2357-3

Innovations in Strongly Correlated Electronic Systems: School and Workshop

6 - 17 August 2012

Mott transition, Hubbard model and superconductivity: an introduction

Andre-Marie TREMBLAY

Departement de Physique and RQMP
Universite de Sherbrooke, QC J1K 281
CANADA

Mott transition, Hubbard model and superconductivity: an introduction

A.-M. Tremblay

G. Sordi, K. Haule, D. Sénéchal,

P. Sémon, B. Kyung, G. Kotliar

CIFAR
CANADIAN INSTITUTE for ADVANCED RESEARCH

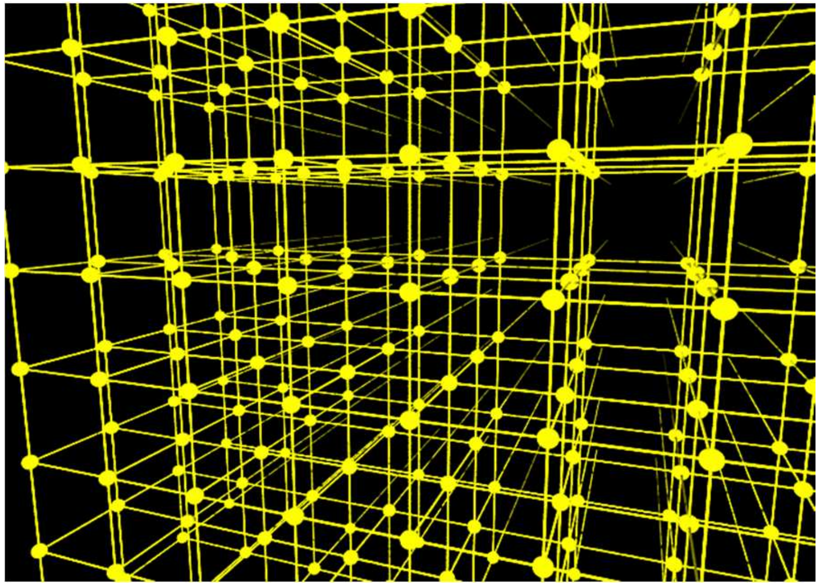
UNIVERSITÉ DE SHERBROOKE

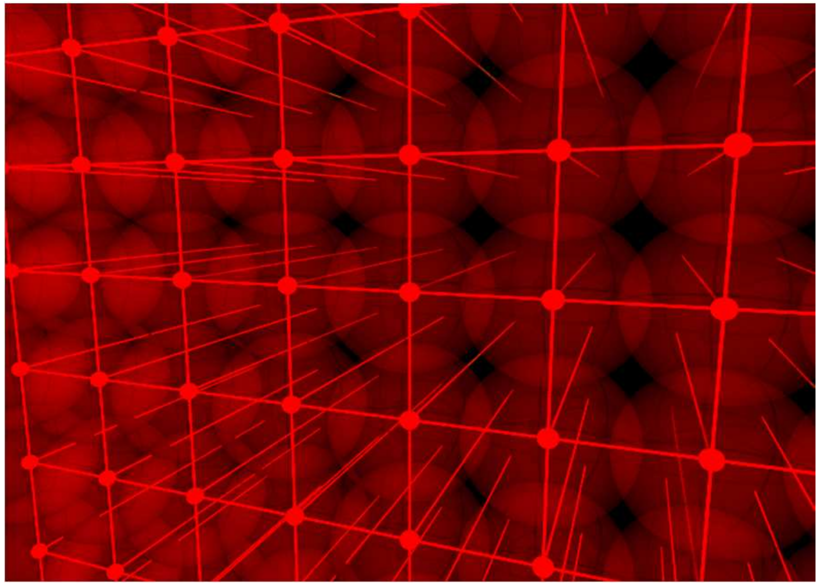
Trieste, 6 August, 2012

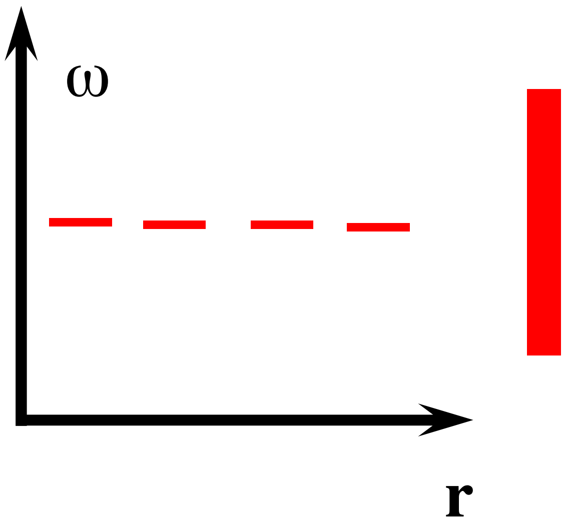
VERITATEM IN CHARITATE

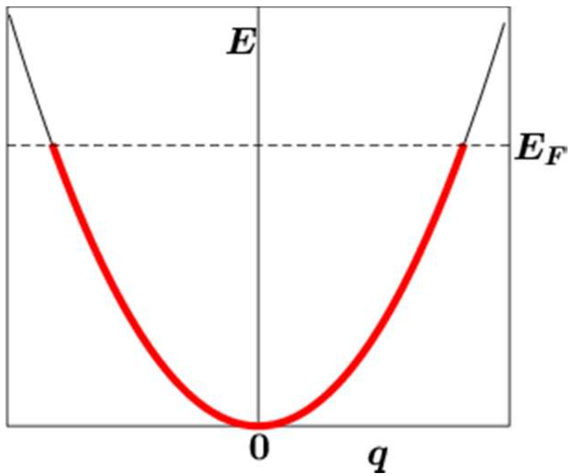
UNIVERSITÉ DE SHERBROOKE

How to make a metal





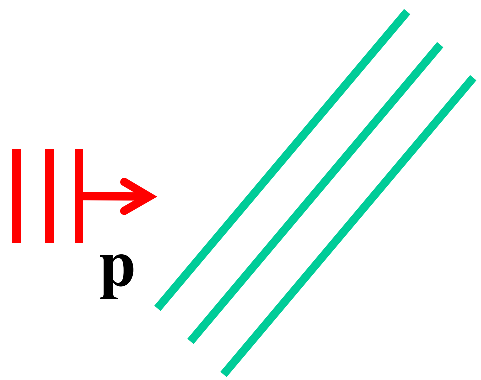




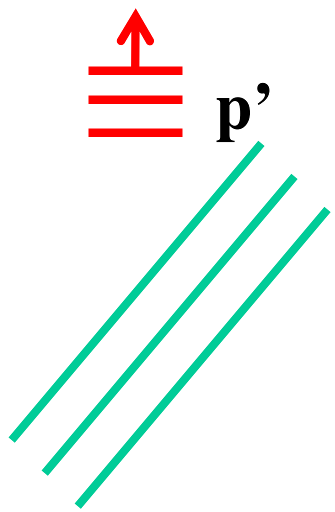
Courtesy, S. Julian

Superconductivity

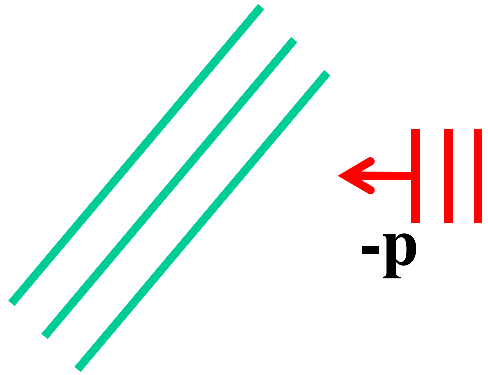
Attraction mechanism in the metallic state



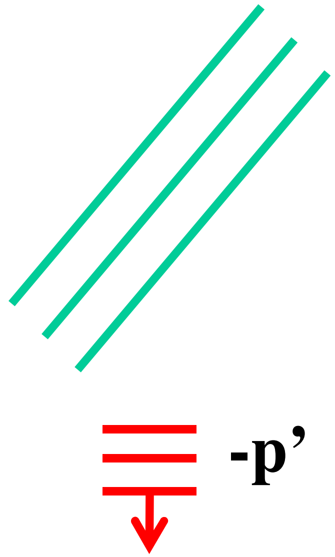
Attraction mechanism in the metallic state



Attraction mechanism in the metallic state

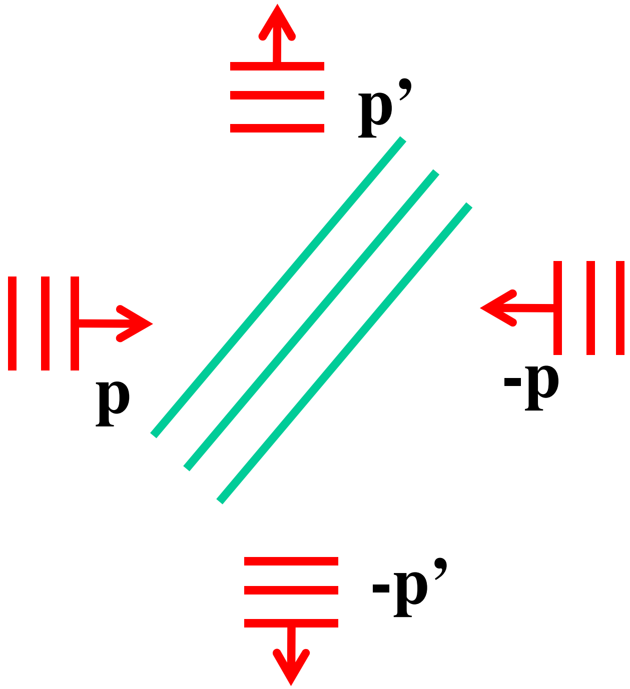


Attraction mechanism in the metallic state



UNIVERSITÉ DE SHERBROOKE

Attraction mechanism in the metallic state



#1 Cooper pair, #2 Phase coherence

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

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

$$|\mathrm{BCS}(\theta)\rangle = \ldots + e^{iN\theta}|N\rangle + e^{i(N+2)\theta}|N+2\rangle + \ldots .$$

UNIVERSITÉ DE SHERBROOKE

Half-filled band is metallic?

Half-filled band: Not always a metal

NiO, Boer and Verway

Peierls, 1937

Mott, 1949

« Conventional » Mott transition

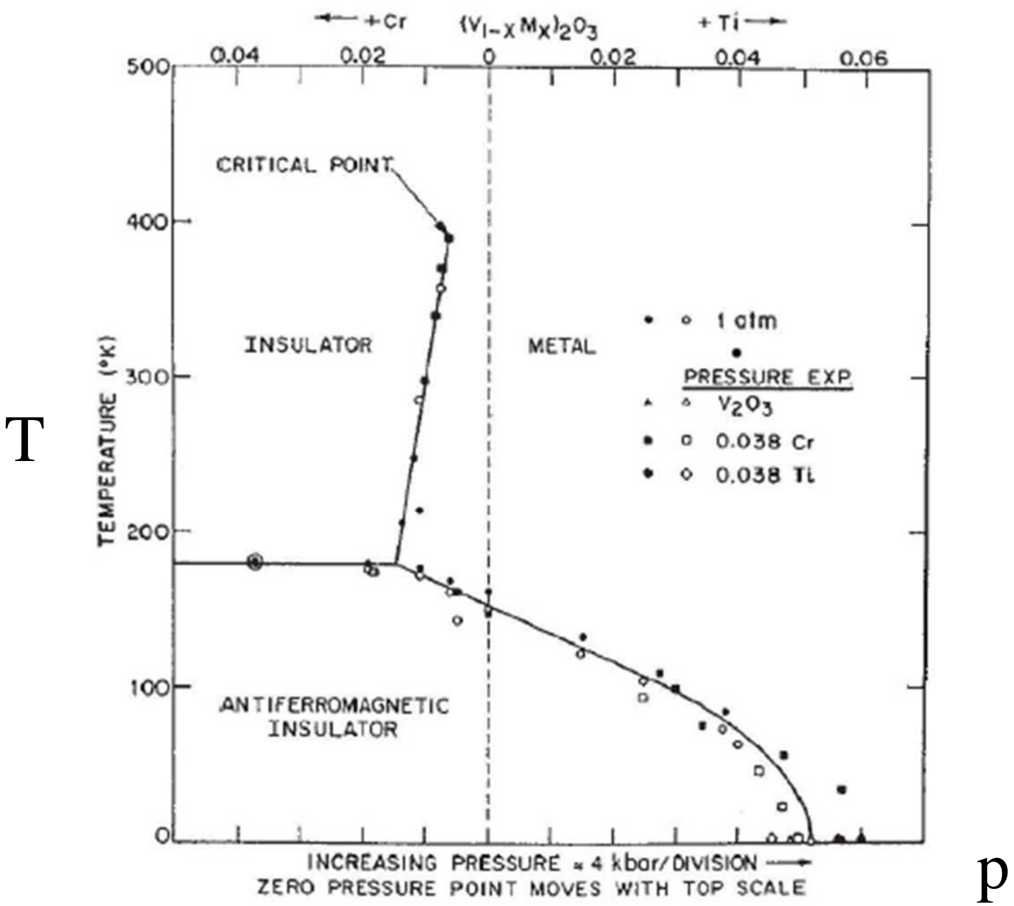
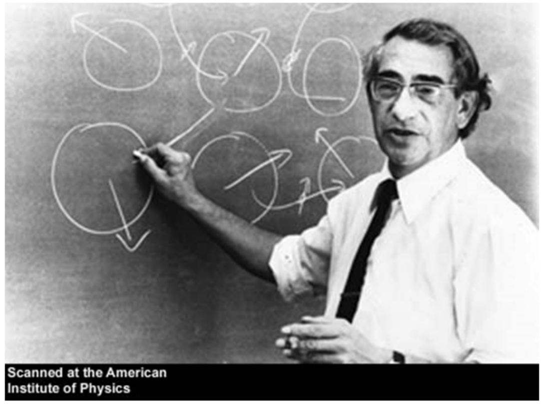
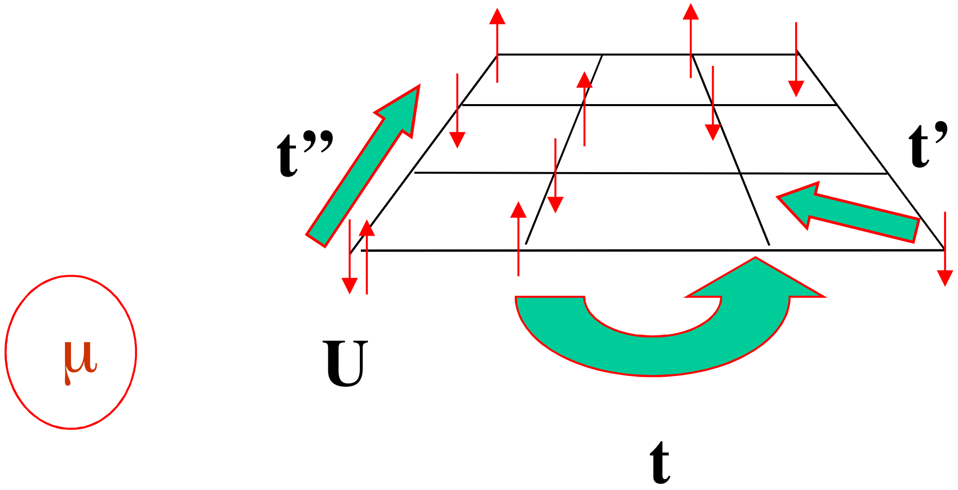


Figure: McWhan, PRB 1970; Limelette, Science 2003

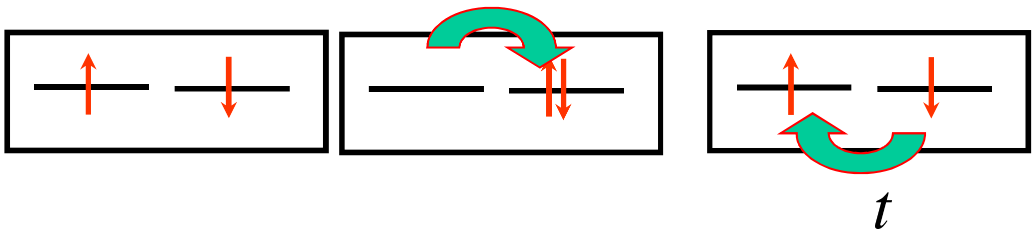
Hubbard model



1931-1980



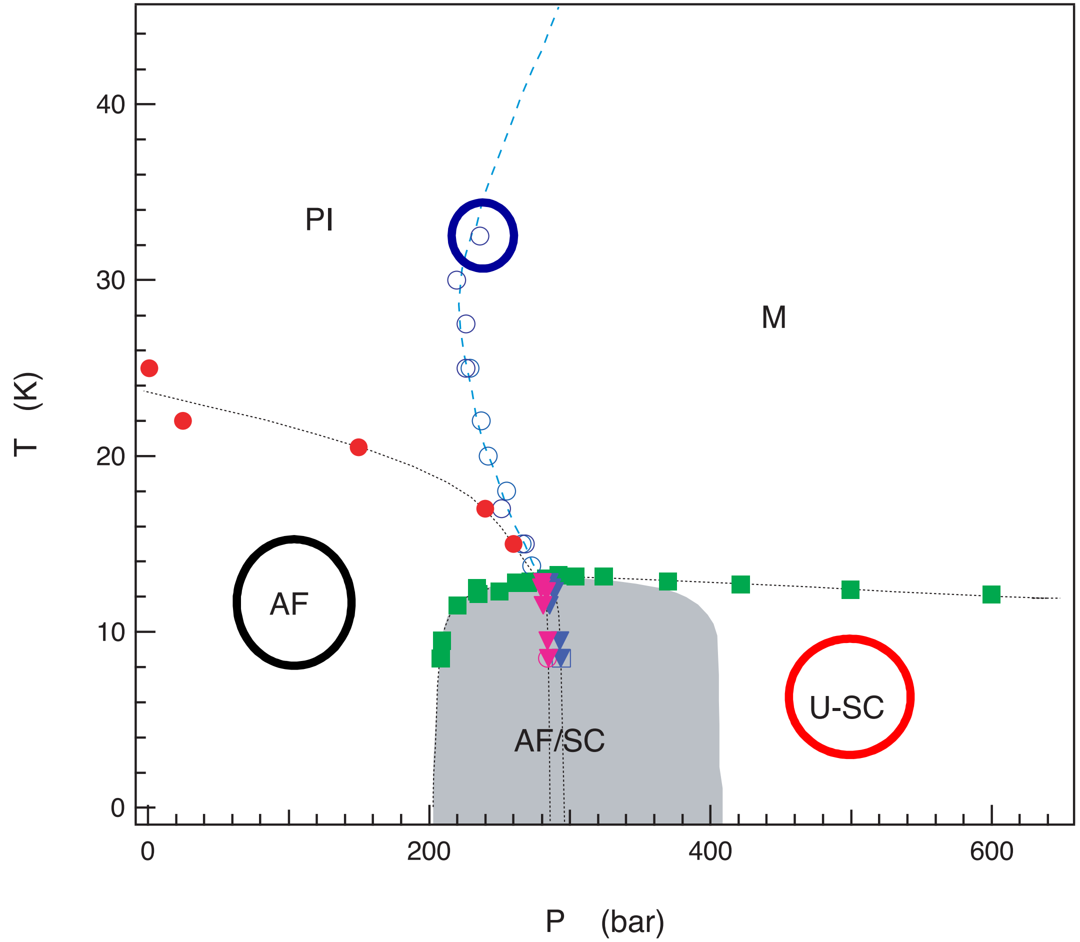
$$H = -\sum_{<ij>\sigma} t_{i,j} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

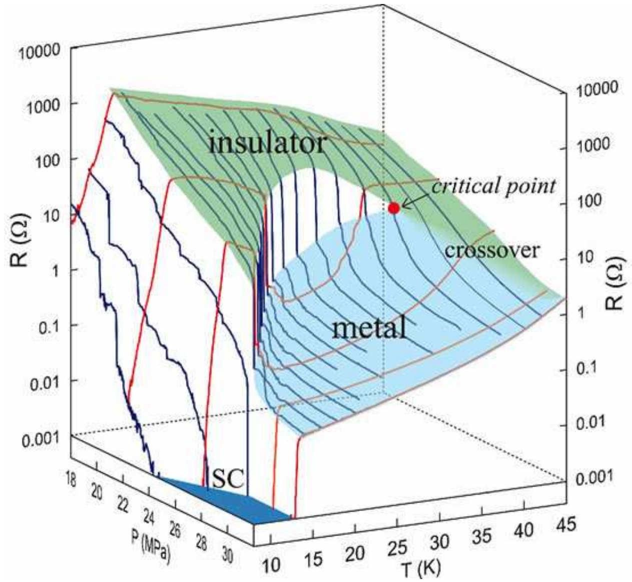


Effective model, Heisenberg: $J = 4t^2 / U$

Superconductivity and attraction?

Bare Mott critical point in organics





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

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

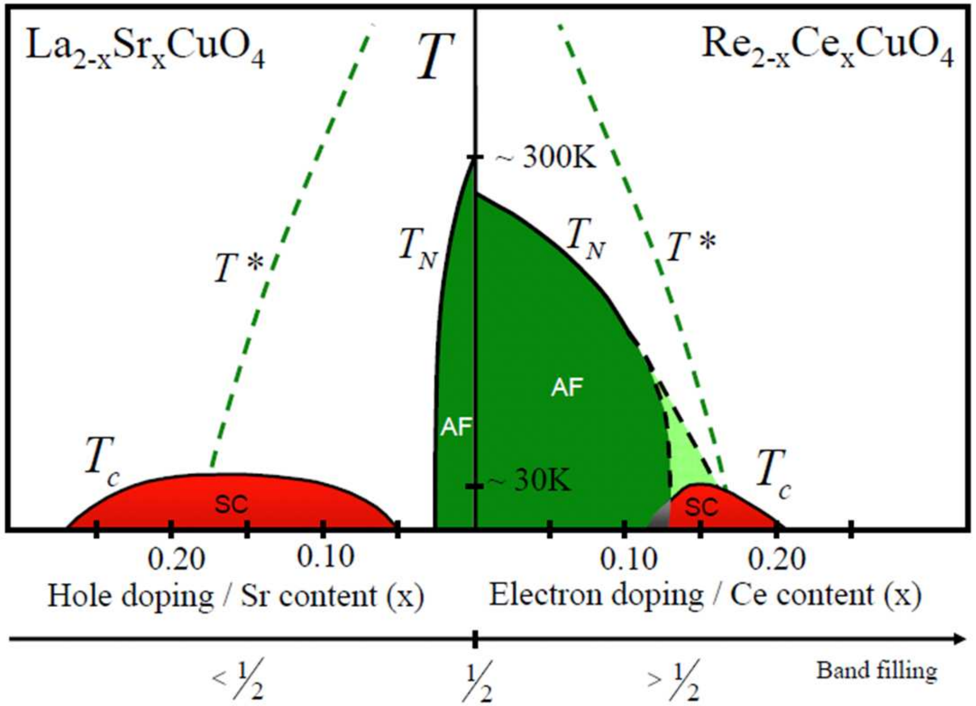
S. Lefebvre et al. PRL **85**, 5420 (2000), P. Limelette, et al. PRL **91** (2003)

CIAR The Canadian Institute for Advanced Research

UNIVERSITÉ DE SHERBROOKE

High-temperature superconductors

Armitage, Fournier, Greene, RMP (2009)

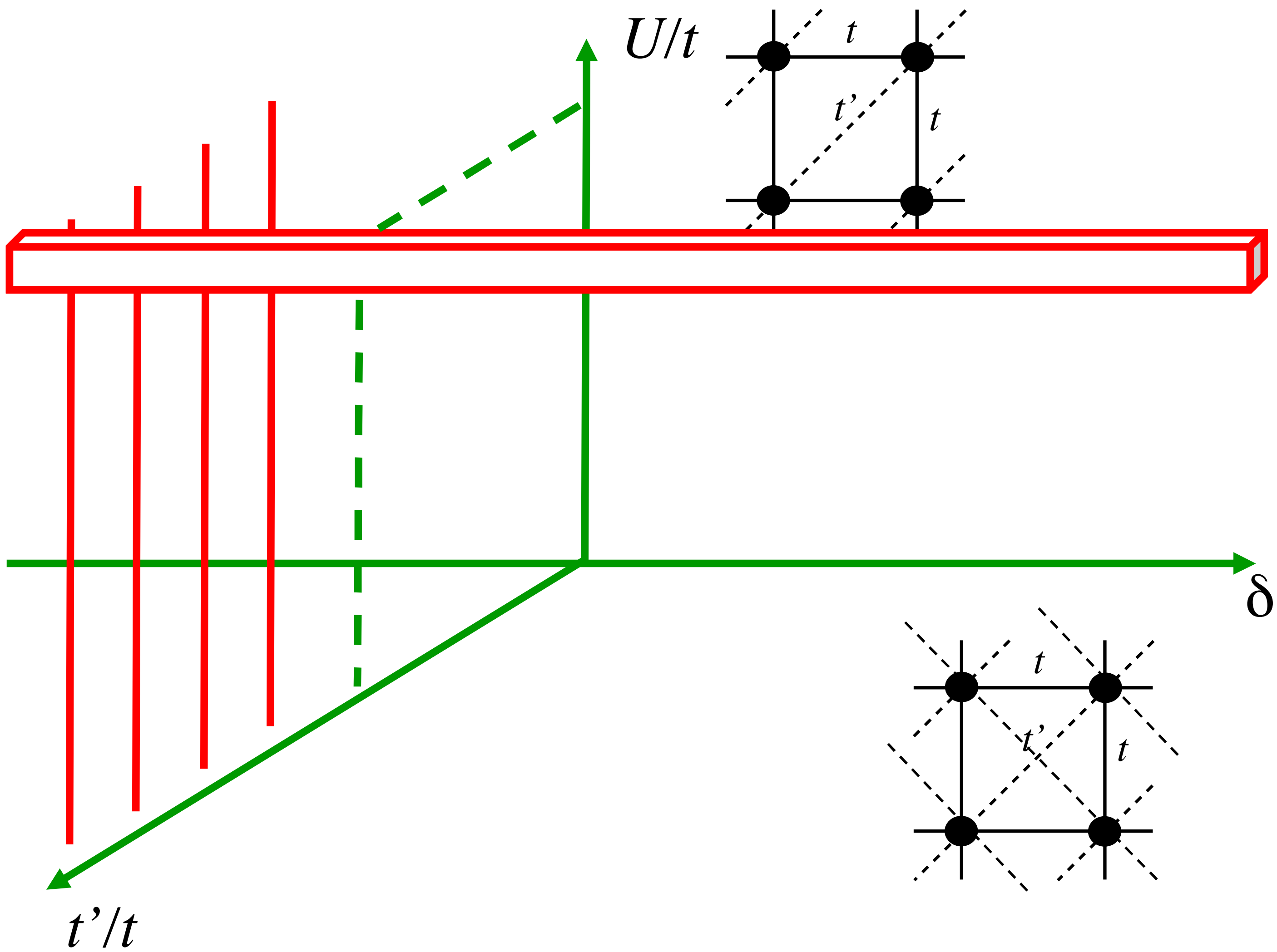


- *n = 1* Mott
- Non-FL (Pseudogap)
- QCP
- non-BCS (phonons? *d*-wave)

- 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

Perspective



UNIVERSITÉ DE SHERBROOKE

« Big things » induced by correlations

- Metal to insulator, heavy fermion behavior, high temperature superconductivity, colossal magnetoresistance, giant thermolectricity ……………
- The Kohn Sham approach cannot possibly describe spectroscopic properties of correlated materials,
  - because these retain atomic physics aspects (Motness, e.g. multiplets, transfer or spectral weight, high Tc's,) which are not perturbative

Theoretical difficulties

- Low dimension
  - (quantum and thermal fluctuations)

- Large residual interactions
  - (Potential ~ Kinetic)
  - Expansion parameter?
  - Particle-wave?

- By now we should be as quantitative as possible!

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 coupling approaches agree at intermediate coupling.
- Compare with experiment

Theoretical Methods

Example of some that have been used
to search for *d*-wave
superconductivity in Hubbard model

d-wave superconductivity

- Weak coupling
  - C. J. Halboth and W. Metzner, Phys. Rev. Lett. 85, 5162 (2000). Functional Renormalization Group
  - B. Kyung, J.-S. Landry, and A. M. S. Tremblay, Phys. Rev. B 68, 174502 (2003). TPSC
  - C. Bourbonnais and A. Sedeki, Physical Review B 80, 085105 (2009). Functional RG
  - D. J. Scalapino, Physica C: Superconductivity 470, Supplement 1, S1 (2010), ISSN 0921-4534, FLEX proceedings of the 9th International Conference on Materials and Mech anisms of Superconductivity.
  - A. Abanov, A. V. Chubukov, and J. Schmalian, Adv. Phys. **52**, 119 (2003). Feynman diagrams
- Renormalized Mean-Field Theory (Gutzwiller)
  - P. W. Anderson, P. A. Lee, M. Randeria, T. M. Rice, N. Trivedi, and F. C. Zhang, Journal of Physics: Condensed Matter 16, R755 (2004).
  - K.-Y. Yang, T. M. Rice, and F.-C. Zhang, Phys. Rev. B 73, 174501 (2006).
- Slave particles (Gauge theories)
  - G. Kotliar, Liu, P.R.B (1988).
  - P. A. Lee, N. Nagaosa, and X.-G. Wen, Rev. Mod. Phys. 78, 17 (2006).
  - M. Imada, Y. Yamaji, S. Sakai, and Y. Motome, Annalen der Physik 523, 629 (2011)
- Variational approaches
  - T. Giamarchi and C. Lhuillier, Phys. Rev. B 43, 12943 (1991).
  - A. Paramekanti, M. Randeria, and N. Trivedi, Phys. Rev. B 70, 054504 (2004).

d-wave superconductivity

- Quantum cluster methods
  - T. Maier, M. Jarrell, T. Pruschke, and J. Keller, Phys. Rev. Lett. 85, 1524 (2000).
  - T. A. Maier, M. Jarrell, T. C. Schulthess, P. R. C. Kent, and J. B. White, Phys. Rev. Lett. 95, 237001 (2005).
  - K. Haule and G. Kotliar, Phys. Rev. B 76, 104509 (2007).
  - + More in this talk

But…

QMC constrained path

S. Zhang, Carlson, Gubernatis Phys. Rev. Lett. 78, 4486 (1997)

Refined variational approach: no

Aimi and Imada, J. Phys. Soc. Jpn (2007)

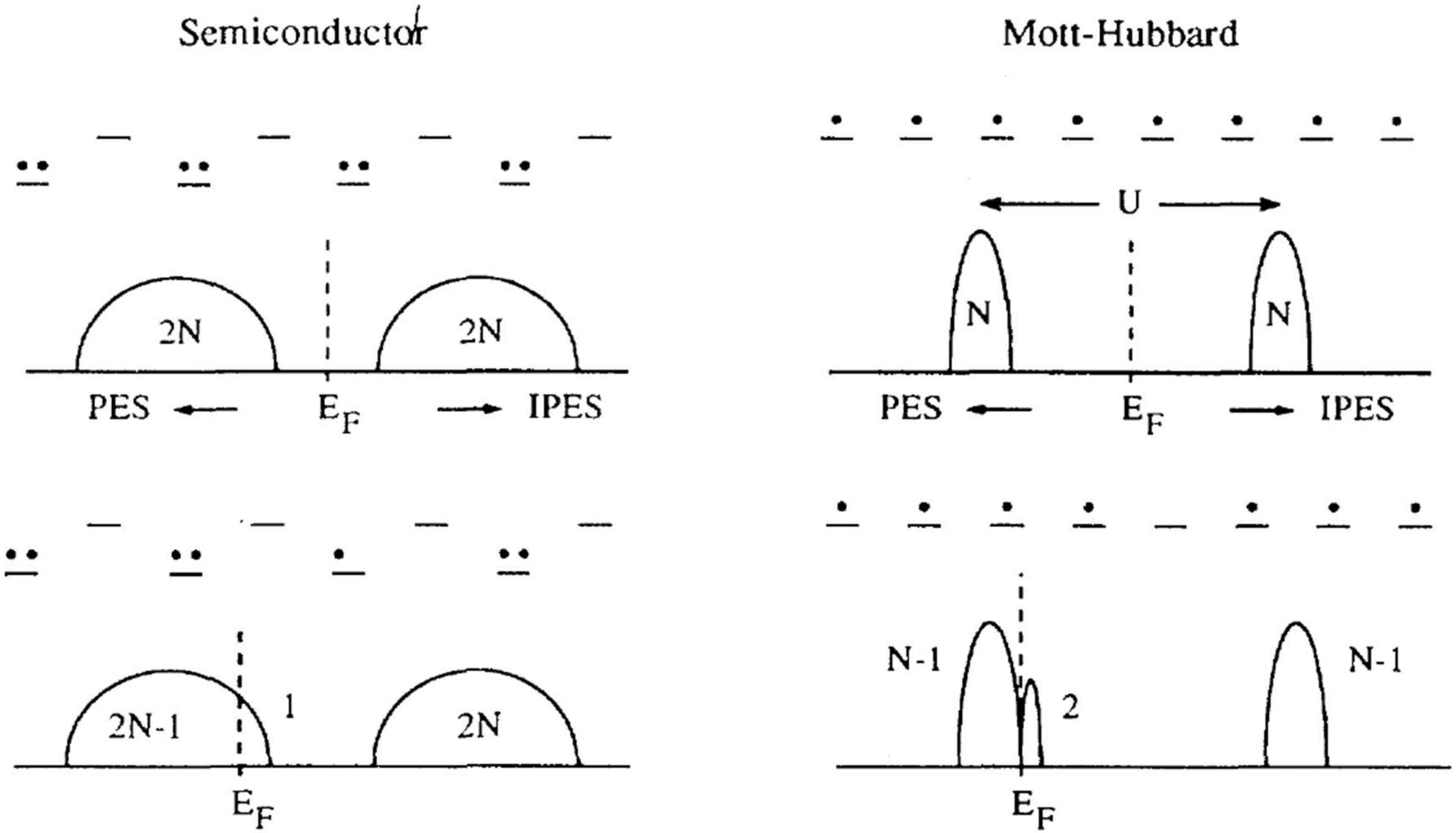
Outline

- More on the model
- Method DMFT
  - Validity
  - Impurity solvers
- Finite *T* phase diagram
  - Normal state
    - First order transition
    - Widom line and pseudogap
- *T=0* phase diagram
  - The « glue »
- Superconductivity *T* finite

The correct model?

Cuprates as doped Mott insulators

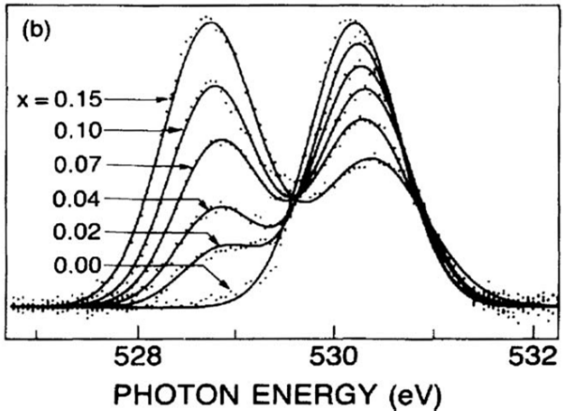
Spectral weight transfer



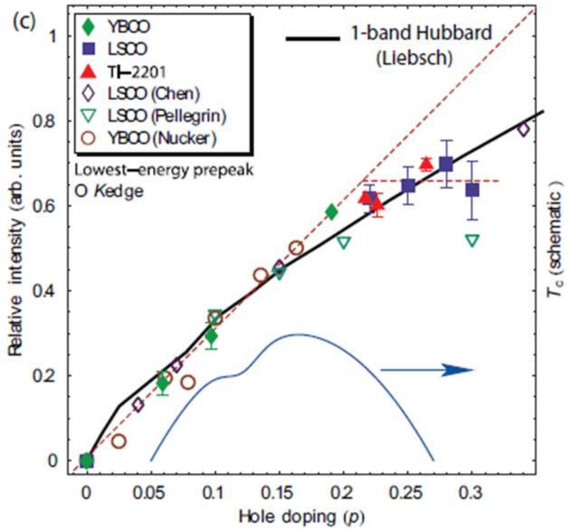
Meinders *et al*. PRB **48**, 3916 (1993)

UNIVERSITÉ DE SHERBROOKE

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

Charge transfer insulator

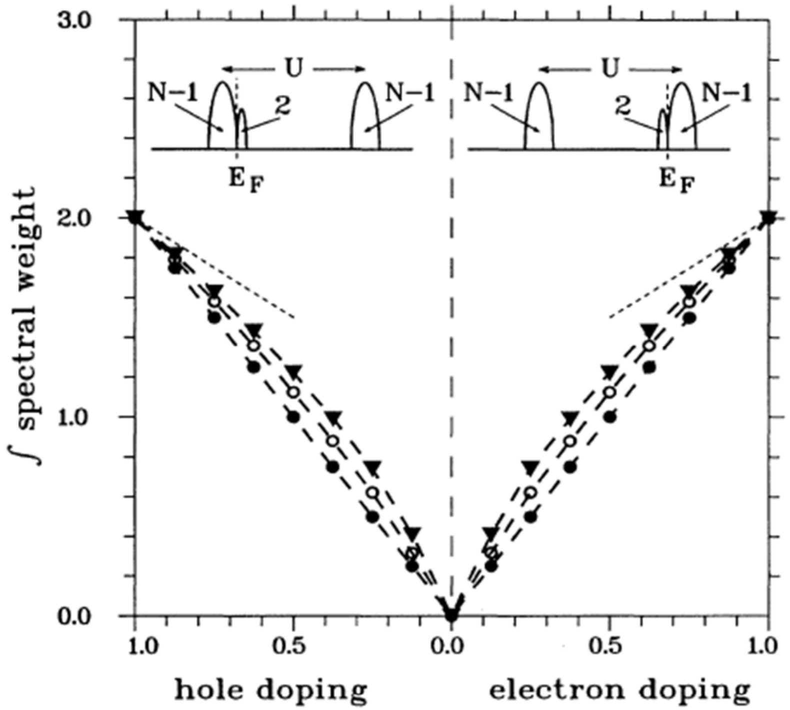


FIG. 2. The integrated low-energy spectral weight divided by the number of sites as a function of doping for the $N=8$ site one-dimensional Hubbard chain with periodic boundary conditions. The curves correspond to the following: ●, $U/t \rightarrow \infty$; ○, $U/t=-10$; and ▼, $U/t=-5$. The dotted line represents the free-particle limit. Inset: The intensities, shown schematically, of the electron-addition and -removal spectra for the Hubbard system with one additional hole (left) and one additional electron (right) in the localized limit.

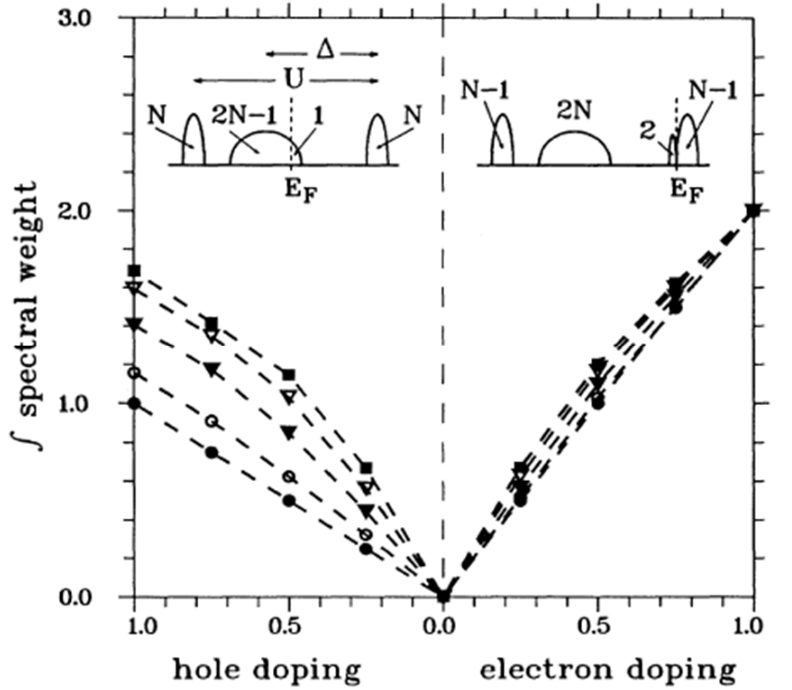


FIG. 3. The integrated low-energy spectral weight divided by the number of unit cells as a function of the doping for the $N=4$ unit-cell charge-transfer system with periodic boundary conditions. The curves correspond to the following: ●, $t_{pd}=0$; ○, $t_{pd}=0.5$; ▼, $t_{pd}=1.0$; ▽, $t_{pd}=1.5$; and ■, $t_{pd}=2.0$ eV. For all curves, $\epsilon_p-\epsilon_d=4$, $U_{dd}=8$, and $t_{pp}=-0.25$ eV. Inset: The intensities, shown schematically, of the electron-addition and -removal spectra for the system with one additional hole (left) and one additional electron (right) in the localized limit.

Eskes, Meinders, Sawatzky, PRL **67**, 1991

UNIVERSITÉ DE SHERBROOKE

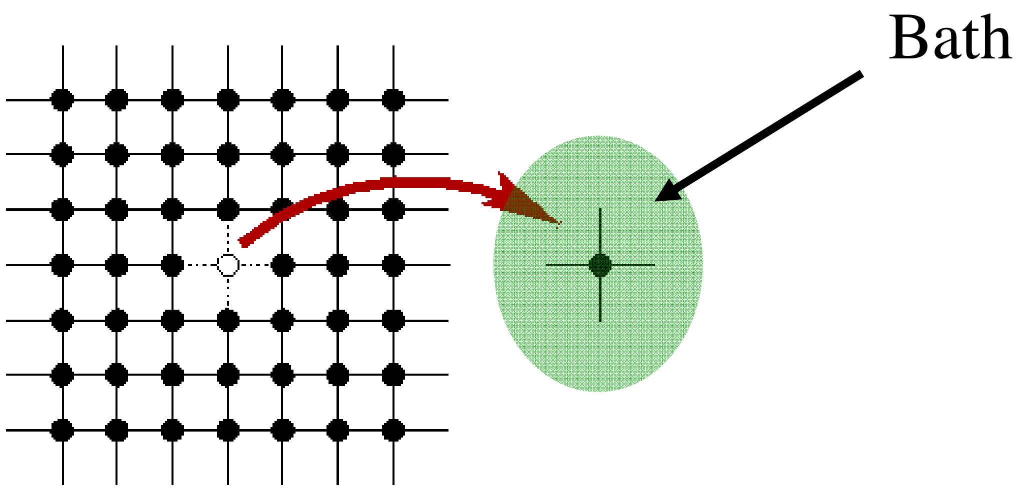
Outline

- More on the model
- Method DMFT
  - Validity
  - Impurity solvers
- Finite *T* phase diagram
  - Normal state
    - First order transition
    - Widom line and pseudogap
- *T=0* phase diagram
  - The « glue »
- Superconductivity *T* finite

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)*

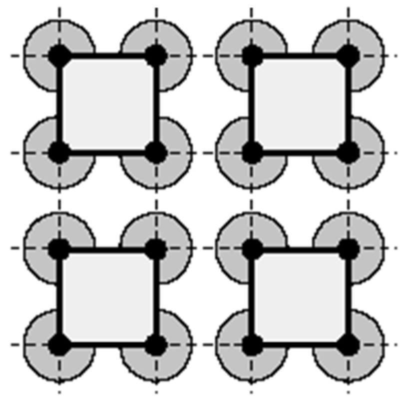
UNIVERSITÉ DE SHERBROOKE

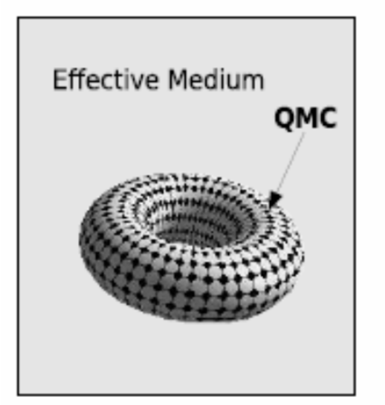
2d Hubbard: Quantum cluster method

REVIEWS

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

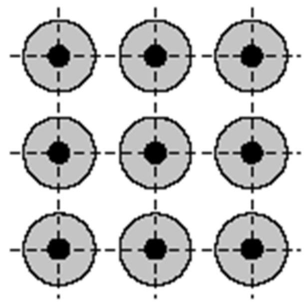
C-DMFT





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)

Self-consistency

$$\mathcal{G}_{\sigma}^{imp}(i\omega_n)^{-1} = \mathcal{G}_{\sigma}^{0-imp}(i\omega_n)^{-1} - \Sigma_{\sigma}(i\omega_n)$$

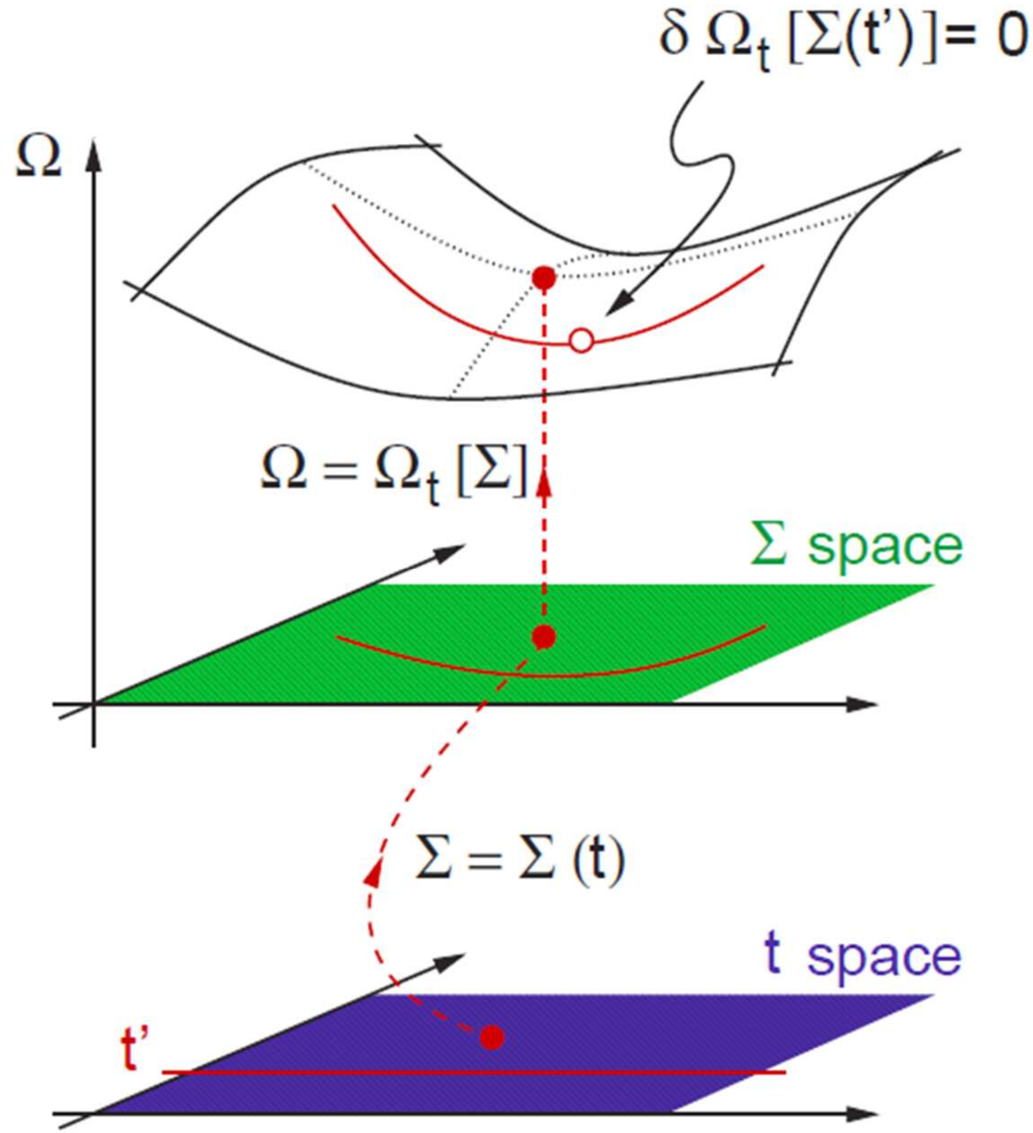
$$N_c \int \frac{d^d\tilde{\mathbf{k}}}{(2\pi)^d} \frac{1}{\mathcal{G}_{\tilde{\mathbf{k}}\sigma}^{0}(i\omega_n)^{-1} - \Sigma_{\sigma}(i\omega_n)} = \mathcal{G}_{\sigma}^{imp}(i\omega_n)$$

Methods of derivation

- Cavity method
- Local nature of perturbation theory in infinite dimensions
- Expansion around the atomic limit
- Effective medium theory
- Potthoff self-energy functional

M. Potthoff, Eur. Phys. J. B **32**, 429 (2003).
A. Georges *et al.*, Rev. Mod. Phys. **68**, 13 (1996).

DMFT as a stationnary point

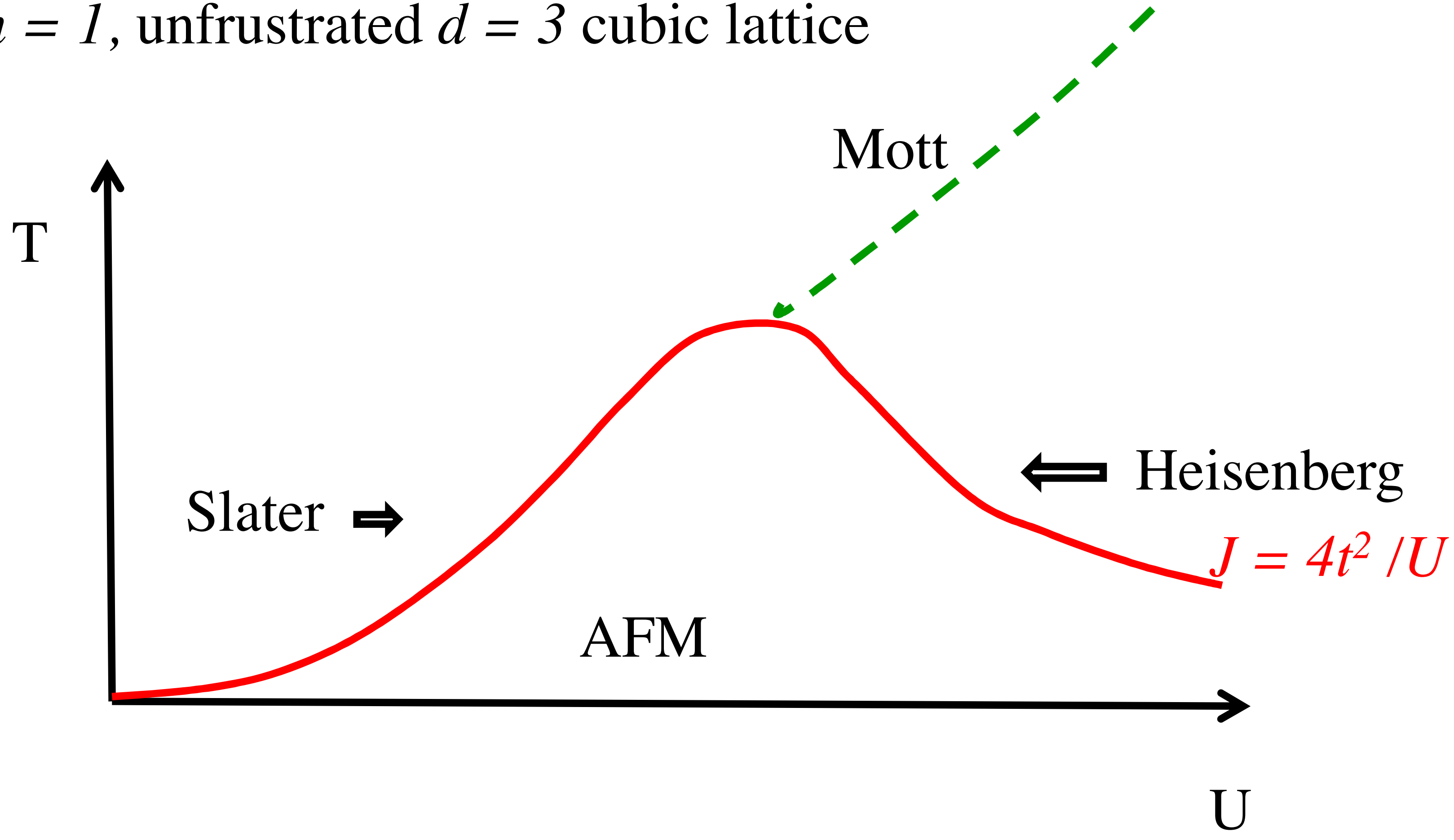


UNIVERSITÉ DE SHERBROOKE

When is cluster DMFT OK?
Example: The Mott transition

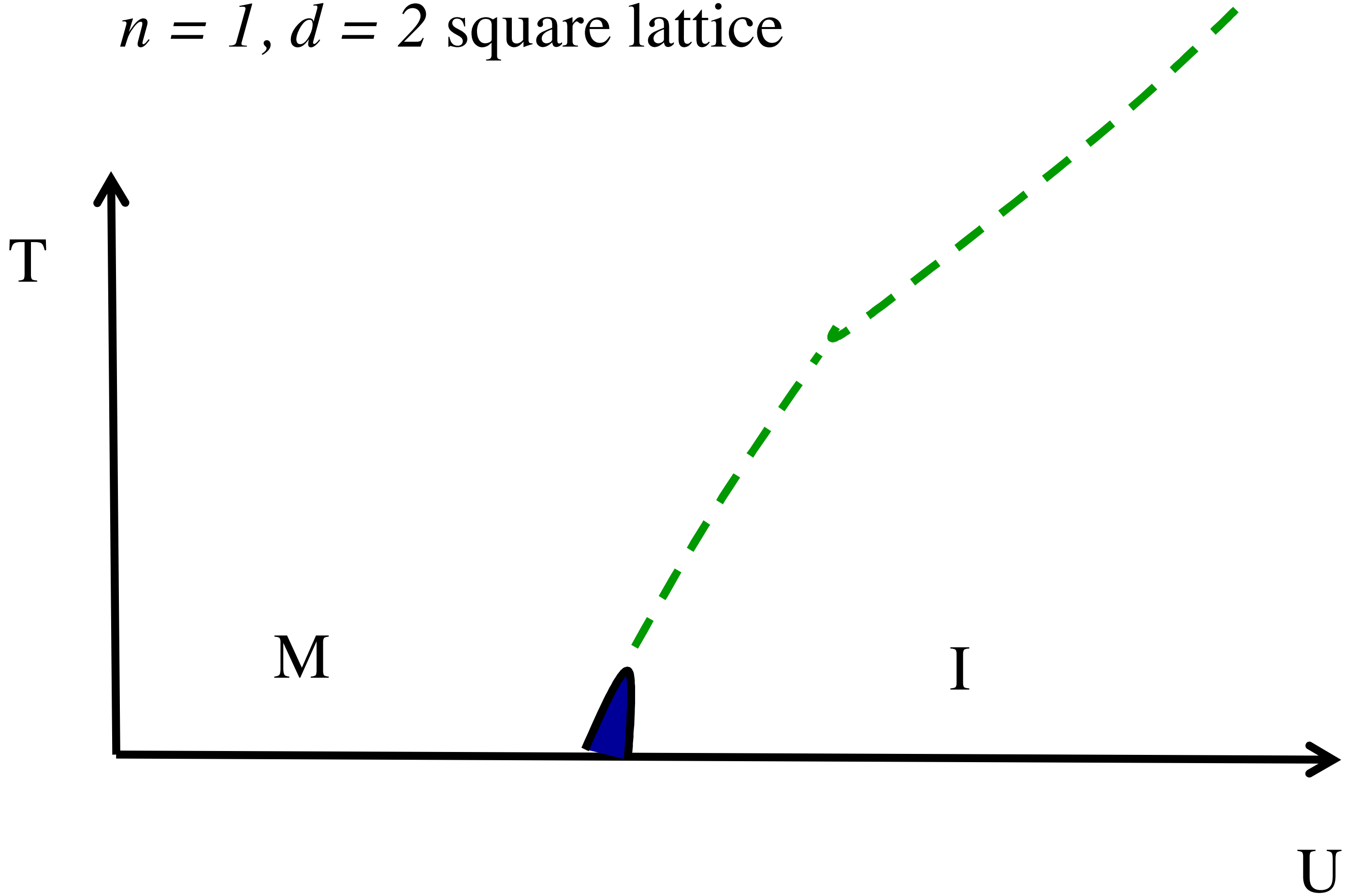
Local moment and Mott transition

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



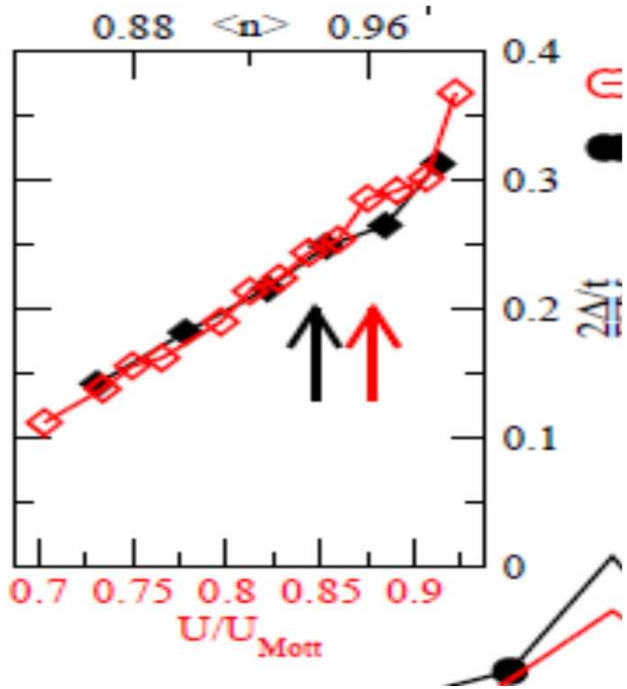
Local moment and Mott transition

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



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

Size dependence



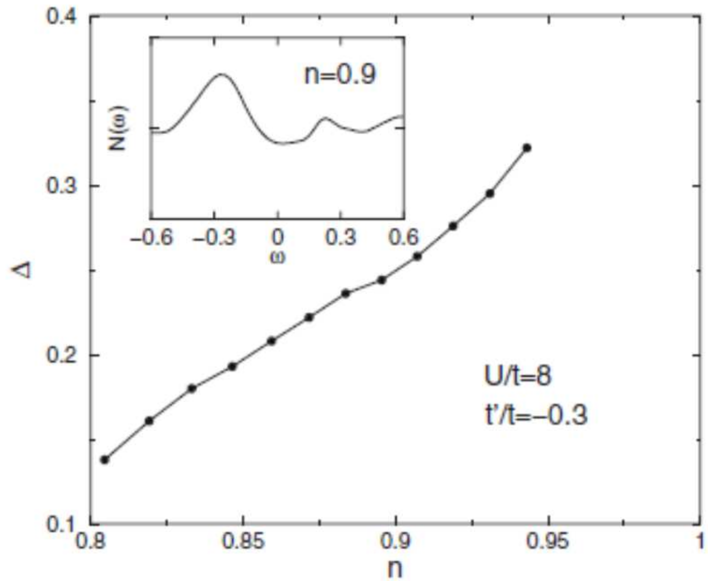
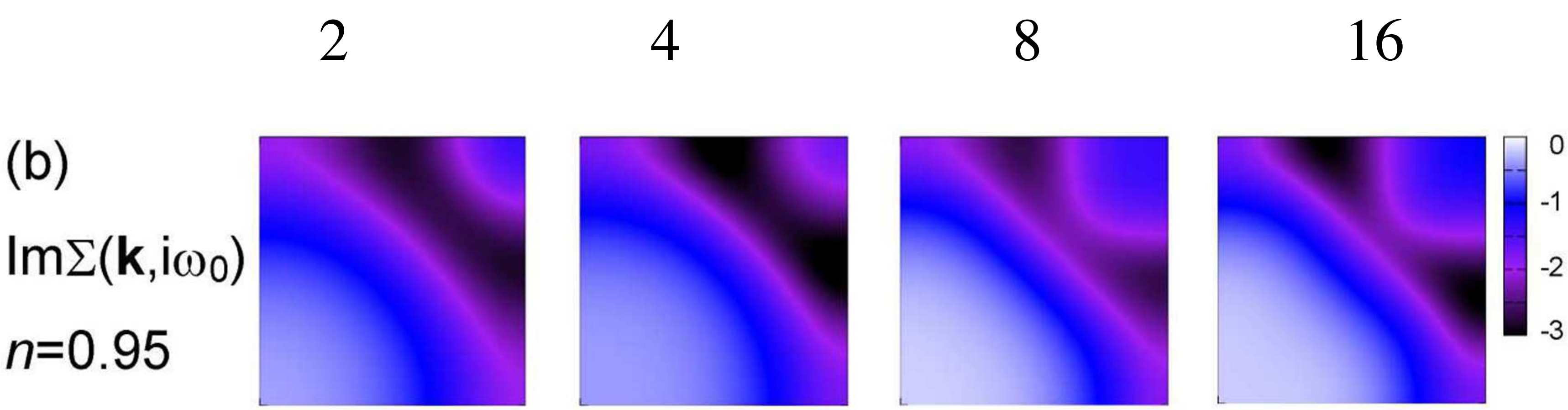


FIG. 5. The gap as a function of filling, for $U=8t$, $t'=-0.3t$. The gap is defined as half the distance between the two peaks on either side of $\omega=0$, as they appear, for example, in the inset.

Gull, Parcollet, Millis
arXiv:1207.2490v1

Kancharla et al. PRB **77**, 184516 (2008)

Size dependence near FS



Sakai et al. arXiv:1112.3227

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
  - Long-wavelength collective modes can become unstable
- 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.
  - Long-wavelength collective modes can become unstable

+ 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

Some many-body theory for the Hubbard model

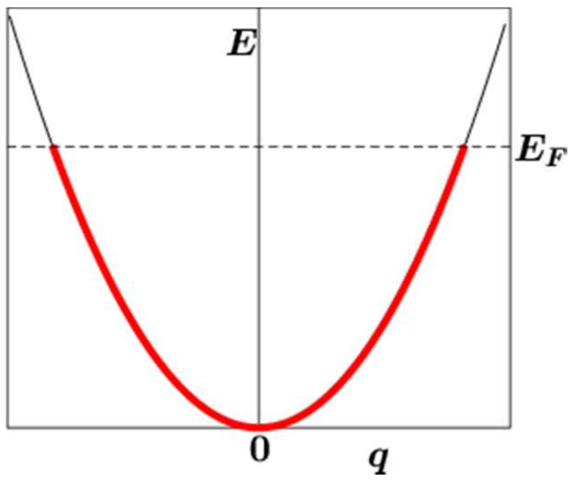
$U = 0$

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

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

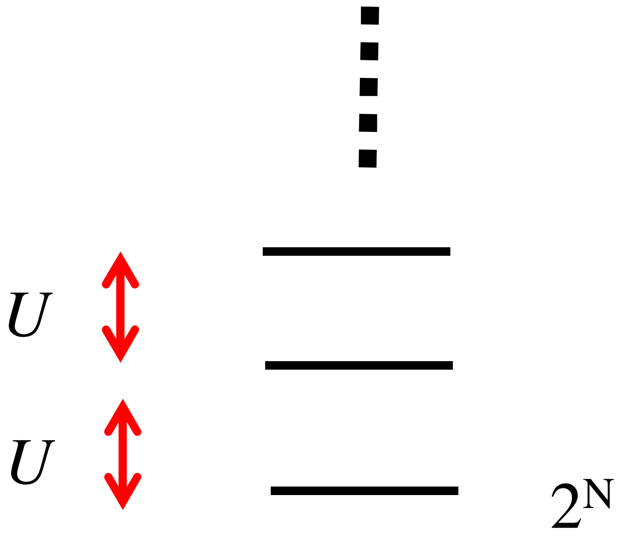
$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

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



$t_{ij} = 0$

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



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

UNIVERSITÉ DE SHERBROOKE

Green's function: free electrons, atomic limit

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

$$\mathcal{G}_{\mathbf{k}\sigma}(i\omega_n) = \frac{1}{i\omega_n - (\varepsilon_{\mathbf{k}} - \mu)}$$

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

$$\langle n \rangle = 1 \qquad \mathcal{G}_{\sigma}(i\omega_n) = \frac{1/2}{i\omega_n + \frac{U}{2}} + \frac{1/2}{i\omega_n - \frac{U}{2}}$$

Self-energy and all that

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

$$\mathcal{G}_{\mathbf{k}\sigma}(i\omega_n) = \frac{1}{i\omega_n - (\varepsilon_{\mathbf{k}} - \mu) - \Sigma_{\mathbf{k}\sigma}(i\omega_n)}$$

$$\mathcal{G}_{\mathbf{k}\sigma}^{-1}(i\omega_n) = \mathcal{G}_{\mathbf{k}\sigma}^{0-1}(i\omega_n) - \Sigma_{\mathbf{k}\sigma}(i\omega_n)$$

Self-energy in the atomic limit for $n = 1$

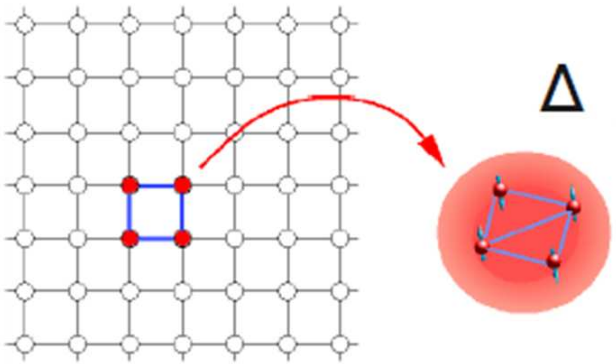
$$\mathcal{G}_{\sigma}(i\omega_n) = \frac{1/2}{i\omega_n + \frac{U}{2}} + \frac{1/2}{i\omega_n - \frac{U}{2}}$$

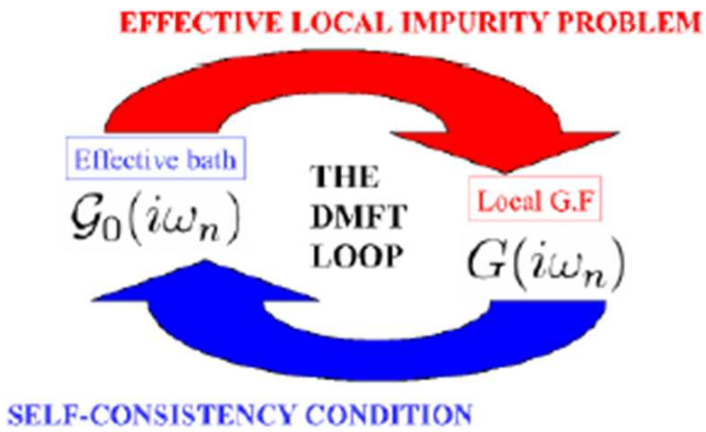
$$\mathcal{G}_{\sigma}(i\omega_n) = \frac{1}{i\omega_n + \frac{U}{2} - \Sigma(i\omega_n)} \qquad \Sigma(i\omega_n) = \frac{U}{2} + \frac{U^2}{i\omega_n}$$

Impurity solvers

C-DMFT

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





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

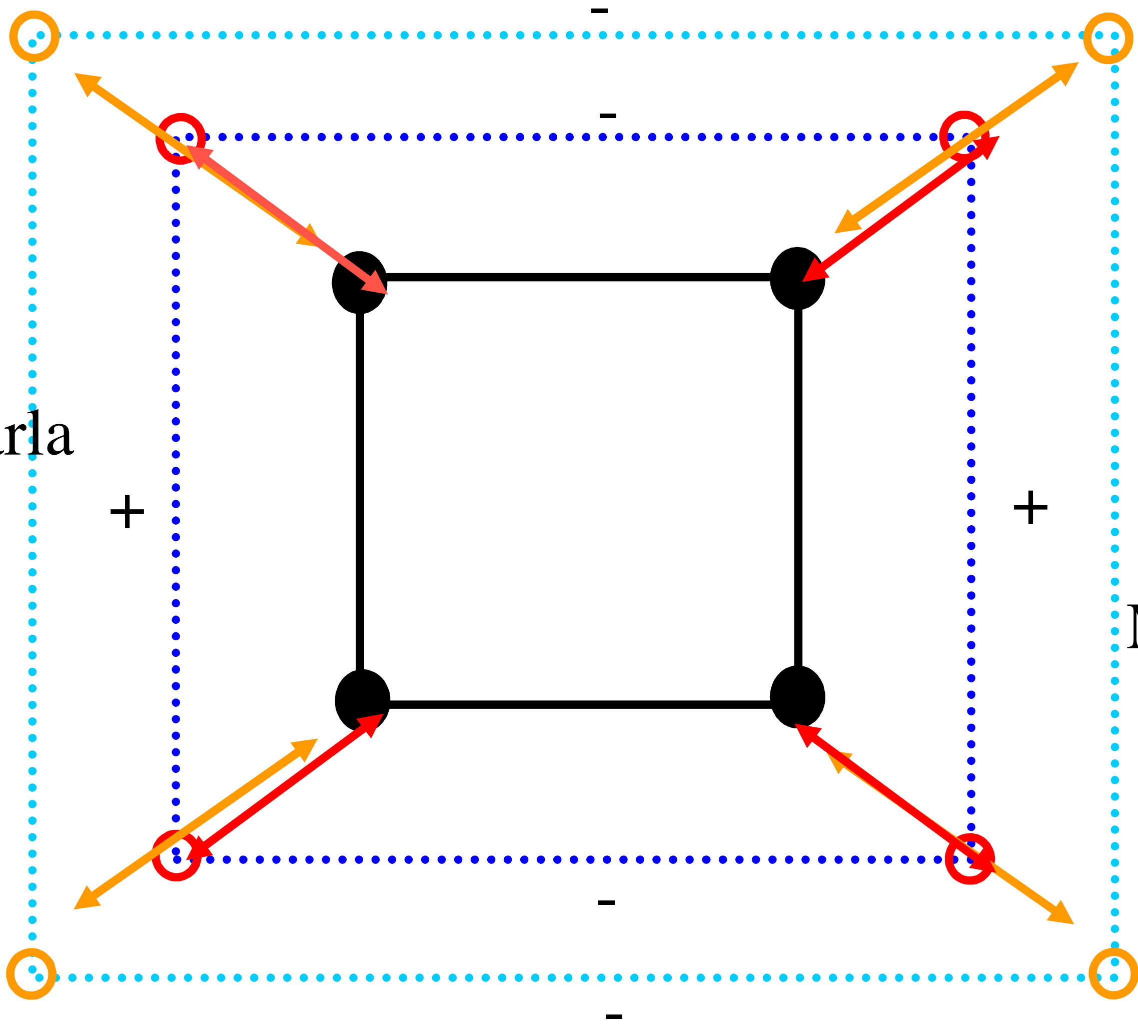
Here: continuous time QMC

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

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

CDMFT + ED

Sarma Kancharla



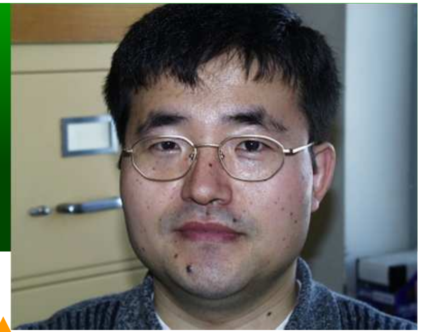
Marcello Civelli

Caffarel and Krauth, PRL (1994)

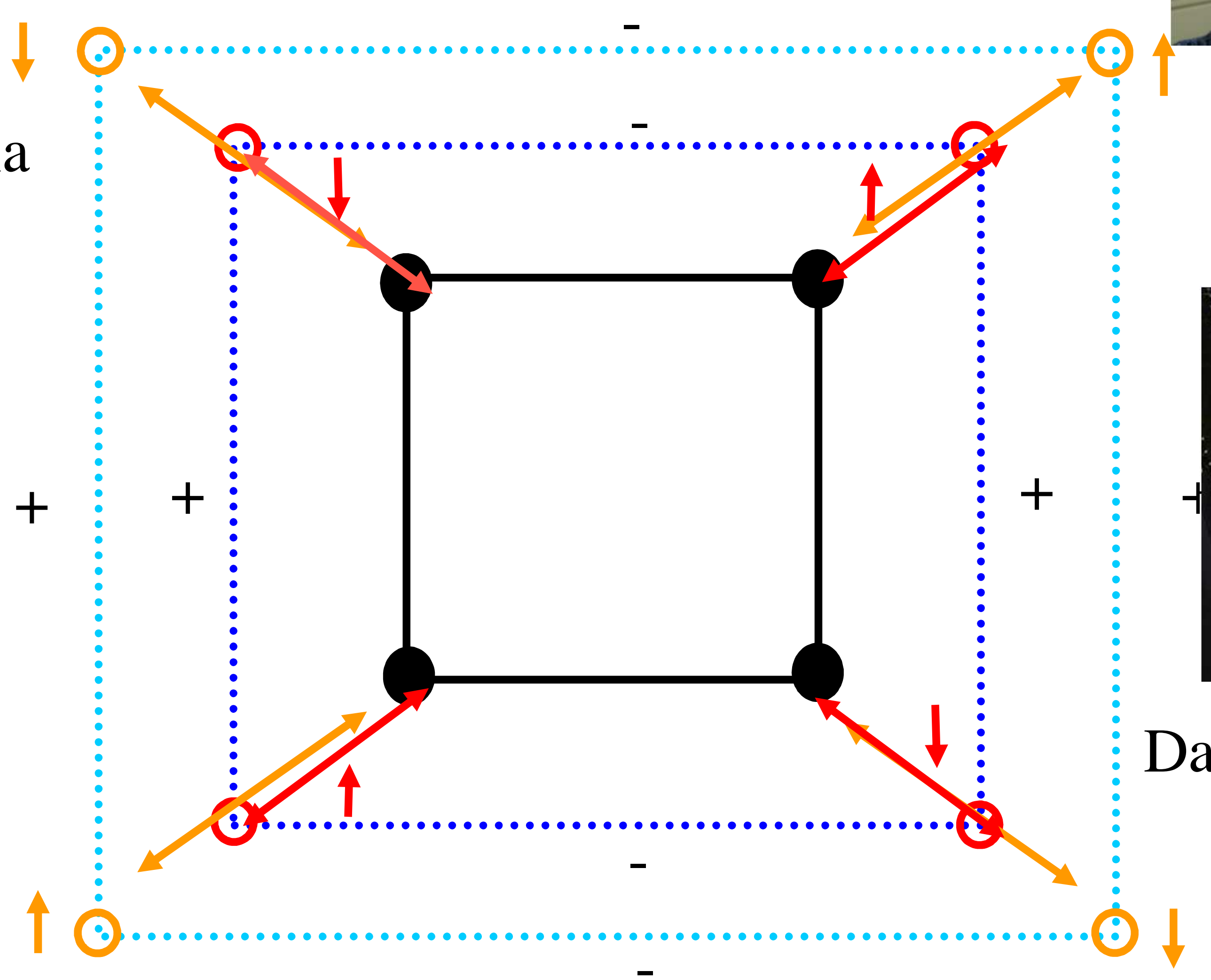
No Weiss field on the cluster!

Competition AFM-dSC

S. Kancharla



B. Kyung



David Sénéchal

See also, Capone and Kotliar, Phys. Rev. B 74, 054513 (2006),
Macridin, Maier, Jarrell, Sawatzky, Phys. Rev. B 71, 134527 (2005)

UNIVERSITÉ DE SHERBROOKE

Monte Carlo method

Gull, Millis, Lichtenstein, Rubtsov, Troyer, Werner,
Rev.Mod.Phys. **83**, 349 (2011)

$$Z = \int_{\mathcal{C}} d\mathbf{x}\, p(\mathbf{x}).$$

$$\langle A \rangle_p = \frac{1}{Z} \int_{\mathcal{C}} d\mathbf{x}\, \mathcal{A}(\mathbf{x}) p(\mathbf{x}).$$

$$\langle A \rangle_p \approx \langle A \rangle_{\mathrm{MC}} \equiv \frac{1}{M} \sum_{i=1}^{M} \mathcal{A}(\mathbf{x}_i).$$

$$\langle A \rangle = \frac{1}{Z} \int_{\mathcal{C}} d\mathbf{x}\, \mathcal{A}(\mathbf{x}) p(\mathbf{x}) = \frac{\int_{\mathcal{C}} d\mathbf{x}\, \mathcal{A}(\mathbf{x})[p(\mathbf{x})/\rho(\mathbf{x})]\rho(\mathbf{x})}{\int_{\mathcal{C}} d\mathbf{x}[p(\mathbf{x})/\rho(\mathbf{x})]\rho(\mathbf{x})} \equiv \frac{\langle A(p/\rho)\rangle_\rho}{\langle p/\rho \rangle_\rho}.$$

Monte Carlo: Markov chain

- Ergodicity
- Detailed balance

$$\frac{W_{\mathbf{xy}}}{W_{\mathbf{yx}}} = \frac{p(\mathbf{y})}{p(\mathbf{x})} \qquad W_{\mathbf{xy}} = W_{\mathbf{xy}}^{\mathrm{prop}} W_{\mathbf{xy}}^{\mathrm{acc}}$$

$$W_{\mathbf{xy}}^{\mathrm{acc}} = \min[1, R_{\mathbf{xy}}] \qquad R_{\mathbf{xy}} = \frac{p(\mathbf{y}) W_{\mathbf{yx}}^{\mathrm{prop}}}{p(\mathbf{x}) W_{\mathbf{xy}}^{\mathrm{prop}}}$$

Reminder on perturbation theory

$$\exp(-\beta(H_a + H_b)) = \exp(-\beta H_a)U(\beta)$$

$$\frac{\partial U(\beta)}{\partial \beta} = -H_b(\beta)U(\beta)$$

$$U(\beta) = 1 - \int_0^\beta d\tau H_b(\tau) + \int_0^\beta d\tau \int_0^\tau d\tau' H_b(\tau)H_b(\tau') + \ldots$$

Partition function as sum over configurations

$$Z = \mathrm{Tr}[\exp(H_a + H_b)]$$

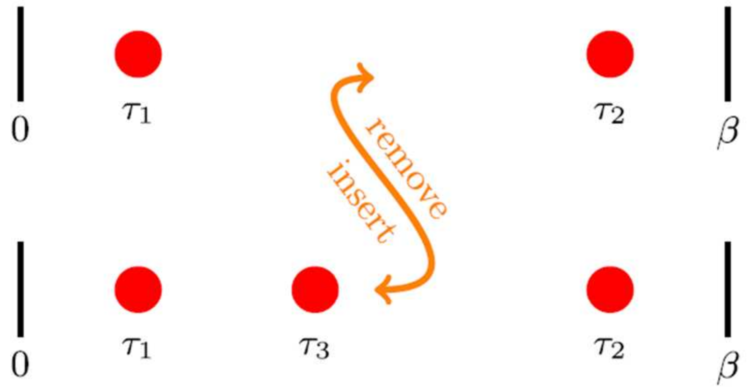
$$= \sum_k (-1)^k \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \, \mathrm{Tr}[e^{-\beta H_a} H_b(\tau_k) \times H_b(\tau_{k-1}) \cdots H_b(\tau_1)].$$

$$Z = \sum_{k=0}^{\infty} \sum_{\gamma \in \Gamma_k} \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k w(k, \gamma, \tau_1, \ldots, \tau_k)$$

$$\mathbf{x} = (k, \gamma, (\tau_1, \ldots, \tau_k)), \qquad p(\mathbf{x}) = w(k, \gamma, \tau_1, \ldots, \tau_k) d\tau_1 \cdots d\tau_k,$$

UNIVERSITÉ DE SHERBROOKE

Updates



$$W^{\text{prop}}_{(k,\vec{\tau}),(k+1,\vec{\tau}')} = \frac{d\tau}{\beta}$$

$$W^{\text{prop}}_{(k+1,\vec{\tau}'),(k,\vec{\tau})} = \frac{1}{k+1}.$$

$$R_{(k,\vec{\tau}),(k+1,\vec{\tau}')} = \frac{p((k+1,\vec{\tau}'))}{p((k,\vec{\tau}))} \frac{W^{\text{prop}}_{(k+1,\vec{\tau}'),(k,\vec{\tau})}}{W^{\text{prop}}_{(k,\vec{\tau}),(k+1,\vec{\tau}')}}$$

$$= \frac{w(k+1)d\tau'_1 \cdots d\tau'_{k+1}}{w(k)d\tau_1 \cdots d\tau_k} \frac{1/(k+1)}{d\tau/\beta}$$

$$= \frac{w(k+1)}{w(k)} \frac{\beta}{k+1}.$$

Beard, B. B., and U.-J. Wiese, 1996, Phys. Rev. Lett. **77**, 5130.
Prokof'ev, N. V., B. V. Svistunov, and I. S. Tupitsyn, 1996, JETP Lett. **64**, 911.

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).

Expansion in powers of the hybridization

$$H_{\text{hyb}} = \sum_{pj}(V_p^j c_p^\dagger d_j + V_p^{j*} d_j^\dagger c_p) = \tilde{H}_{\text{hyb}} + \tilde{H}_{\text{hyb}}^\dagger$$

$$Z = \sum_{k=0}^{\infty} \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \int_0^\beta d\tau'_1 \cdots \int_{\tau'_{k-1}}^\beta d\tau'_k$$

$$\times \sum_{\substack{j_1,\ldots,j_k \\ j'_1,\ldots,j'_k}} \sum_{\substack{p_1,\ldots,p_k \\ p'_1,\ldots,p'_k}} V_{p_1}^{j_1} V_{p'_1}^{j'_1 *} \cdots V_{p_k}^{j_k} V_{p'_k}^{j'_k *}$$

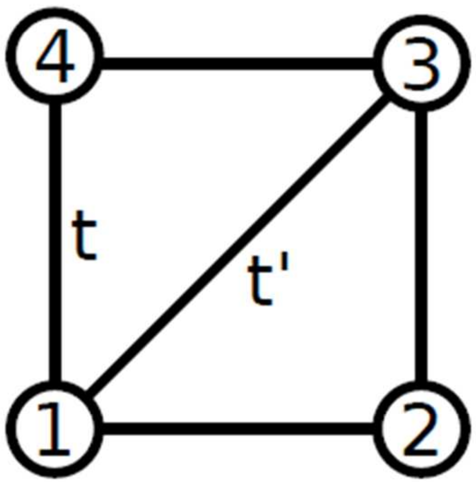
$$\times \mathrm{Tr}_d[T_\tau e^{-\beta H_{\text{loc}}} d_{j_k}(\tau_k) d^\dagger_{j'_k}(\tau'_k) \cdots d_{j_1}(\tau_1) d^\dagger_{j'_1}(\tau'_1)]$$

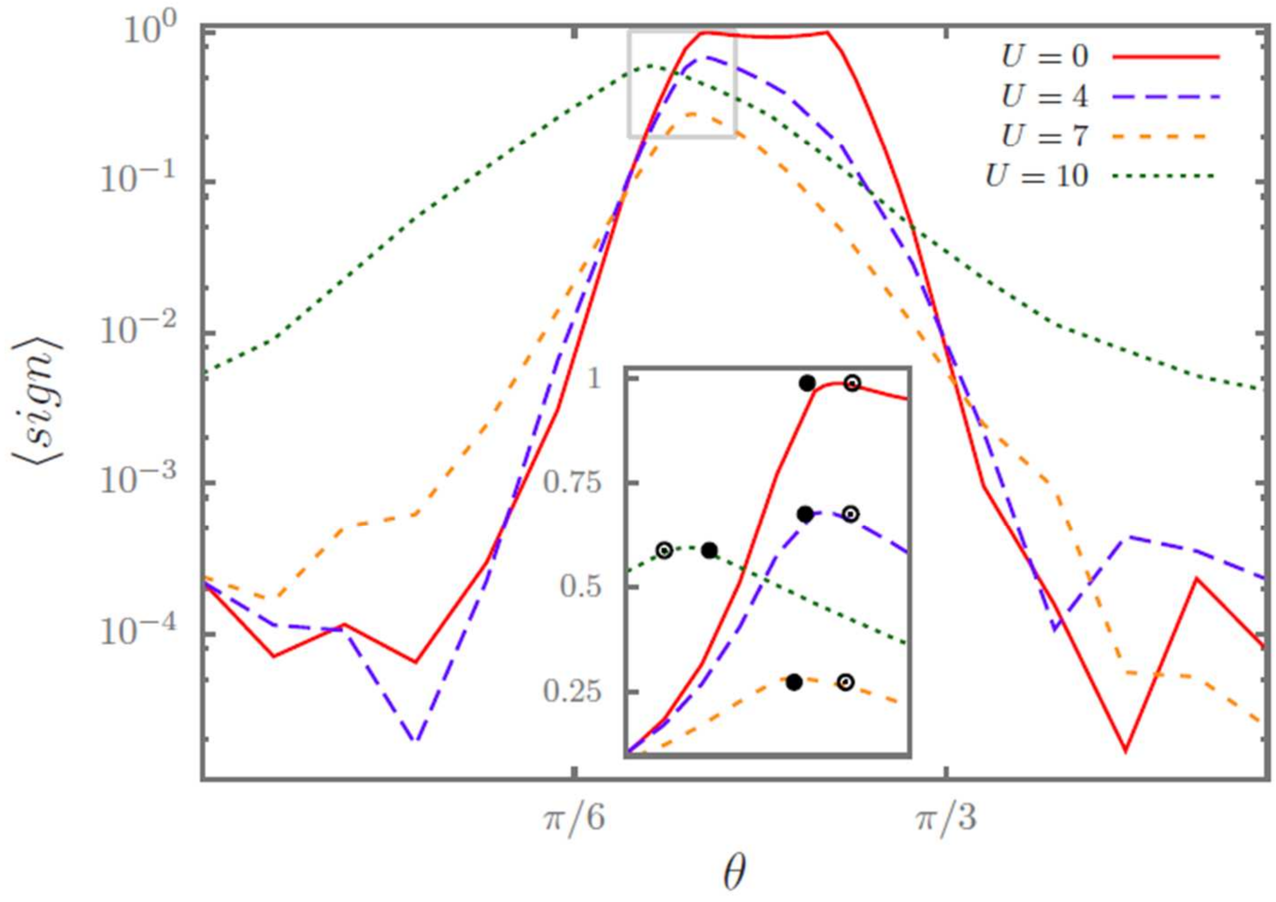
$$\times \mathrm{Tr}_c[T_\tau e^{-\beta H_{\text{bath}}} c^\dagger_{p_k}(\tau_k) c_{p_{k'}}(\tau'_k) \cdots c^\dagger_{p_1}(\tau_1) c_{p'_1}(\tau'_1)].$$

$$P_m = \frac{\langle m| e^{-\beta H_{loc}} d_{j_k}(\tau_k) d^\dagger_{j'_k}(\tau'_k) \ldots d_{j_1}(\tau_1) d^\dagger_{j'_1}(\tau'_1) |m\rangle}{\sum_n \langle n| e^{-\beta H_{loc}} d_{j_k}(\tau_k) d^\dagger_{j'_k}(\tau'_k) \ldots d_{j_1}(\tau_1) d^\dagger_{j'_1}(\tau'_1) |n\rangle}$$

Sign problem

$$S = S_{\rm cl}(\boldsymbol{c}^\dagger, \boldsymbol{c}) + \int_0^\beta d\tau d\tau' \boldsymbol{c}^\dagger(\tau')\boldsymbol{\Delta}(\tau'-\tau)\boldsymbol{c}(\tau)$$





P. Sémon, A.-M.S. Tremblay, (unpub.)

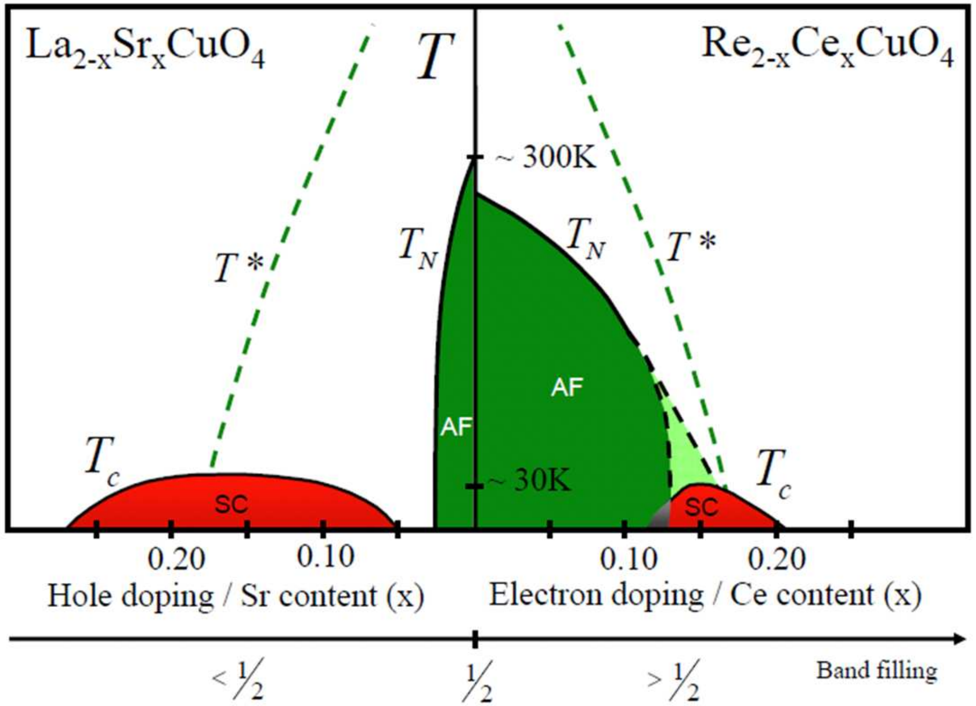
Outline

- More on the model
- Method DMFT
  - Validity
  - Impurity solvers
- Finite *T* phase diagram
  - Pseudogap normal state
    - First order transition
    - Widom line and pseudogap
- *T=0* phase diagram
  - The « glue »
- Superconductivity *T* finite

The normal state pseudogap

High-temperature superconductors

Armitage, Fournier, Greene, RMP (2009)



- 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)

What is under the dome?

Mott Physics away from $n = 1$

UNIVERSITÉ DE SHERBROOKE

Three broad classes of mechanisms for pseudogap

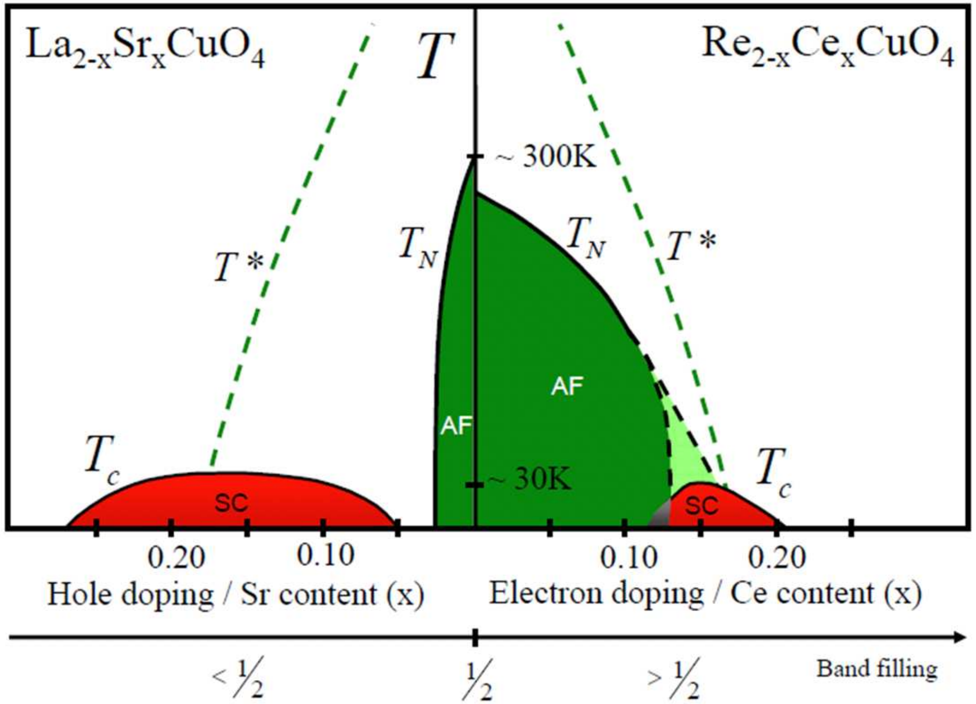
- Rounded first order transition
- Precursor to a lower temperature broken symmetry phase
- Mott physics

- 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

Normal state of high-temperature superconductors

Armitage, Fournier, Greene, RMP (2009)



$$\Delta\varepsilon = k_B T = \hbar v_F \Delta k$$

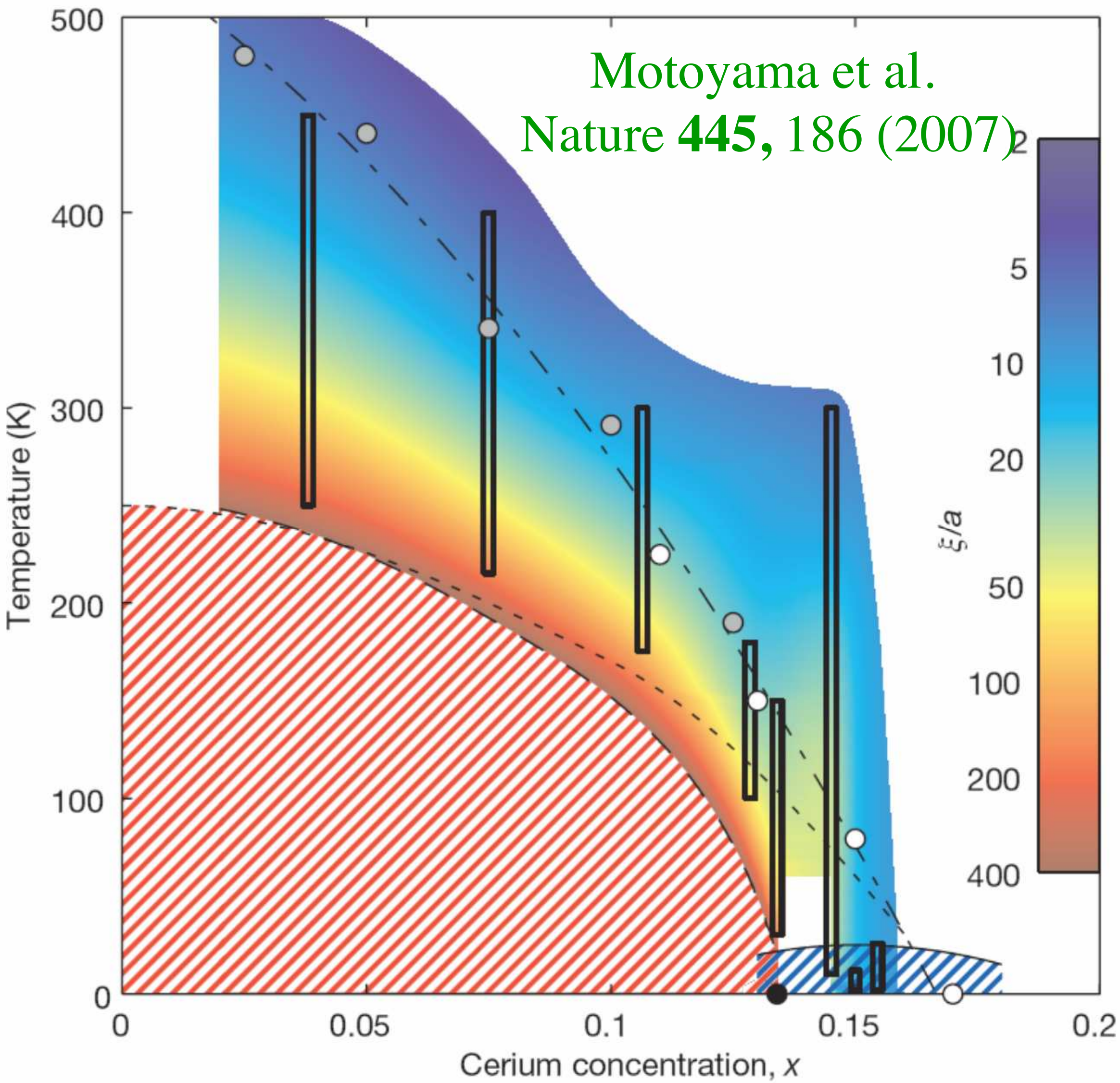
$$(\hbar v_F / k_B T^*) \sim \xi_{th}(T^*) \sim \xi_{AFM}(T^*)$$

- Vilk, AMST J. Phys. France **7**, 1309 (1997)

- e-doped more weakly coupled
  - Sénéchal, AMST, PRL **92**, 126401 (2004)
  - Weber et al. Nature Phys. **6**, 574 (2010)
- e-doped T* from precursors of AFM
  - Kyung et al. PRL **93**, 147004 (2004).
  - Motoyama et al. Nature **445**, 186 (2007).

UNIVERSITÉ DE SHERBROOKE

$d = 2$ precursors, e-doped



$$\xi^{\star} = 2.6(2)\xi_{\text{th}}.$$

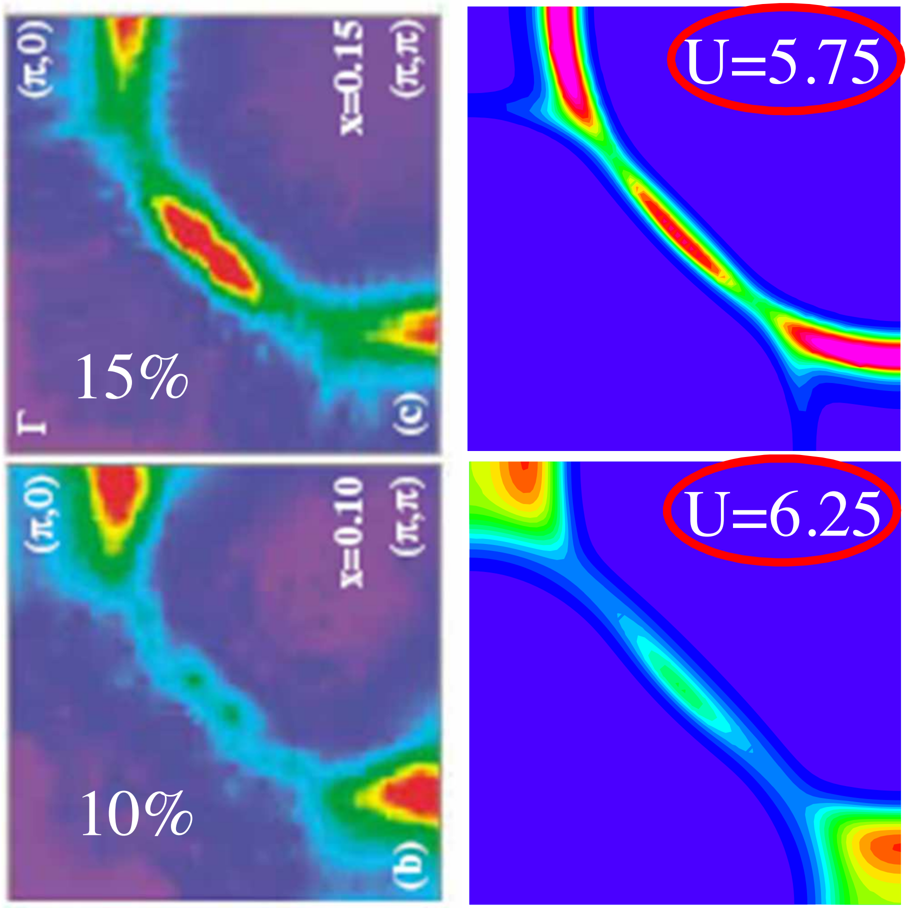
Vilk, A.-M.S.T (1997)

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

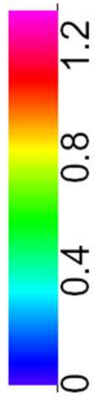
Semi-quantitative fits of both ARPES and neutron

Fermi surface plots

Hubbard repulsion *U* has to…



be not too large

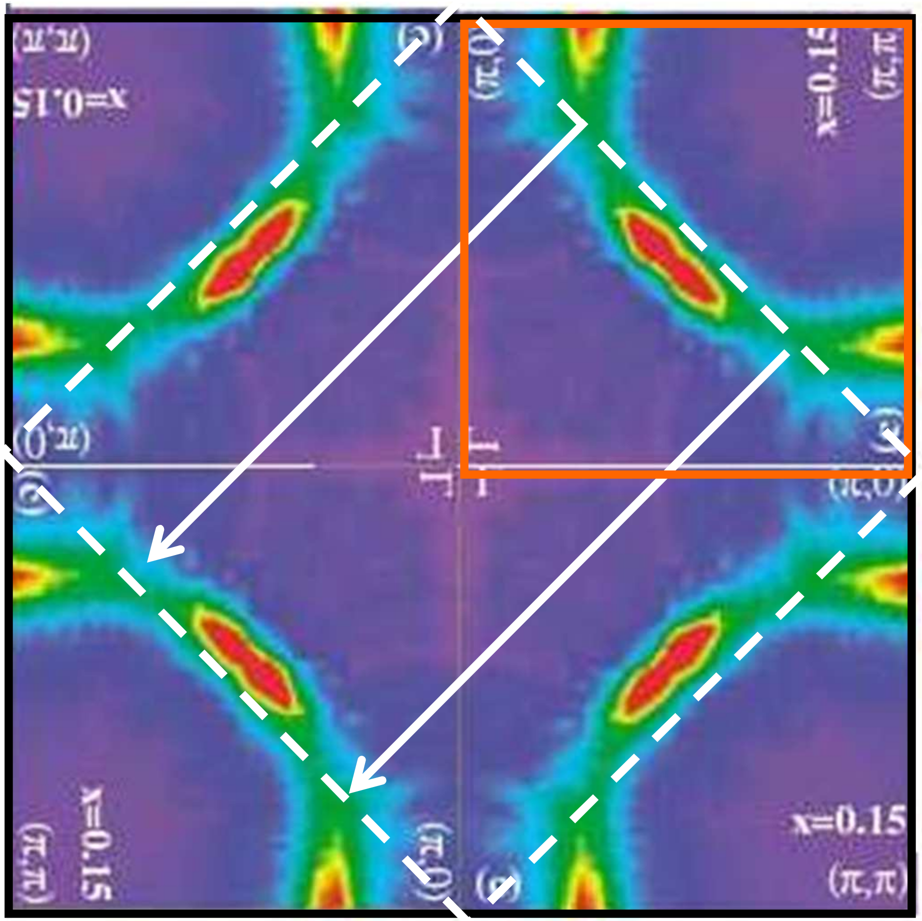


increase for
smaller doping

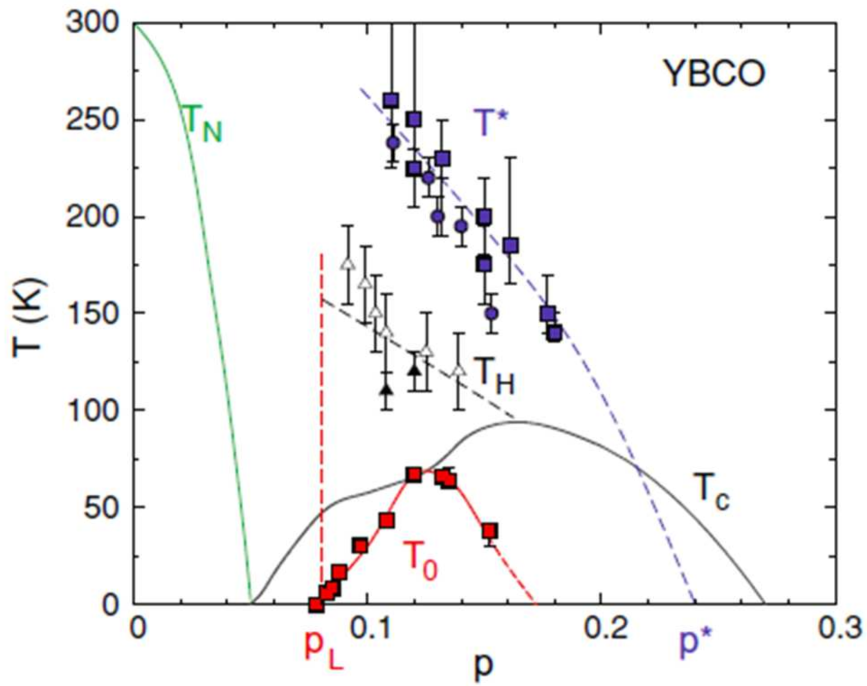
B.Kyung *et al.*,PRB **68**, 174502 (2003)

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

Hot spots from AFM quasi-static scattering

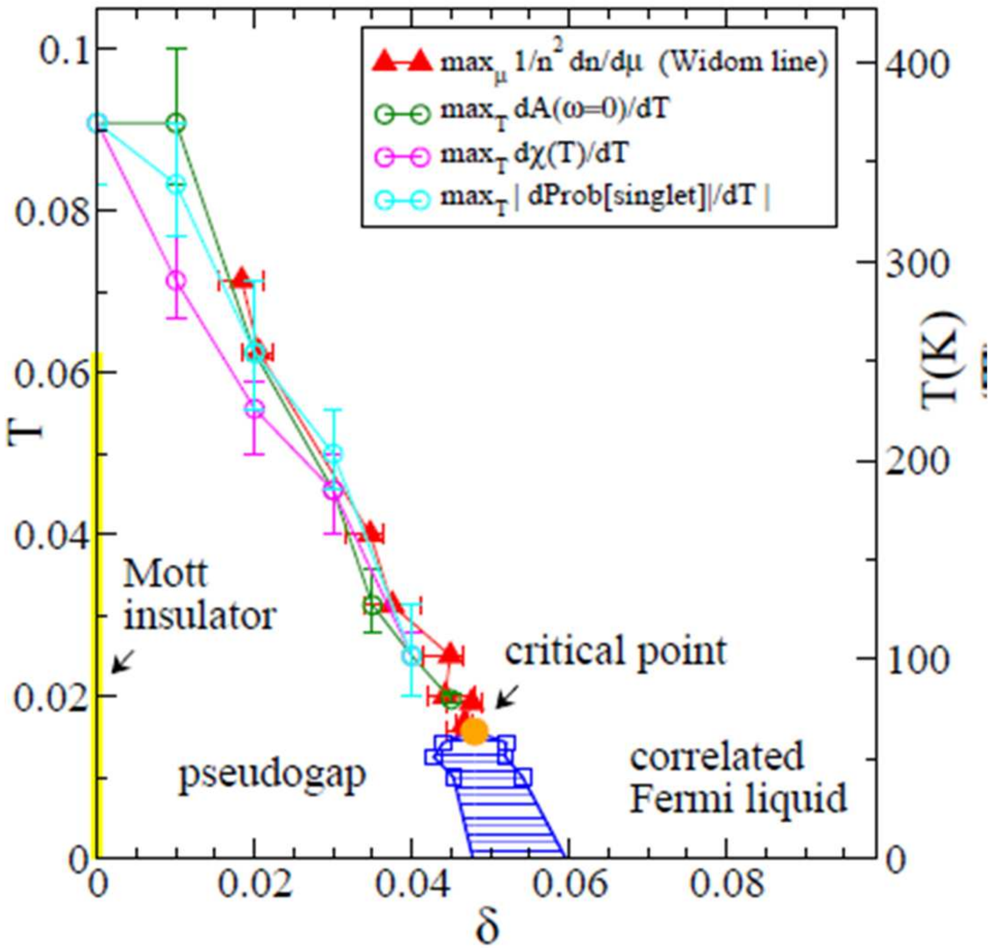


Hole-doped case: Competing phases?



Leboeuf, Doiron-Leyraud et al. PRB **83,** 054506 (2011)

Pseudogap from Mott physics



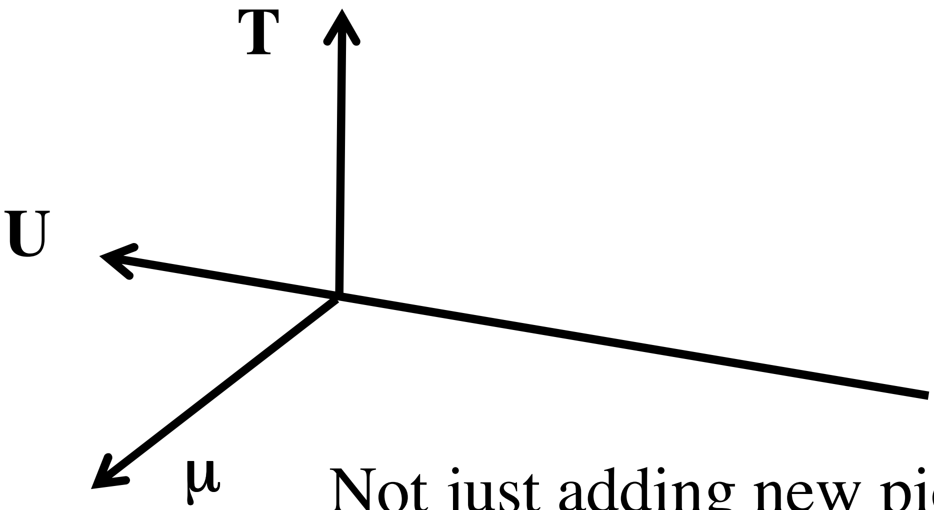
G. Sordi, *et al*. Scientific Reports 2, 547 (2012)

Competing order is a consequence of the pseudogap, not its cause:
Parker et al. Nature 468, 677 (2010)

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*)

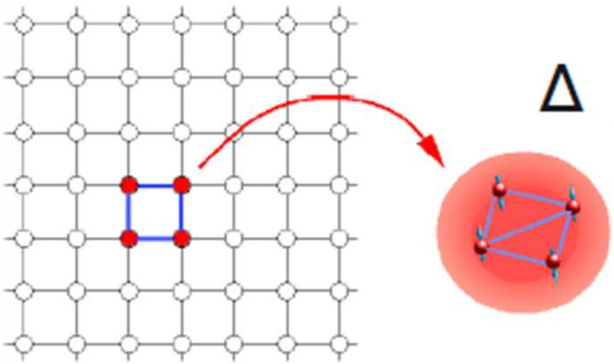


Kristjan Haule

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

UNIVERSITÉ DE SHERBROOKE

C-DMFT



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

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

Here: continuous time QMC

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

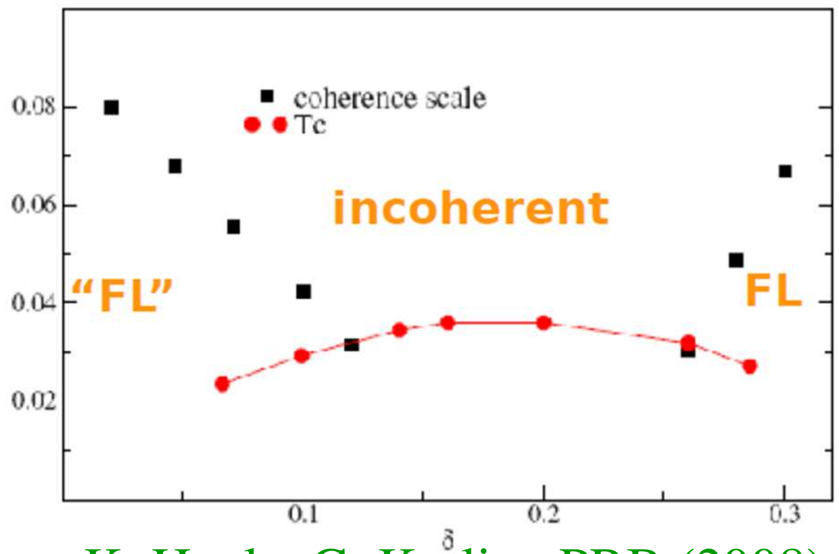
Continuous-time Quantum Monte Carlo calculations to sum all diagrams generated from expansion in powers of hybridization.

P. Werner, A. Comanac, L. de' Medici, M. Troyer, and A. J. Millis, Phys. Rev. Lett. **97**, 076405 (2006).

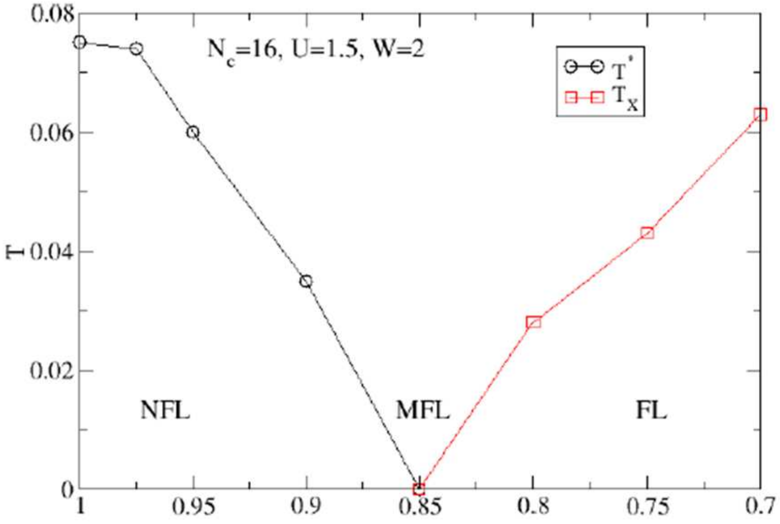
K. Haule, Phys. Rev. B **75**, 155113 (2007).

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)

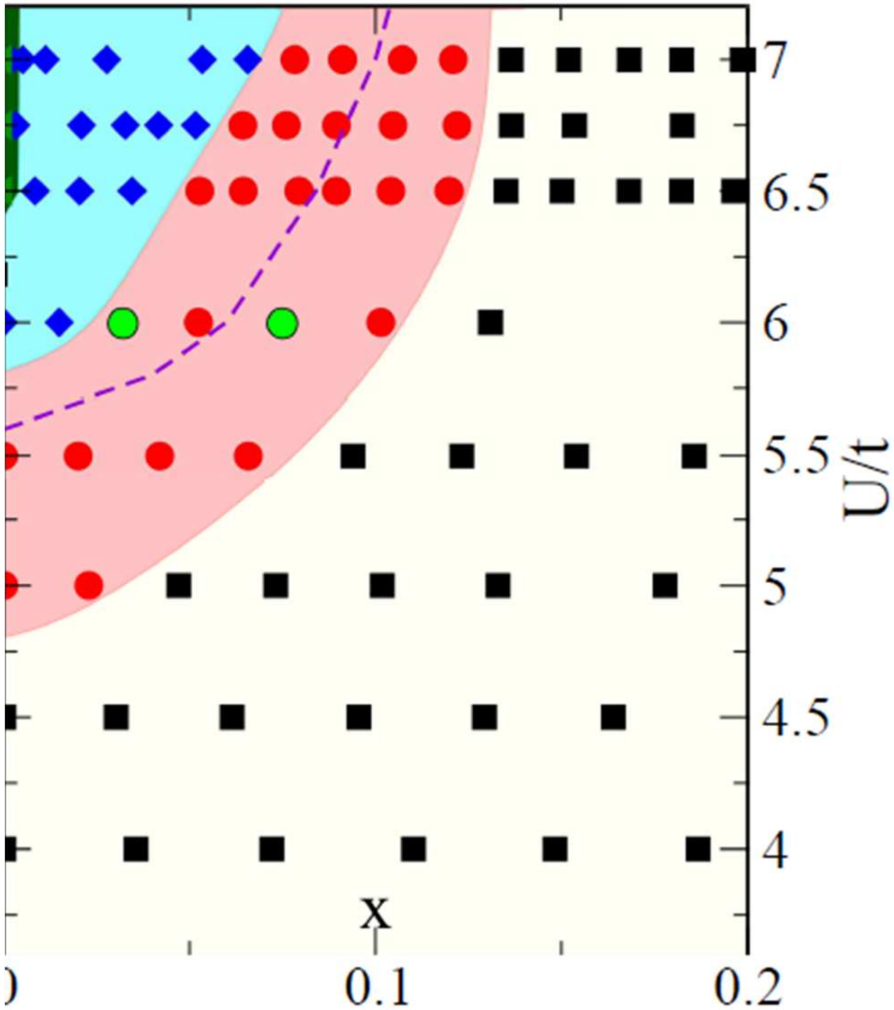


K. Haule, G. Kotliar, PRB (2008)



Vildhyadhiraja, PRL (2009)

Doping driven Mott transition



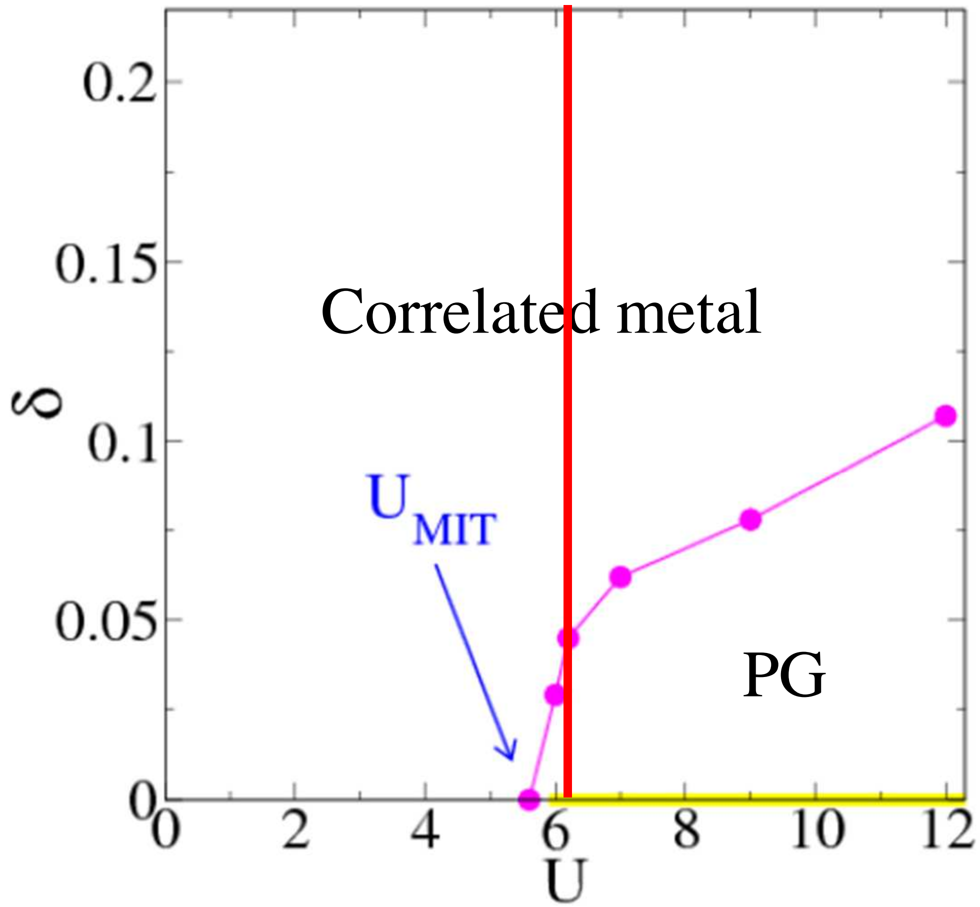
T = 0.25 t

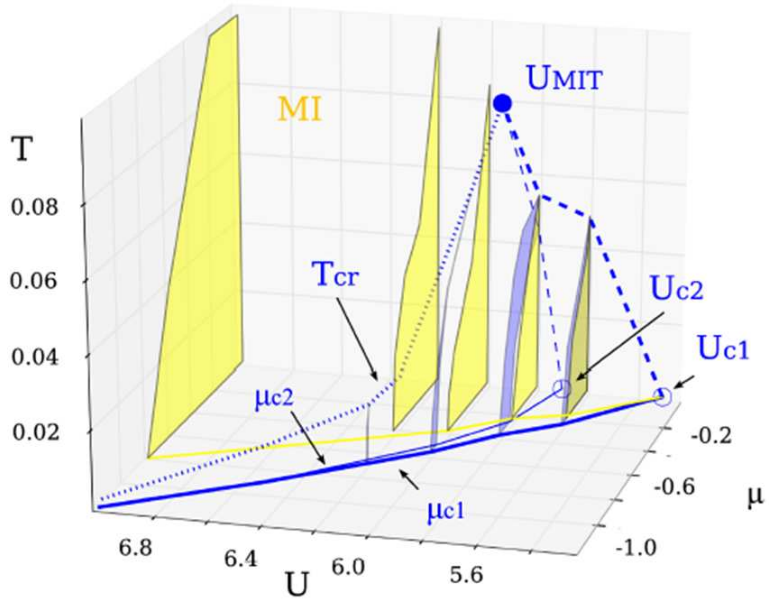
Gull, Parcollet, Millis
arXiv:1207.2490v1

Gull, Werner, Millis, (2009)
E. Gull, M. Ferrero, O. Parcollet, A. Georges, and A. J. Millis (2010)

Link to Mott transition up to optimal doping

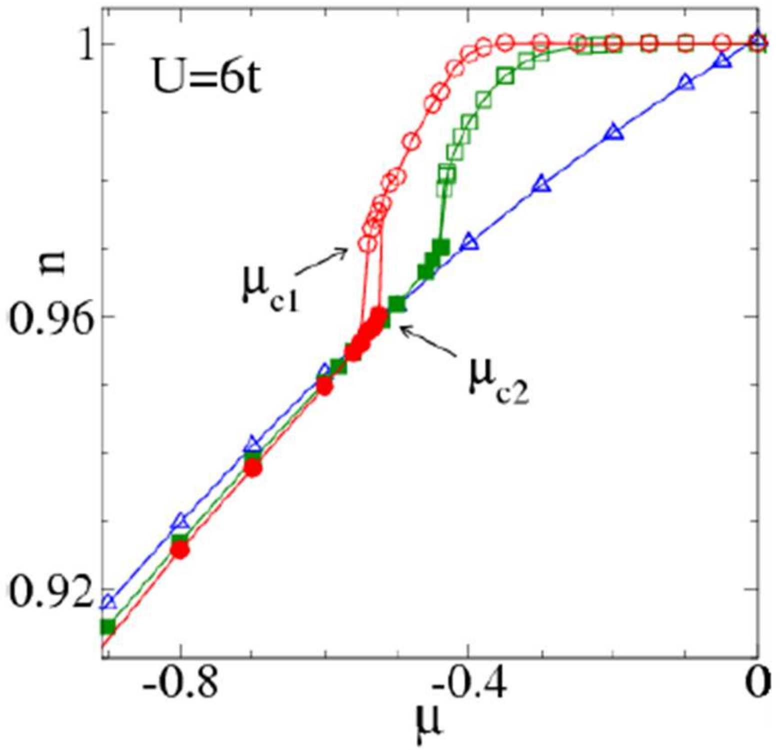
Doping dependence of critical point as a function of *U*





UNIVERSITÉ DE SHERBROOKE

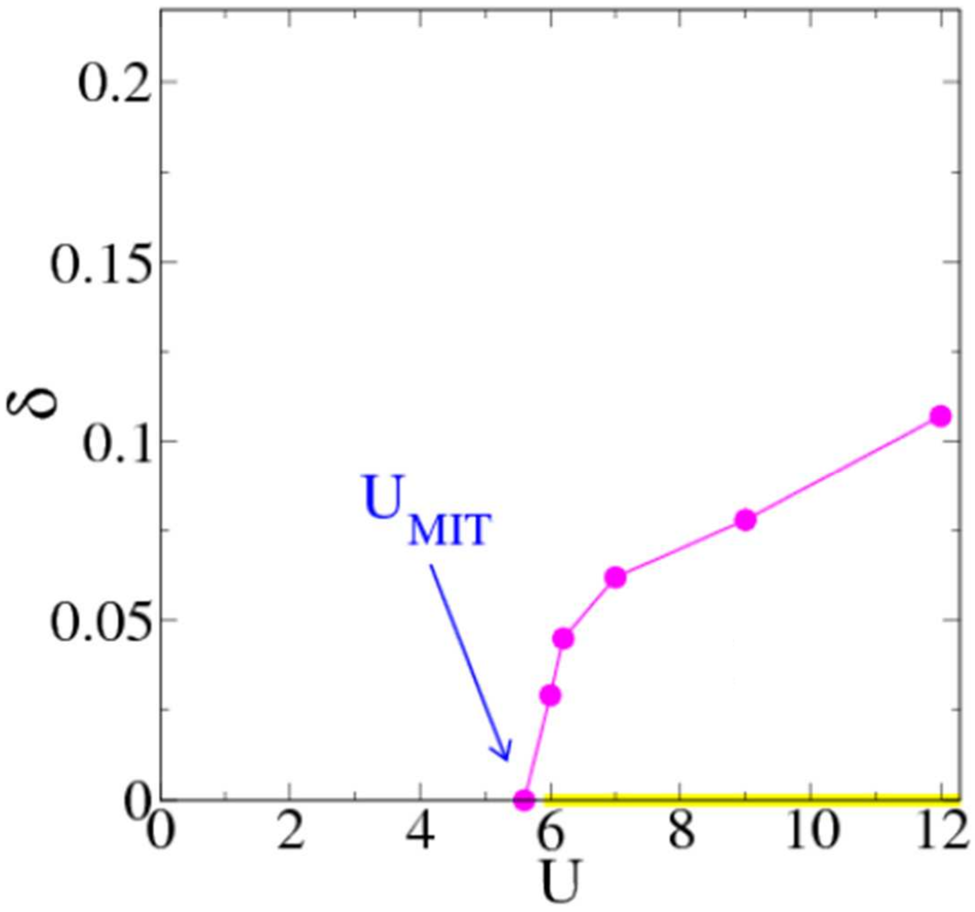
First order transition at finite doping



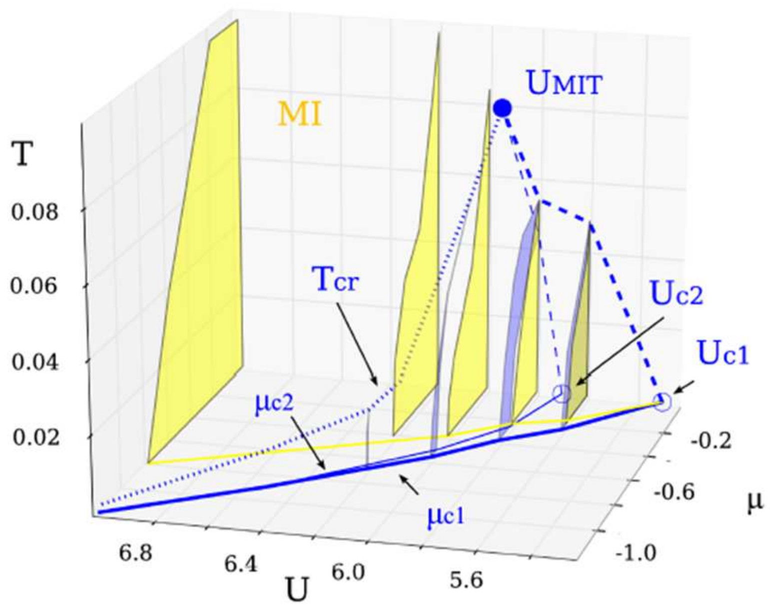
$n(\mu)$ for several temperatures:
$T/t =$1/10, 1/25, 1/50

Link to Mott transition up to optimal doping

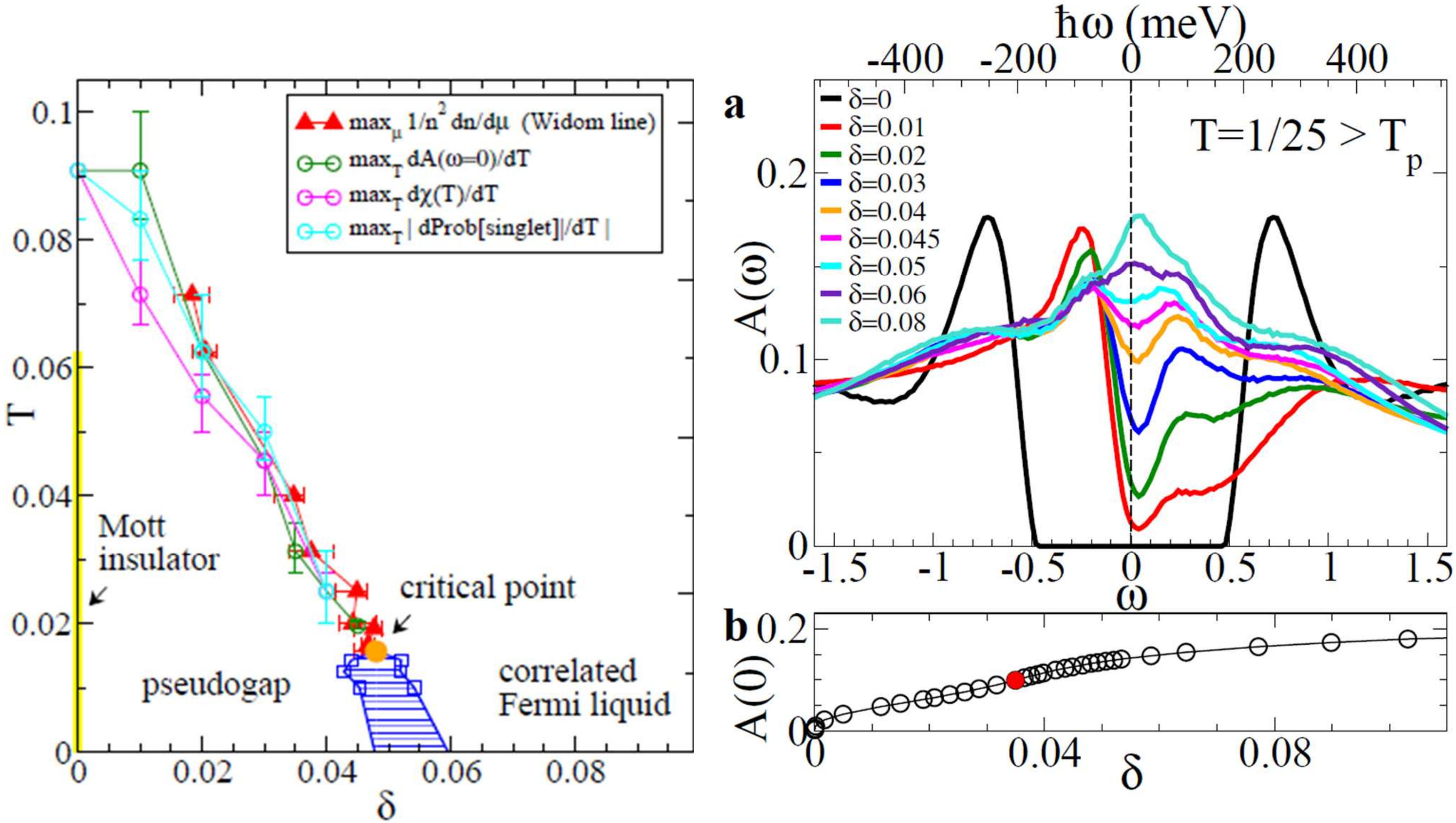
Doping dependence of critical point as a function of *U*



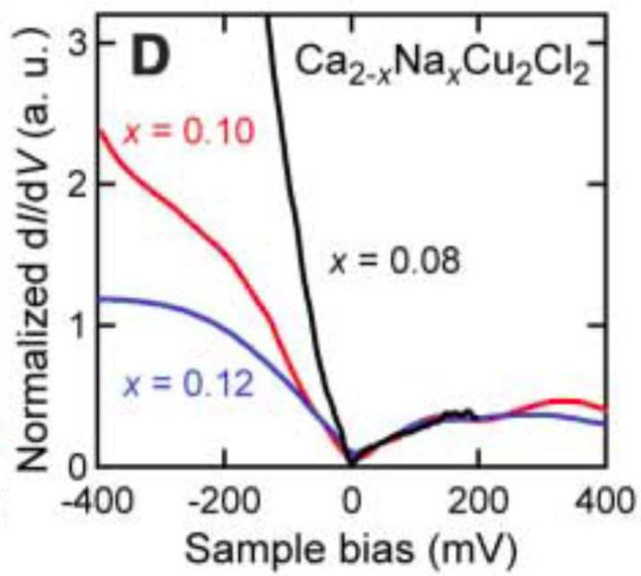
Smaller *D* and *S*

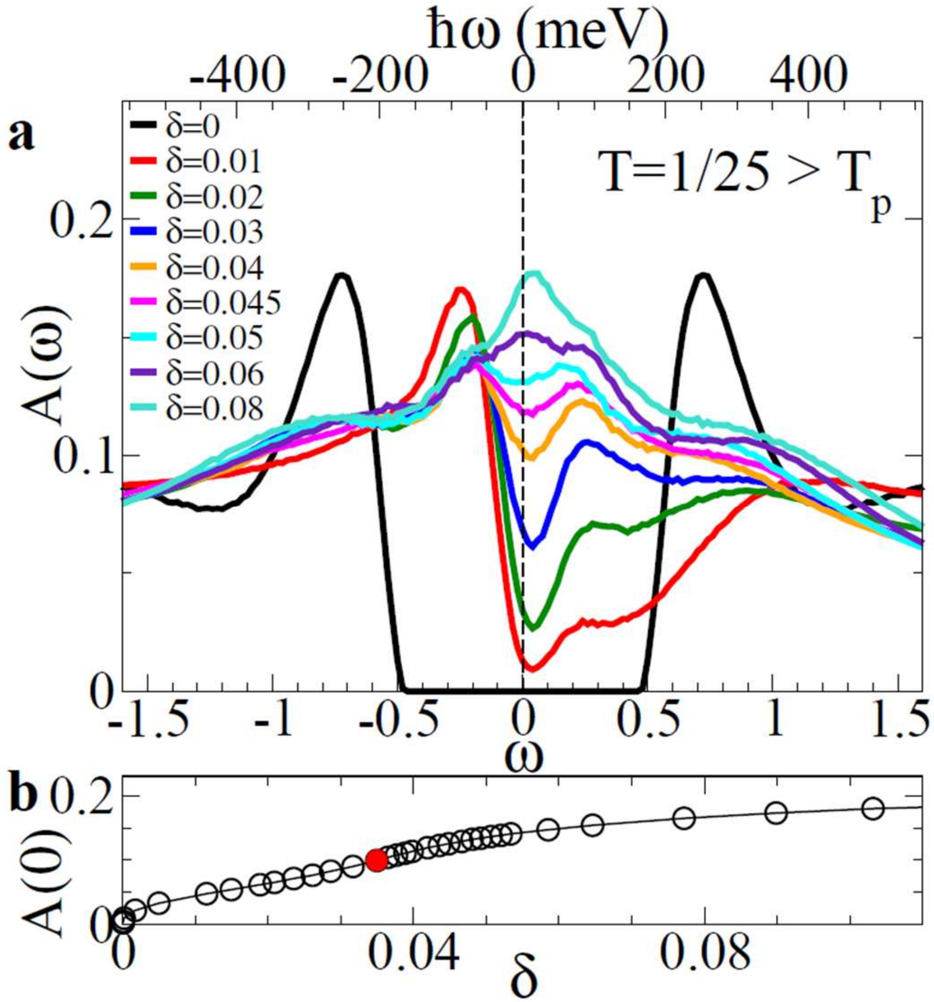


Density of states



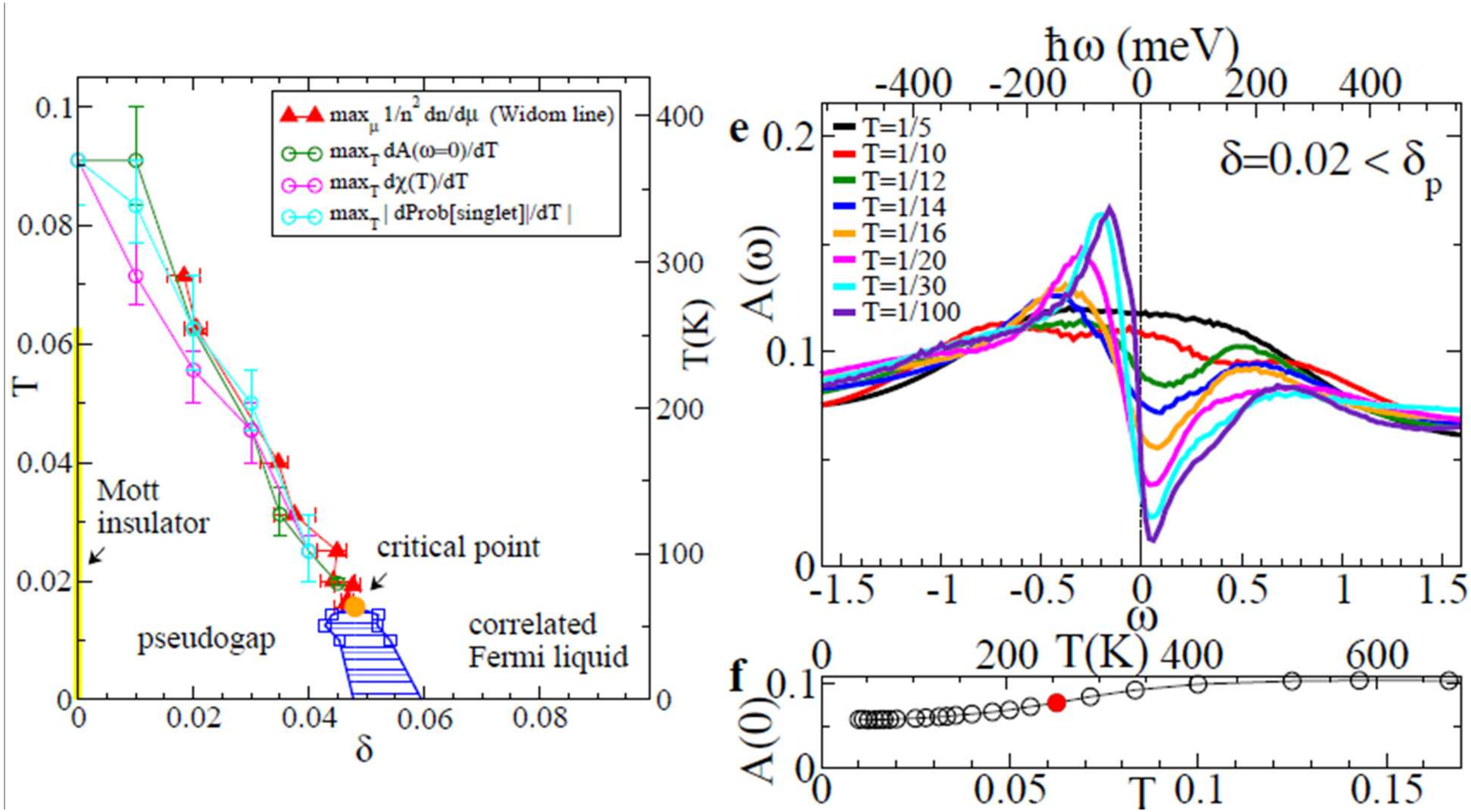
Density of states



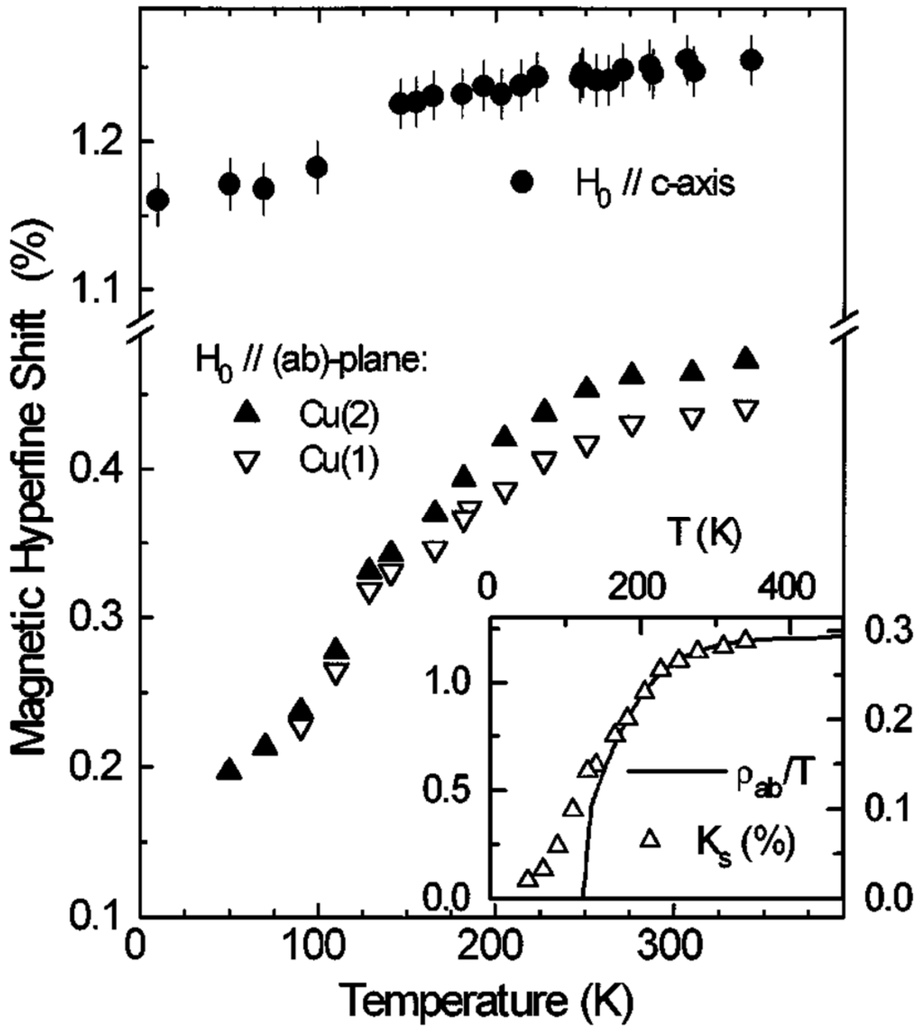


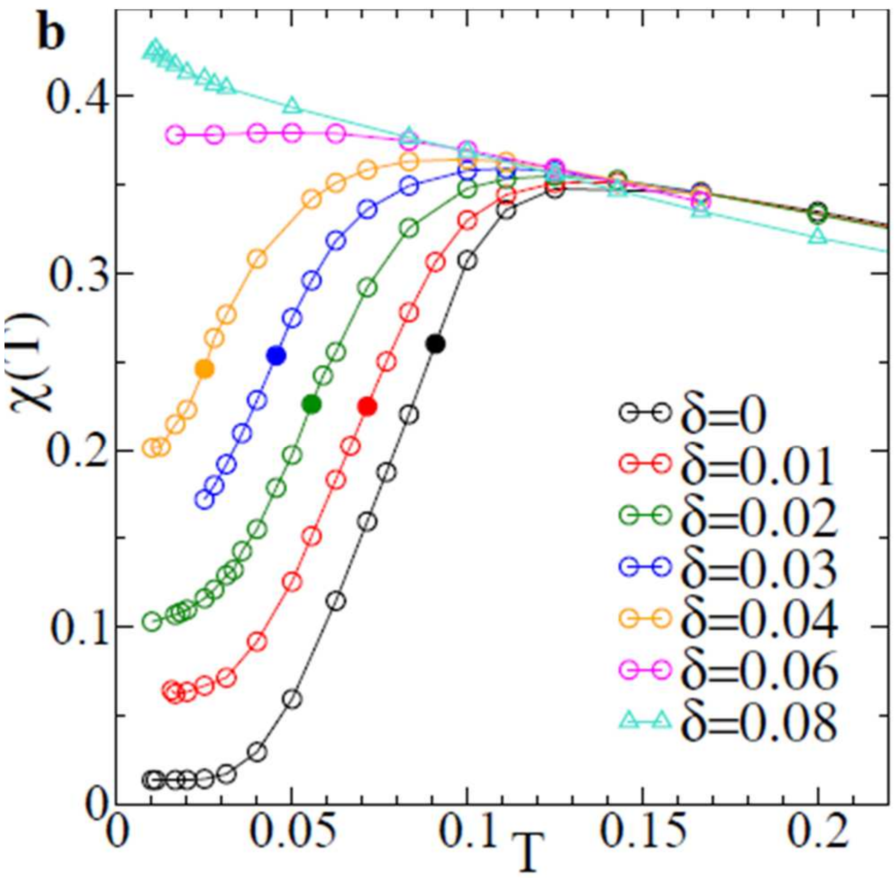
Khosaka et al. *Science* **315**, 1380 (2007);

Density of states



Spin susceptibility



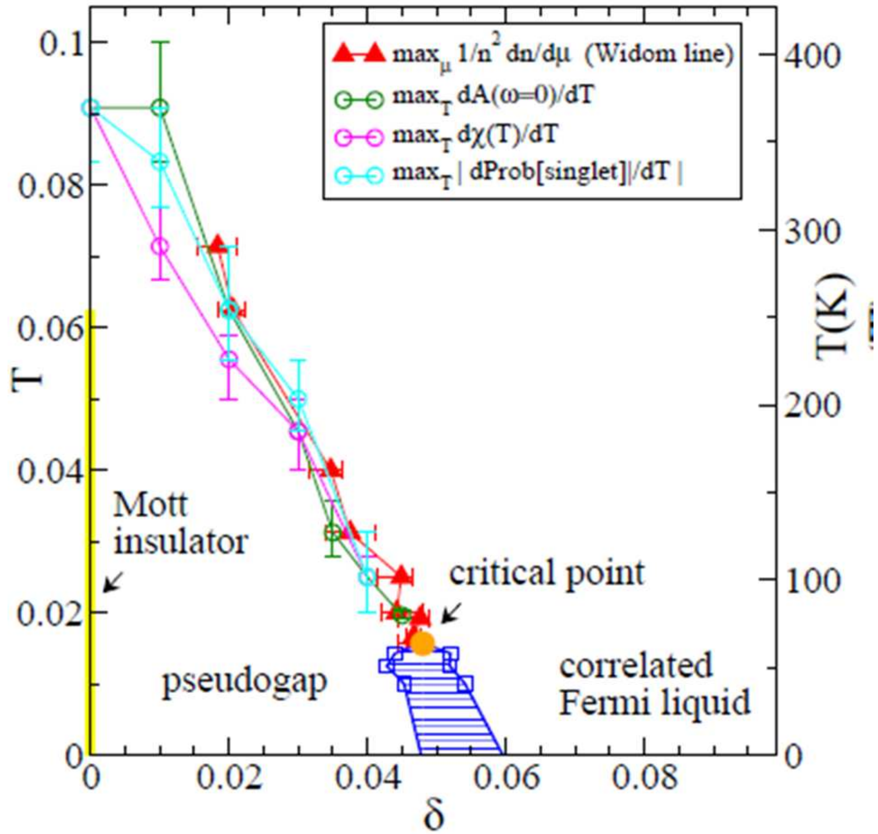


Underdoped Hg1223

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

UNIVERSITÉ DE SHERBROOKE

Pseudogap *T** along the Widom line



Giovanni Sordi

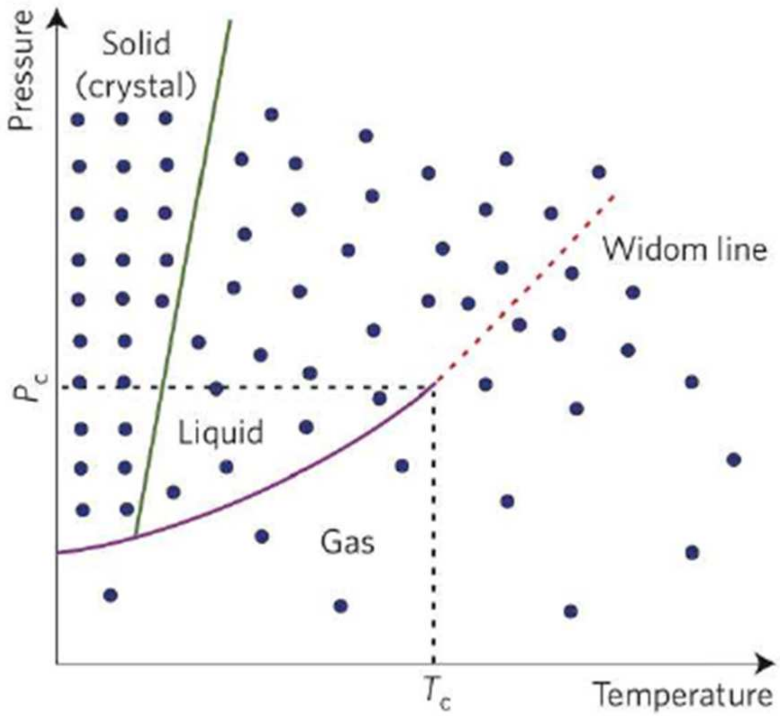
Patrick Sémon

Kristjan Haule

The Widom line

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

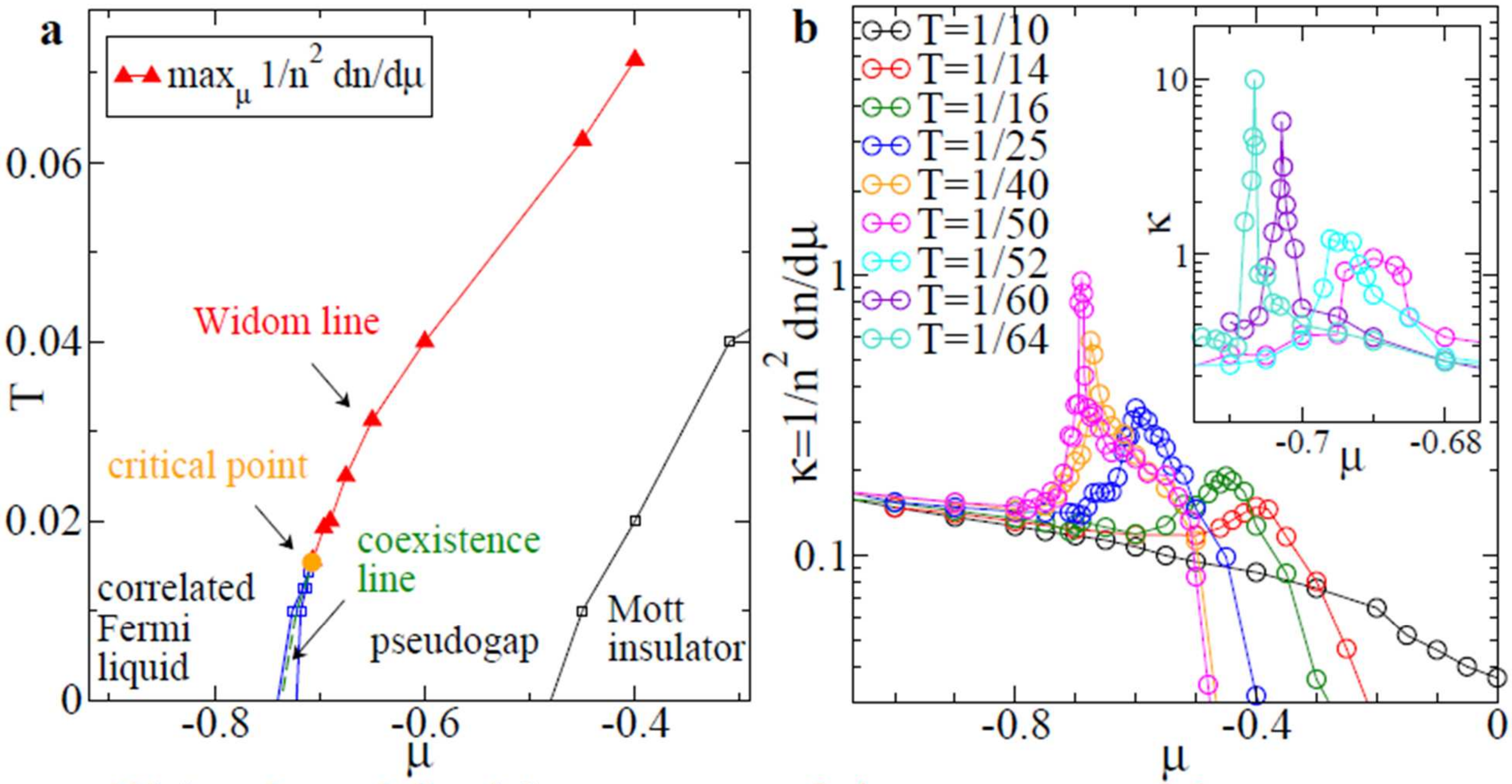
What is the Widom line?



McMillan and Stanley, Nat Phys 2010

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

Pseudogap *T** along the Widom line

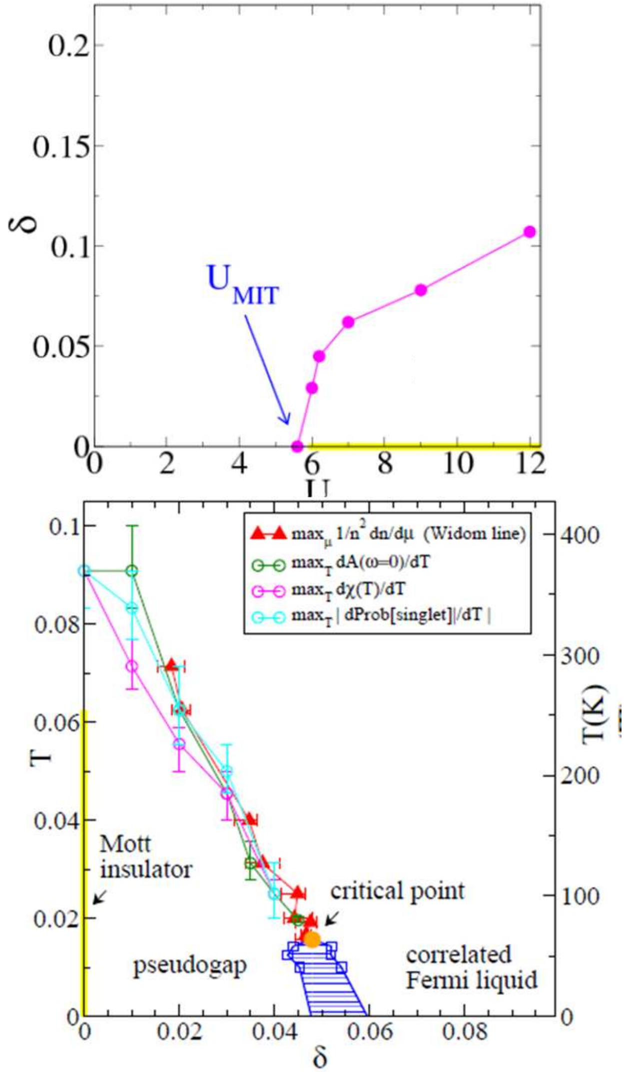


Widom line: defined from maxima of charge compressibility

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

divergence of κ at the (classical) critical point!

Summary: normal state



- Mott physics extends way beyond half-filling
- Pseudogap is a phase
- Pseudogap *T** is a Widom line
- High compressibility (stripes?)

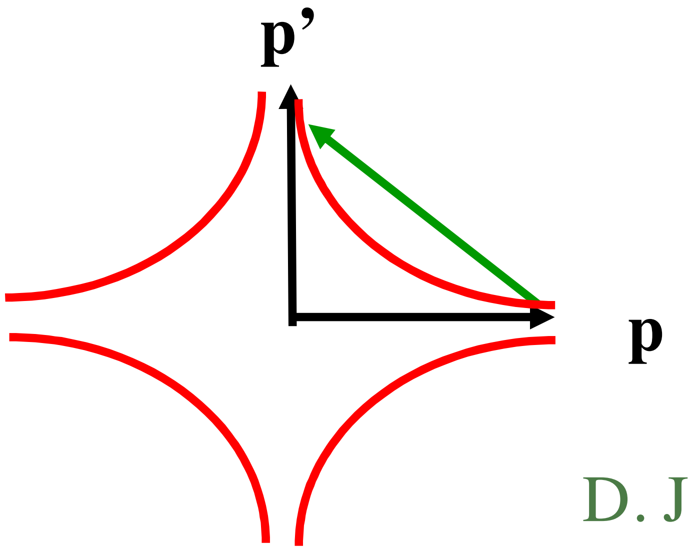
Outline

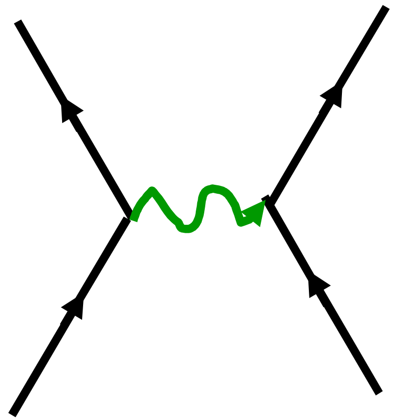
- More on the model
- Method DMFT
  - Validity
  - Impurity solvers
- Finite *T* phase diagram
  - Normal state
    - First order transition
    - Widom line and pseudogap
- Superconductivity *T=0* phase diagram
  - The « glue »
- Superconductivity *T* finite

A bit of physics: superconductivity and repulsion

Cartoon « BCS » weak-coupling picture

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





Exchange of spin waves?

Kohn-Luttinger

T_c with pressure

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

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

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

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

A cartoon strong coupling picture

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

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

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

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

Pitaevskii Brückner:

Pair state orthogonal to repulsive core of Coulomb interaction

Kotliar and Liu, P.R. B **38,** 5142 (1988)

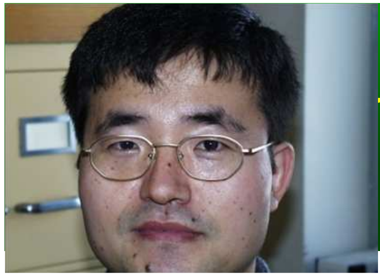
Miyake, Schmitt–Rink, and Varma

P.R. B **34**, 6554-6556 (1986)

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

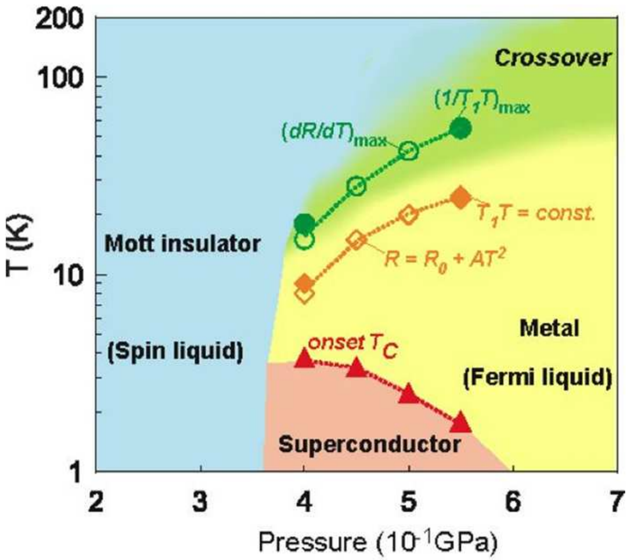
Phase diagram

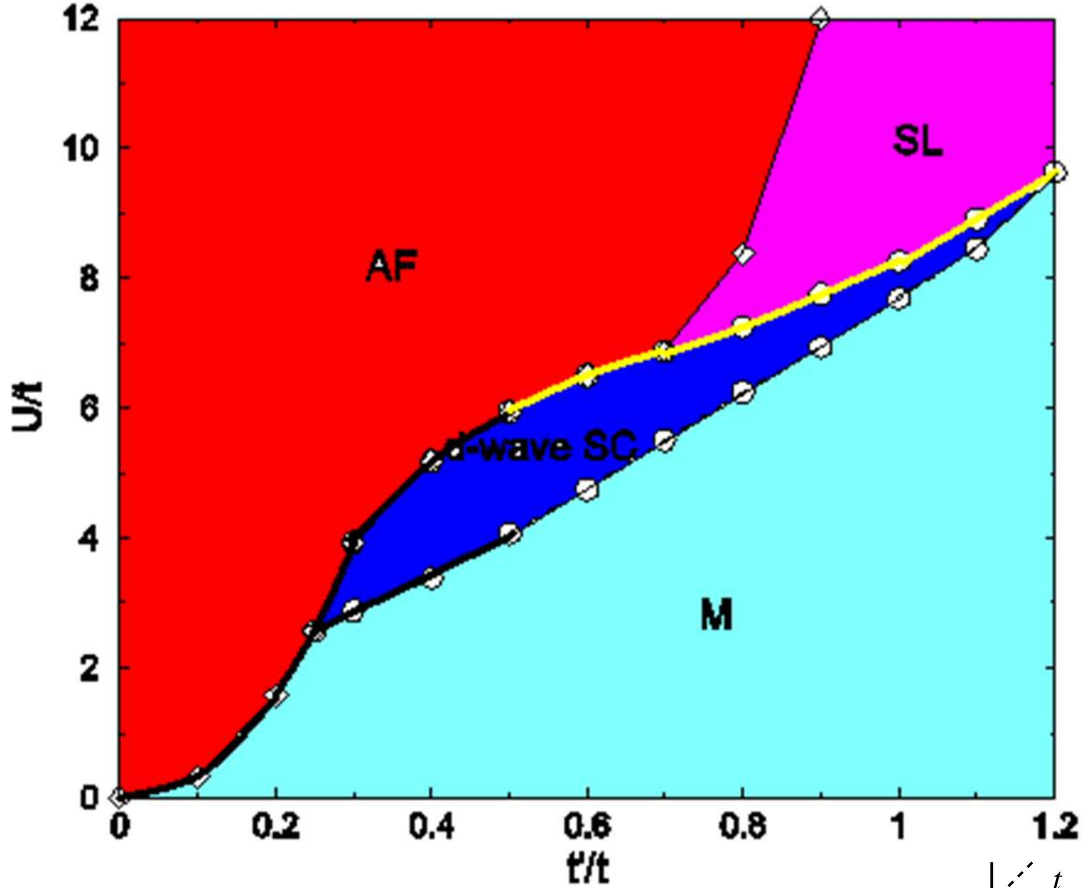
Exact diagonalization as impurity solver ($T=0$).

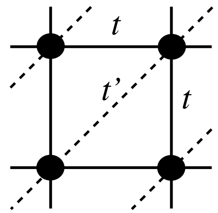


Theoretical phase diagram BEDT

X= $Cu_2(CN)_3$ (t′~ t)







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

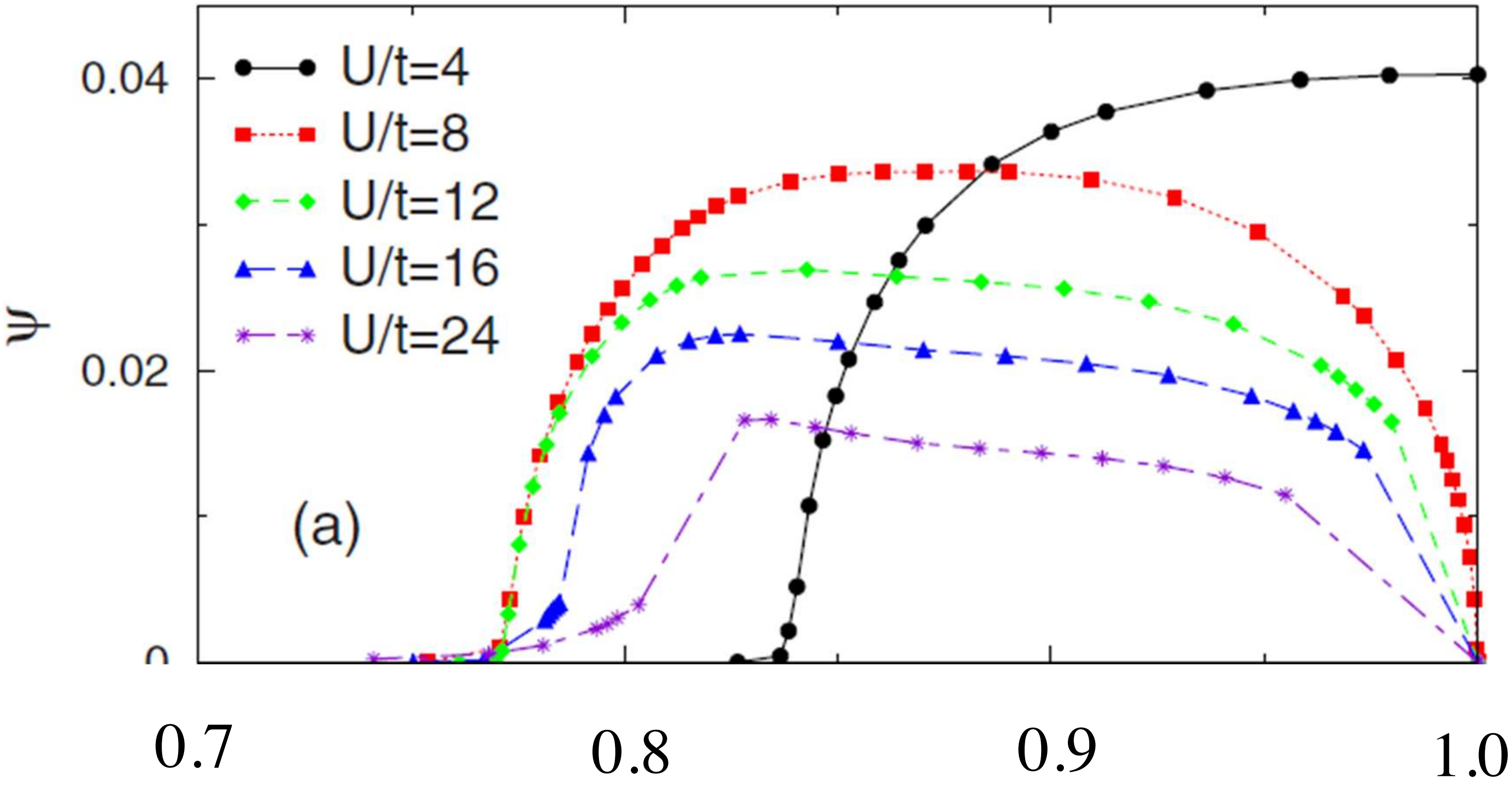
Y. Kurisaki, et al.
Phys. Rev. Lett. **95**, 177001(2005)   Y. Shimizu, et al. Phys. Rev. Lett. **91**, (2003)

T = 0 phase diagram: cuprates

Phase diagram

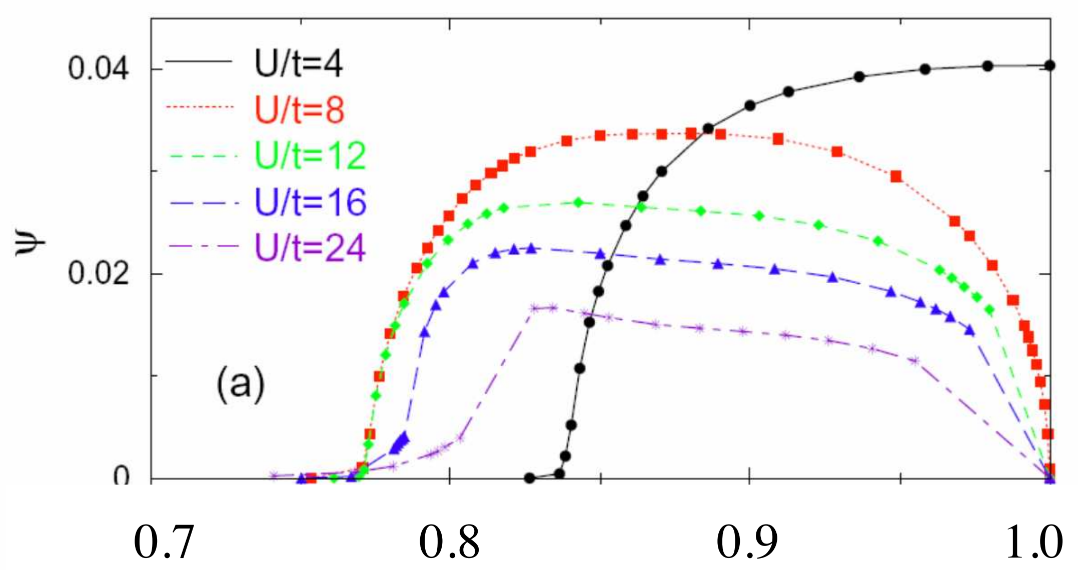
Exact diagonalization as impurity solver ($T=0$).

Theory: T_c down vs Mott



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

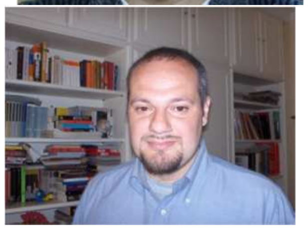
Dome vs Mott (CDMFT)



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

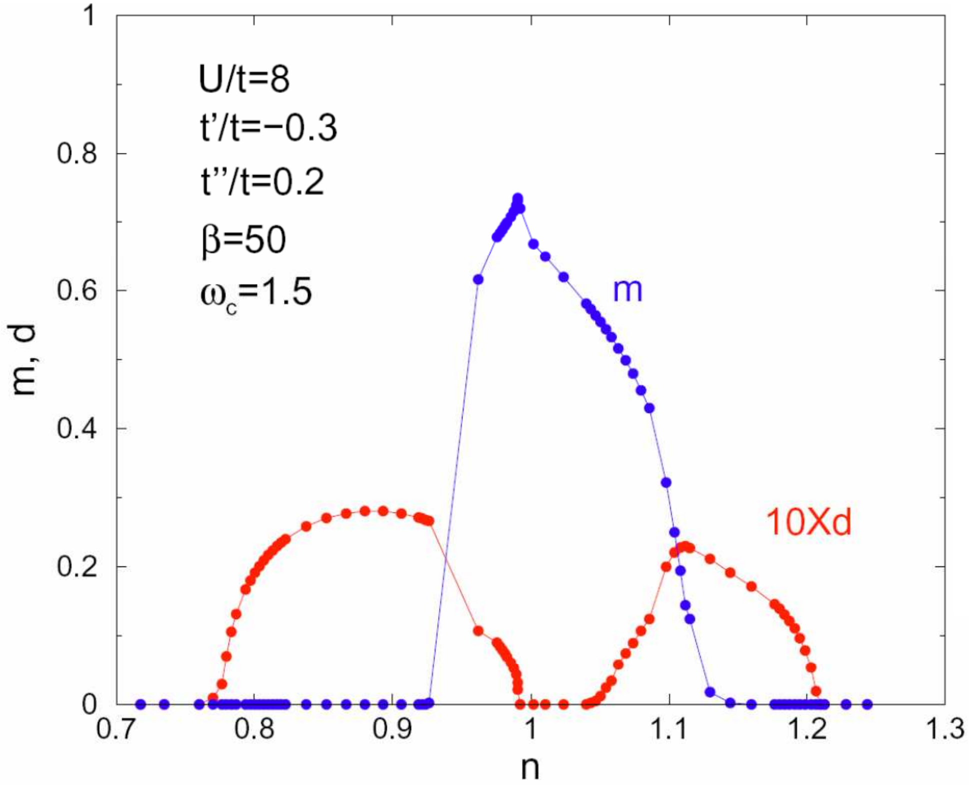




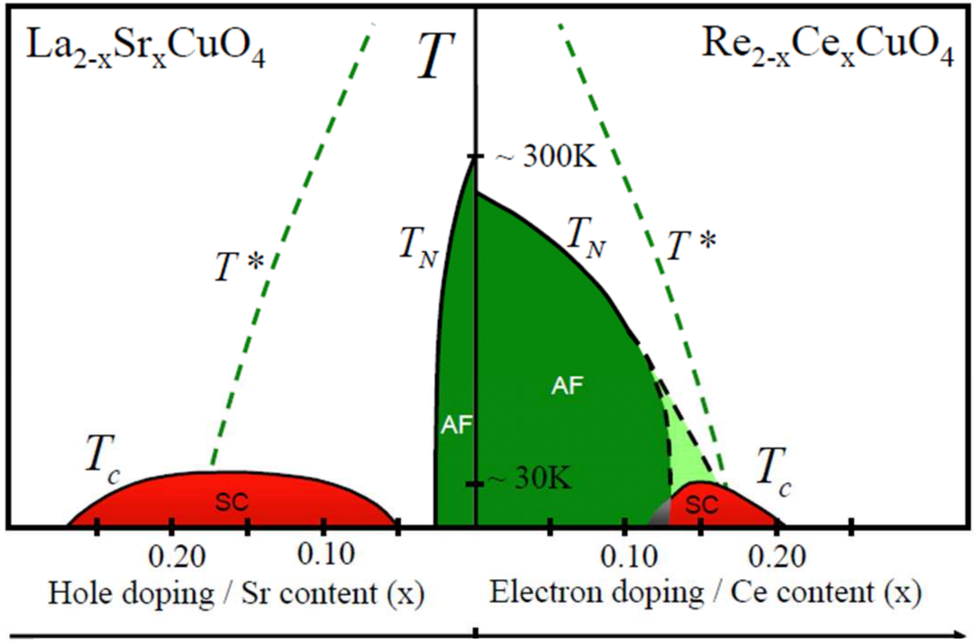



SHERBROOKE

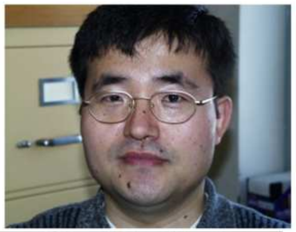
CDMFT global phase diagram



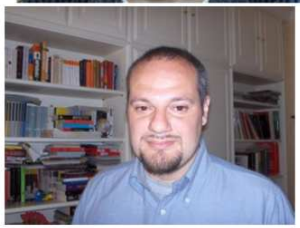
Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008) AND Capone, Kotliar PRL (2006)



Armitage, Fournier, Greene, RMP (2009)

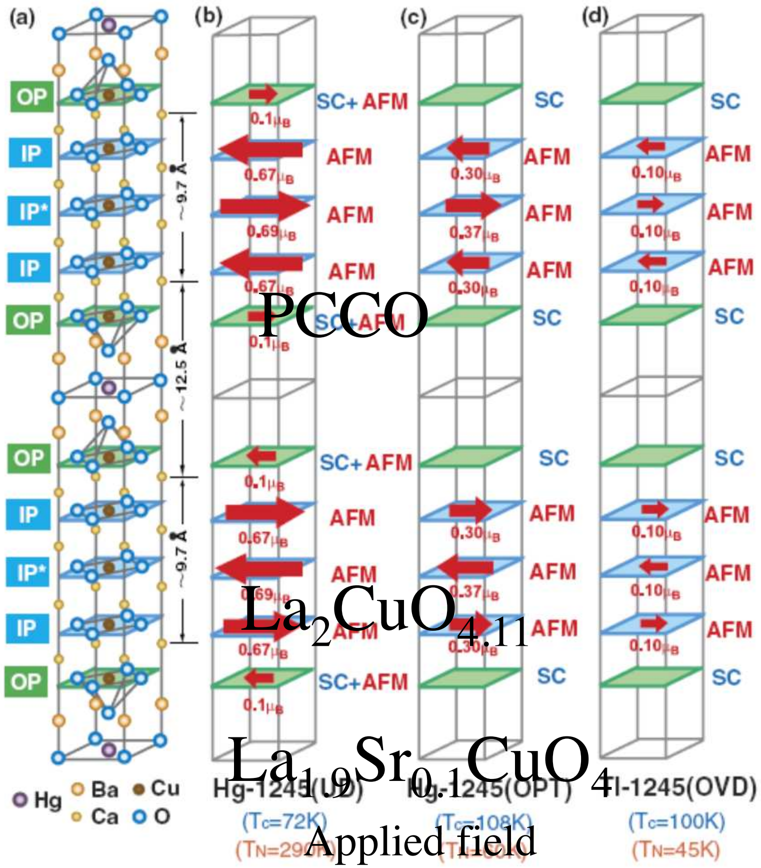







UNIVERSITÉ DE SHERBROOKE

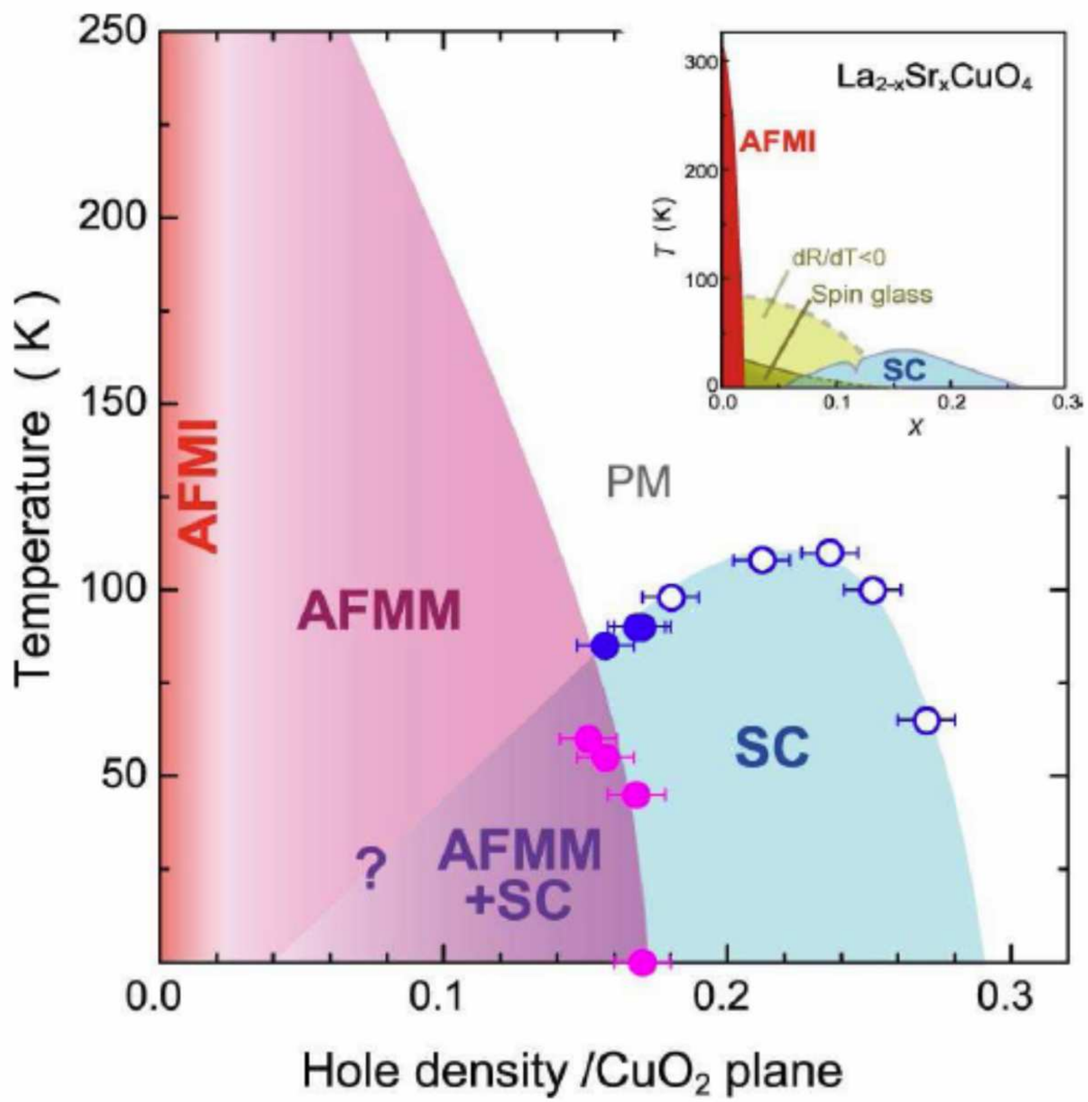
Homogeneous coexistence (experimental)

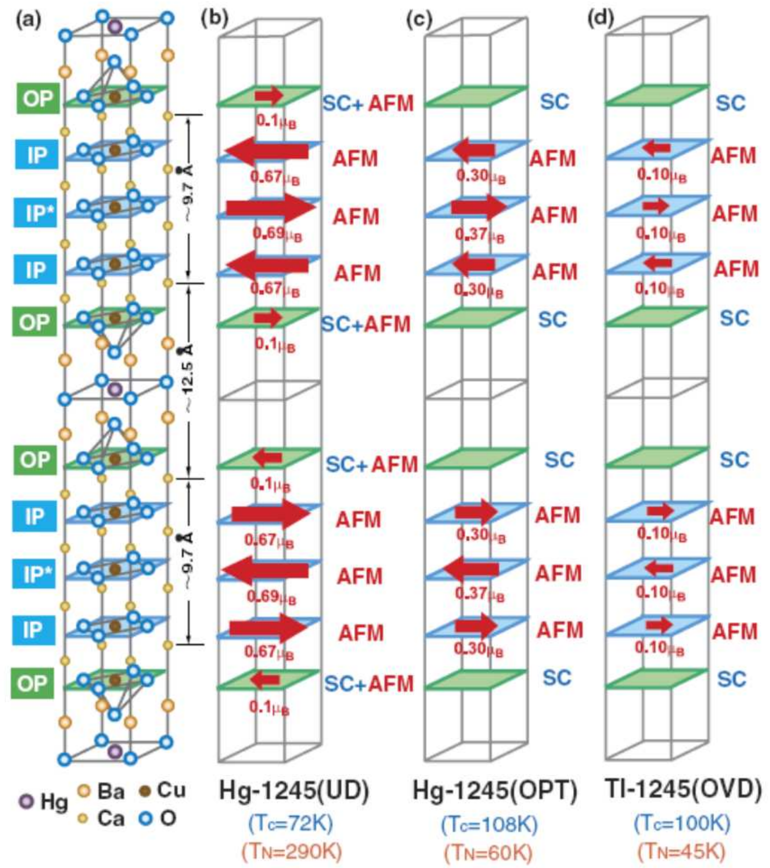


- H. Mukuda, M. Abe, Y. Araki, Y. Kitaoka, K. Tokiwa, T. Watanabe, A. Iyo, H. Kito, and Y. Tanaka, Phys. Rev. Lett. **96**, 087001 (2006).
- Pengcheng Dai, H. J. Kang, H. A. Mook, M. Matsuura, J. W. Lynn, Y. Kurita, Seiki Komiya, and Yoichi Ando, Phys. Rev. B **71**, 100502 R (2005).
- Robert J. Birgeneau, Chris Stock, John M. Tranquada and Kazuyoshi Yamada, J. Phys. Soc. Japan, **75**, 111003 (2006).
- Chang, … Mesot PRB **78**, 104525 (2008).

Consistent with following experiments

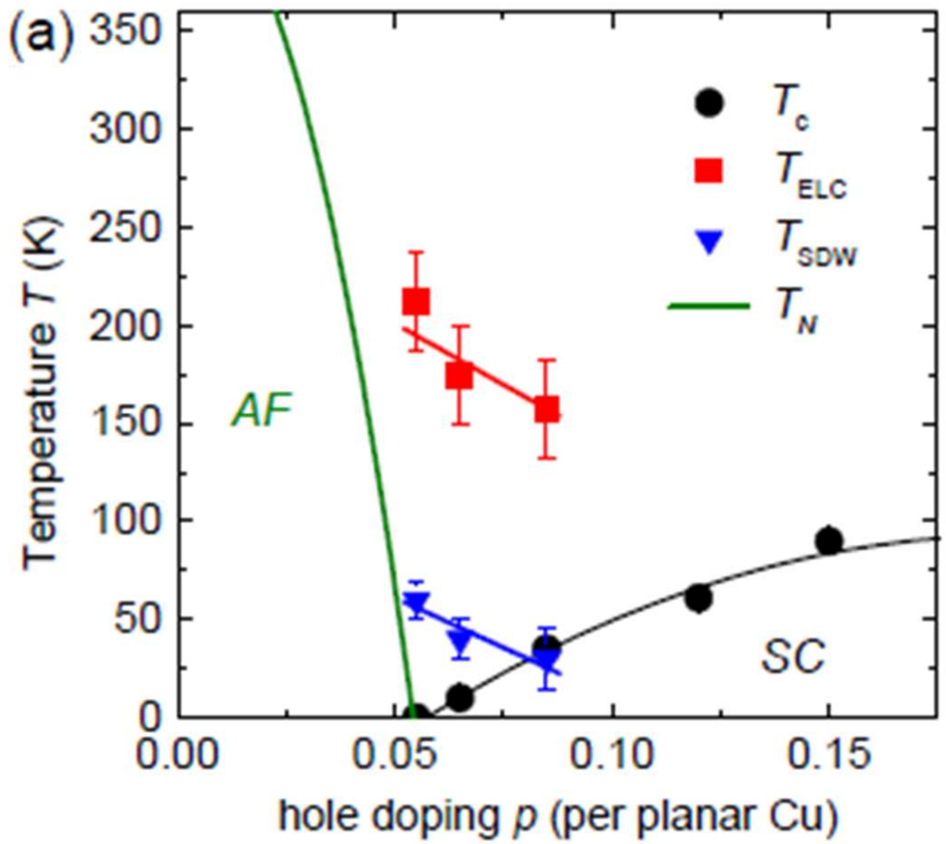
H. Mukuda, Y. Yamaguchi, S. Shimizu, … A. Iyo JPSJ **77**, 124706 (2008)





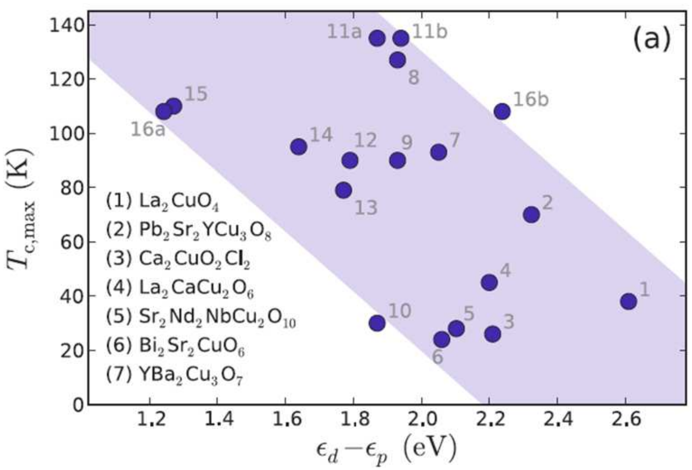
UNIVERSITÉ DE SHERBROOKE

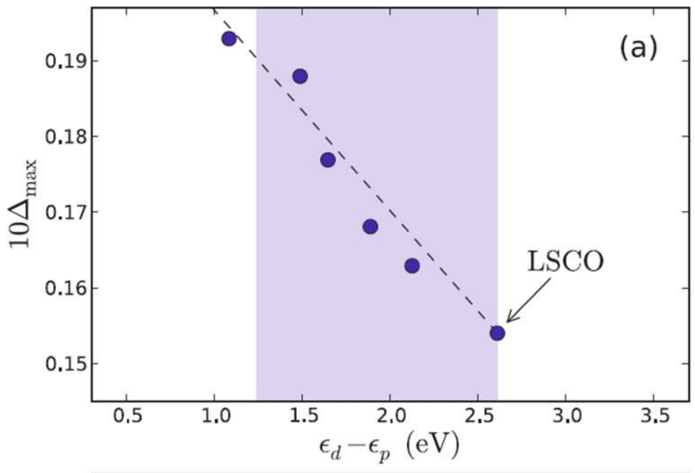
Magnetic phase diagram of YBCO



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

Materials dependent properties





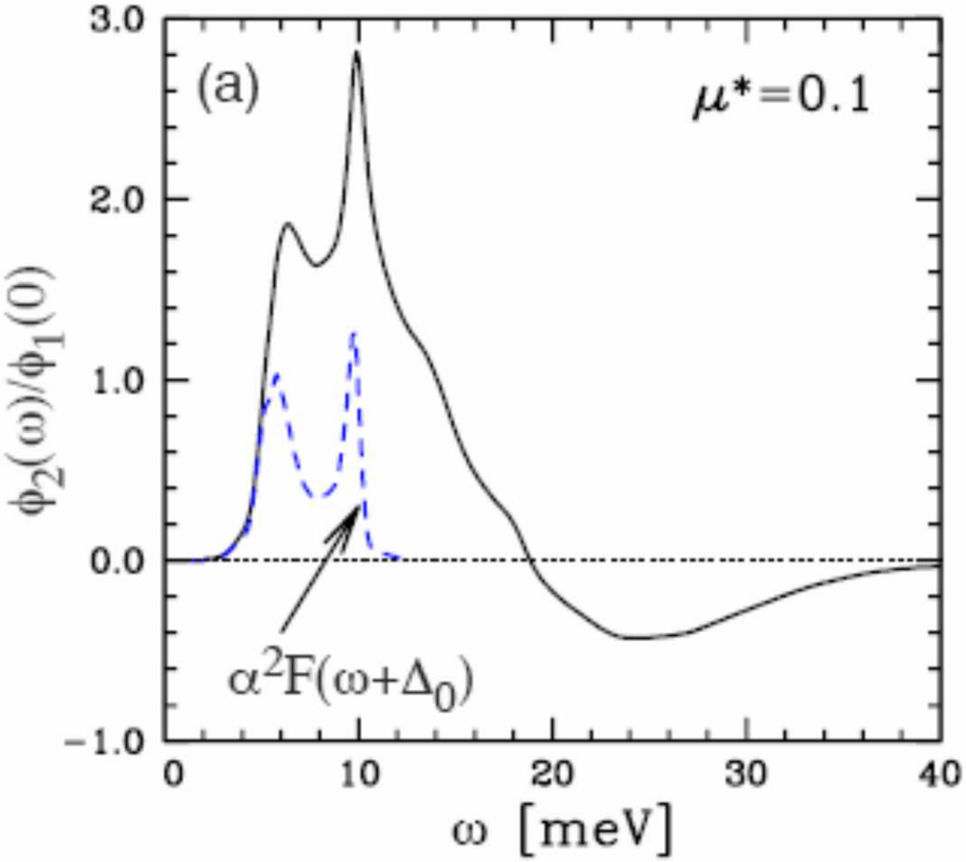
C. Weber, C.-H. Yee, K. Haule, and G. Kotliar, ArXiv e-prints (2011), 1108.3028.

$T = 0$ phase diagram

The glue

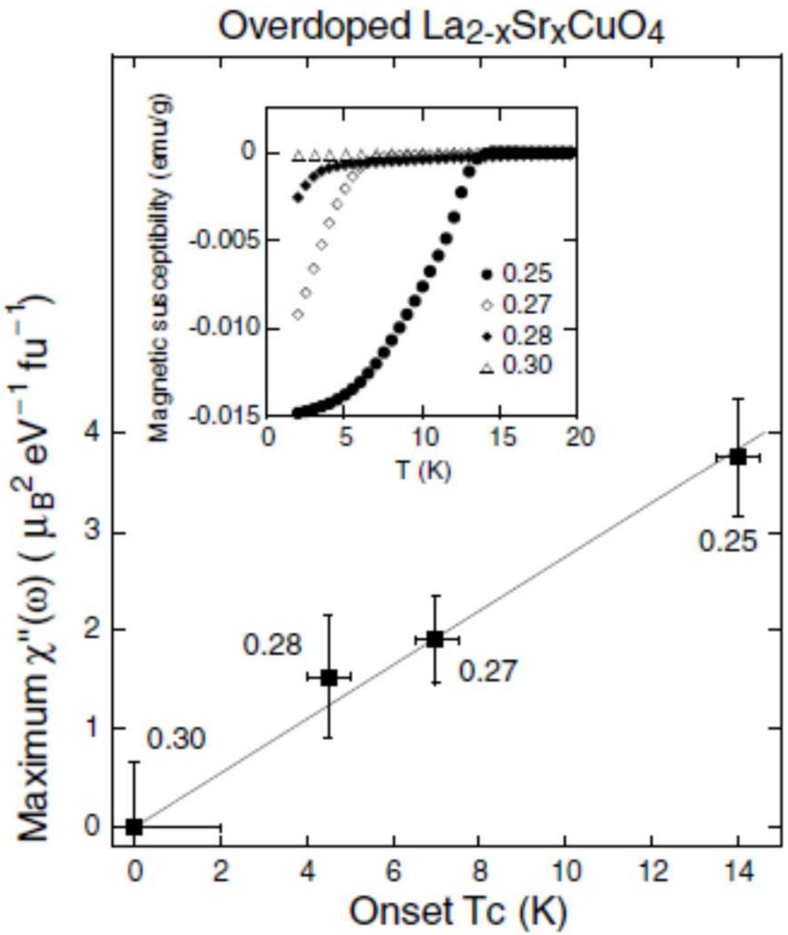
Im Σ_{an} and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

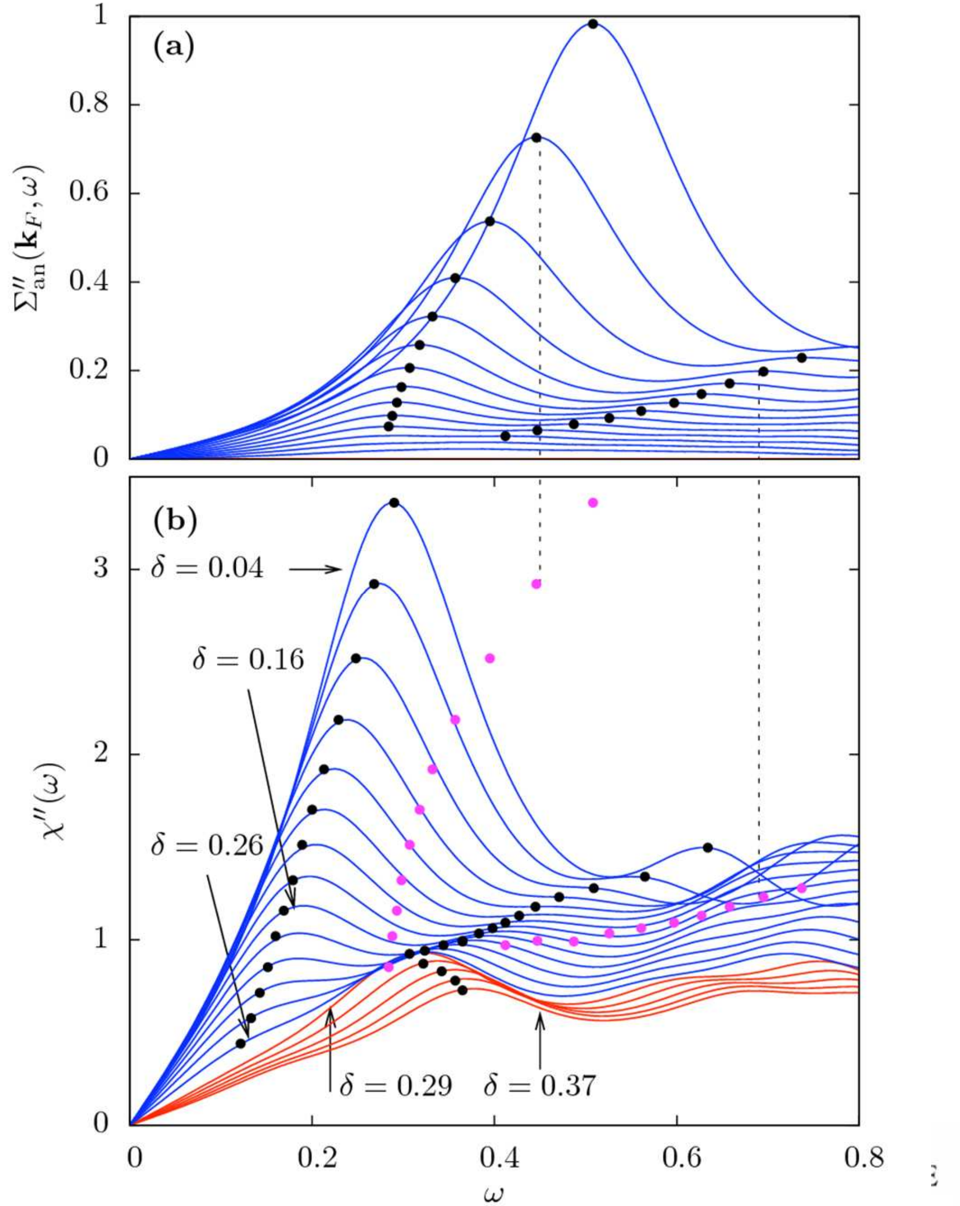


The glue

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



Wakimoto … Birgeneau PRL (2004)



The glue and neutrons

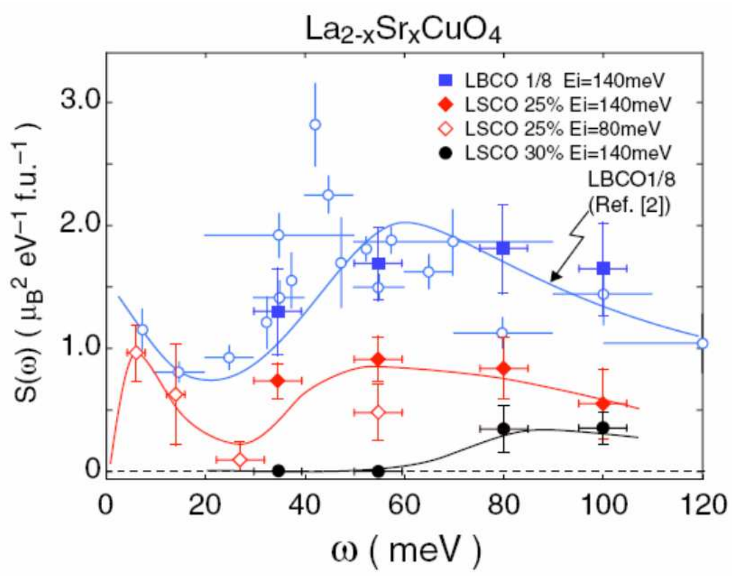
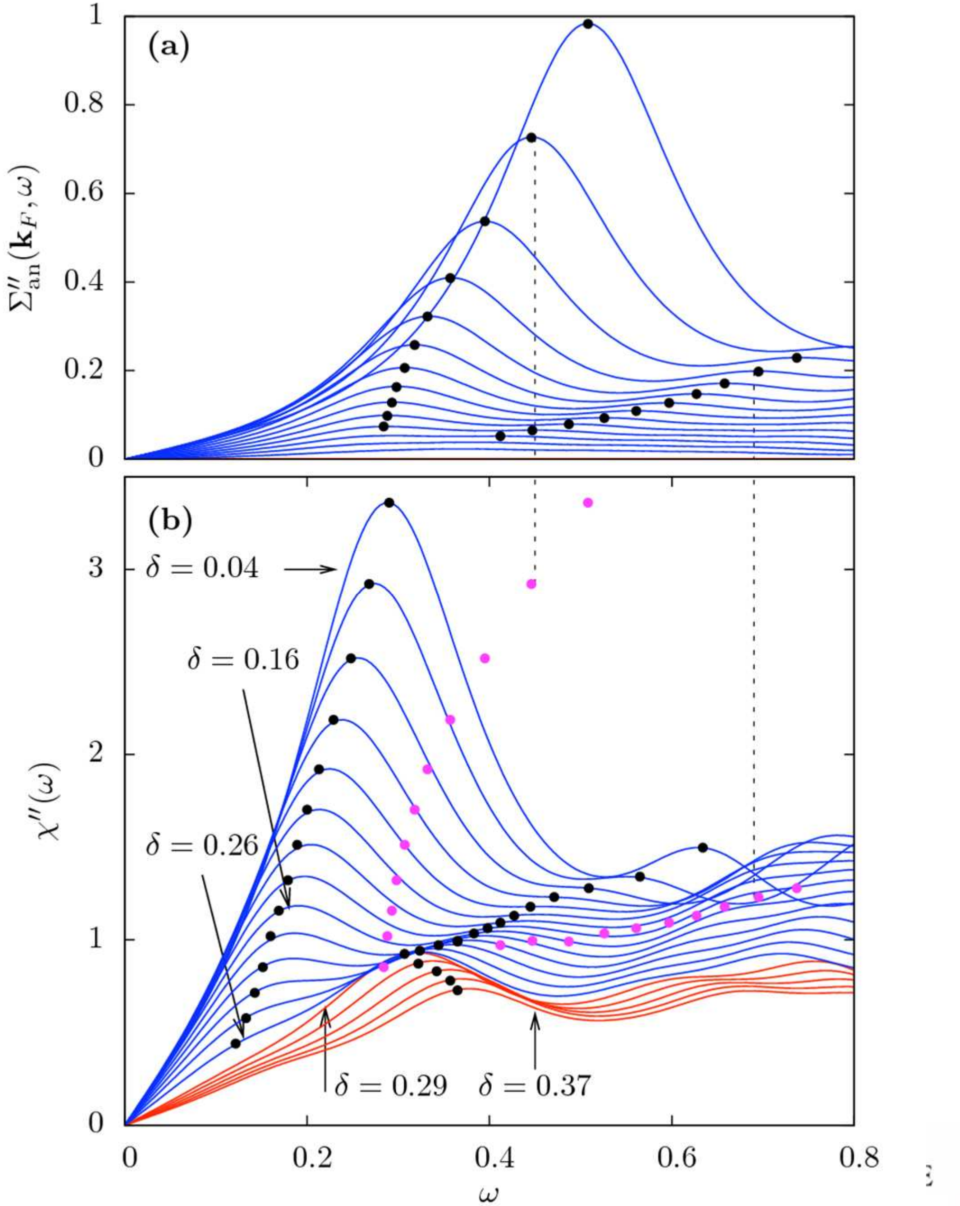


FIG. 3 (color online). **Q**-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i = 140$ meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO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

Outline

- More on the model
- Method DMFT
  - Validity
  - Impurity solvers
- Finite *T* phase diagram
  - Normal state
    - First order transition
    - Widom line and pseudogap
- *T=0* phase diagram
  - The « glue »
- Superconductivity *T* finite

Giovanni Sordi

Patrick Sémon

Kristjan Haule

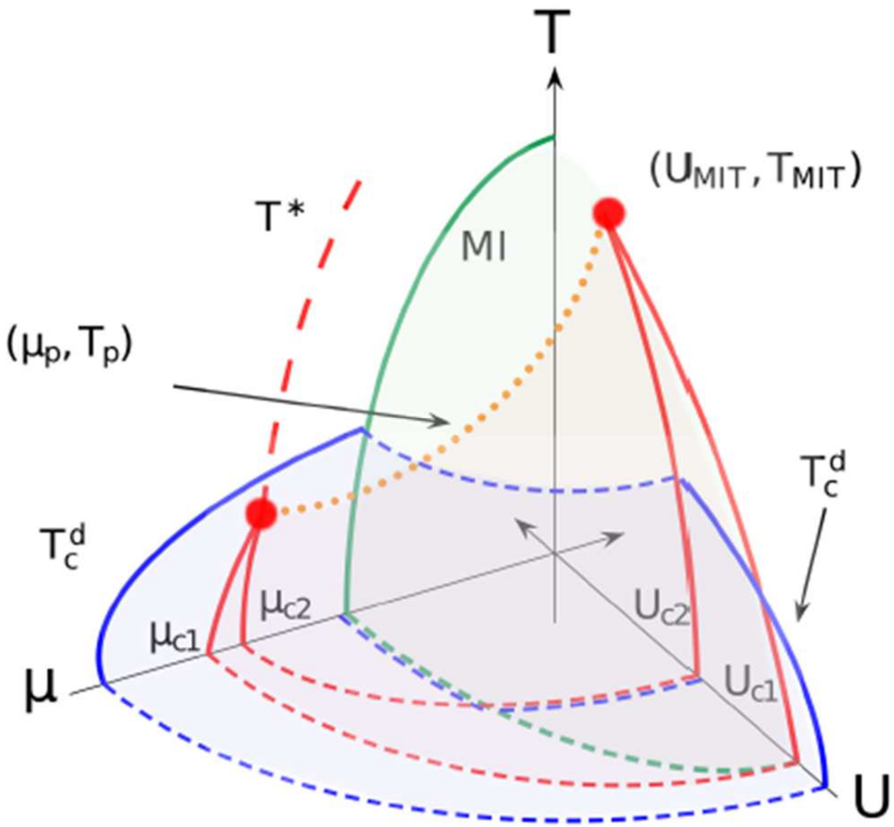
Finite *T* phase diagram

Superconductivity

Sordi et al. PRL **108**, 216401 (2012)

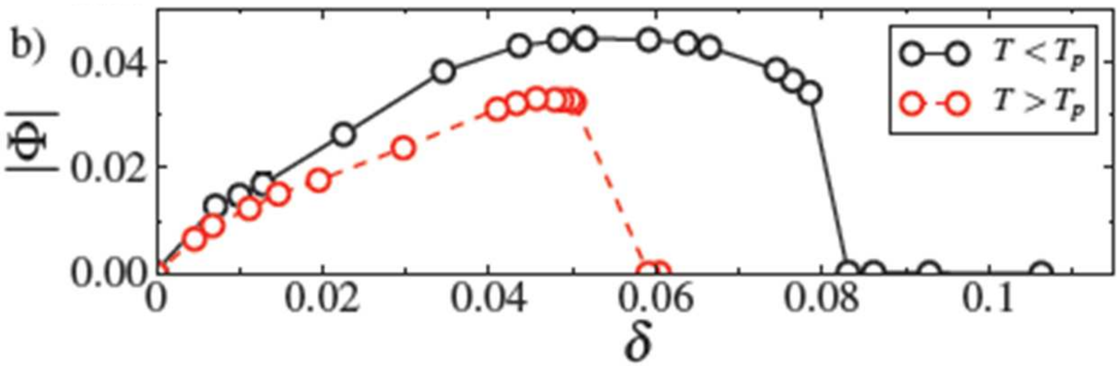
UNIVERSITÉ DE SHERBROOKE

Unified phase diagram



UNIVERSITÉ DE SHERBROOKE

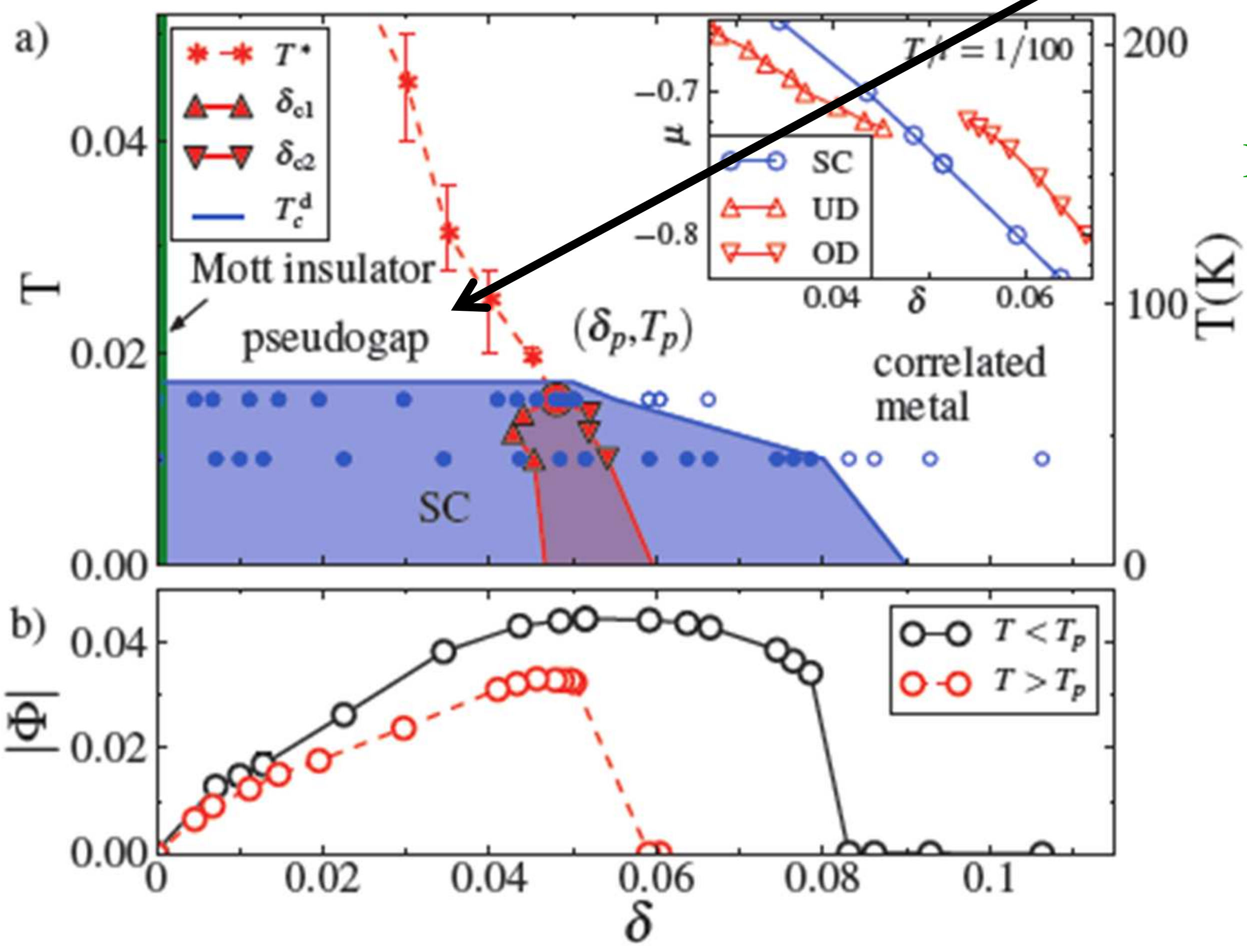
Cuprates (doping driven transition)



UNIVERSITÉ DE SHERBROOKE

Cuprates (doping driven transition)

Pseudogap vs pair



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

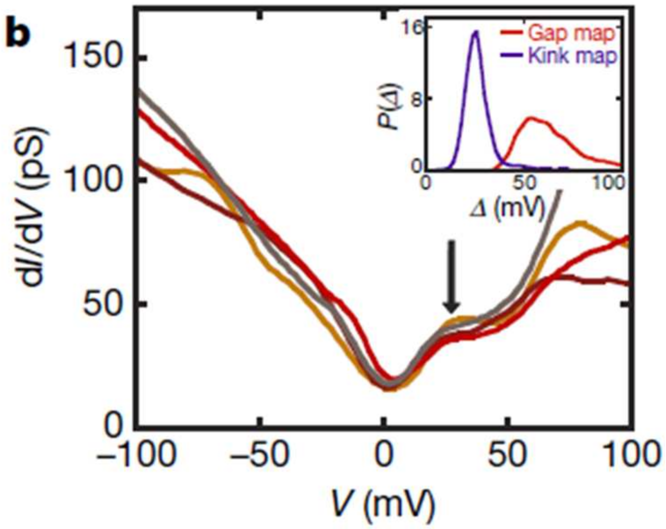
UNIVERSITÉ DE SHERBROOKE

Larger clusters

- Is there a minimal size cluster where T_c vanishes before half-filling?
- Learn something from small clusters as well
- Local pairs in underdoped

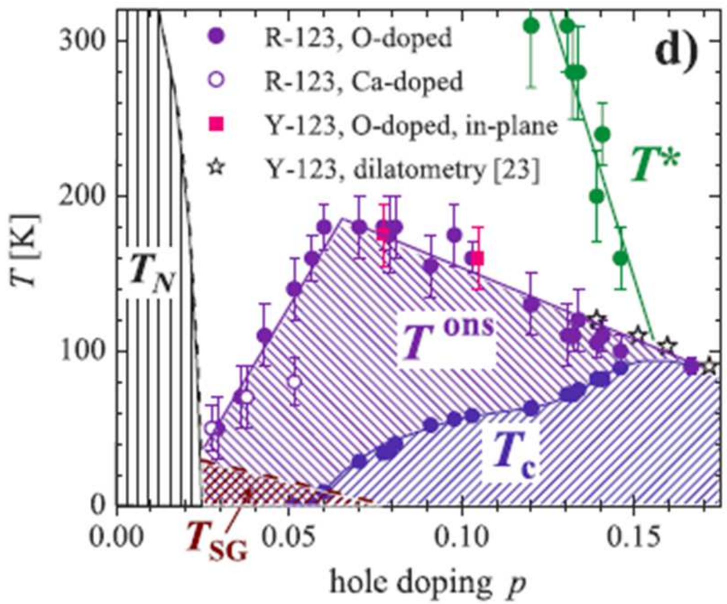
Meaning of T_c^d

- Local pair formation



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

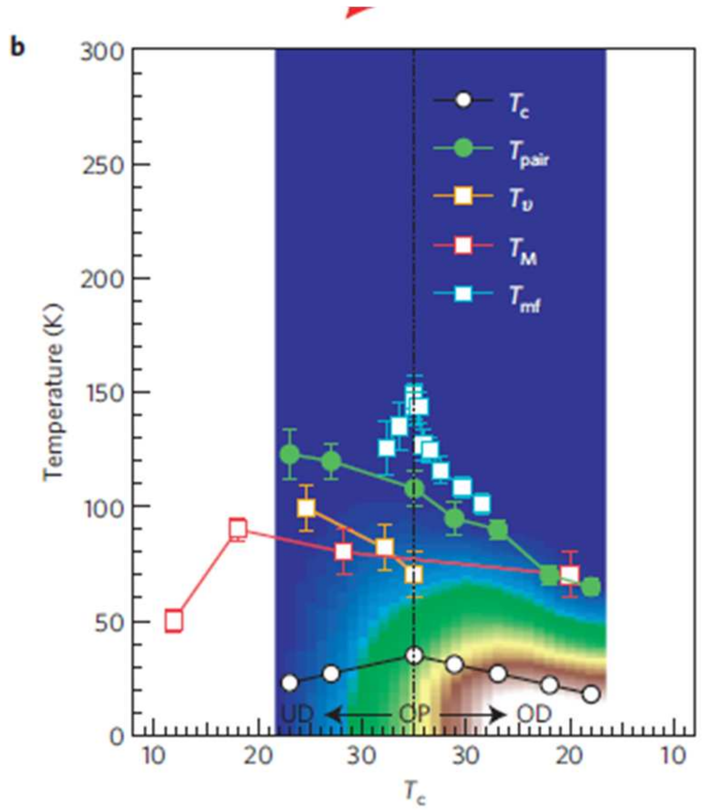
Fluctuating region



Infrared response

Dubroka et al. 106, 047006 (2011)

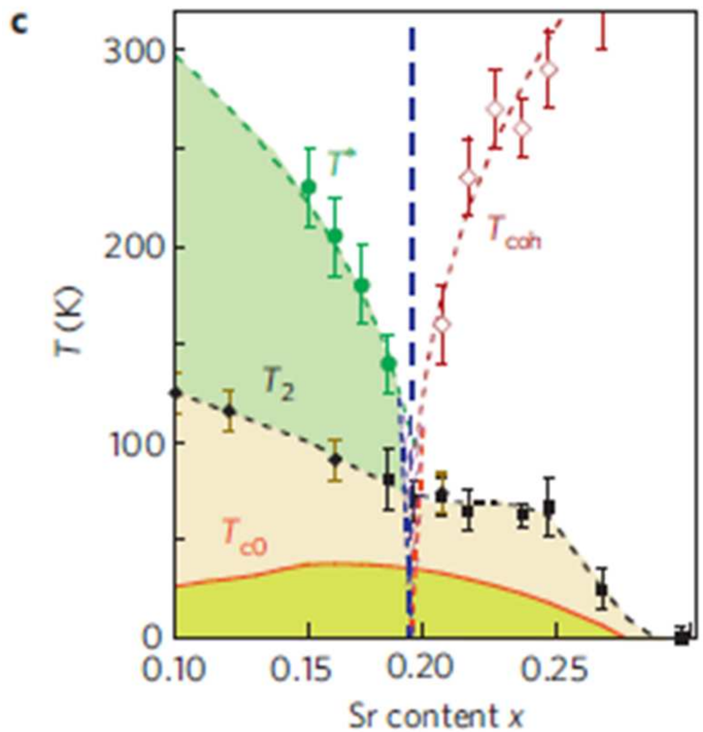
Tpair



ARPES
Bi2212

Kondo, Takeshi, et al. Kaminski Nature Physics **2011**, *7*, 21-25

T_2



Magnetoresistance, LSCO
Fluctuating vortices

Patrick M. Rourke, et al. Hussey Nature Physics 7, 455–458 (2011)

Giant proximity effect

$T_c = 32\ K$
$T_c < 5K$

Morenzoni et al.,
Nature Comms. **2** (2011)

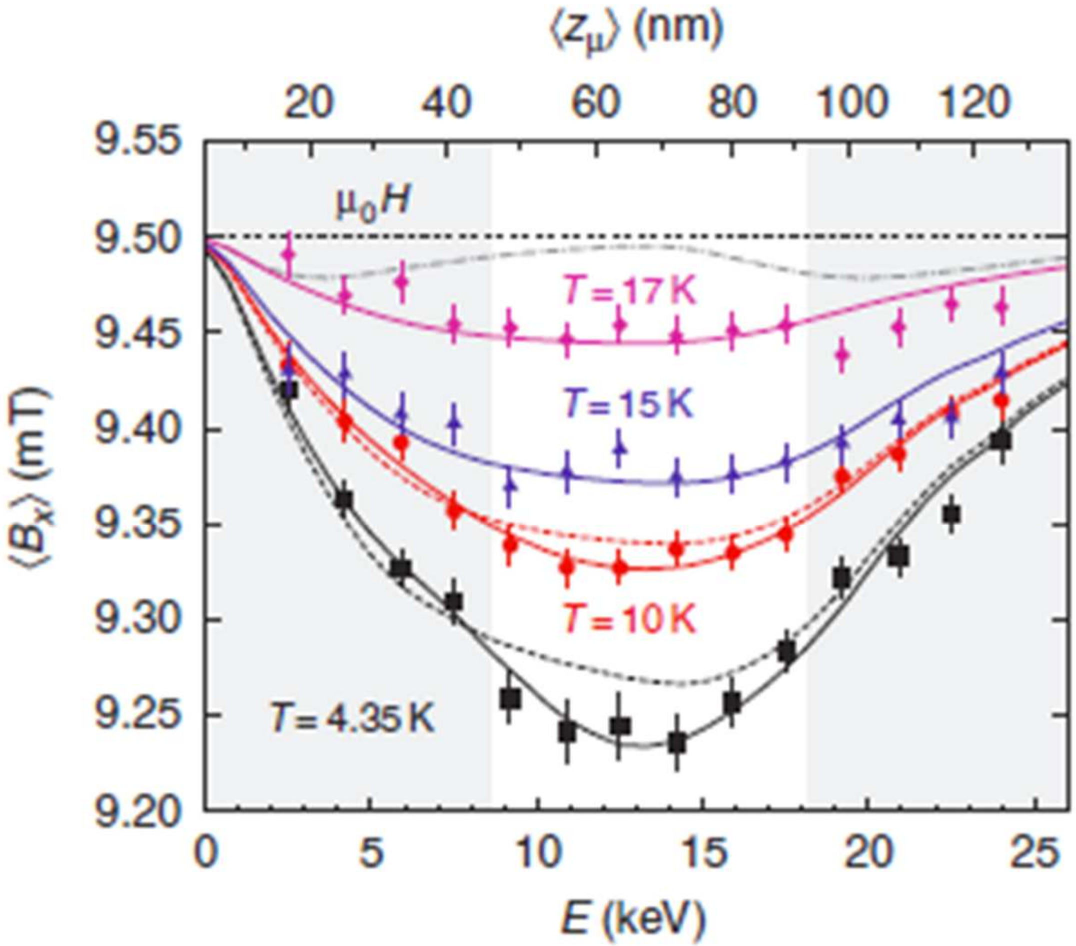
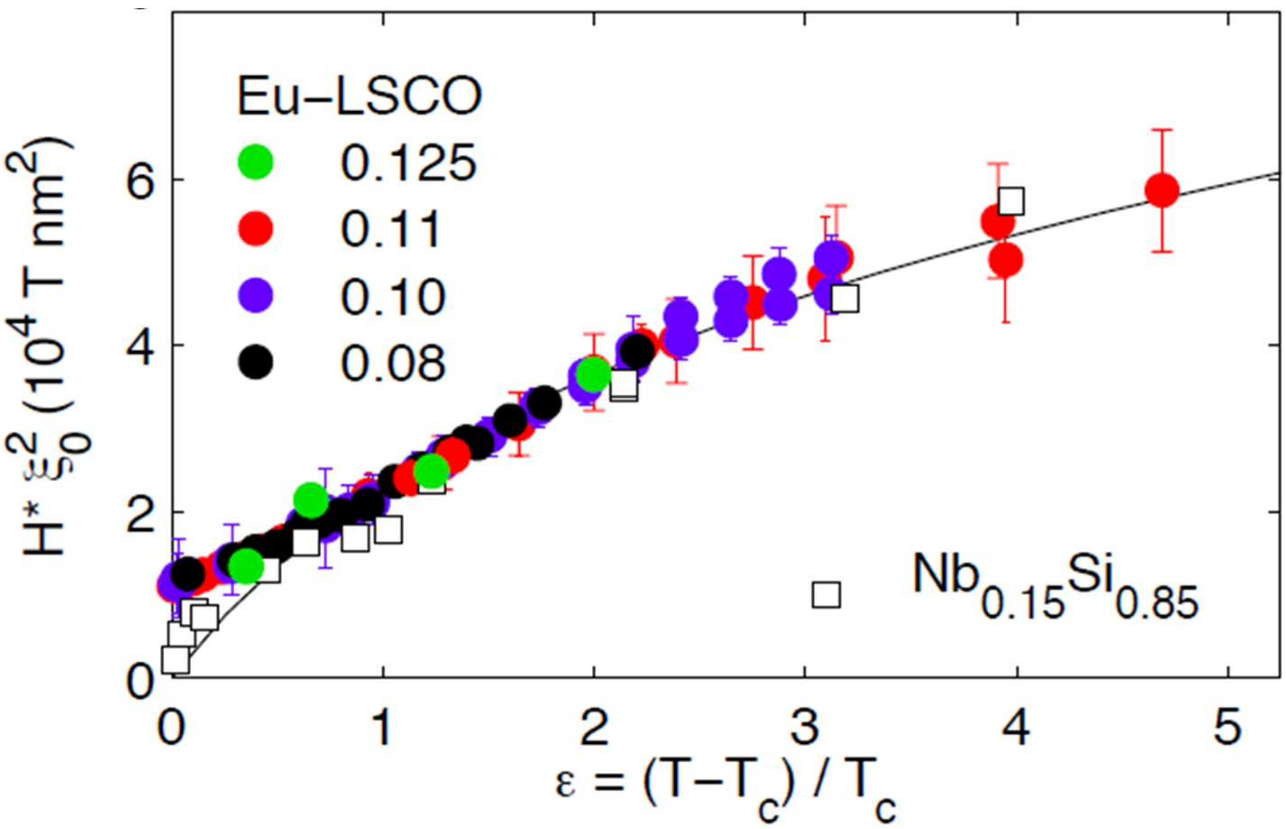


Figure 6 | Depth profile of the local field at different temperatures. The

Actual T_c in underdoped

- Quantum and classical phase fluctuations
  - V. J. Emery and S. A. Kivelson, Phys. Rev. Lett. **74**, 3253 (1995).
  - V. J. Emery and S. A. Kivelson, Nature **374**, 474 (1995).
  - D. Podolsky, S. Raghu, and A. Vishwanath, Phys. Rev. Lett. **99**, 117004 (2007).
  - Z. Tesanovic, Nat Phys **4**, 408 (2008).
- Magnitude fluctuations
  - I. Ussishkin, S. L. Sondhi, and D. A. Huse, Phys. Rev. Lett. **89**, 287001 (2002).
- Competing order
  - E. Fradkin, S. A. Kivelson, M. J. Lawler, J. P. Eisenstein, and A. P. Mackenzie, Annual Review of Condensed Matter Physics **1**, 153 (2010).
- Disorder
  - F. Rullier-Albenque, H. Alloul, F. Balakirev, and C. Proust, EPL (Europhysics Letters) **81**, 37008 (2008).
  - H. Alloul, J. Bobro, M. Gabay, and P. J. Hirschfeld, Rev. Mod. Phys. **81**, 45 (2009).

Gaussian amplitude fluctuations in Eu-LSCO



Chang, Doiron-Leyraud et al.

Phase fluctuations and disorder?

Monolayer LSCO, field doped

A. T. Bollinger et al. & I. Božović, Nature **472**, 458–460

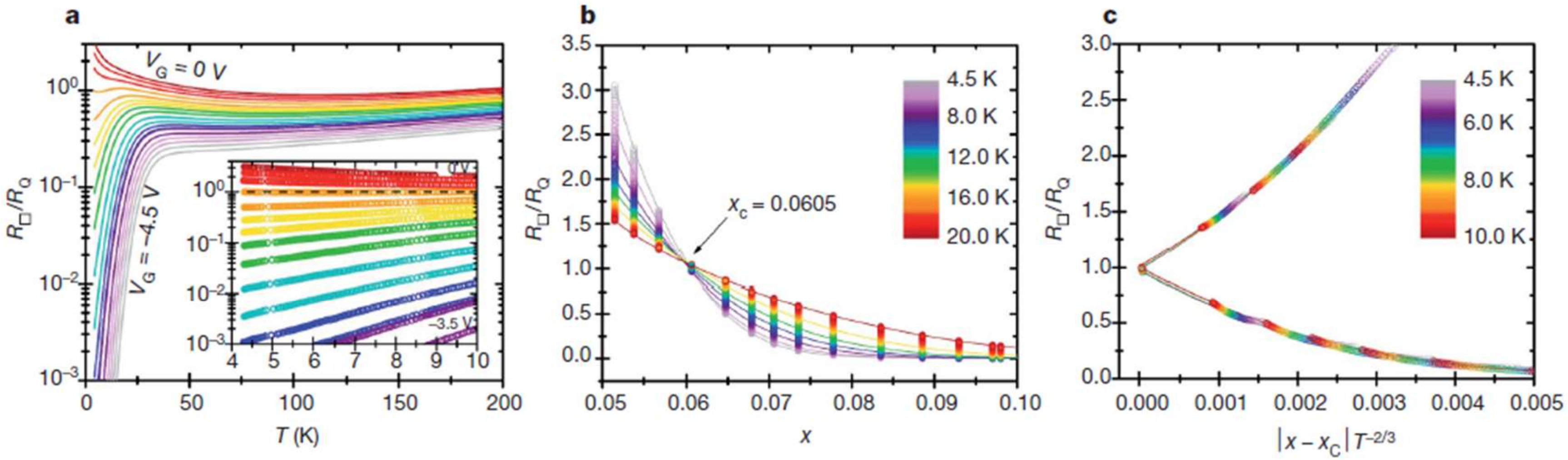
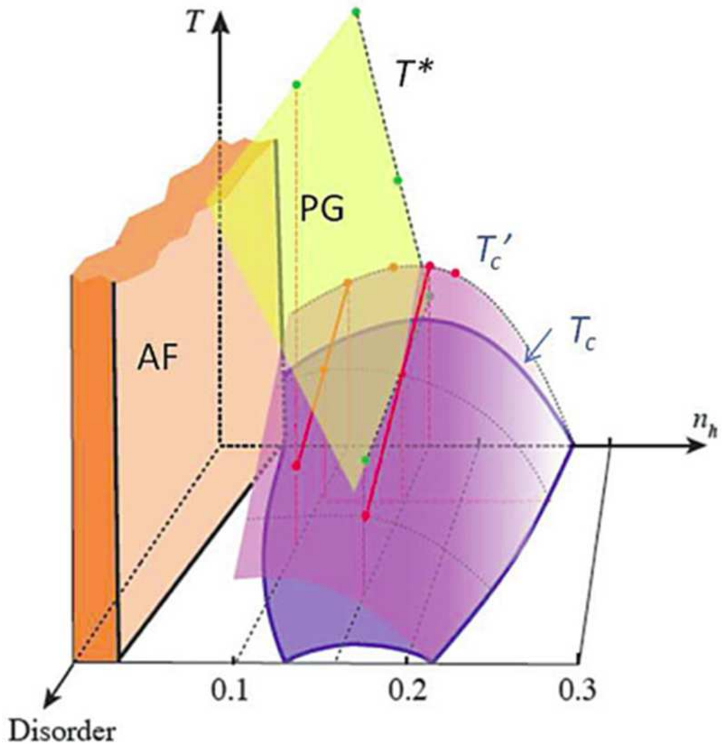


Figure 2 | Superconductor–insulator transition driven by electric field. **a**, Temperature dependence of normalized resistance $r = R_\square(x,T)/R_Q$ of an initially heavily underdoped and insulating film (see Supplementary Fig. 12 for linear scale). The device (Supplementary section B) employs a coplanar Au gate and DEME-TFSI ionic liquid. The carrier density, fixed for each curve, is tuned by varying the gate voltage from 0 V to −4.5 V in 0.25 V steps; an insulating film becomes superconducting via a QPT. The inset highlights a separatrix independent of temperature below 10 K. The open circles are the actual raw data points; the black dashed line is $R_\square(x_c,T) = R_Q = 6.45$ kΩ. **b**, The inverse representation of the same data, that is, the $r_T(x)$ dependence at fixed temperatures below 20 K. Each vertical array of (about 100) data points corresponds to one fixed carrier density, that is, to one $r_x(T)$ curve in Fig. 2a. The colours refer to the temperature, and the continuous lines are interpolated for selected temperatures (4.5, 6.0, 8.0, 10.0, 12.0, 15.0 and 20.0 K). The crossing point defines the critical carrier concentration $x_c = 0.06 \pm 0.01$, and the critical resistance $R_c = 6.45 \pm 0.10$ kΩ. **c**, Scaling of the same data with respect to a single variable $u = |x - x_c|T^{-1/z\nu}$, with $z\nu = 1.5$. This figure is derived by folding panel **b** at x_c and scaling the abscissa of each $r_T(|x - x_c|)$ curve by $T^{-2/3}$. For 4.3 K < T < 10 K, the discrete groups of points of Fig. 2b collapse accurately onto a two-valued function, with one branch corresponding to x larger and the other to x smaller than x_c. The critical exponents are identical on both sides of the superconductor–insulator transition. The raw data points cover the interpolation lines almost completely, except close to the origin.

E

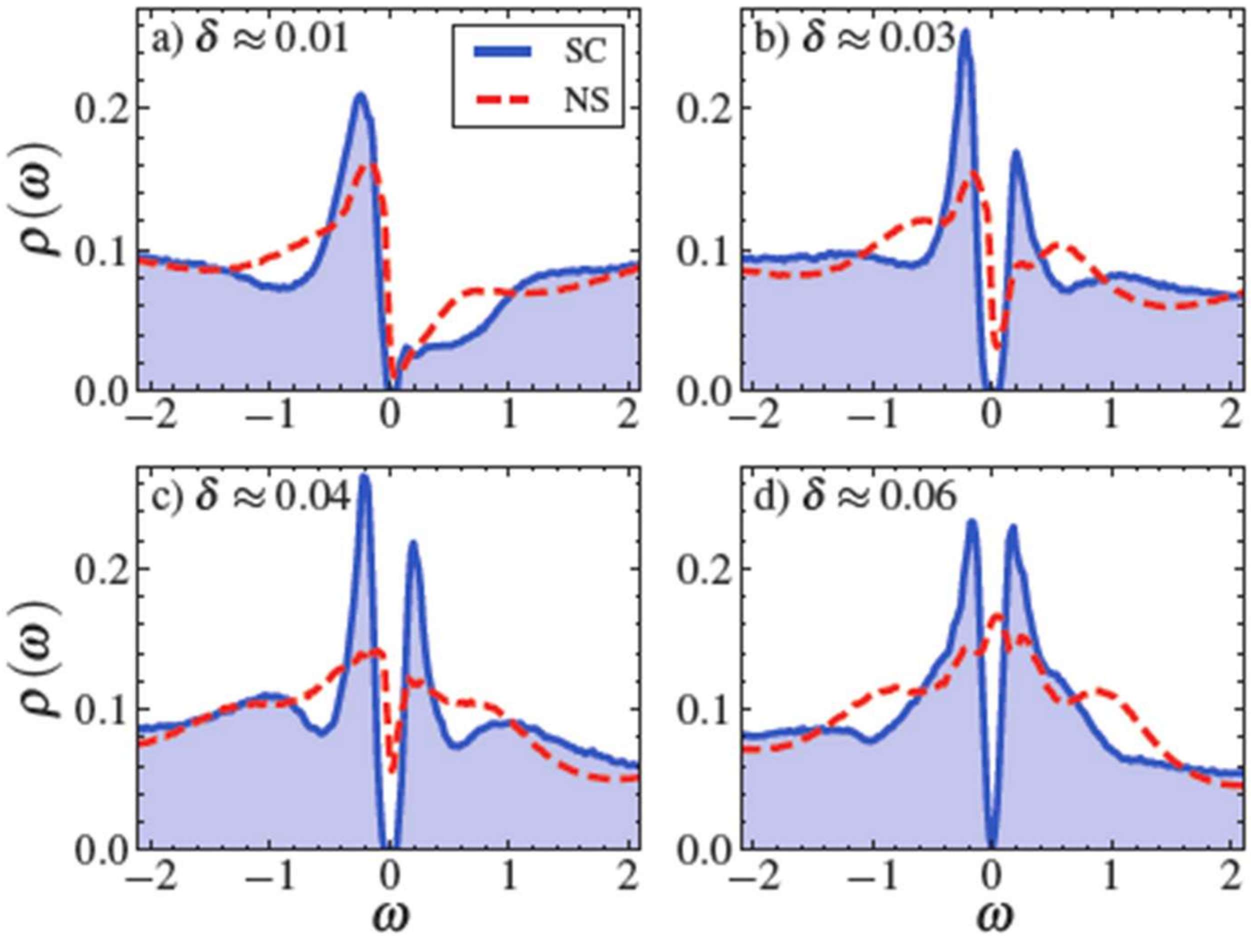
Effect of disorder



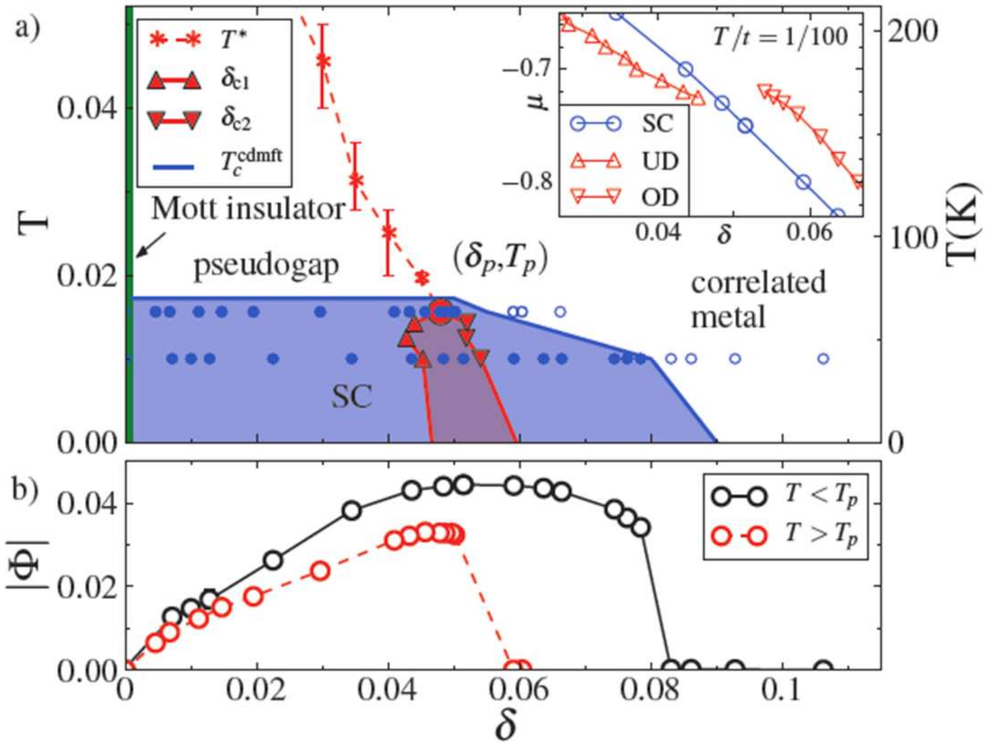
F. Rullier-Albenque, H. Alloul, and G.Rikken,
Phys. Rev. B **84**, 014522 (2011).

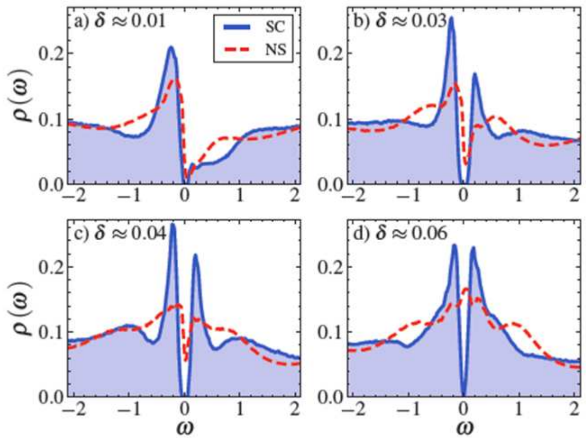
Superconductivity in underdoped vs BCS

First-order transition leaves its mark

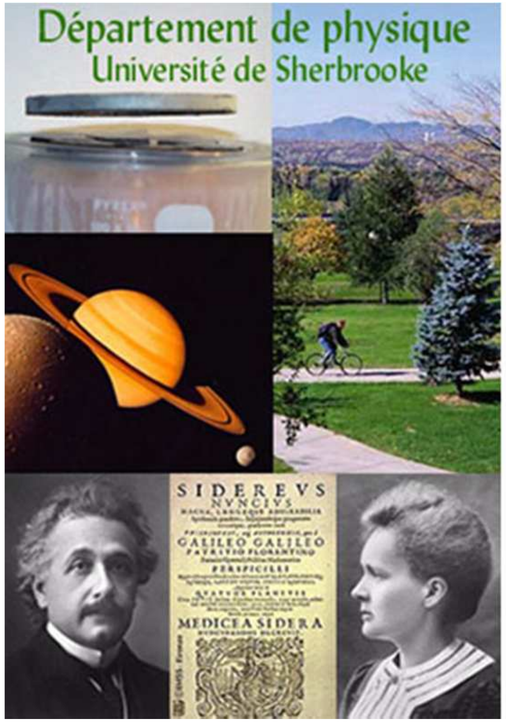


Summary





- Below the dome finite T critical point (not QCP) controls normal state
- First-order transition destroyed but traces in the dynamics
- Pseudogap different from pairing.
- Actual T_c in underdoped
  - Competing order
  - Long wavelength fluctuations (see O.P.)
  - Disorder



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

Merci

Thank you