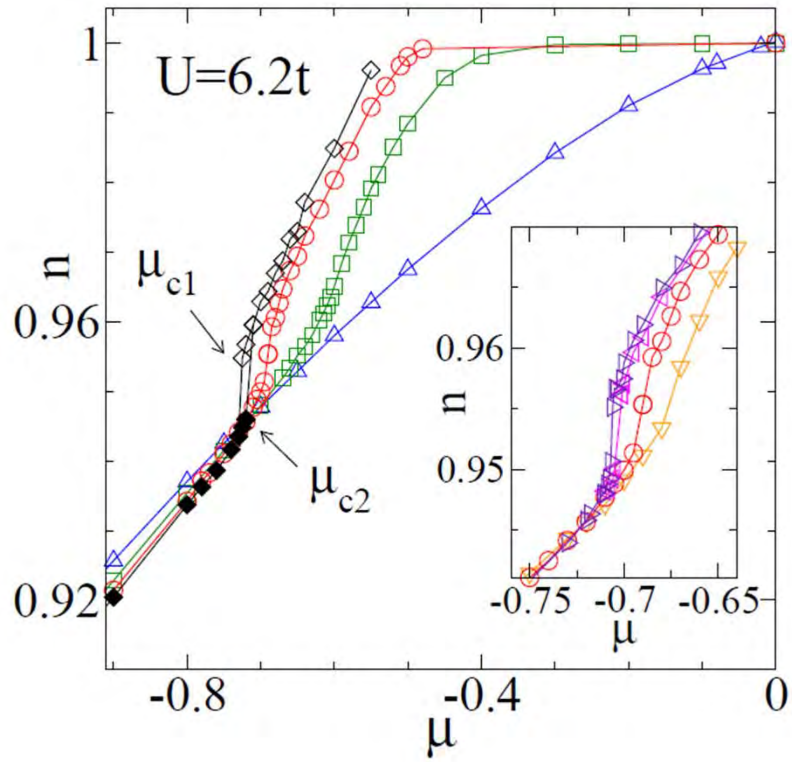
Gull, Werner, Millis, (2009)

First order transition at finite doping



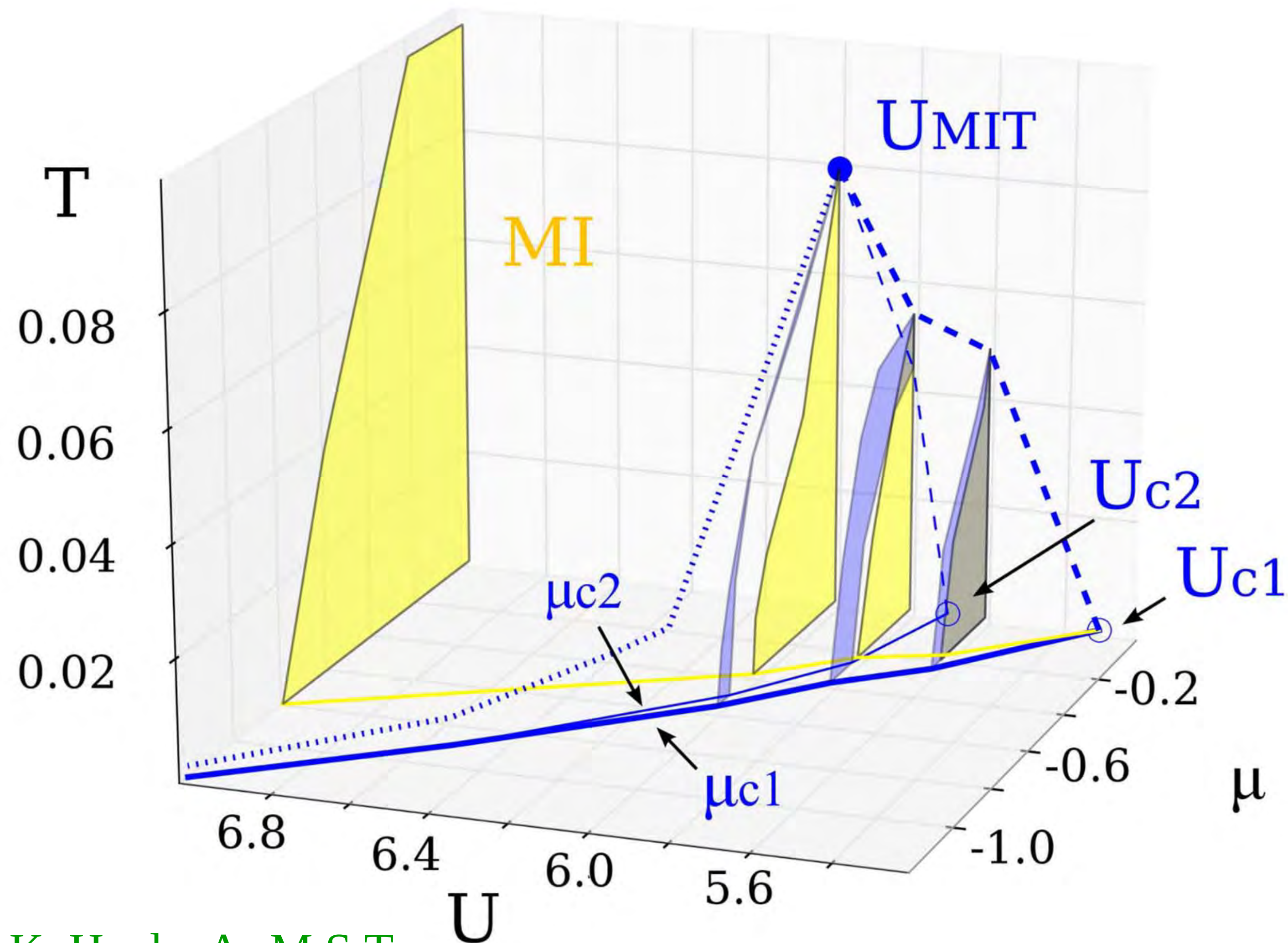
$n(\mu)$ for several temperatures:
T/t =1/10, 1/25, 1/50

The critical point



UNIVERSITÉ DE SHERBROOKE

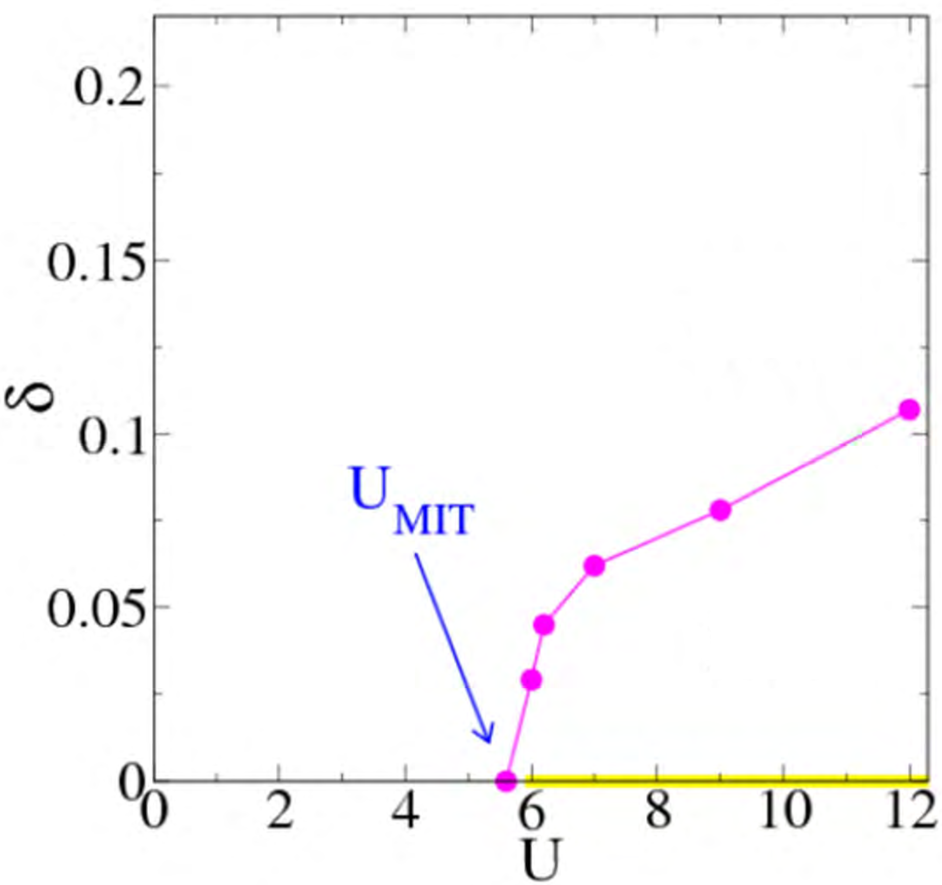
Normal state phase diagram

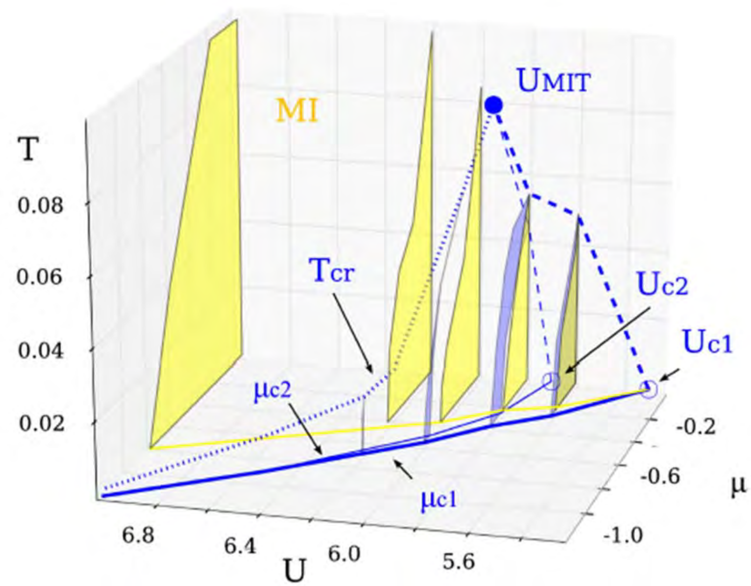


G. Sordi, K. Haule, A.-M.S.T
PRL, **104**, 226402 (2010)

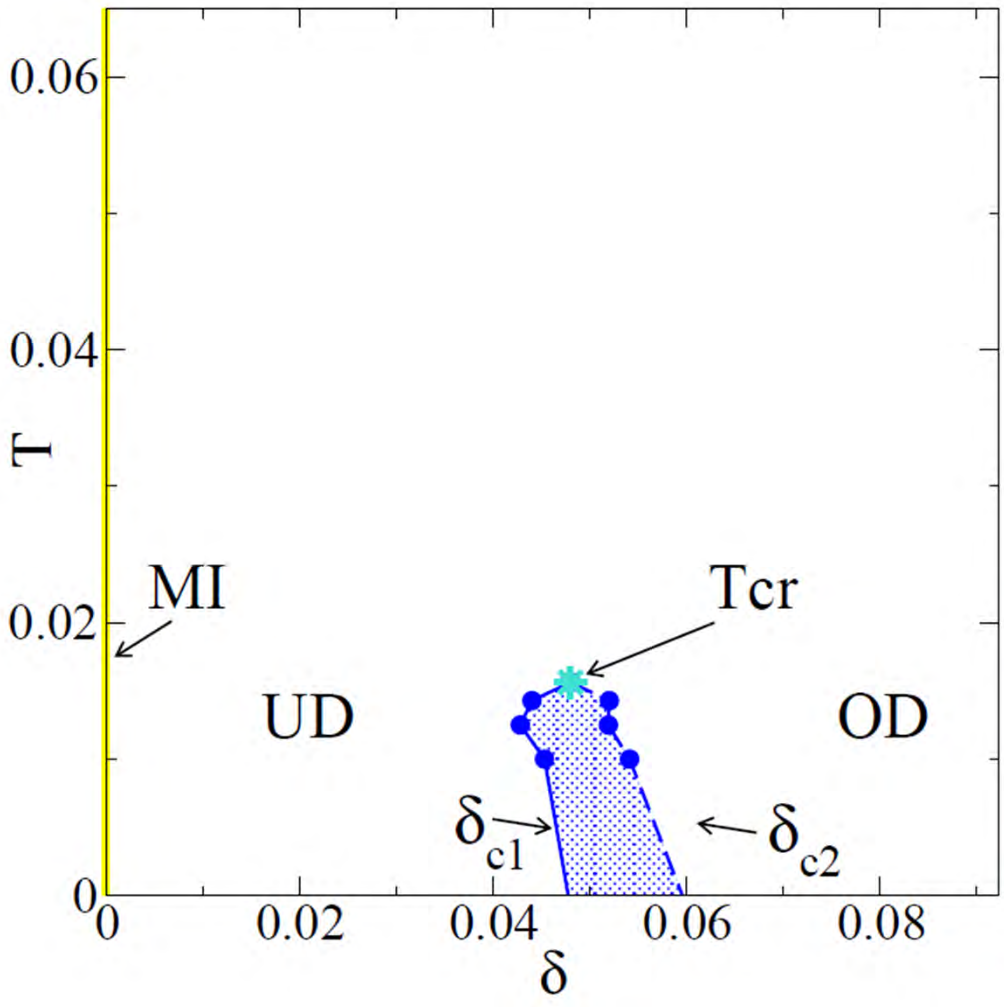
Link to Mott transition up to optimal doping

Doping dependence of critical point as a function of U





Characterisation of the phases (U=6.2t)



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

1. Mott insulator (MI)
2. Underdoped phase (UD): $\delta < \delta_c$
3. Overdoped phase (OD): $\delta > \delta_c$
4. Coexistence/forbidden region

Here "optimal doping" δ_c = doping at which the 1st order transition occurs

How does the UD phase differ from the OD phase?

UNIVERSITÉ DE SHERBROOKE

Giovanni Sordi

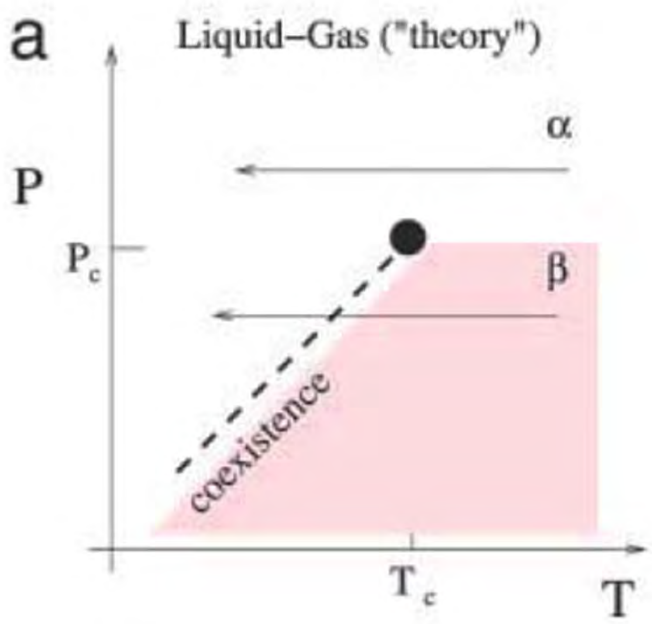
Patrick Sémon

Kristjan Haul

Pseudogap and the Widom line

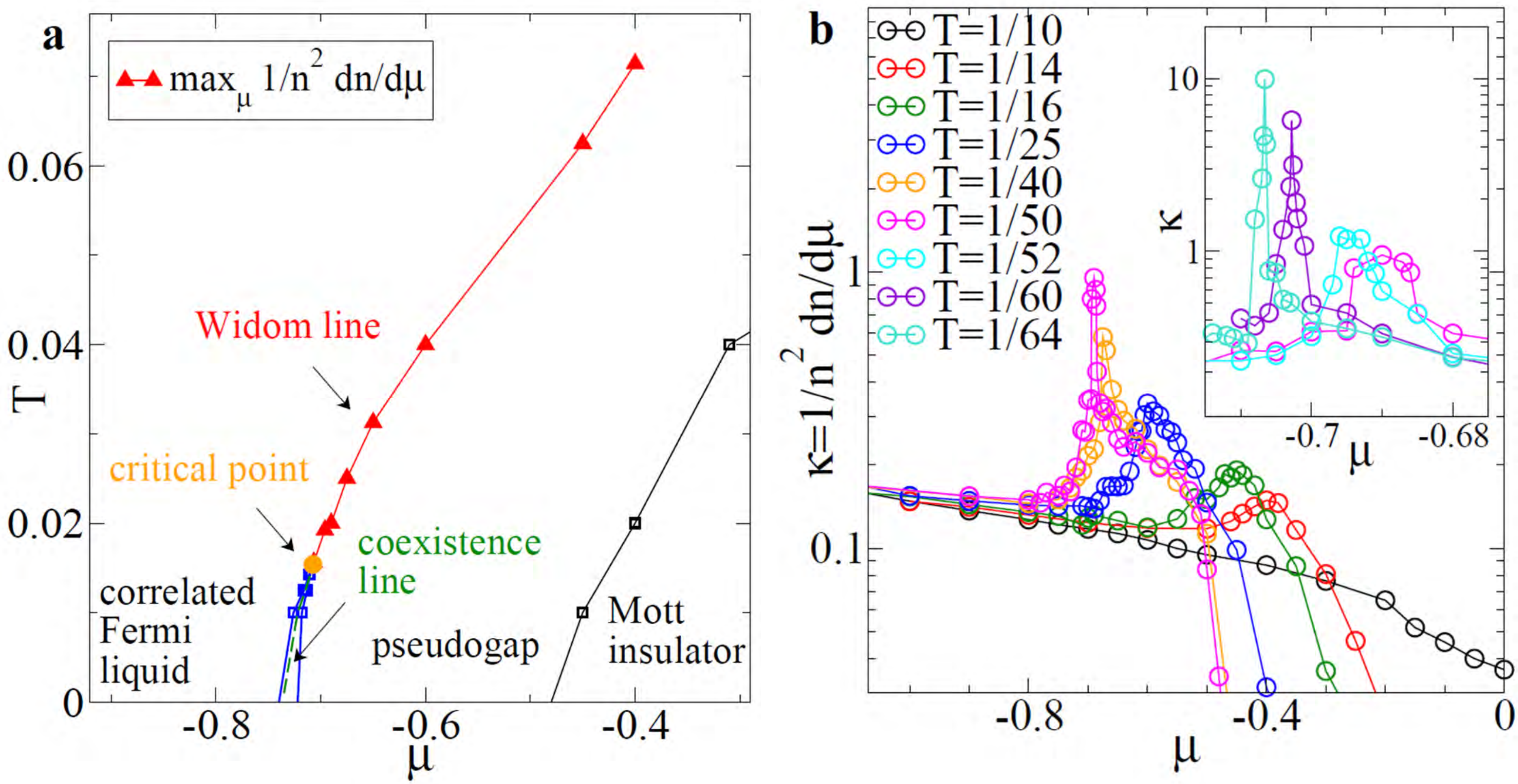
UNIVERSITÉ DE SHERBROOKE

The Widom line

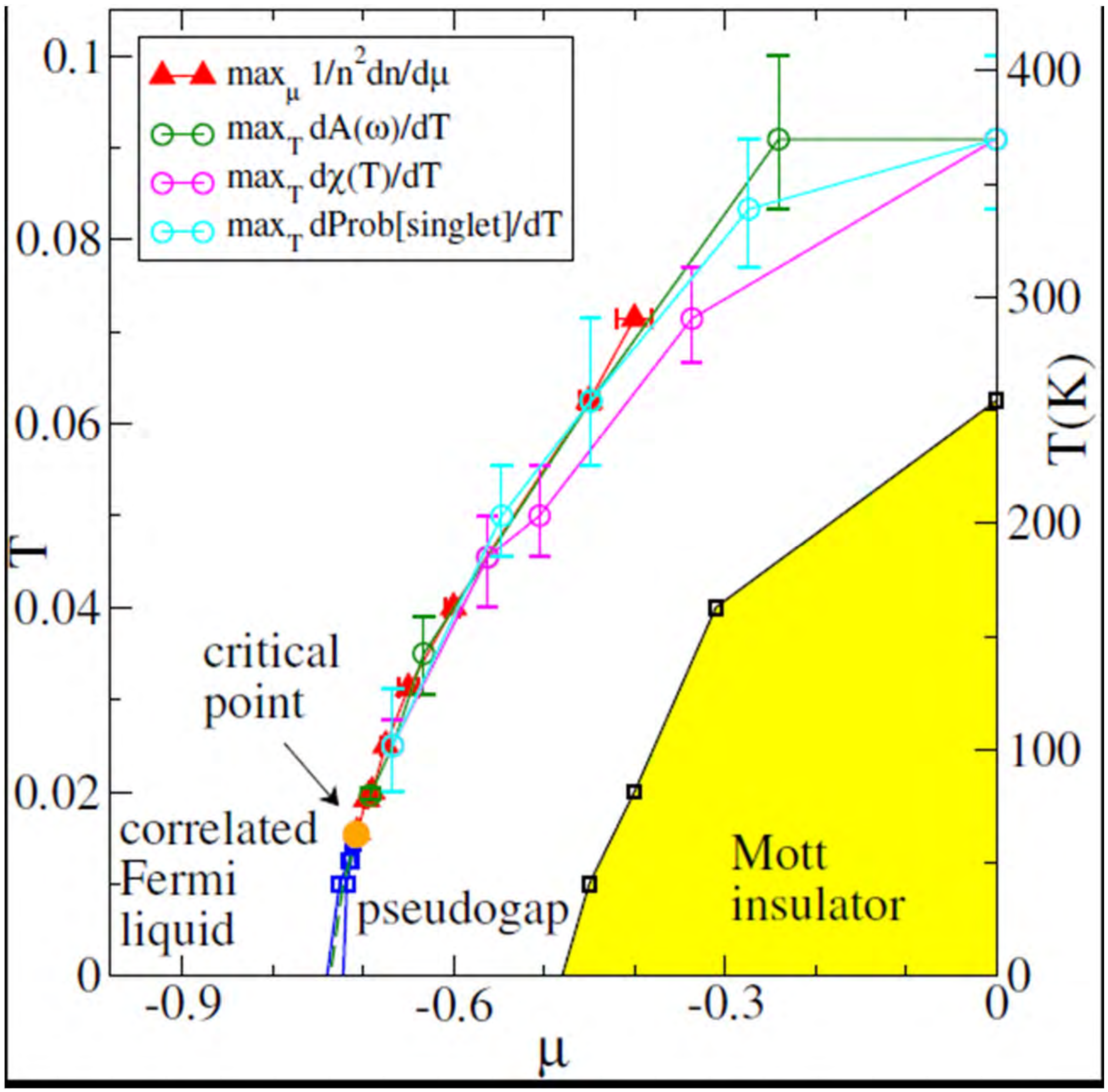


Xu et al. PNAS, **102**, 46 (2005)
Simeoni et al., Nature Physics **6**, 503 (2010)

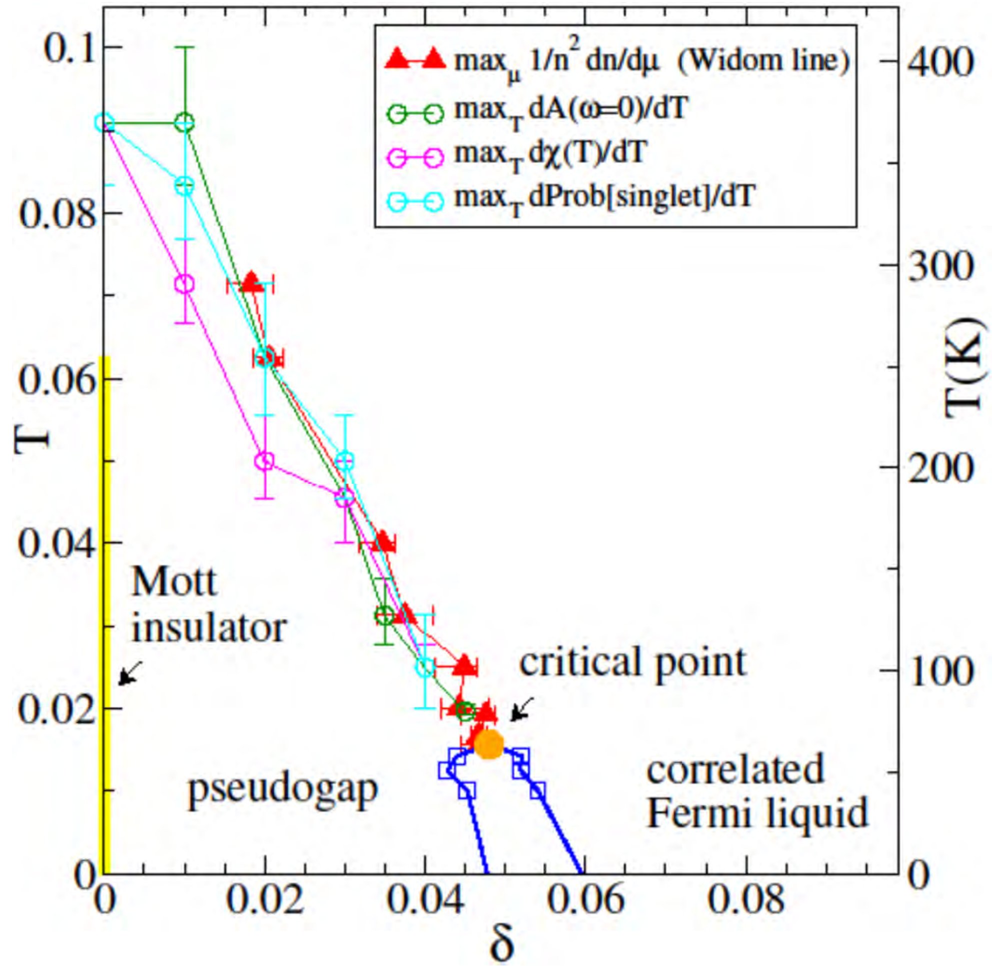
The Widom line



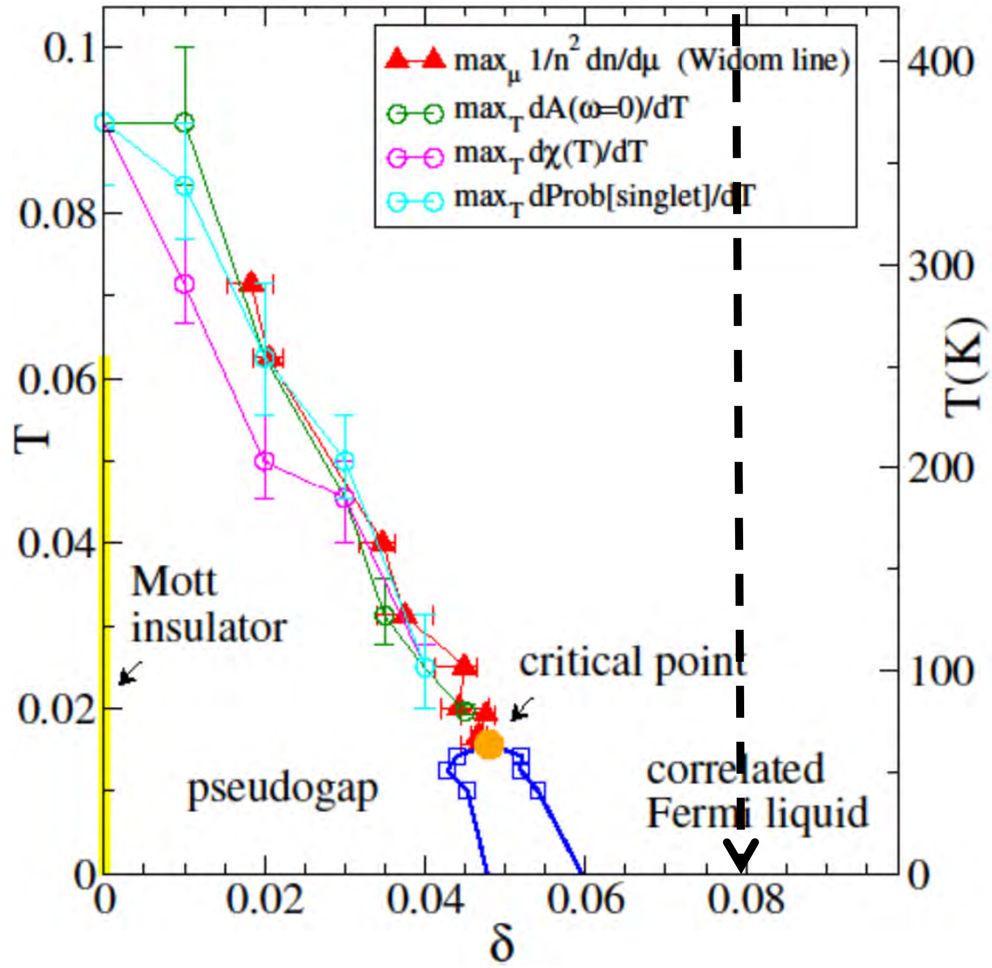
Rapid change also in dynamical quantities

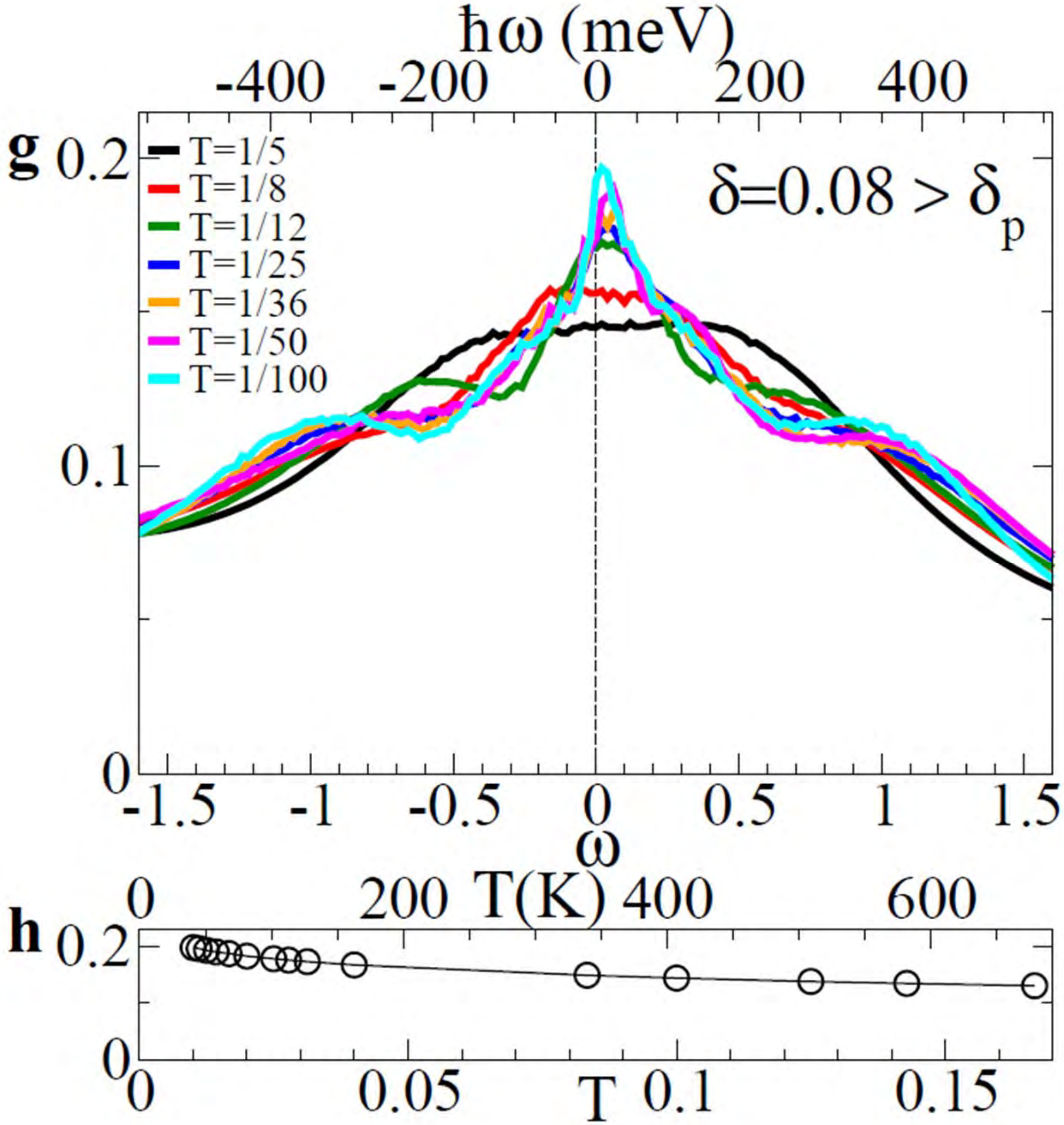


Phase diagram



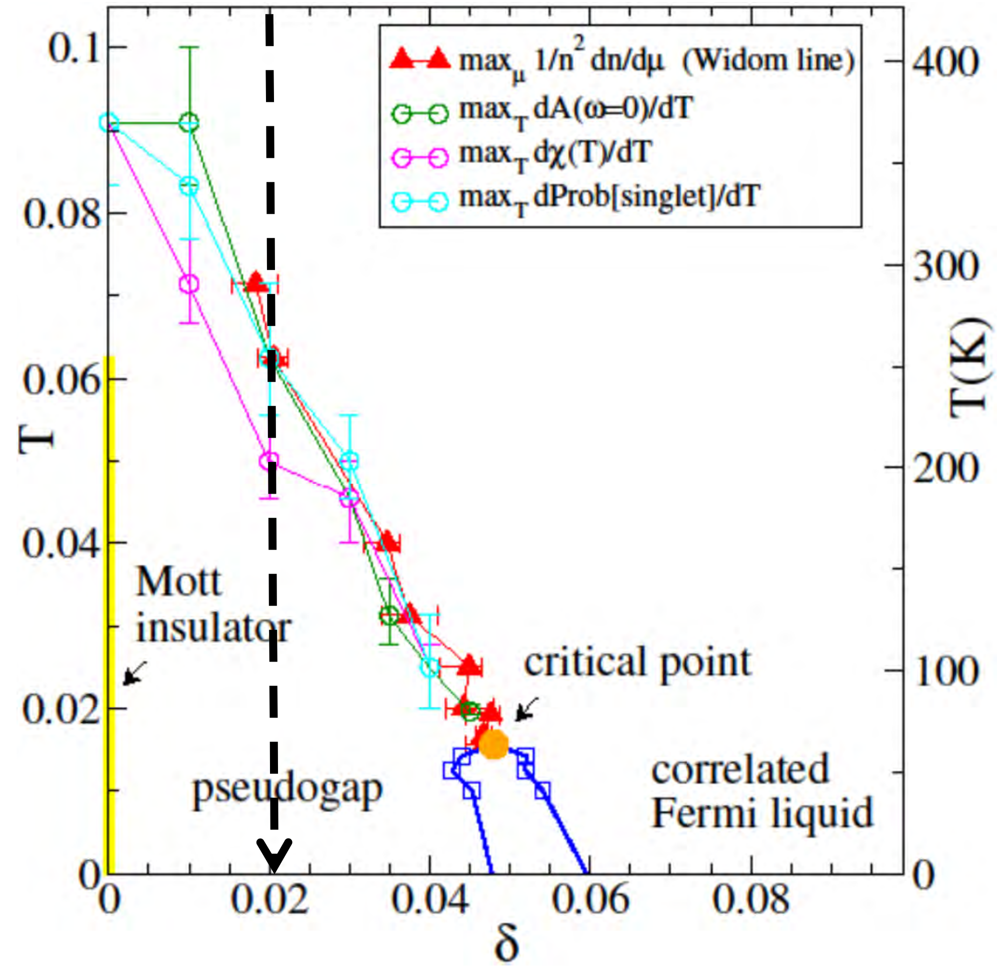
Phase diagram



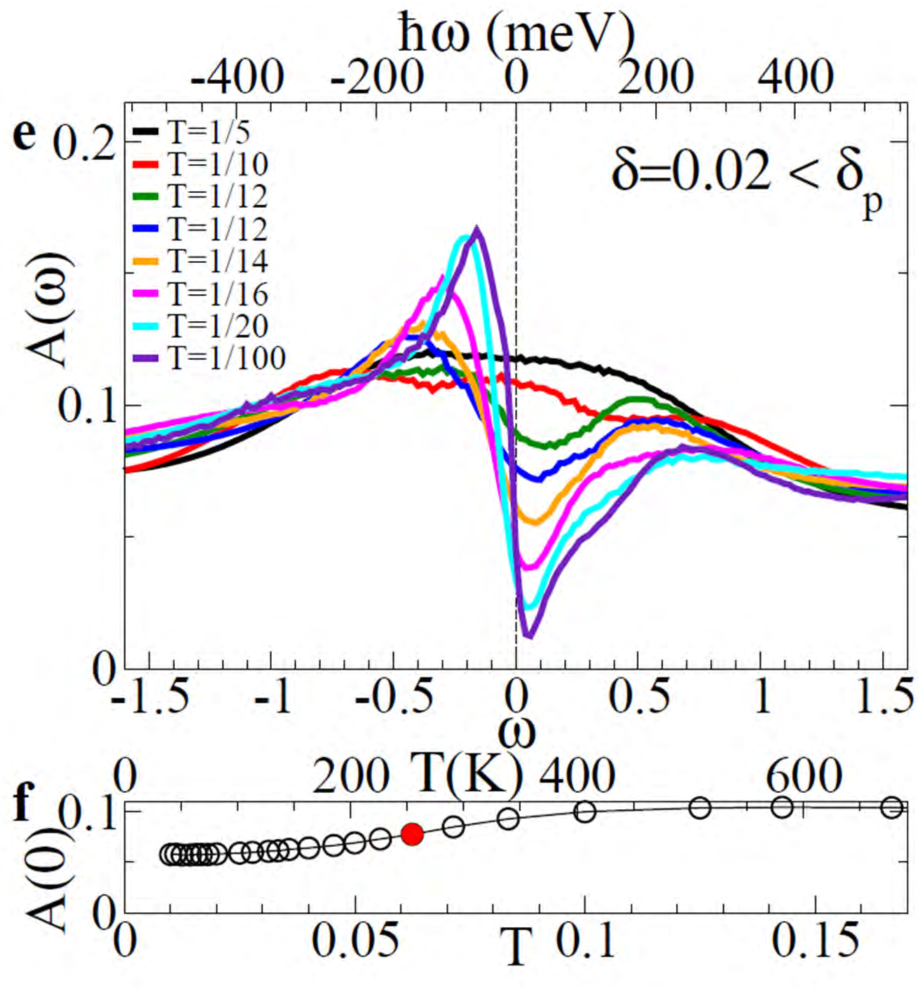


UNIVERSITÉ DE SHERBROOKE

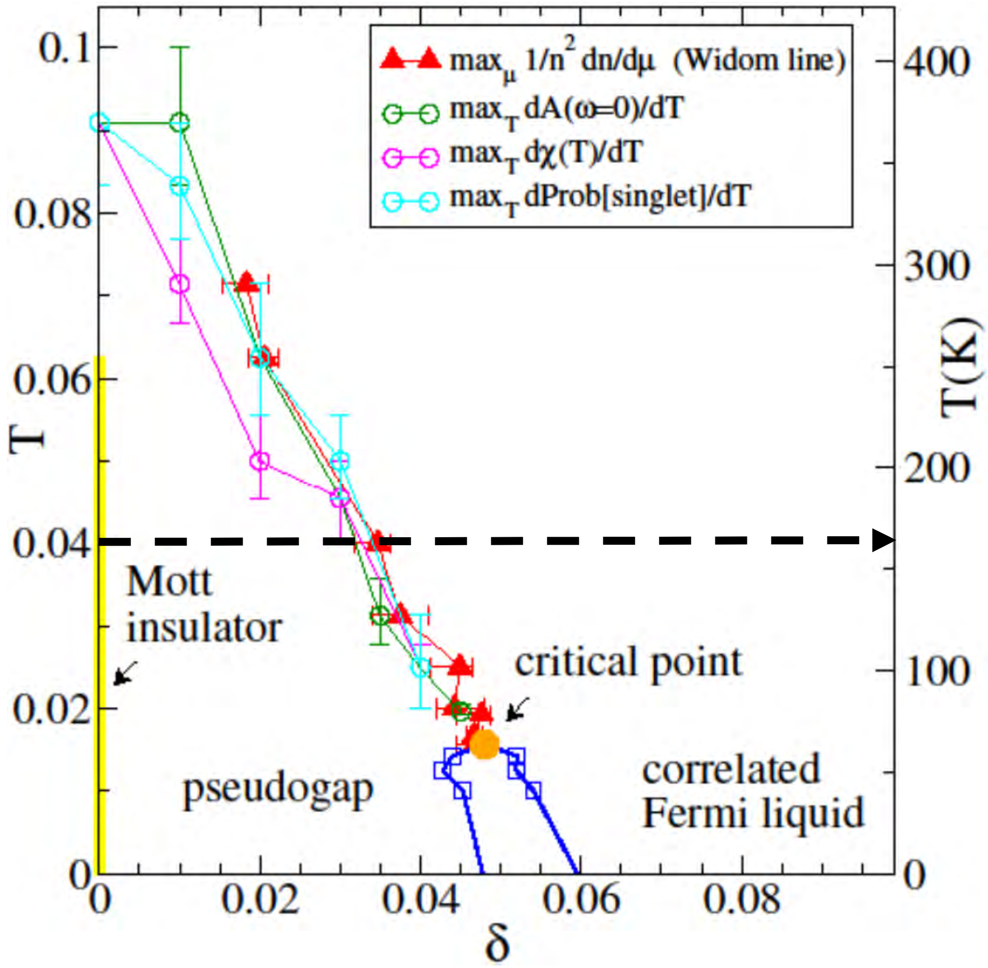
Phase diagram



T dependence of the DOS

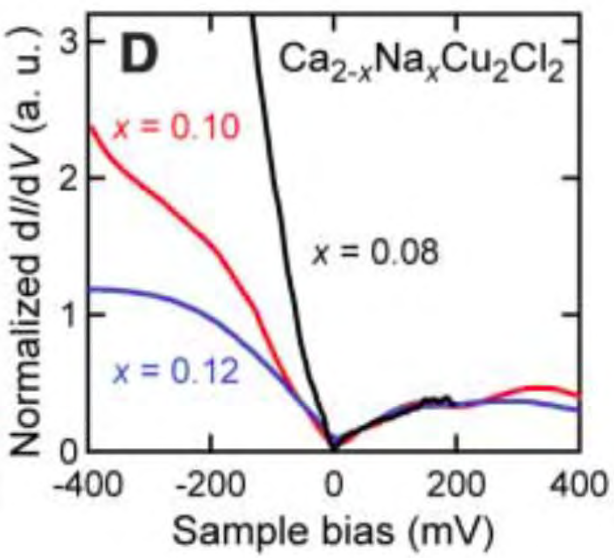


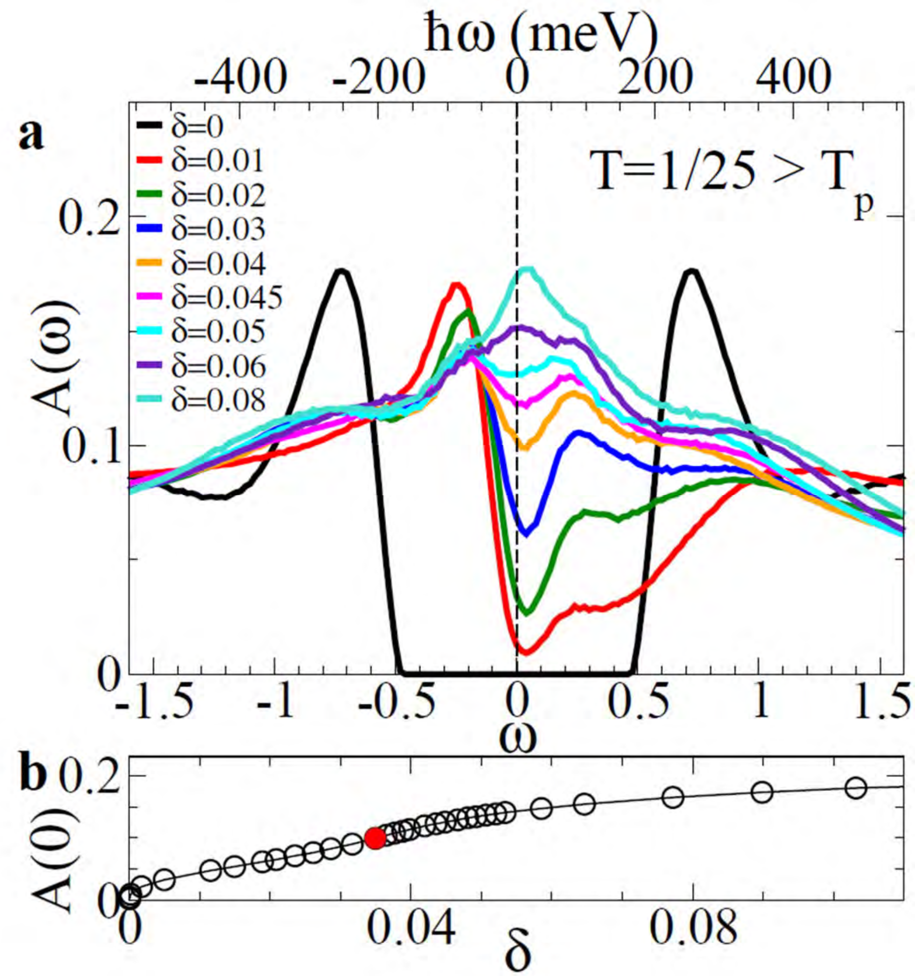
Phase diagram



UNIVERSITÉ DE SHERBROOKE

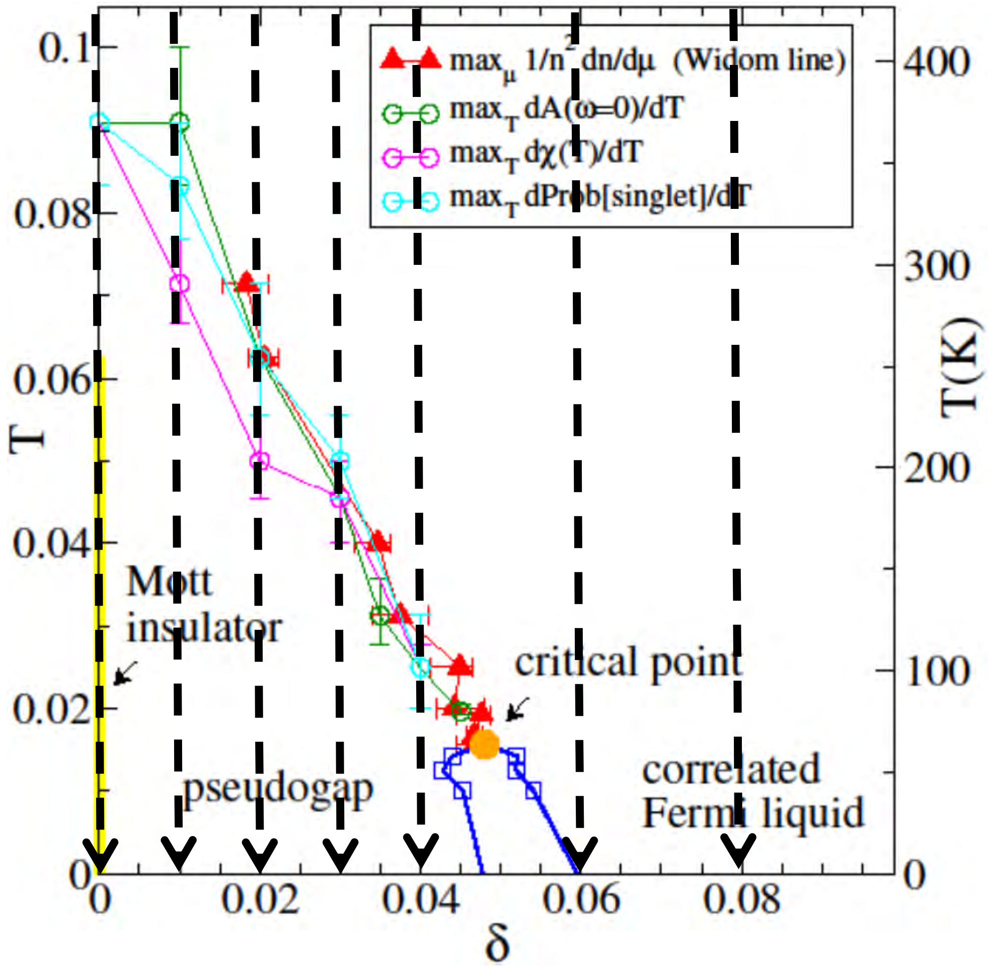
Tunneling DOS



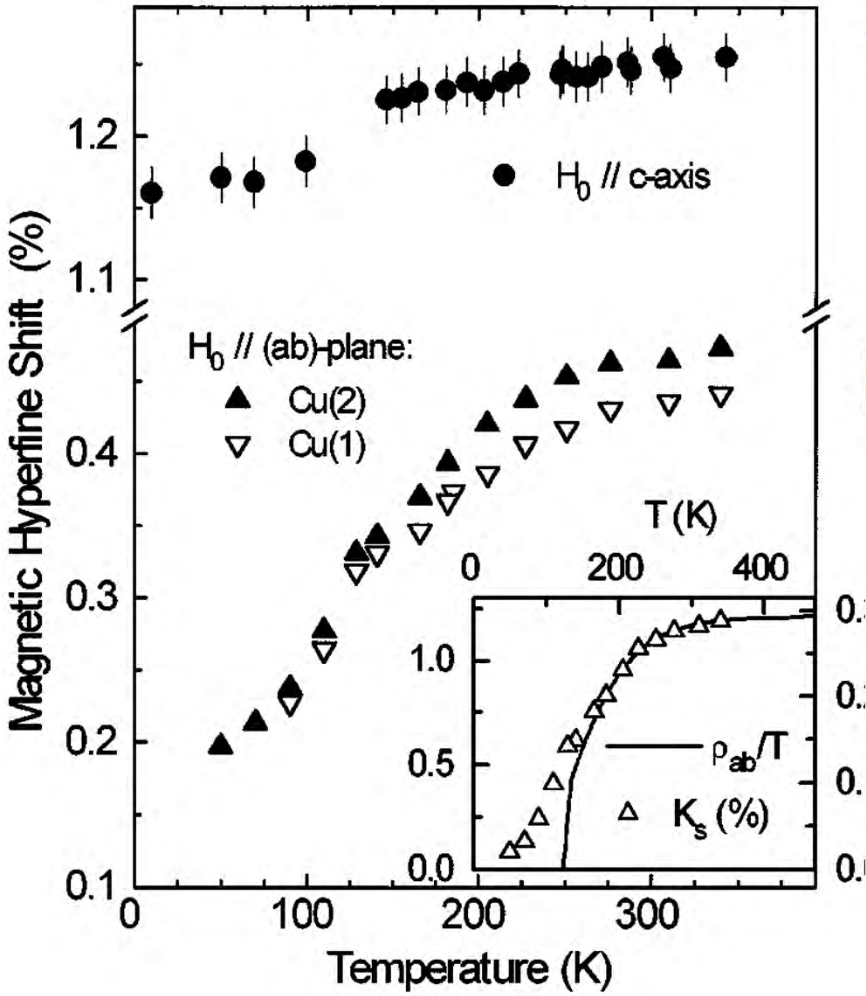


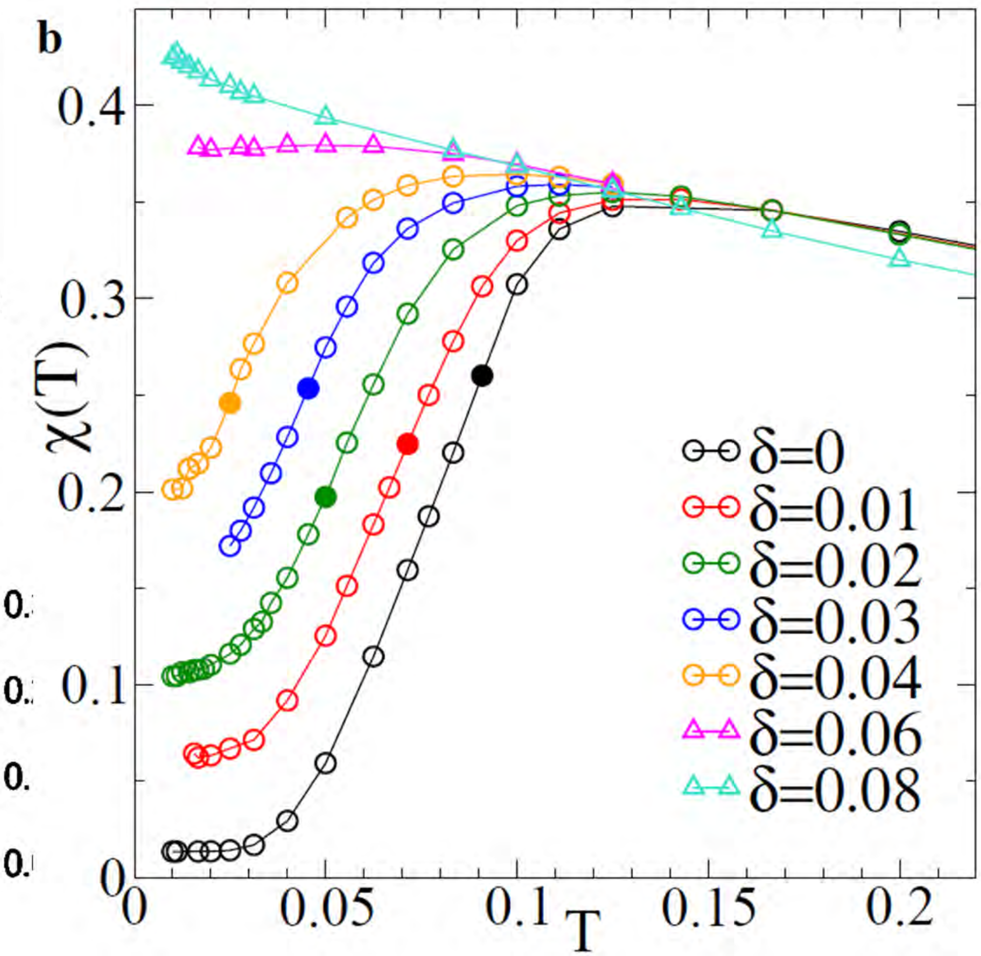
Khosaka et al. *Science* **315**, 1380 (2007);

Phase diagram



Spin susceptibility

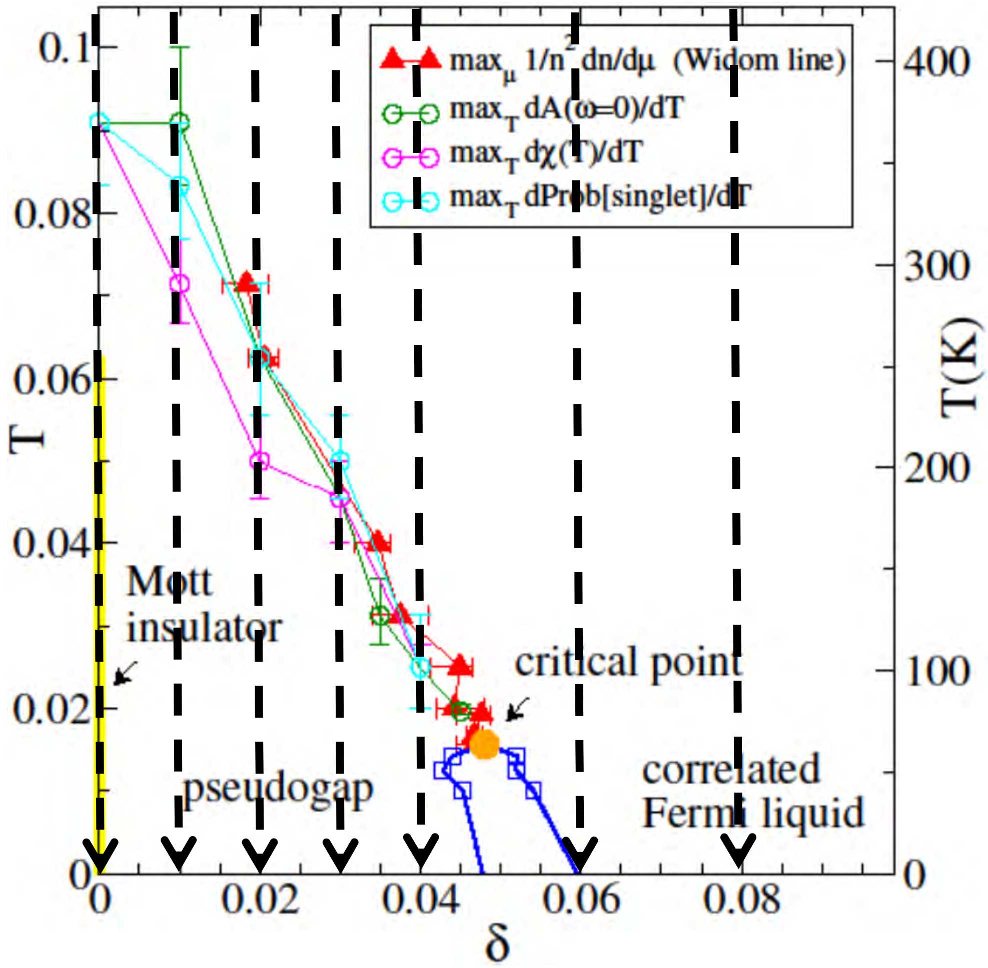




Underdoped Hg1223

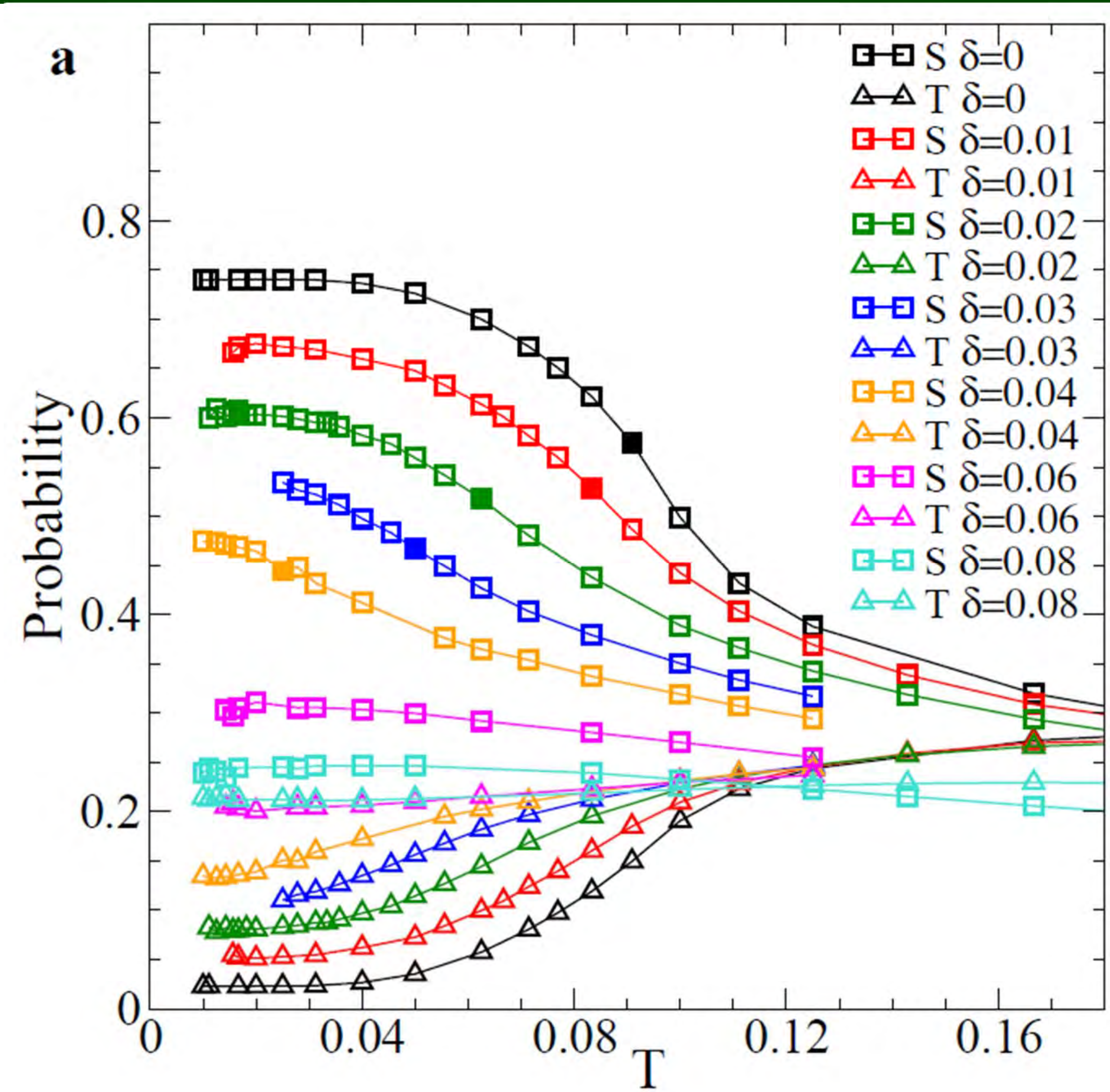
Julien et al. PRL **76,** 4238 (1996)

Phase diagram



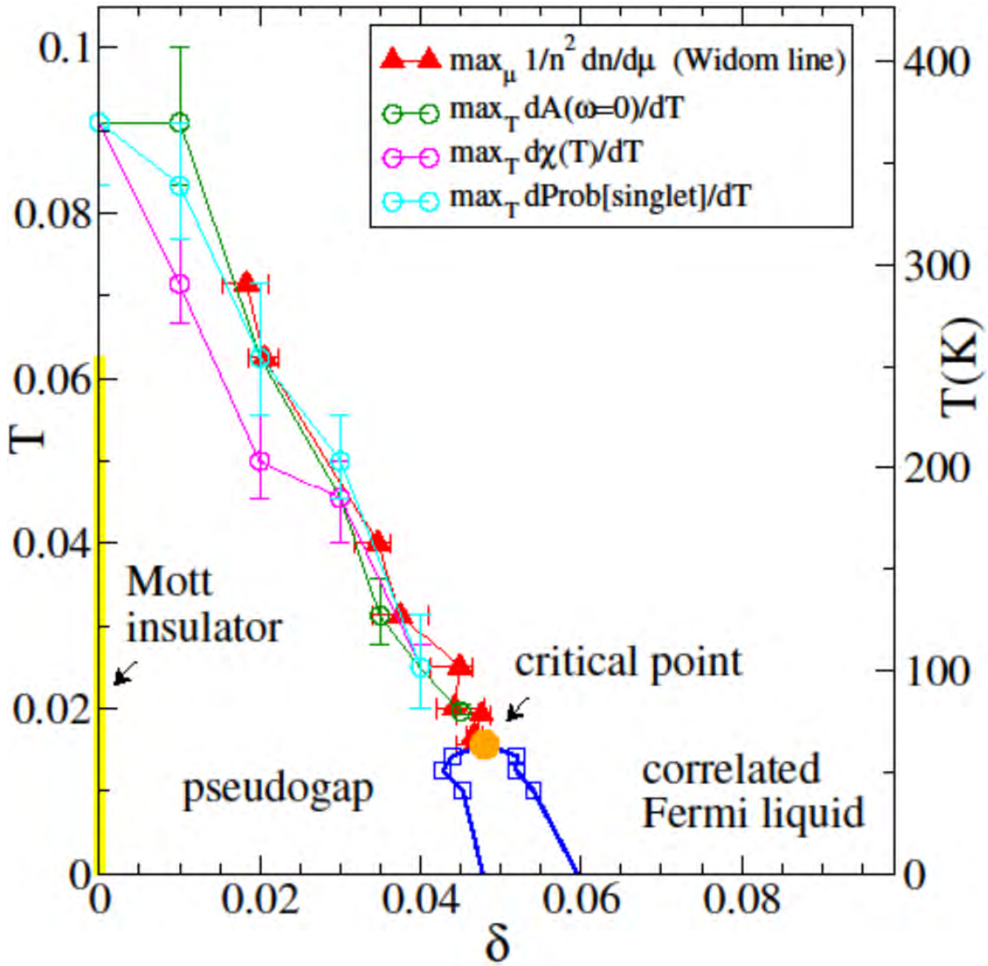
UNIVERSITÉ DE SHERBROOKE

Plaquette eigenstates



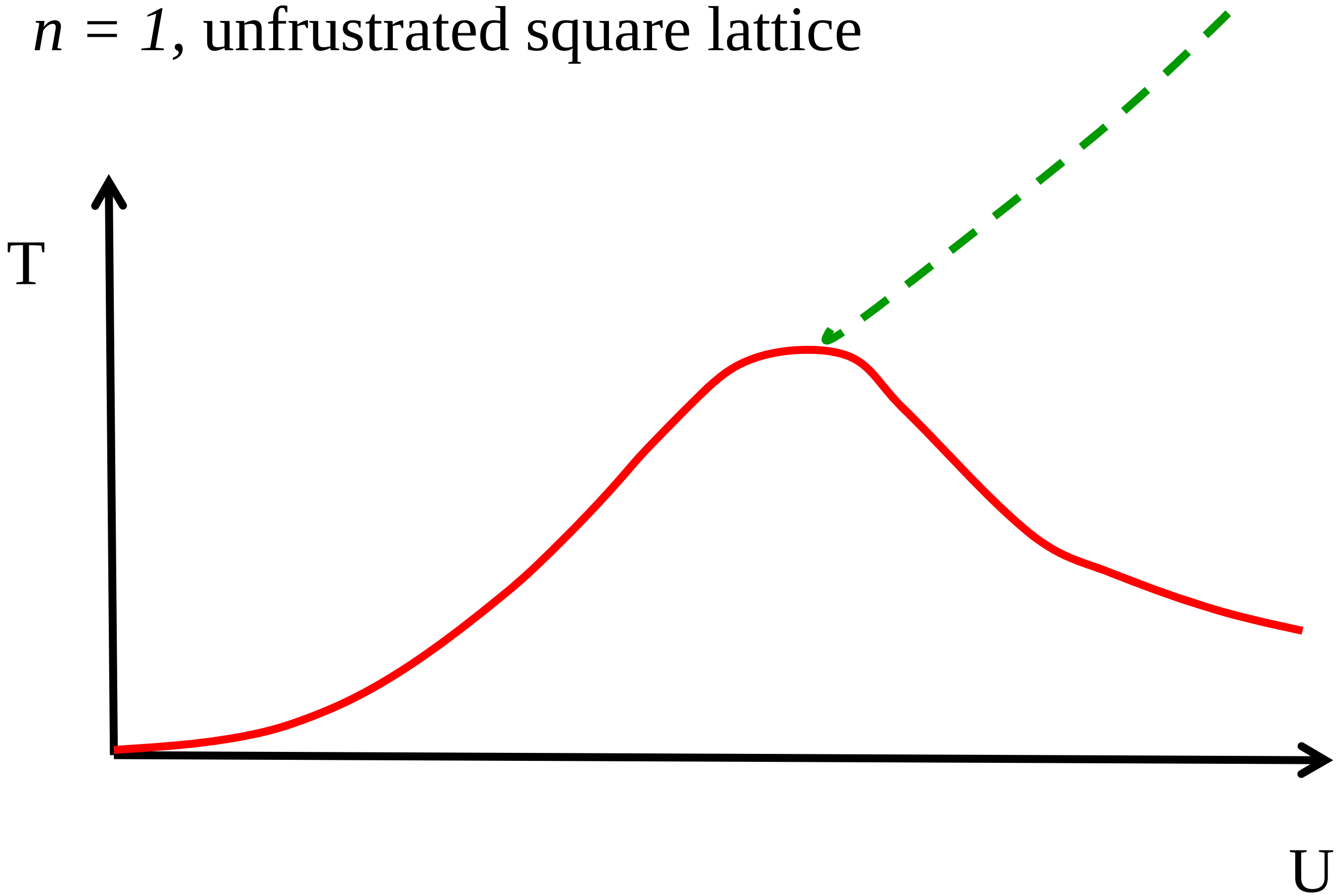
UNIVERSITÉ DE SHERBROOKE

Phase diagram



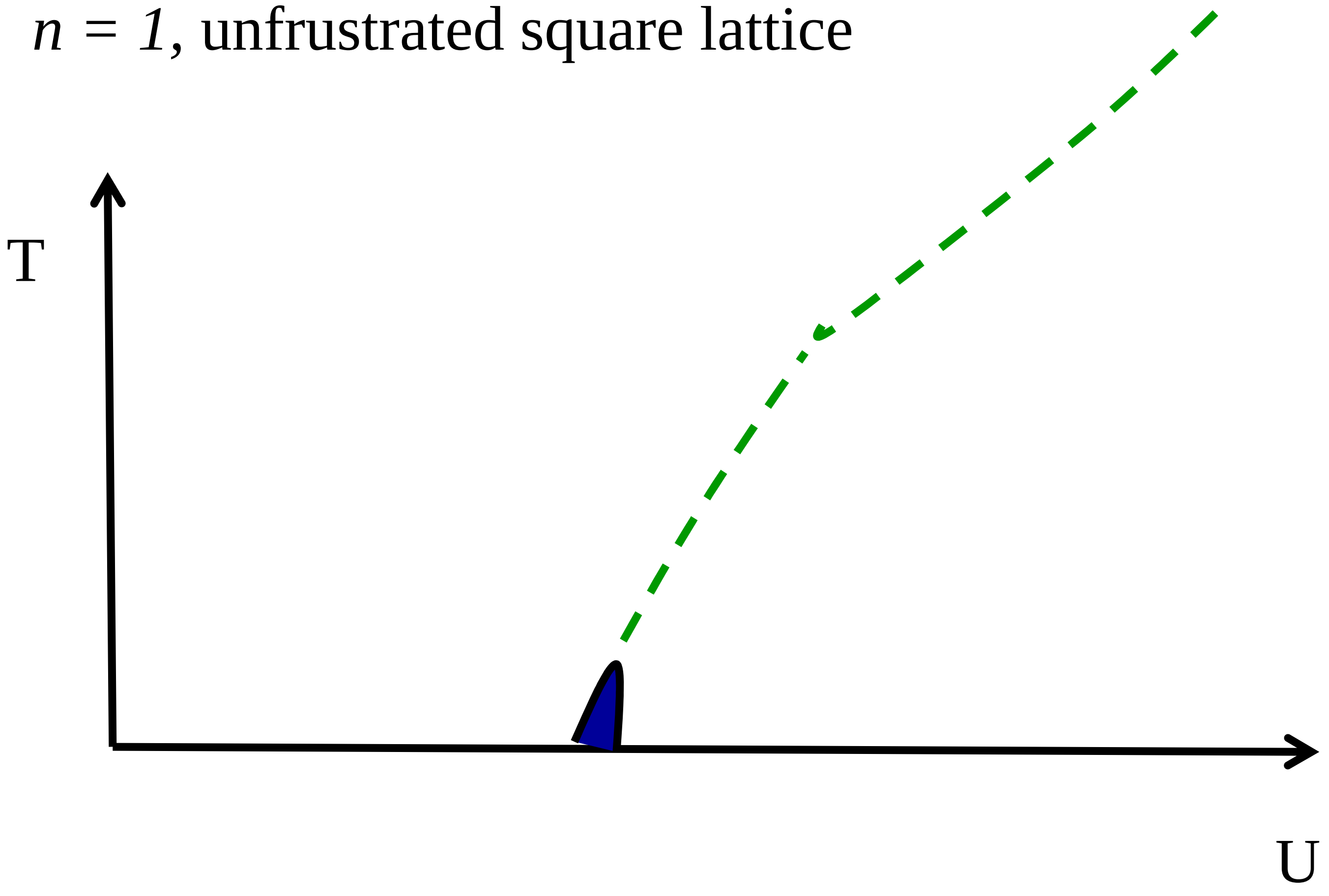
Local moment and Mott transition

n = 1, unfrustrated square lattice

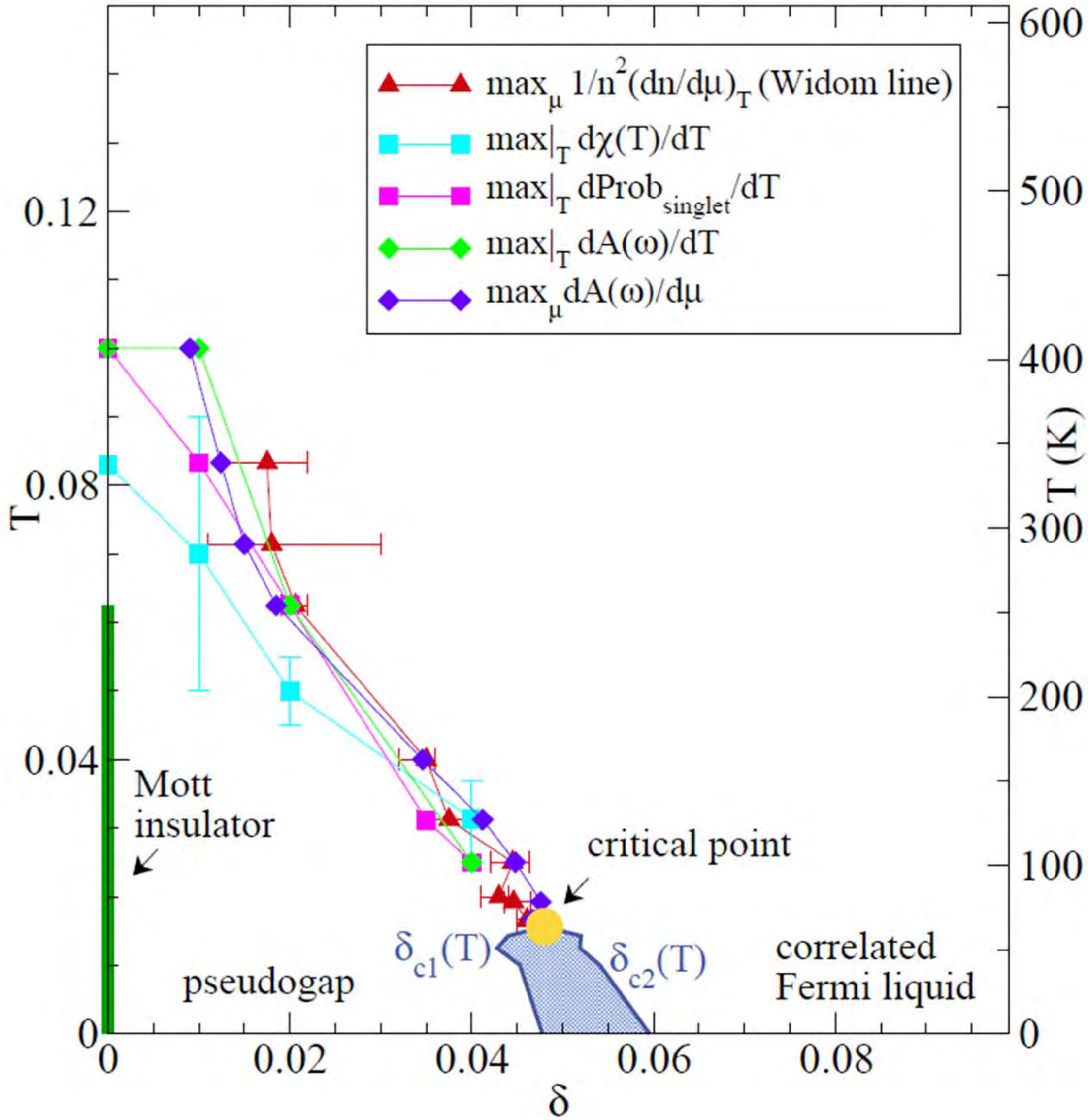


Local moment and Mott transition

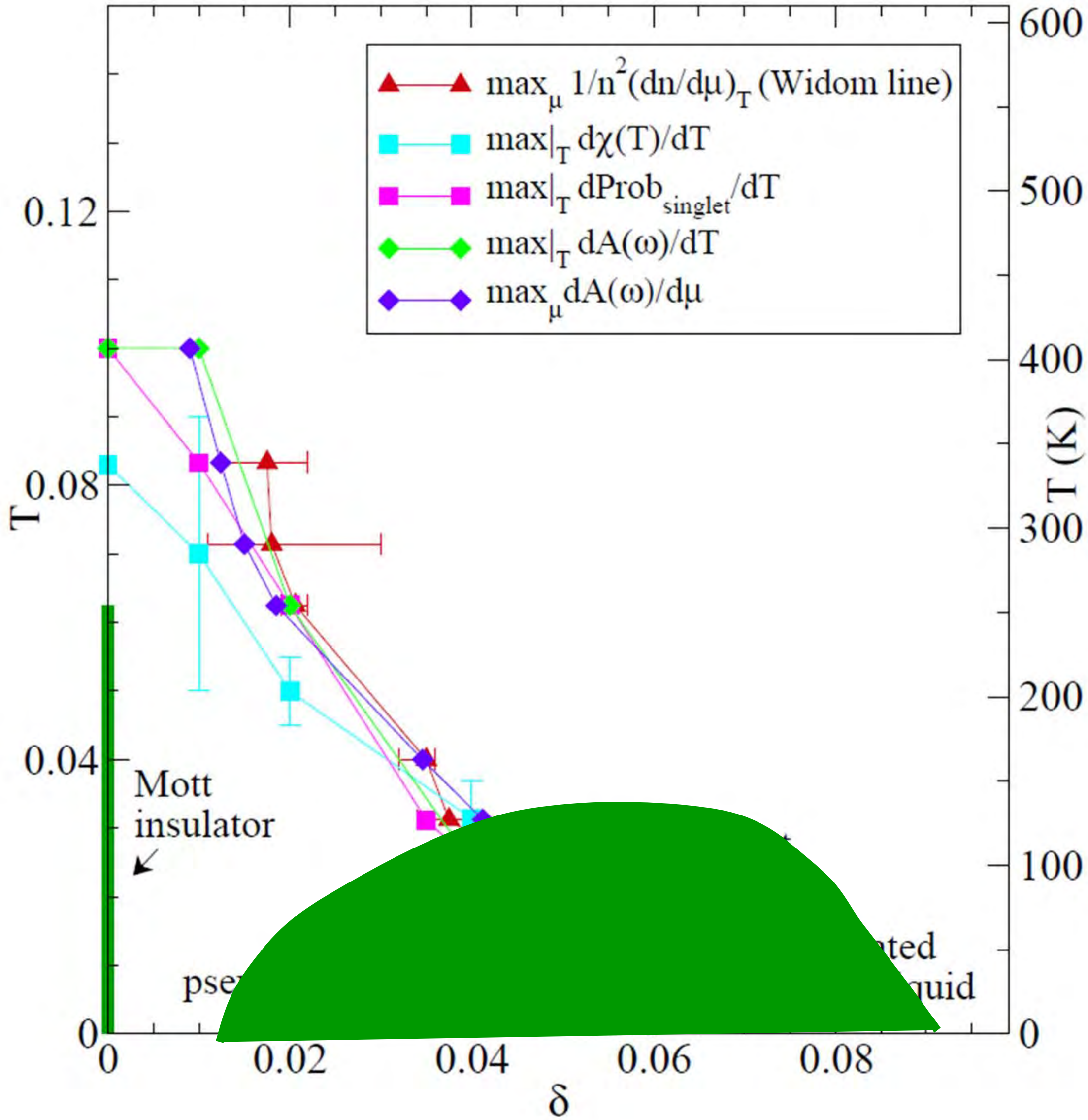
n = 1, unfrustrated square lattice



Local singlet and pseudogap transition



Local singlet and pseudogap transition



Another property of the UD phase

Underdoped metal very sensitive to anisotropy

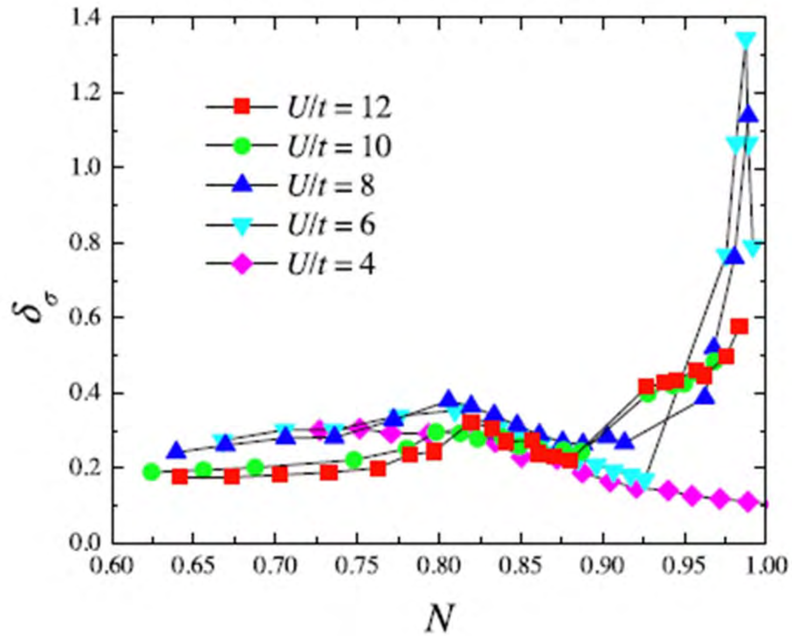
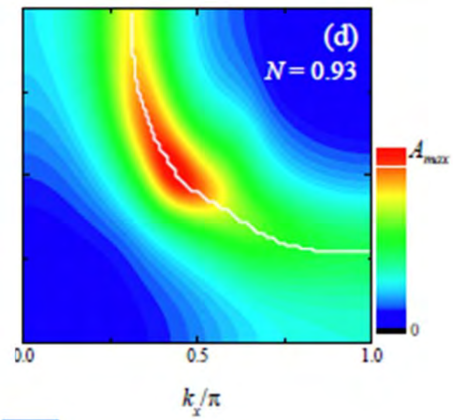
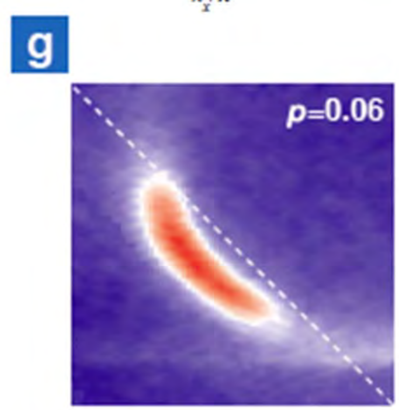


FIG. 3: (Color online) Anisotropy in the CDMFT conductivity $\delta_\sigma = 2\left[\sigma_x(0) - \sigma_y(0)\right] / \left[\sigma_x(0) + \sigma_y(0)\right]$ as a function of filling N for various values of U and $\eta = 0.1$, $\delta_0 = 0.04$.





Satoshi Okamoto

David Sénéchal

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

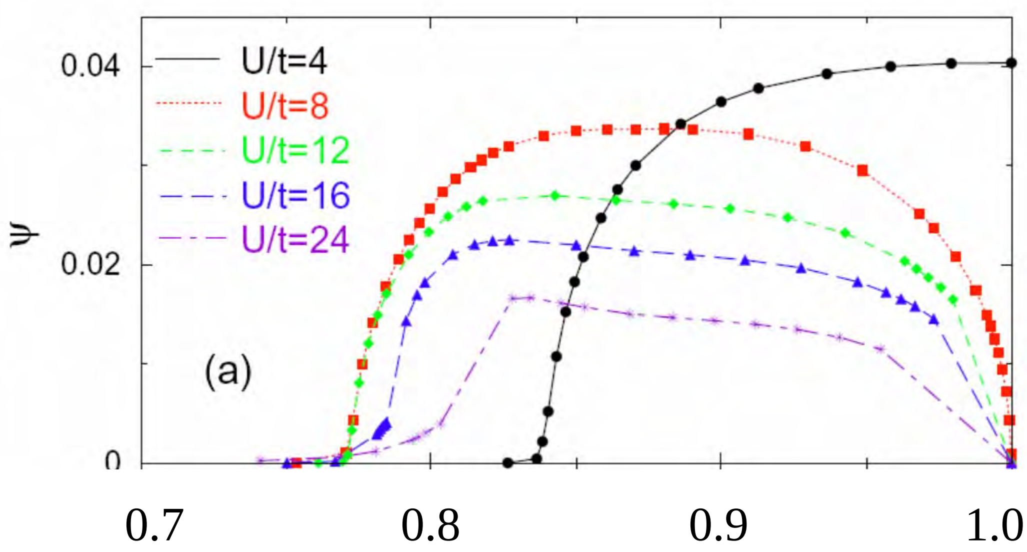
D. Fournier *et al.* Nature Physics (Marcello Civelli

Superconductivity

Phase diagram

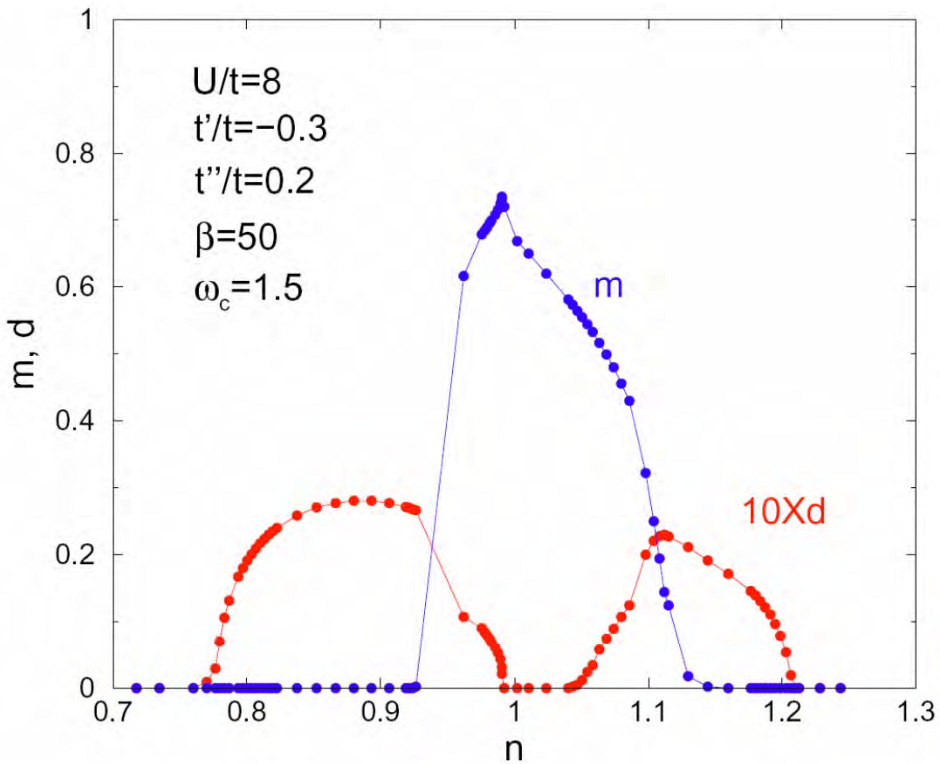
Exact diagonalization as impurity solver ($T=0$).

Dome vs Mott (CDMFT)

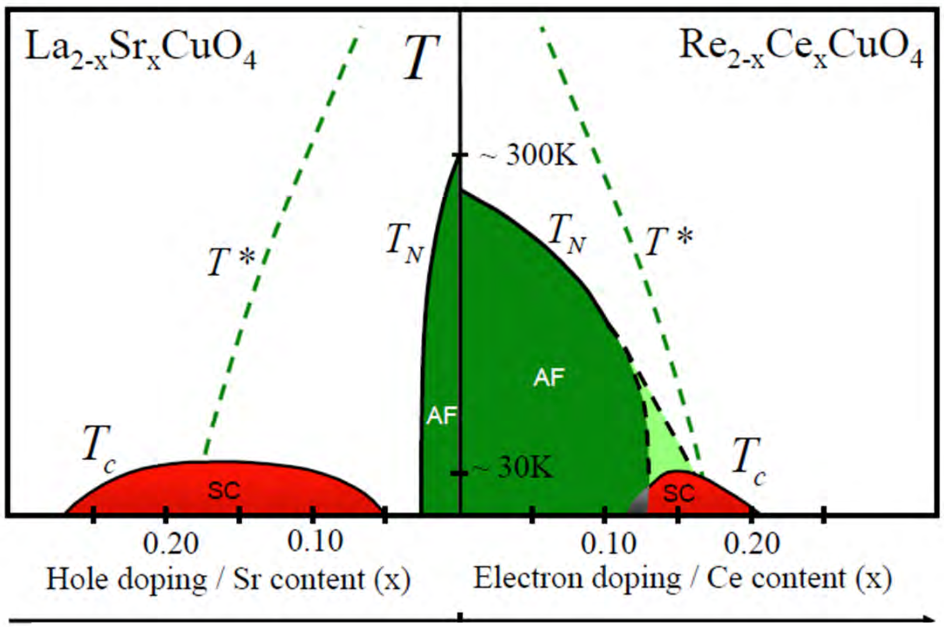


Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008)

CDMFT global phase diagram



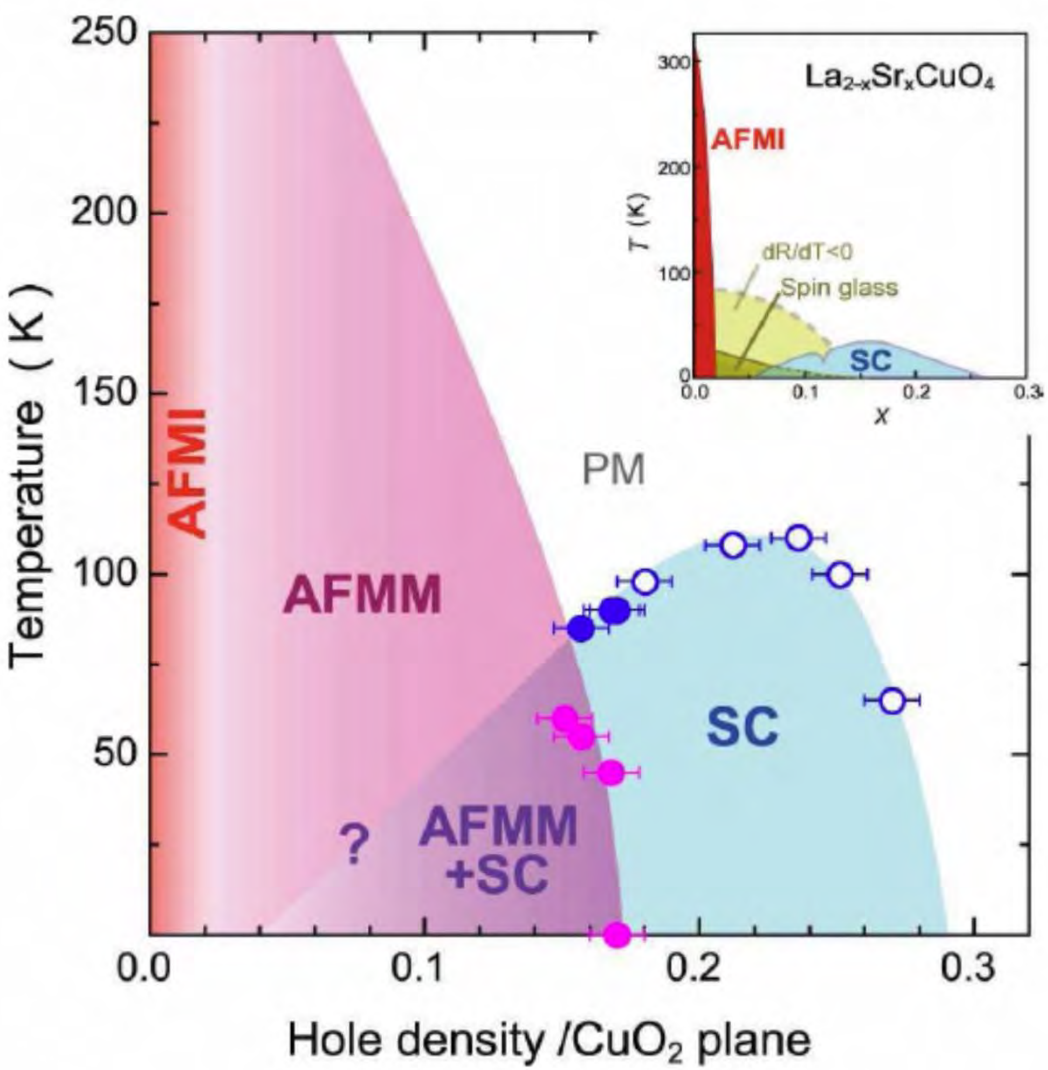
Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008)

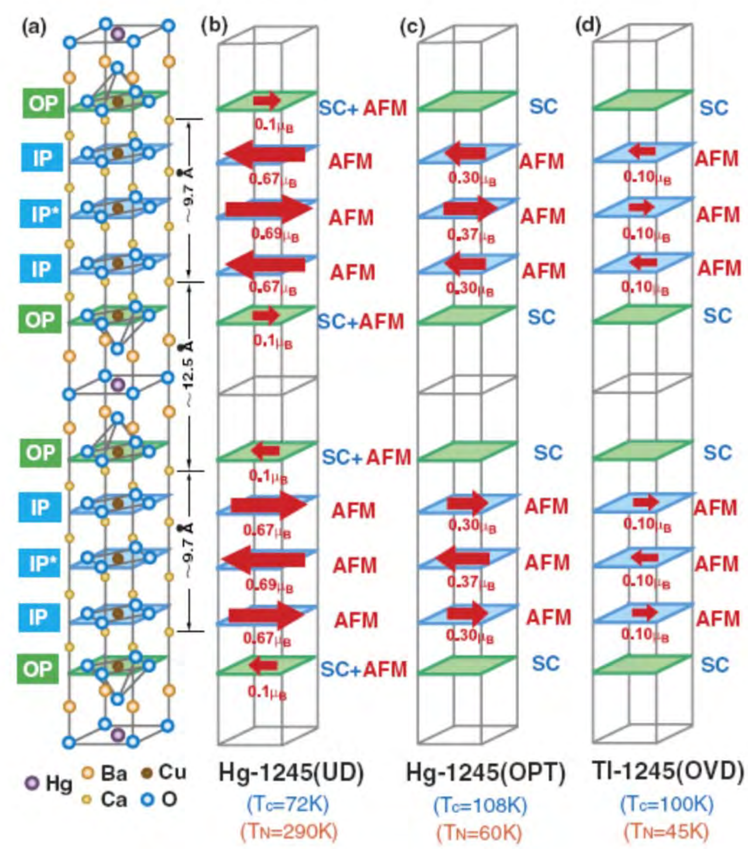


Armitage, Fournier, Greene, RMP (2009)

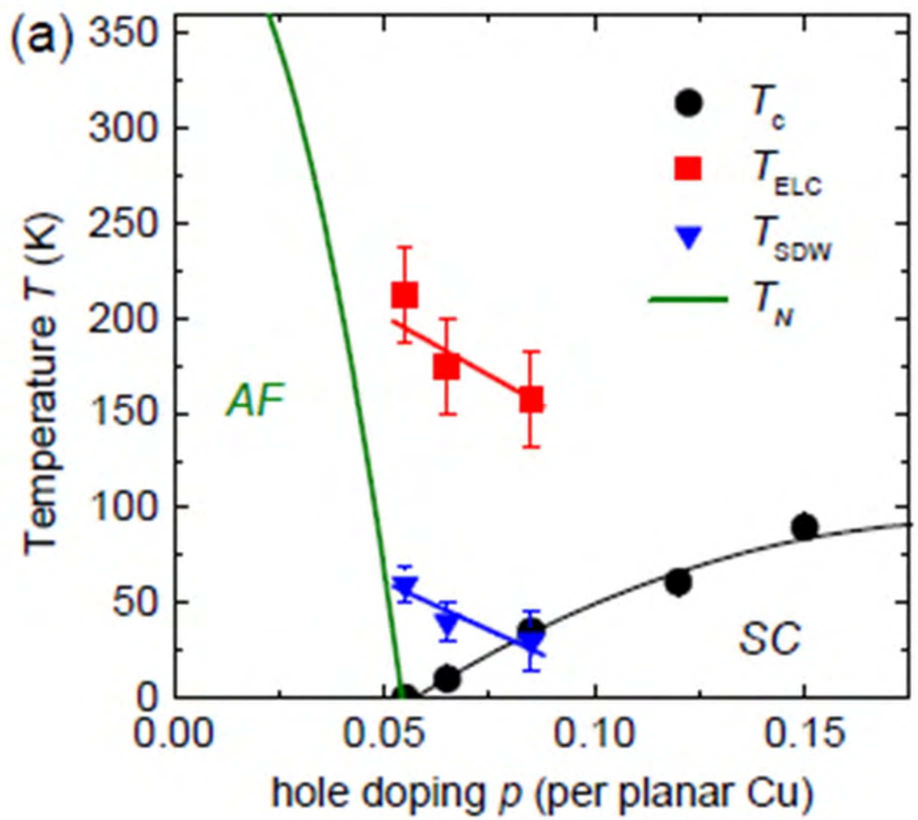
Consistent with following experiment

H. Mukuda, Y. Yamaguchi, S. Shimizu, … A. Iyo JPSJ **77**, 124706 (2008)



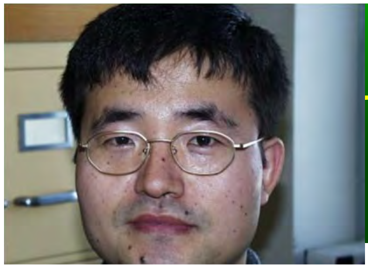


Magnetic phase diagram of YBCO



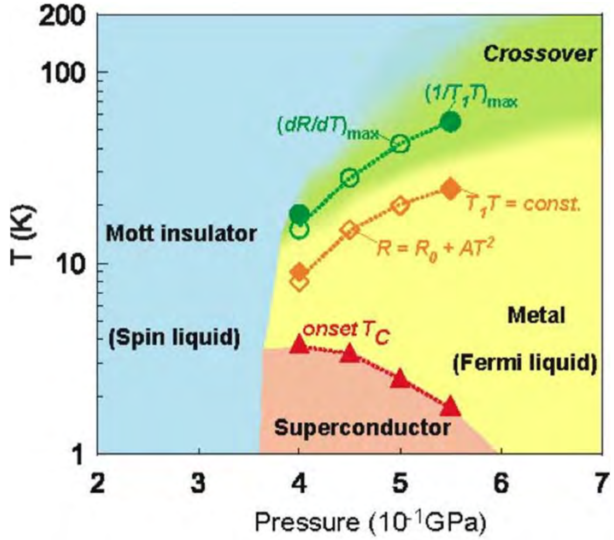
Haug, … Keimer, New J. Phys. 12, 105006 (2010)

UNIVERSITÉ DE SHERBROOKE



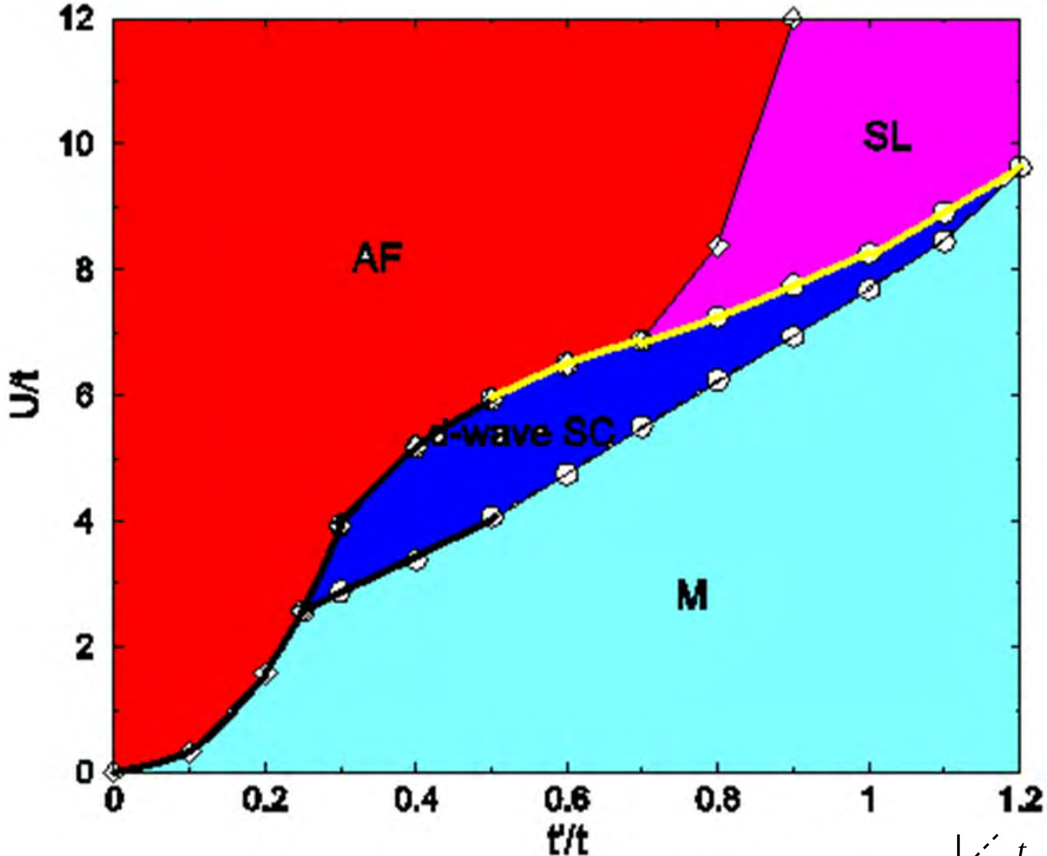
Theoretical phase diagram BEDT

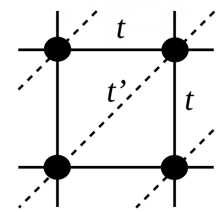
X= $Cu_2(CN)_3$ (t'~ t)



Y. Kurisaki, et al.

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





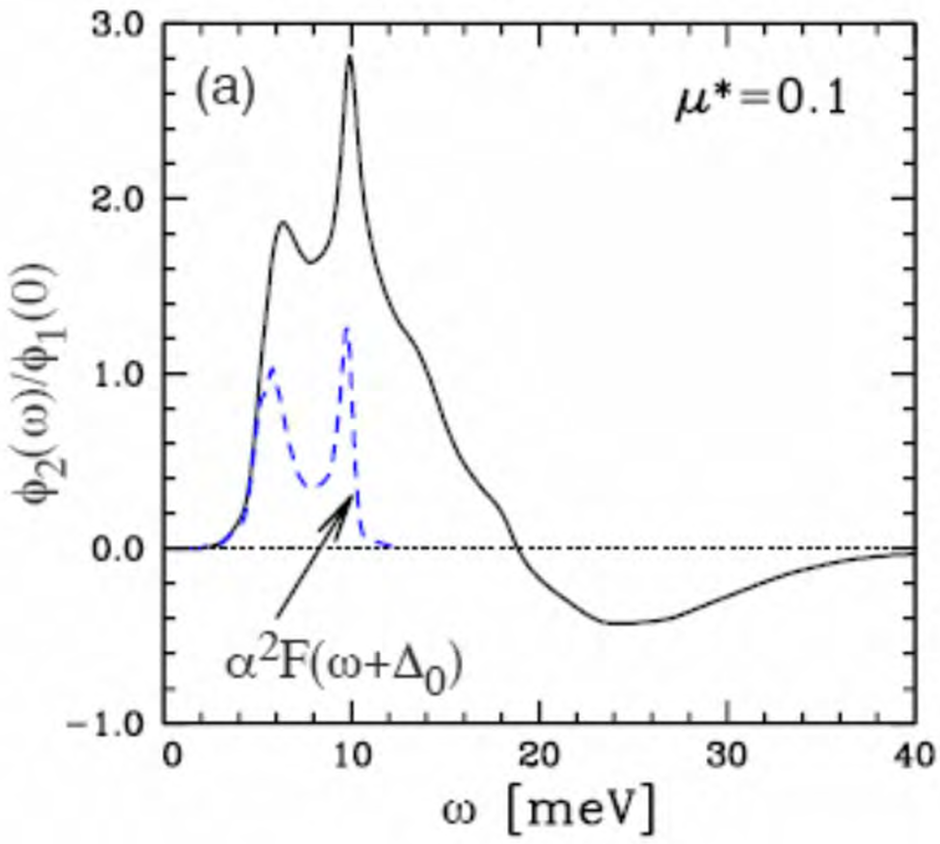
Kyung, A.-M.S.T. PRL 97, 046402 (2006)

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

The glue

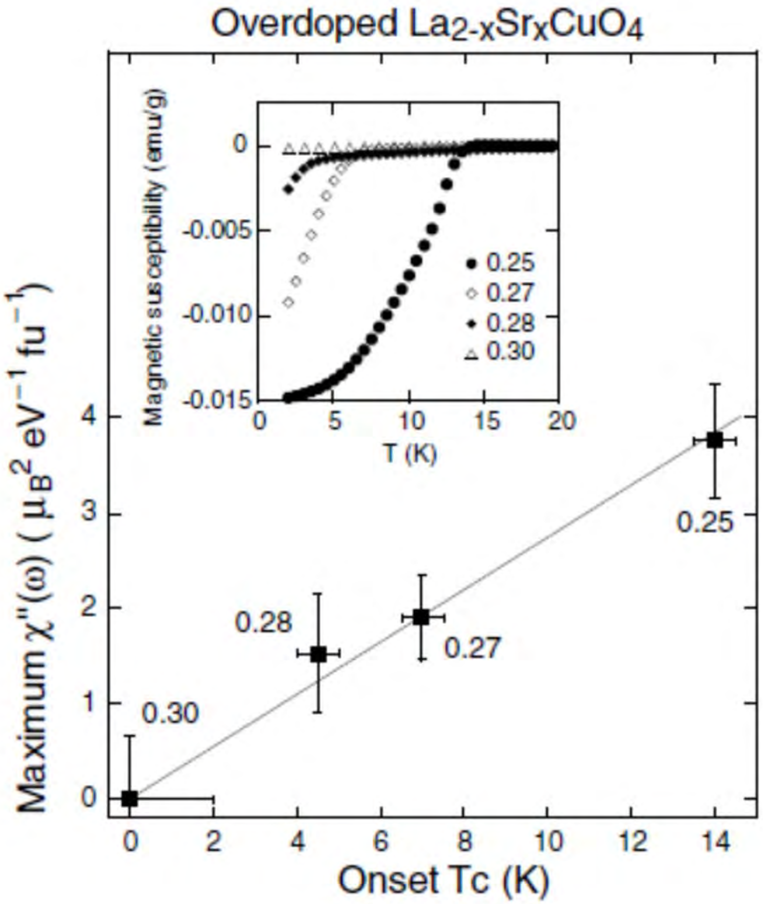
Im Σ_{an} and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

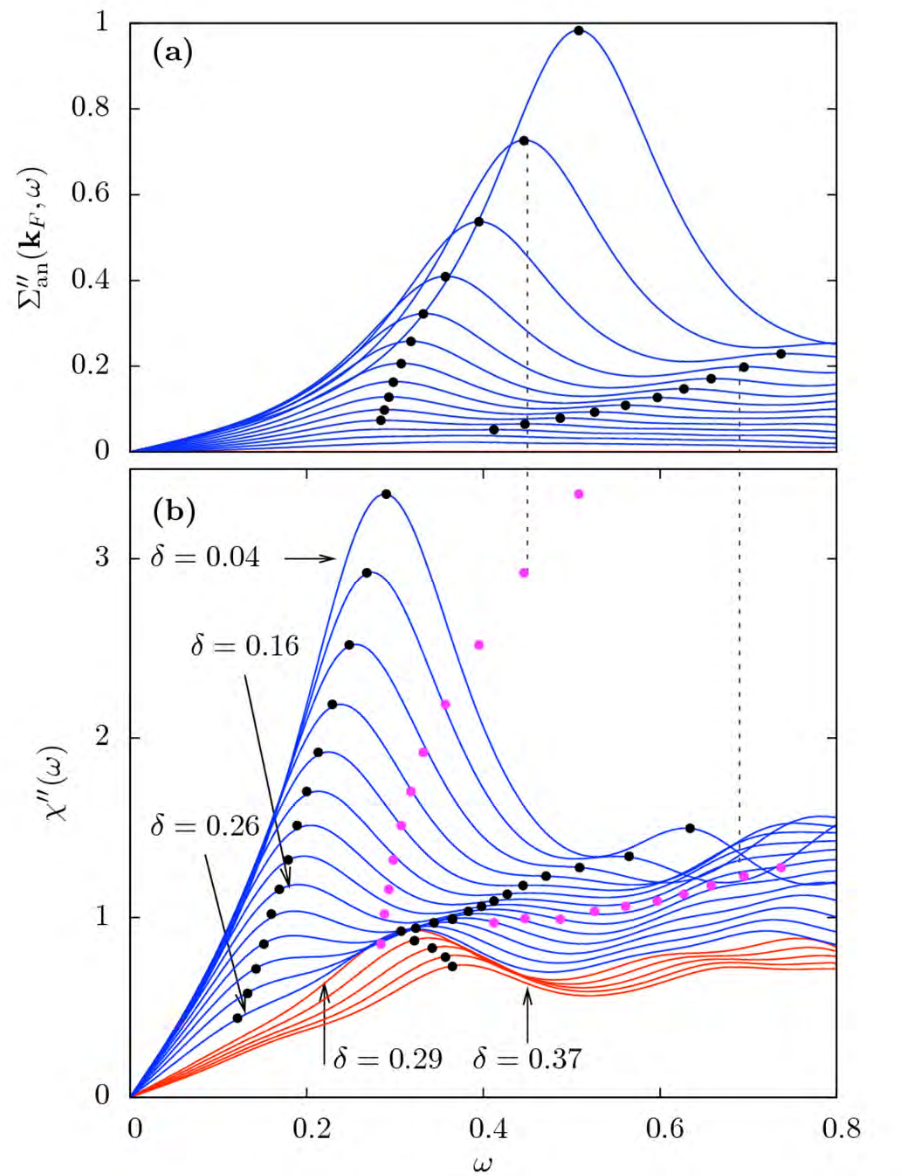


The glue

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



Wakimoto … Birgeneau PRL (2004)



The glue and neutrons

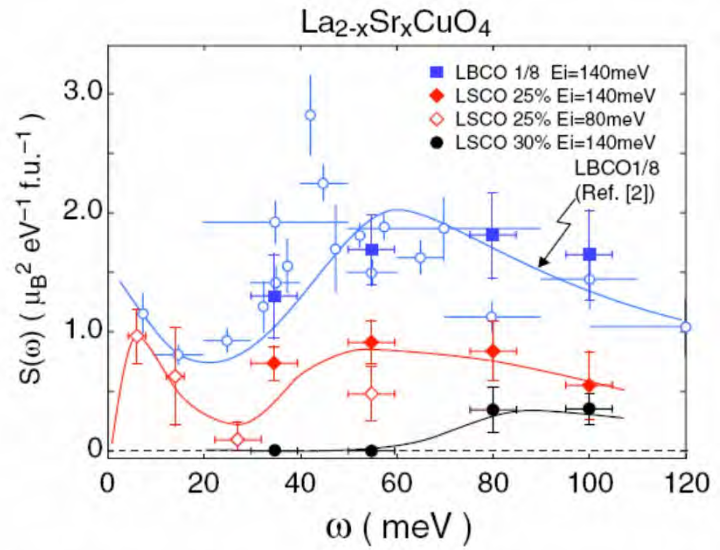
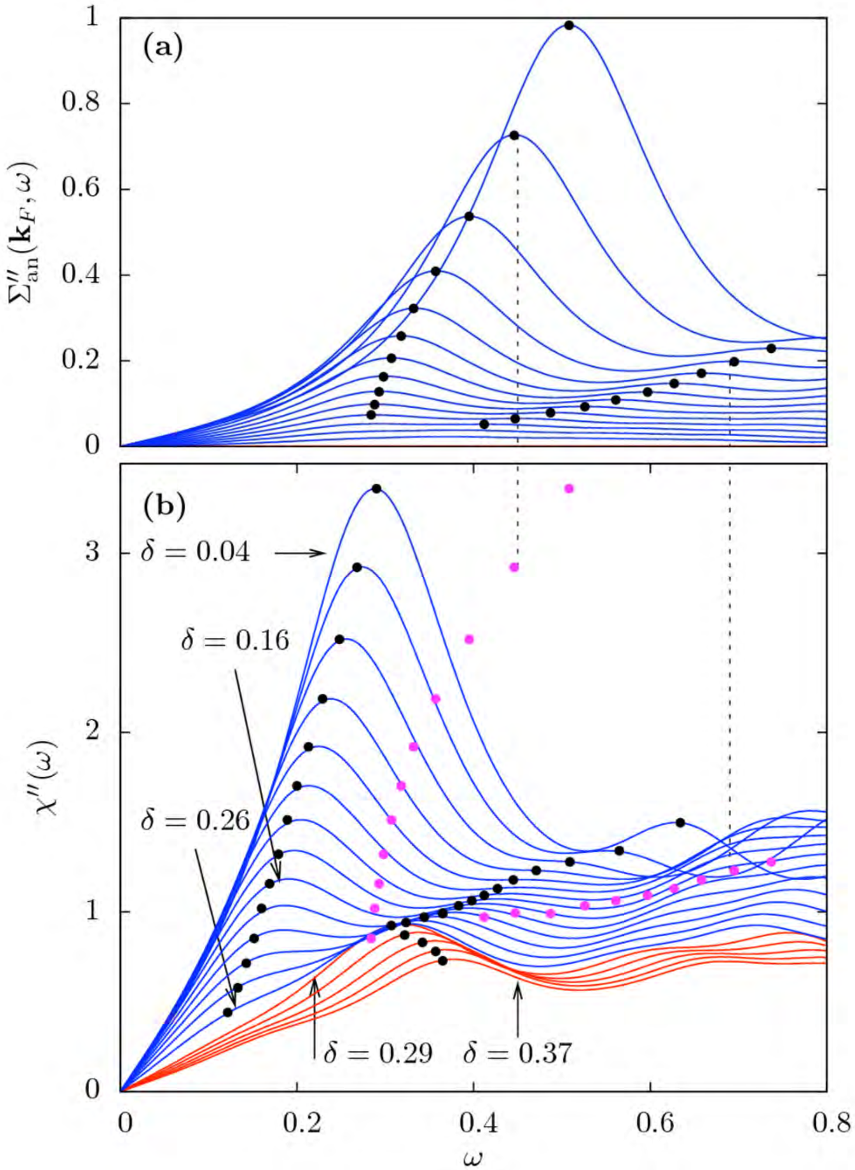


FIG. 3 (color online). **Q**-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i = 140$ meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO 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)



Main collaborators

Giovanni Sordi

David Sénéchal

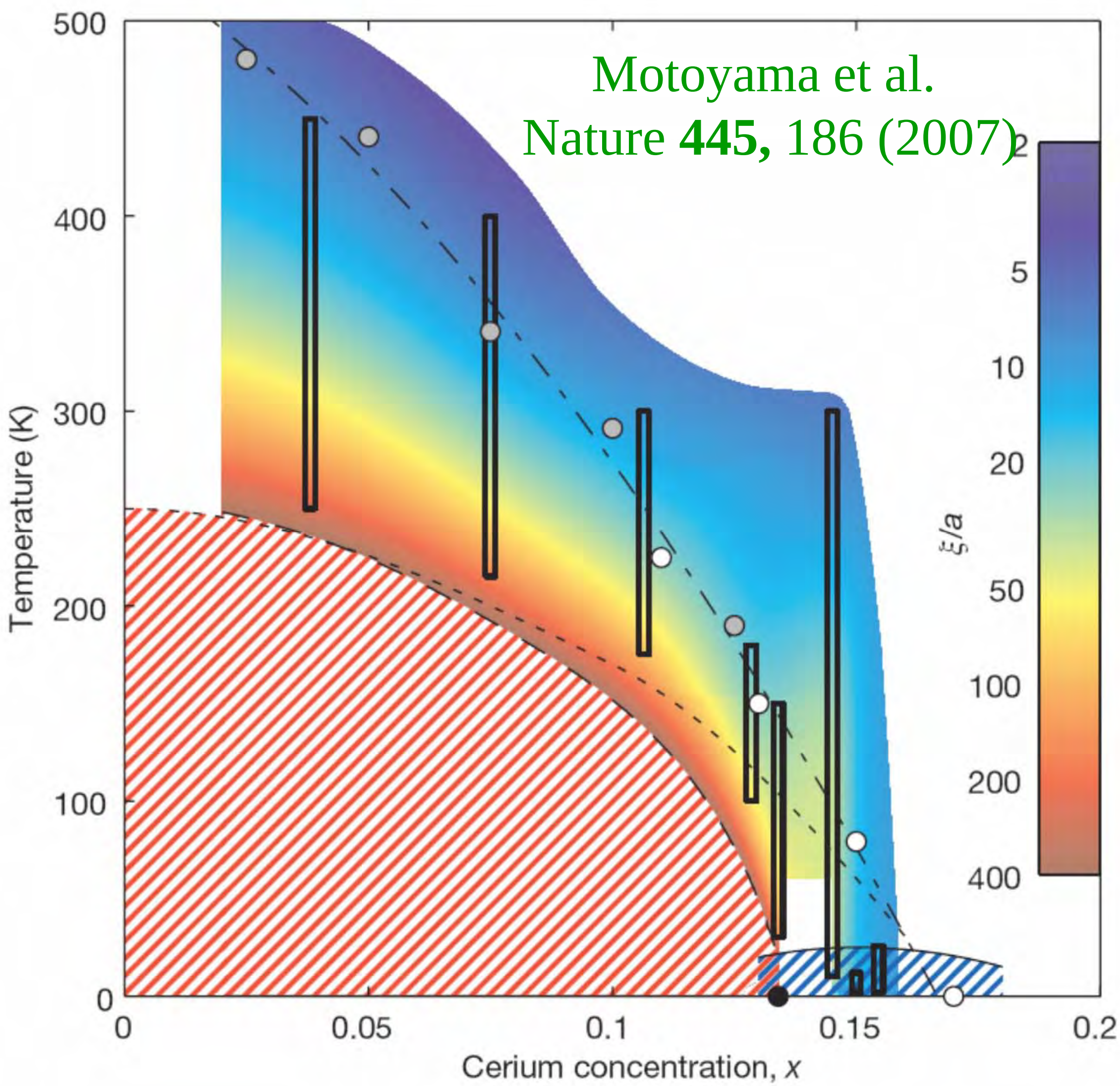
Kristjan Haule

Bumsoo Kyung

Marcello Civelli

Satoshi Okamoto

d = 2 precursors, e-doped



Motoyama et al.
Nature **445,** 186 (2007)

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

Vilk, A.-M.S.T (1997)

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

Semi-quantitative fits of both ARPES and neutron

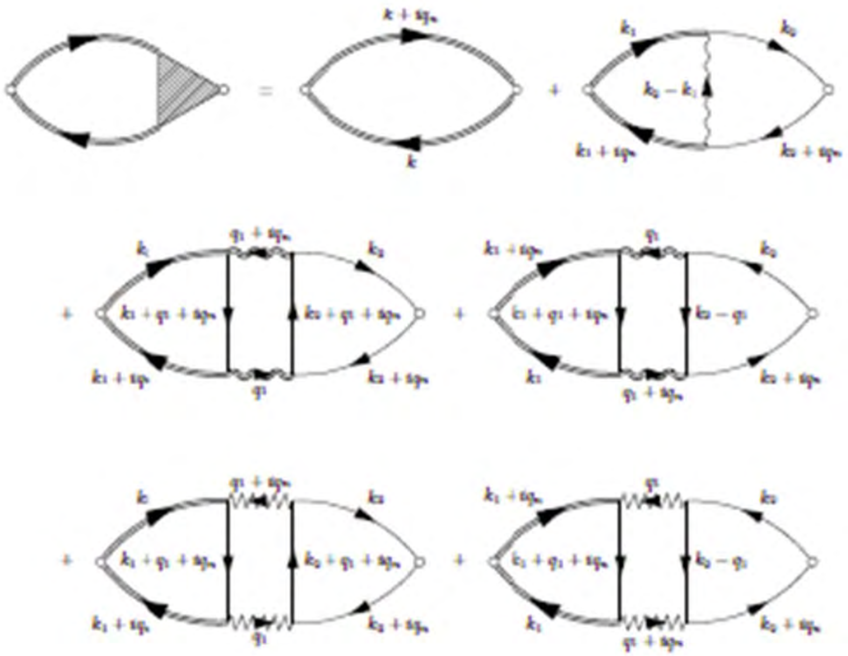
TPSC: general ideas

- 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)

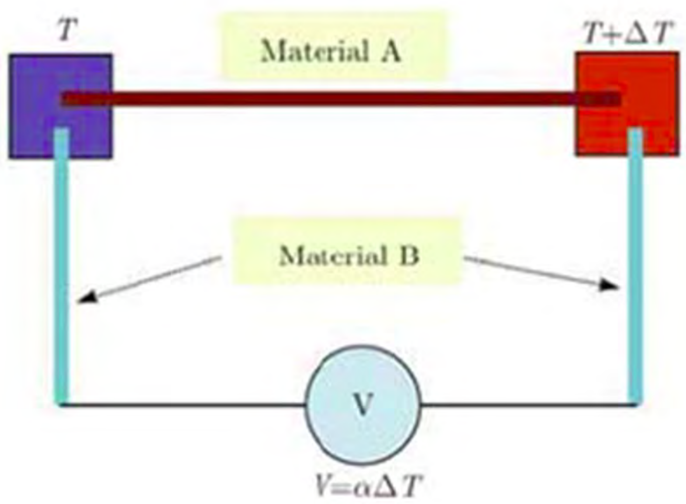
UNIVERSITÉ DE SHERBROOKE

Resistivity (TPSC)



Dominic Bergeron

Thermoelectric power



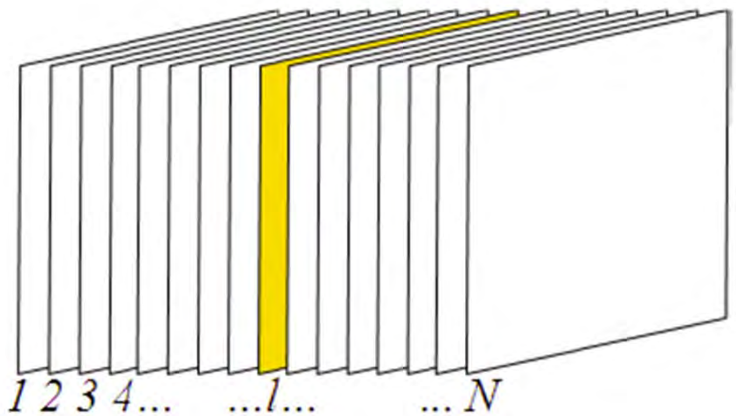
Louis-François Arsenault

Sriram Shastry

Patrick Sémon

UNIVERSITÉ DE SHERBROOKE

Heterostructures



Maxime Charlebois

David Sénéchal

Syed Hassan

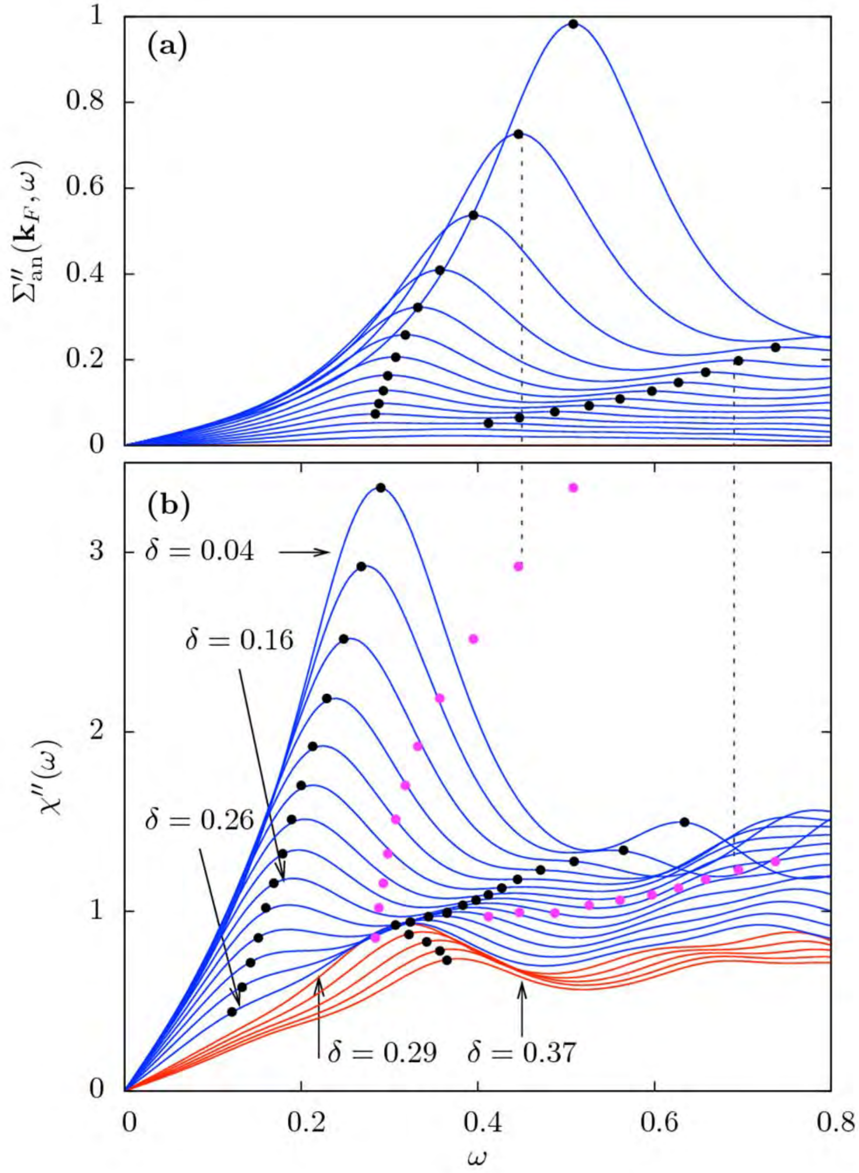
Patrick Fournier

Maxime Dion

Simon Verret

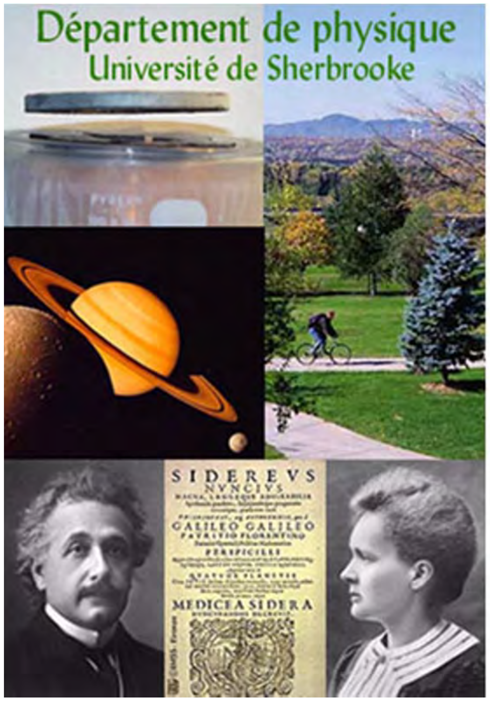
UNIVERSITÉ DE SHERBROOKE

Retardation effects



David Sénéchal

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, série

Réseau Québécois
de Calcul de Haute
Performance

Éducation,
Loisir et Sport
Québec

Canada Foundation for Innovation
Fondation canadienne pour l'innovation

UNIVERSITÉ DE
SHERBROOKE

Conclusions

- Tools for Hubbard model, high Tc.
- The influence of Mott Physics extends way beyond half-filling
  - Pseudogap as a phase
  - Effects of critical point at high temperature (Widom line)
  - Superconductivity
    - Dome
    - Retardation effects in pairing come from spin fluctuations.

Merci

Thank you