Strongly correlated superconductivity: cuprates and organics

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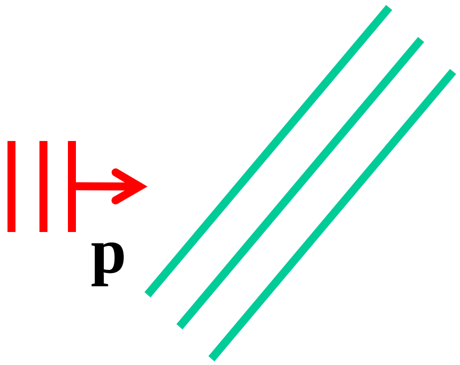
VERITATEM IN CHARITATE

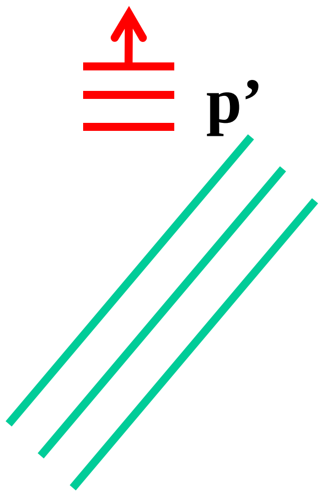
Advances in strongly correlated electronic systems
Minneapolis - 13 June 2016

Superconductivity

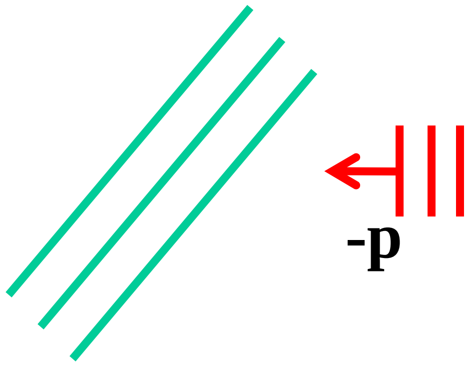
Attraction mechanism in the metallic state



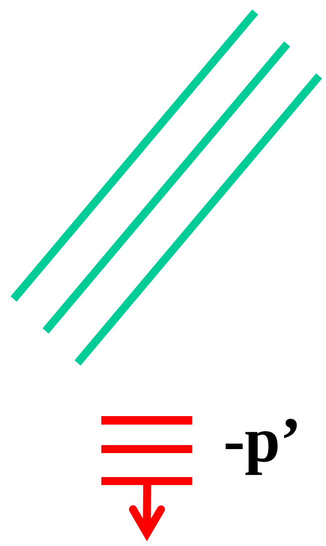
Attraction mechanism in the metallic state



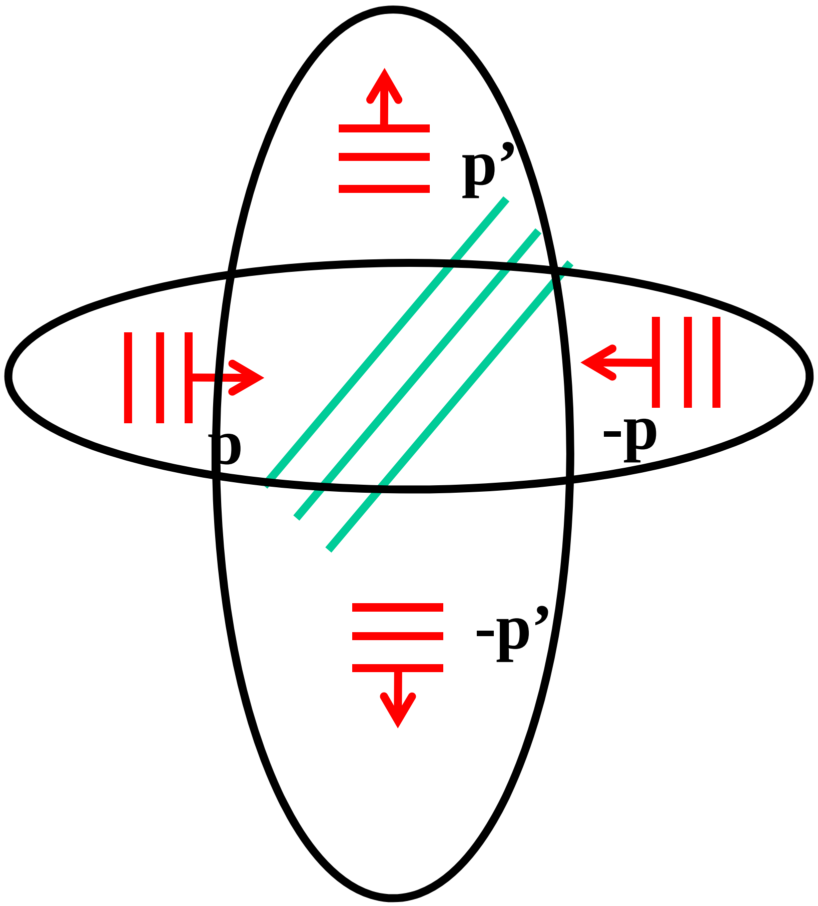
Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



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#1 Cooper pair, #2 Phase coherence

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

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

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

Half-filled band is metallic?

Half-filled band: Not always a metal

NiO, Boer and Verway

Peierls, 1937

Mott, 1949

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« Conventional » Mott transition

T

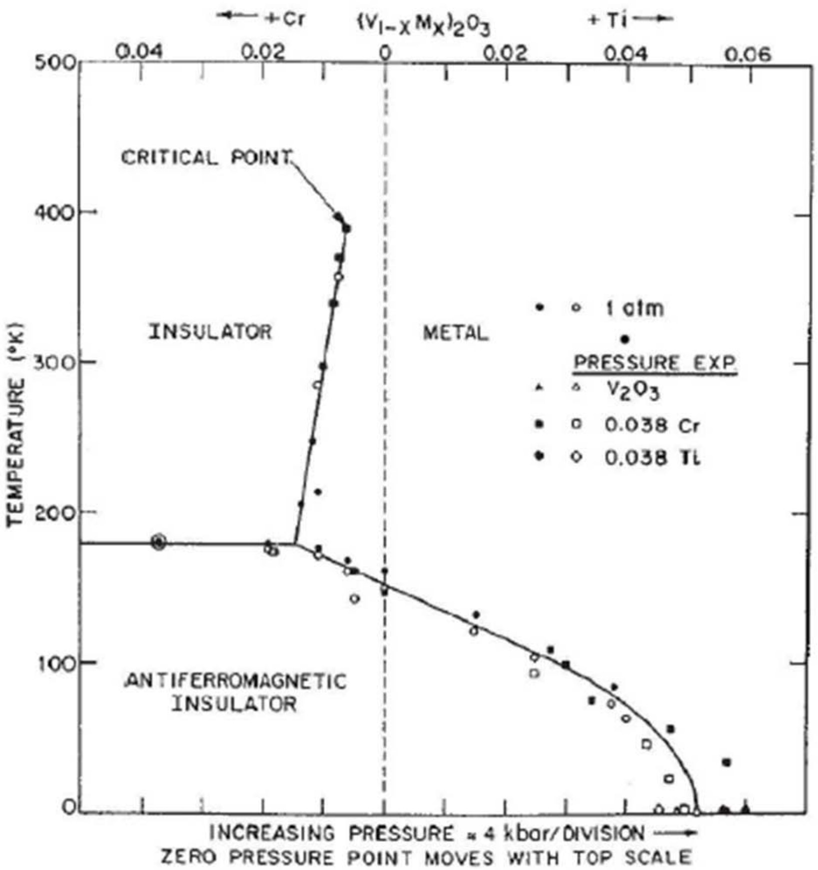

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Figure: McWhan, PRB 1970; Limelette, Science 2003

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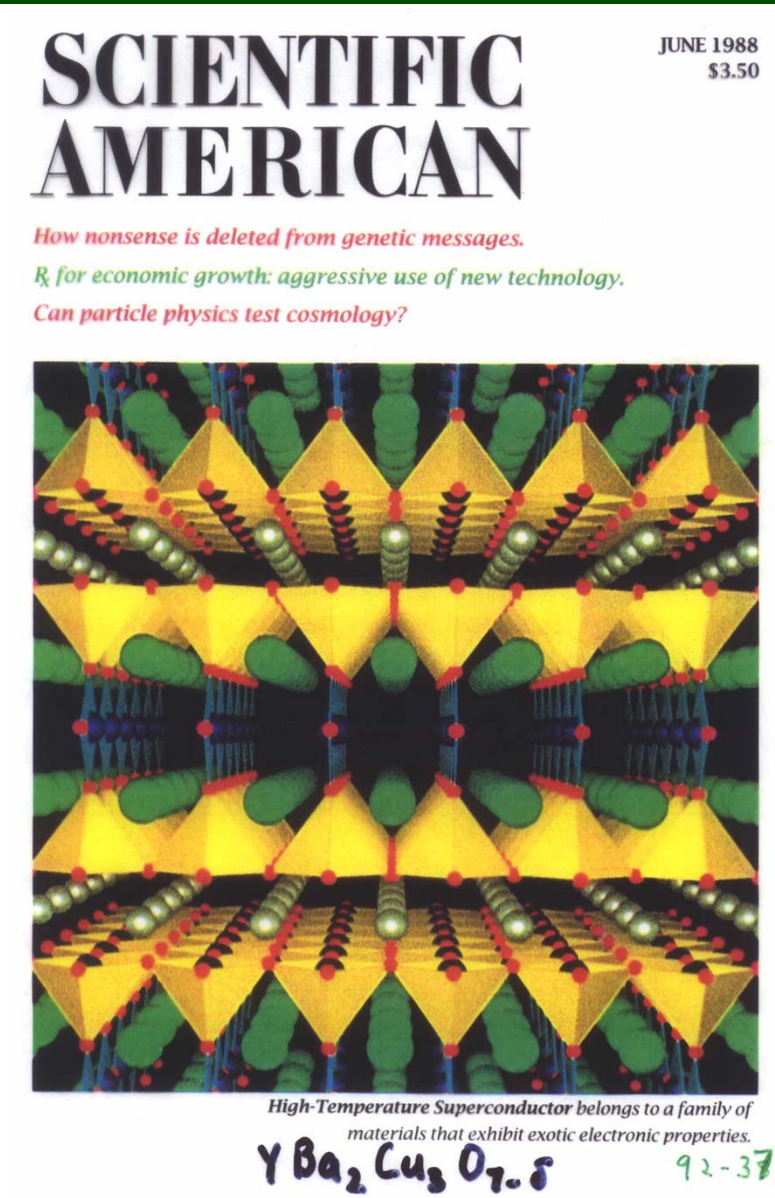
Two pillars of Condensed Matter Physics

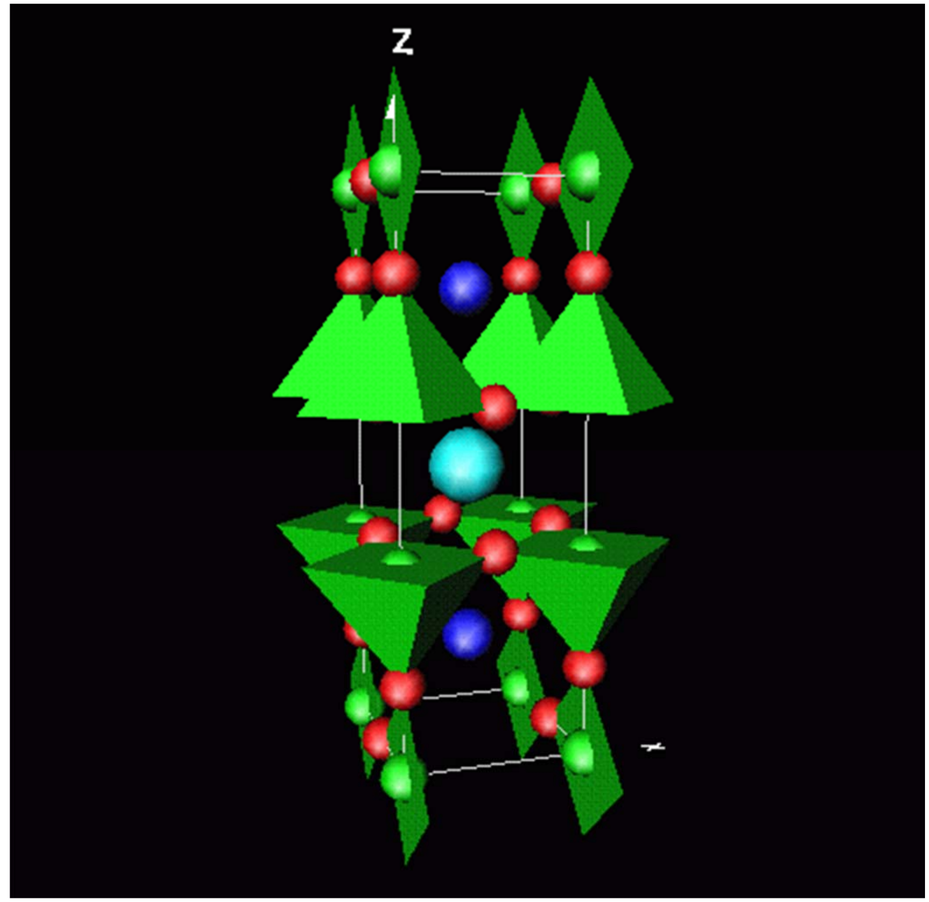
- Band theory
  - DFT
  - Fermi liquid Theory
    - Metals
    - Semiconductors: transistor
- BCS theory of superconductivity
  - Broken symmetry
  - Emergent phenomenon
    - Also in particle physics, astrophysics…

« Phase » and emergent properties

- Emergent properties
  - e.g. Fermi surface
    - Shiny
    - Quantum oscillations (in B field)
- Many microscopic models will do the same
  - Electrons in box or atoms in solid, Fermi surface
  - Concept of Fermi liquid
  - Often hard to « derive » from first principles (fractionalization - gauge theories)

Atomic structure





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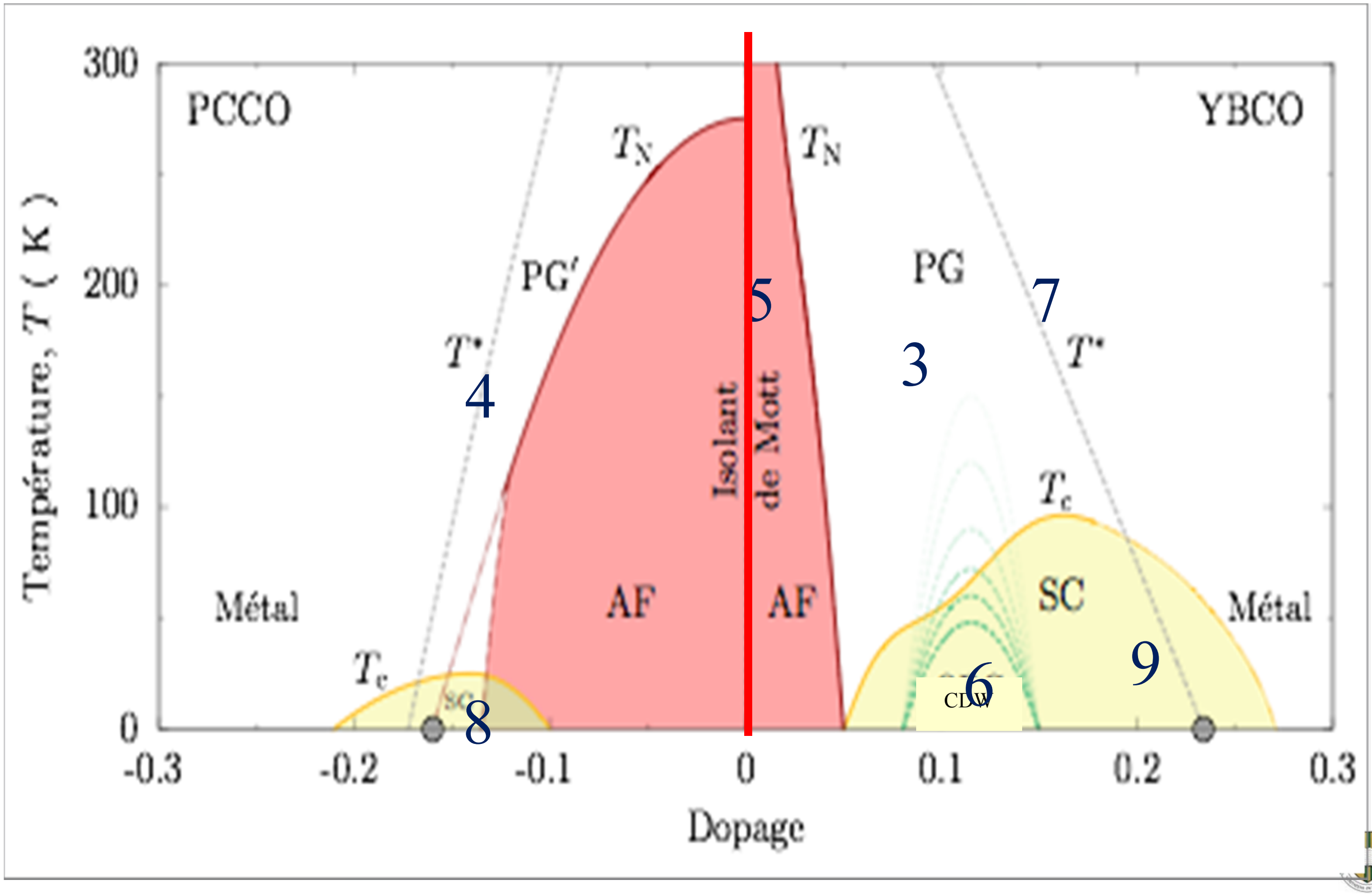
Breakdown

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



2. The model

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

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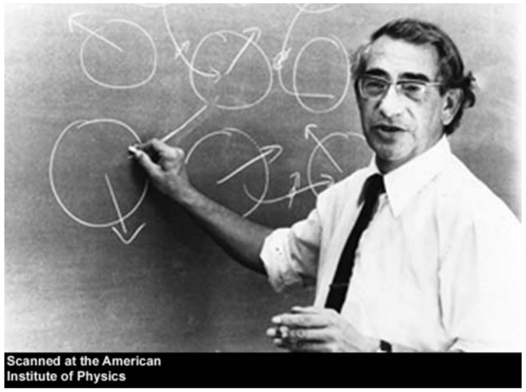
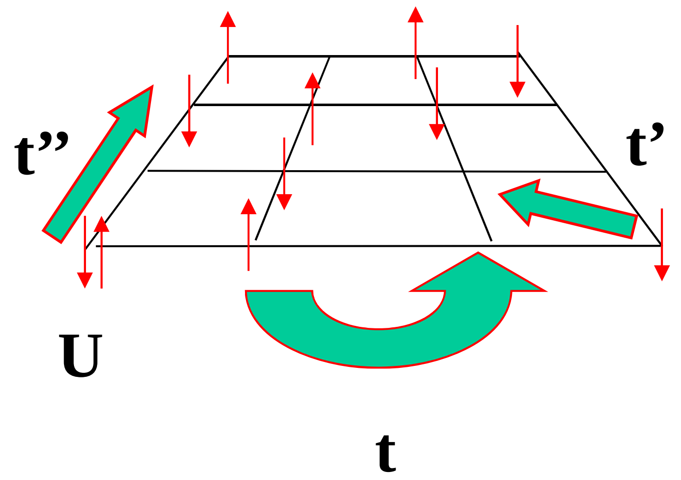
Hubbard model



1931-1980

μ



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

Attn: Charge transfer insulator

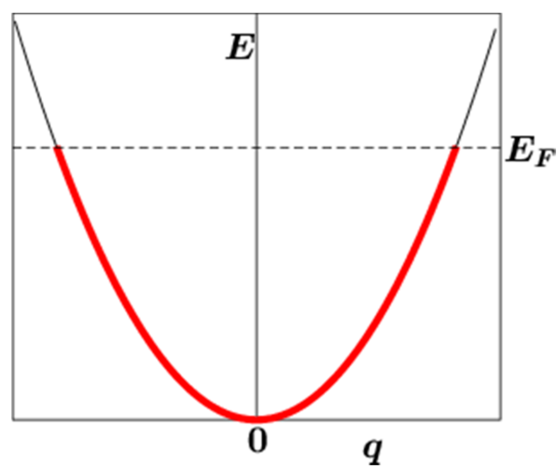
$U = 0$

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

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

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

$$|\Psi\rangle = \prod_{\mathbf{k},\sigma} c_{\mathbf{k}\sigma}^{\dagger} |0\rangle$$



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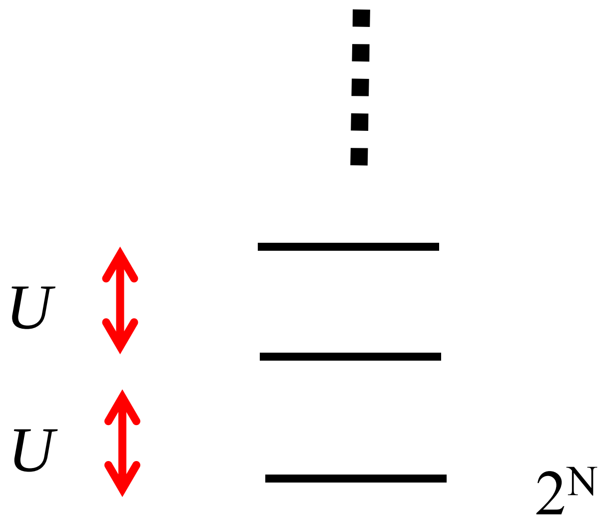
$t_{ij} = 0$

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

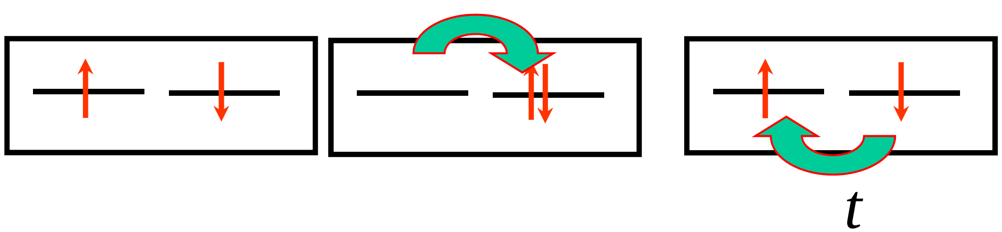


$$|\Psi\rangle = \prod_{\mathbf{i}} c^\dagger_{\mathbf{i}\uparrow} \prod_{\mathbf{j}} c^\dagger_{\mathbf{j}\downarrow} |0\rangle$$

Interesting in the general case

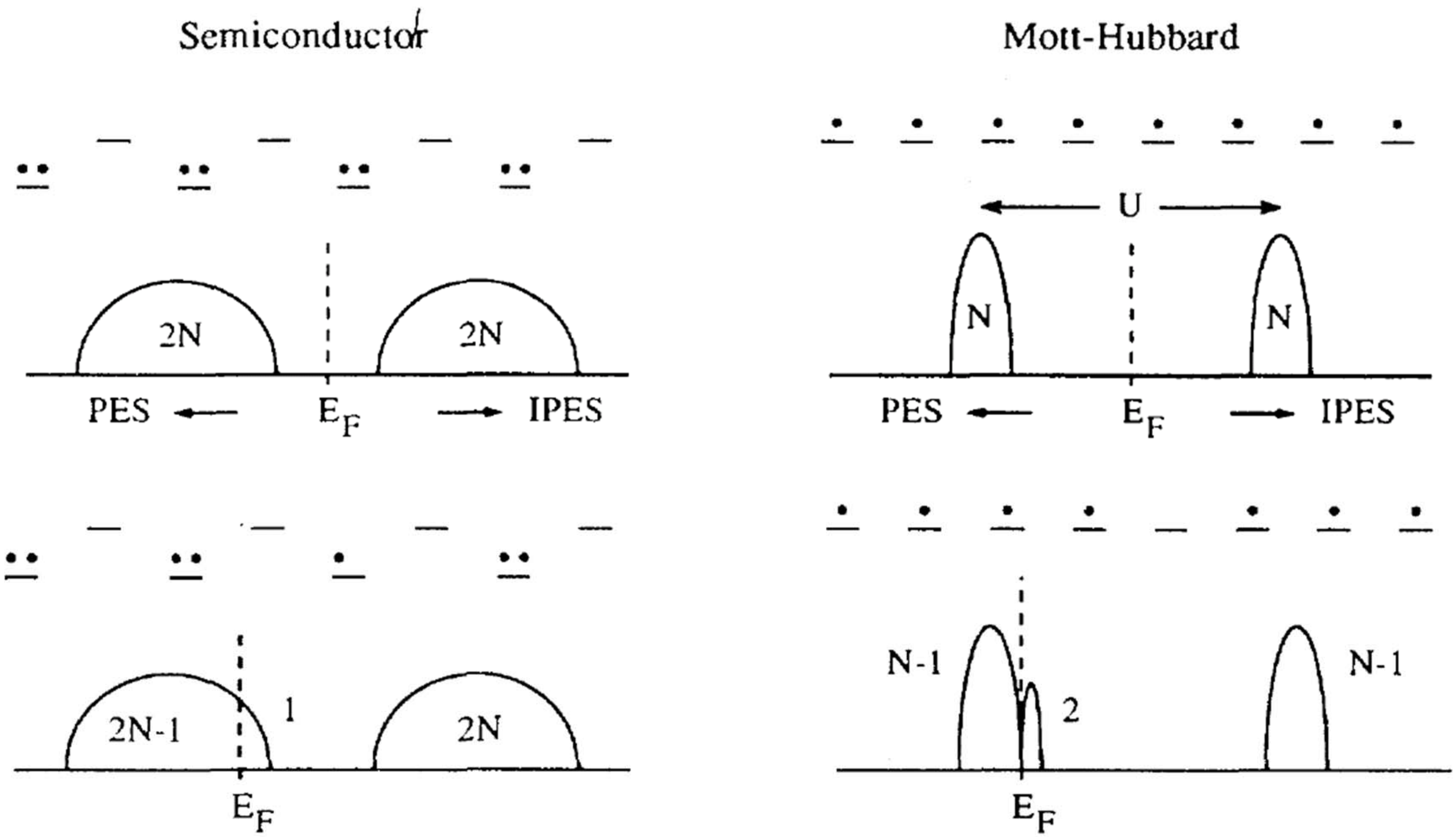
$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}\right) + U\sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Mott transition



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

Spectral weight transfer



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

Outline

1. Introduction
2. The model
3. Weakly and strongly correlated antiferromagnets
    1. Qualitative
    2. Contrasting methods for weak and strong coupling

Outline

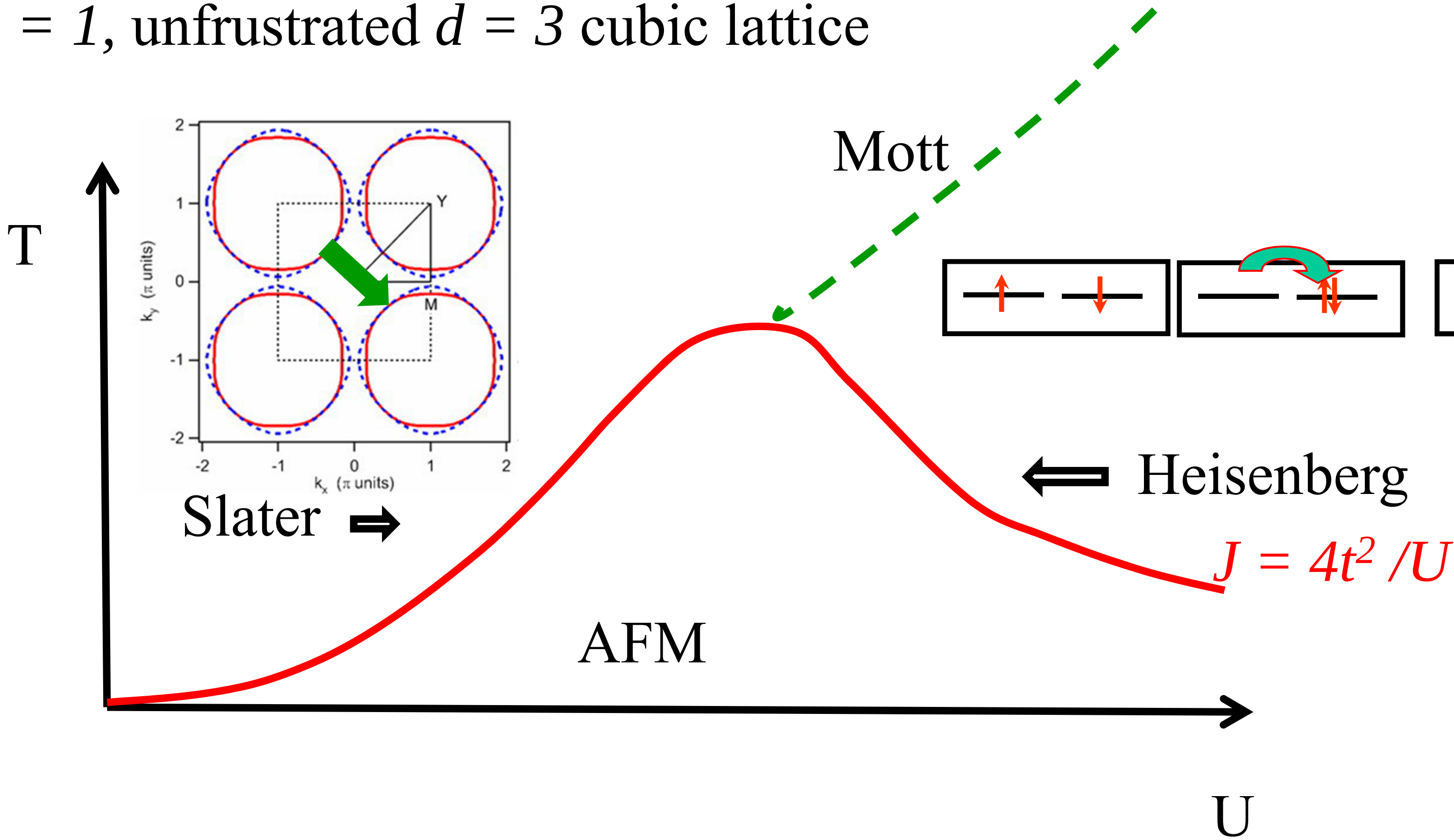
4. Weakly and strongly correlated superconductivity
    1. Qualitative
    2. Contrasting methods
5. High Tc the view from DMFT
    1. Quantum clusters
    2. Normal state and pseudogap
    3. SC state
6. Organics
7. Methods, 2 of them: C-DMFT and TPSC
8. Conclusion

3. Strong vs weak correlations for an antiferromagnet

3.1 Qualitative

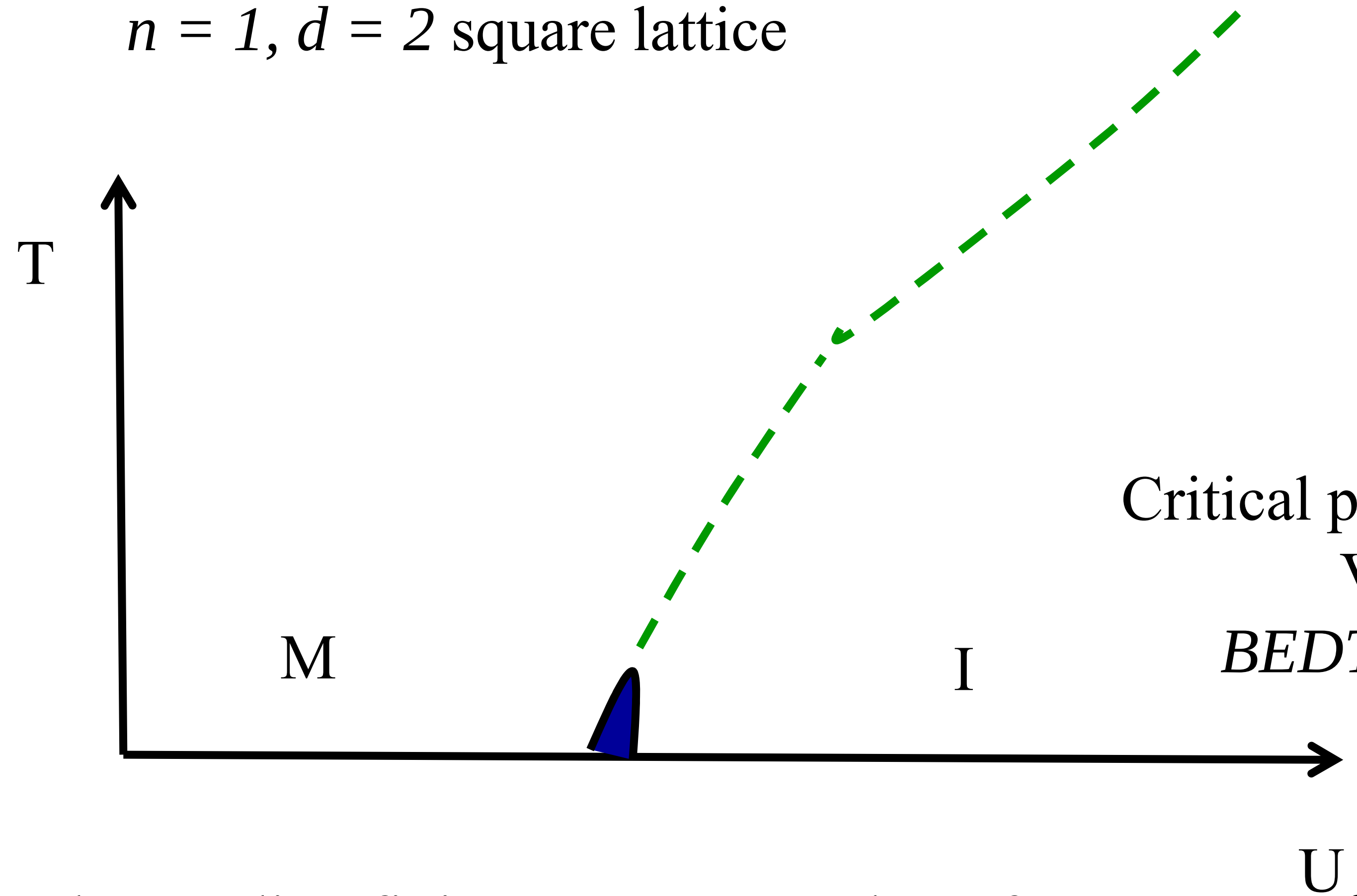
Weak vs Strong correlations

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



Local moment and Mott transition

n = 1, d = 2 square lattice



Critical point visible in V_2O_3, *BEDT* organics

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

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Antiferromagnetic phase: emergent properties

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

Differences between weakly and strongly correlated

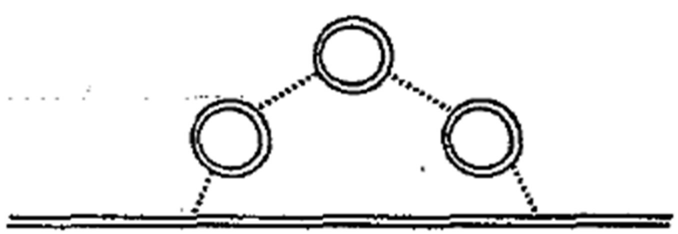
- Different in ordered phase (finite frequency)
  - Ordered moment
  - Landau damping
    - Spin waves all the way or not to J
- Different, even more, in the normal state:
  - metallic in $d = 3$ if weakly correlated
  - Insulating if strongly correlated
  - Pressure dependence of T_N

Strong vs weak correlations

Contrasting methods

Ordered state

- Mean-field (Hartree-Fock) for AFM



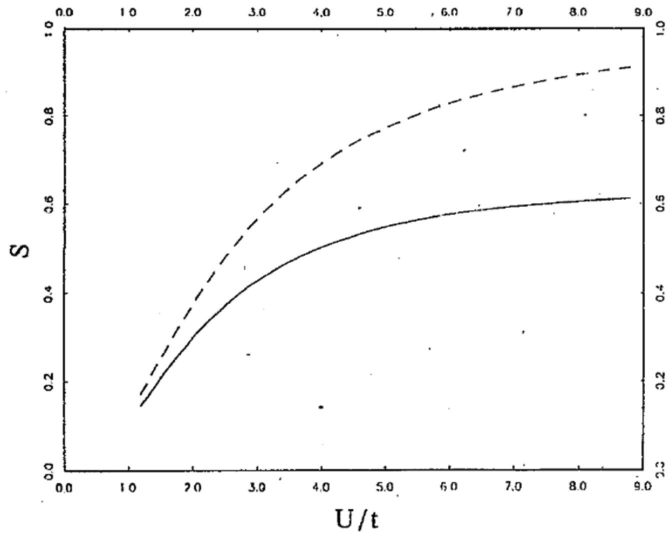


FIG. 7. The solid line represents the sublattice magnetization including the fluctuation effects. The dashed line is the mean-field result.

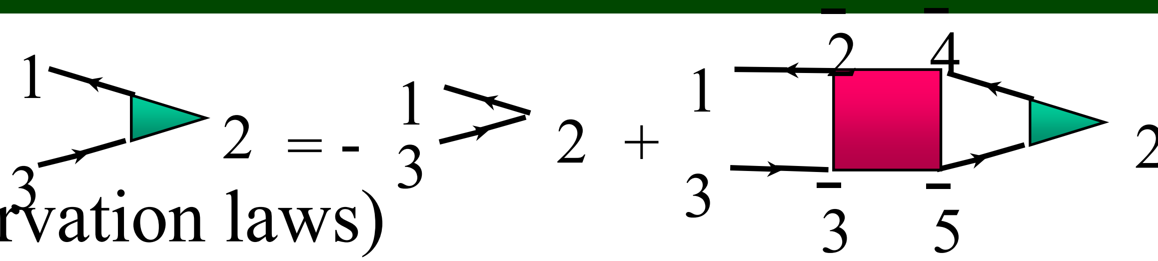
Schrieffer, Wen, Zhang, PRB 1989

More methods for ordered states, n=1

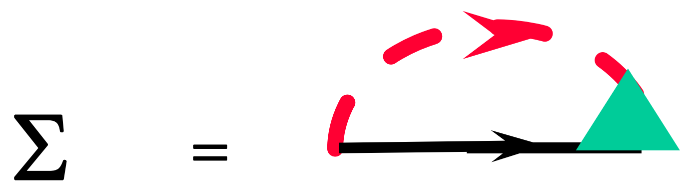
  - Numerically, stochastic series expansion,
  - High-temperature series expansion,
  - Quantum Monte Carlo
  - World-line
  - Worm algorithms
  - Variational methods
- Ground state of S=1/2 in *d=2* is AFM, not spin liquid

In paramagnetic state

Theory difficult even at weak to intermediate correlation!



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



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

Two-Particle Self-Consistent (idea)

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

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

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Doped Mott insulator : strong correlations

Normal state

Emergence and slave particle approaches

$$H = \sum_{\langle ij \rangle} J\left(\boldsymbol{S}_i \cdot \boldsymbol{S}_j - \frac{1}{4} n_i n_j \right) - \sum_{ij,\sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + \mathrm{H.c.})$$

$$\sum_\sigma c_{i\sigma}^\dagger c_{i\sigma} \leqslant 1$$

$$c_{i\sigma}^\dagger = f_{i\sigma}^\dagger b_i \qquad f_{i\uparrow}^\dagger f_{i\uparrow} + f_{i\downarrow}^\dagger f_{i\downarrow} + b_i^\dagger b_i = 1$$

$$\boldsymbol{S}_i \cdot \boldsymbol{S}_j = -\frac{1}{4} f_{i\alpha}^\dagger f_{j\alpha} f_{j\beta}^\dagger f_{i\beta} - \frac{1}{4} (f_{i\uparrow}^\dagger f_{j\downarrow}^\dagger - f_{i\downarrow}^\dagger f_{j\uparrow}^\dagger)(f_{j\downarrow} f_{i\uparrow} - f_{j\uparrow} f_{i\downarrow}) + \frac{1}{4} (f_{i\alpha}^\dagger f_{i\alpha}). \qquad (35)$$

$$n_i n_j = (1 - b_i^\dagger b_i)(1 - b_j^\dagger b_j)$$

P.A. Lee, N. Nagaosa, and X.-G. Wen, Rev. Mod. Phys. 78, 17 (2006)

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Lagrangian after HS transformation

$$Z = \int DfDf^{\dagger}DbDb^{*}D\lambda D\chi D\Delta \exp\left(-\int_0^{\beta} d\tau L_1\right)$$

$$\begin{aligned} L_1 = {} & \tilde{J}\sum_{\langle ij\rangle} (|\chi_{ij}|^2 + |\Delta_{ij}|^2) + \sum_{i\sigma} f_{i\sigma}^{\dagger}(\partial_\tau - i\lambda_i)f_{i\sigma} \\ & - \tilde{J}\left[\sum_{\langle ij\rangle} \chi_{ij}^{*}\left(\sum_{\sigma} f_{i\sigma}^{\dagger}f_{j\sigma}\right) + \text{c.c.}\right] \\ & + \tilde{J}\left[\sum_{\langle ij\rangle} \Delta_{ij}(f_{i\uparrow}^{\dagger}f_{j\downarrow}^{\dagger} - f_{i\downarrow}^{\dagger}f_{j\uparrow}^{\dagger}) + \text{c.c.}\right] \\ & + \sum_{i} b_i^{*}(\partial_\tau - i\lambda_i + \mu_B)b_i - \sum_{ij} t_{ij}b_i b_j^{*} f_{i\sigma}^{\dagger}f_{j\sigma} \end{aligned}$$

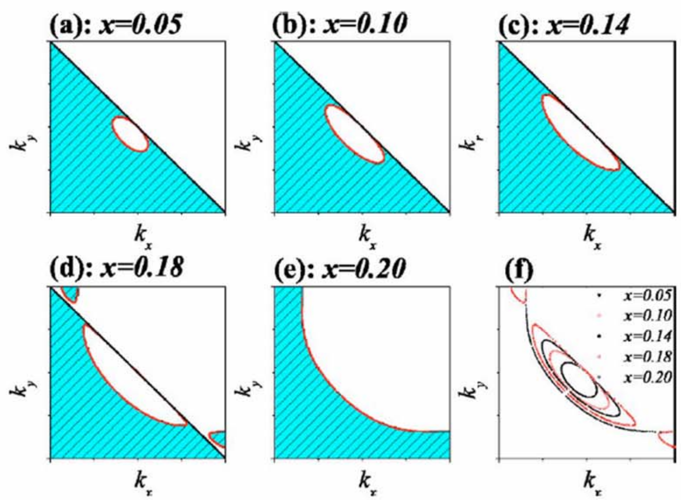
For strong correlations

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

YRZ

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

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



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

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

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

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

4. Weakly and strongly correlated superconductivity (cuprates, normal state)

Analog to weakly and strongly correlated antiferromagnets

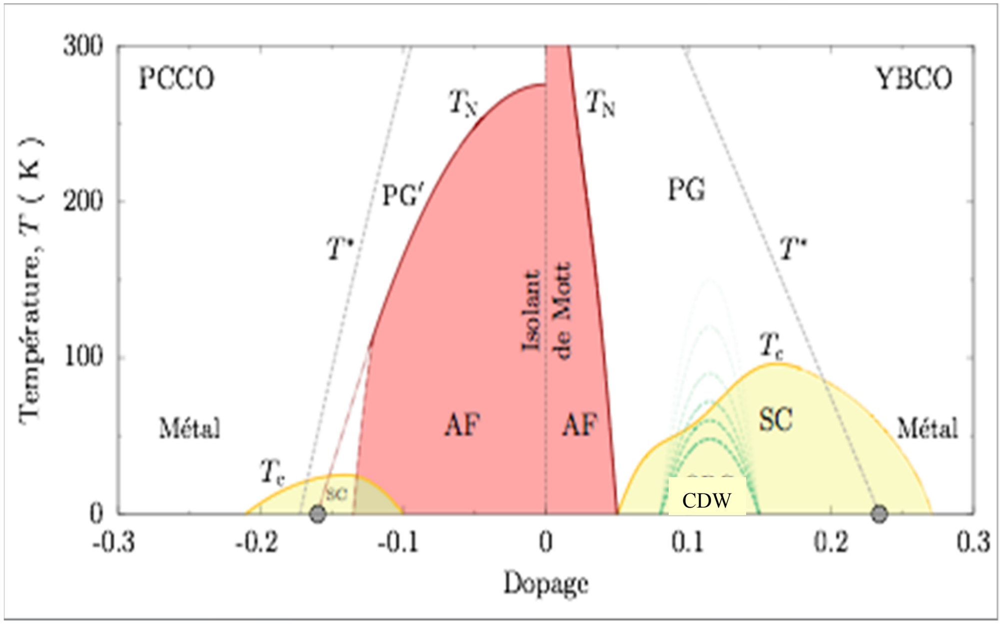
Superconducting phase: identical properties

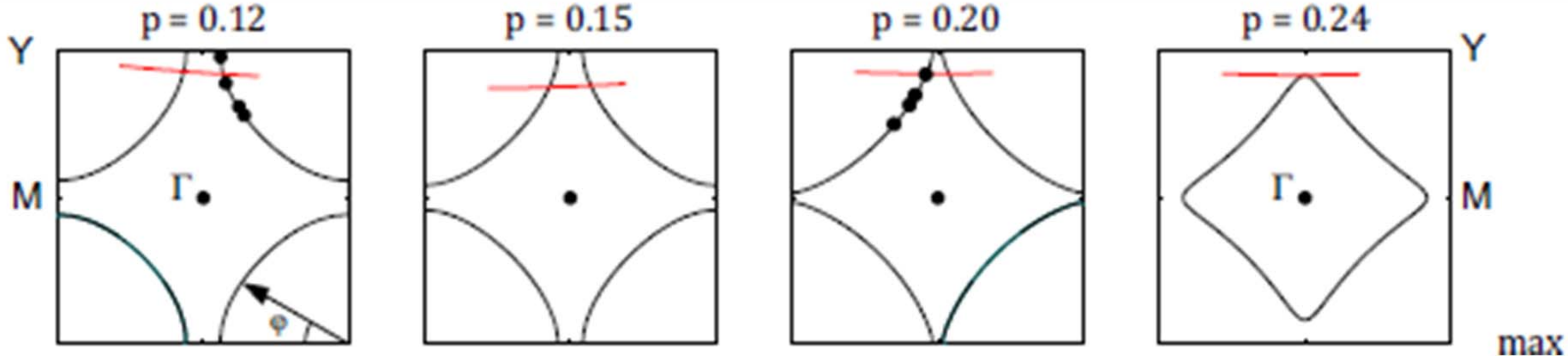
- Emergent:
  - Same broken symmetry *U(1)* for s-wave,
  - *U(1)* and C_{4v} for d-wave
  - Single-Particle gap, point or line node.
    - *T* dependence of C_p and κ at low *T*
  - Goldstone modes (+Higgs)

Superconductivity not universal even with phonons: weak or strong coupling

- In BCS universal ratios: e.g. $\Delta/k_B T_c$
  - Would never know the mechanism for sure if only BCS!
  - N.B. Strong coupling in a different sense

Phase diagram: hole and electron doping





Strongly correlated superconductors

- T_c does not scale like order parameter
- Superfluid stiffness scales like doping
- Superconductivity can be largest close to the metal-insulator transition
- Resilience to near-neighbor repulsion

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

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Mott-Ioffe-Regel limit

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

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

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

Mott-Ioffe-Regel limit

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

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

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

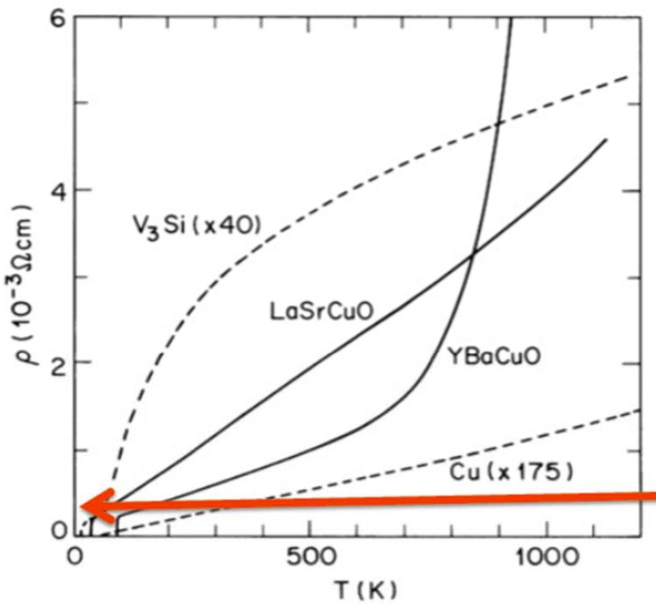
$$\ell = \left(\frac{\hbar k_F}{m}\right)\tau$$

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

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

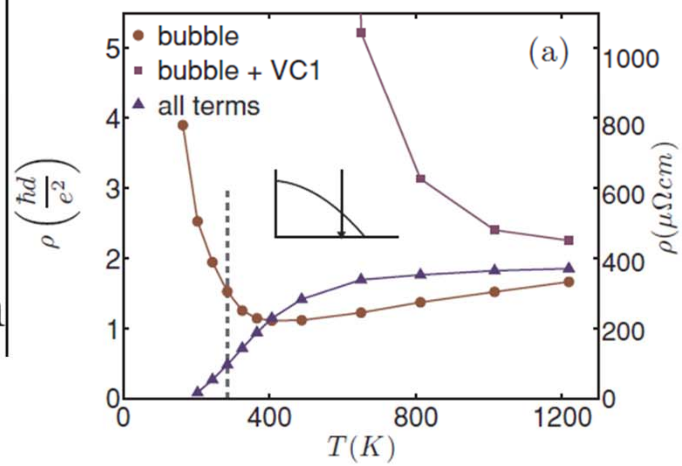
$$\sigma_{MIR} = \frac{e^2}{\hbar d}$$

Hole-doped cuprates and MIR limit



Gurvitch & Fiory
PRL 59, 1337
(1987)

MIR limit
Mean-free path
~ Fermi wavelength



LSCO 17%, YBCO optimal

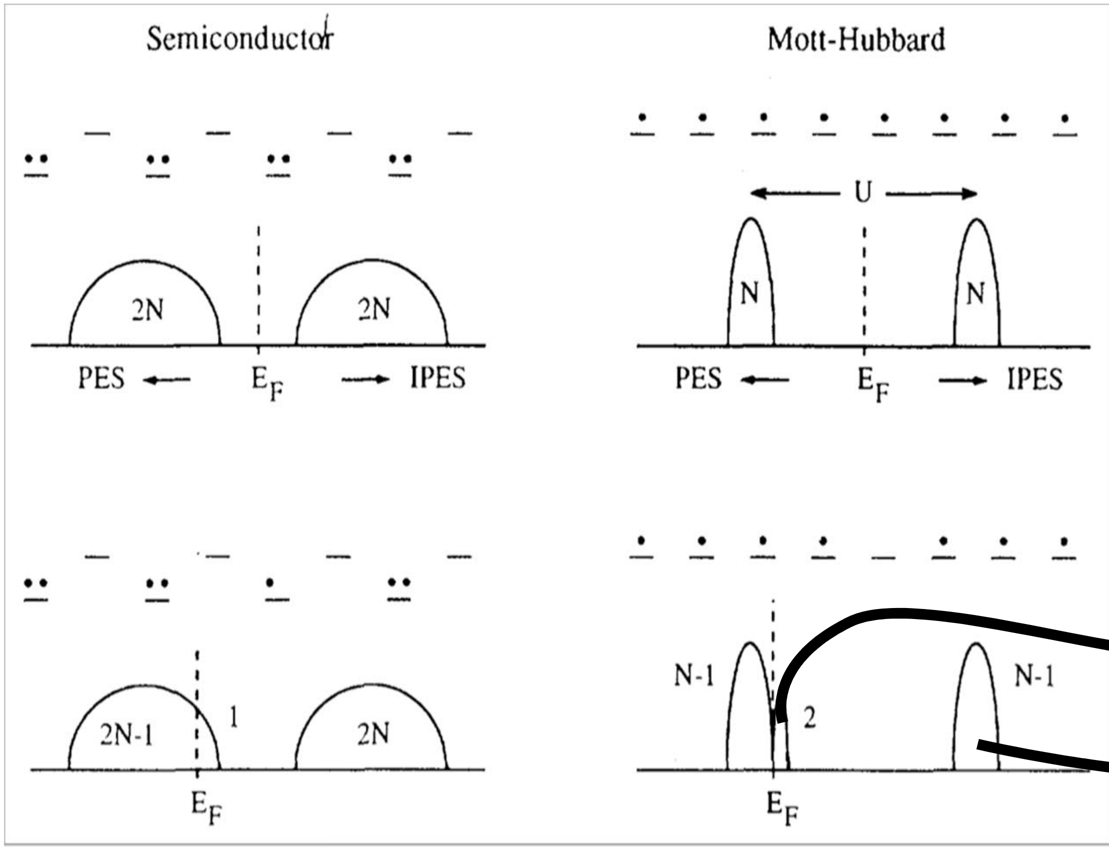
Dominic Bergeron & AMST
PRB 2011
TPSC

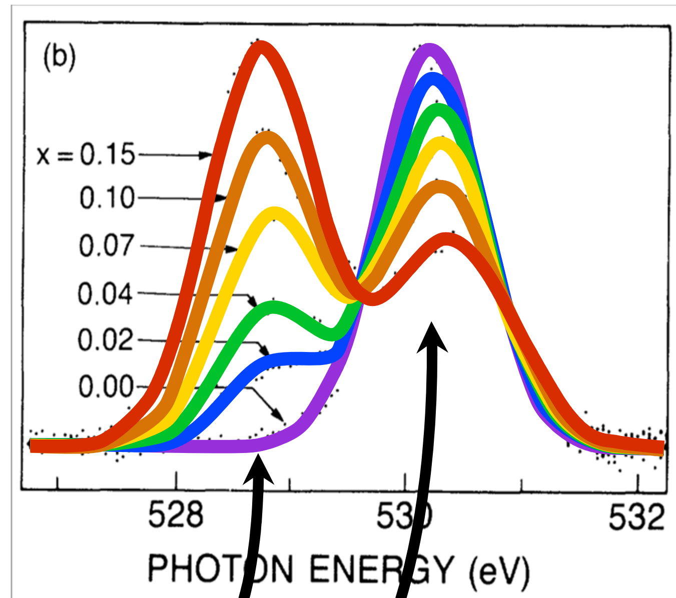
PHYSICAL REVIEW B **84**, 085128 (2011)

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

Experiment, X-Ray absorption

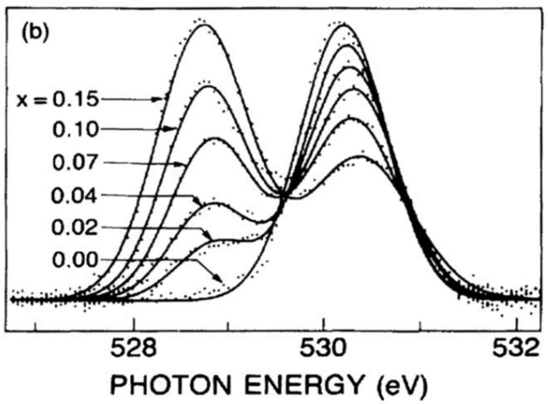
Meinders *et al*. PRB **48**, 3916 (1993)



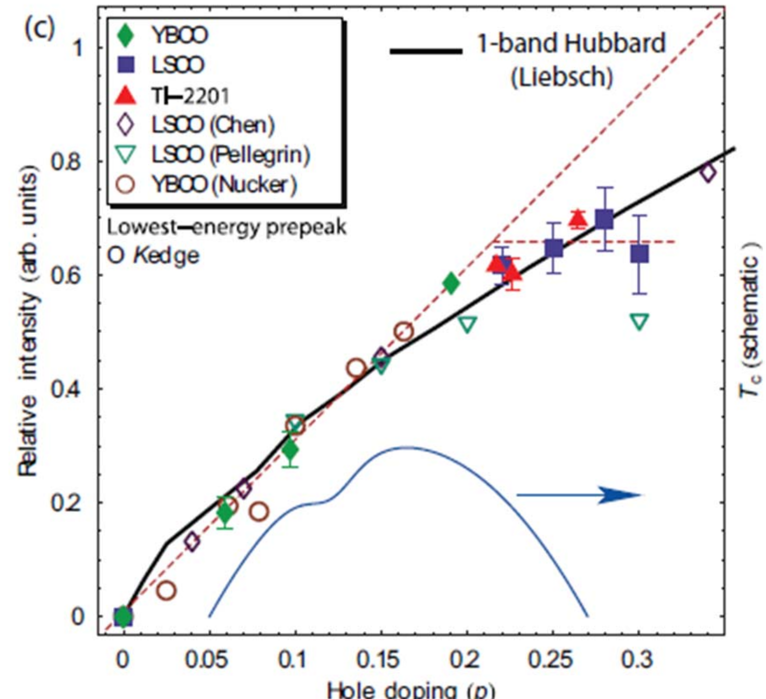


Chen et al. PRL **66**, 104 (1991)

Experiment: X-Ray absorption



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



Peets et al. PRL **103**, (2009),

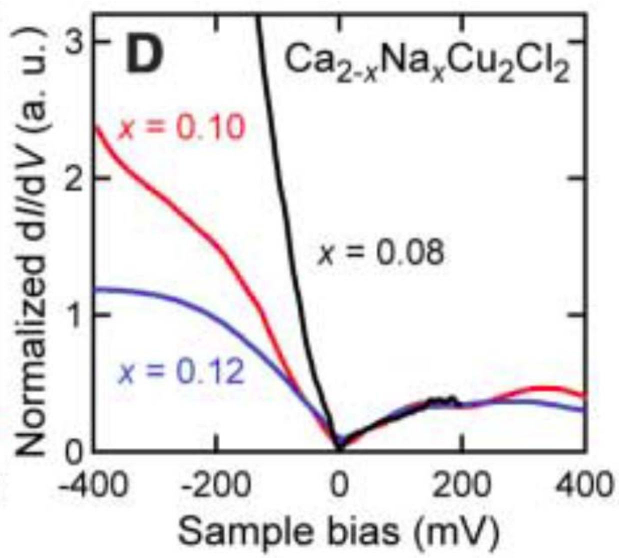
Phillips, Jarrell PRL , vol. **105**, 199701 (2010)

Number of low energy states above ω = 0 scales as *2x* +

Not as 1+x as in Fermi liquid

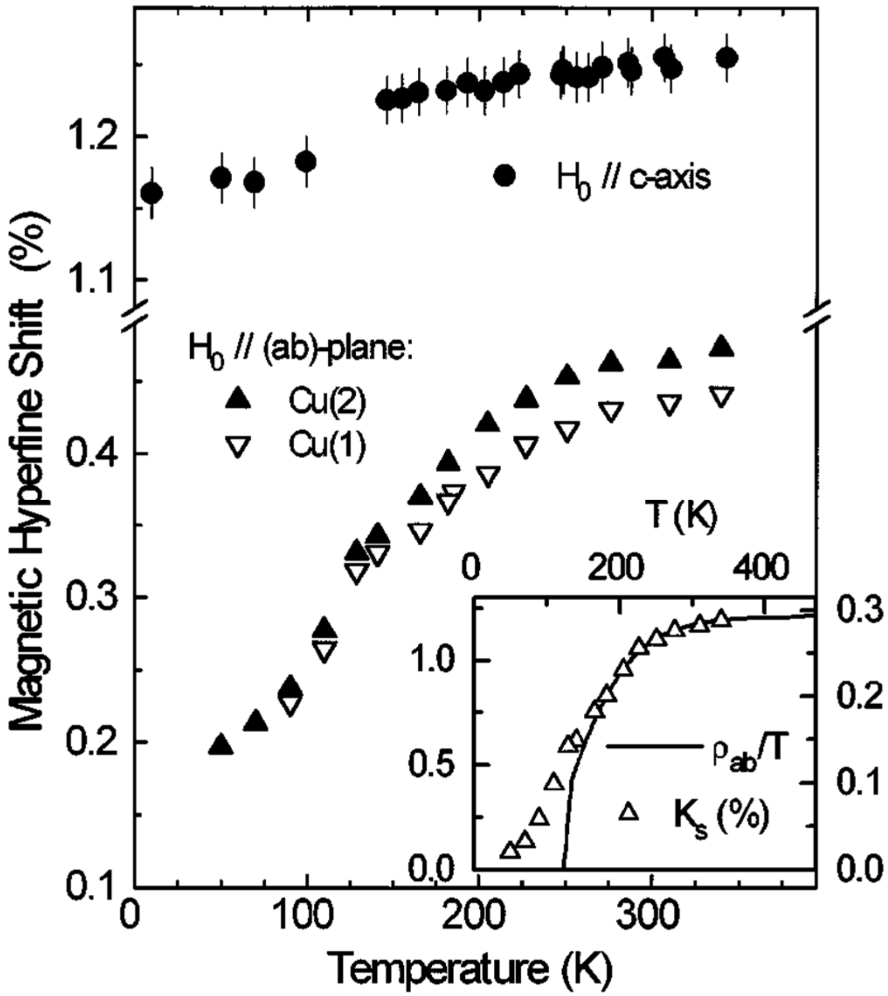
Meinders *et al.* PRB **48**, 3916 (1993)

Density of states (STM)



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

Spin susceptibility (Knight shift): Pseudogap

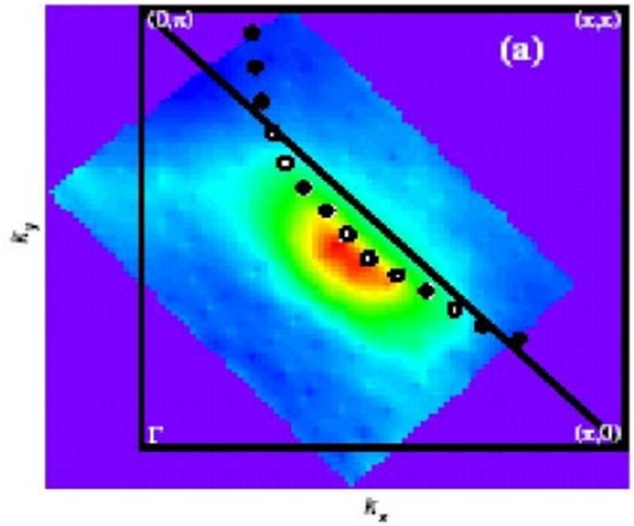


Underdoped Hg1223

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

ARPES: (Pseudogap)

Hole-doped, 10%



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

Ronning *et al.* (PRB 2003)

e-doped cuprates

Less strongly coupled: evidence from the normal state (MIR, pseudogap)

Sénéchal, A.-M.S. T. PRL (2004)

C. Weber, K. Haule, and G. Kotliar, Nature Physics 6, 574 (2010)

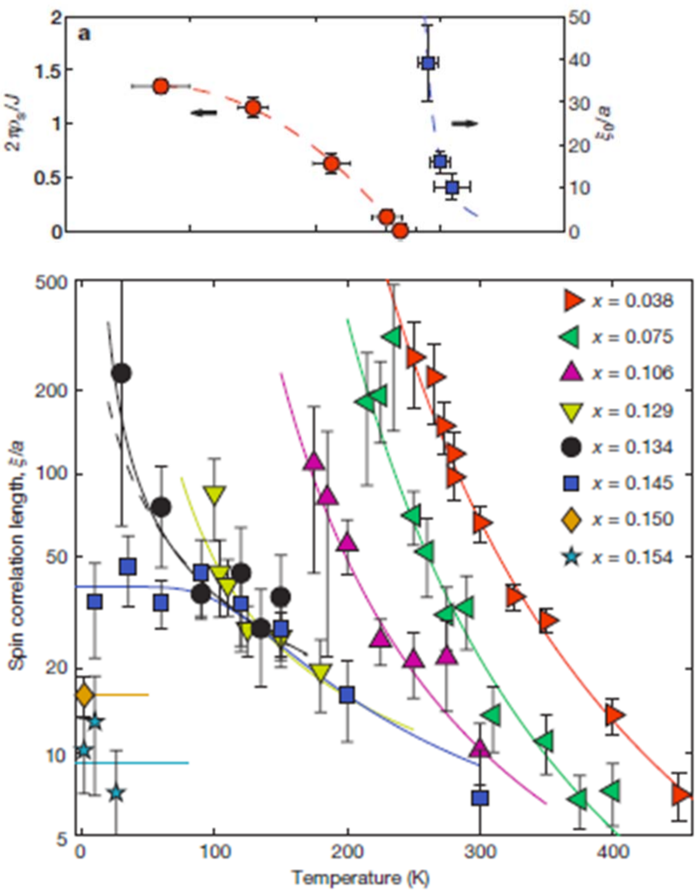
Less strongly correlated

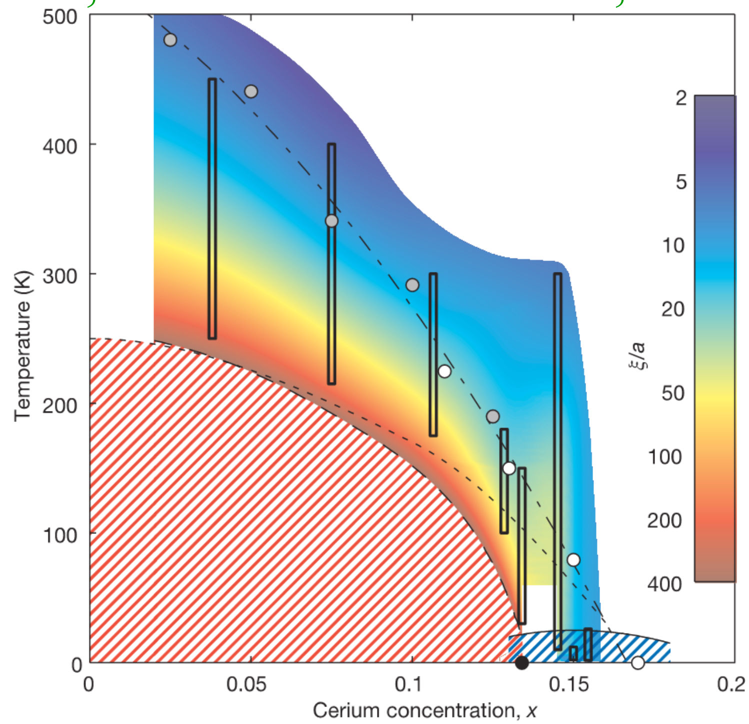
- MIR
- Shape of hot spots
- Pressure dependence of T_c
- Size of the optical gap

e-doped cuprates: precursors

NCCO

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

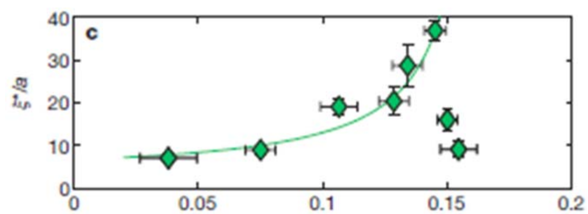




$z = 1$

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

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



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

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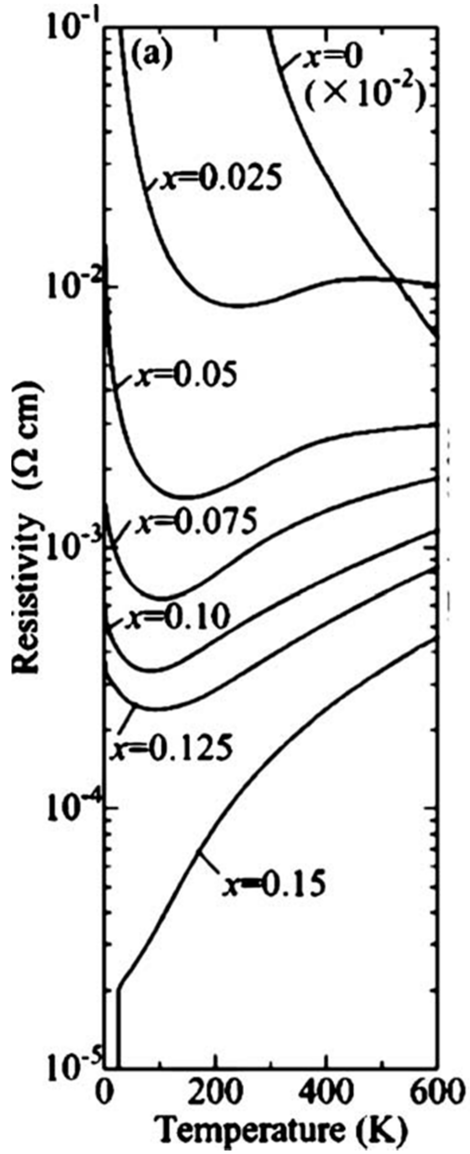
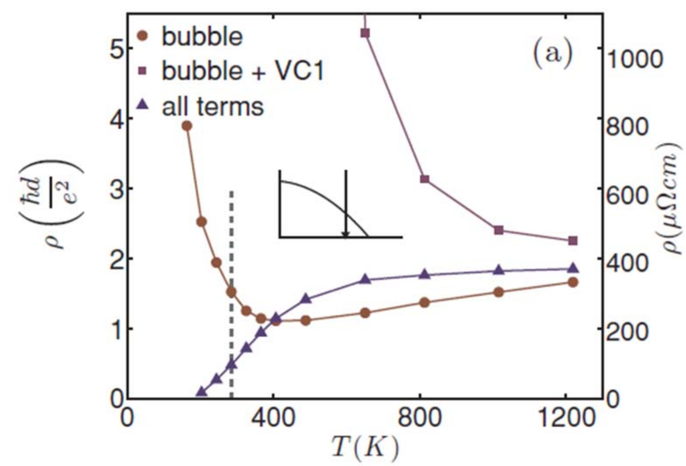
Electron-doped and MIR limit



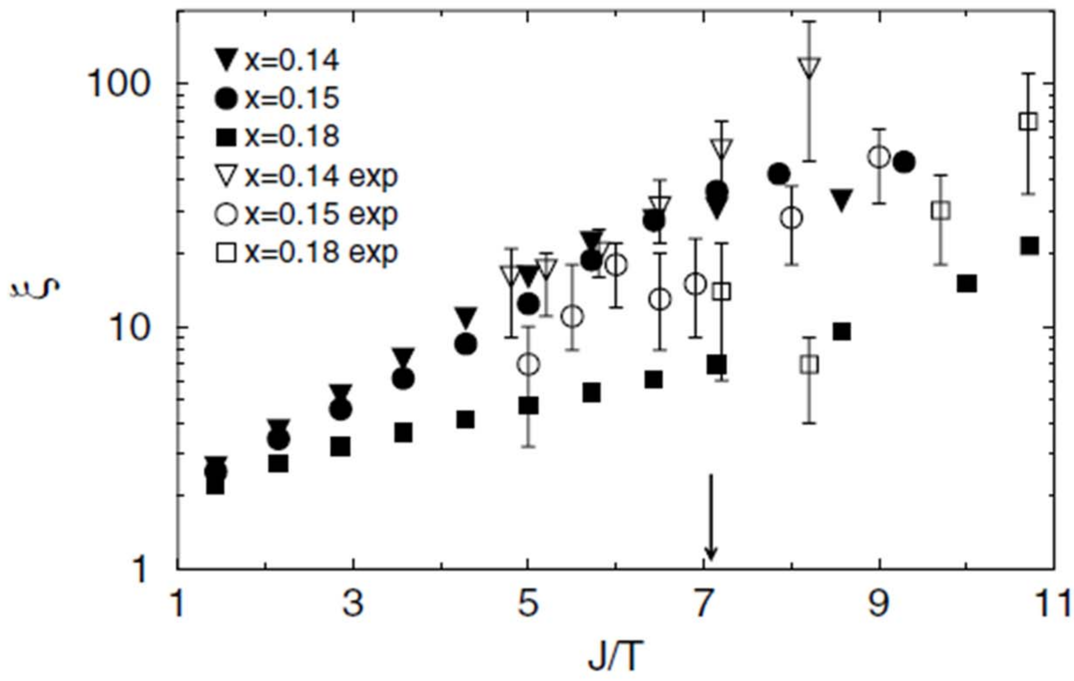
NCCO



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

Onose et al. 2004

TPSC vs experiment for ξ



Kyung et al. PRL **93**, 147004 (2004)

P. K. Mang et al., Phys. Rev. Lett. 93, 027002 (2004).
M. Matsuda et al., Phys. Rev. B 45, 12 548 (1992).

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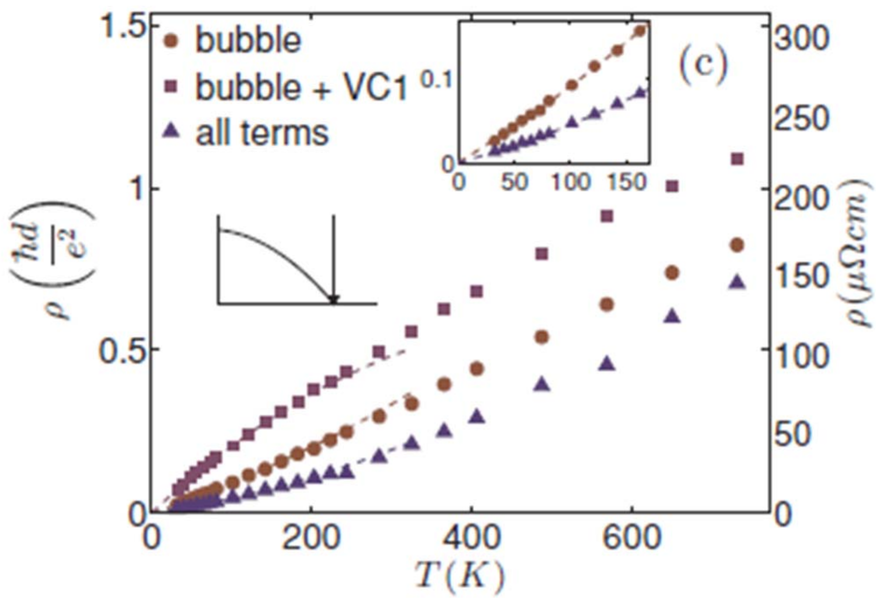
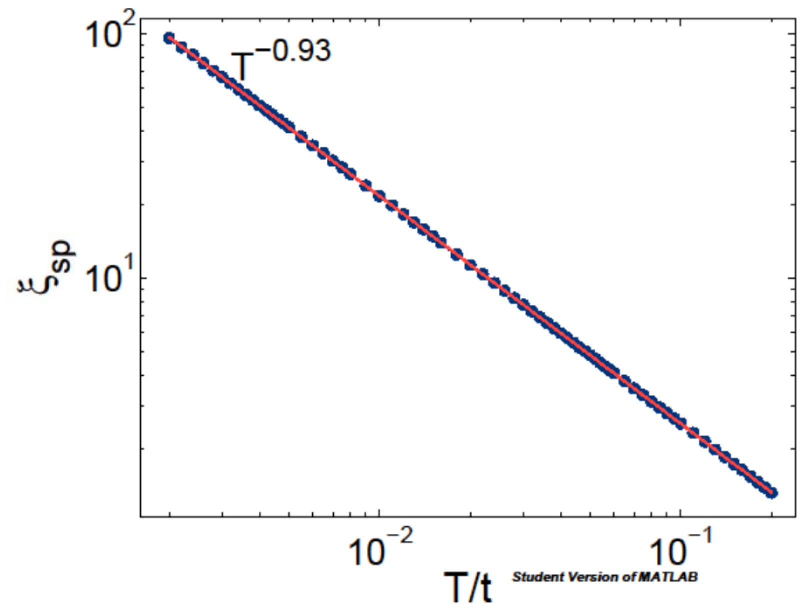
ξ(T) at the QCP

NCCO

Matsui et al. PRB 2007





z = 1

Motoyama, Nature 2007

U=6, t'=-0.175, t"=0.05, n=1.2007

Dominic Bergeron TPSC

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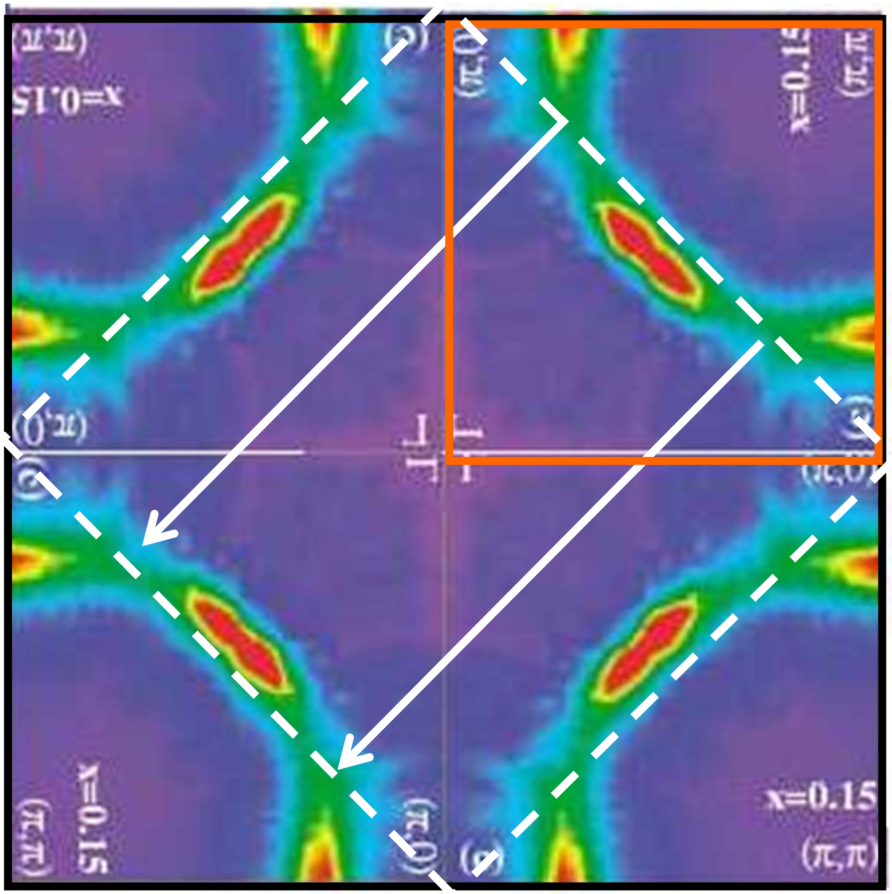
Hot spots from AFM quasi-static scattering

Mermin-Wagner

$d = 2$

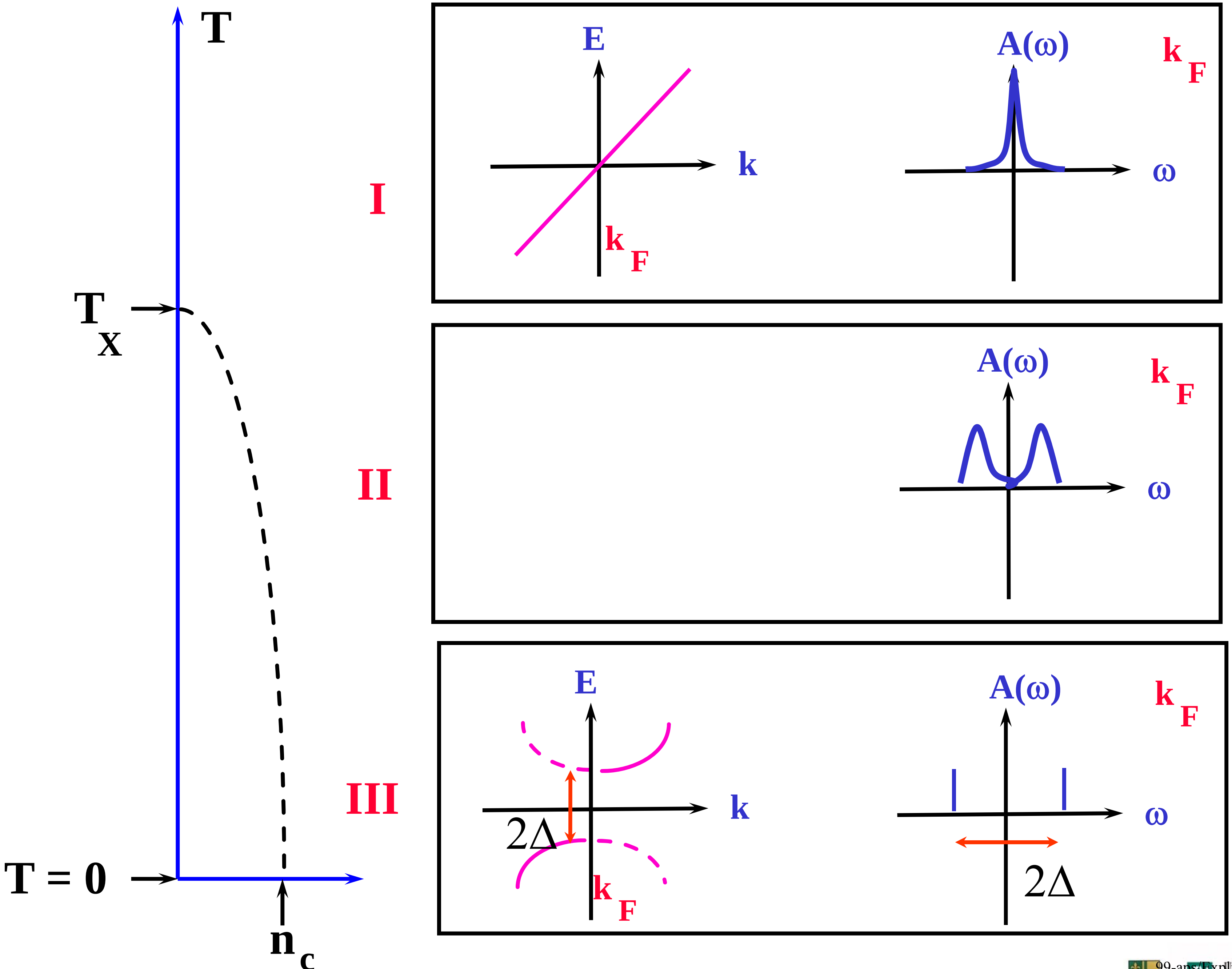


Armitage et al. PRL 2001

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

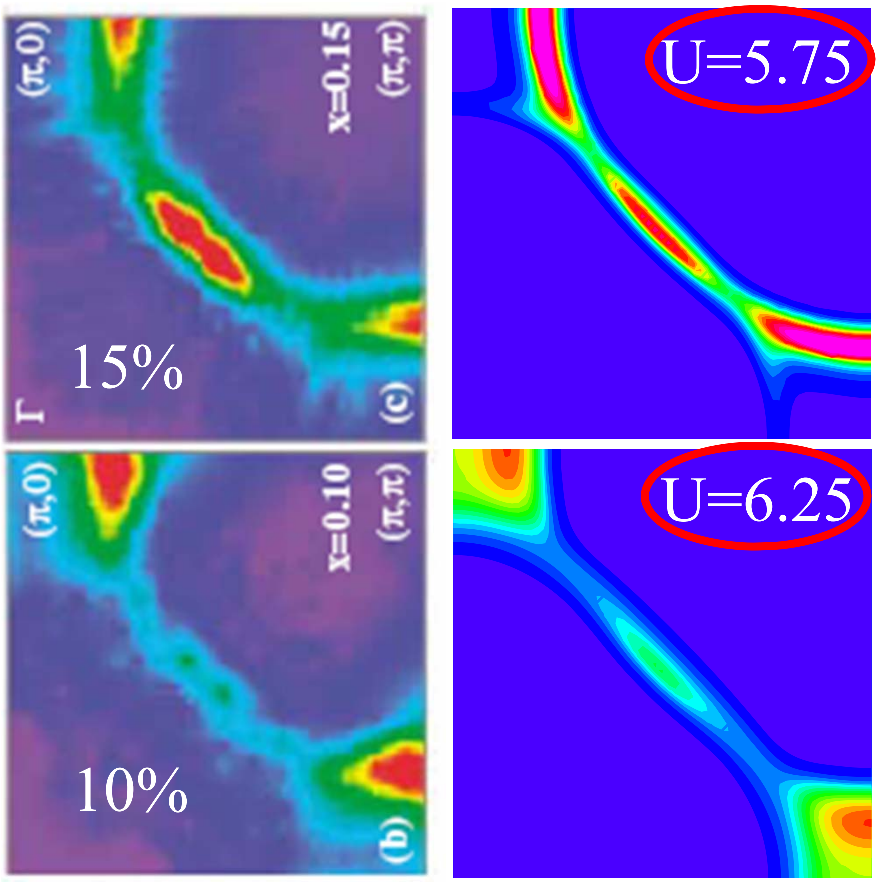
$\xi^{*} = 2.6(2)\xi_{th}$.

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

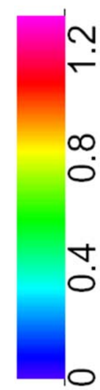

T
T_X
T = 0
n_c
I
II
III
E
k
k_F
A(ω)
ω
2Δ

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

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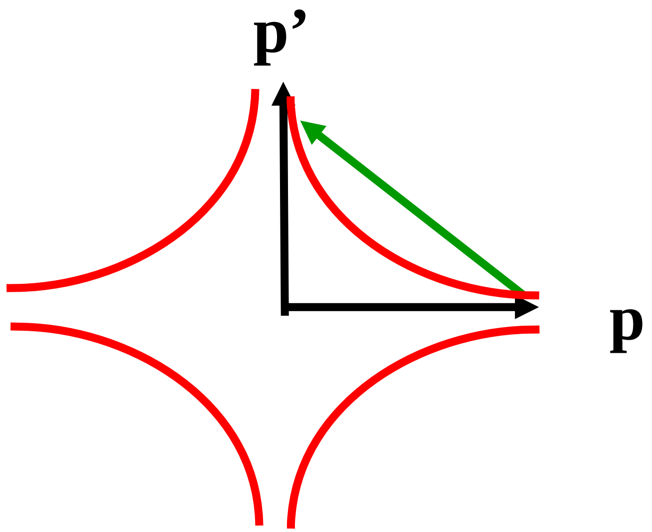
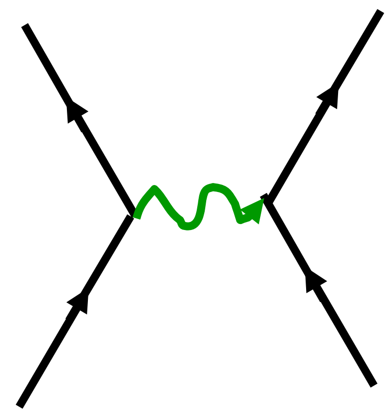
4. Weakly and strongly correlated superconductivity

Weakly correlated case

Cartoon « BCS » weak-coupling picture

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





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

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

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

Exchange of spin waves?
Kohn-Luttinger
T_c with pressure

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

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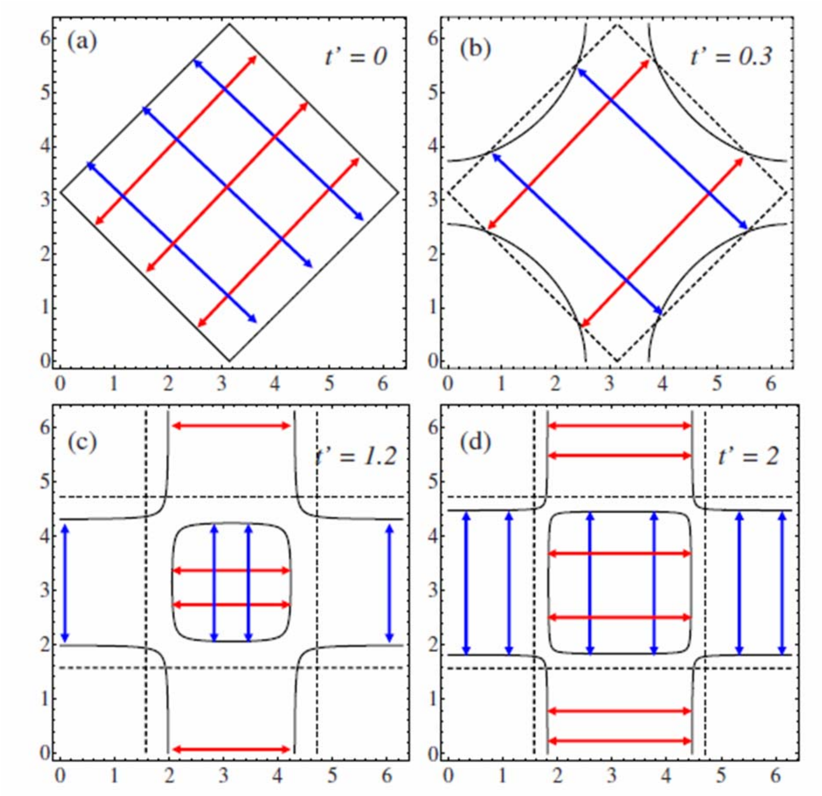
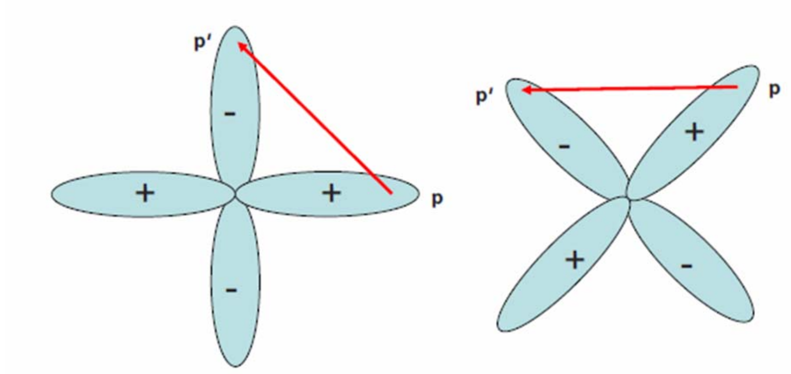
Results from TPSC

Satisfies Mermin-Wagner

Relation between symmetry and wave vector of AFM fluctuations





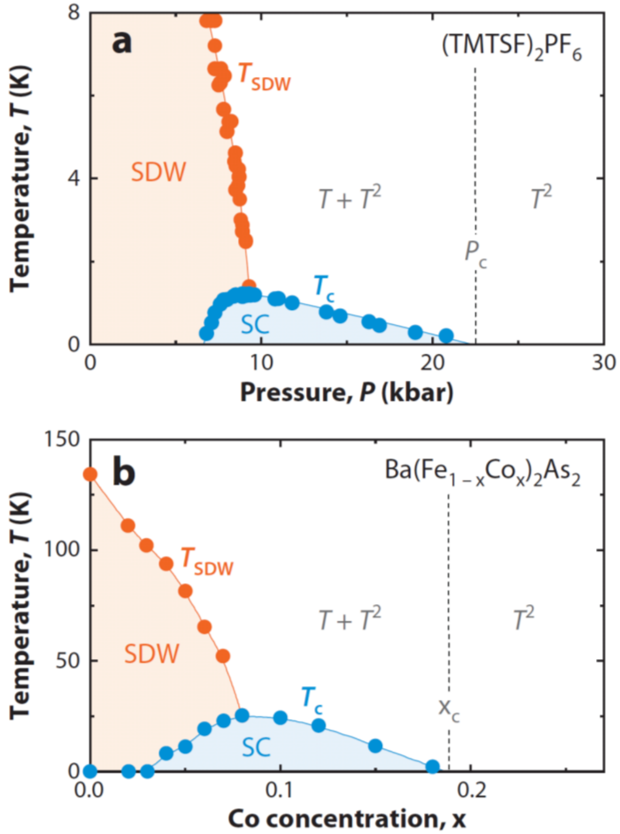
Hassan et al. PRB 2008

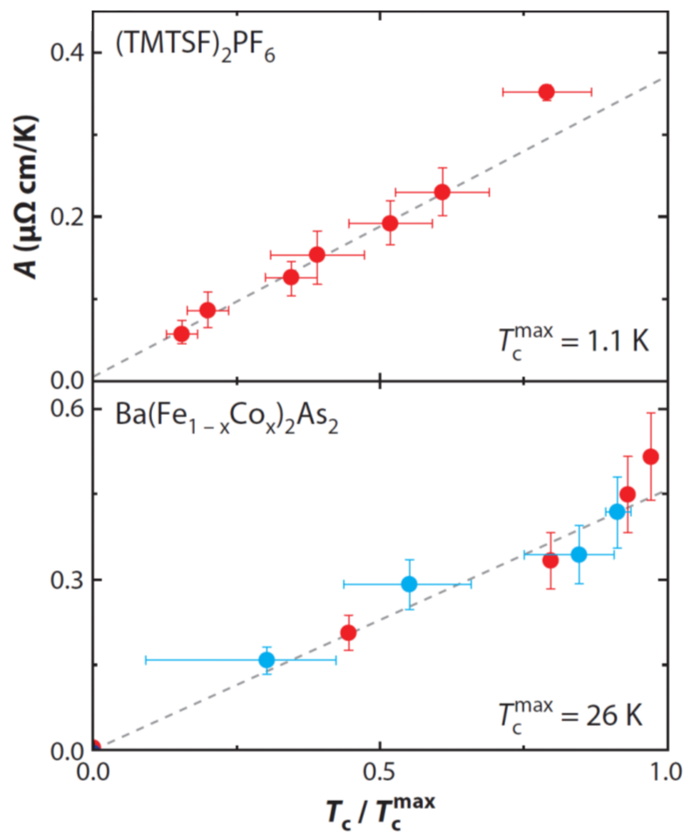
Organics & Pnictides

Bourbonnais, Sedeki, 2012

Organic

Pnictide





*Doiron-Leyraud et al., PRB **80**, 214531 (2009)*

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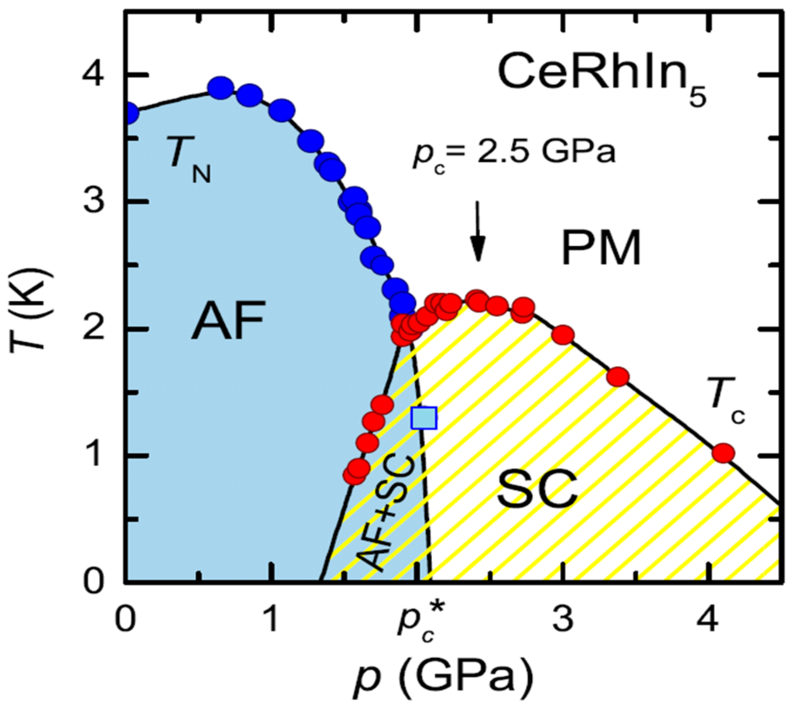
Heavy fermions

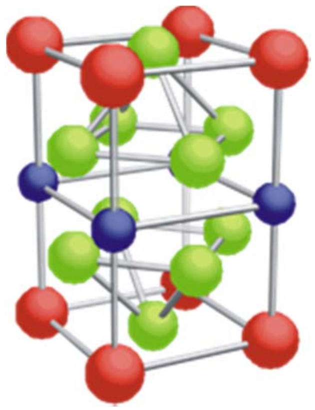
Heavy fermions **3D metals tuned by pressure, field or concentration**



Knebel et al. (2009)

Quantum criticality

$CeRhIn_5$



Magnetic superconductivity

Mathur et al., Nature 1998

4. Weakly and strongly correlated superconductivity

Strong correlations point of view

A cartoon strong coupling picture

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

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

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

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

Pitaevskii Brückner:
Pair state orthogonal to repulsive core of Coulomb interaction

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

5. High-temperature superconductors the view from dynamical mean-field theory

5.1: Quantum cluster approaches

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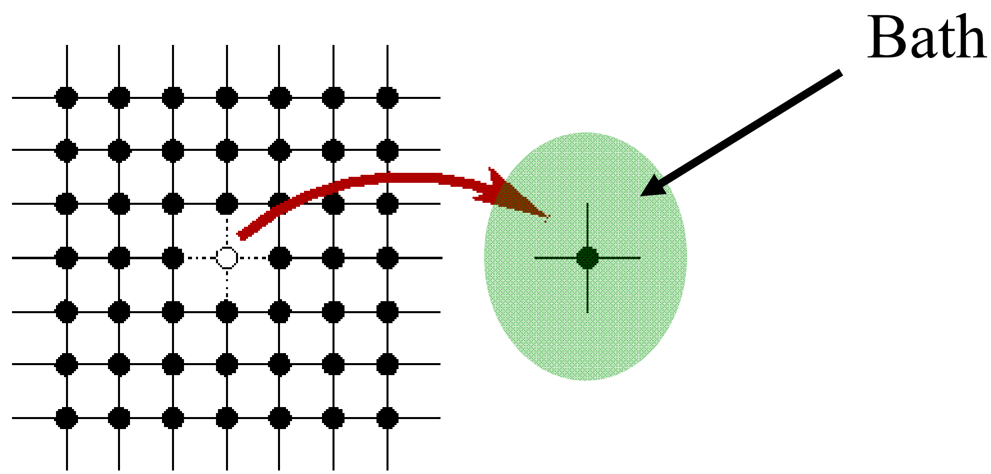
Mott transition and Dynamical Mean-Field Theory. The beginnings in *d = infinity*

- 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.

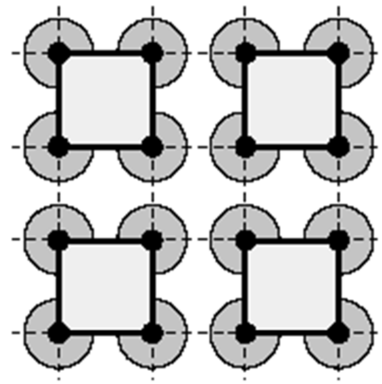


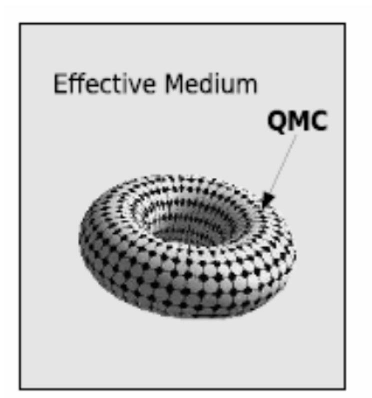
W. Metzner and D. Vollhardt, PRL (1989)
A. Georges and G. Kotliar, PRB (1992)
M. Jarrell PRB (1992)

DMFT, ($d = 3$)

2d Hubbard: Quantum cluster method

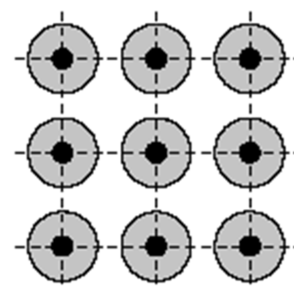
C-DMFT





DCA

DMFT



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

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

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+ and -

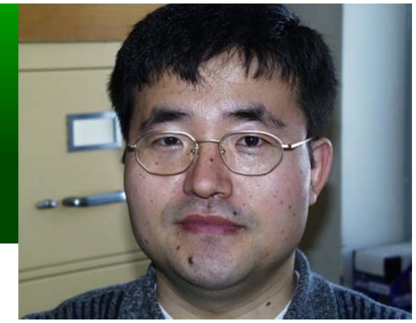
- Long range order:
  - Allow symmetry breaking in the bath (mean-field)
- Included:
  - Short-range dynamical and spatial correlations

- Missing:
  - Long wavelength p-h and p-p fluctuations

Two solvers for the cluster-in-a-bath problem

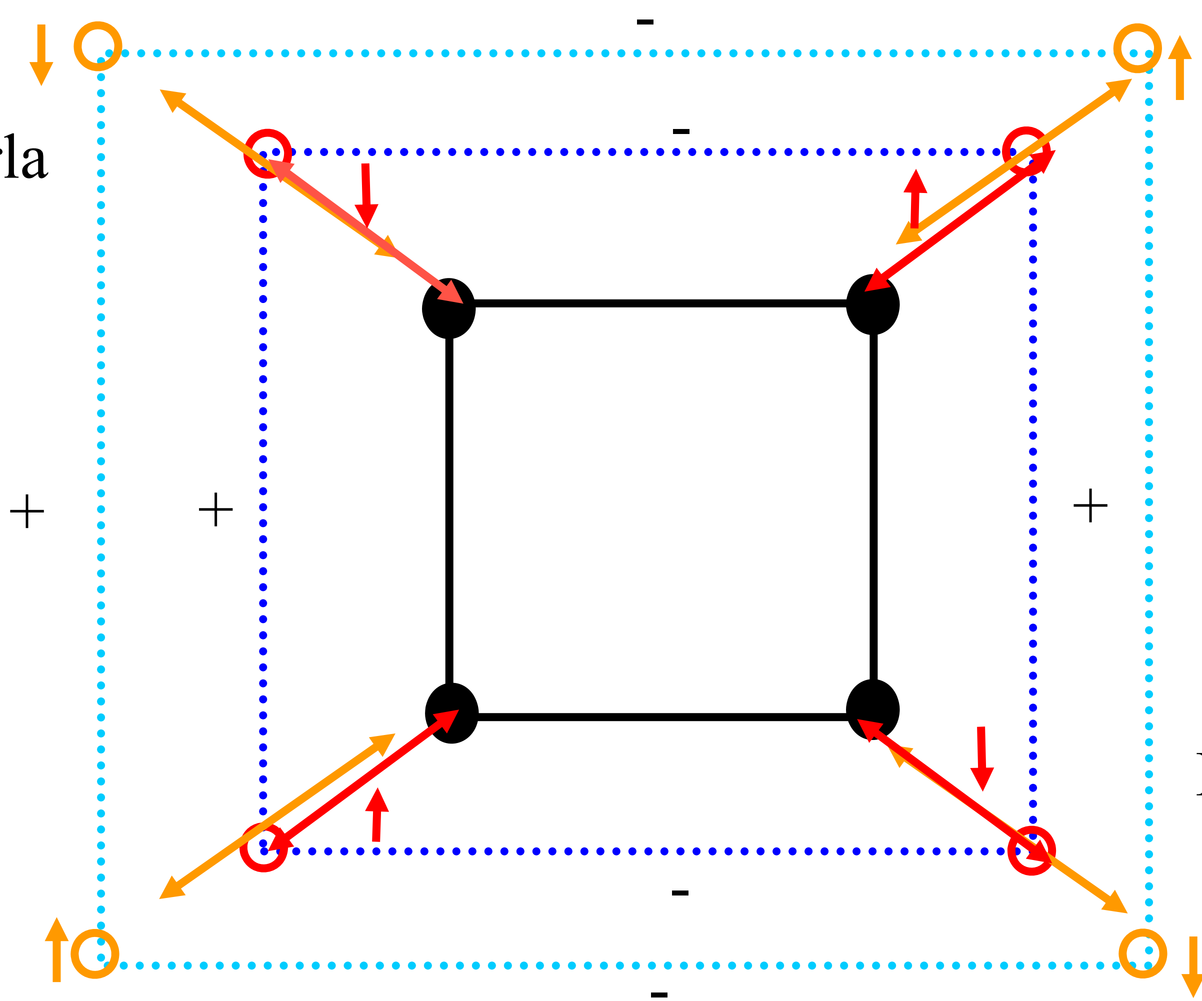
Competition AFM-dSC

S. Kancharla



B. Kyung

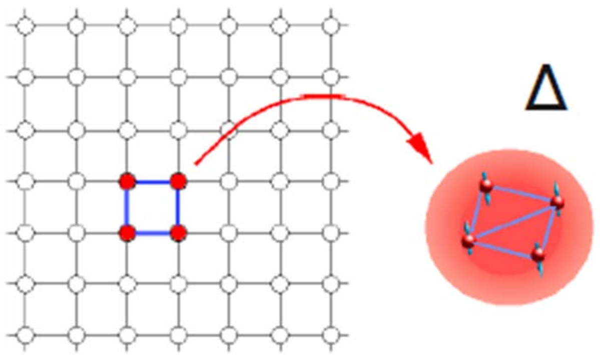
David Sénéchal

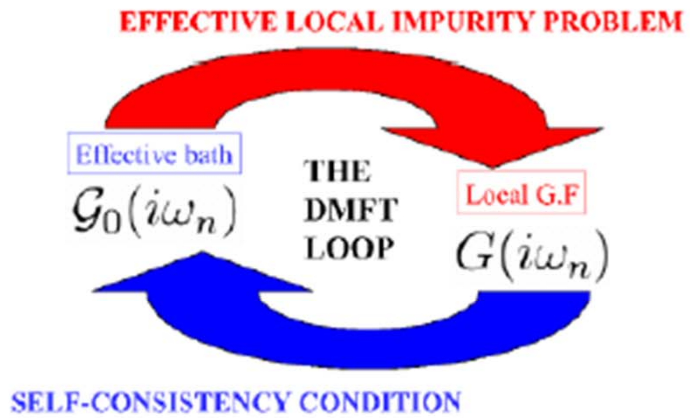


See also, Capone and Kotliar, Phys. Rev. B 74, 054513 (2006),
Macridin, Maier, Jarrell, Sawatzky, Phys. Rev. B 71, 134527 (2005)

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

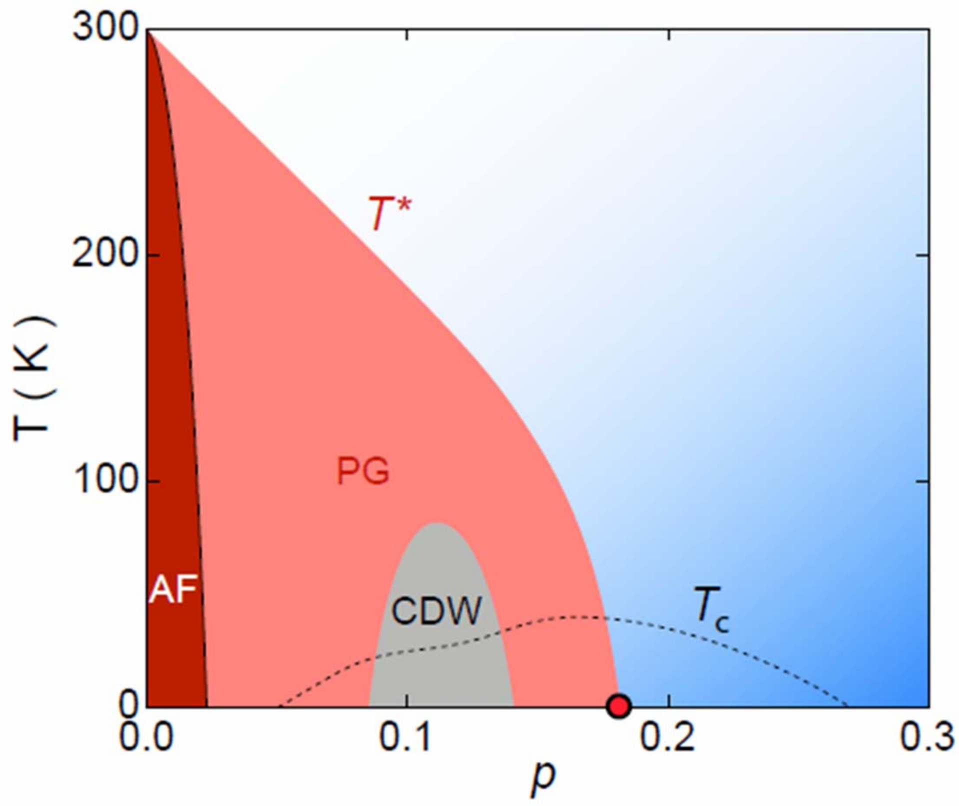
$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n) - \left[\sum_{\tilde{k}} \frac{1}{i\omega_n + \mu - t_c(\tilde{k}) - \Sigma_c(i\omega_n)} \right]^{-1}$$

At finite T, 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).

5.2 Normal state and pseudogap
The view from quantum clusters

Phase diagram, hole-doped (YBCO)



Laliberté, …. Taillefer (2016)

Three broad classes of mechanisms for pseudogap

- Rounded first order transition
- *d* =*2* 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)

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Underdoped metal very sensitive to anisotropy

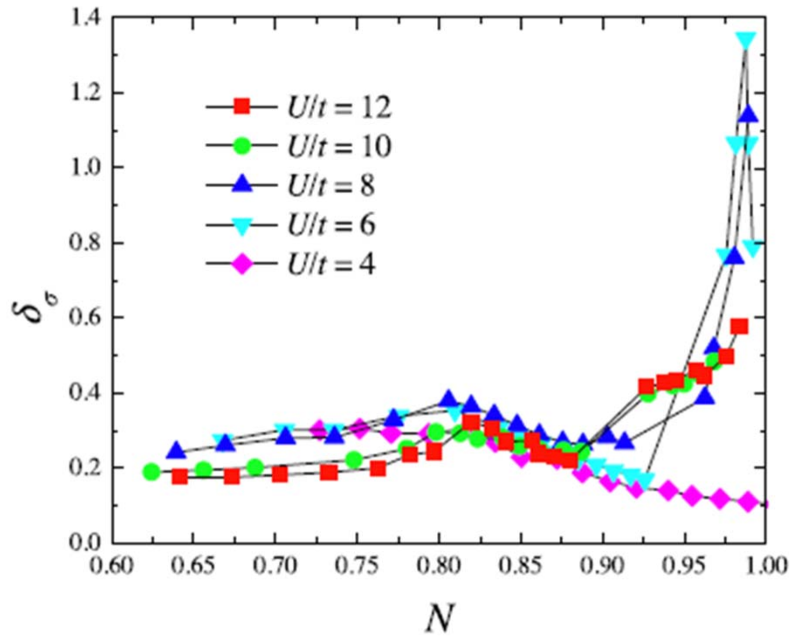
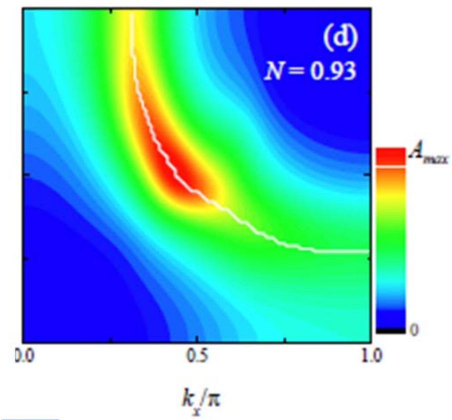
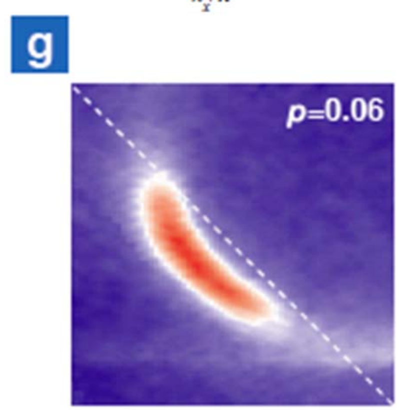


FIG. 3: (Color online) Anisotropy in the CDMFT conductivity $\delta_\sigma = 2\,[\sigma_x(0) - \sigma_y(0)]\,/\,[\sigma_x(0) + \sigma_y(0)]$ as a function of filling N for various values of U and $\eta = 0.1$, $\delta_0 = 0.04$.





Satoshi Okamoto

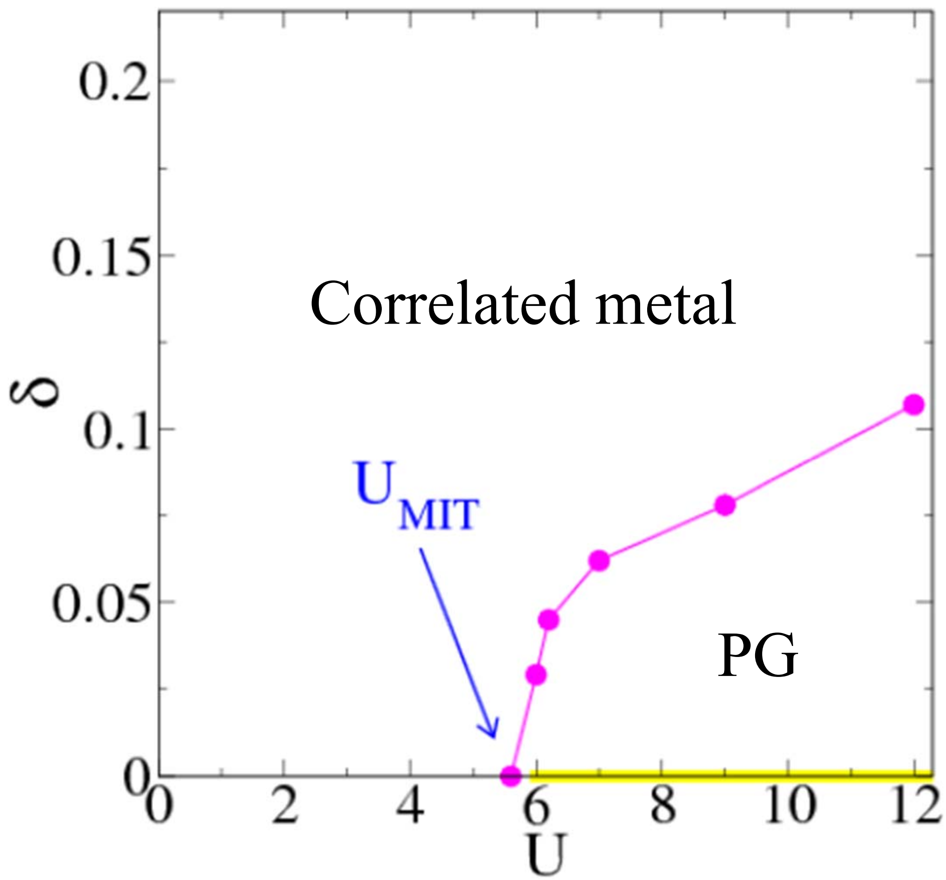
David Sénéchal

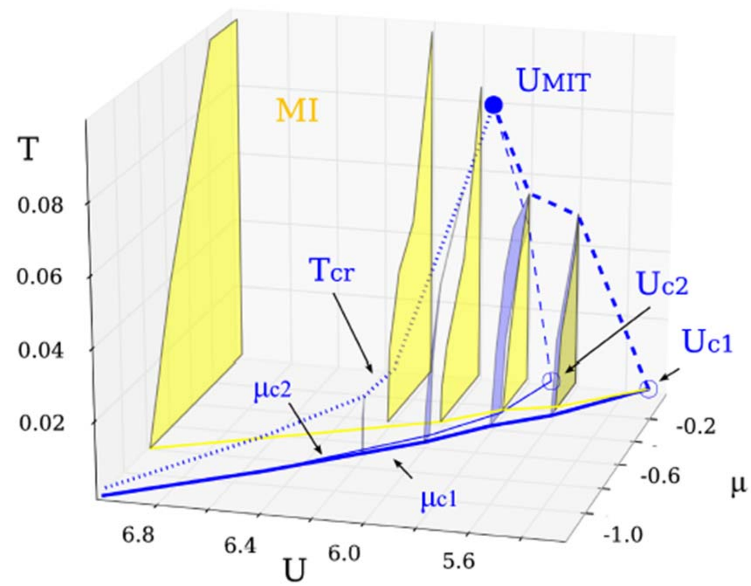
Okamoto, Sénéchal, Civelli, AMST
Phys. Rev. B **82**, 180511R 2010

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

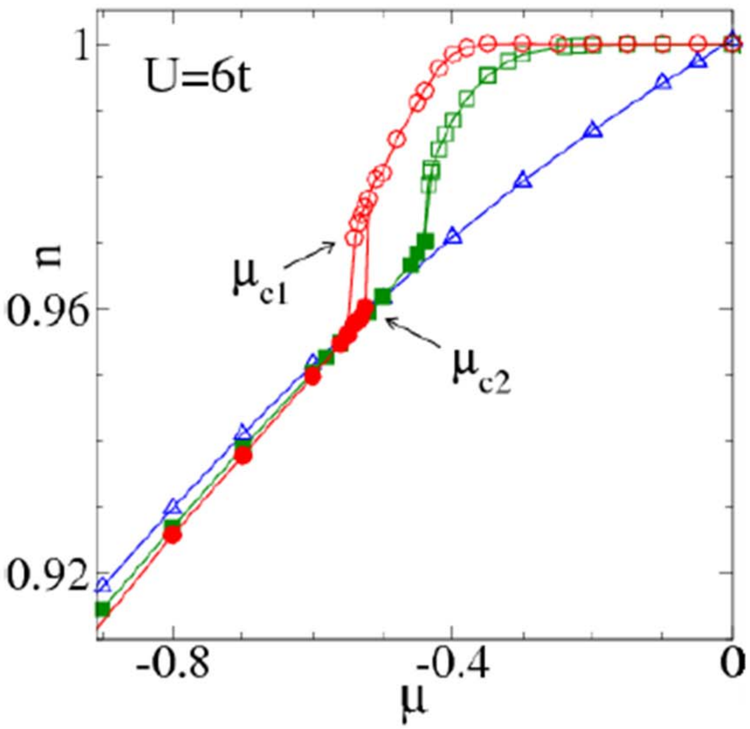
Link to Mott transition up to optimal doping

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





First order transition at finite doping

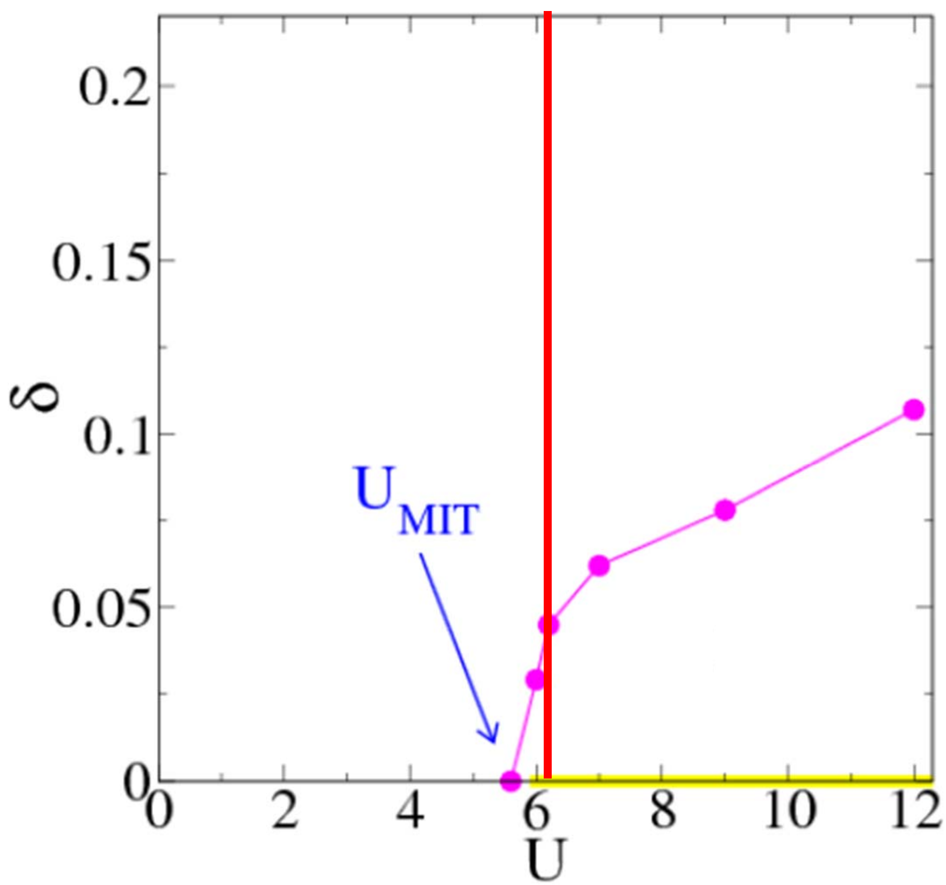


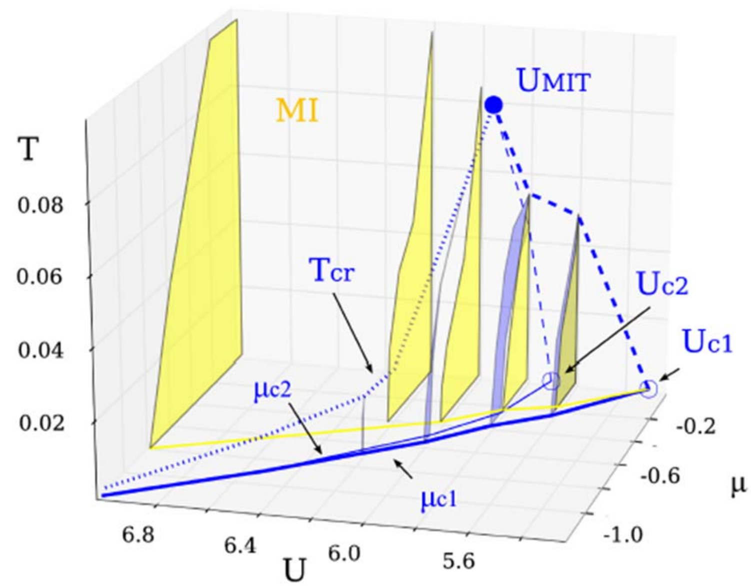
$n(\mu)$ for several temperatures:
T/t =1/10, 1/25, 1/50

Also, A. Liebsch and N.-H. Tong,
Phys. Rev. B **80**, 165126 (2009).

Link to Mott transition up to optimal doping

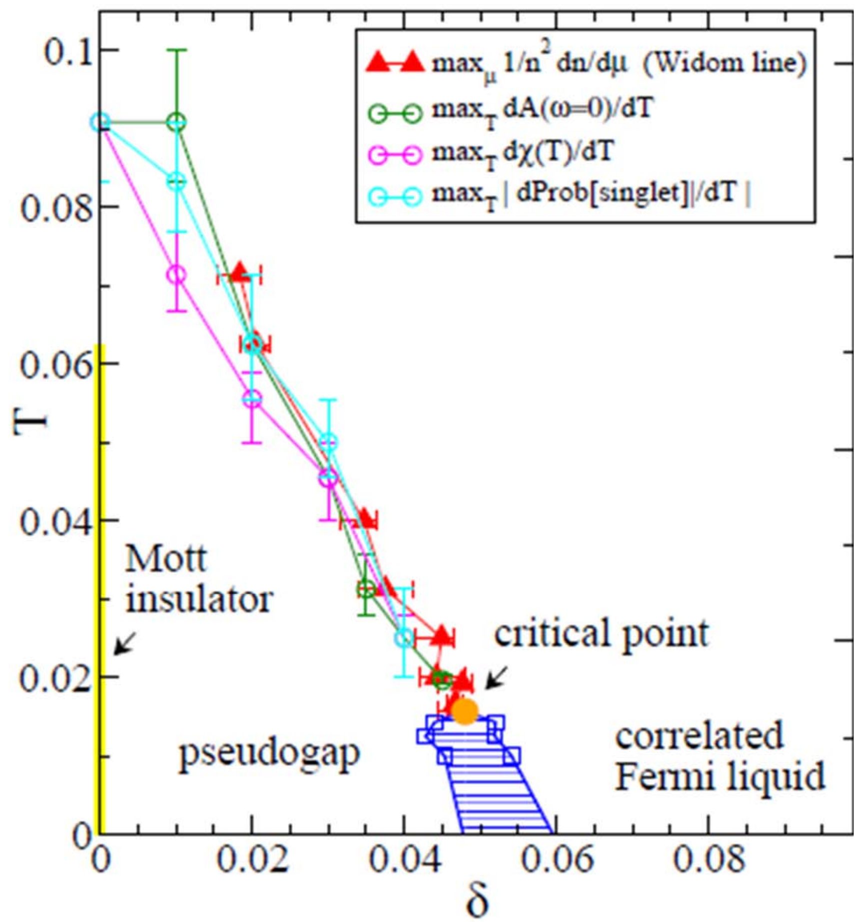
Doping dependence of critical point as a function of *U*

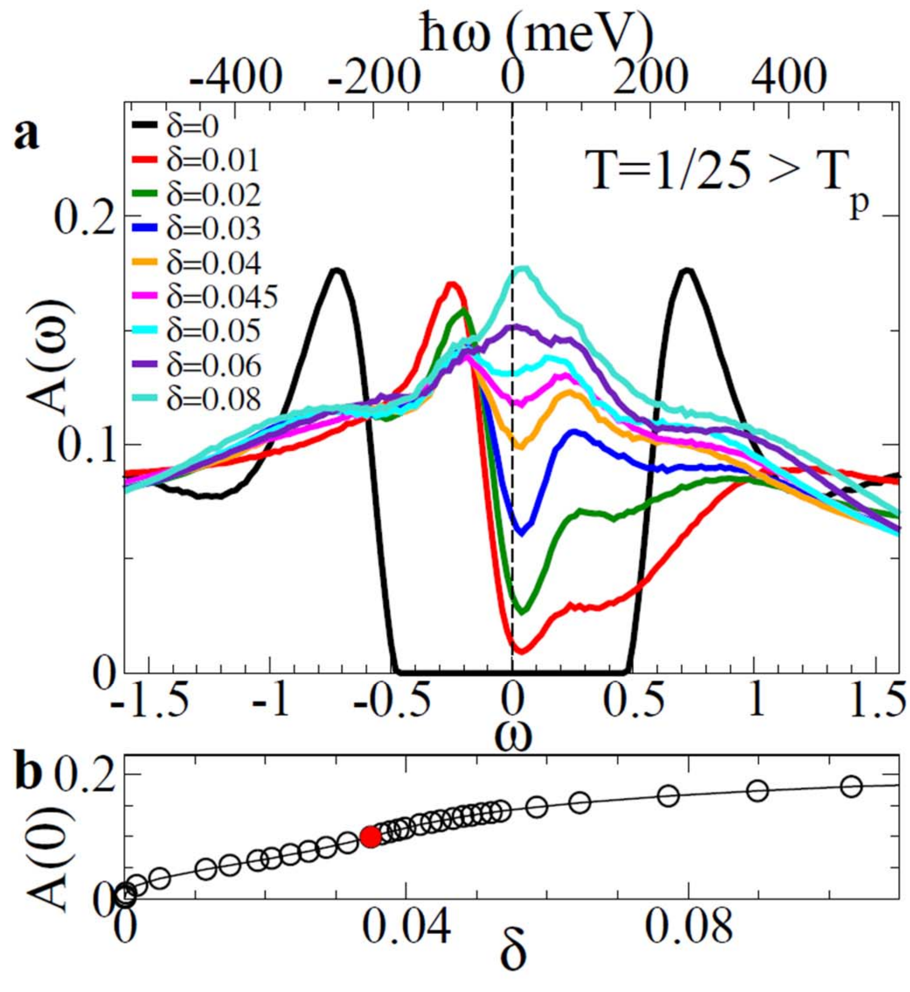




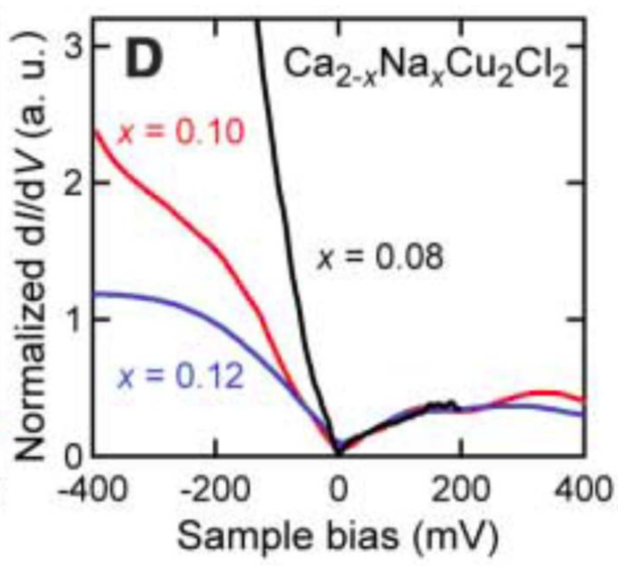
Smaller *D* and *S*

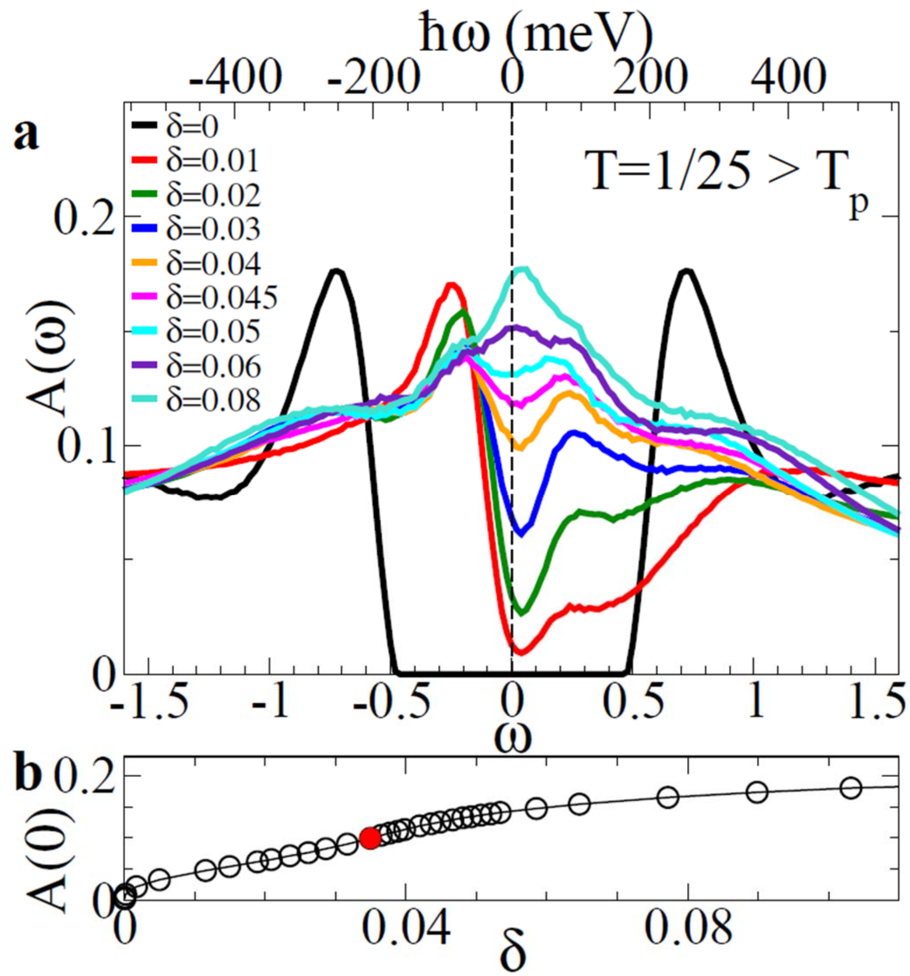
Density of states





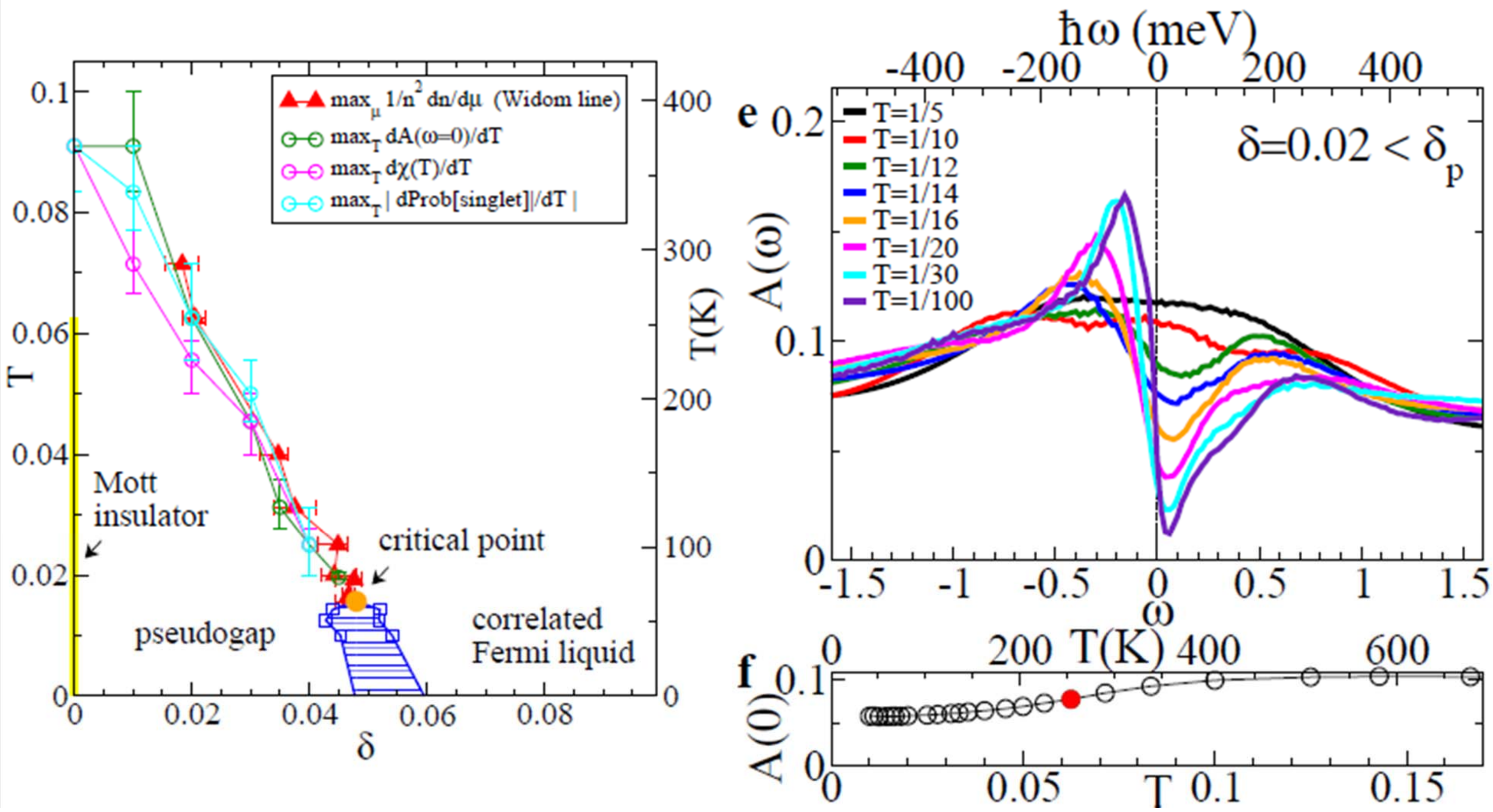
Density of states



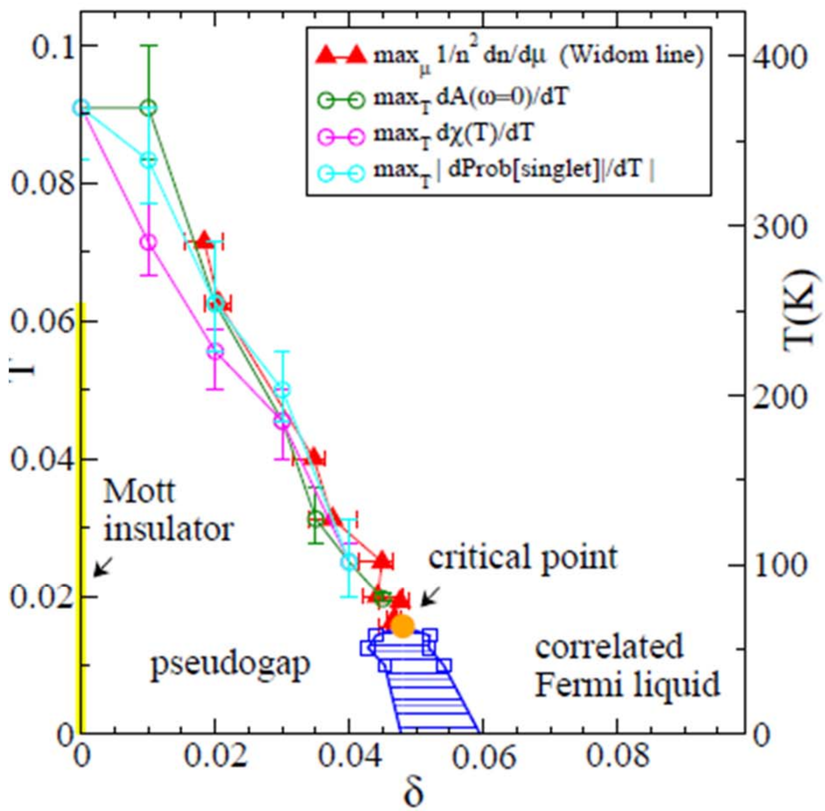


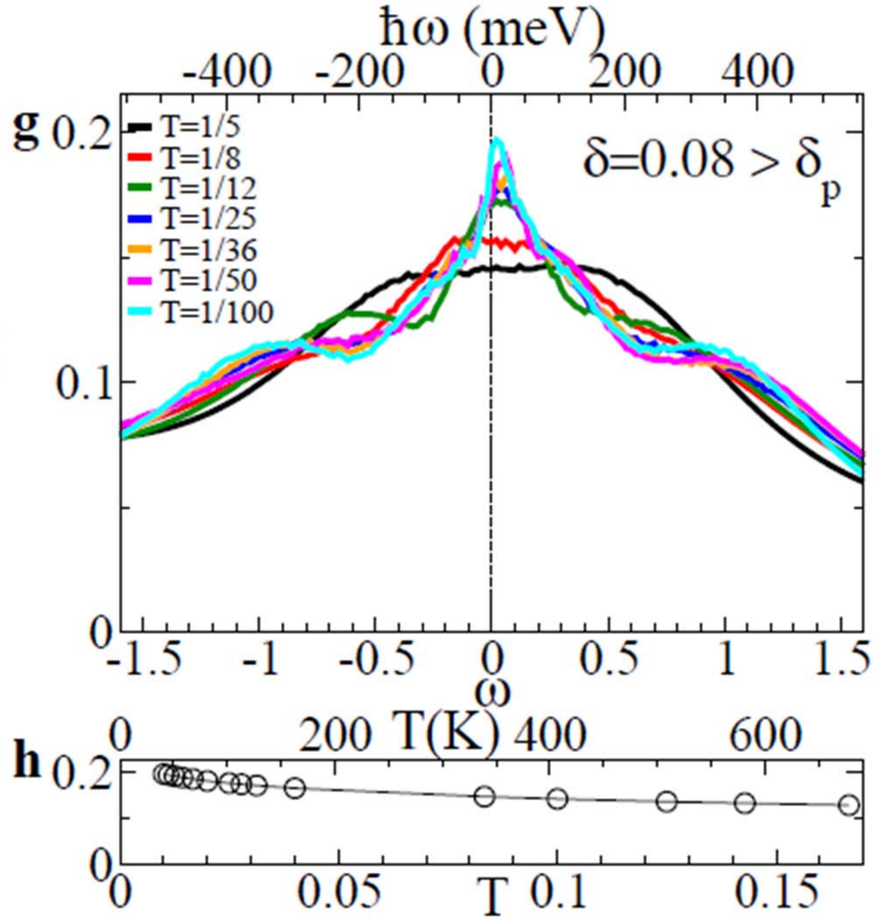
Khosaka et al. *Science* **315**, 1380 (2007);

Density of states

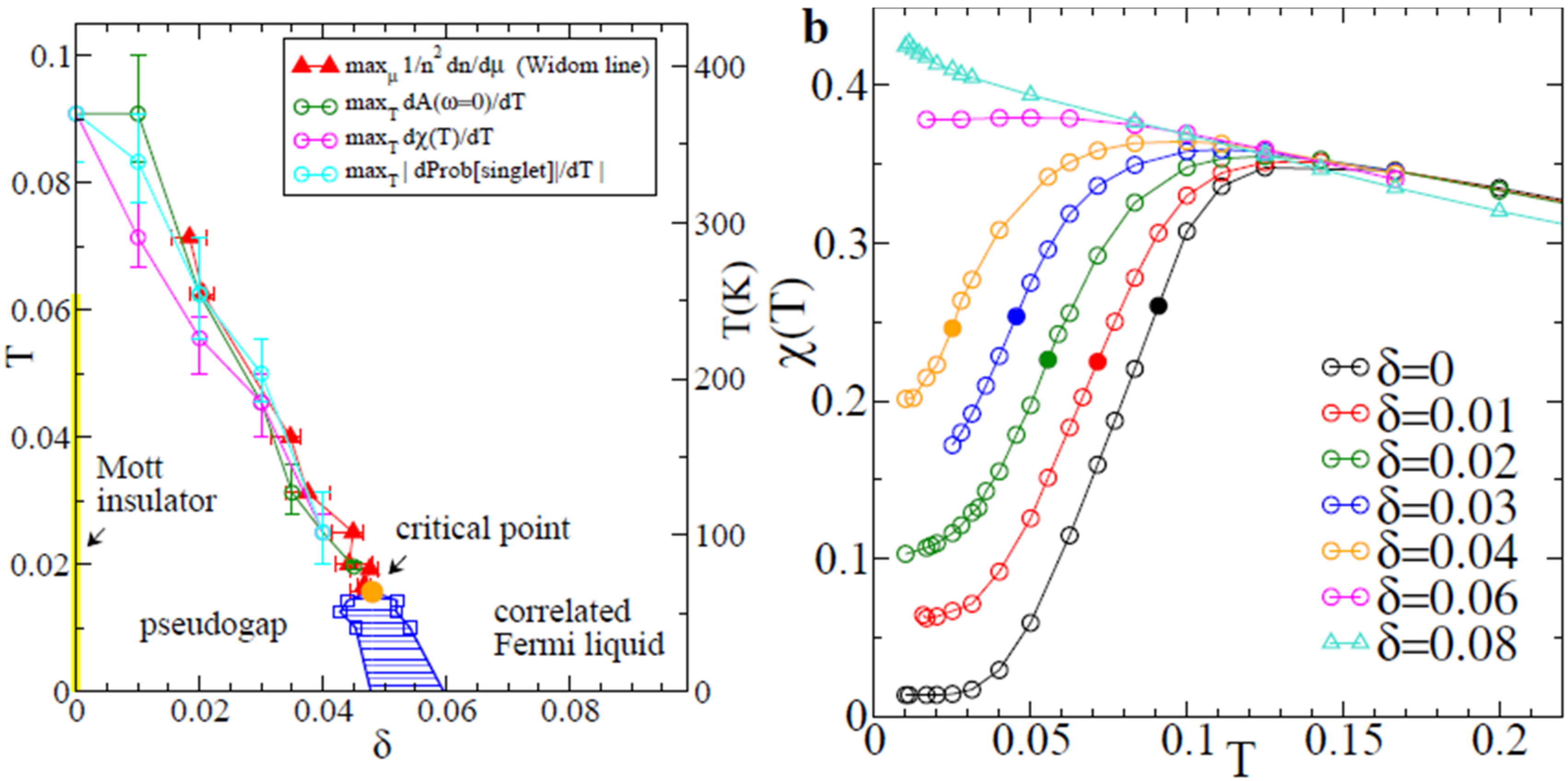


Density of states

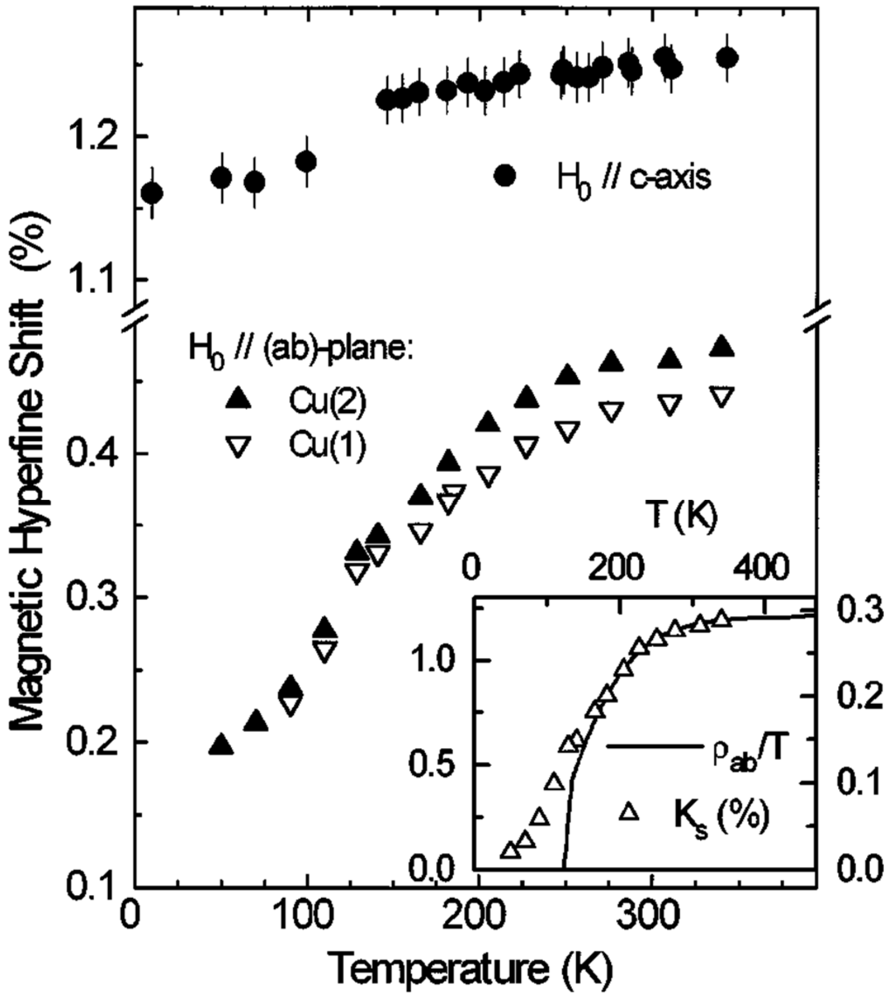


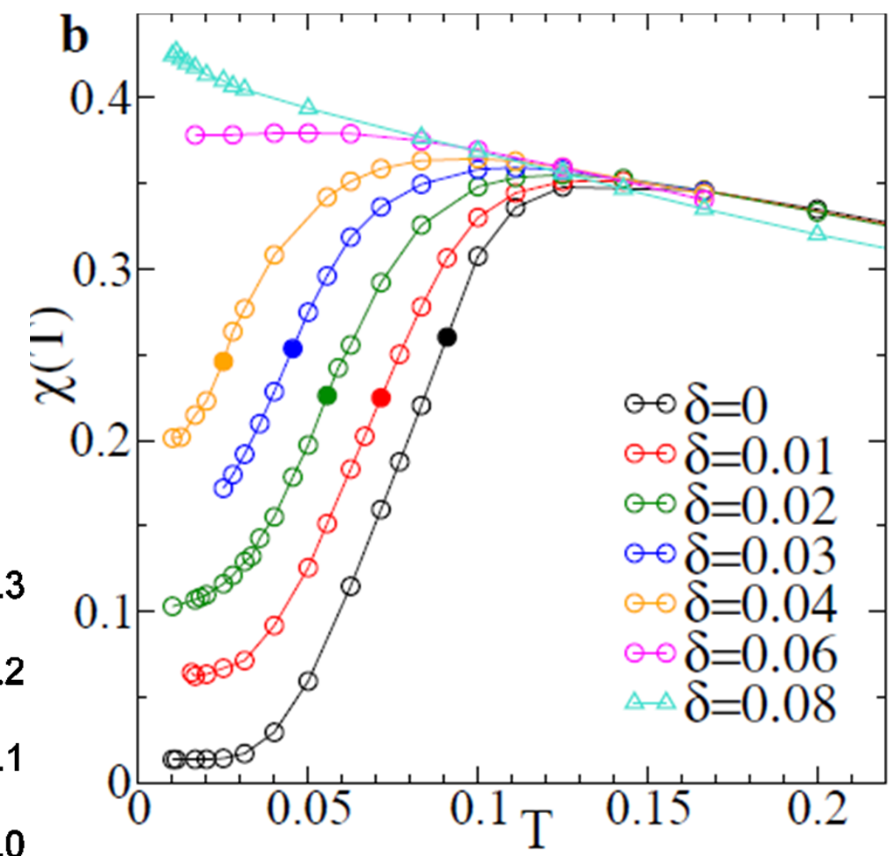


Spin susceptibility



Spin susceptibility

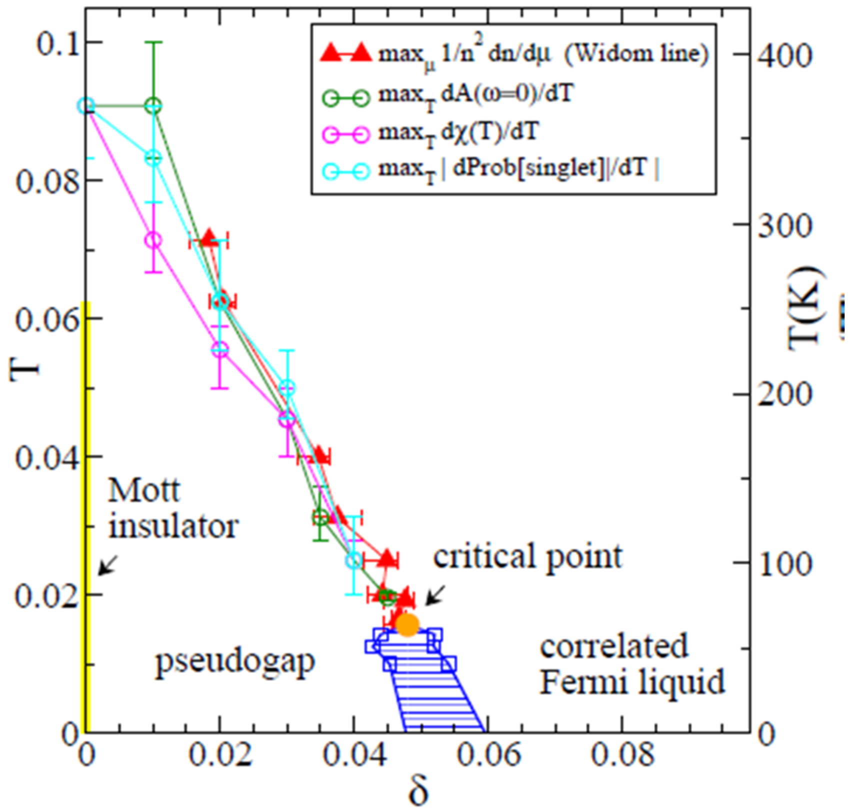


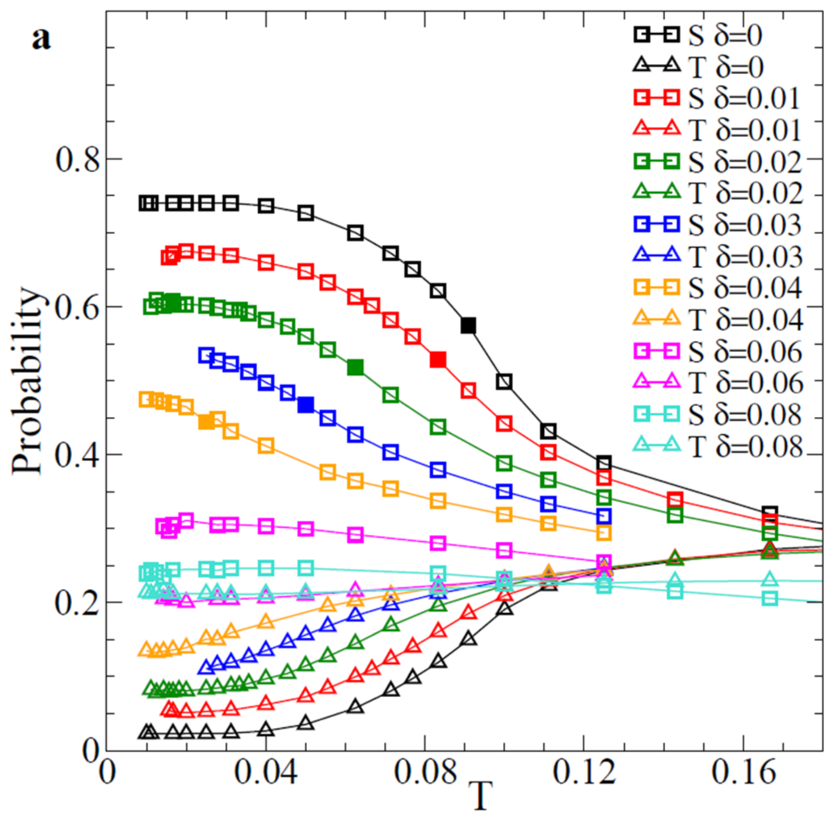


Underdoped Hg1223

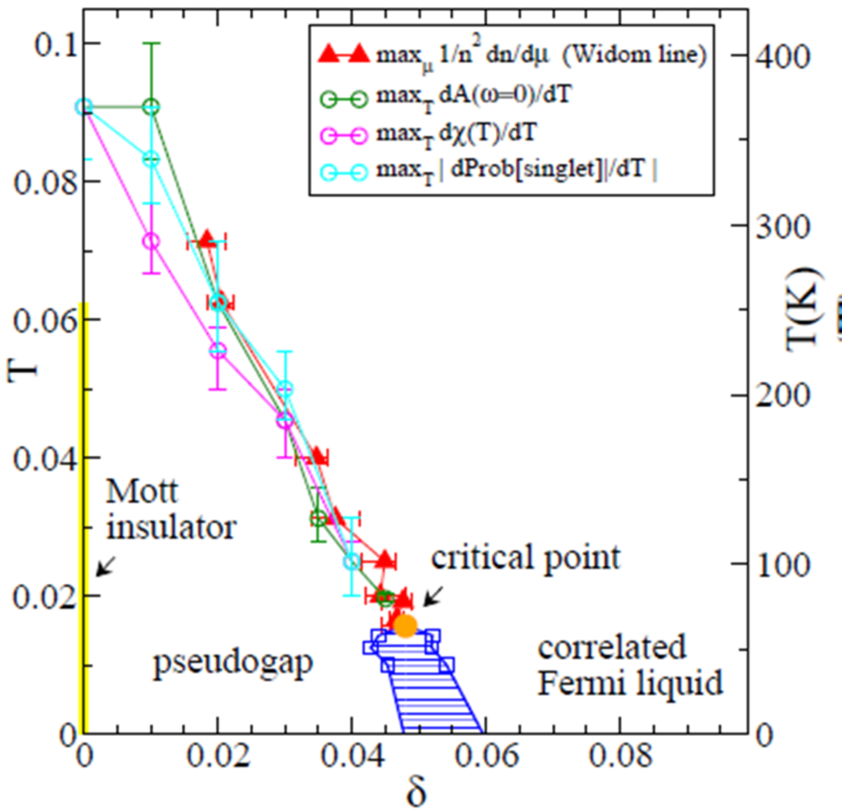
Julien et al. PRL **76,** 4238 (1996)

Plaquette eigenstates





Pseudogap *T** along the Widom line



Giovanni Sordi

Patrick Sémon

Kristjan Haule

The Widom line

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

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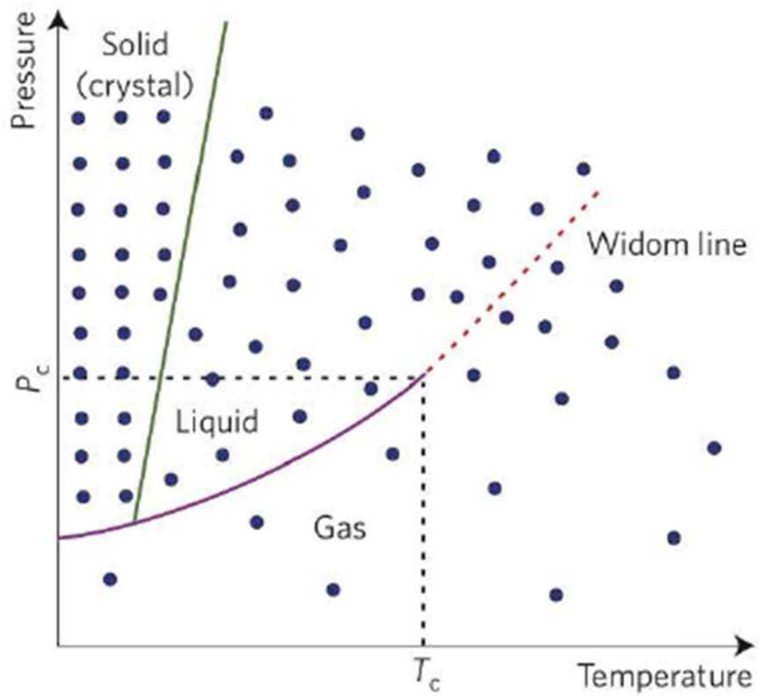
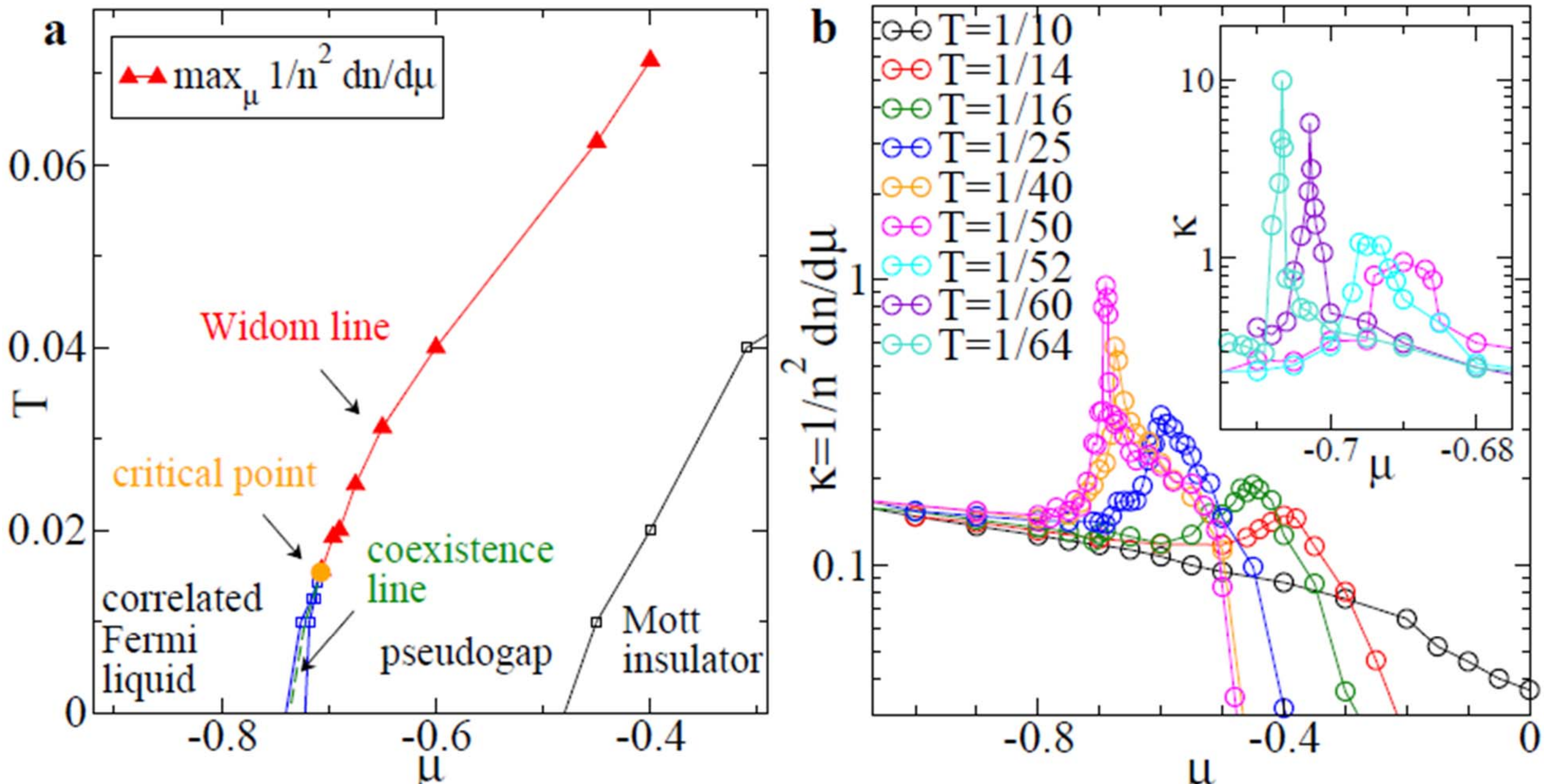
What is the Widom line?



McMillan and Stanley, Nat Phys 2010

- it is the continuation of the coexistence line in the supercritical region
- line where the maxima of different response functions touch each other asymptotically as $T \to T_p$
- 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

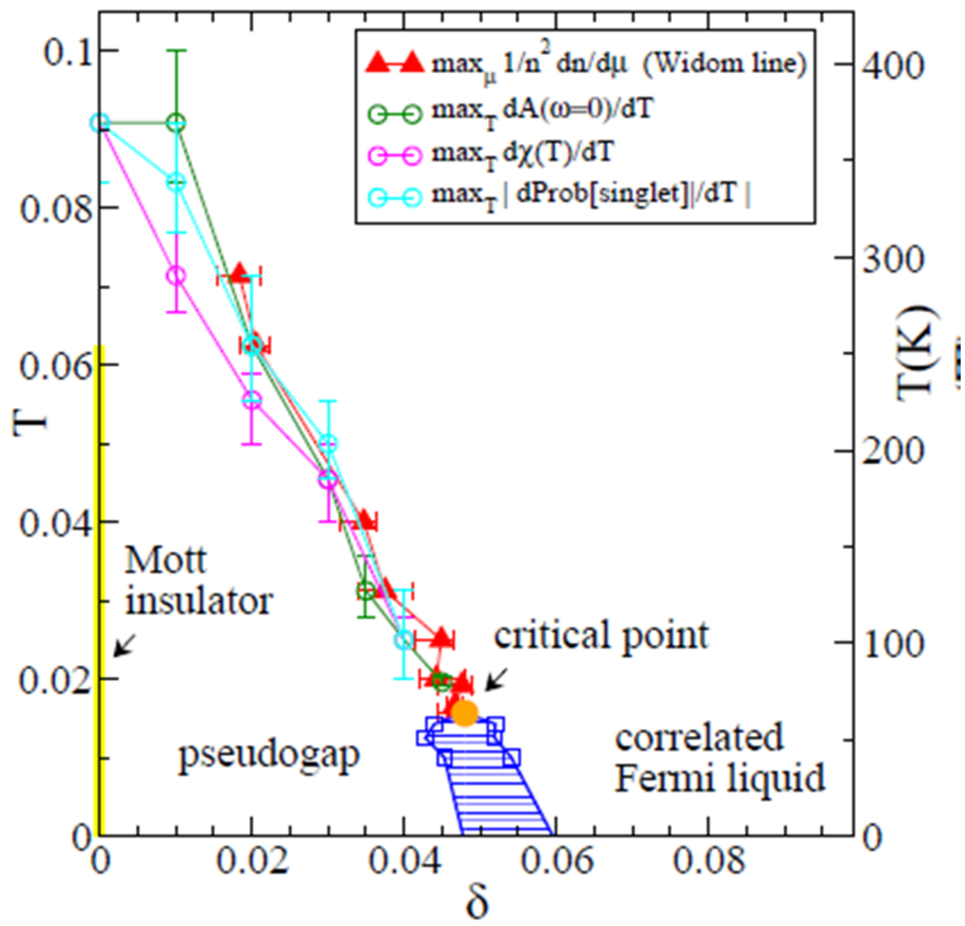


Widom line: defined from maxima of charge compressibility

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

divergence of κ at the (classical) critical point!

Phase diagram



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What is the minimal model?

H. Alloul arXiv:1302.3473

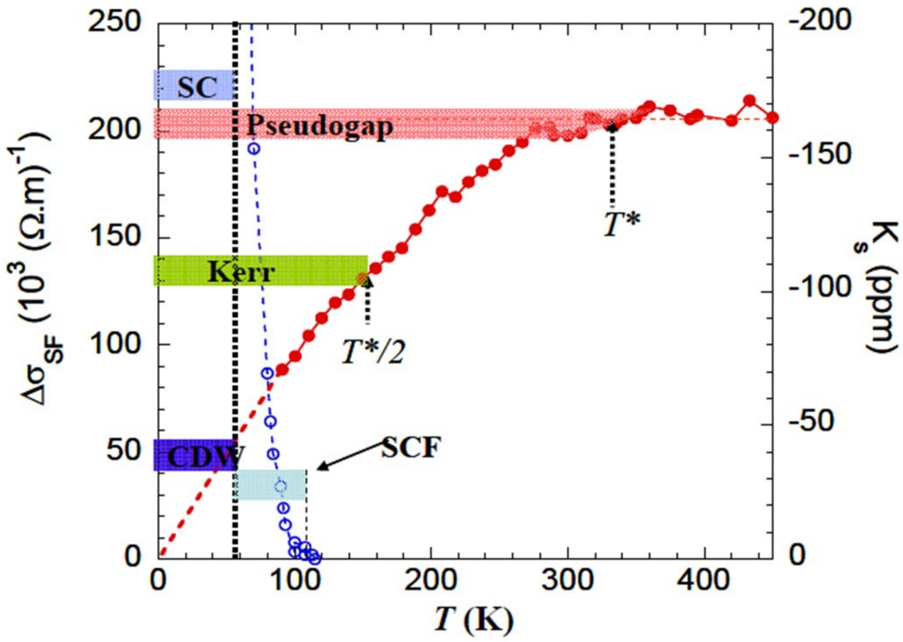

Fig 1 Spin contribution K_s to the ^{89}Y NMR Knight shift [11] for $YBCO_{6.6}$ permit to define the PG onset T^*. Here K_s is reduced by a factor two at $T \sim T^*/2$. The sharp drop of the SC fluctuation conductivity (SCF) is illustrated (left scale) [23]. We report as well the range over which a Kerr signal is detected [28], and that for which a CDW is evidenced in high fields from NMR quadrupole effects [33] and ultrasound velocity data [30]. (See text).

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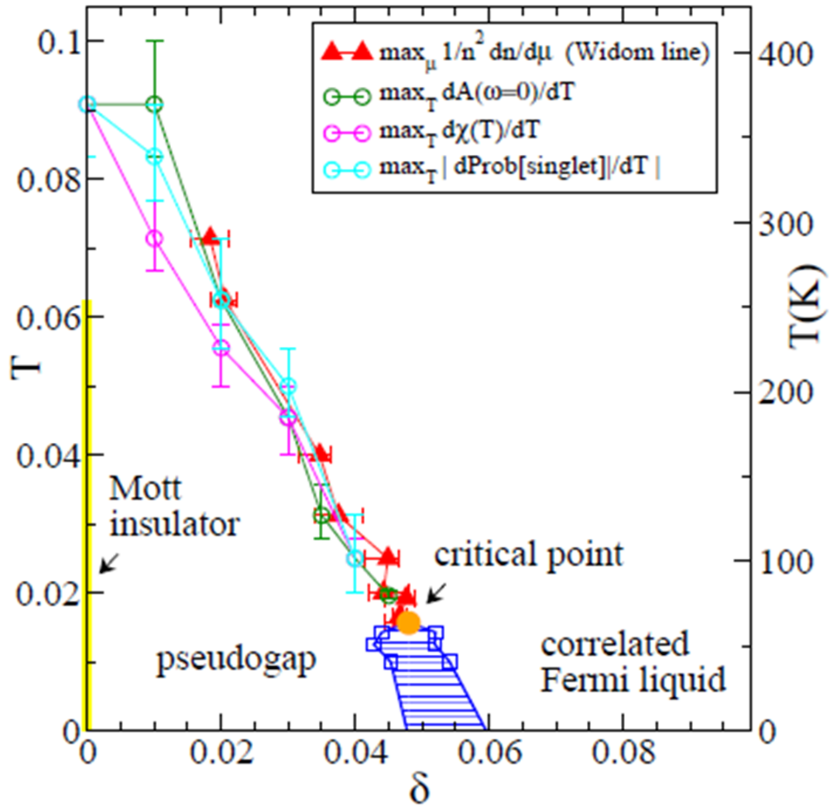
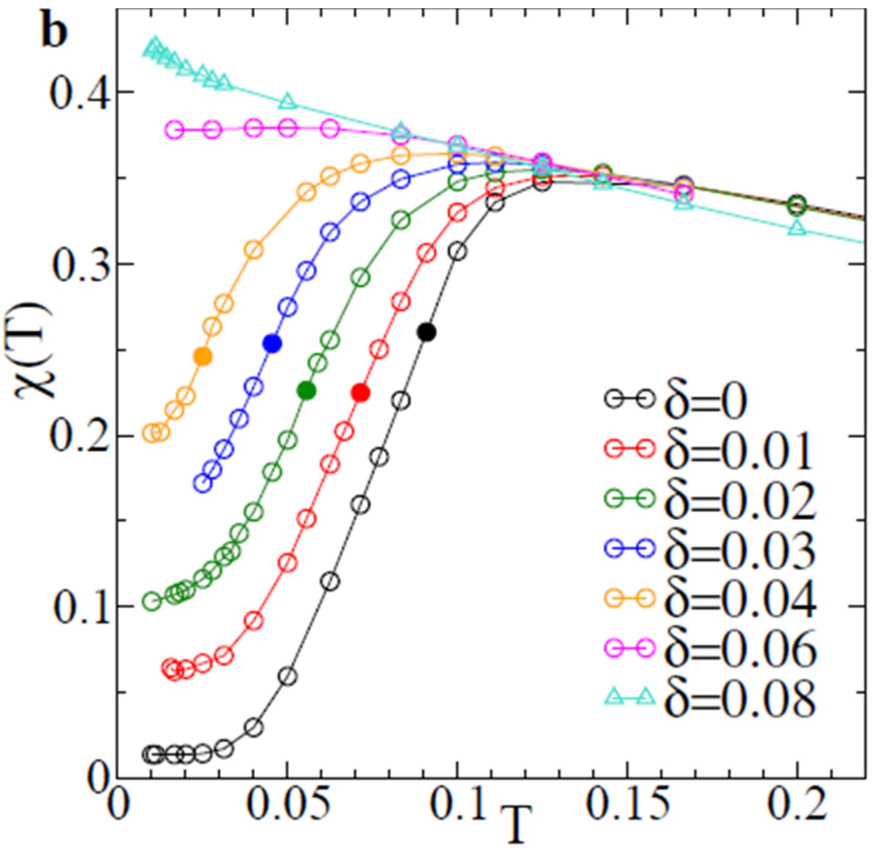
Spin susceptibility





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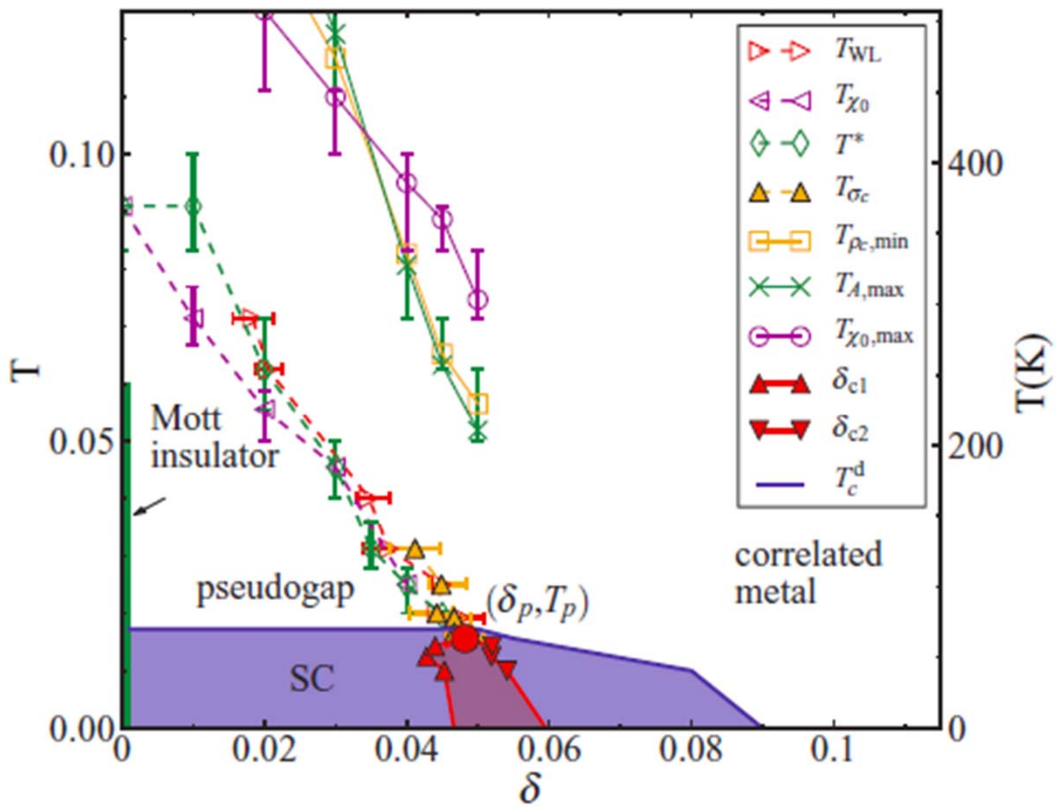
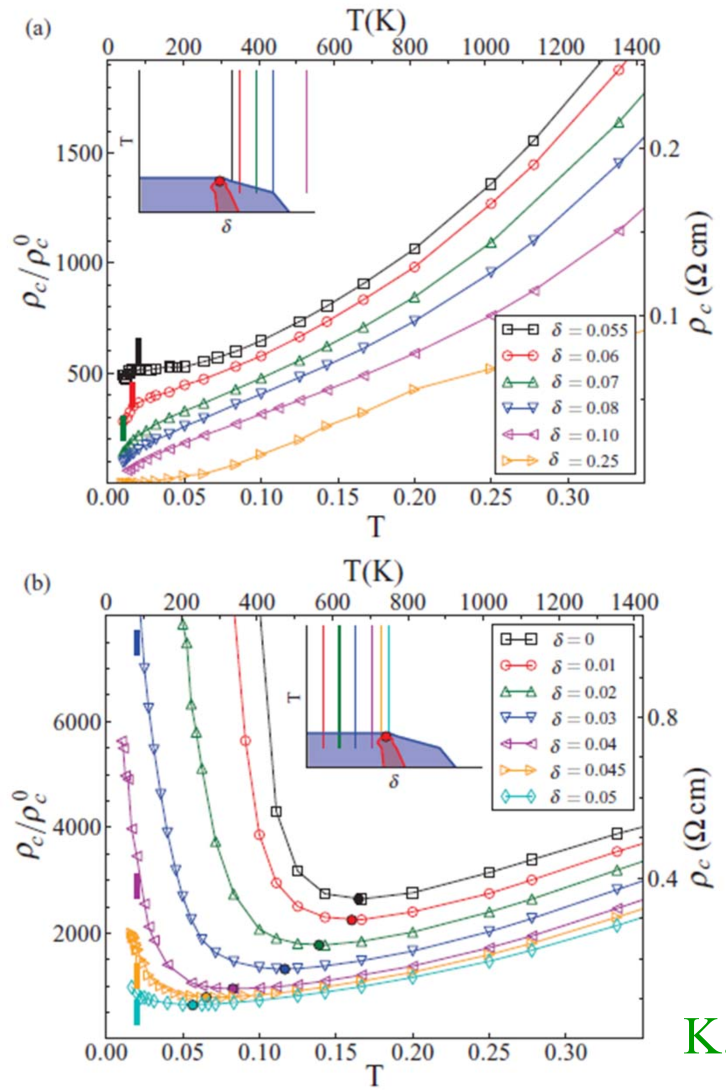
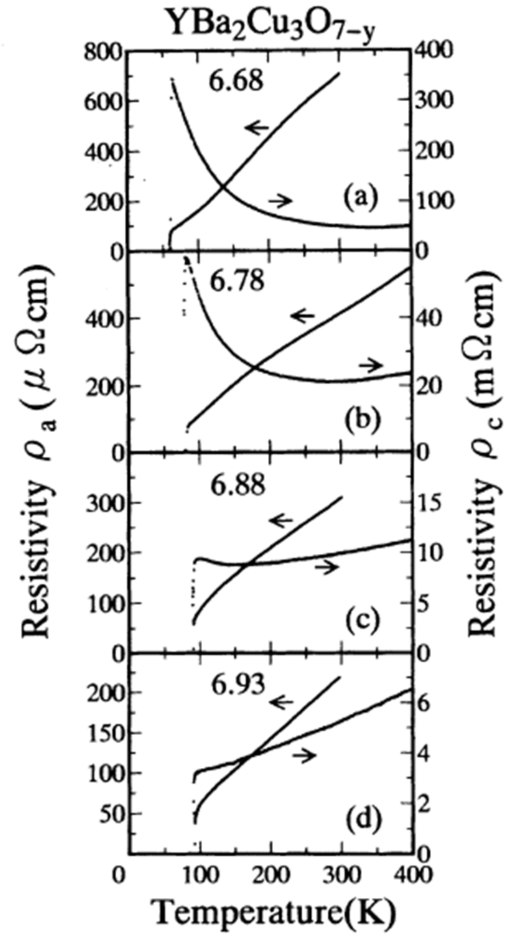
Two crossover lines



Sordi et al. PRL 108, 216401 (2012)
PRB **87**, 041101(R) (2013)

c-axis resistivity





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

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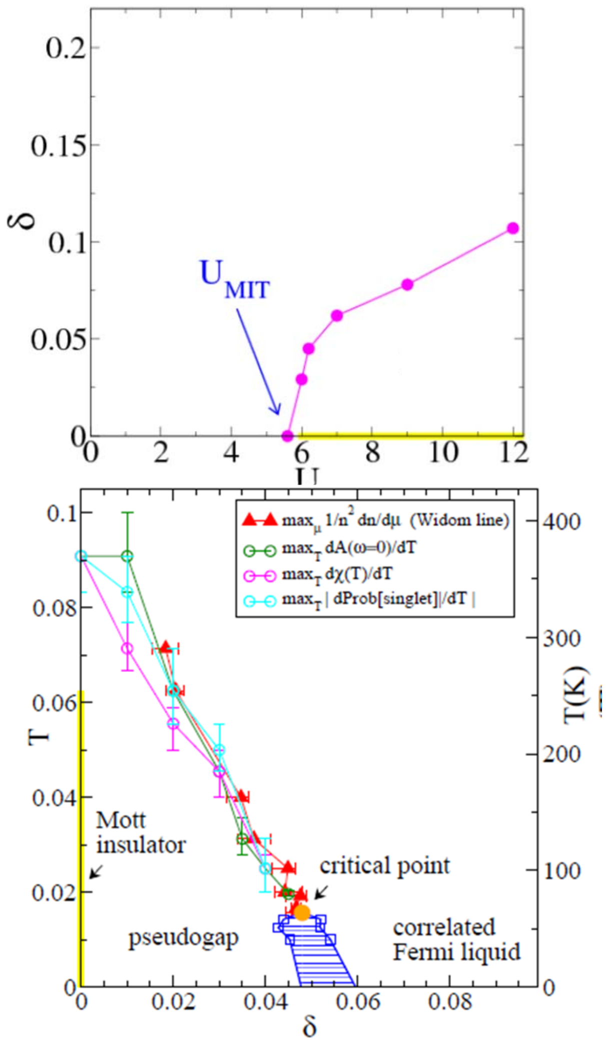
Summary: normal state



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

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Giovanni Sordi

Patrick Sémon

Lorenzo Fratino

Kristjan Haule

Finite *T* phase diagram Superconductivity

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

Fratino et al.

Sci. Rep. **6**, 22715

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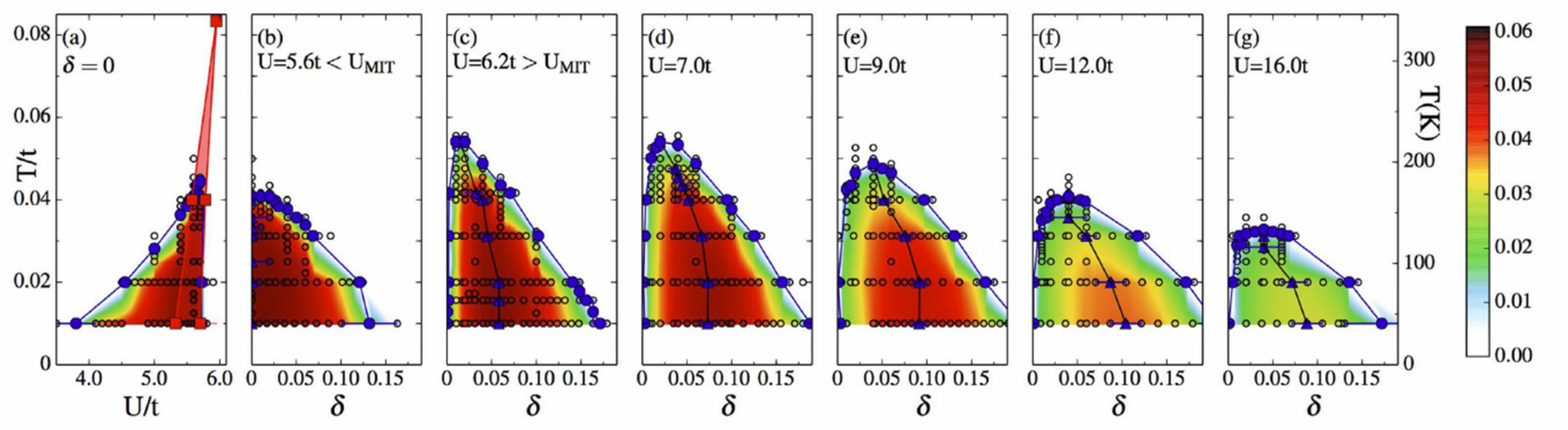
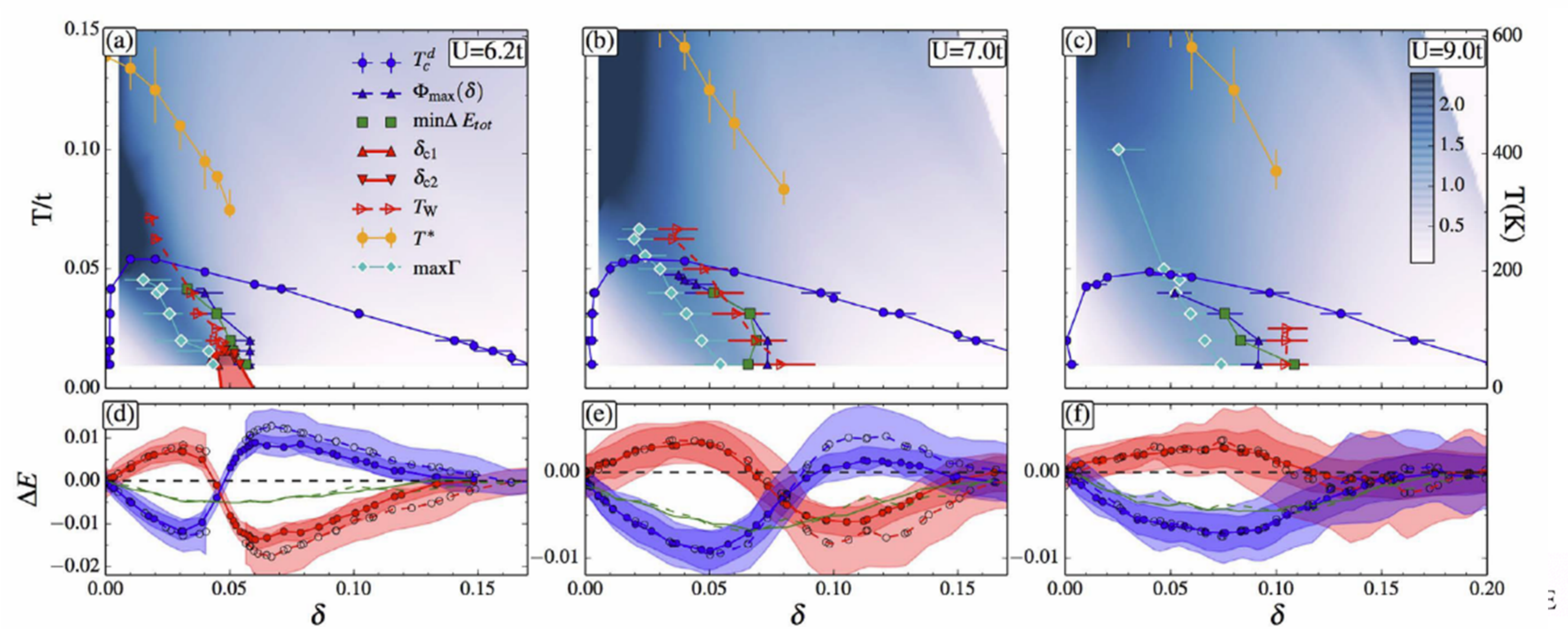
An organizing principle





Fratino et al.
Sci. Rep. **6**, 22715

3 bands, charge transfer insulator

Fratino et al. Phys. Rev. B in press

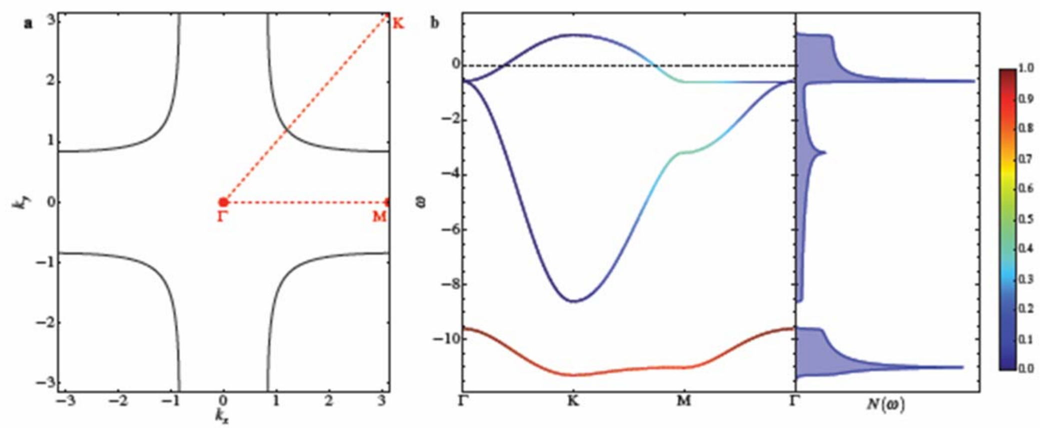
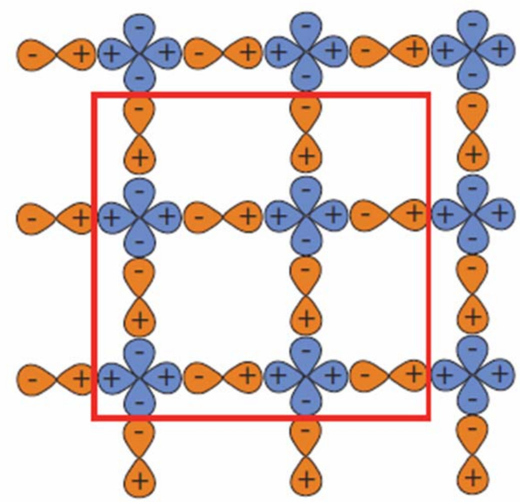


FIG. 2. (a) Noninteracting Fermi surface for the model parameter investigated in Fig. 1a of main text, namely $\epsilon_p = 9$, $t_{pp} = 1$, $t_{pd} = 1.5$, which gives a total occupation n_{tot} equal to five. (b) Non-interacting band structure for the same model parameter along with the resulting total density of states. Color corresponds to the d-character of the hybridised bands. The band crossing the Fermi level has mostly oxygen character.



Giovanni Sordi

Lorenzo Fratino

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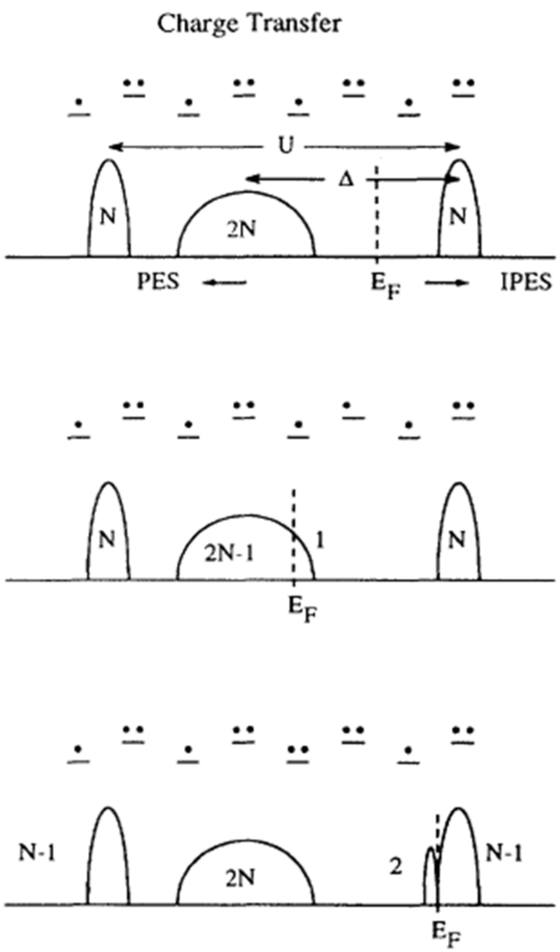
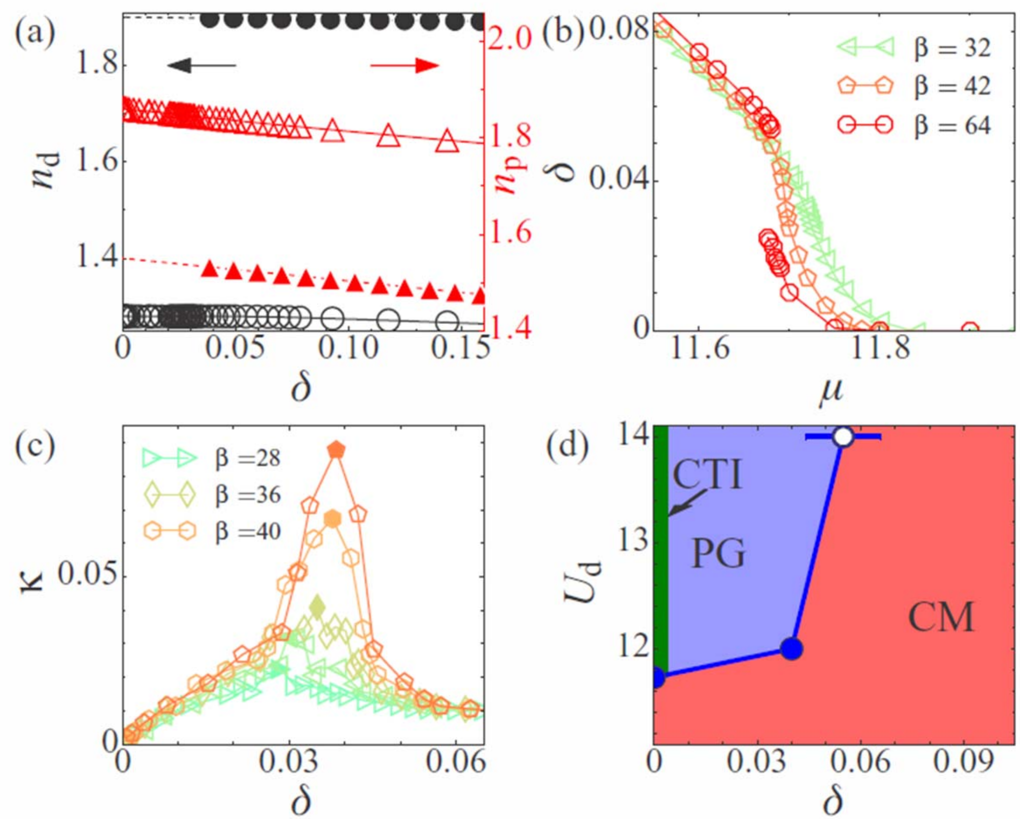
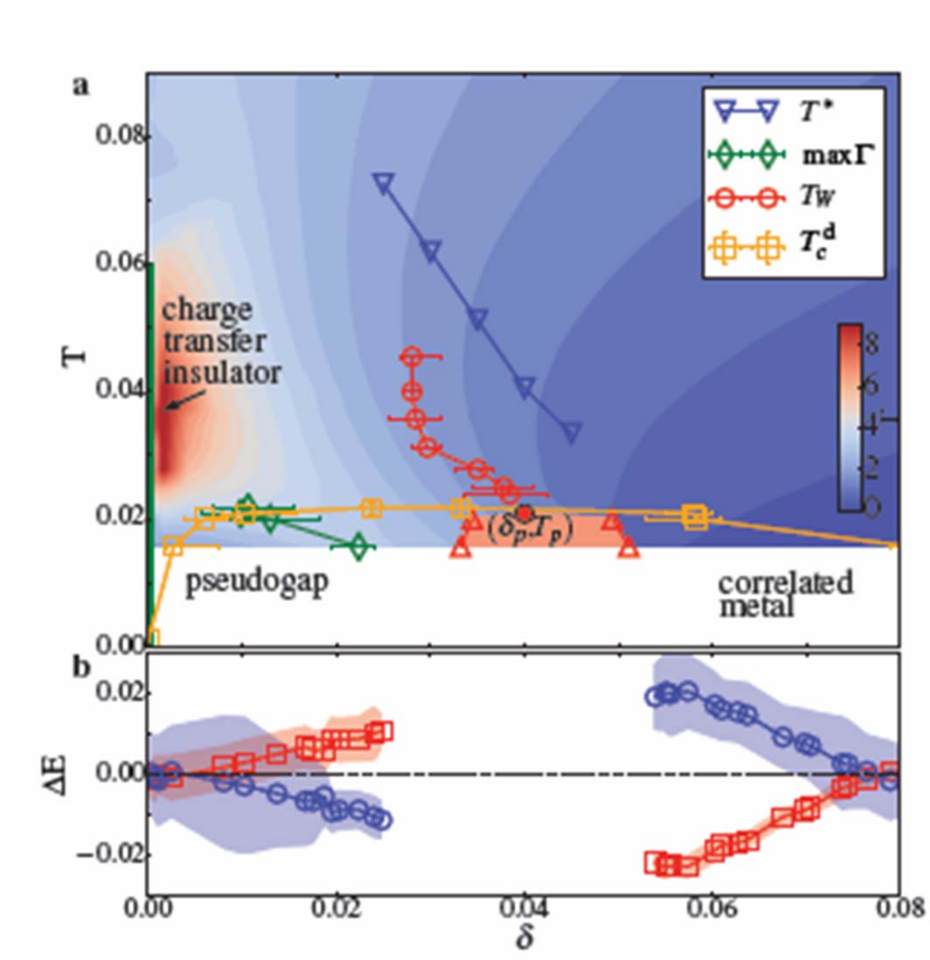
3 bands, charge transfer insulator





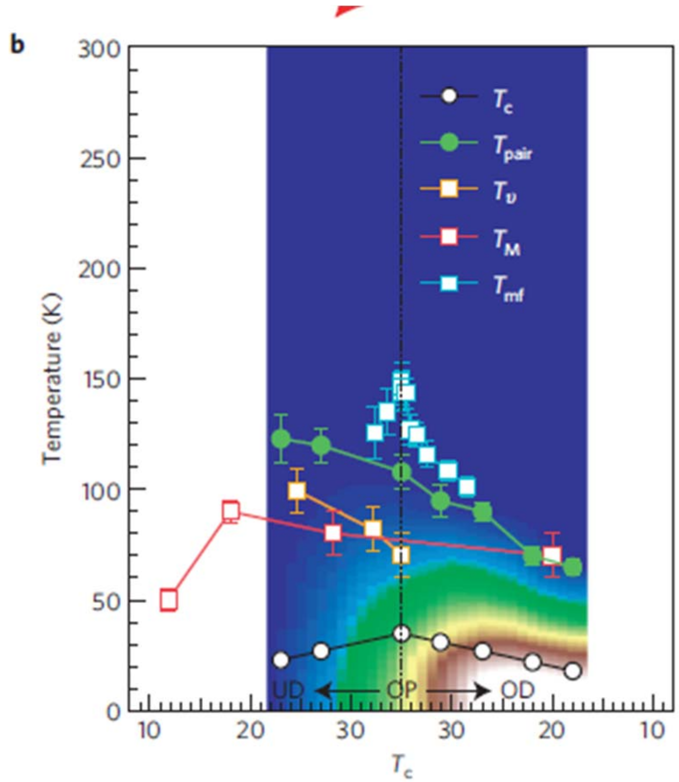
Fratino et al. Phys. Rev. B in press

3 bands, charge transfer insulator



Fratino et al. Phys. Rev. B in press

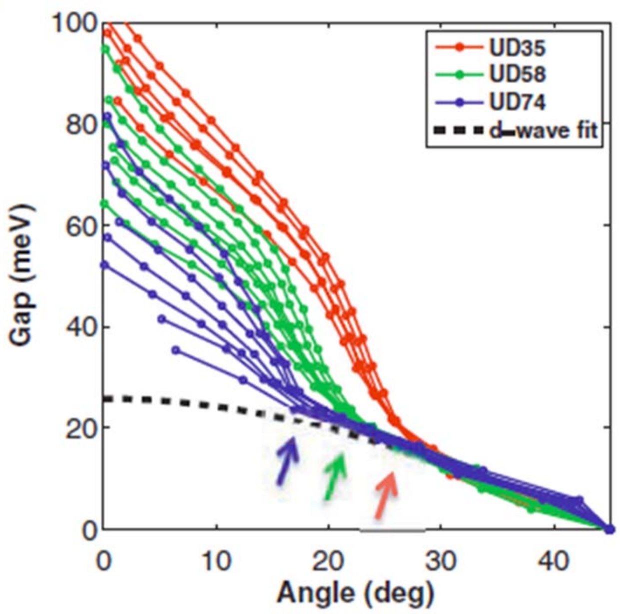
Tpair



ARPES
Bi2212

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

Meaning of T_c^d : Local pair formation



A. Pushp, Parker, … A. Yazdani, Science **364**, 1689 (2009)

However, our measurements demonstrate that the nodal gap does not change with reduced doping. The pairing strength does not get weaker or stronger as the Mott insulator is approached; rather, it saturates.

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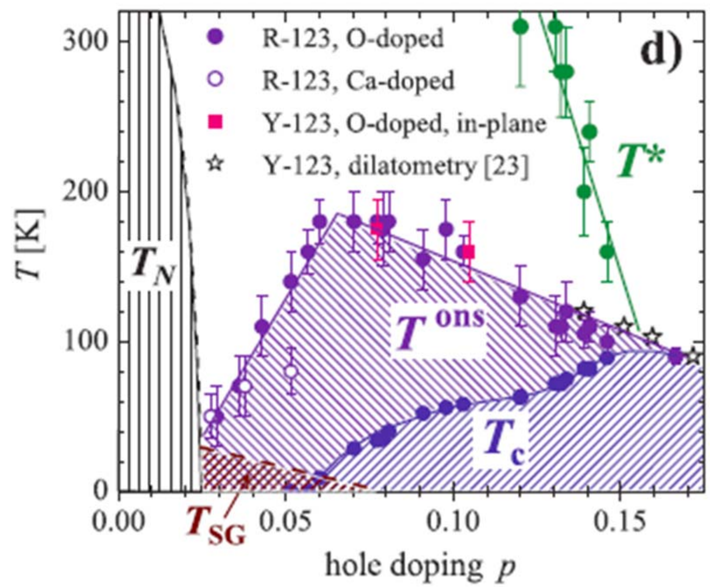
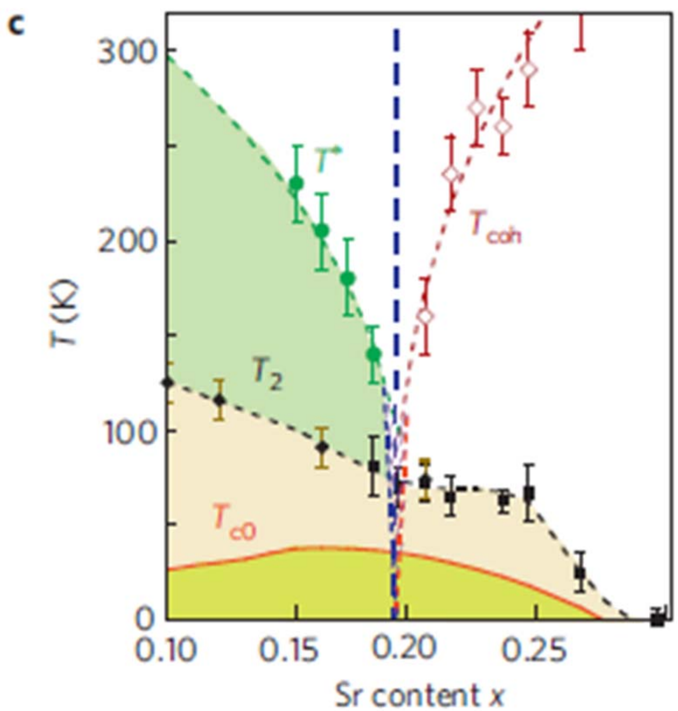
Fluctuating region



Infrared response

Dubroka et al. PRL 106, 047006 (2011)

T_2



Magnetoresistance, LSCO
Fluctuating vortices

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

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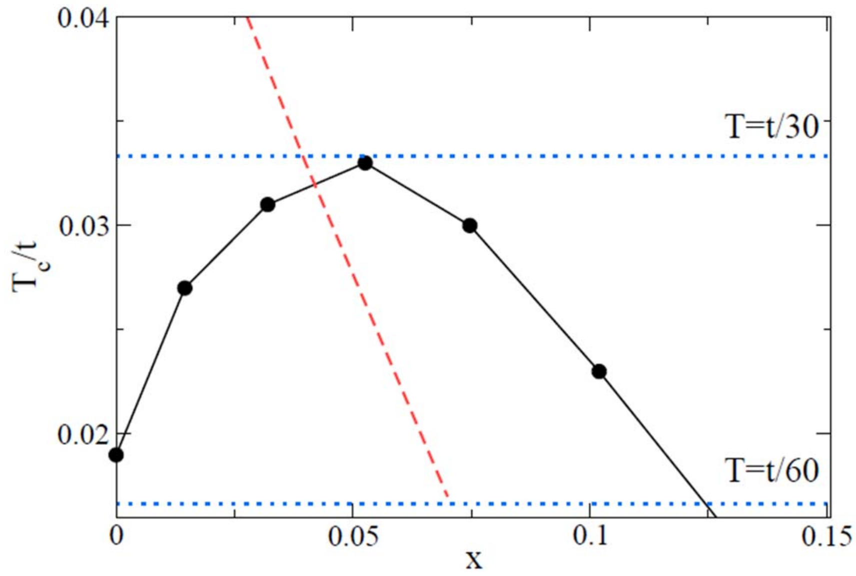
Actual T_c in underdoped

- 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).

Larger clusters

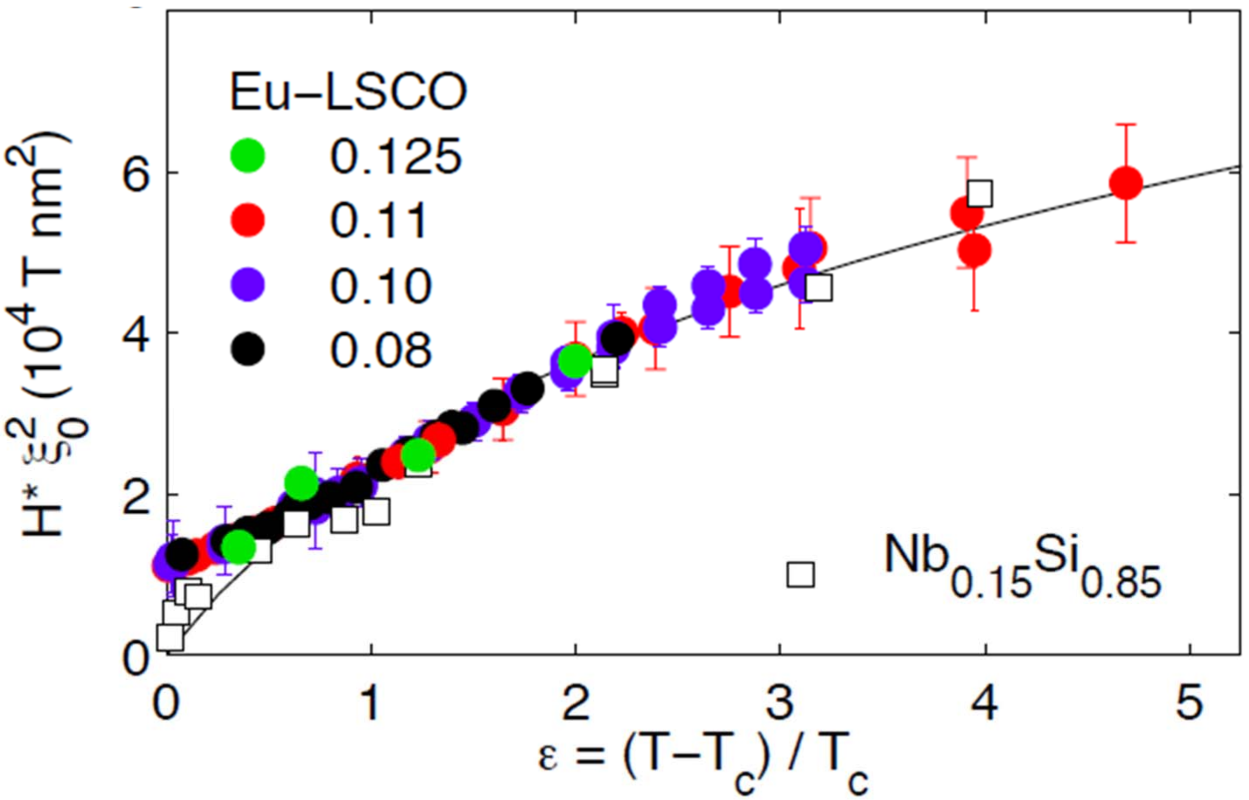
- Is there a minimal size cluster where T_c vanishes before half-filling?
- Learn something from small clusters as well
- Local pairs in underdoped

Larger cluster 8 site DCA



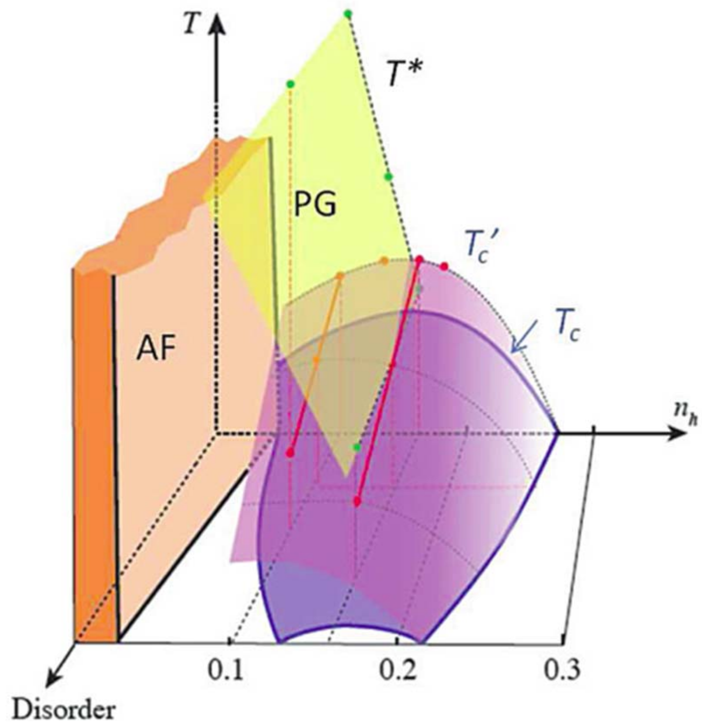
Gull, Millis, arxiv.org:1304.6406

Gaussian amplitude fluctuations in Eu-LSCO



Chang, Doiron-Leyraud et al.

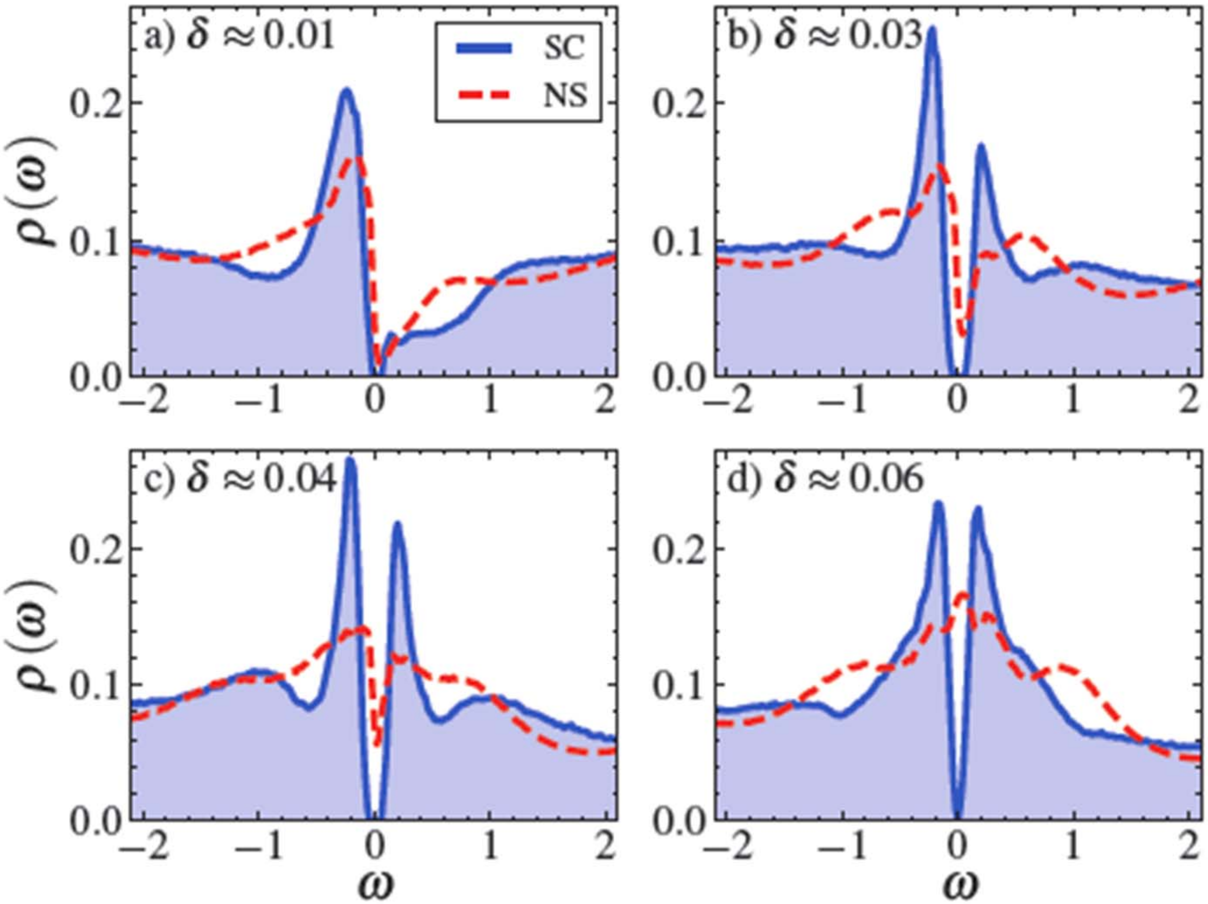
Effect of disorder



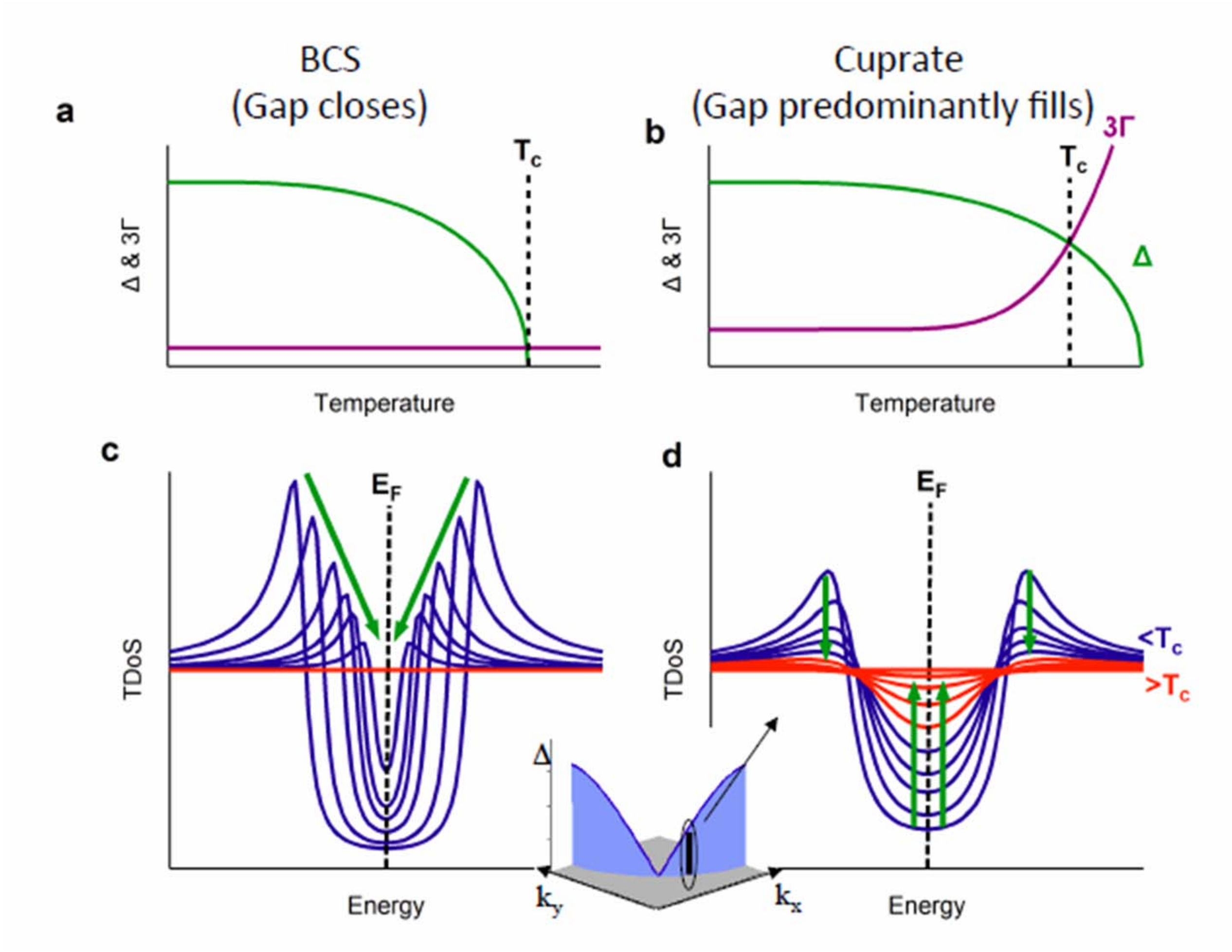
F. Rullier-Albenque, H. Alloul, and G.Rikken,
Phys. Rev. B **84**, 014522 (2011).

Superconductivity in underdoped vs BCS

First-order transition leaves its mark



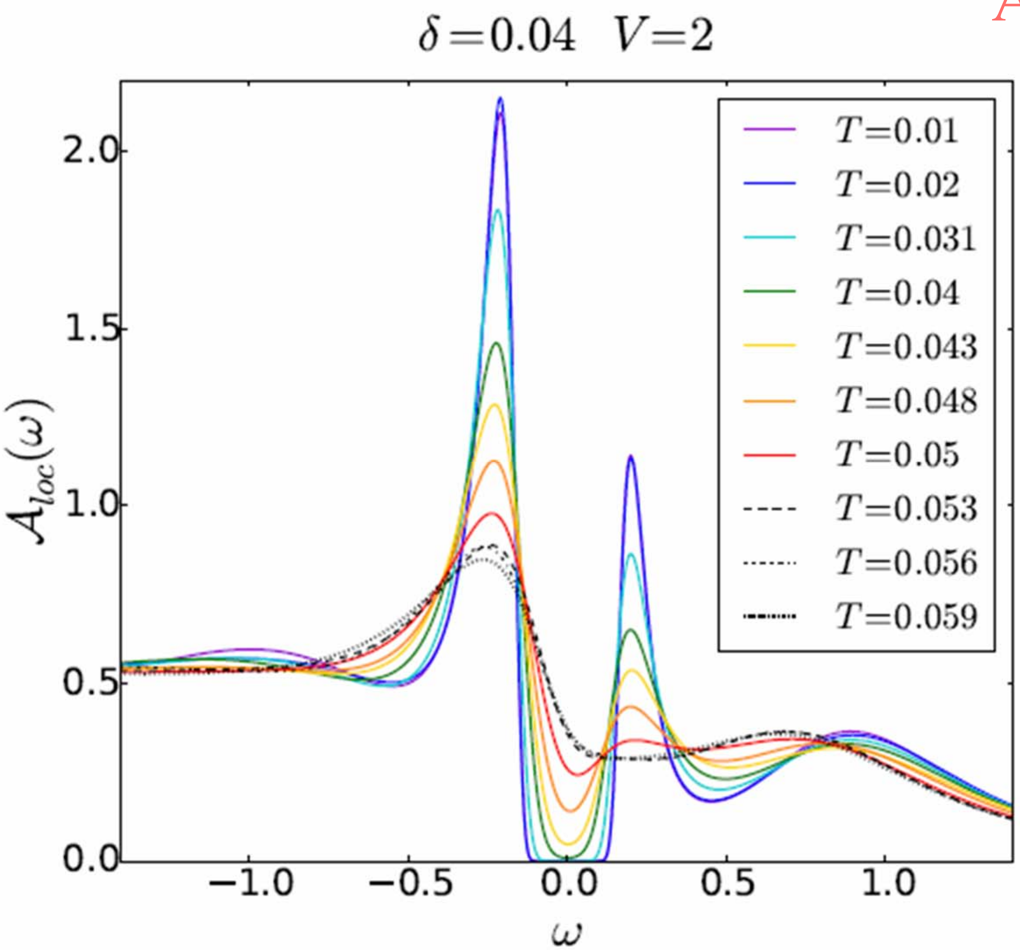
Schematic *T* dependence of the gap



T.J. Reber, … D.S. Dessau, arXiv:1508.06252

T dependence of the gap underdoped

Alexis Reymbaut



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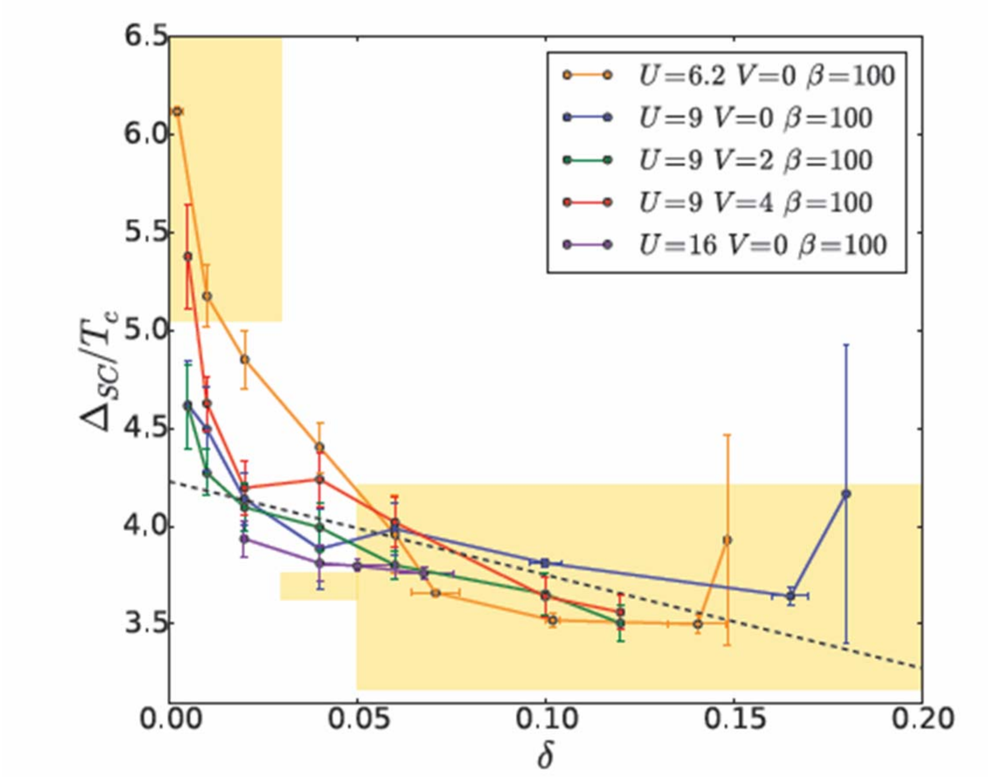
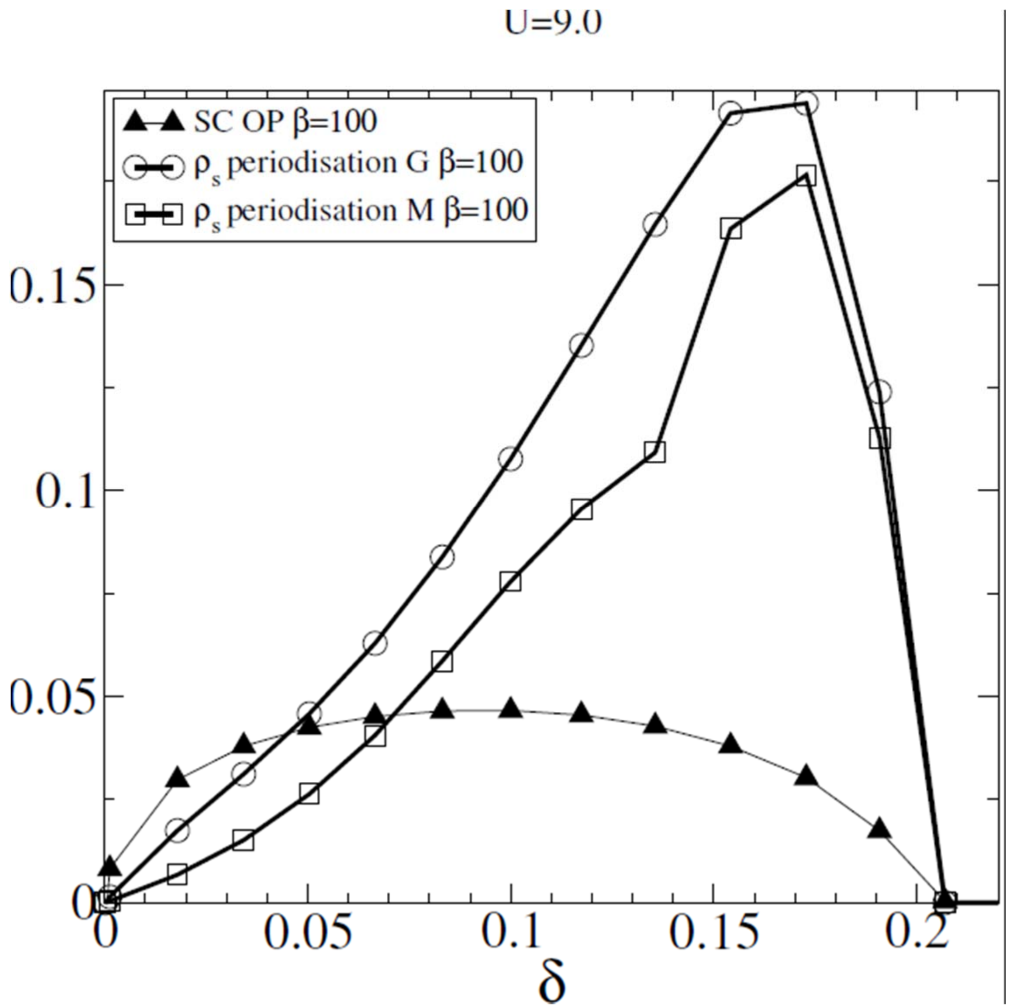
Δ/T_c

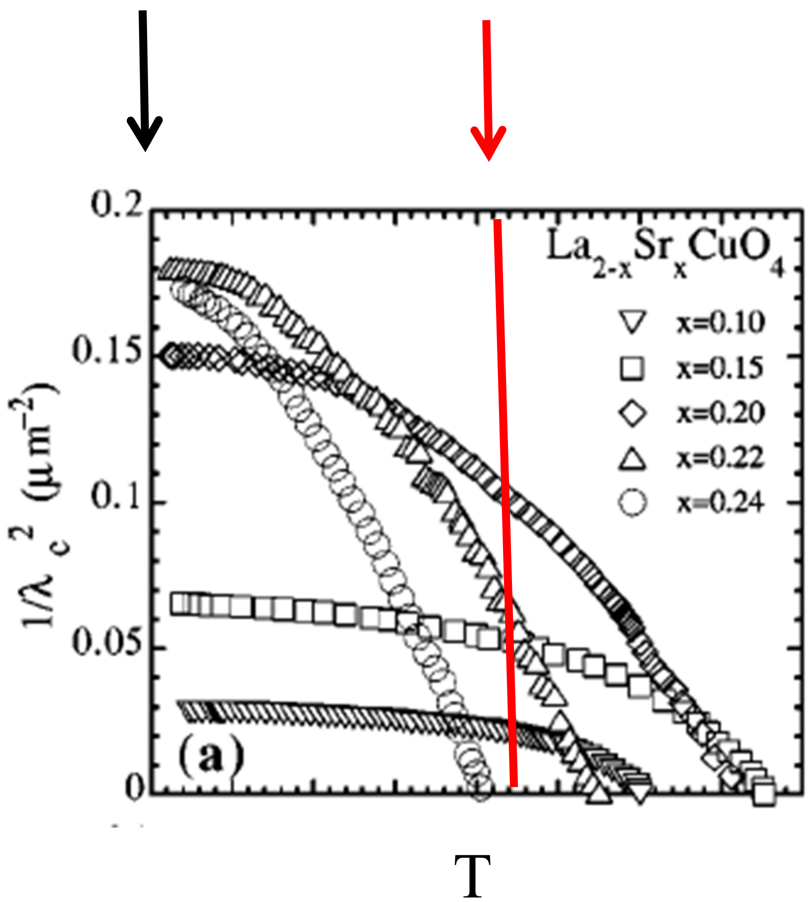


A. Reymbaut, PhD thesis, Sherbrooke 2016

c-axis Superfluid stiffness *U = 9t, T=1/100*

Fratino, Sordi, unpubllished





Panagopoulos et al. PRB 2000

See also, Gull Millis, PRB, 2013

Also from 8 site DCA

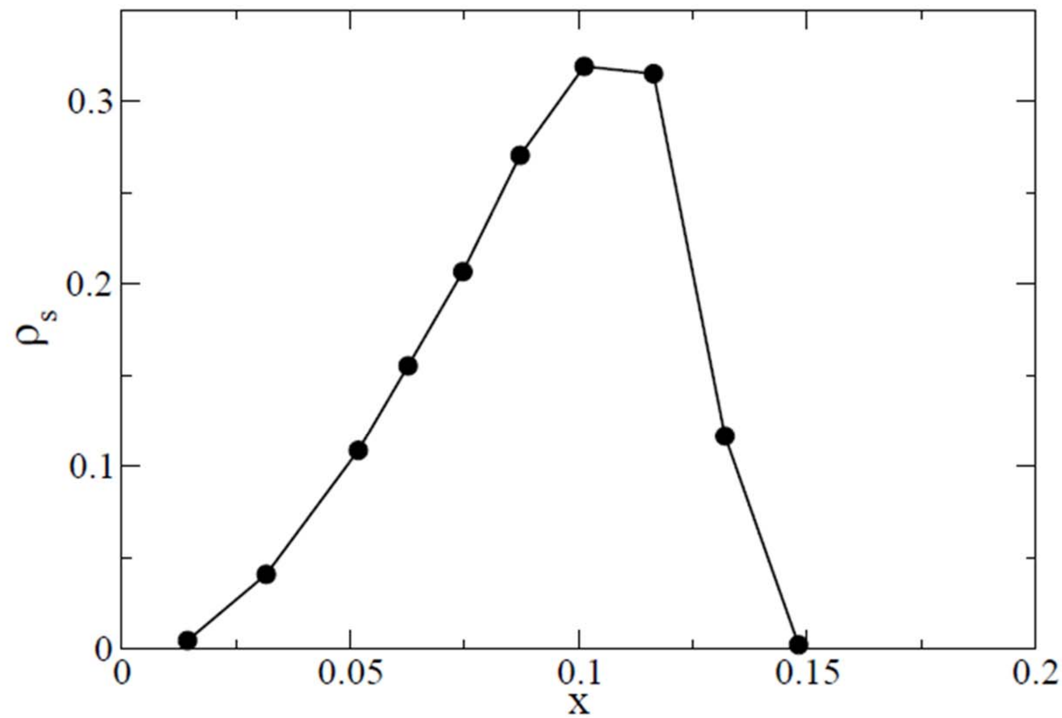


FIG. 8. Superfluid stiffness ρ_s determined in the superconducting state at $T = t/60$ from Eq. 15, as a function of doping.

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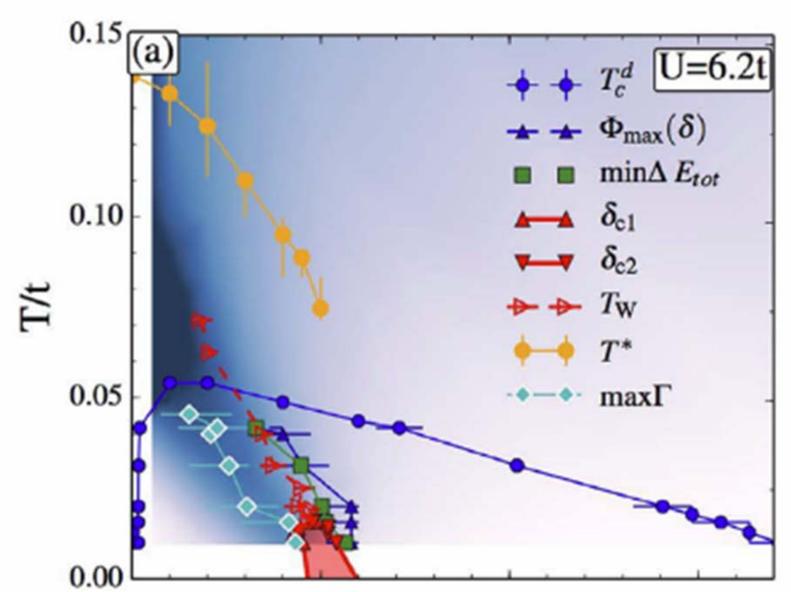
Summary



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

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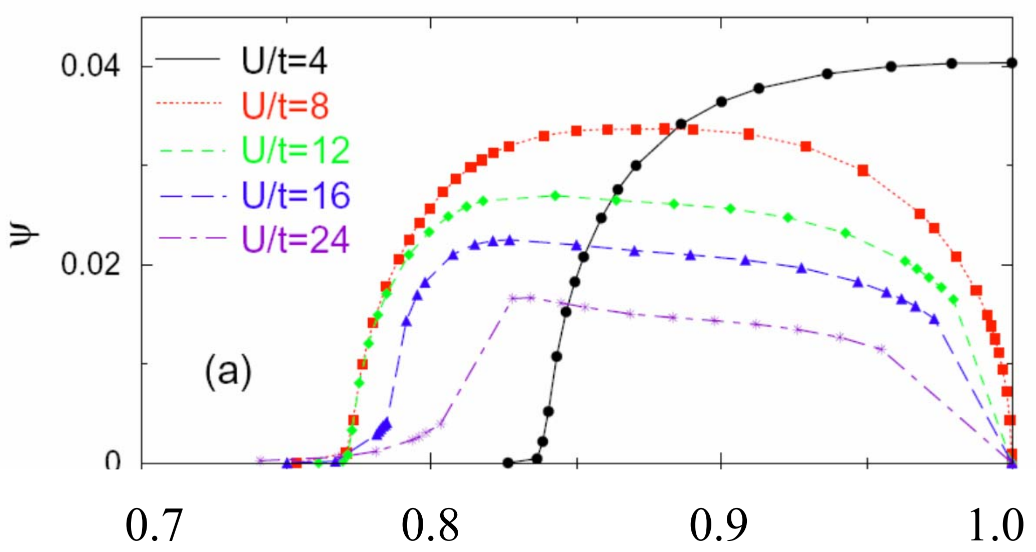
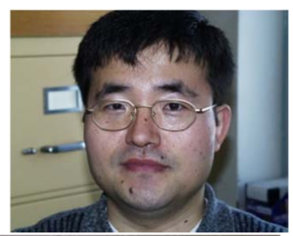
T = 0 phase diagram: superconductivity

Mechanism in the presence of strong correlation

Dome vs Mott (CDMFT)



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



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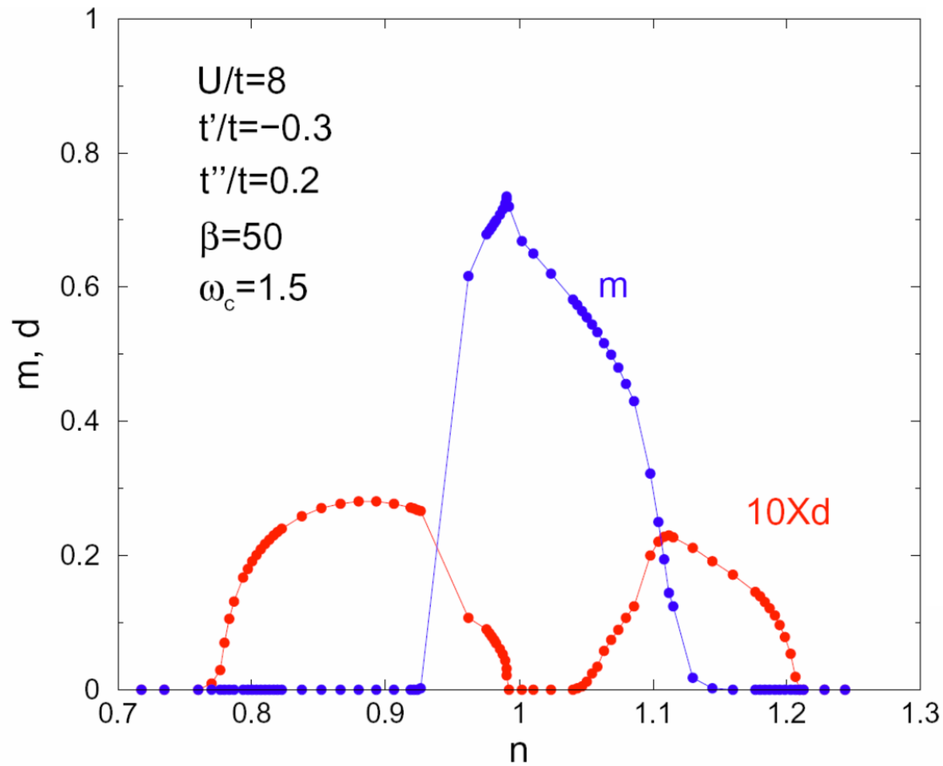
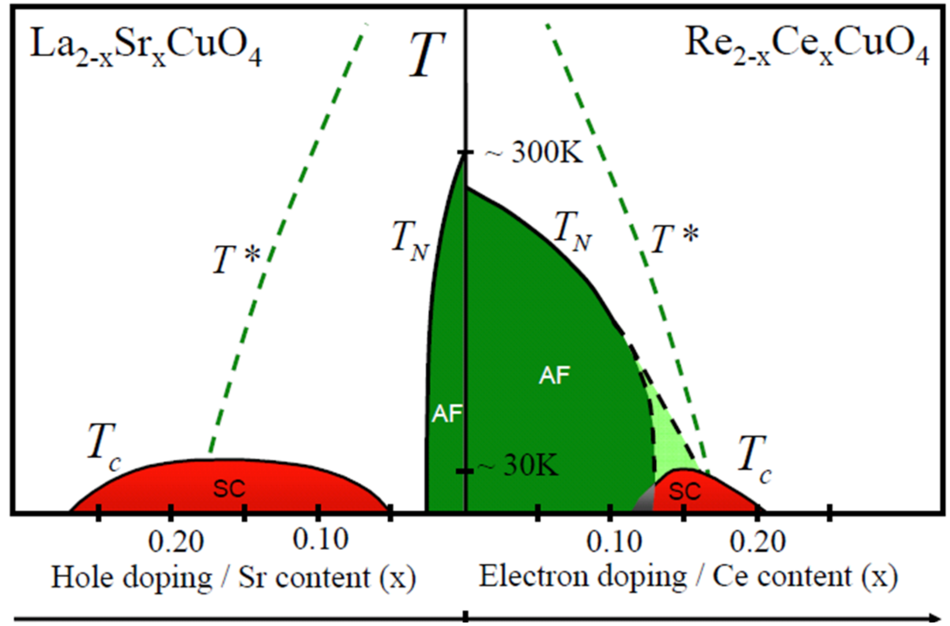
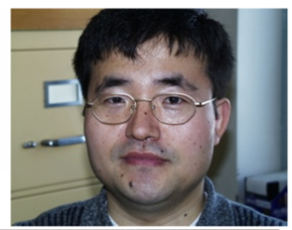
CDMFT global phase diagram

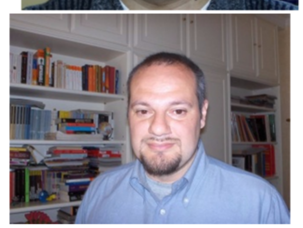


Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008)
AND Capone, Kotliar PRL (2006)



Armitage, Fournier, Greene, RMP (2009)





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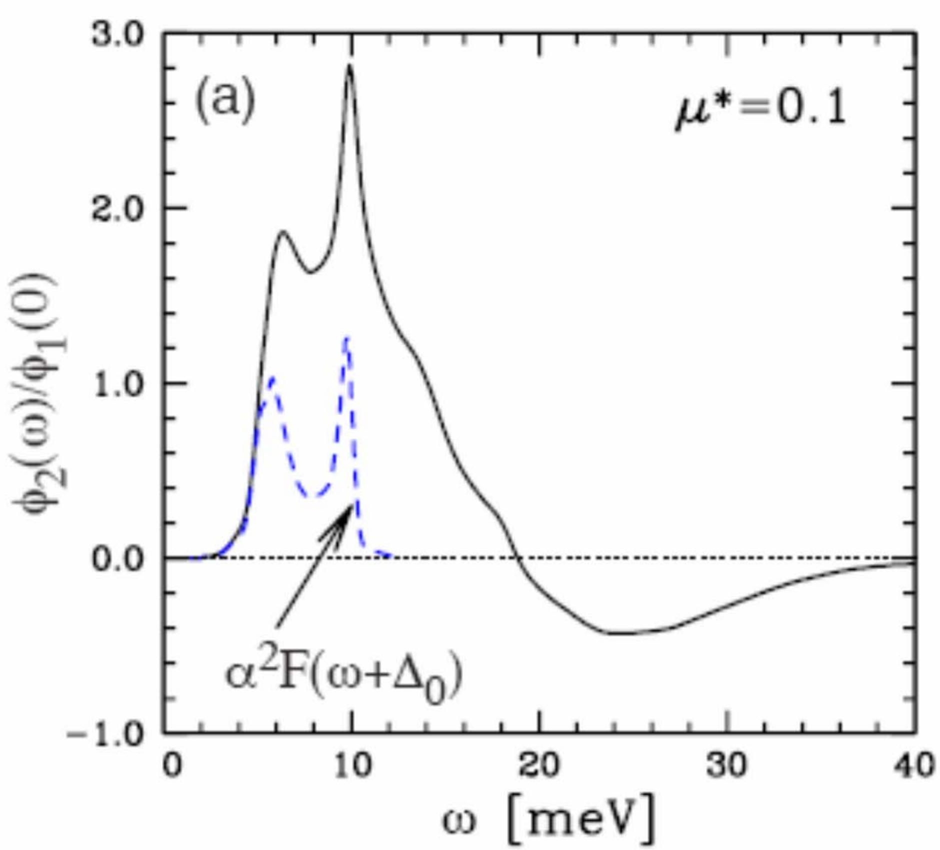
The glue

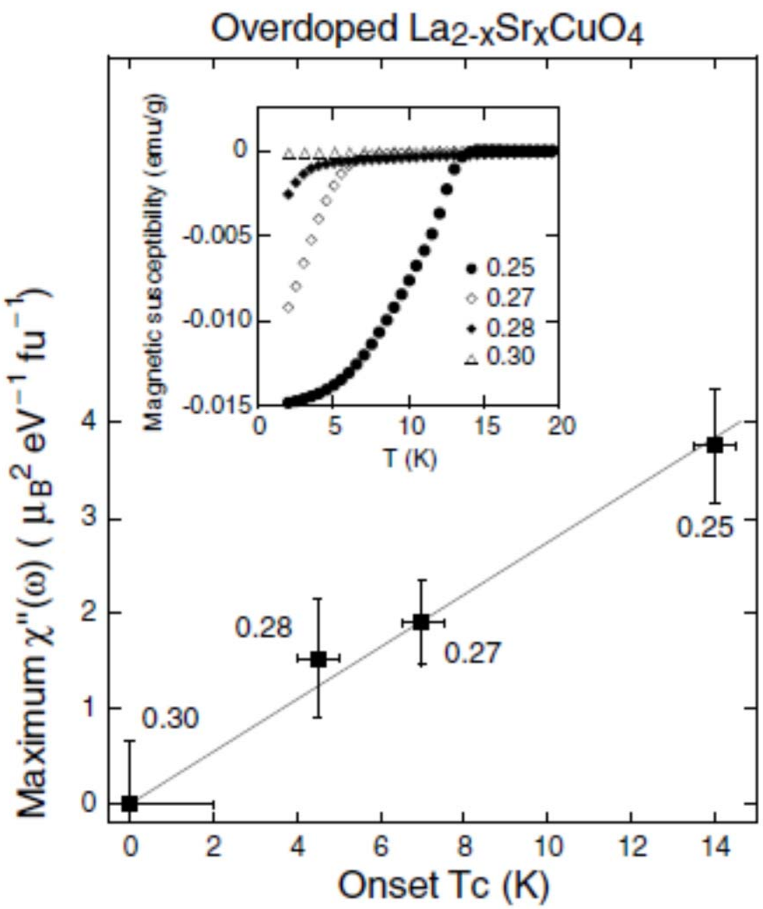
Im Σ_{an} and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

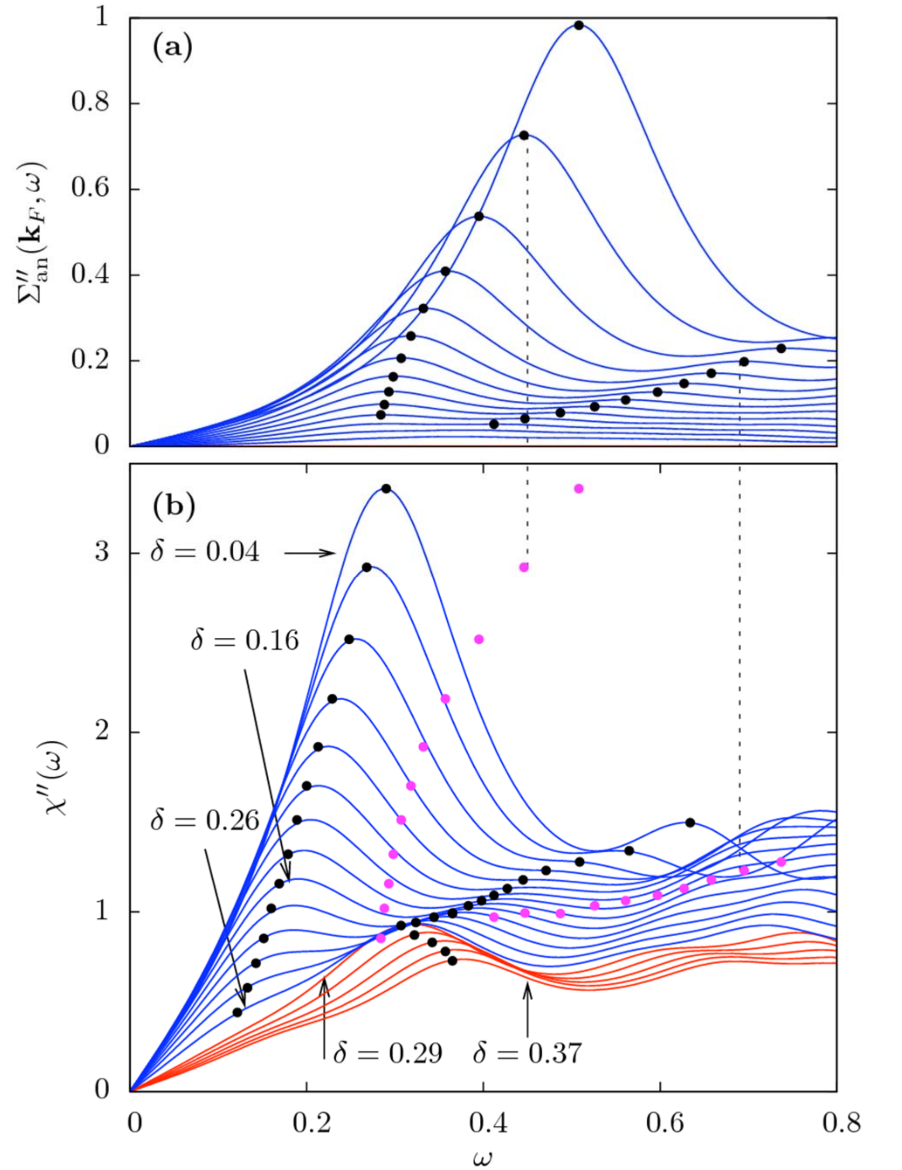


The glue

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



Wakimoto … Birgeneau PRL (2004)



The glue and neutrons

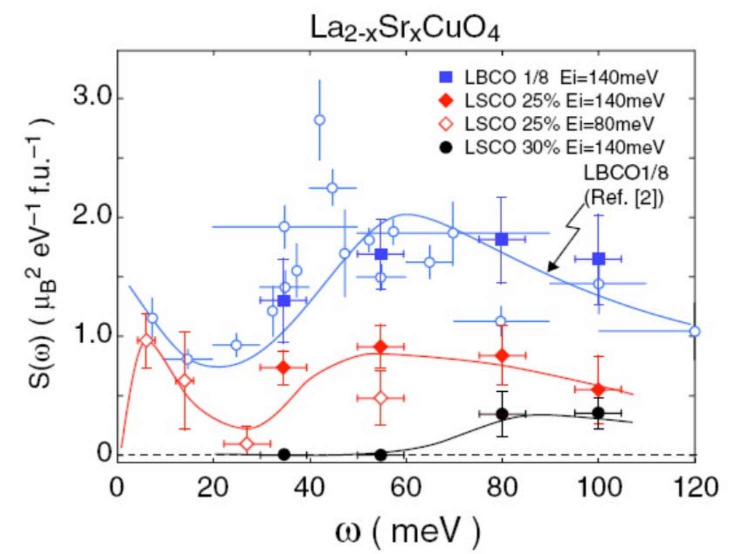
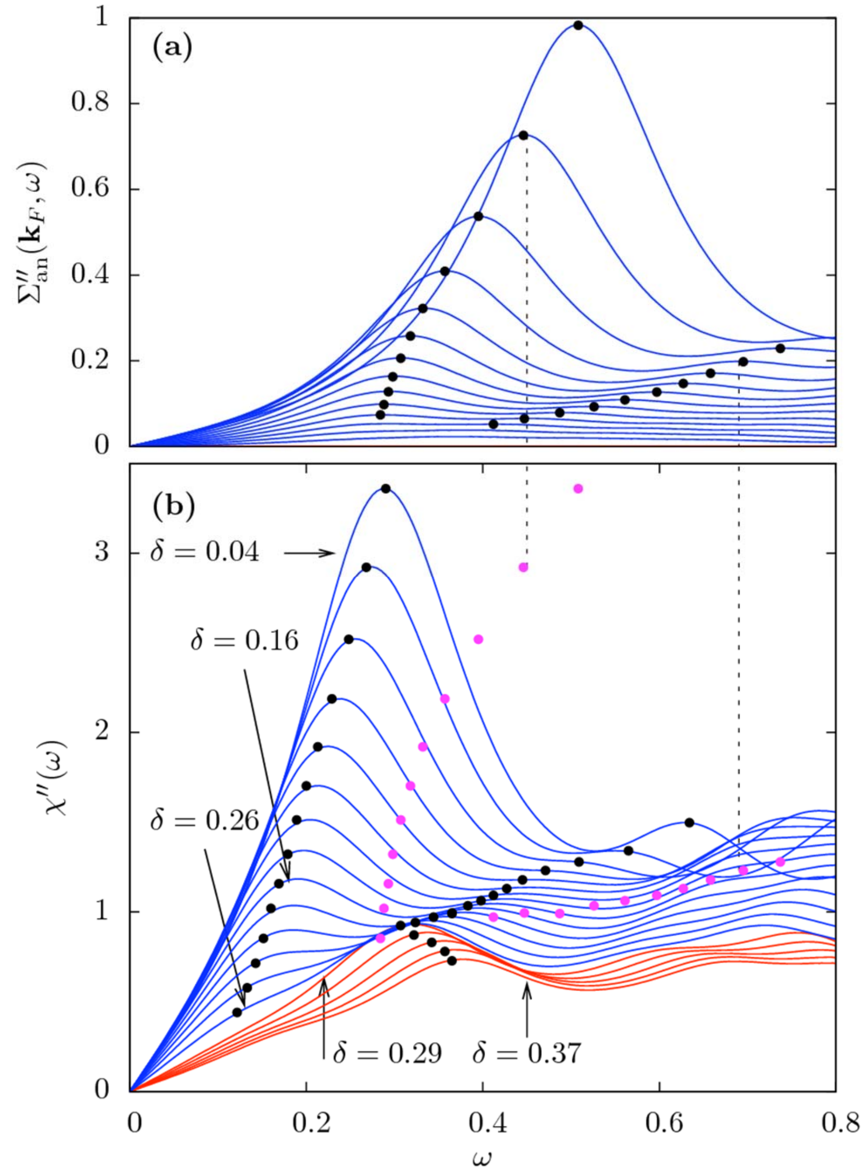


FIG. 3 (color online). **Q**-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-H integrated profiles for LBCO $1/8$ (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i = 140$ meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO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



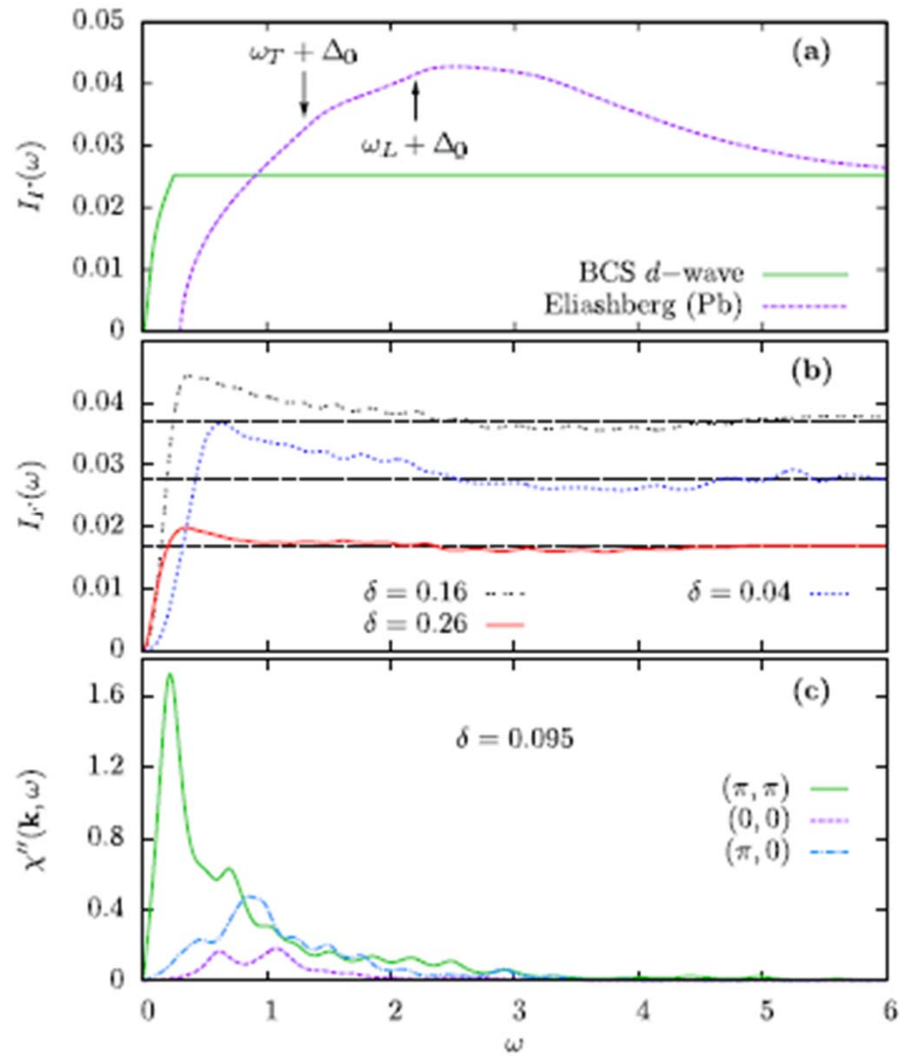
Frequencies important for pairing

Bumsoo Kyung

David Sénéchal

$$I_F(\omega) \equiv -\int_0^{\omega} \frac{d\omega'}{\pi} \mathrm{Im}\, F^R_{ij}(\omega').$$

$\langle c_{i\uparrow} c_{j\downarrow} \rangle$ for $\omega \rightarrow \infty$



B. Kyung, D. Sénéchal, and A.-M. S.T, Phys. Rev. B **80**, 205109 (2009).

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Resilience to near-neighbor repulsion *V*

In mean-field, $J - V$

$J = 130\ meV$

$V = 400\ meV$

The $\ln(E_F/\omega_D)$ necessary to screen *V*, for μ^* not enough

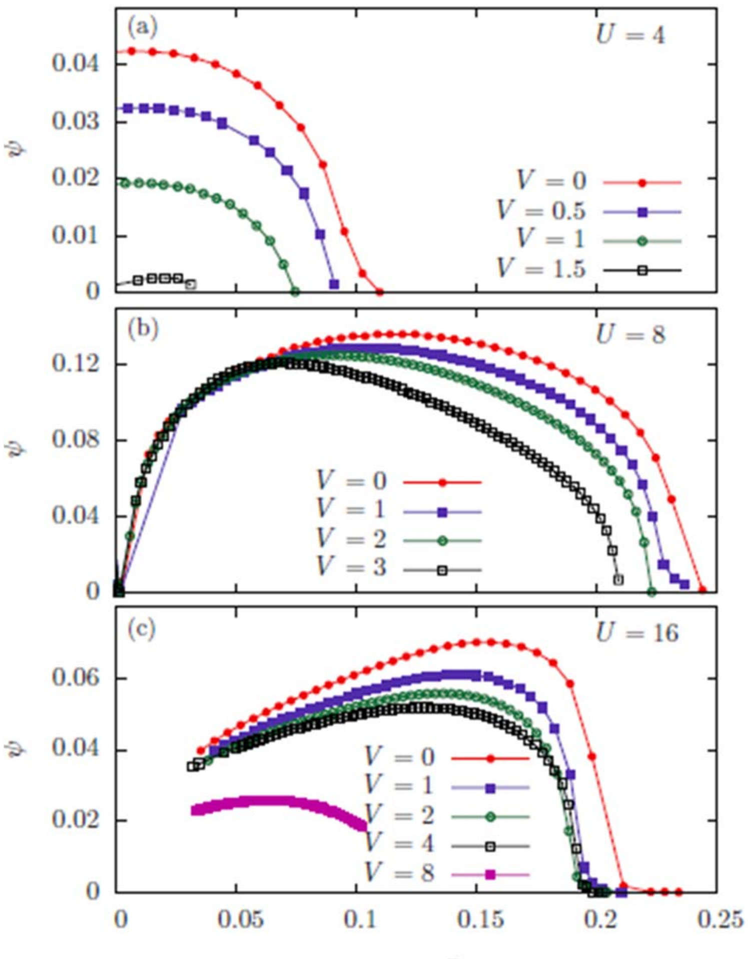
Weak-coupling: $V < U\ (U/W)$ for survival of d-wave

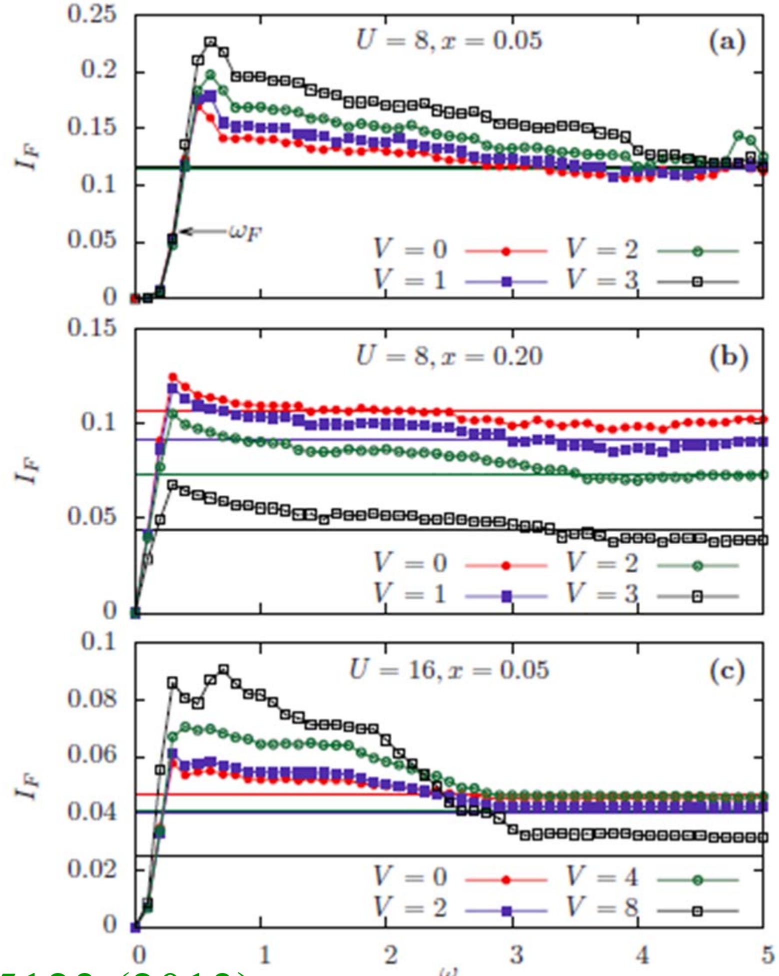
S. Raghu, E. Berg, A. V. Chubukov, and S. A. Kivelson, PRB **85**, 024516 (2012).
S. Onari, R. Arita, K. Kuroki, and H. Aoki, PRB **70**, 094523 (2004).

Resilience to near-neighbor repulsion

David Sénéchal

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





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

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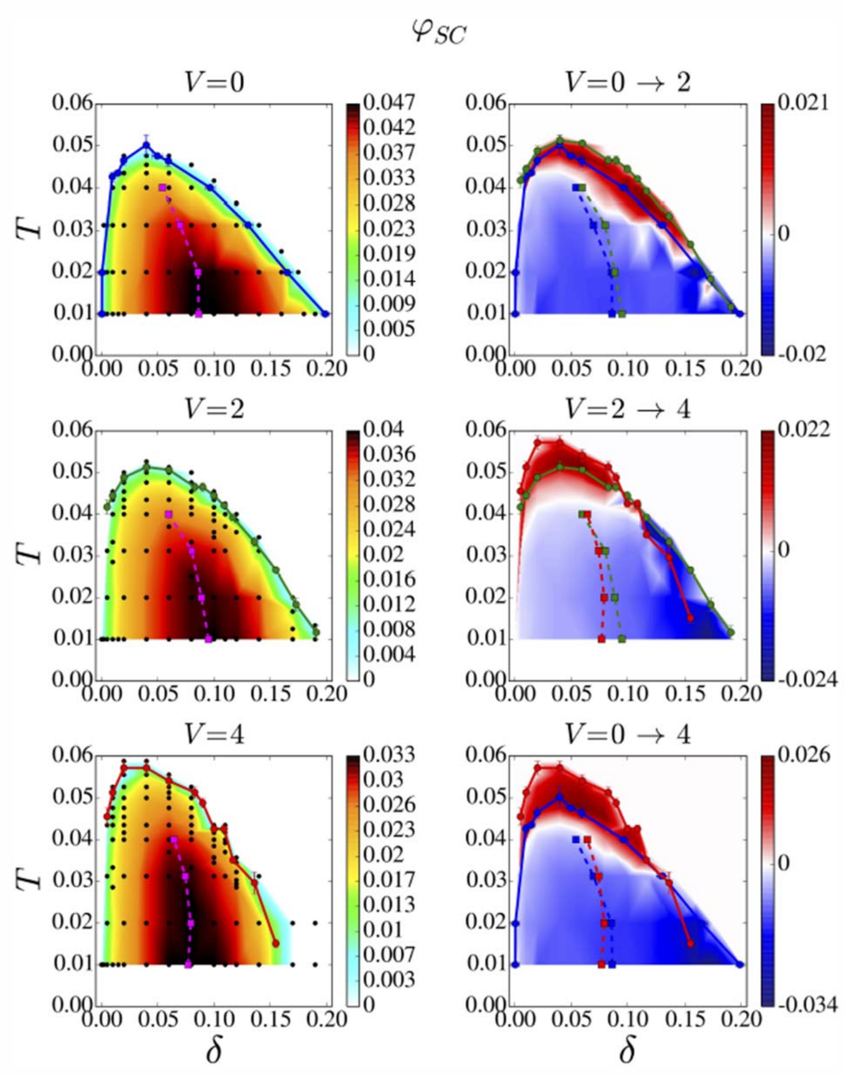
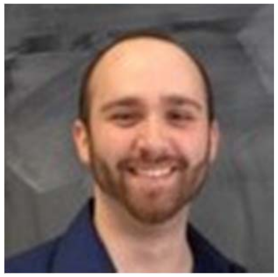
Effect of *V*, finite temperature, *U* = 9*t*



Thesis, Alexis Reymbaut

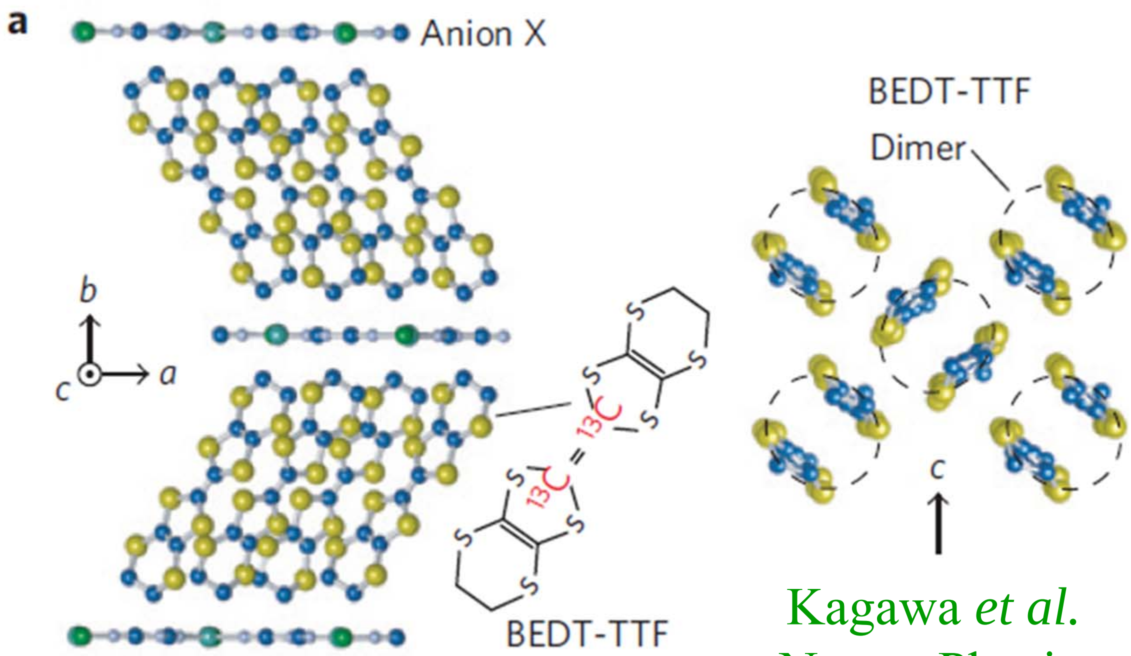


Alexis Reymbaut

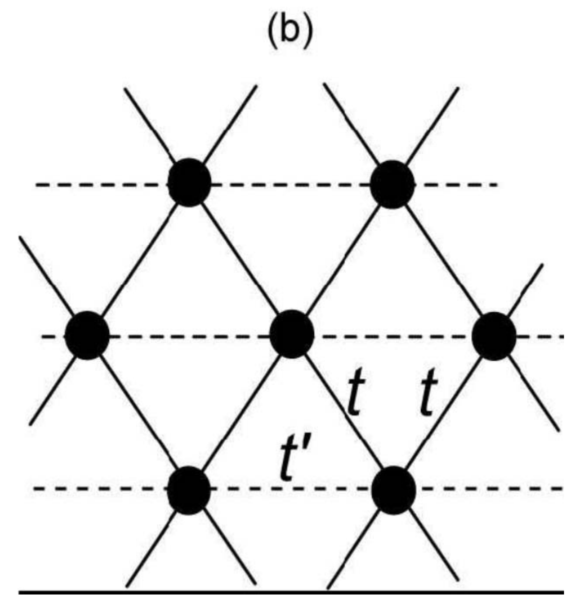
6. Superconductivity in the organics

Hubbard on anisotropic triangular lattice

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



Kagawa *et al.*
Nature Physics
5, 880 (2009)



n=1, varying *t'/t*

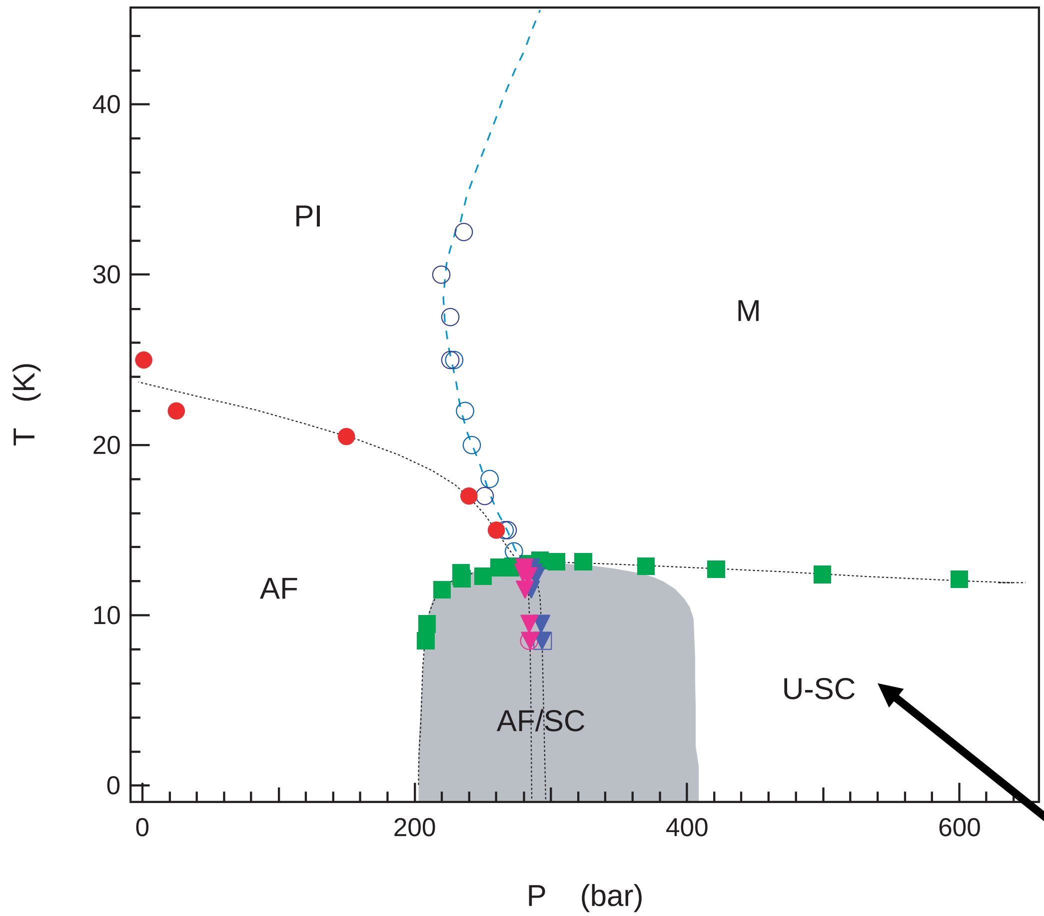
$$H = \sum_{ij\sigma}(t_{ij} - \delta_{ij}\mu)c^\dagger_{i\sigma}c_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}$$

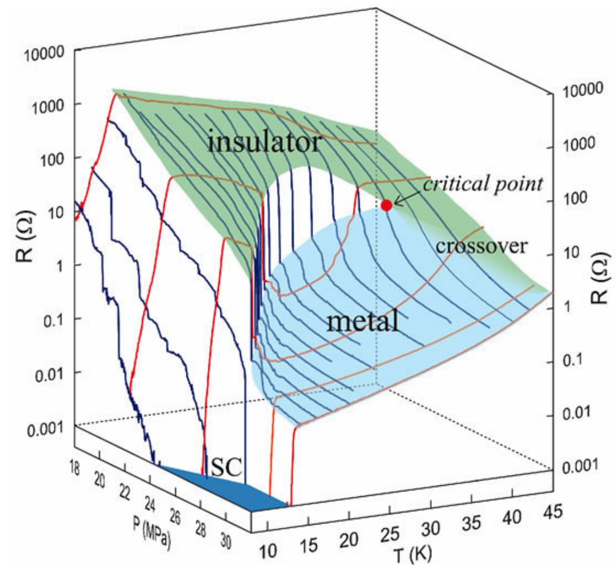
$t \approx 50\,\mathrm{meV}$

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

t'/t ~ 0.6 - 1.1

Phase diagram for organics





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

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

Powell, McKenzie cond-mat/0607078

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

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

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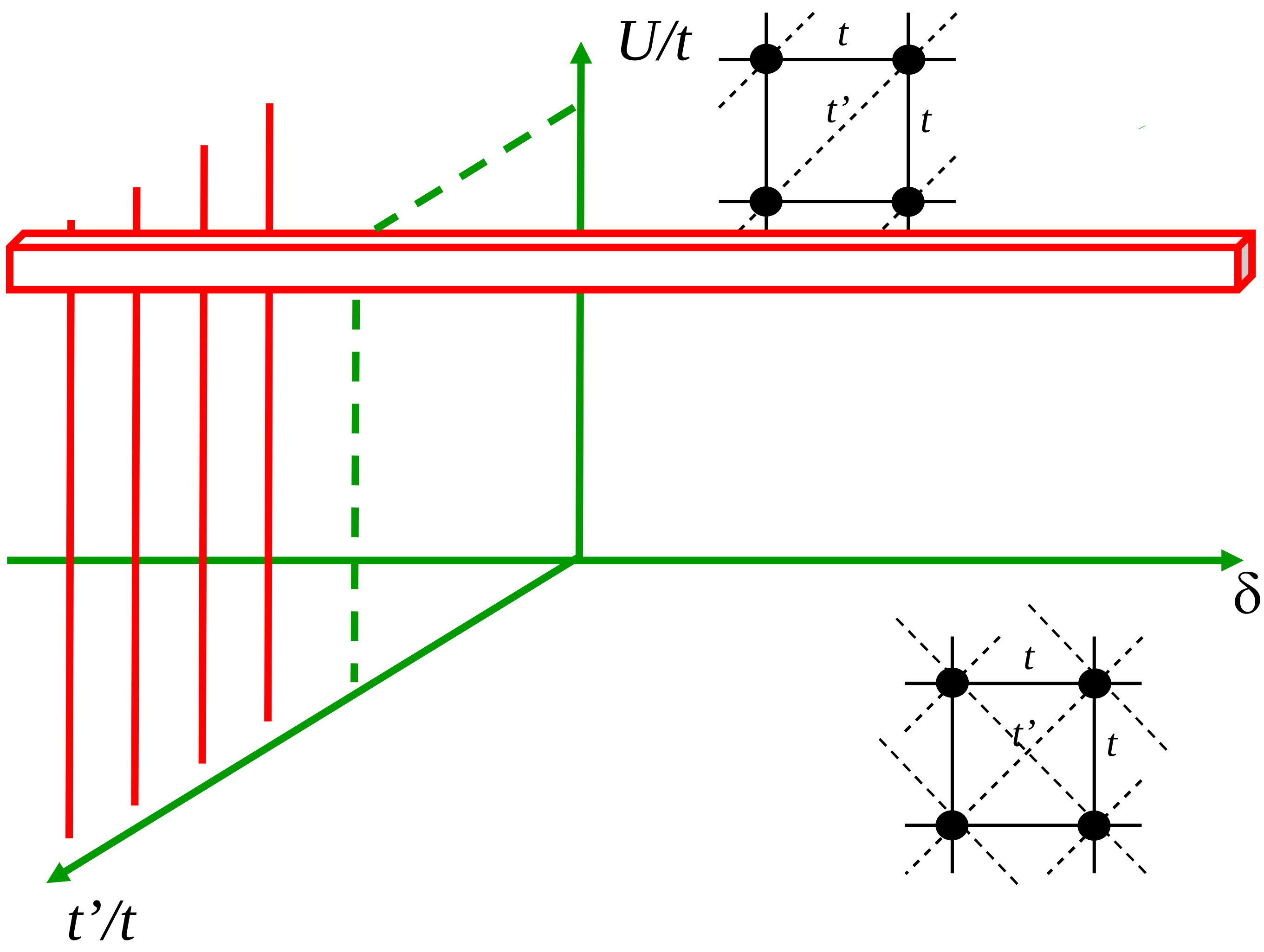
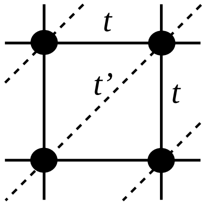
Perspective

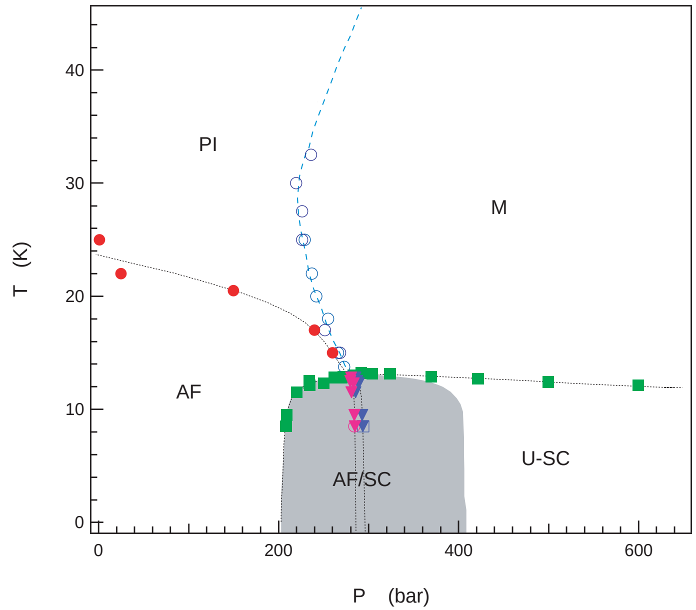


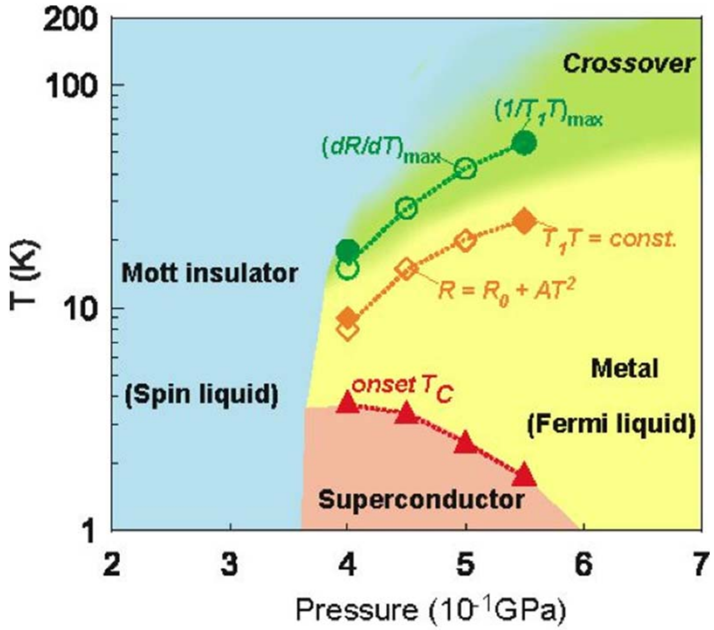
Phase diagram BEDT



$t' = 0.6t$

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





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

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

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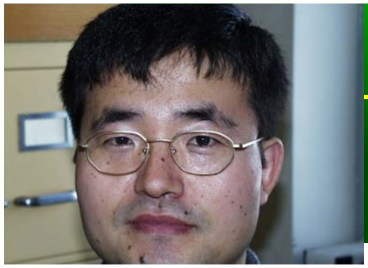
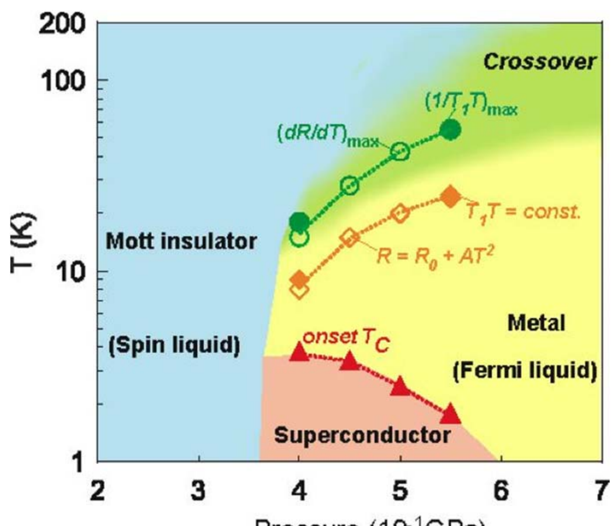
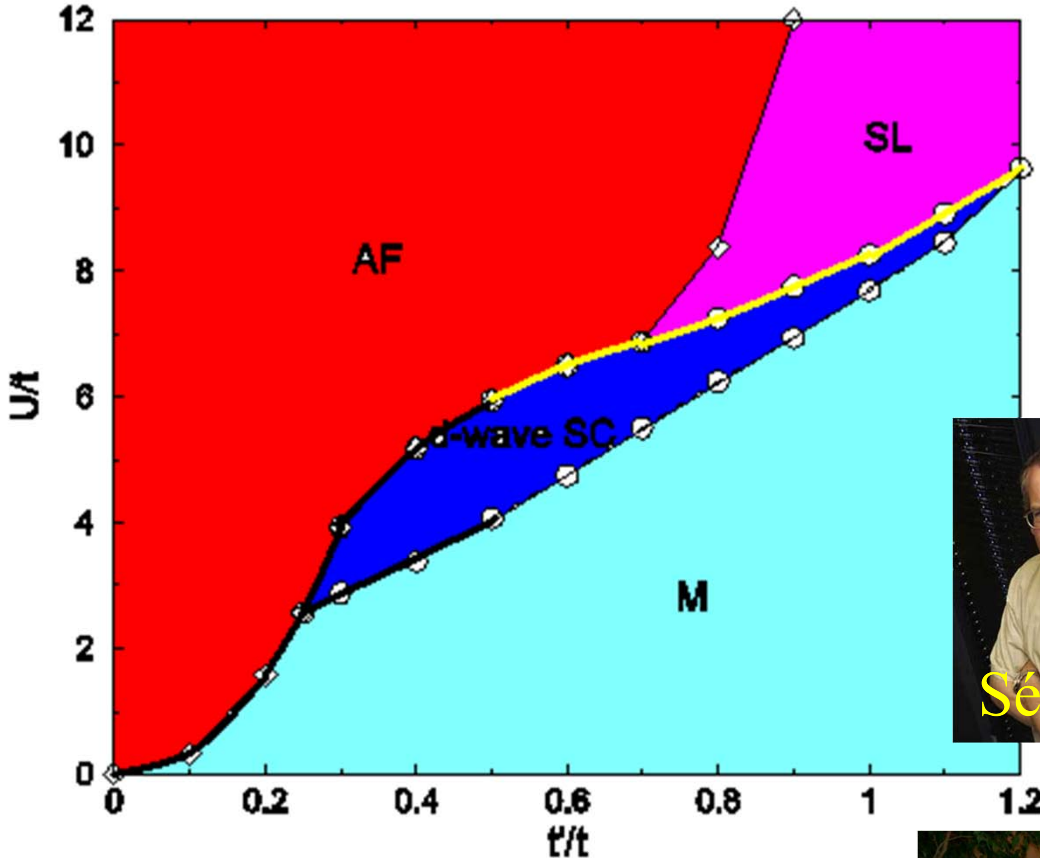


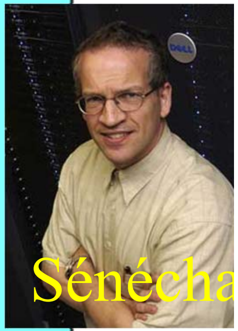
Theoretical phase diagram BEDT

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)

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

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

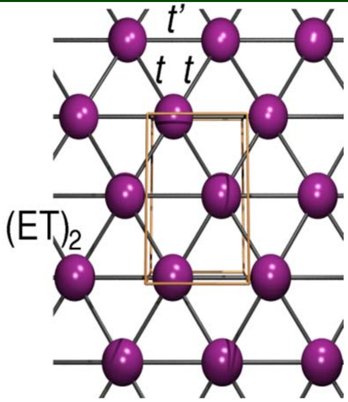
Other compounds (R. Valenti et al.)

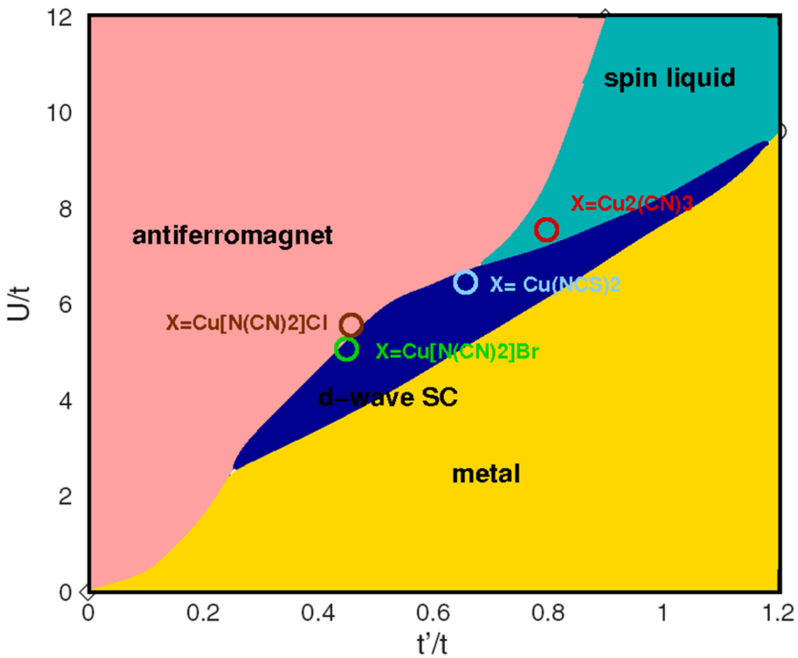
	Hueckel		DFT	
X	t'/t	U/t	t'/t	U/t
CN	1.06	8.2	0.83 (0.85)	7.3 (12)
SCN	0.84	6.8	0.58 (0.83)	6.0
Cl	0.75	7.5	0.44	7.5
Br	0.68	7.2	0.42	5.1

Kandpal et al. PRL (2009)

Nakamura et al. JPSJ (2009)

Komatsu et al. JPSJ (1996)



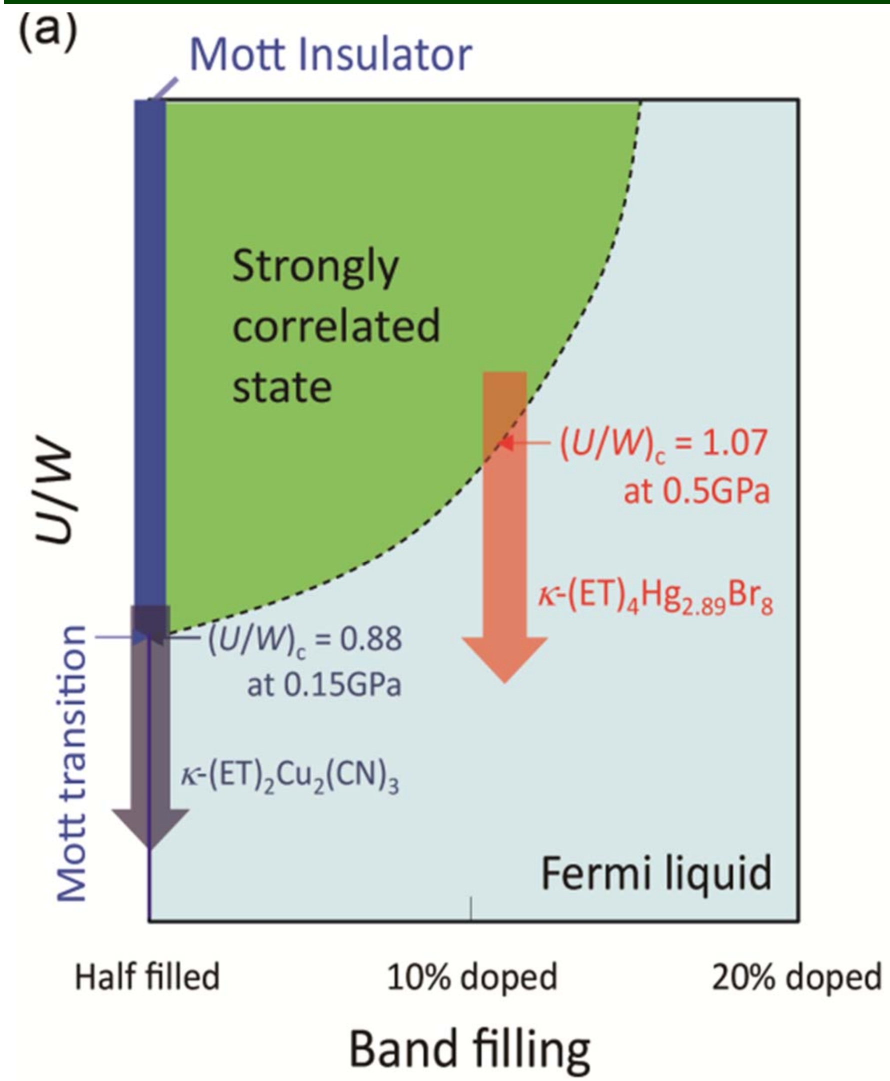


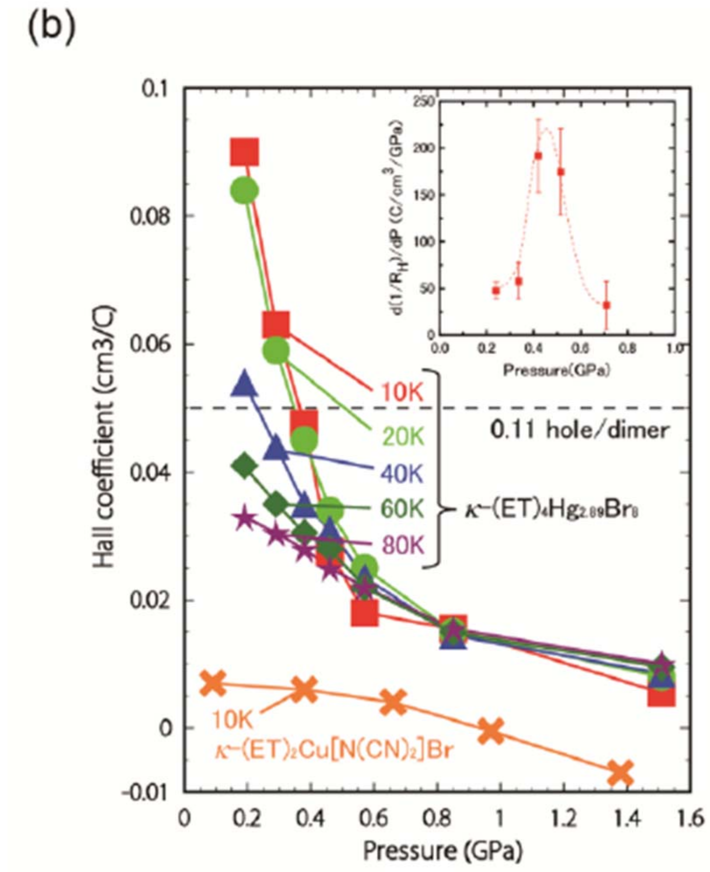
Kyung, Tremblay PRL (2006)

Tocchio, Parola, Gros, Becca PRB (2009)

Doped organic: experiment

Doped BEDT





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

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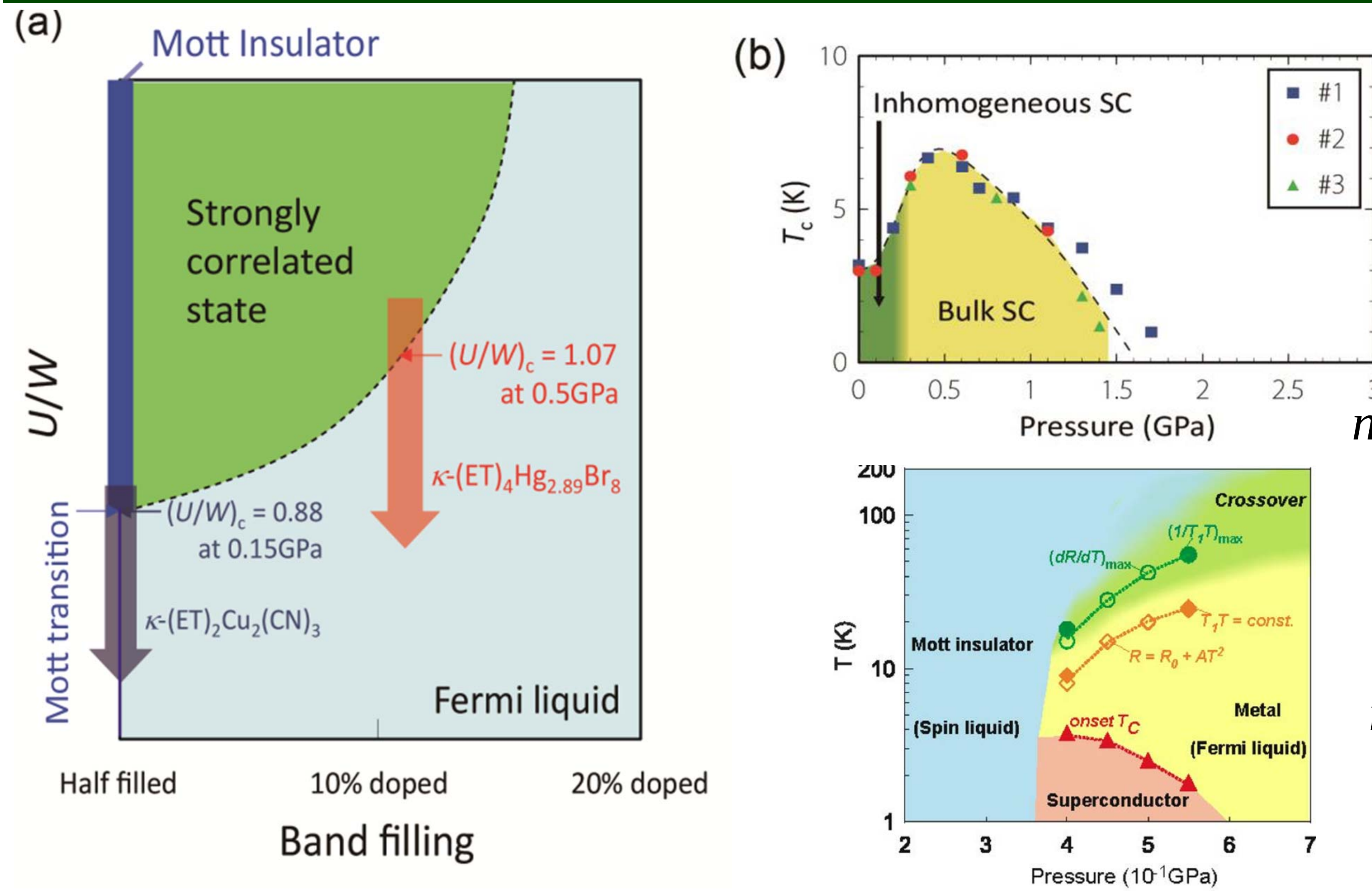
Doped BEDT



n = 0.90

n = 1

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

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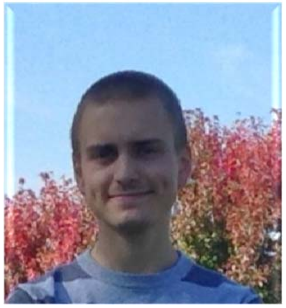

Charles-David Hébert

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)

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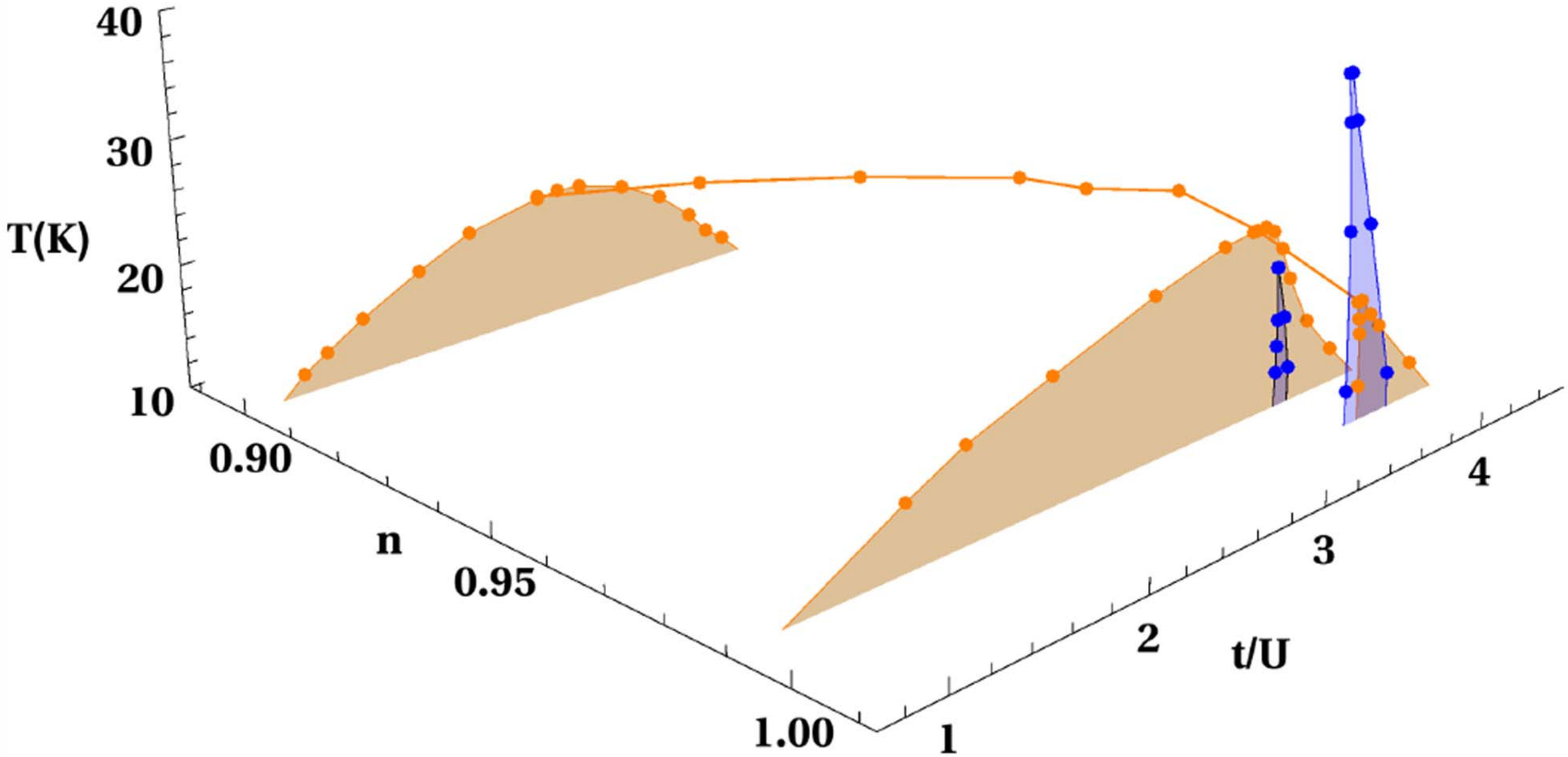
t' = 0.4t overview



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

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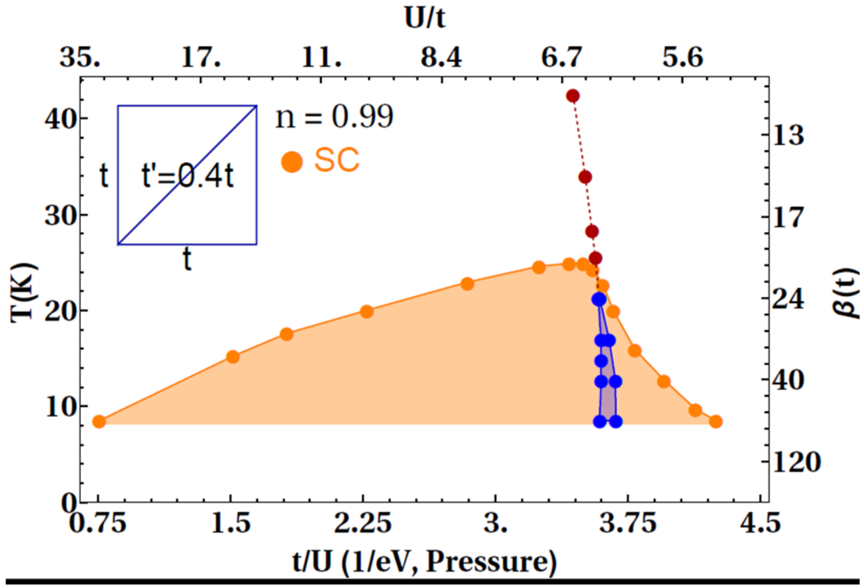
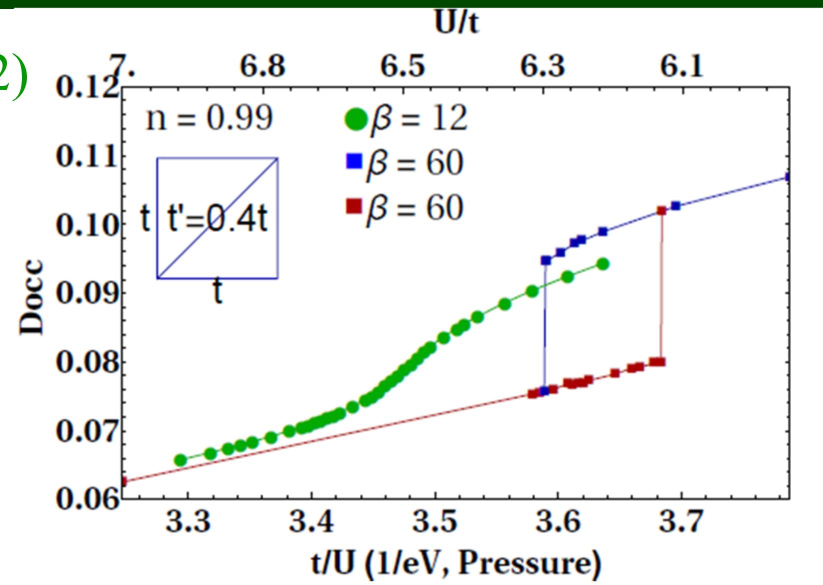
First order and Widom line in organics

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





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)

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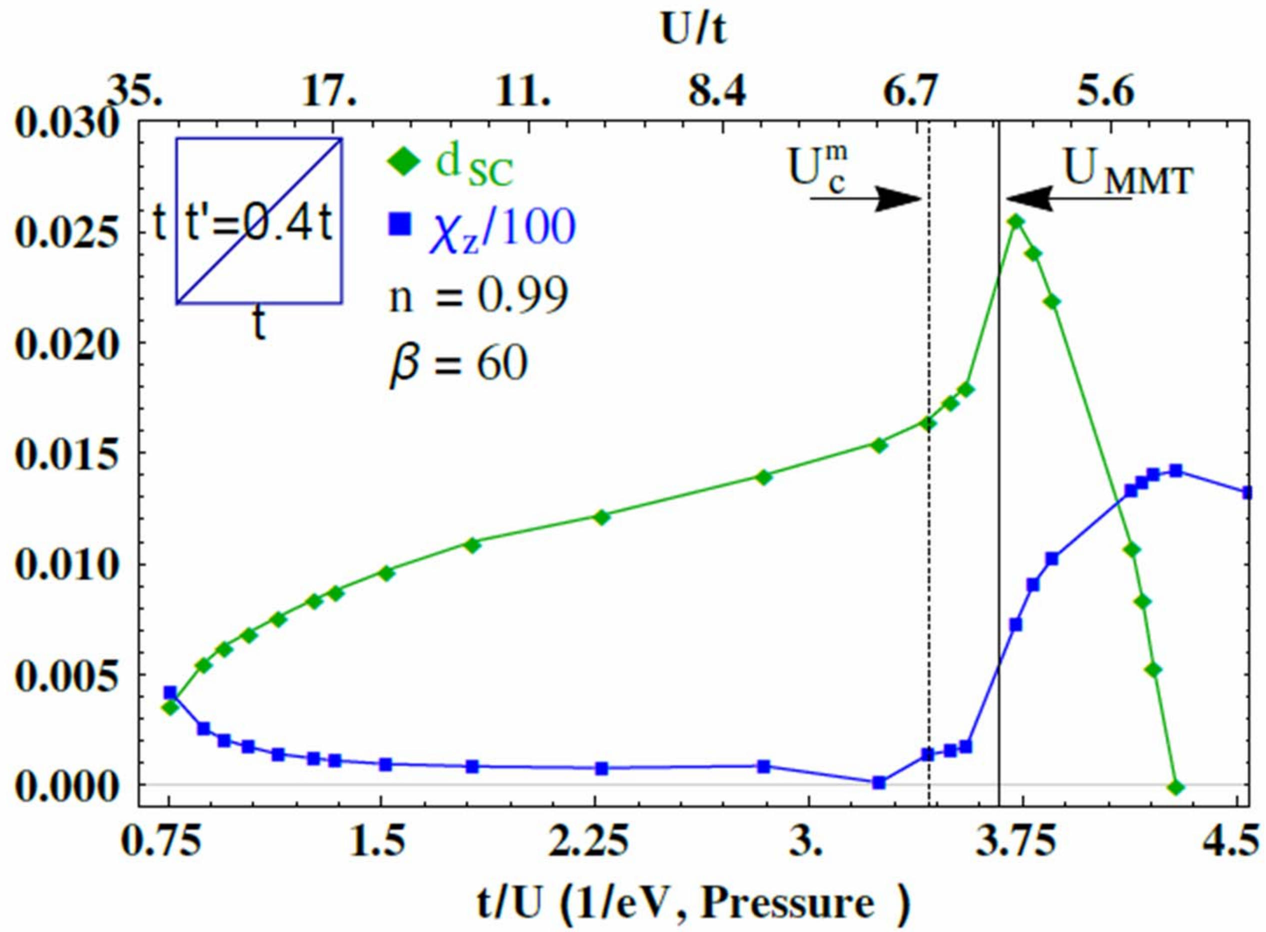
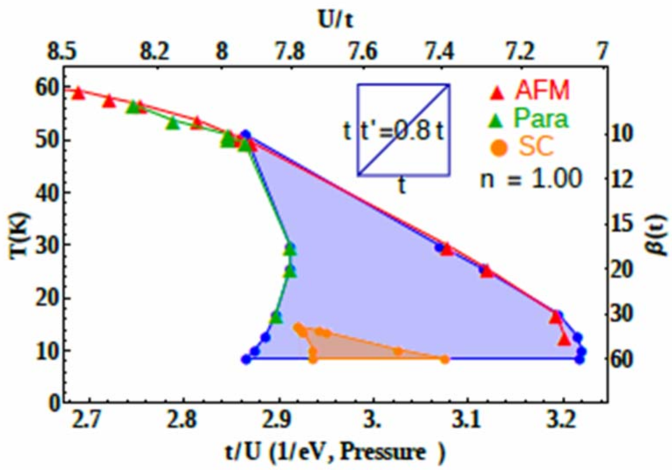
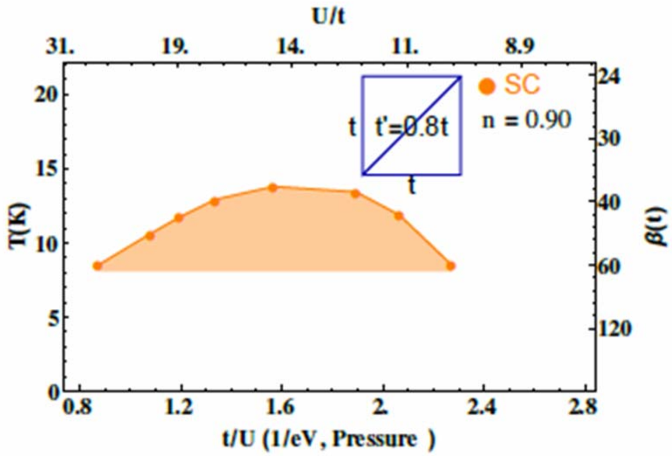
Signatures of Widom line in the superconducting state



t' = 0.8 t



(a)



(b)

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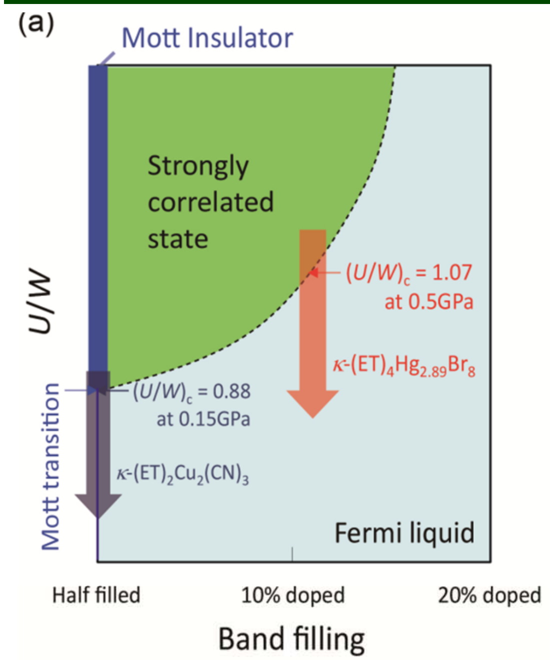
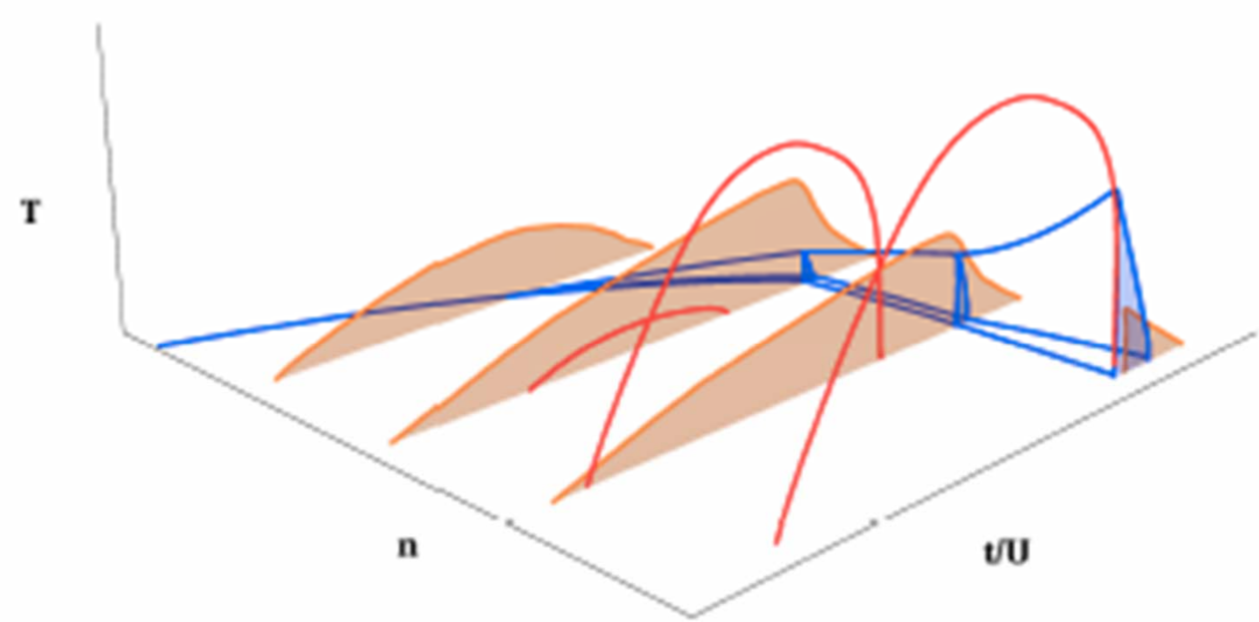
Generic case highly frustrated case





Wei Wu

AFM quantum critical point in heavy fermions (with same category of methods)

W. Wu A.-M.S.T. Phys. Rev. X, 2015

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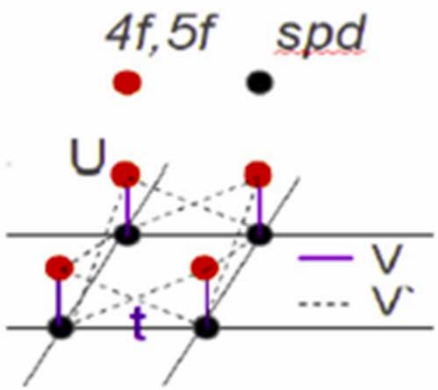
Heavy fermions

$$H = \sum_{k,\sigma} \epsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{k,\sigma} \epsilon^f f^\dagger_{k,\sigma} f_{k,\sigma}$$

$$+ \sum_{k,\sigma} V_k (f^\dagger_{k,\sigma} c_{k,\sigma} + \text{H.c.}) + \sum_i U \left(n_f^\uparrow - \frac{1}{2}\right)\left(n_f^\downarrow - \frac{1}{2}\right)$$

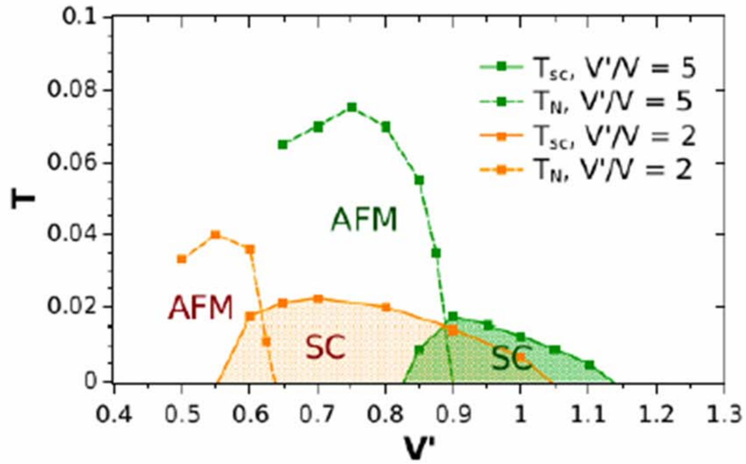


$$V_k = V + 2V'[cos(k_x) + cos(k_y)]$$

U=4

AFM: antiferro-magnetism
SC: superconducting

V'/V = 2 : more frustrated case
V'/V = 5 : less frustrated case



W. Wu A.-M.S.T. Phys. Rev. X, 2015

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Summary : organics

- Agreement with experiment
  - SC: larger T_c and broader P range if doped
  - Larger frustration: Decrease T_N and T_c
  - Normal state metal to pseudogap crossover
- Predictions
  - First order transition at low T in normal state
    - (or remnants in SC state)
- Physics
  - SC dome without an AFM QCP. Extension of Mott
  - SC from short range J.
  - T_c decreases at Widom line

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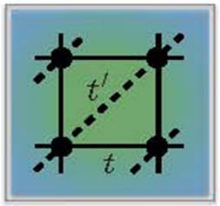
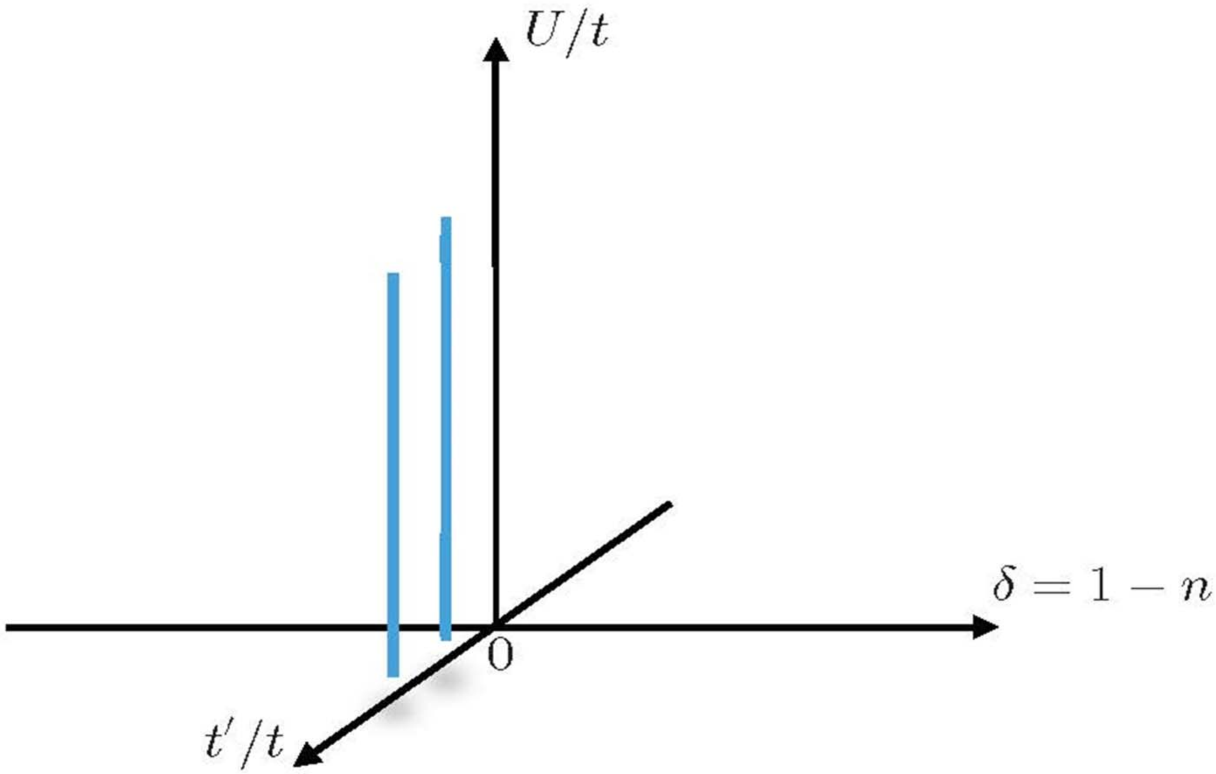
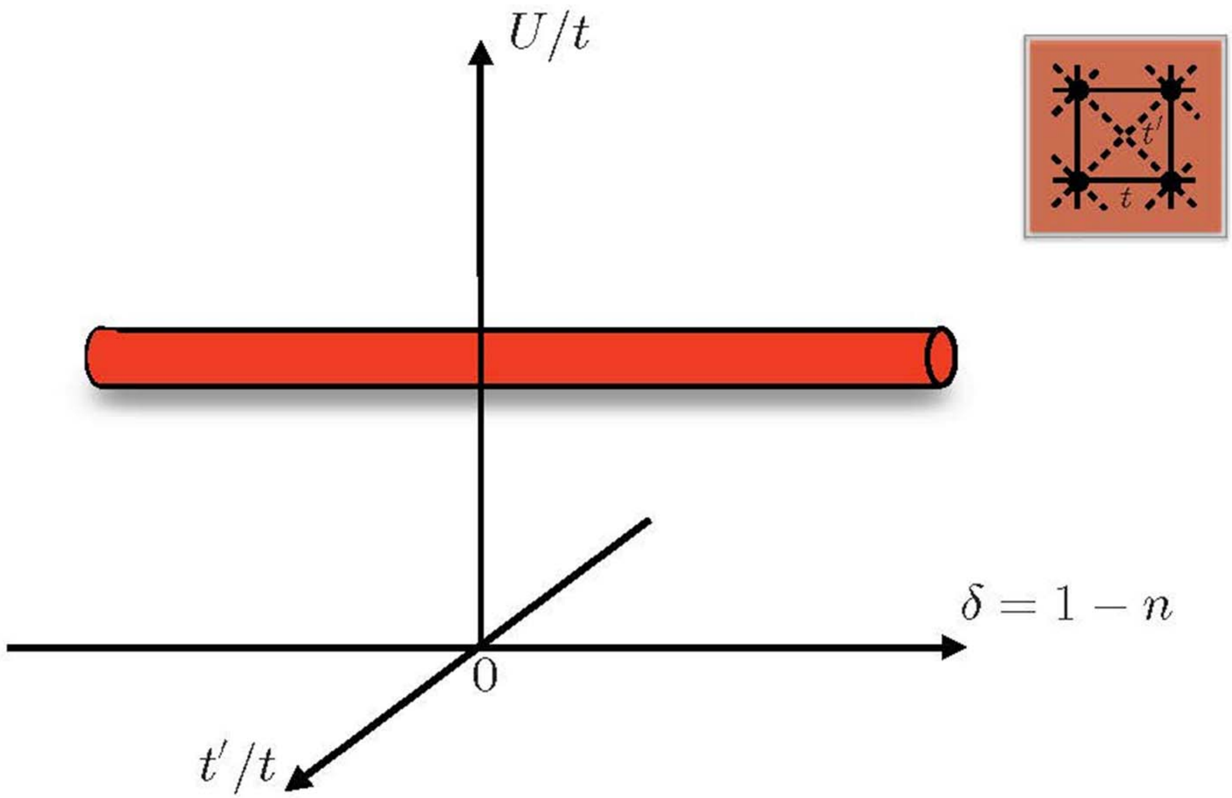
Perspective





Perspective



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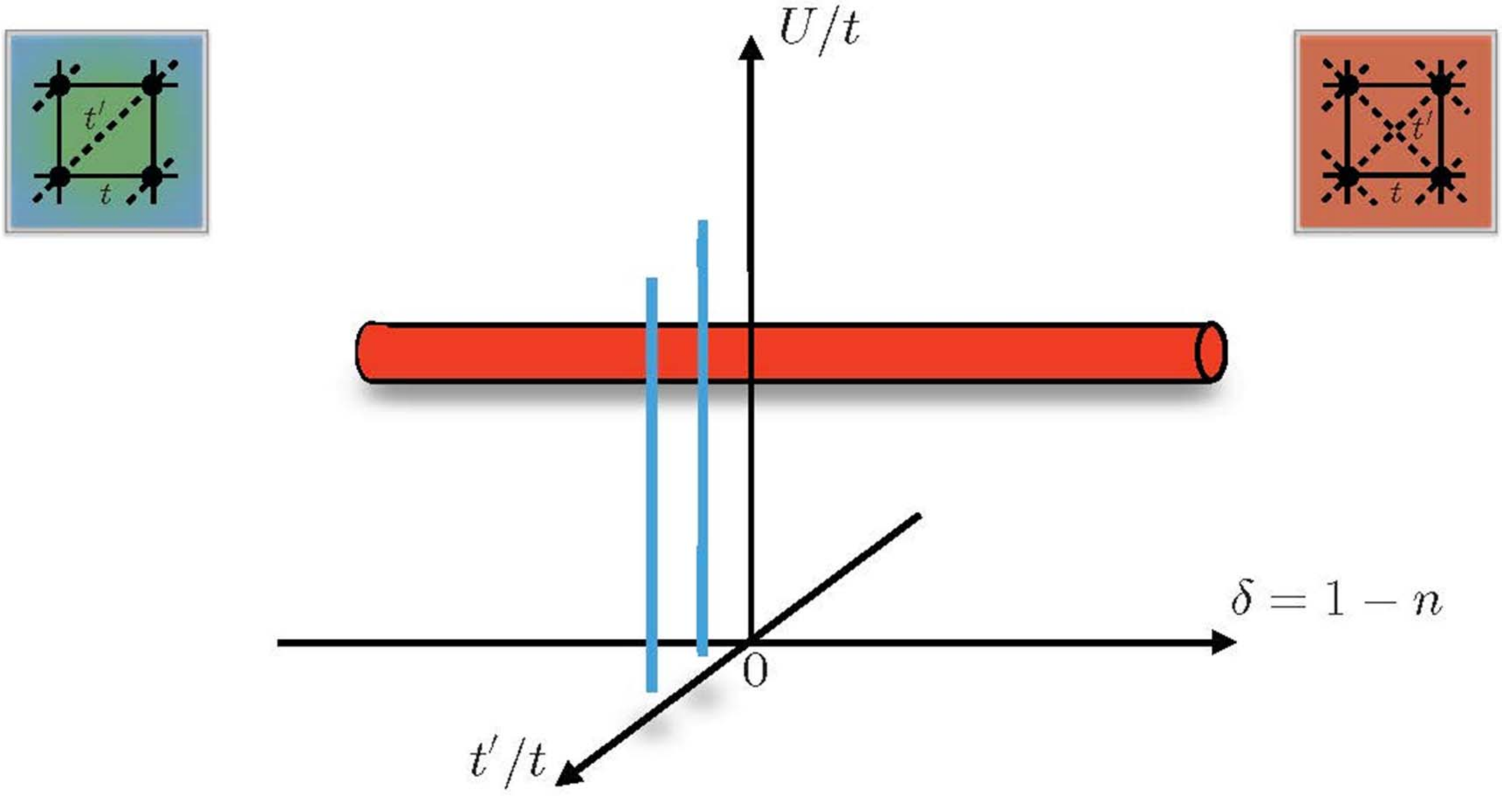
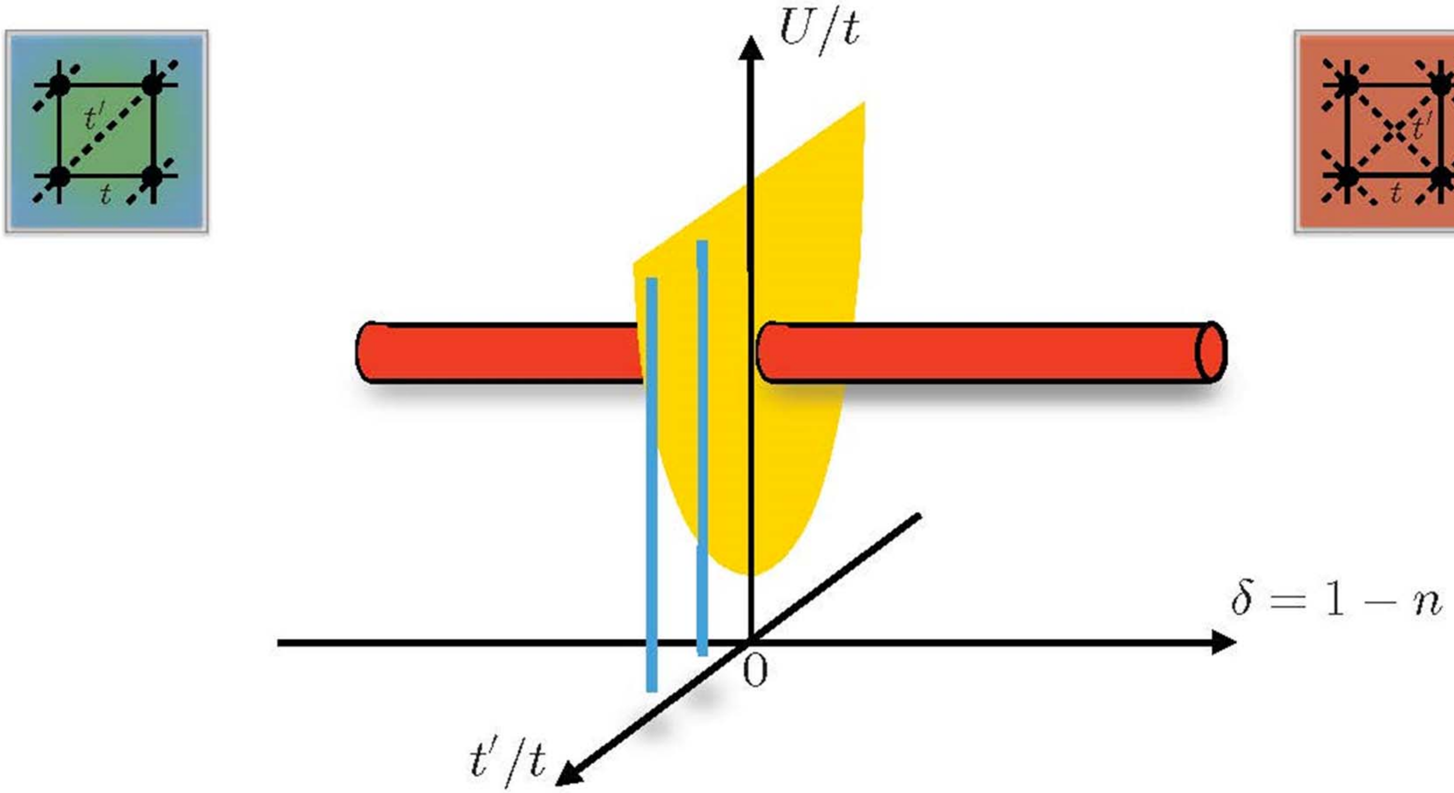
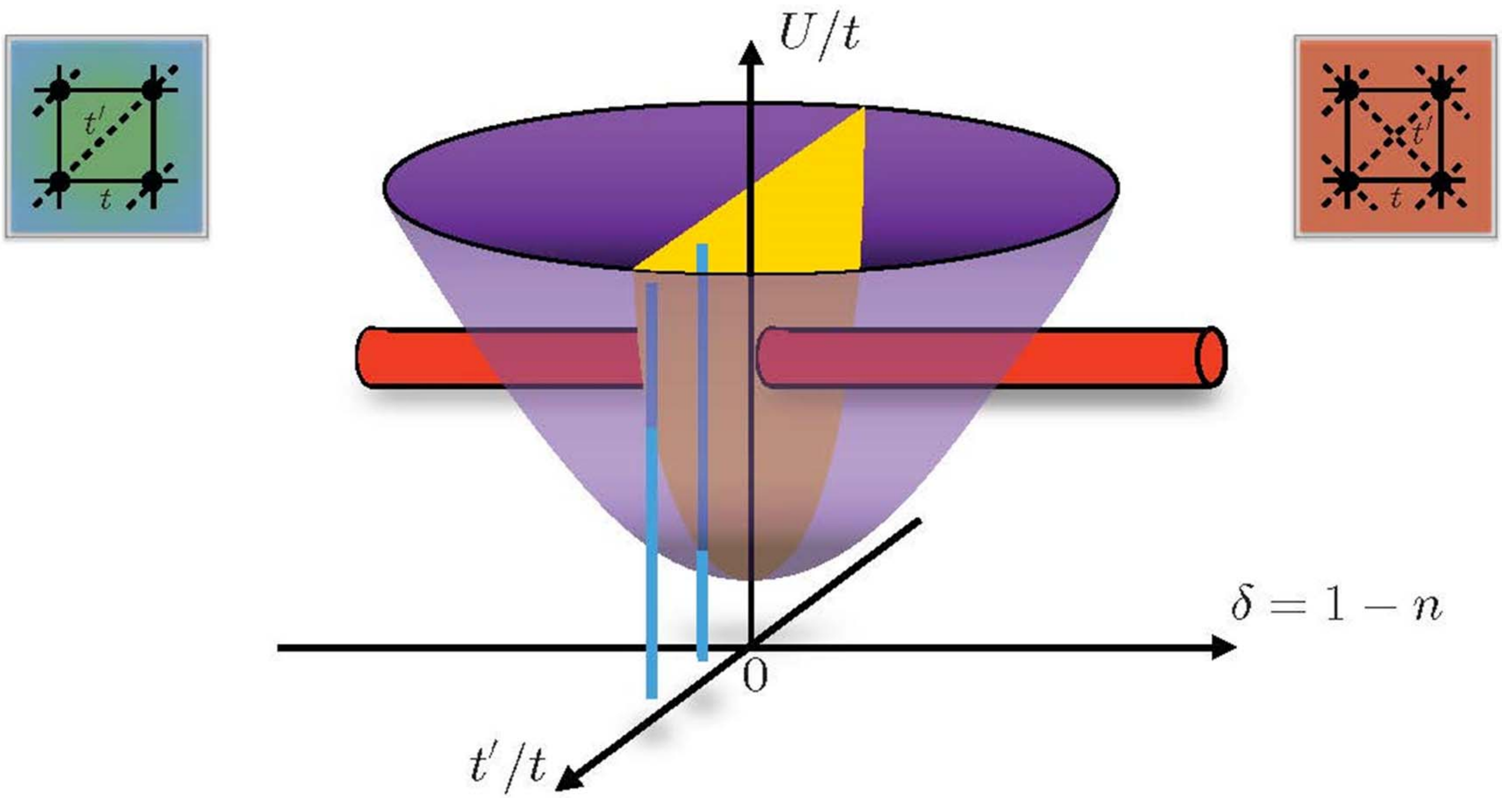
Perspective



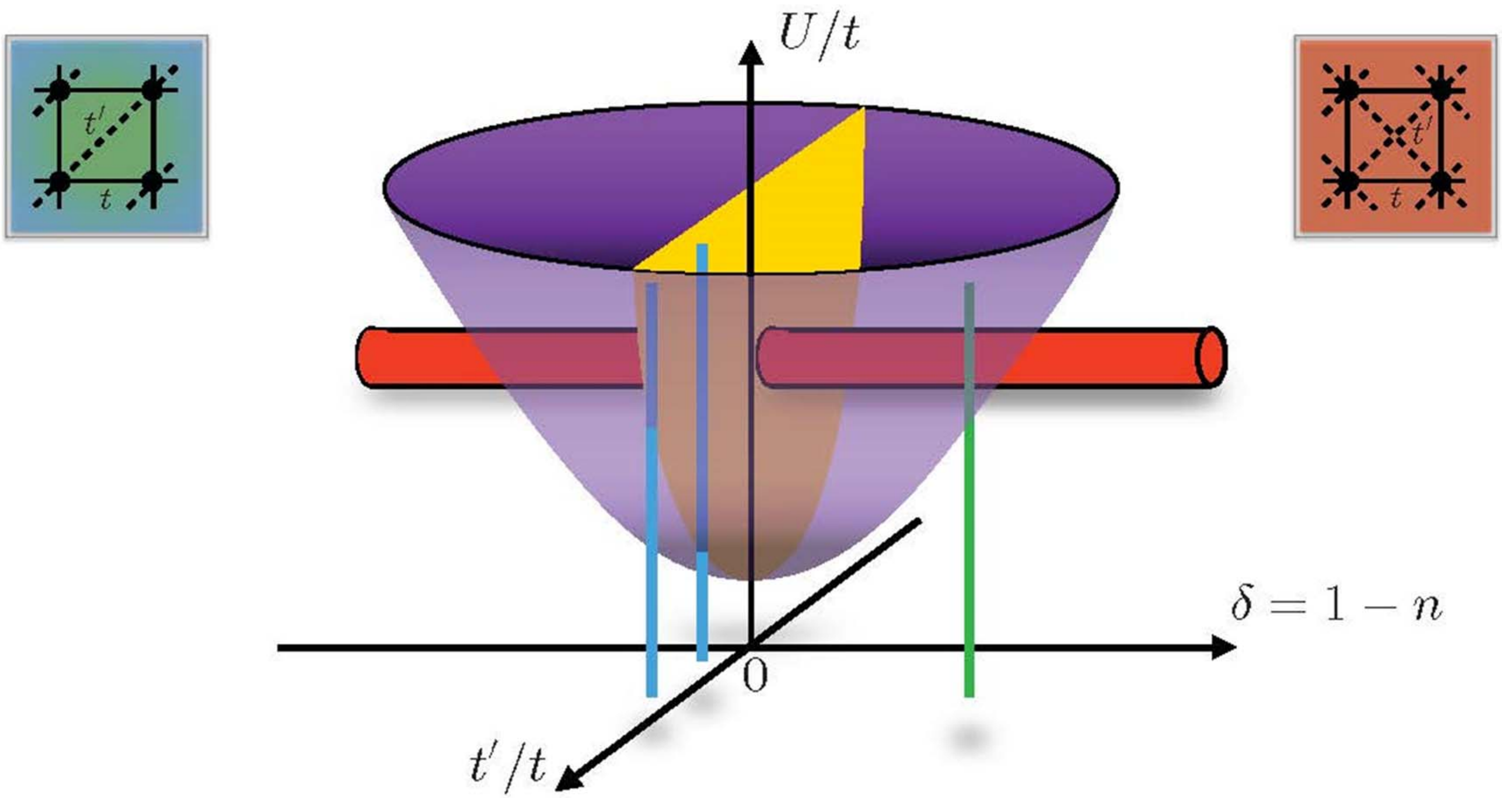
Perspective



Perspective



Perspective



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Main collaborators

Giovanni Sordi

Kristjan Haule

David Sénéchal

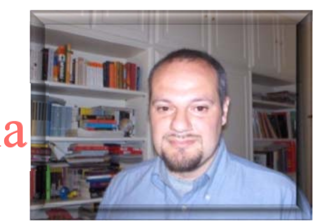
Bumsoo Kyung

Patrick Sémon

Dominic Bergeron

Sarma Kancharla

Marcello Civelli



Massimo Capone

Gabriel Kotliar

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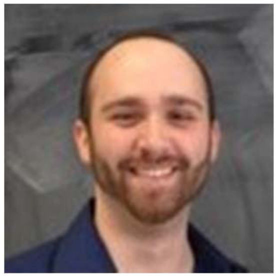
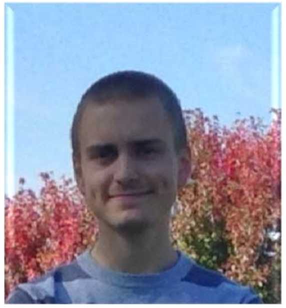
Main collaborators, continued

Lorenzo Fratino

Wei Wu



Alexis Reymbaut



Charles-David Hébert

Maxime Charlebois

Alexandre Day

Vincent Bouliane

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Mammouth

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

Éducation, Loisir et Sport Québec

Canada Foundation for Innovation
Fondation canadienne pour l'innovation

Calcul Québec

Université de Sherbrooke

Further references

For references, September 2013 Julich summer school
Strongly Correlated Superconductivity

http://www.cond-mat.de/events/correl13/manuscripts/tremblay.pdf

Lecture notes

http://www.physique.usherbrooke.ca/tremblay/cours/phy-892/N-corps.pdf

Merci

Thank you

Methods

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Measurable quantities : Green's functions

$$\langle \mathcal{O} \rangle \equiv \frac{Tr\left[e^{-\beta(H-\mu N)}\mathcal{O}\right]}{Tr\left[e^{-\beta(H-\mu N)}\right]}$$

$$\mathcal{G}_{\mathbf{k}\sigma}(\tau) = -\langle T_\tau[c_{\mathbf{k}\sigma}(\tau)c^\dagger_{\mathbf{k}\sigma}]\rangle$$

$$= -\theta(\tau)\langle c_{\mathbf{k}\sigma}(\tau)c^\dagger_{\mathbf{k}\sigma}\rangle + \theta(-\tau)\langle c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}(\tau)\rangle.$$

$$c_{\mathbf{k}\sigma}(\tau) = e^{(H-\mu N)\tau}c_{\mathbf{k}\sigma}e^{-(H-\mu N)\tau}$$

$$\mathcal{G}_{\mathbf{k}\sigma}(i\omega_n) = \int_0^\beta d\tau e^{i\omega_n\tau}\mathcal{G}_{\mathbf{k}\sigma}(\tau)$$

$$\omega_n = (2n+1)\pi T$$

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Green's function: free electrons, atomic limit

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

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

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

$$\langle n \rangle = 1$$

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

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 $n = 1$

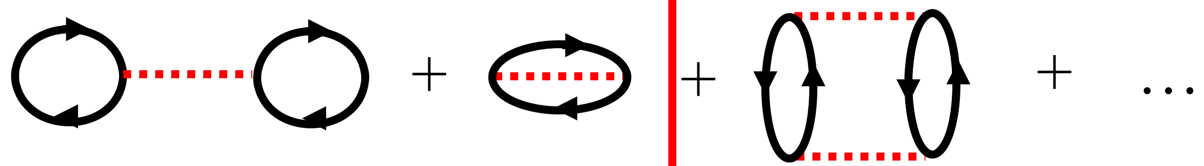
$$\mathcal{G}_{\sigma}(i\omega_n) = \frac{1/2}{i\omega_n + \frac{U}{2}} + \frac{1/2}{i\omega_n - \frac{U}{2}}$$

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

Dynamical "variational" principle

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

$$\Phi[G] =$$



Universality

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

$$\frac{\delta\Omega_{\mathbf{t}}[G]}{\delta G} = \Sigma - G_{0\mathbf{t}}^{-1} + G^{-1} = 0$$

$$G = \frac{1}{G_{0\mathbf{t}}^{-1} - \Sigma}$$

Then Ω is grand potential

Related to dynamics (cf. Ritz)

H.F. if approximate Φ by first order

FLEX higher order

Luttinger and Ward 1960, Baym and Kadanoff (1961)

Self-consistency condition

- Obtain Green's function for the « impurity » (cluster) in a bath
- Extract Σ
- Substitute Σ in lattice Green's function
- Project lattice Green's function on impurity (cluster).
- If the two Green's functions are not equal, modify the bath until they are.

Self-consistency

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

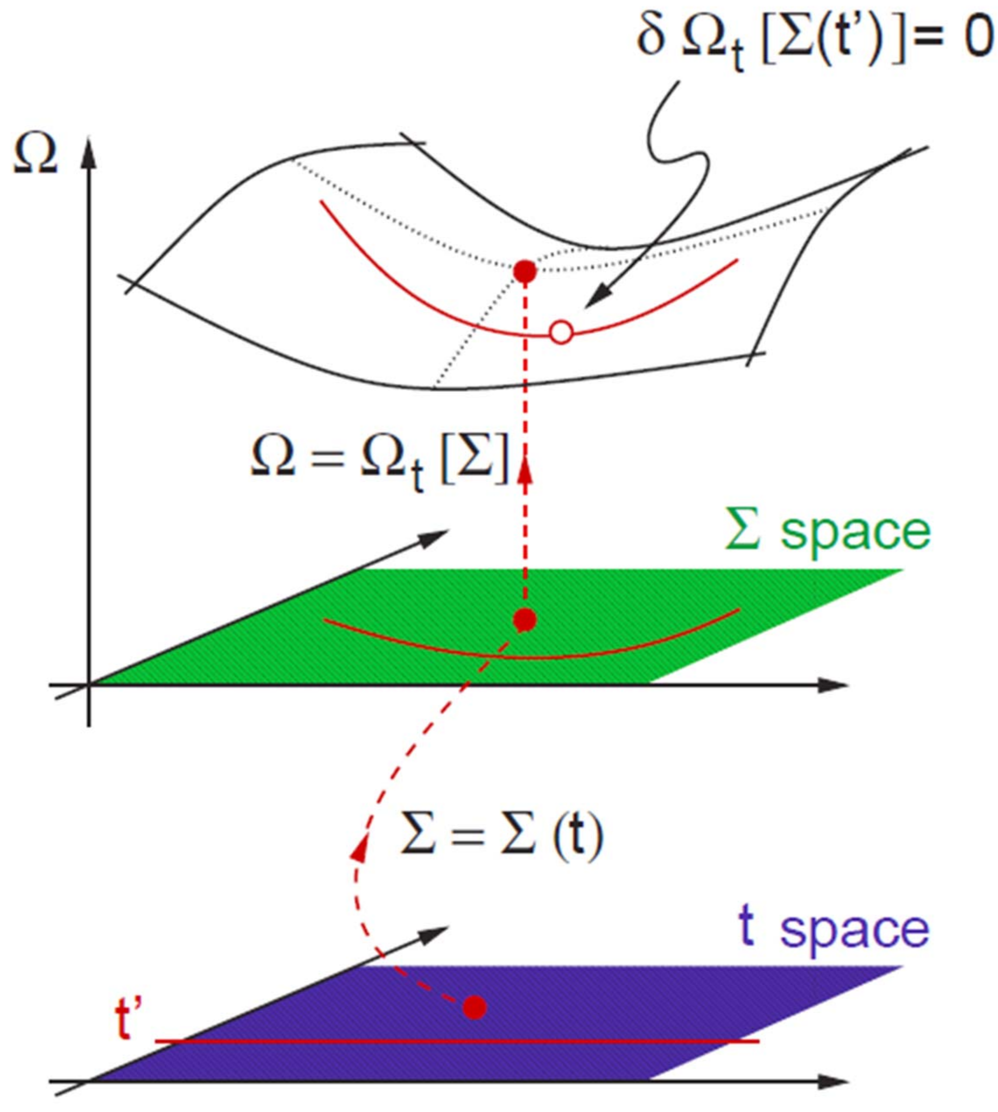
$$N_c \int \frac{d^d\tilde{\mathbf{k}}}{(2\pi)^d} \frac{1}{\mathcal{G}^0_{\tilde{\mathbf{k}}\sigma}(i\omega_n)^{-1} - \Sigma_\sigma(i\omega_n)} = \mathcal{G}_\sigma^{imp}(i\omega_n)$$

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



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Another way to look at this (Potthoff)

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

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

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

Still stationary (chain rule)

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

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

SFT : Self-energy Functional Theory

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

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

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

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

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).

CT-QMC impurity solver

Monte Carlo method

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

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

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

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

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

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Monte Carlo: Markov chain

- Ergodicity
- Detailed balance

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

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

Reminder on perturbation theory

$$
\begin{aligned}
\exp(-\beta(H_a + H_b)) &= \exp(-\beta H_a)U(\beta) \\
\frac{\partial U(\beta)}{\partial \beta} &= -H_b(\beta)U(\beta) \\
U(\beta) &= 1 - \int_0^\beta d\tau H_b(\tau) + \int_0^\beta d\tau \int_0^\tau d\tau' H_b(\tau)H_b(\tau') + \ldots
\end{aligned}
$$

Partition function as sum over configurations

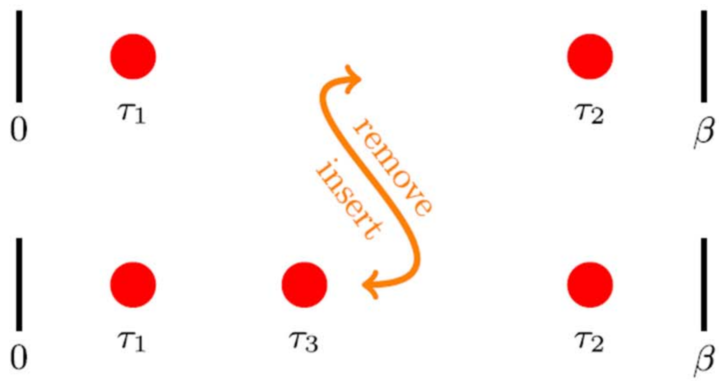
$$Z = \mathrm{Tr}[\exp(H_a + H_b)]$$

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

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

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

Updates



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

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

$$\begin{aligned} R_{(k,\vec{\tau}),(k+1,\vec{\tau}')} &= \frac{p((k+1,\vec{\tau}'))}{p((k,\vec{\tau}))} \frac{W^{\mathrm{prop}}_{(k+1,\vec{\tau}'),(k,\vec{\tau})}}{W^{\mathrm{prop}}_{(k,\vec{\tau}),(k+1,\vec{\tau}')}} \\ &= \frac{w(k+1)d\tau'_1 \cdots d\tau'_{k+1}}{w(k)d\tau_1 \cdots d\tau_k} \frac{1/(k+1)}{d\tau/\beta} \\ &= \frac{w(k+1)}{w(k)} \frac{\beta}{k+1}. \end{aligned}$$

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

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

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

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

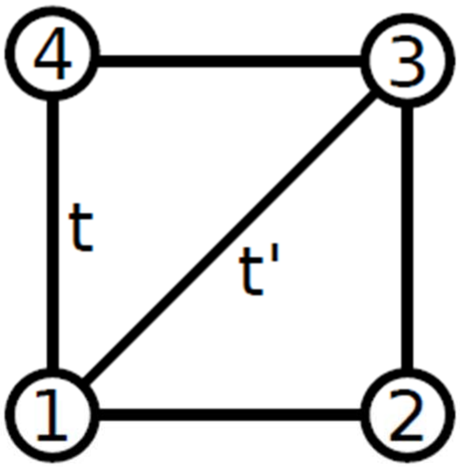
$$\times \mathrm{Tr}_d[T_\tau e^{-\beta H_{\mathrm{loc}}} d_{j_k}(\tau_k) d_{j'_k}^\dagger(\tau'_k) \cdots d_{j_1}(\tau_1) d_{j'_1}^\dagger(\tau'_1)]$$

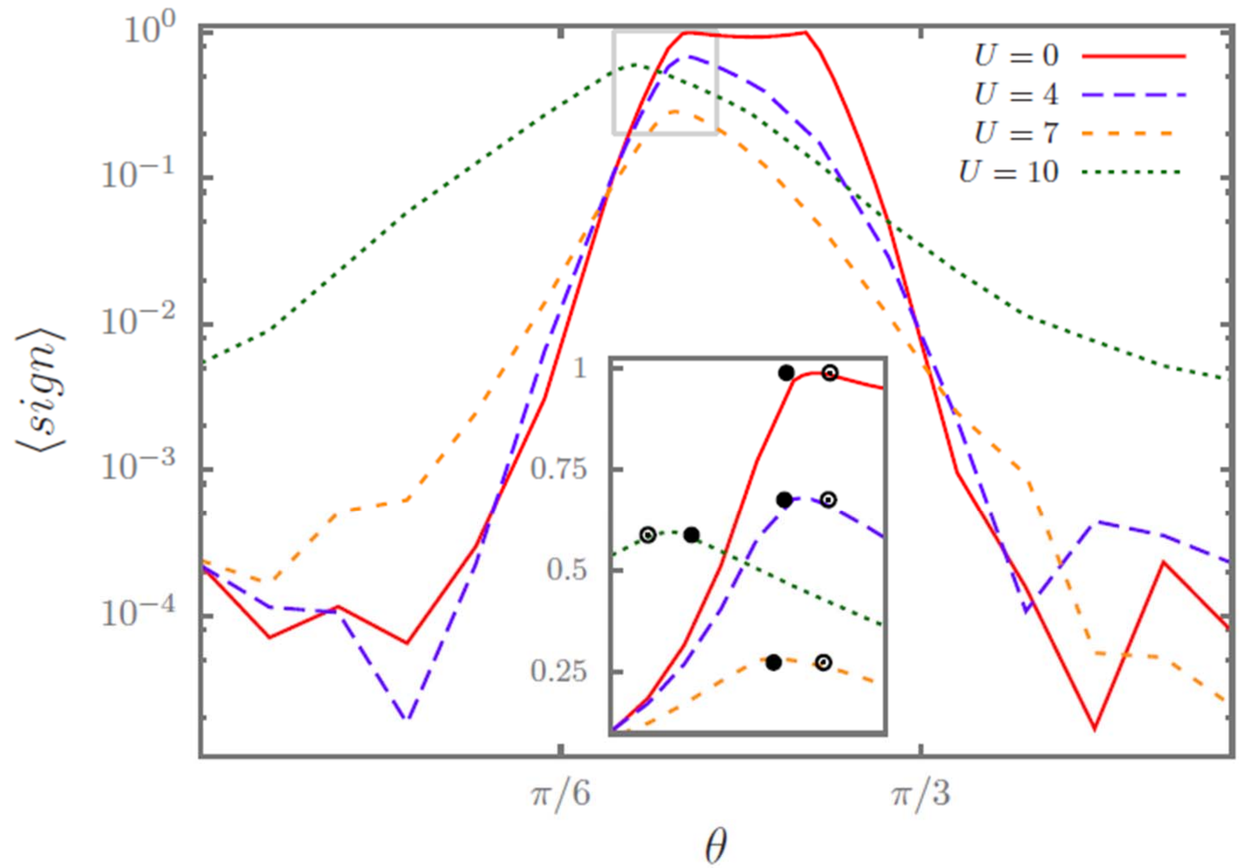
$$\times \mathrm{Tr}_c[T_\tau e^{-\beta H_{\mathrm{bath}}} c_{p_k}^\dagger(\tau_k) c_{p_{k'}}(\tau'_k) \cdots c_{p_1}^\dagger(\tau_1) c_{p'_1}(\tau'_1)].$$

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

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.)

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Two-Particle Self-Consistent Approach (U < 8t)
- How it works

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

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

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

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

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

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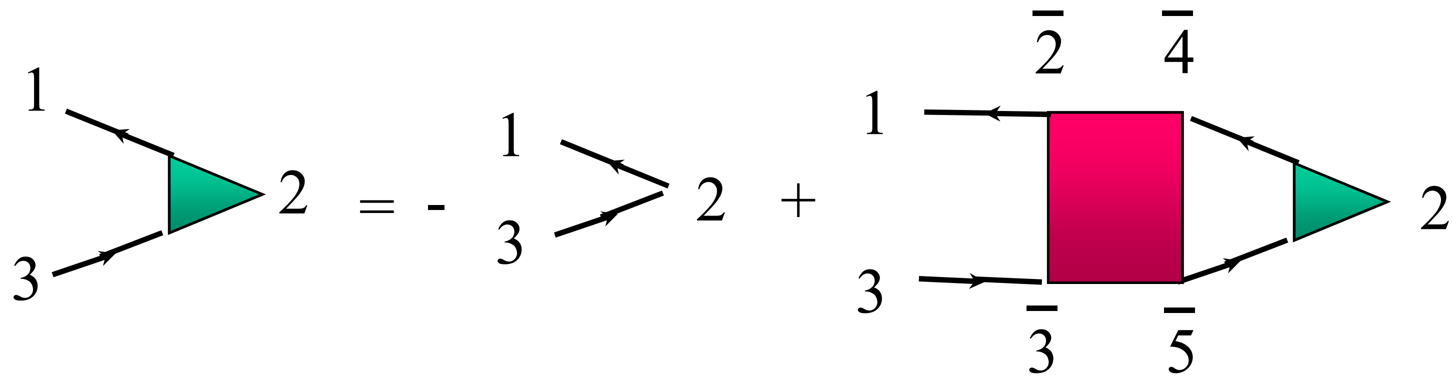
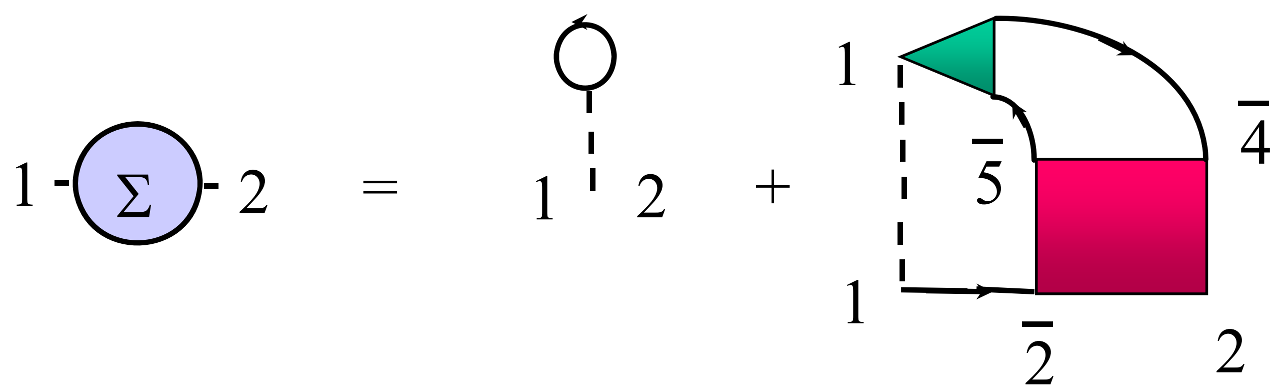
A better approximation for single-particle properties (Ruckenstein)





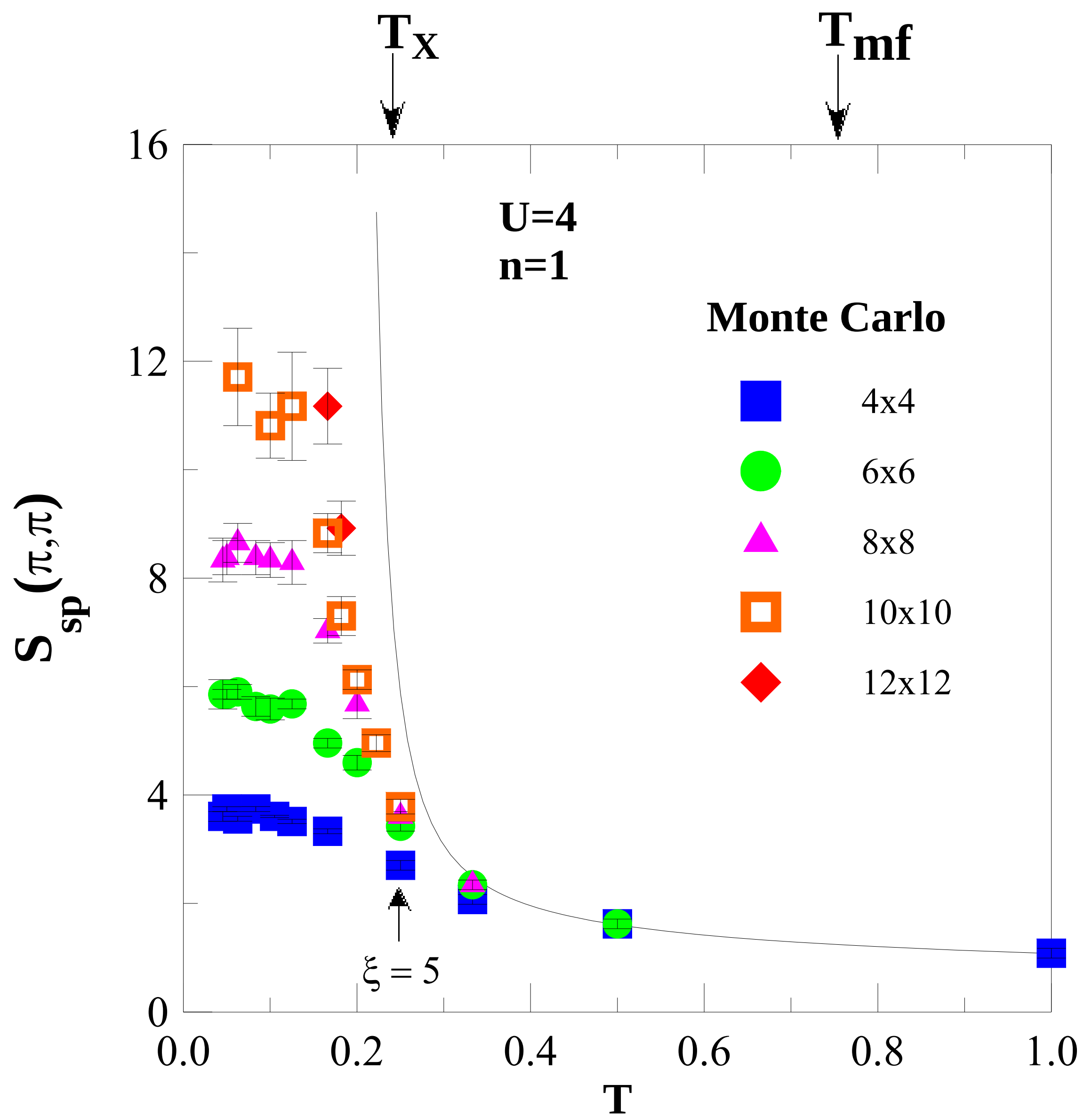
Y.M. Vilk and A.-M.S. Tremblay, J. Phys. Chem. Solids **56**, 1769 (1995).
Y.M. Vilk and A.-M.S. Tremblay, Europhys. Lett. **33**, 159 (1996);

N.B.: No Migdal theorem

Benchmarks for TPSC

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)

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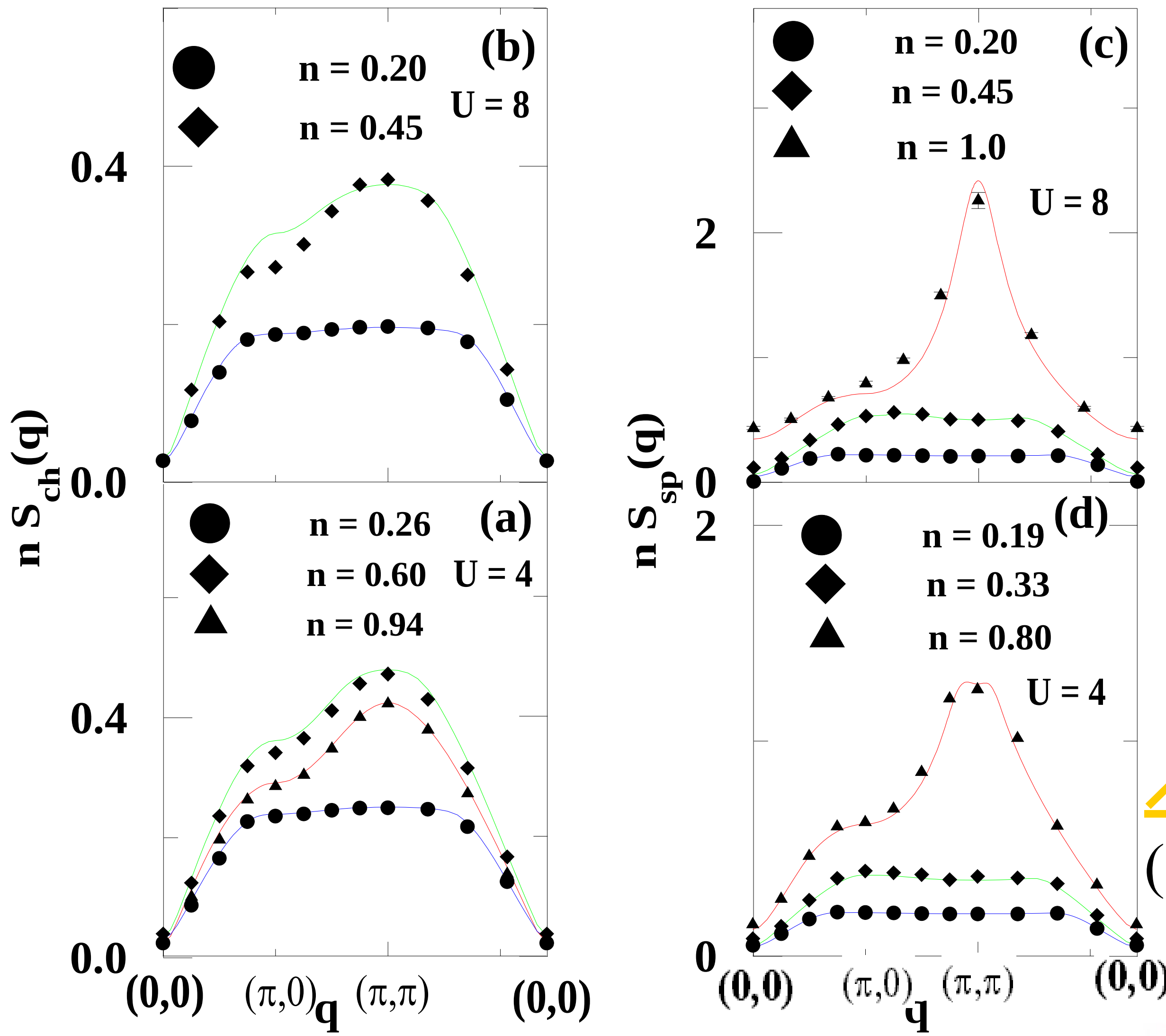
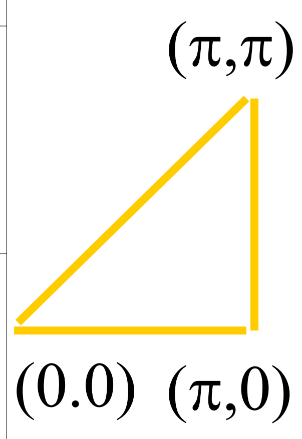
Check on accuracy

Notes:
-F.L. parameters

-Self also Fermi-liquid



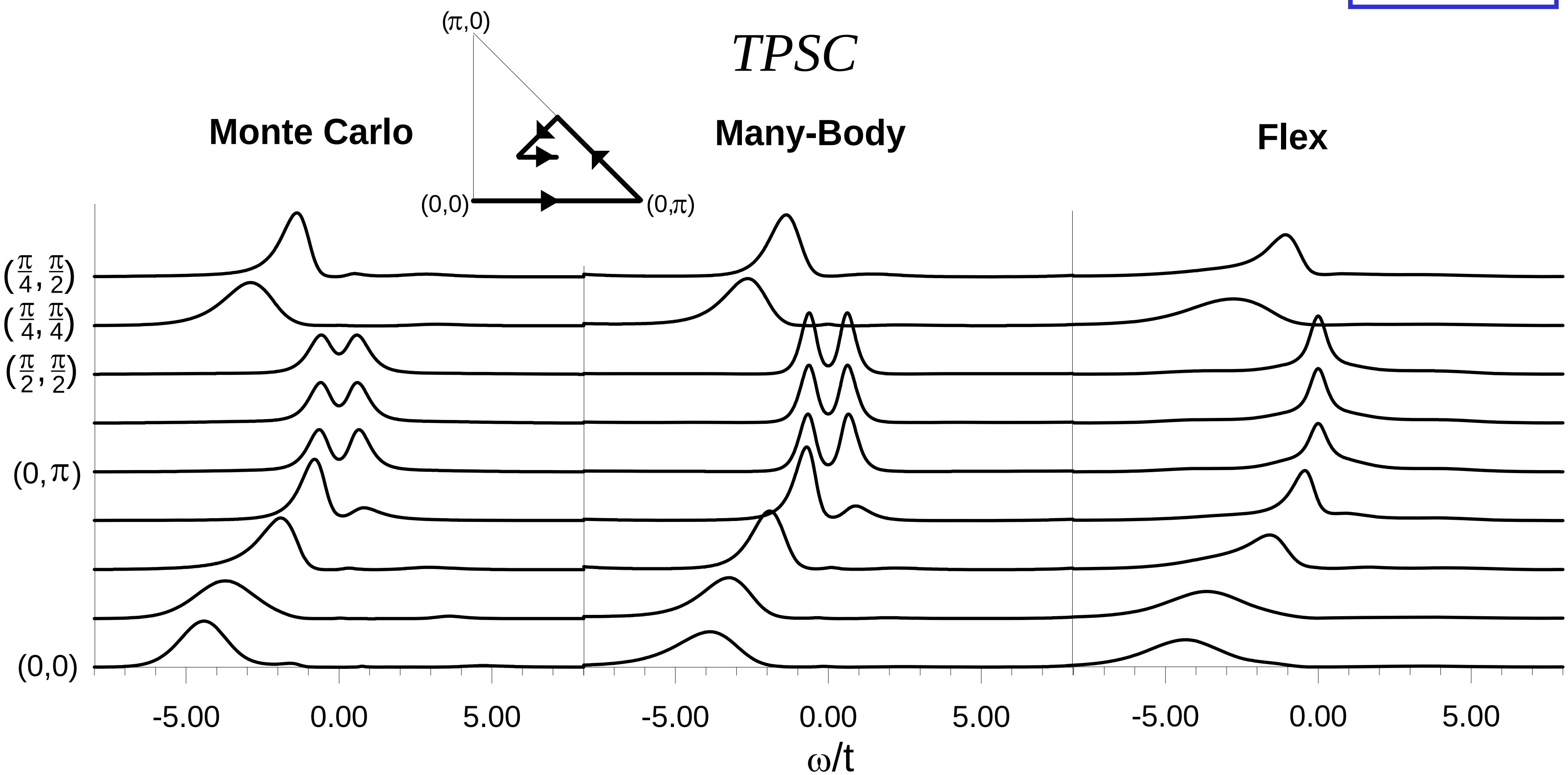
U > 0
β = 5
8 X 8



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

Proofs...

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

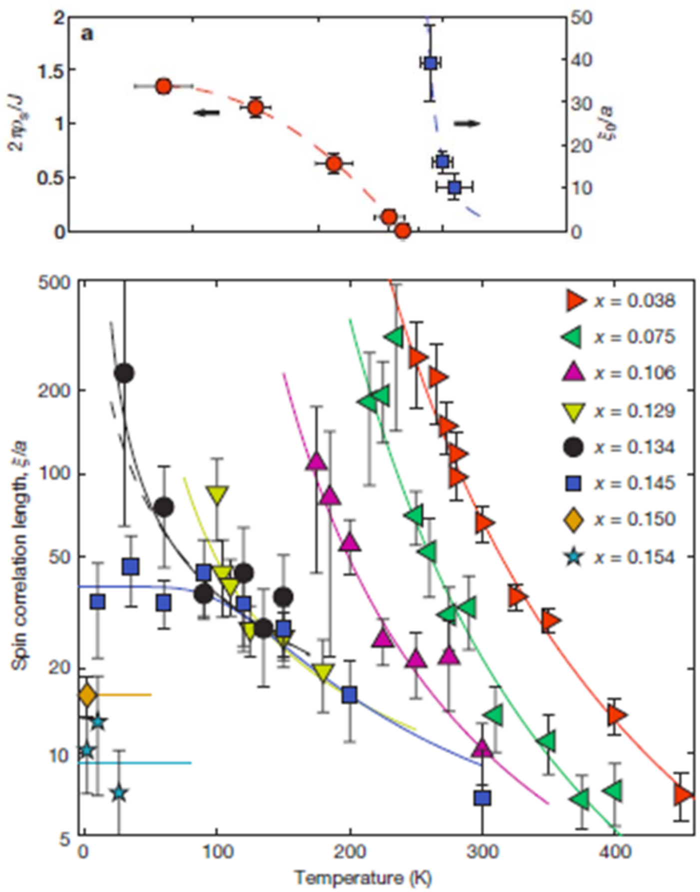


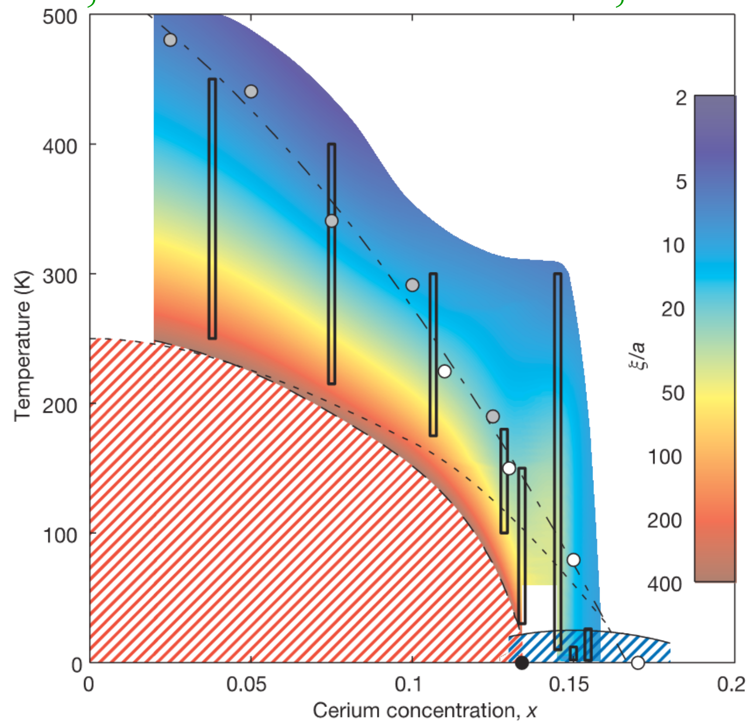
Calc. + QMC: Moukouri et al. P.R. B 61, 7887 (2000).

e-doped cuprates: precursors

NCCO

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

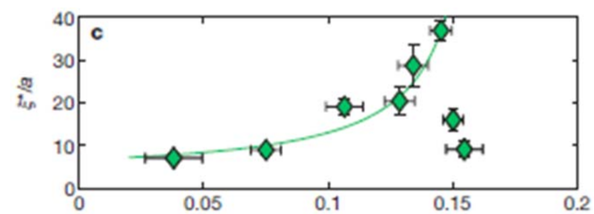




z = 1

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

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



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

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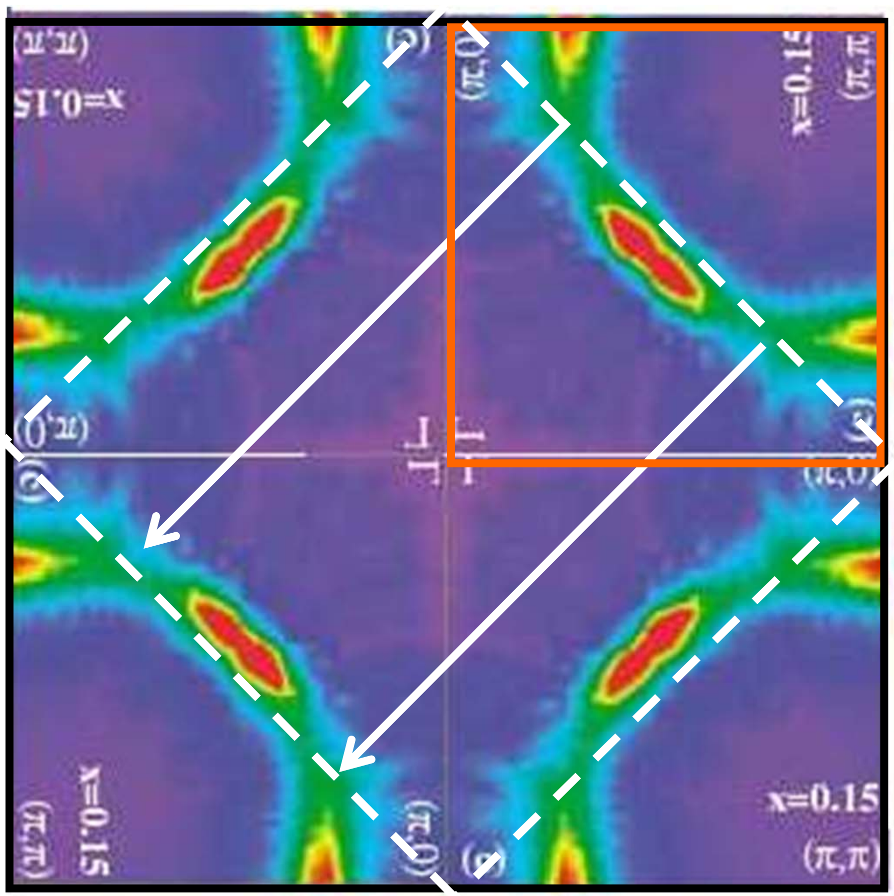
Hot spots from AFM quasi-static scattering

Mermin-Wagner

$d = 2$



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

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

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

Armitage et al. PRL 2001

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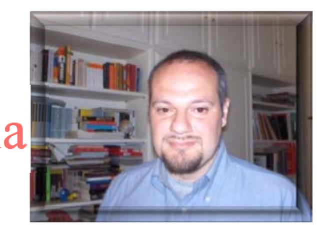
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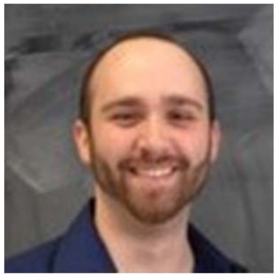

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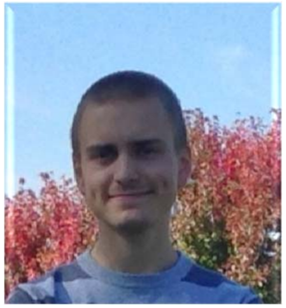

Charles-David Hébert

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Alexandre Day

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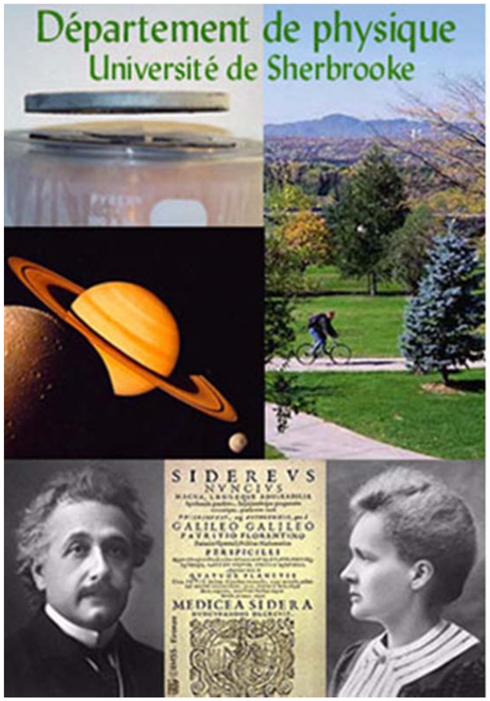
Further references

For references, September 2013 Julich summer school
Strongly Correlated Superconductivity

http://www.cond-mat.de/events/correl13/manuscripts/tremblay.pdf

Lecture notes

http://www.physique.usherbrooke.ca/tremblay/cours/phy-892/N-corps.pdf



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Merci

Thank you