

Strongly correlated superconductivity

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Jülich summer school, 25 Sept. 2013

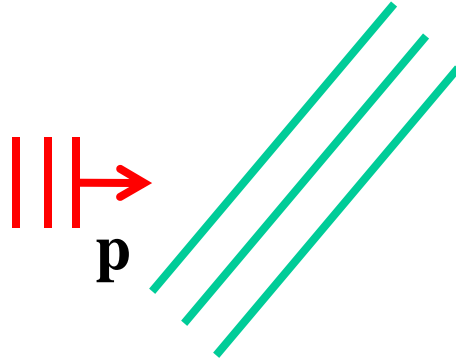


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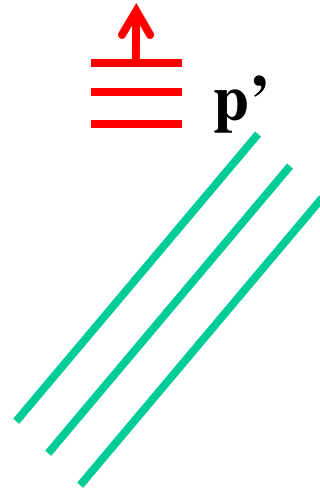
Superconductivity



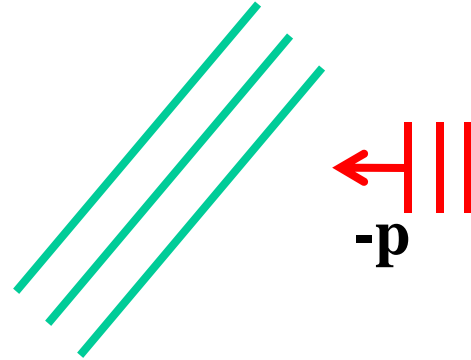
Attraction mechanism in the metallic state



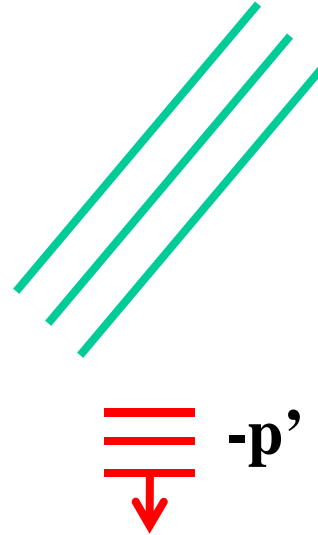
Attraction mechanism in the metallic state



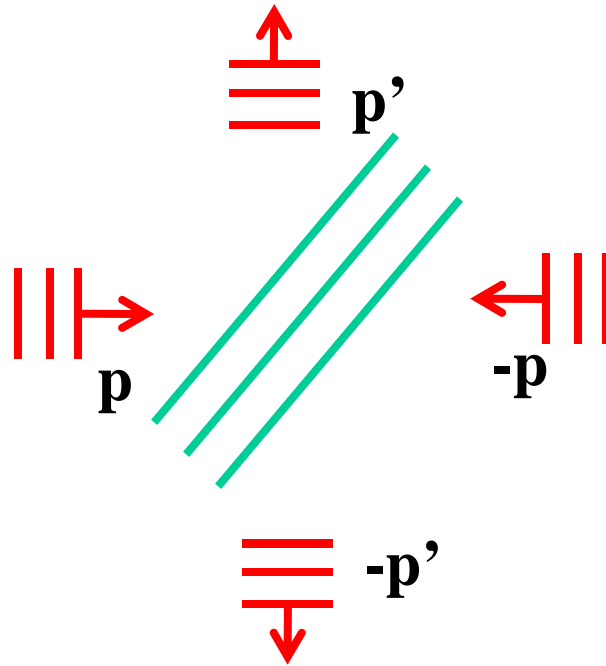
Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



#1 Cooper pair, #2 Phase coherence

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

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

$$|\text{BCS}(\theta)\rangle = \dots + e^{iN\theta} |N\rangle + e^{i(N+2)\theta} |N+2\rangle + \dots$$



Breakdown of band theory

Half-filled band is metallic?



Half-filled band: Not always a metal

NiO, Boer and Verwey



Peierls, 1937



Mott, 1949



« Conventional » Mott transition

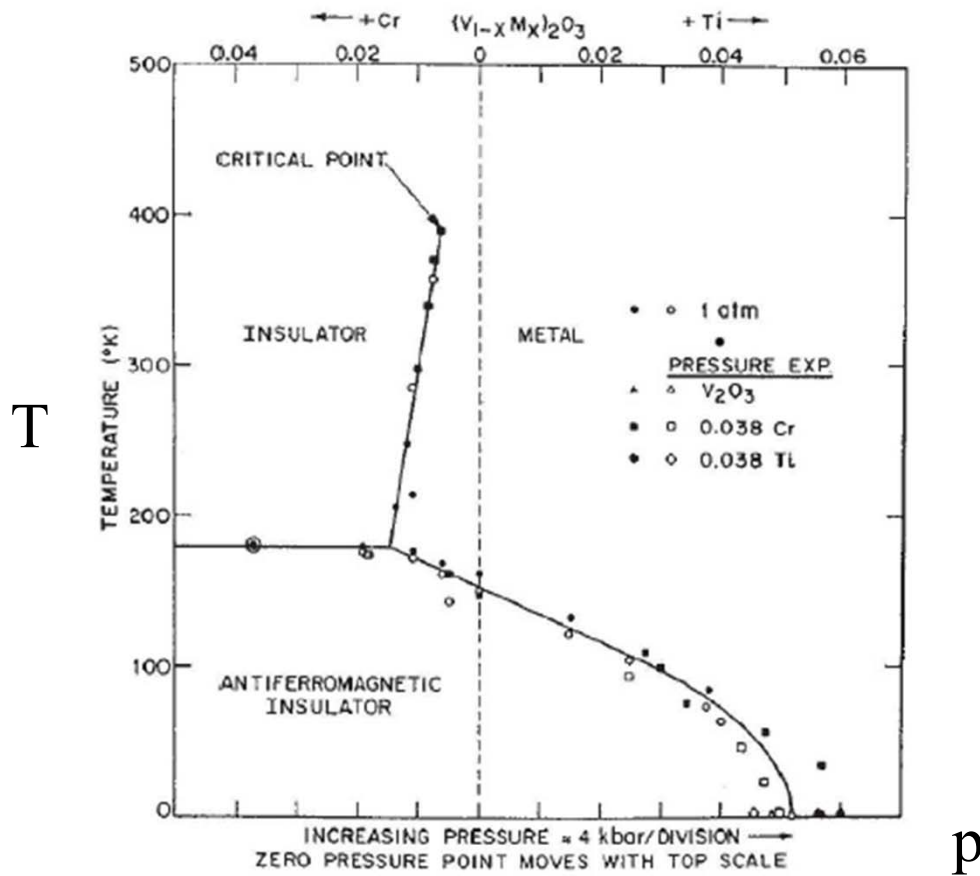


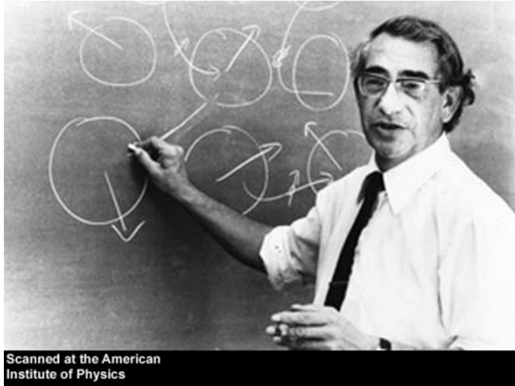
Figure: McWhan, PRB 1970; Limelette, Science 2003

2. The model

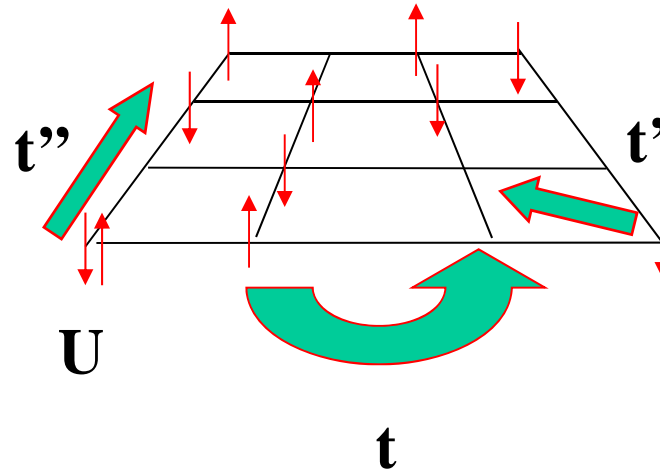
$$H = - \sum_{\langle ij \rangle \sigma} t_{i,j} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



Hubbard model



1931-1980



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

Attn: Charge transfer insulator



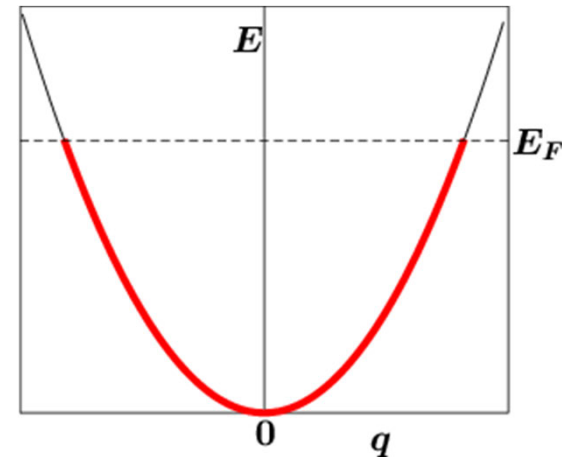
$$U = 0$$

$$H = -\sum_{\langle ij \rangle \sigma} t_{i,j} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma})$$

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

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

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



$$t_{ij} = 0$$

$$H =$$

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

⋮

U



U



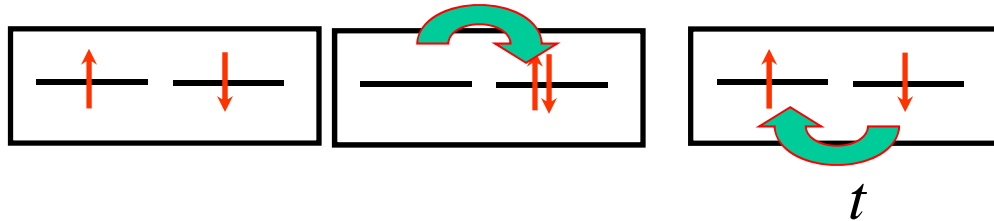
2^N

$$|\Psi\rangle = \prod_i c_{i\uparrow}^\dagger \prod_j c_{j\downarrow}^\dagger |0\rangle$$



Interesting in the general case

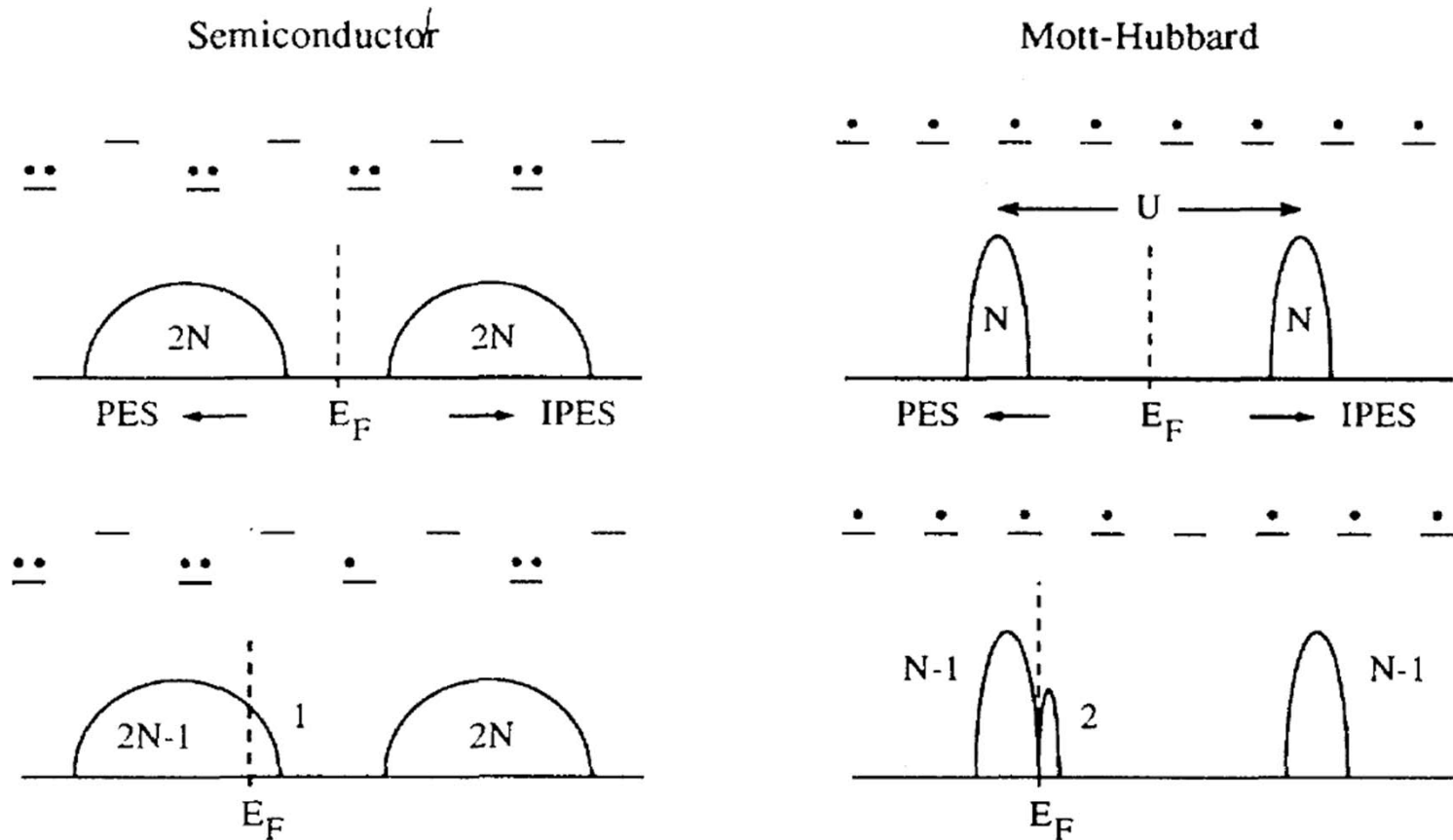
$$H = -\sum_{\langle ij \rangle \sigma} t_{i,j} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



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 T_c and organics, the view from DMFT
 1. Quantum clusters
 2. Normal state and pseudogap
 3. SC state
6. Methods, 2 of them: C-DMFT and TPSC
7. Conclusion



3. Weakly and strongly correlated antiferromagnets

What is a phase?



« 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
 - Often hard to « derive » from first principles (fractionalization - gauge theories)



Antiferromagnetic phase: emergent properties

- Some broken symmetries
 - Time reversal symmetry
 - Translation by one lattice spacing
 - Unbroken Time-reversal times translation by lattice vector \mathbf{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



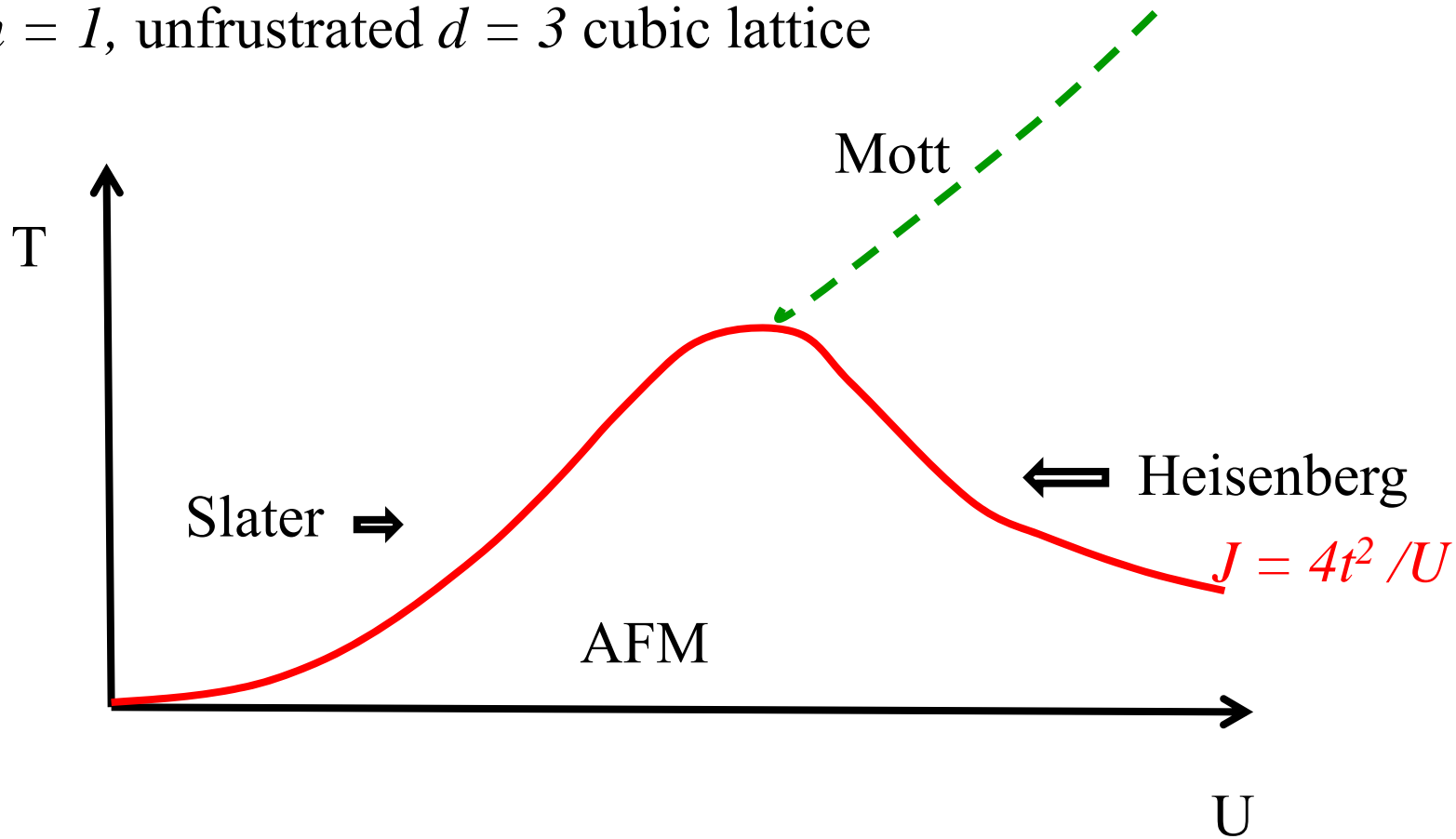
3. Strong vs weak coupling for an antiferromagnet

3.1 Qualitative



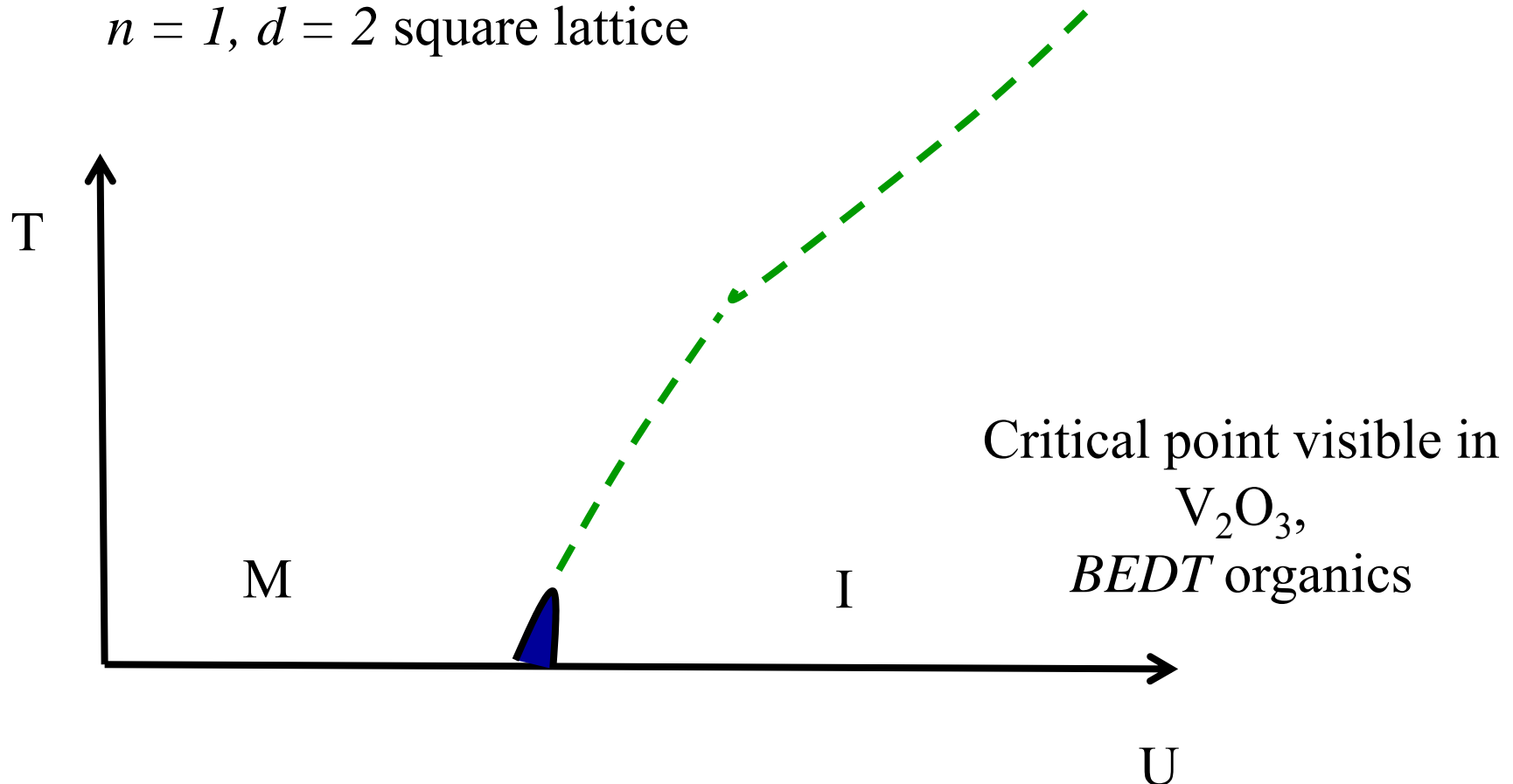
Local moment and Mott transition

$n = 1$, 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 $T = 0$



4. Weakly and strongly correlated superconductivity

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)



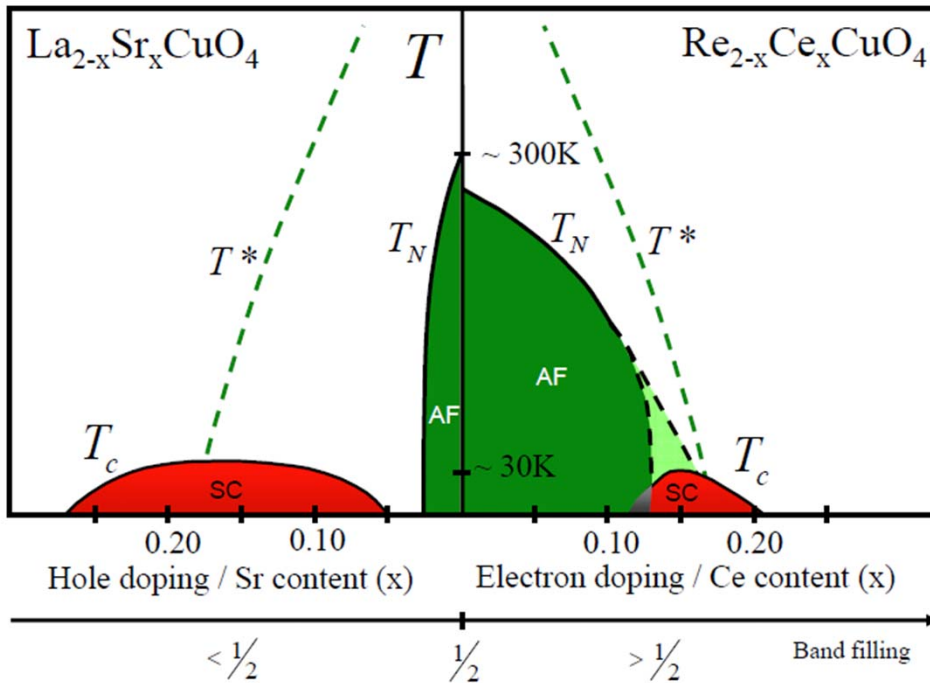
Superconductivity not universal even with phonons: weak or strong coupling

- 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



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) ...

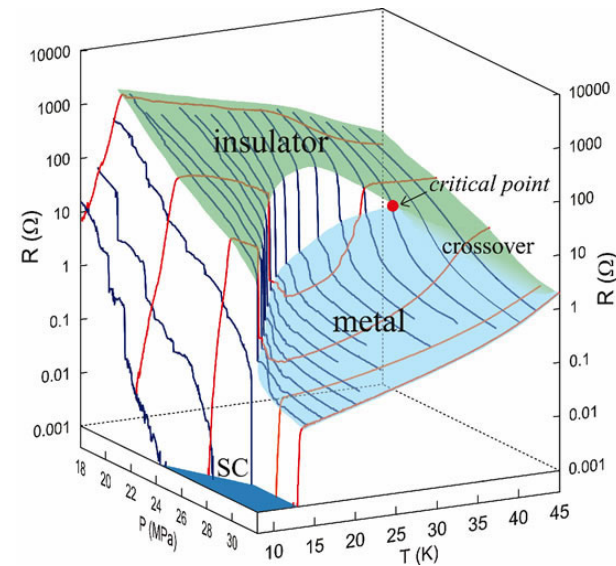
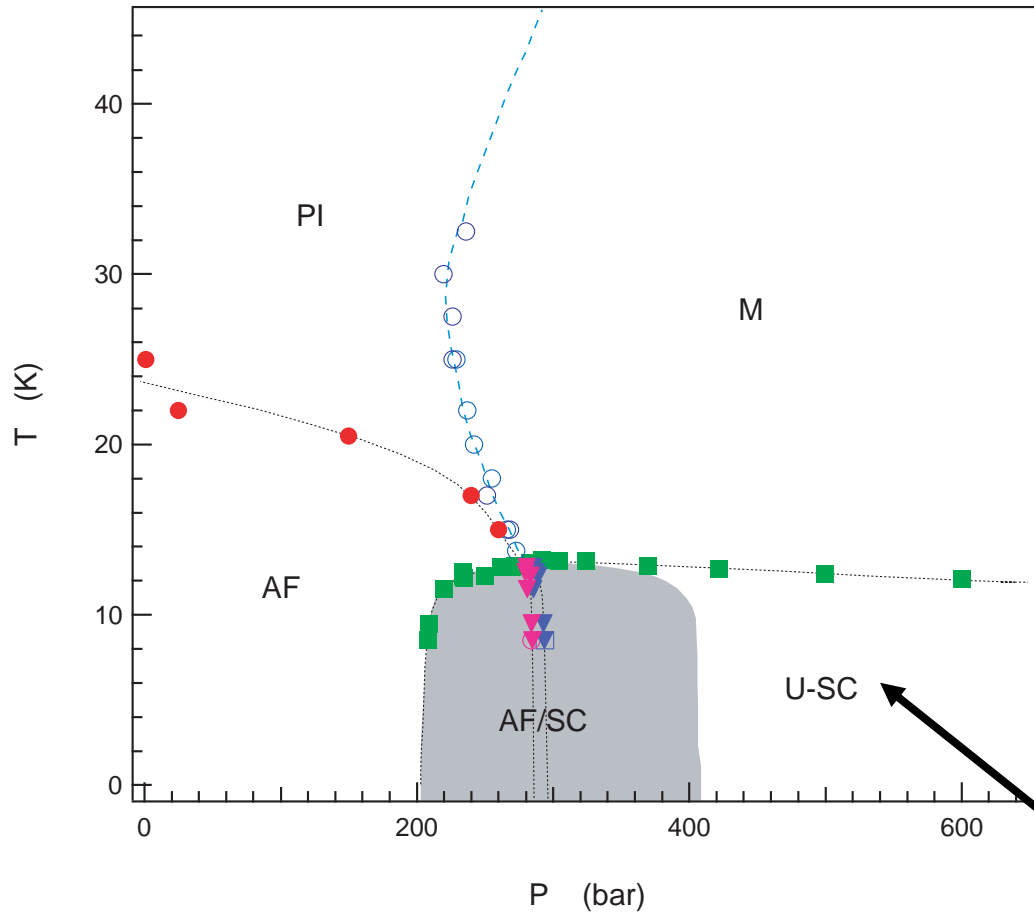
- Or Mott Physics?

- RVB: P.A. Lee Rep. Prog. Phys. **71**, 012501 (2008)

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



Other class of strongly correlated SC



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 ($X=\text{Cu}[\text{N}(\text{CN})_2]\text{Cl}$)

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



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**



Mott-Ioffe-Regel limit

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

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

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

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

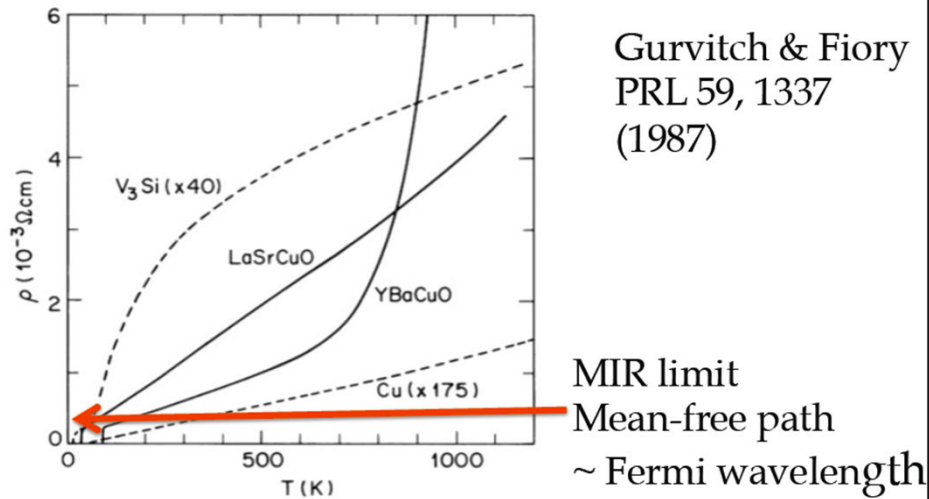
$$\sigma = \frac{1}{2\pi d} k_F e^2 \left(\frac{\ell}{\hbar} \right)$$

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

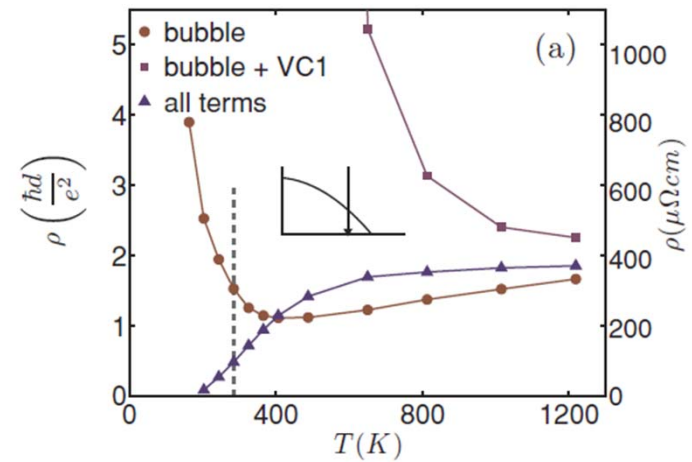
$$\sigma_{MIR} = \frac{e^2}{\hbar d}$$



Hole-doped cuprates and MIR limit



LSCO 17%, YBCO optimal



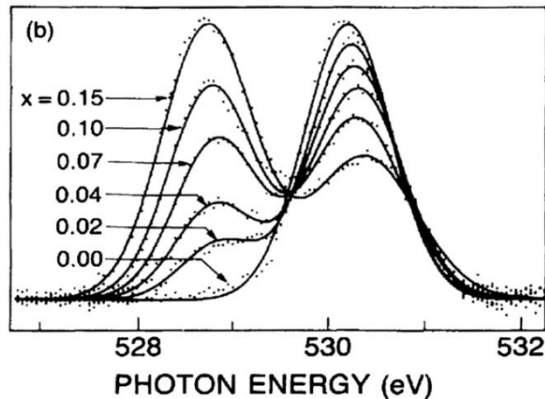
Dominic Bergeron TPSC

PHYSICAL REVIEW B 84, 085128 (2011)

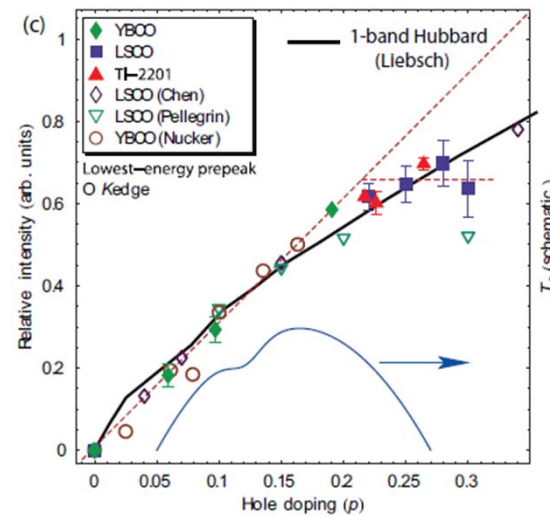
Optical and dc conductivity of the two-dimensional Hubbard model in the pseudogap regime and across the antiferromagnetic quantum critical point including vertex corrections



Experiment: X-Ray absorption



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



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

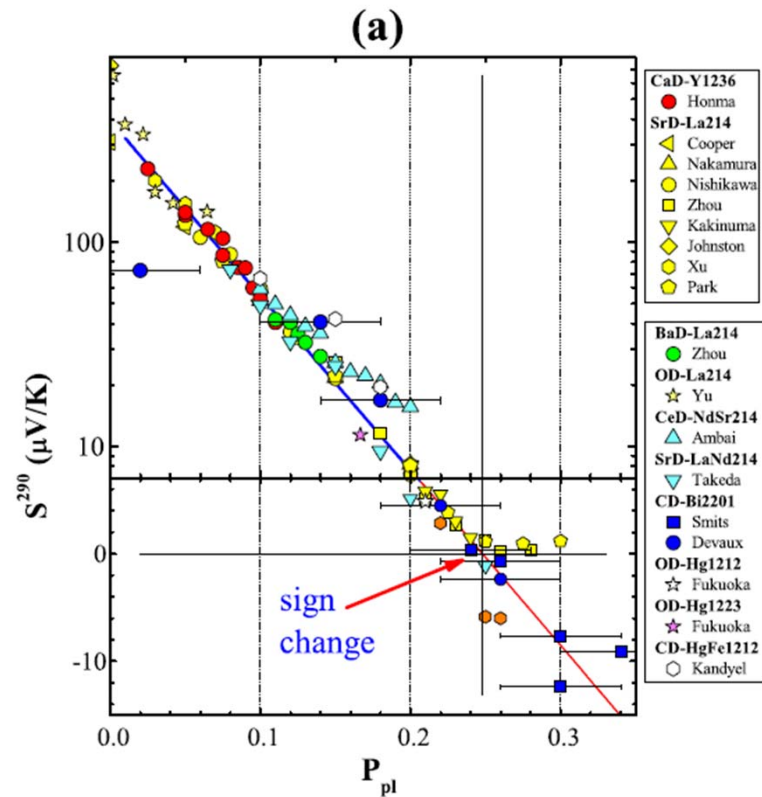
Phillips, Jarrell PRL , vol. **105**, 199701 (2010)

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

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



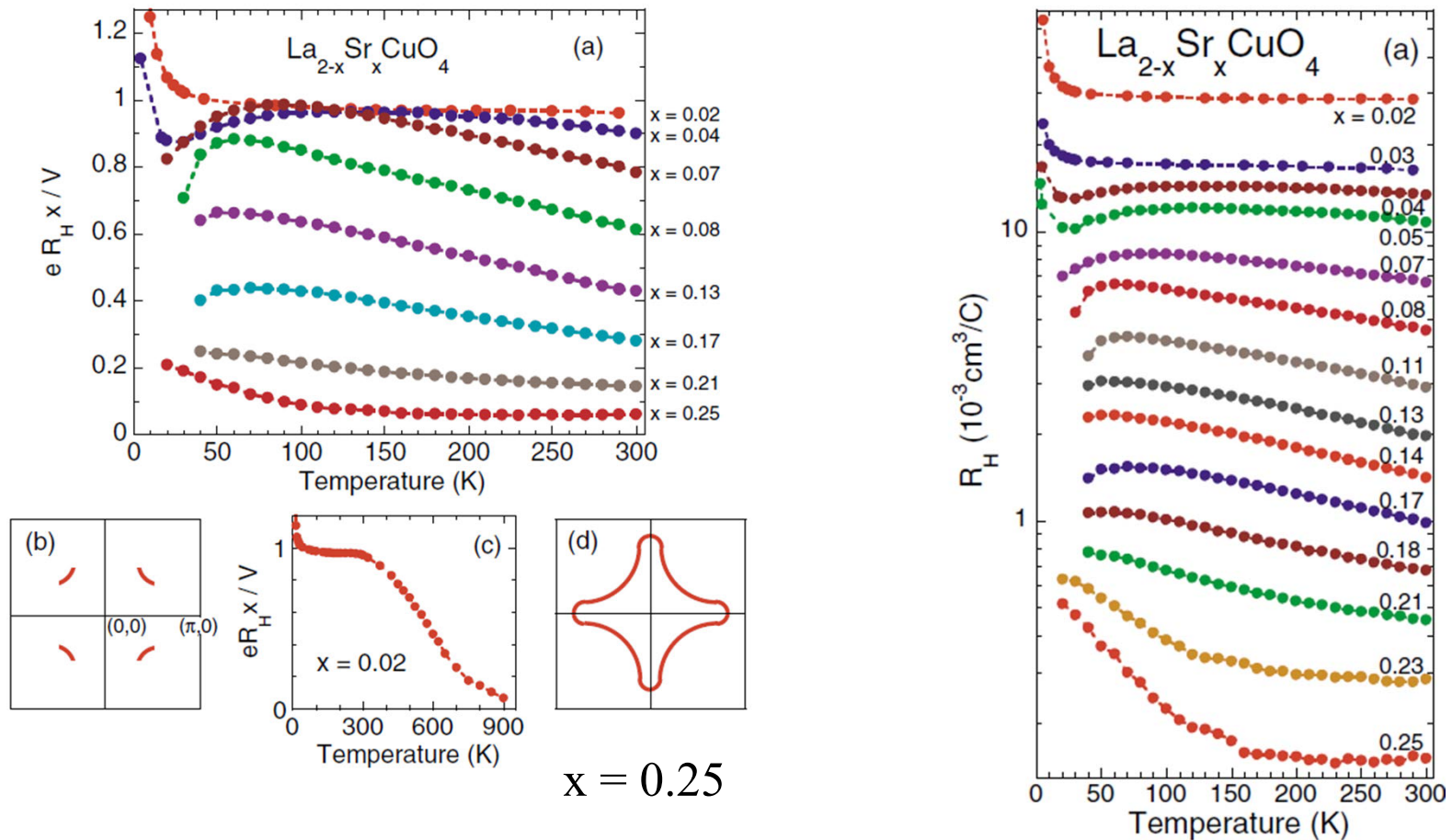
Thermopower



T. Honma and P. H. Hor, Phys. Rev. B **77**,
184520 (2008).

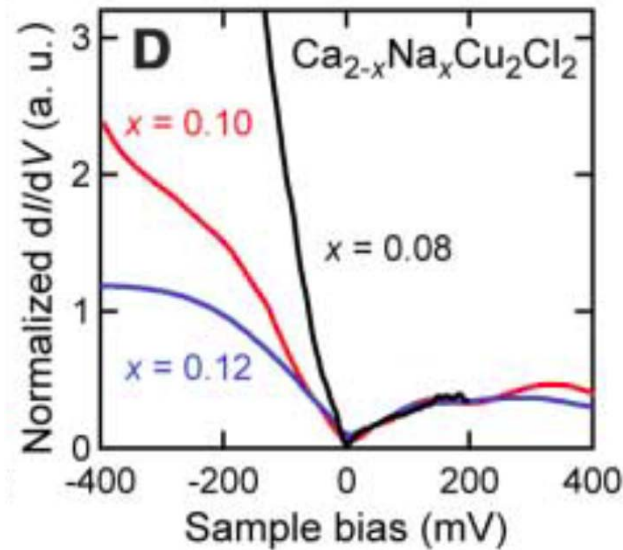


Hall coefficient



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

Density of states (STM)



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

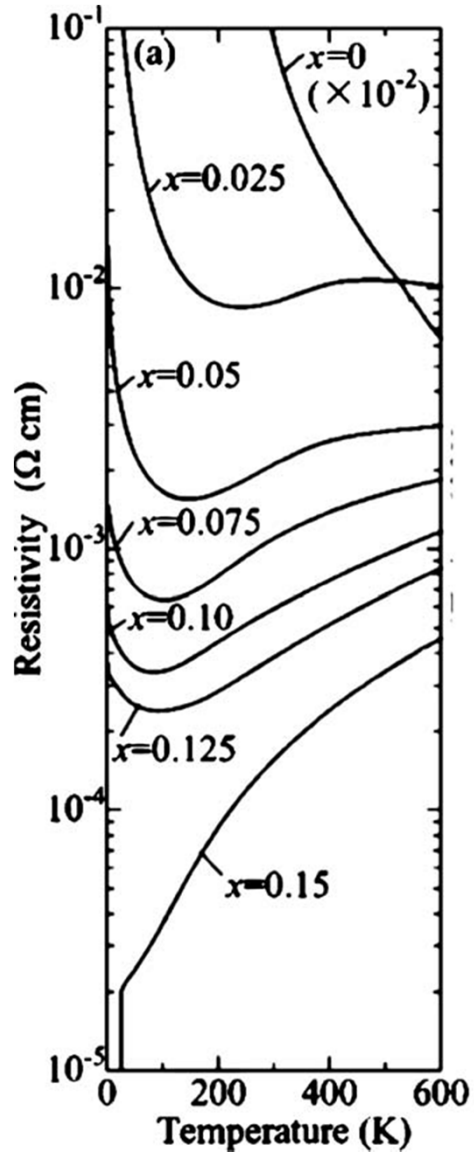


e-doped cuprates

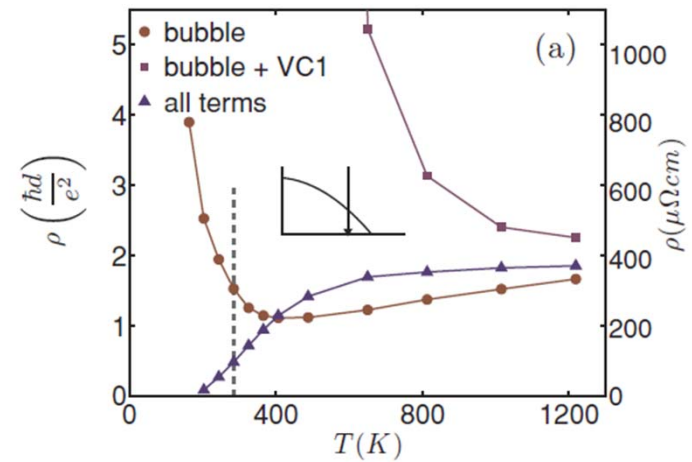
Less strongly coupled: evidence from
the normal state



Electron-doped and MIR limit



NCCO

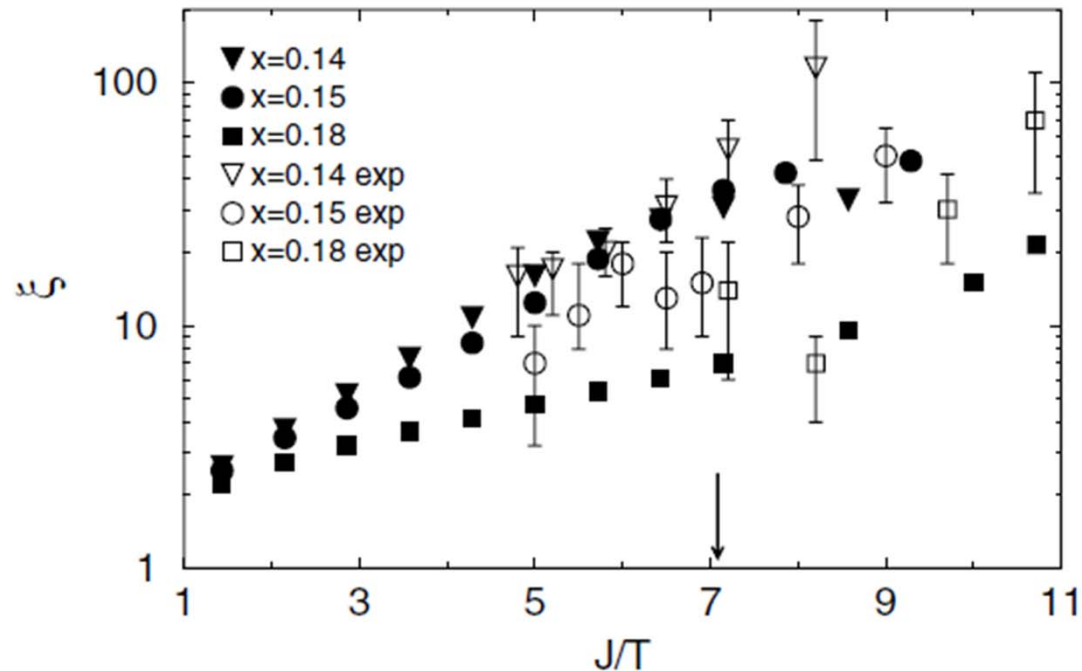


Dominic Bergeron et al. TPSC
PRB **84**, 085128 (2011)

Onose et al. 2004



TPSC vs experiment for ξ



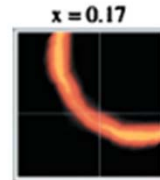
Kyung et al. PRL **93**, 147004 (2004)

P. K. Mang et al., Phys. Rev. Lett. **93**, 027002 (2004).

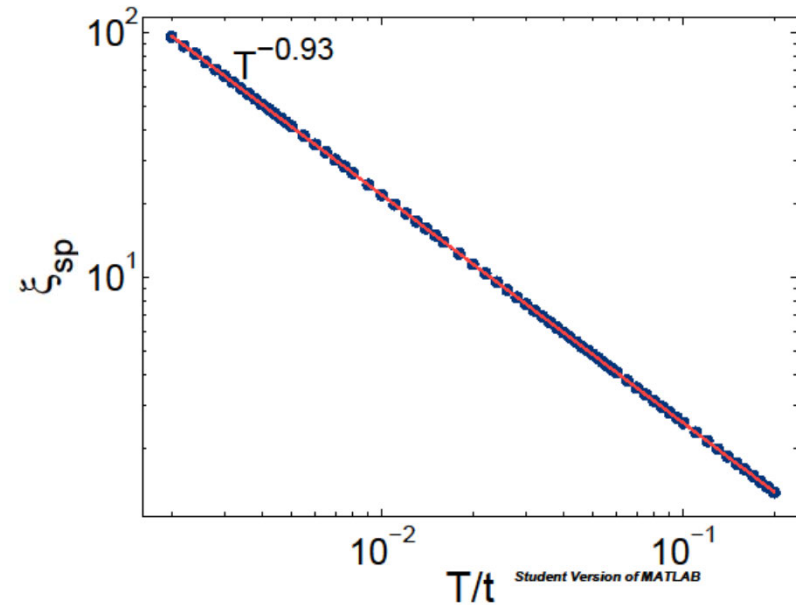
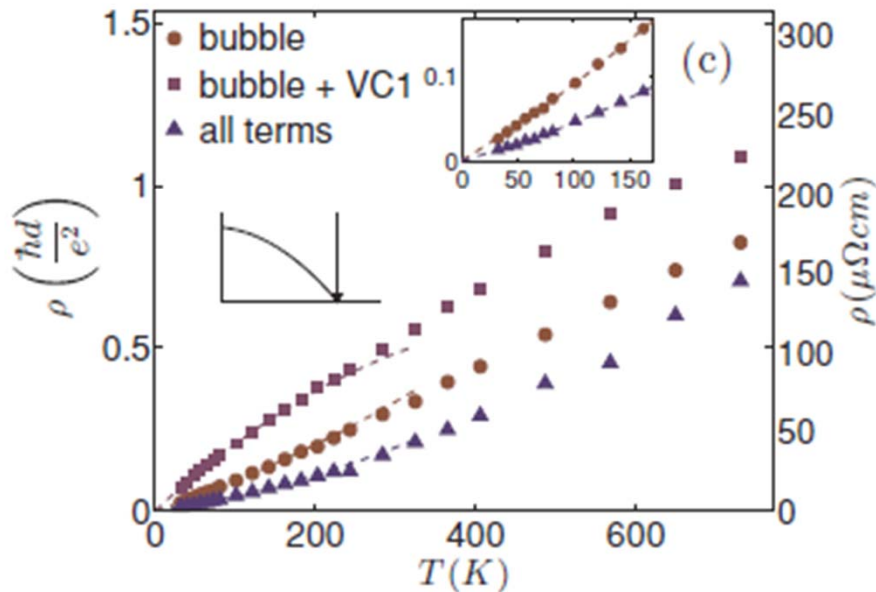
M. Matsuda et al., Phys. Rev. B **45**, 12 548 (1992).



$\xi(T)$ at the QCP



NCCO
Matsui et al. PRB 2007



$z = 1$ Motoyama, Nature 2007

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

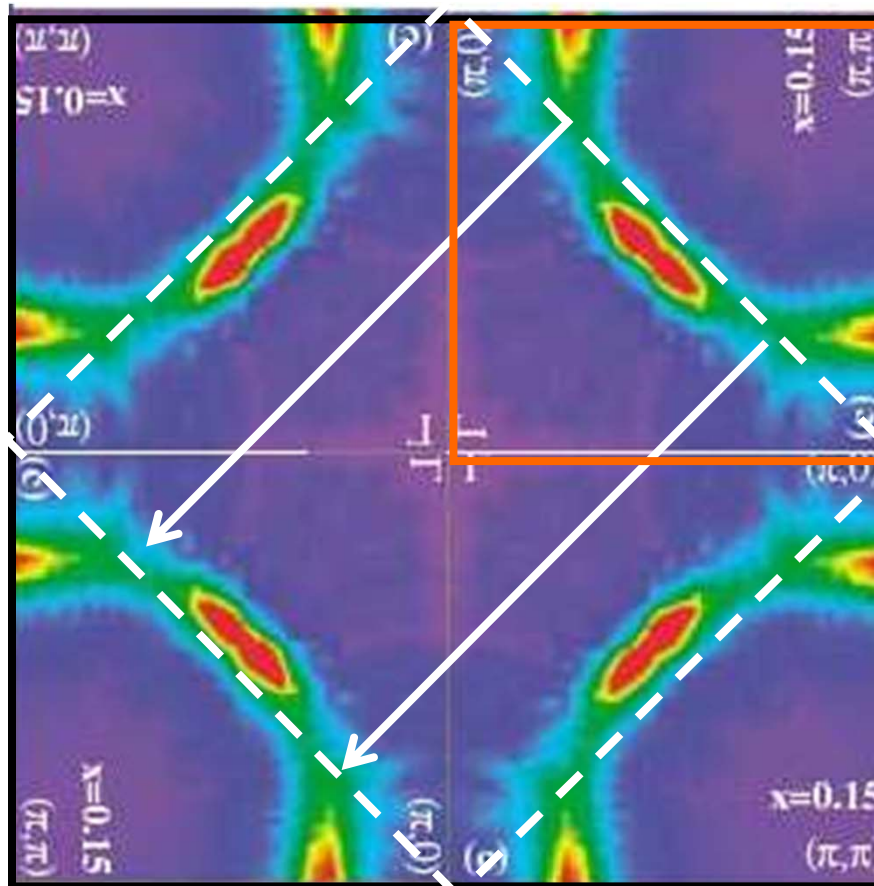
Dominic Bergeron TPSC



Hot spots from AFM quasi-static scattering

Mermin-Wagner

$d = 2$

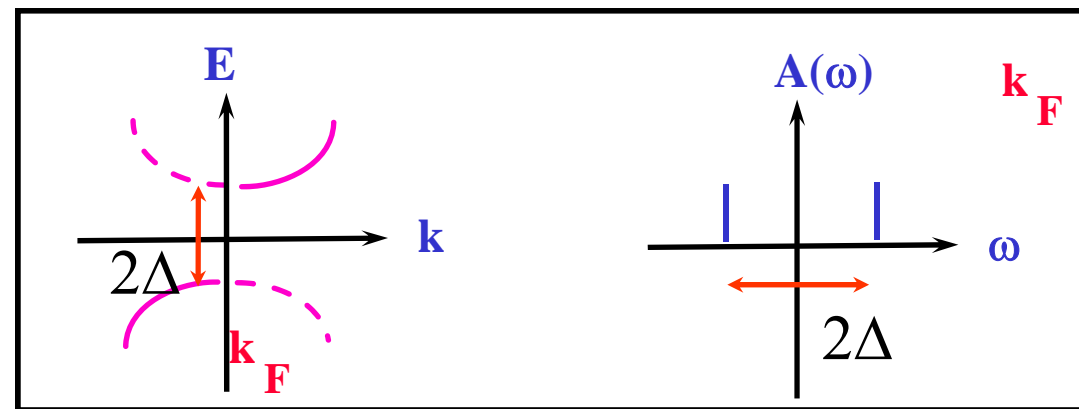
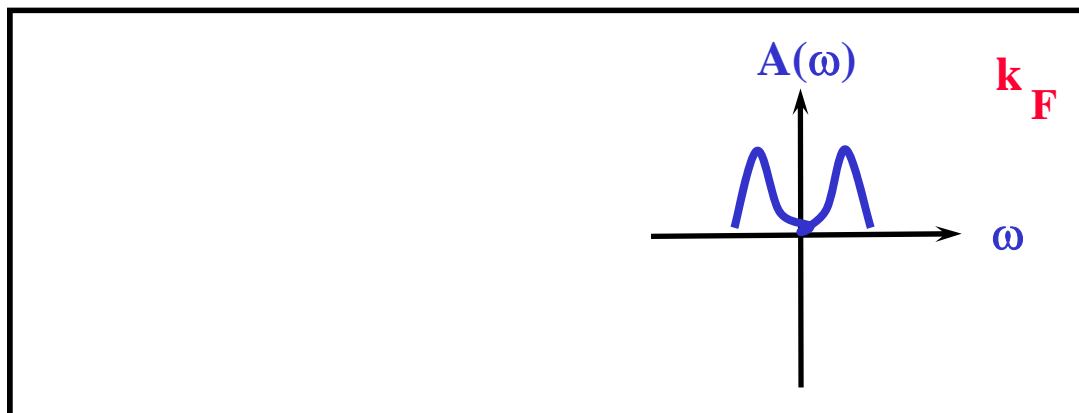
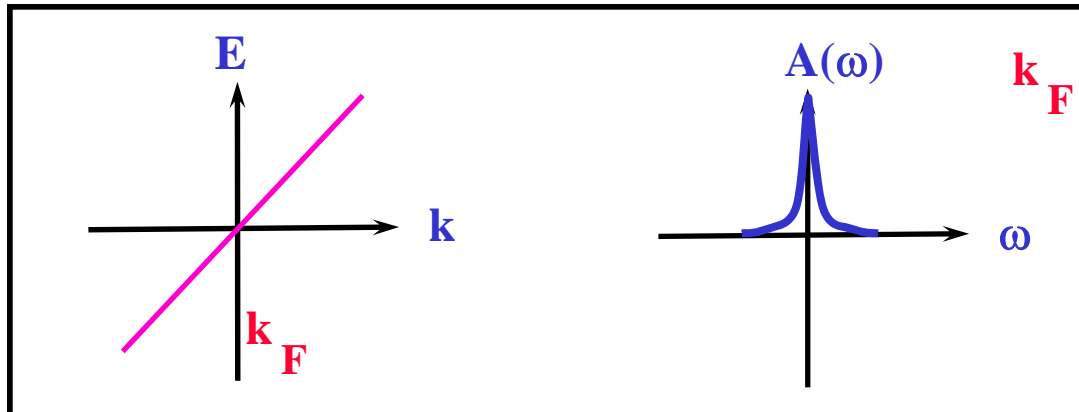
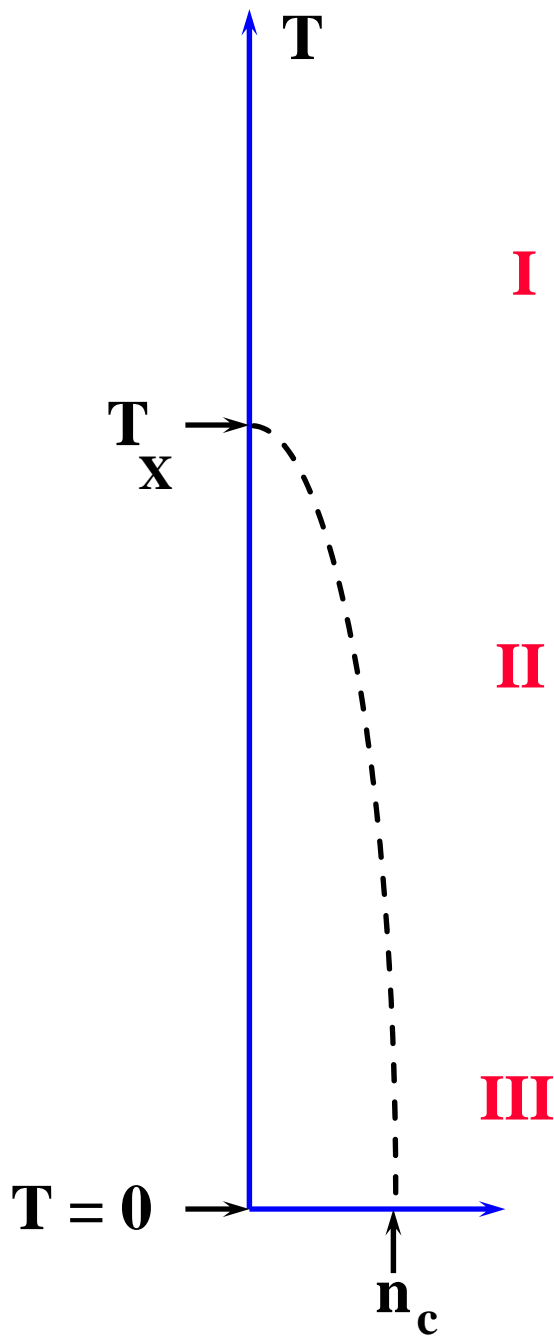


Vilk, A.-M.S.T (1997)
Kyung, Hankevych,
A.-M.S.T., PRL, 2004

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

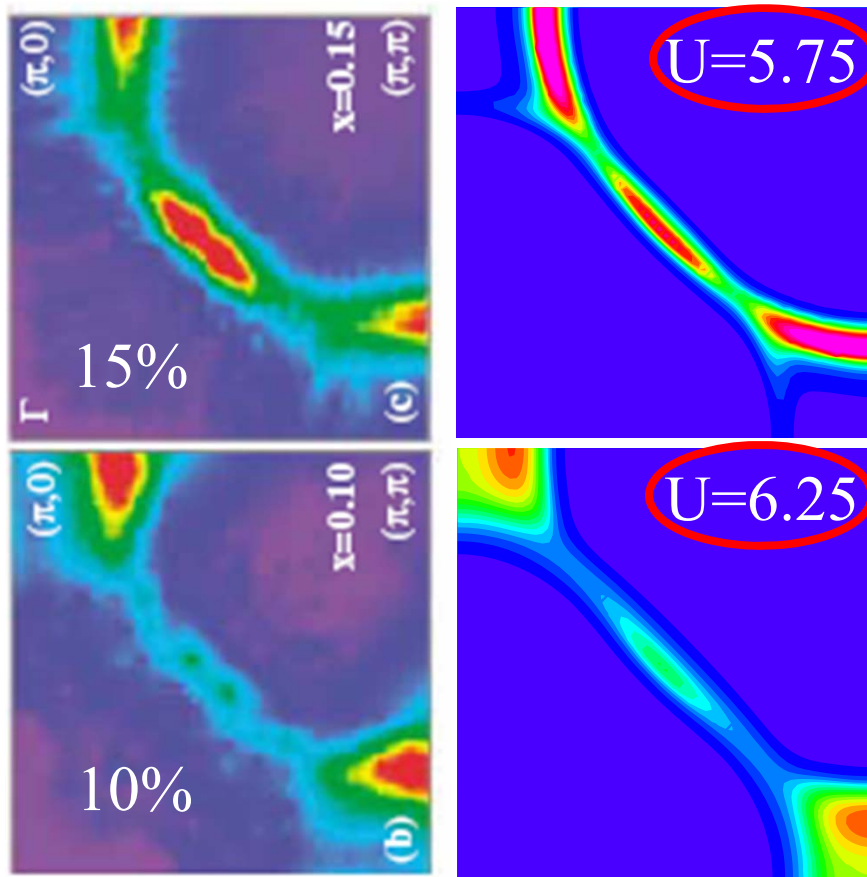
Motoyama, E. M. et al..
445, 186–189 (2007).

Armitage et al. PRL 2001

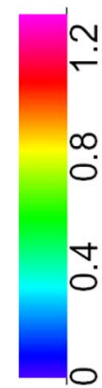


Fermi surface plots

Hubbard repulsion U has to...



be not too large



increase for
smaller doping

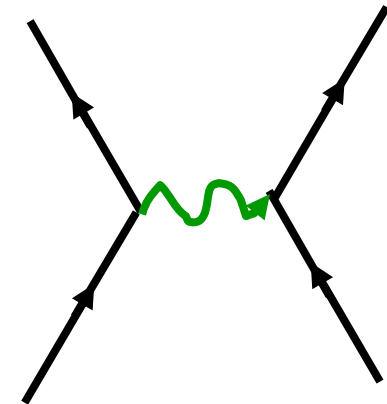
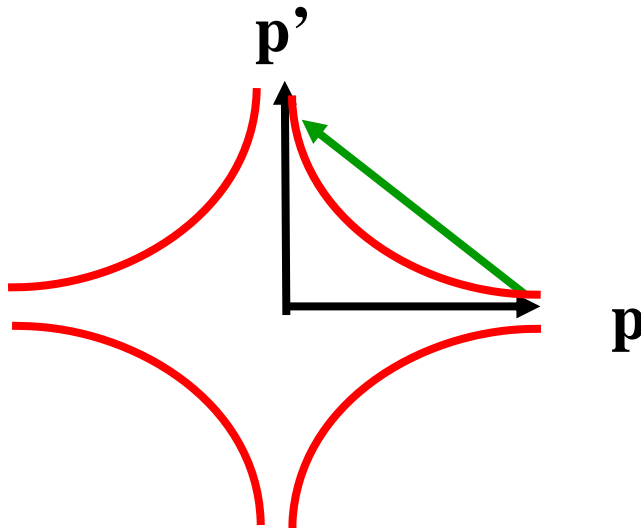
4. Weakly and strongly correlated superconductivity

Weakly correlated case



Cartoon « BCS » weak-coupling picture

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



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

Exchange of spin waves?
Kohn-Luttinger

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

T_c with pressure

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

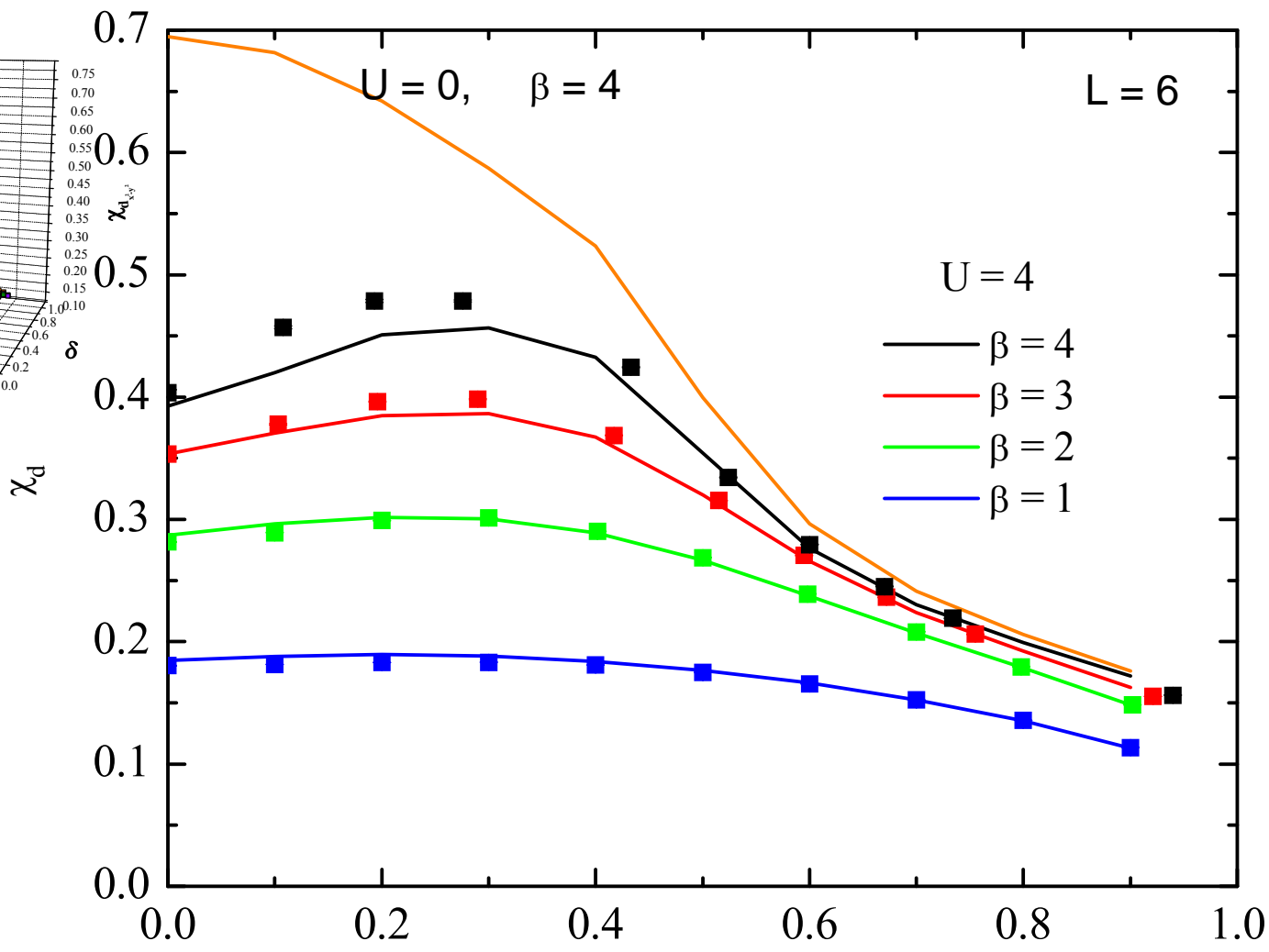
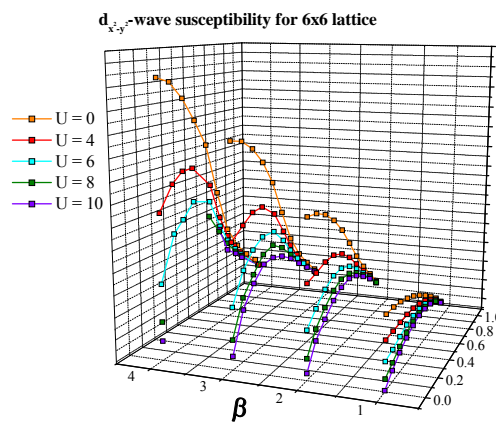
P.W. Anderson *Science* **317**, 1705 (2007)



Results from TPSC

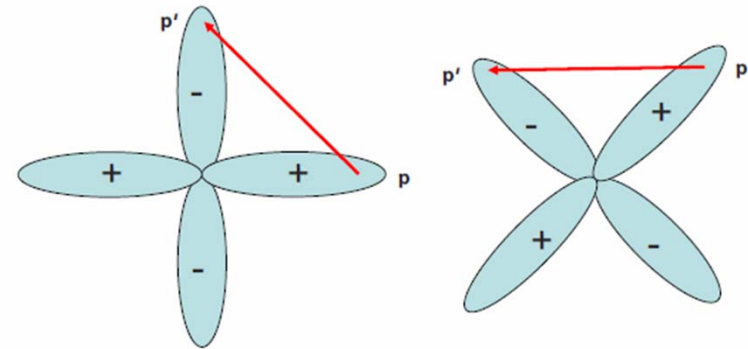
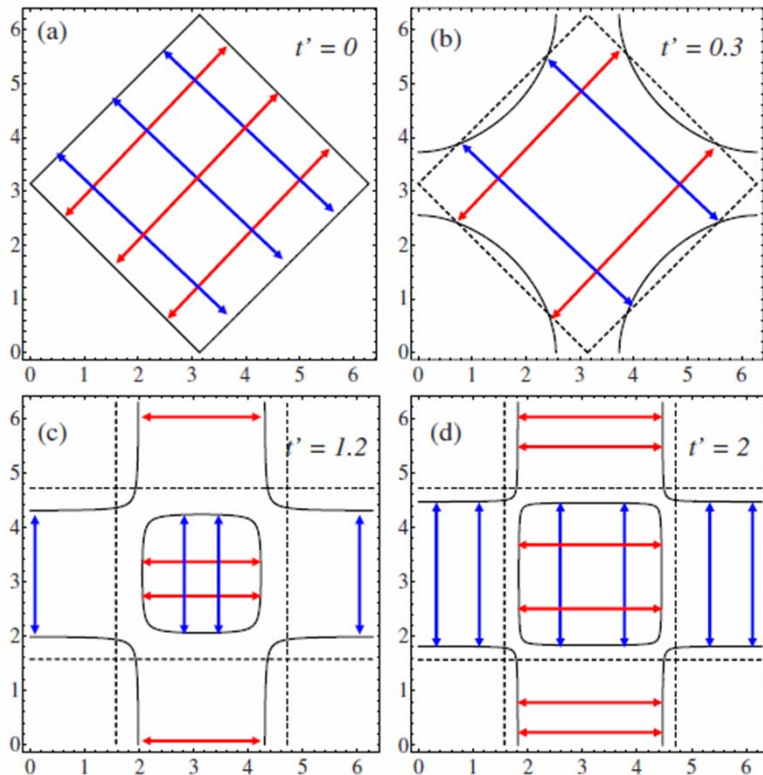
Satisfies Mermin-Wagner





QMC: symbols.
 Solid lines analytical.

Relation between symmetry and wave vector of AFM fluctuations



Hassan et al. PRB 2008



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T_c depends on t'

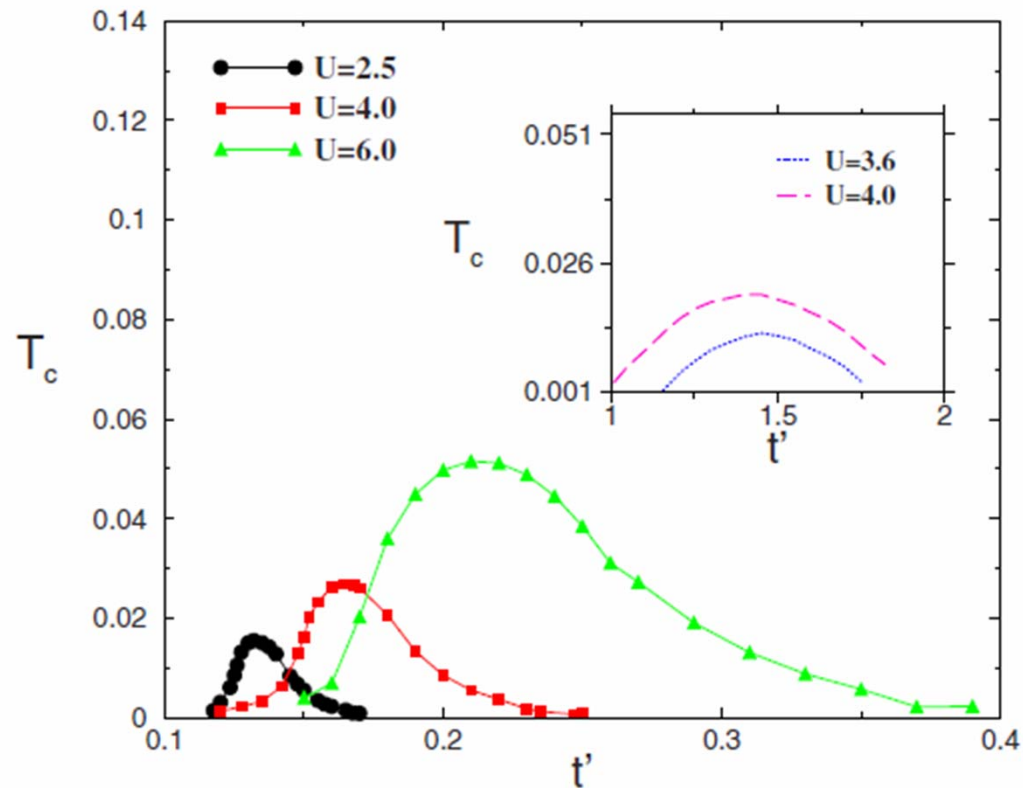


FIG. 5. (Color online) The $d_{x^2-y^2}$ superconducting critical temperature T_c as a function of t' at $U=2.5, 3$, and 4 for $n=1$. The inset shows the d_{xy} superconducting critical temperature T_c as a function of t' for $U=3.6$ and 4 .

Hassan et al. PRB 2008



Tc in RC regime or not

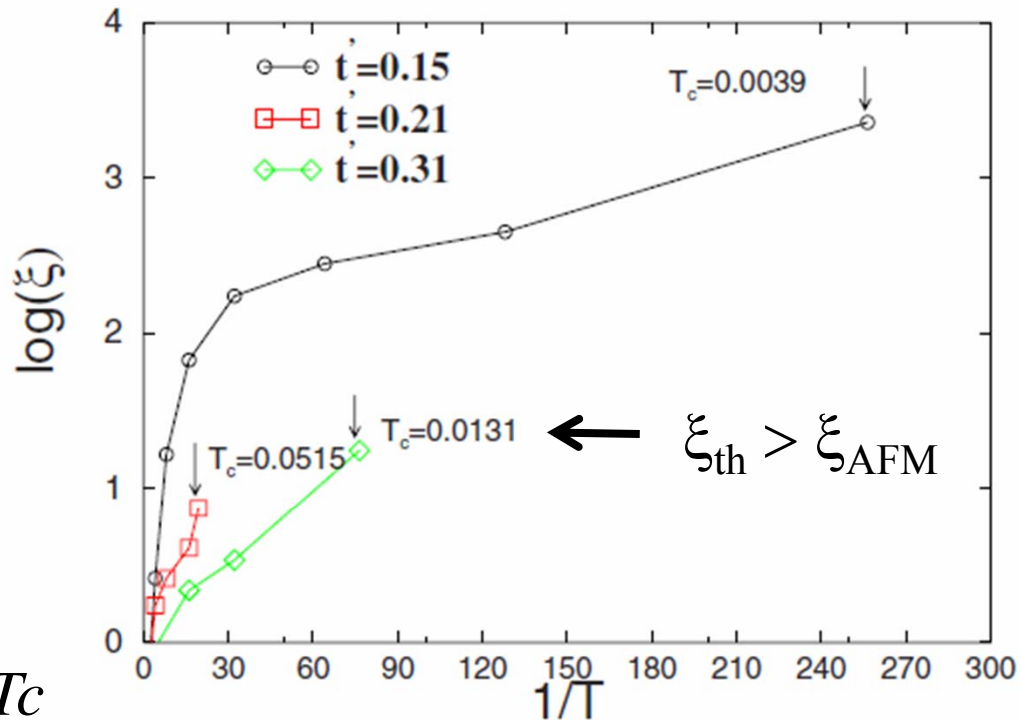


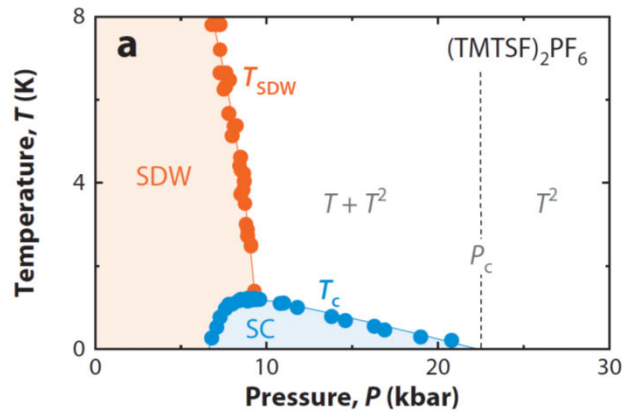
FIG. 6. (Color online) Logarithm base ten of the antiferromagnetic correlation length (in units of the lattice spacing) as a function of inverse temperature for three values of $t'=0.15, 0.21, 0.31$ at $U=4$ for $n=1$. The value of T_c for the corresponding t' is shown on the plot.

Hassan et al. PRB 2008

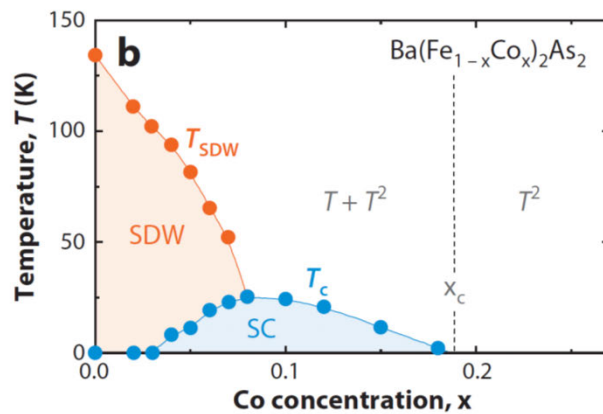


Organics & Pnictides

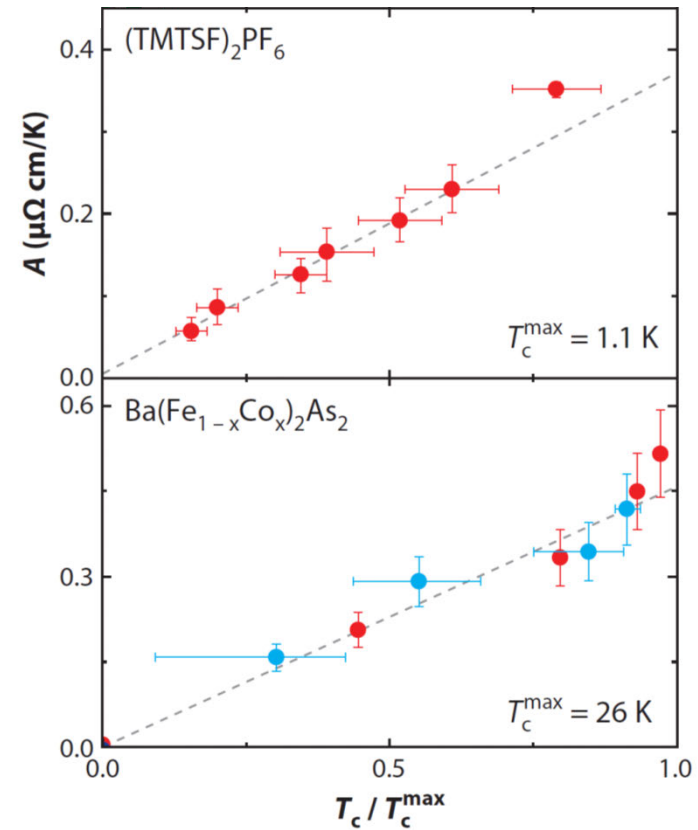
Organic



Pnictide

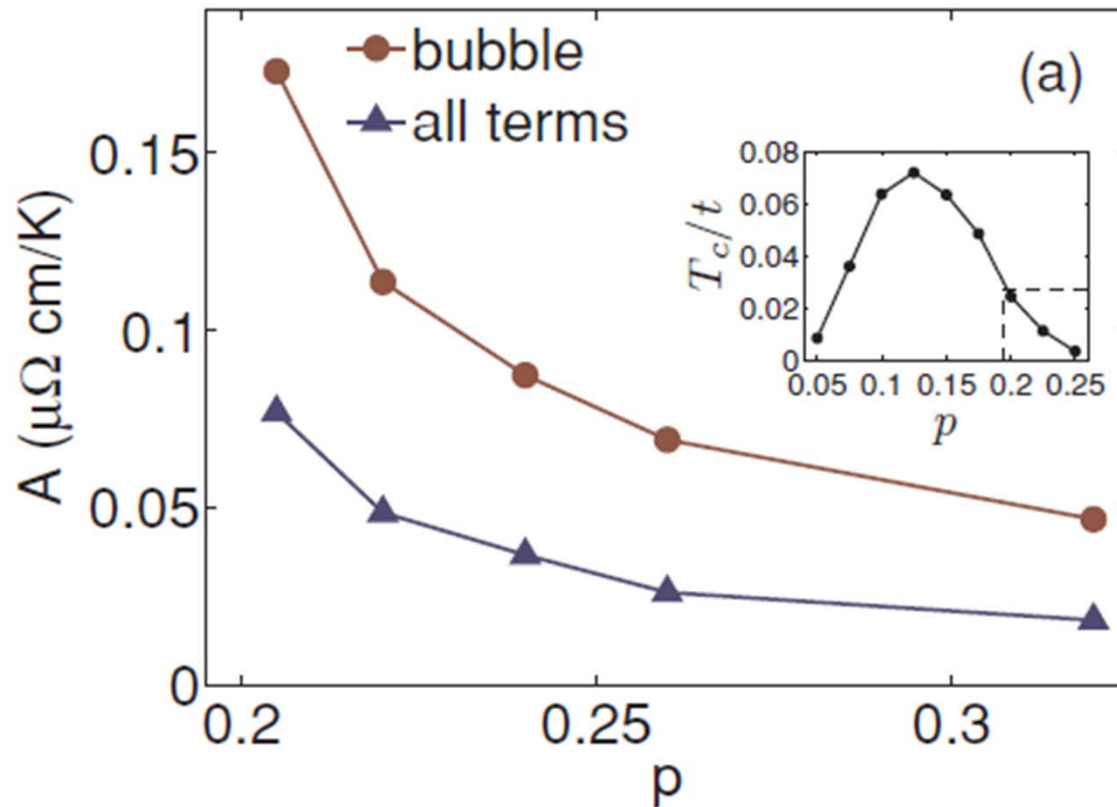


Bourbonnais, Sedeki, 2012



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

Correlation resistivity vs T_c



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



4. Weakly and strongly correlated superconductivity

Strong coupling 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 and organics: the view from dynamical mean-field theory

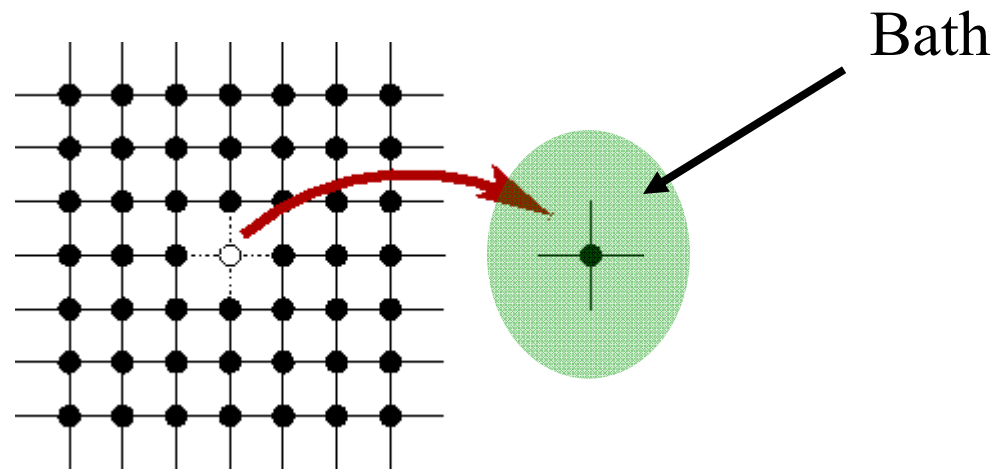
5.1: Quantum cluster approaches



Mott transition and Dynamical Mean-Field Theory.

The beginnings in $d = \text{infinity}$

- 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.

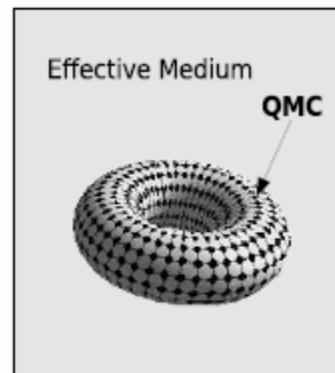


W. Metzner and D. Vollhardt, PRL (1989)
A. Georges and G. Kotliar, PRB (1992)
M. Jarrell PRB (1992)

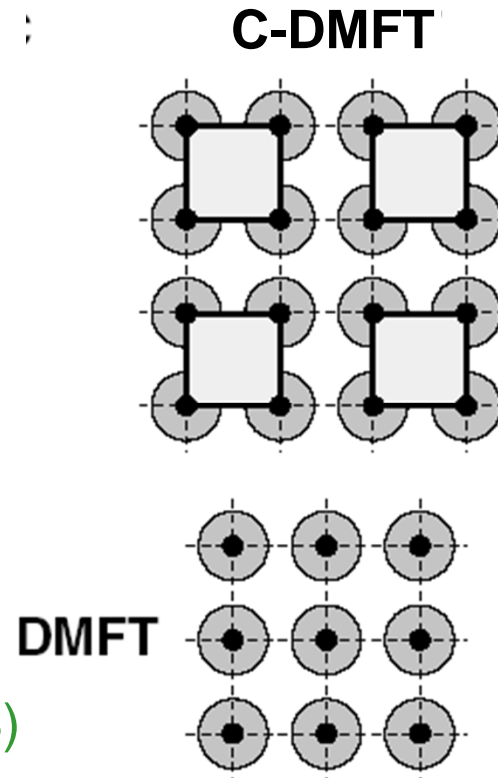
DMFT, ($d = 3$)



2d Hubbard: Quantum cluster method



DCA



Hettler ...Jarrell...Krishnamurty PRB **58** (1998)

Kotliar et al. PRL **87** (2001)

M. Potthoff *et al.* PRL **91**, 206402 (2003).

REVIEWS

Maier, Jarrell et al., RMP. (2005)

Kotliar *et al.* RMP (2006)

AMST *et al.* LTP (2006)



+ and -

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

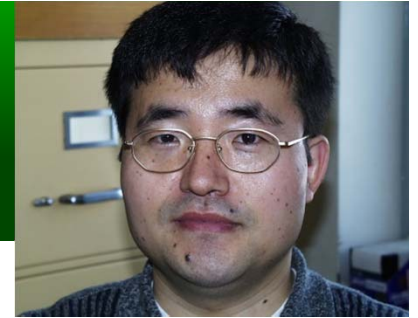


Two solvers for the cluster-in-a-bath problem

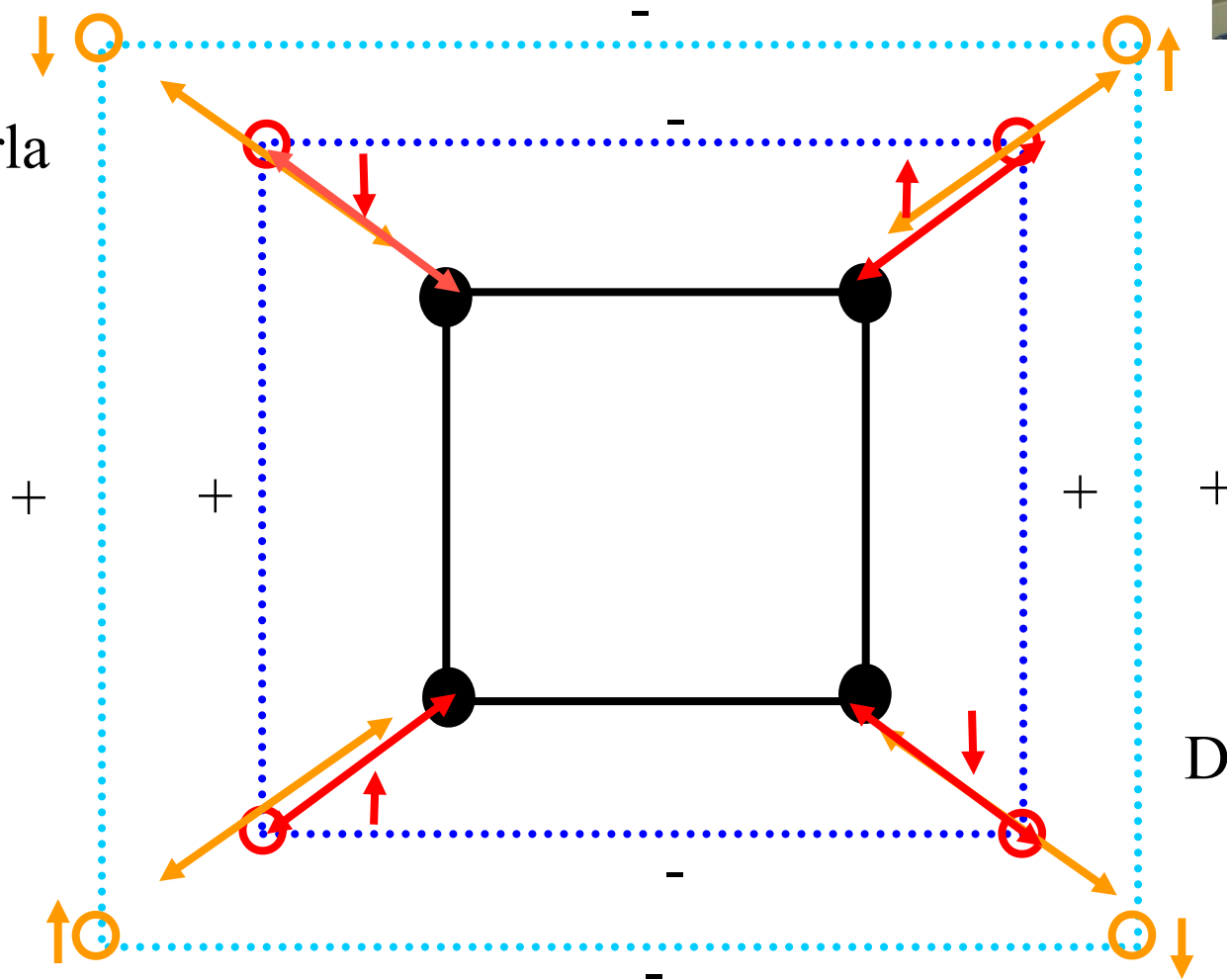
Competition AFM-dSC



S. Kancharla



B. Kyung

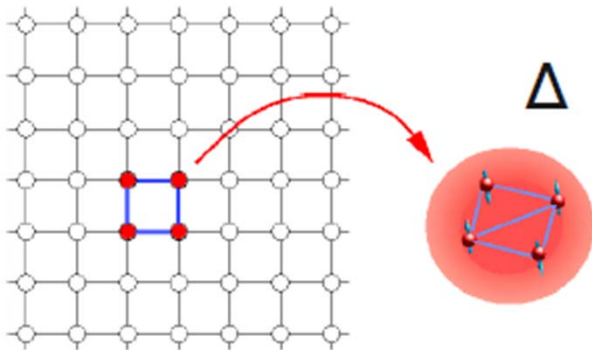


David Sénéchal

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



C-DMFT

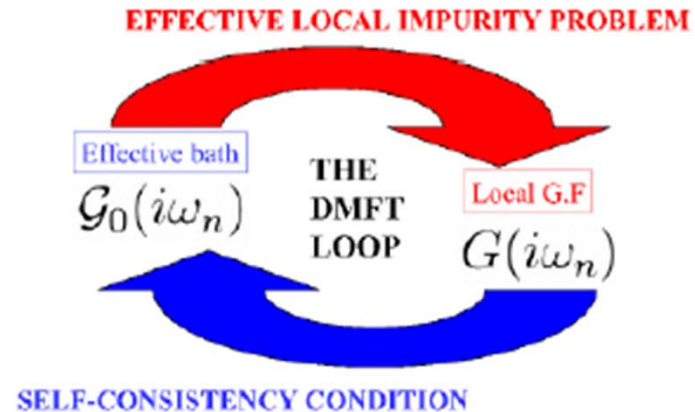


Mean-field is not a trivial problem! Many impurity solvers.

Here: continuous time QMC

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

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



$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n)$$

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

At finite T , solving cluster in a bath problem

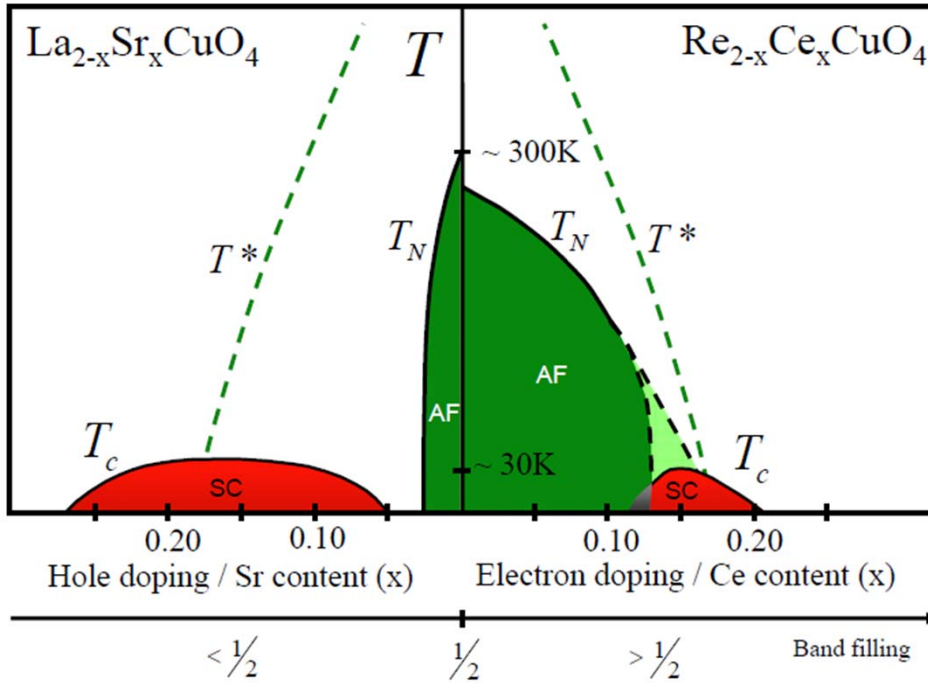
- Continuous-time Quantum Monte Carlo calculations to sum all diagrams generated from expansion in powers of hybridization.
 - P. Werner, A. Comanac, L. de' Medici, M. Troyer, and A. J. Millis, Phys. Rev. Lett. **97**, 076405 (2006).
 - K. Haule, Phys. Rev. B **75**, 155113 (2007).



5.2 Normal state and pseudogap

High-temperature superconductors

Armitage, Fournier, Greene, RMP (2009)



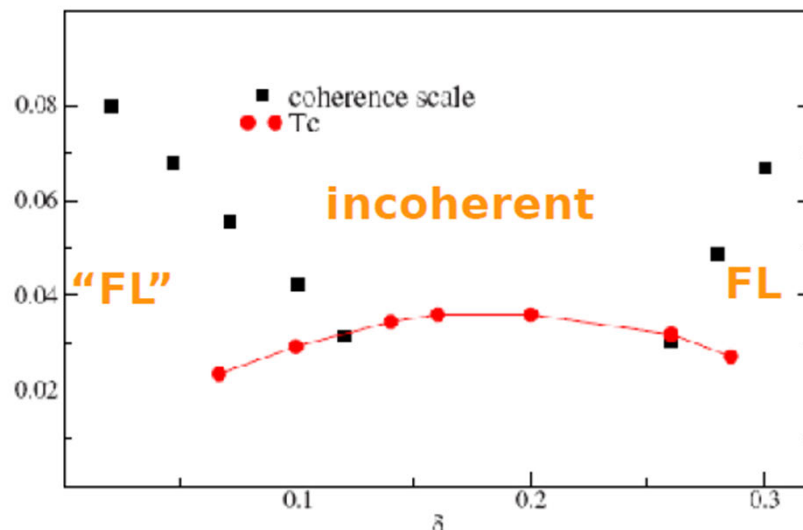
Three broad classes of mechanisms for pseudogap

- 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)

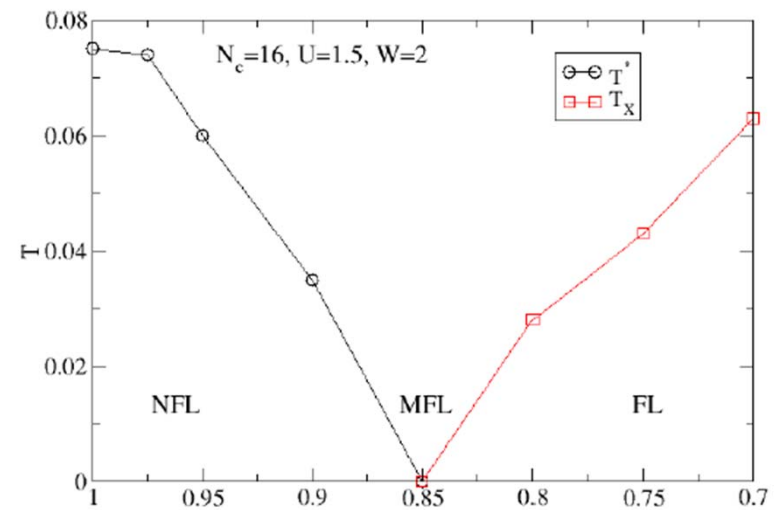


Doping driven Mott transition, $t' = 0$

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)

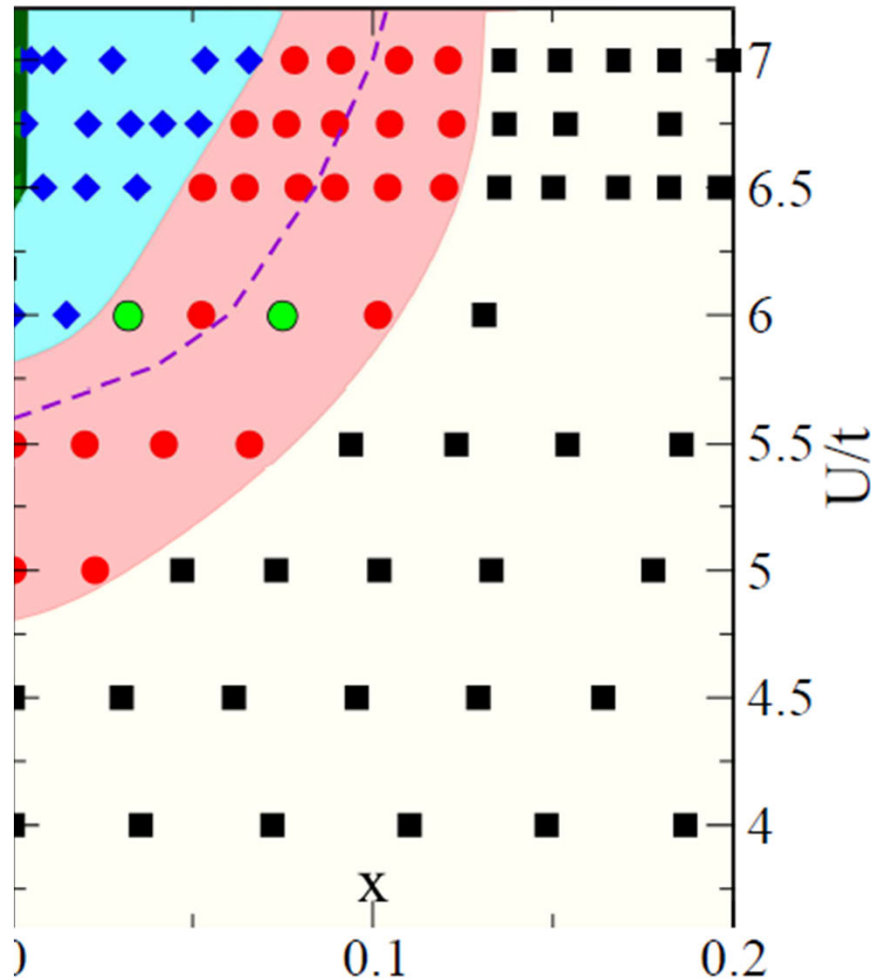


K. Haule, G. Kotliar, PRB (2007)



Vildhyadhiraja, PRL (2009) 3

Doping driven Mott transition



$$T = 0.25 t$$

Gull, Parcollet, Millis
arXiv:1207.2490v1

Gull, Werner, Millis, (2009)

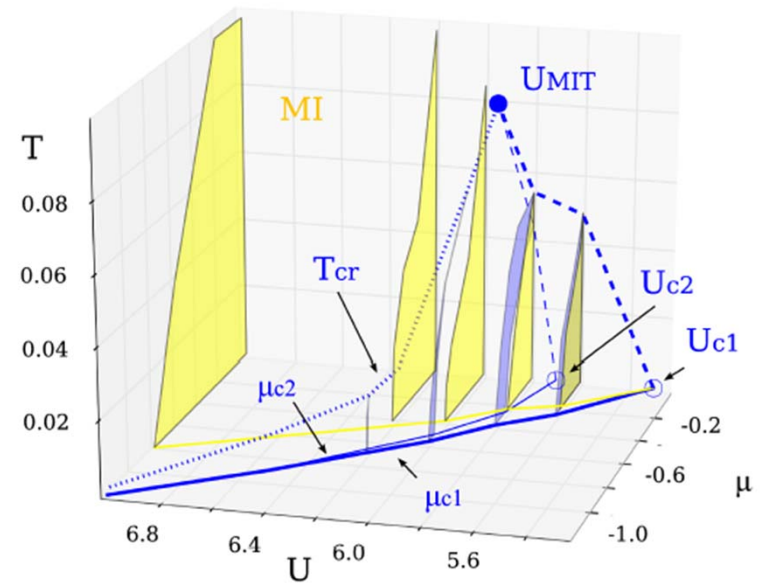
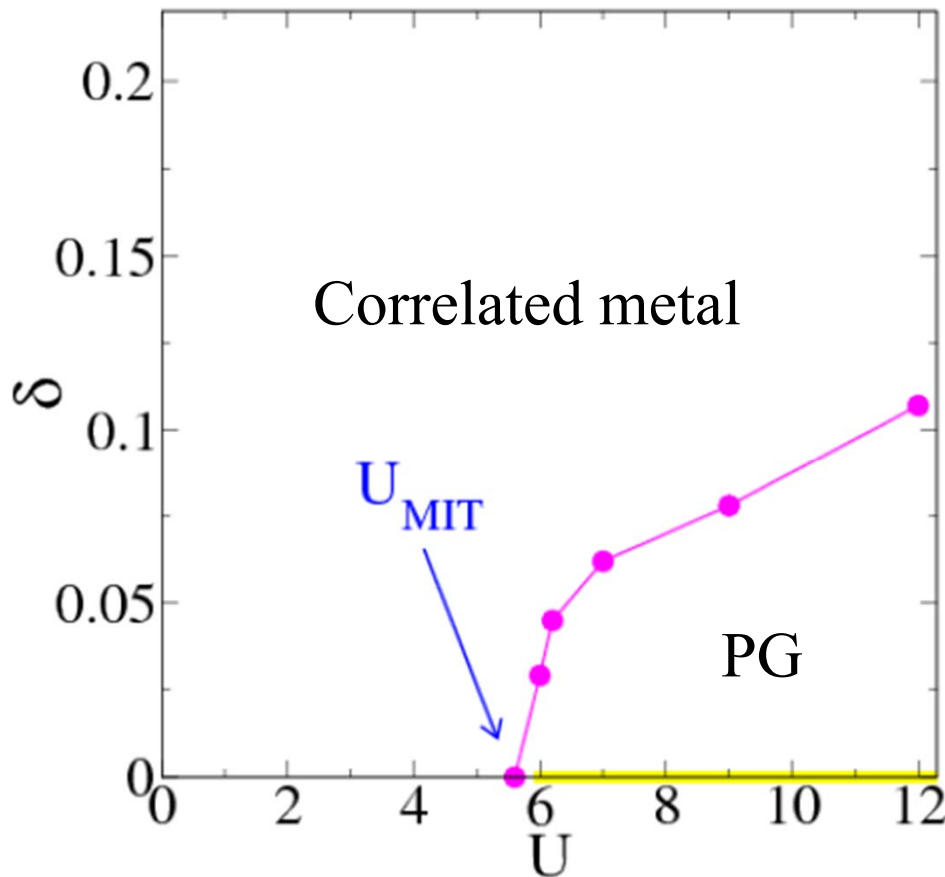
E. Gull, M. Ferrero, O. Parcollet, A. Georges, and A. J. Millis (2010)



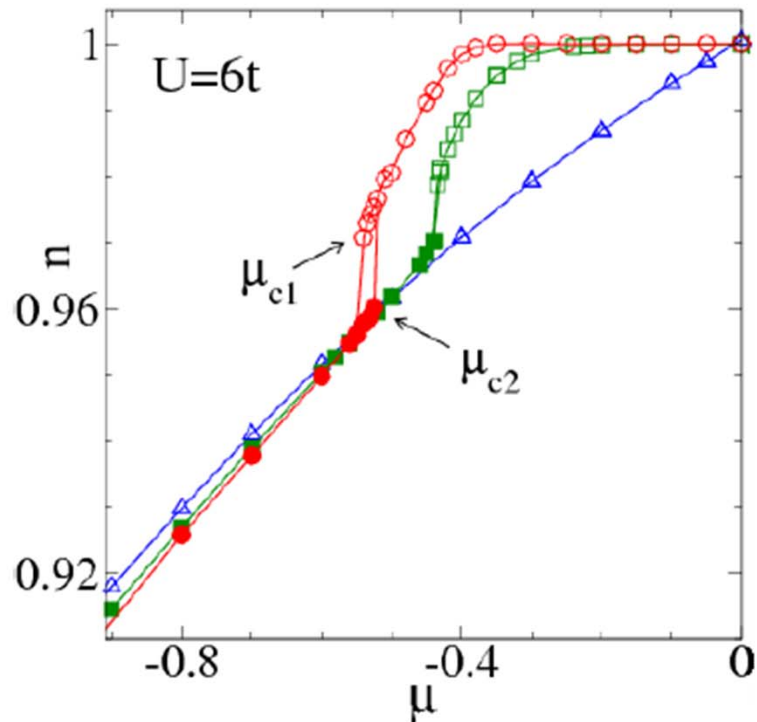
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Link to Mott transition up to optimal doping

Doping dependence of critical point as a function of U



First order transition at finite doping



$n(\mu)$ for several temperatures:

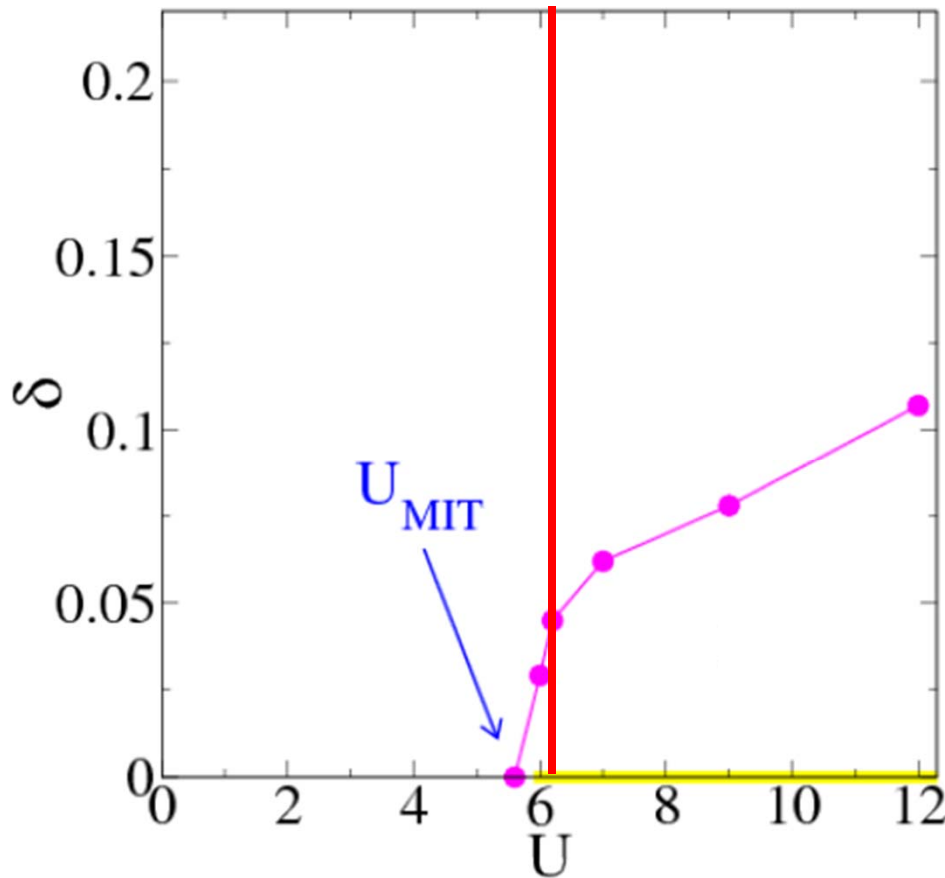
$T/t = 1/10, 1/25, 1/50$

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

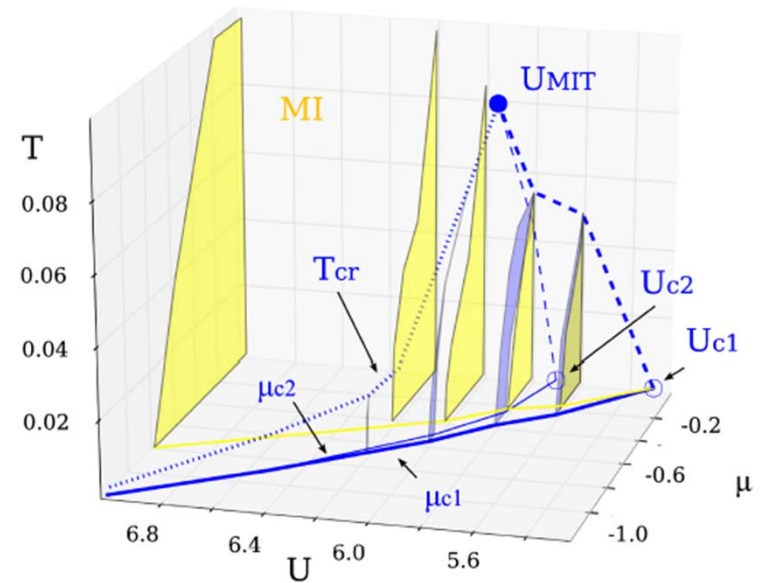


Link to Mott transition up to optimal doping

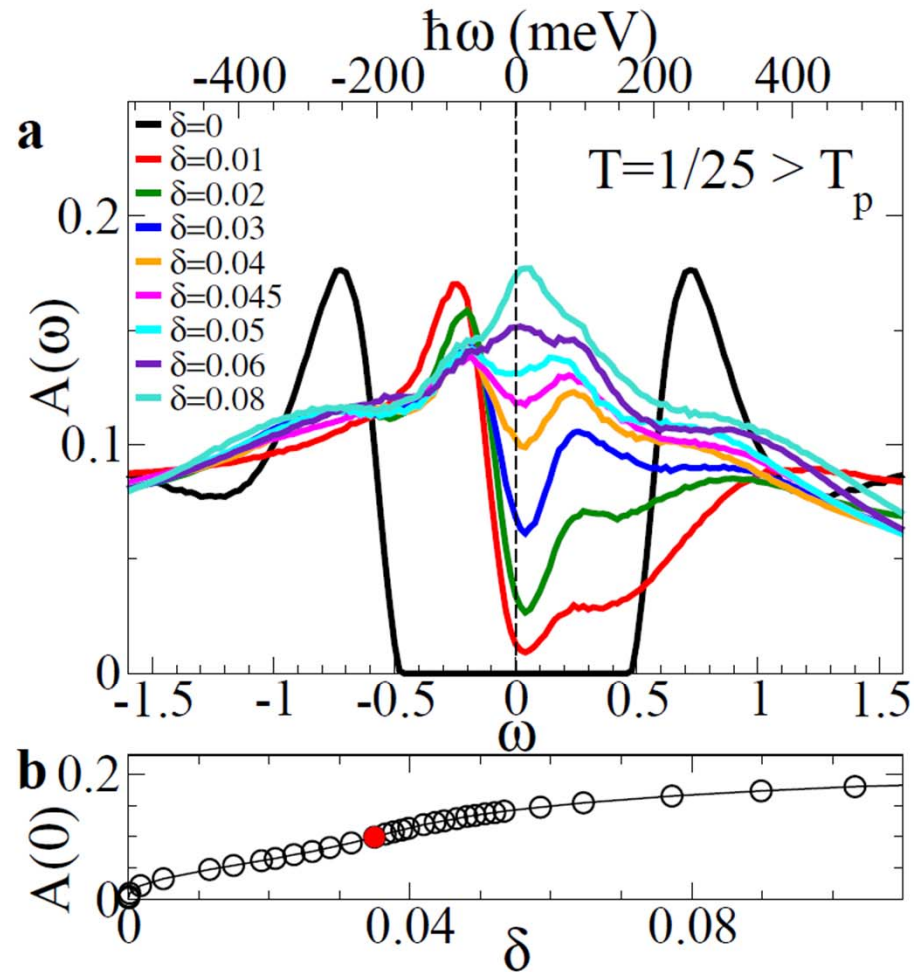
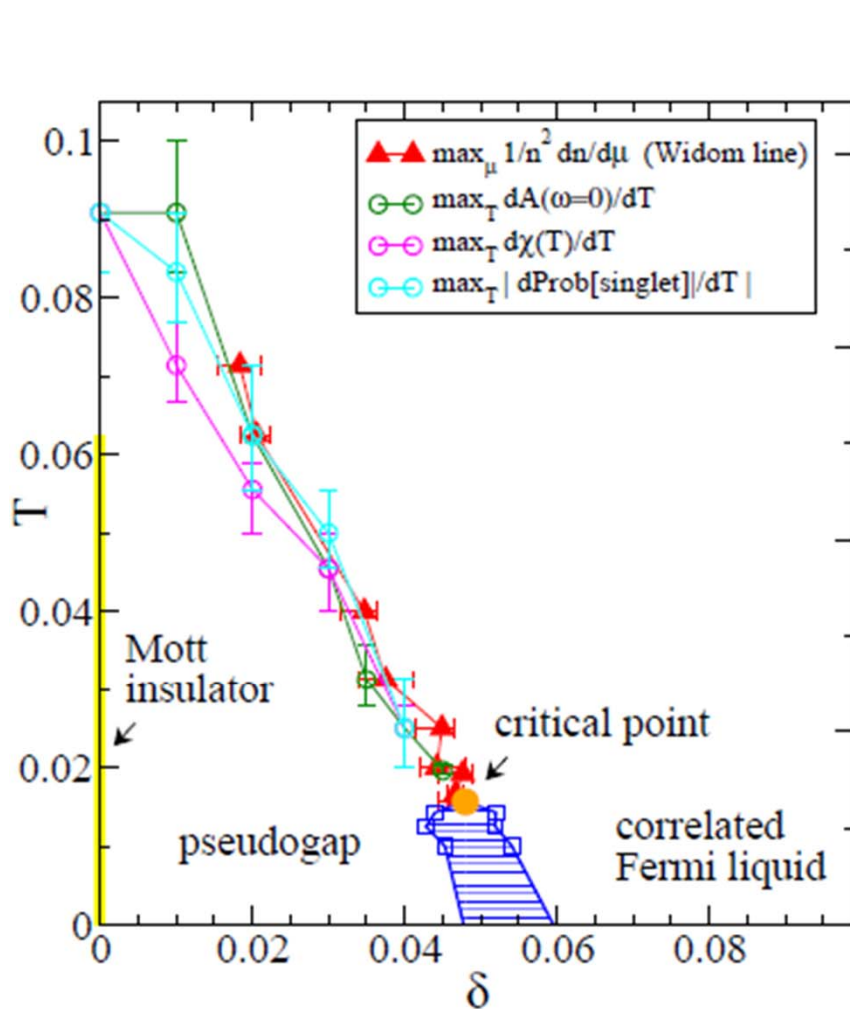
Doping dependence of critical point as a function of U



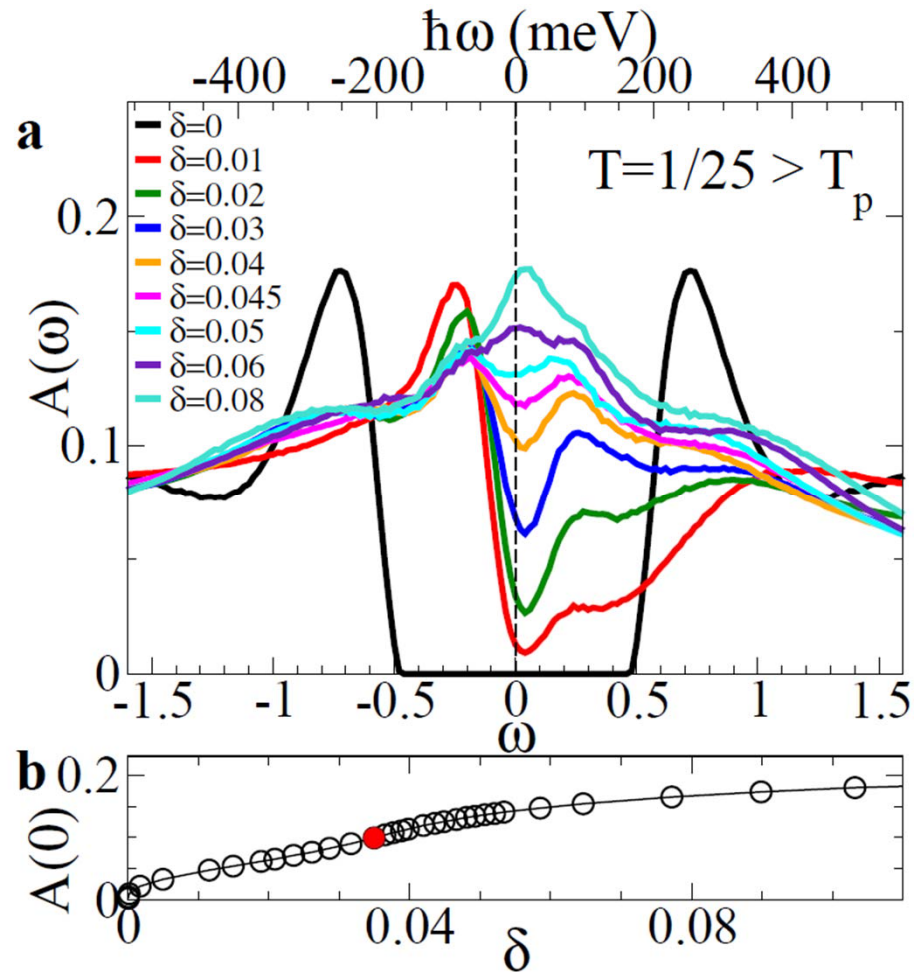
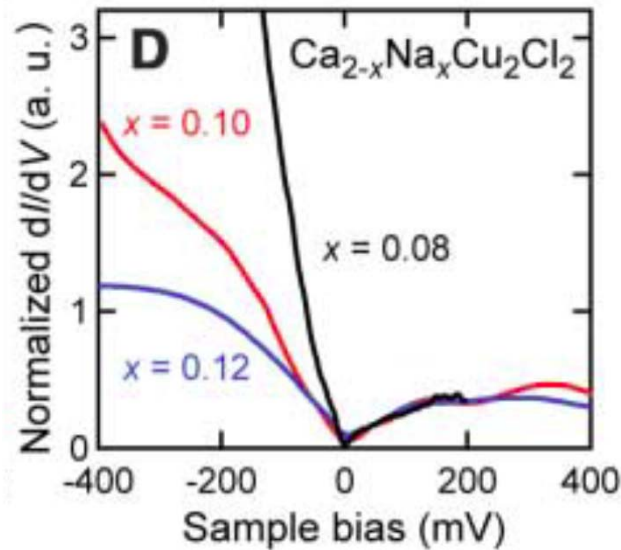
Smaller D and S



Density of states



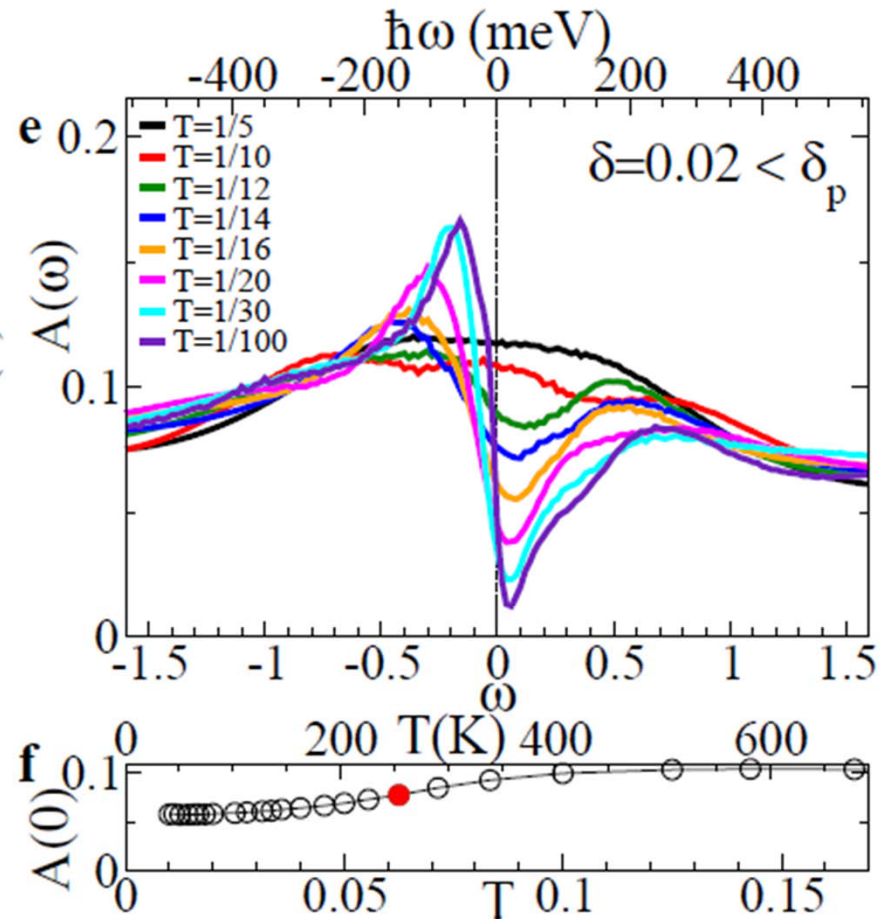
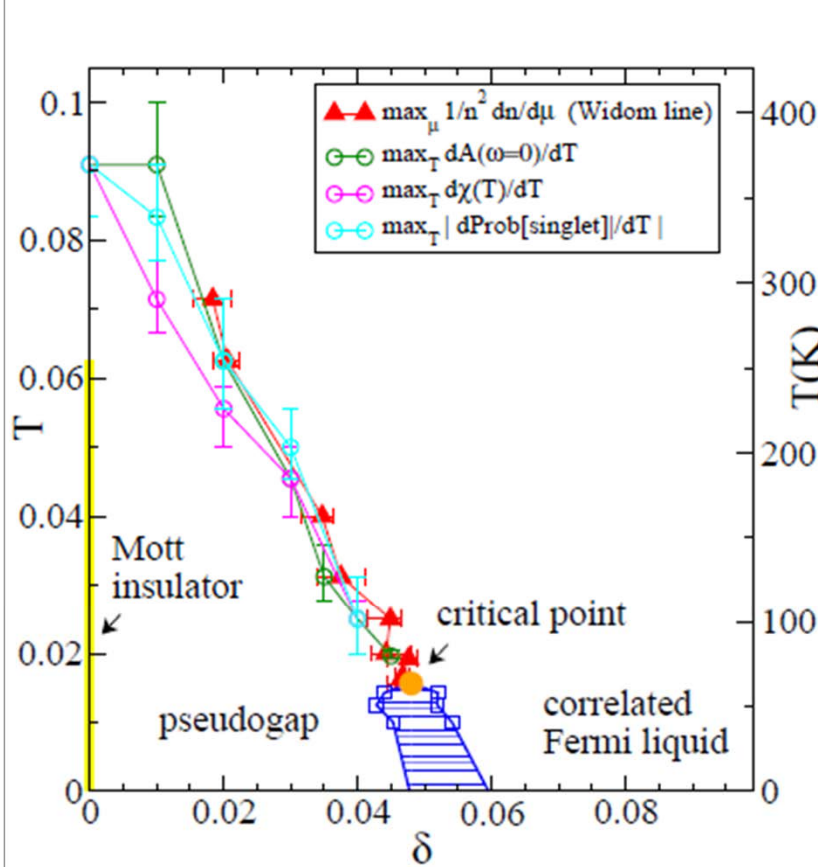
Density of states



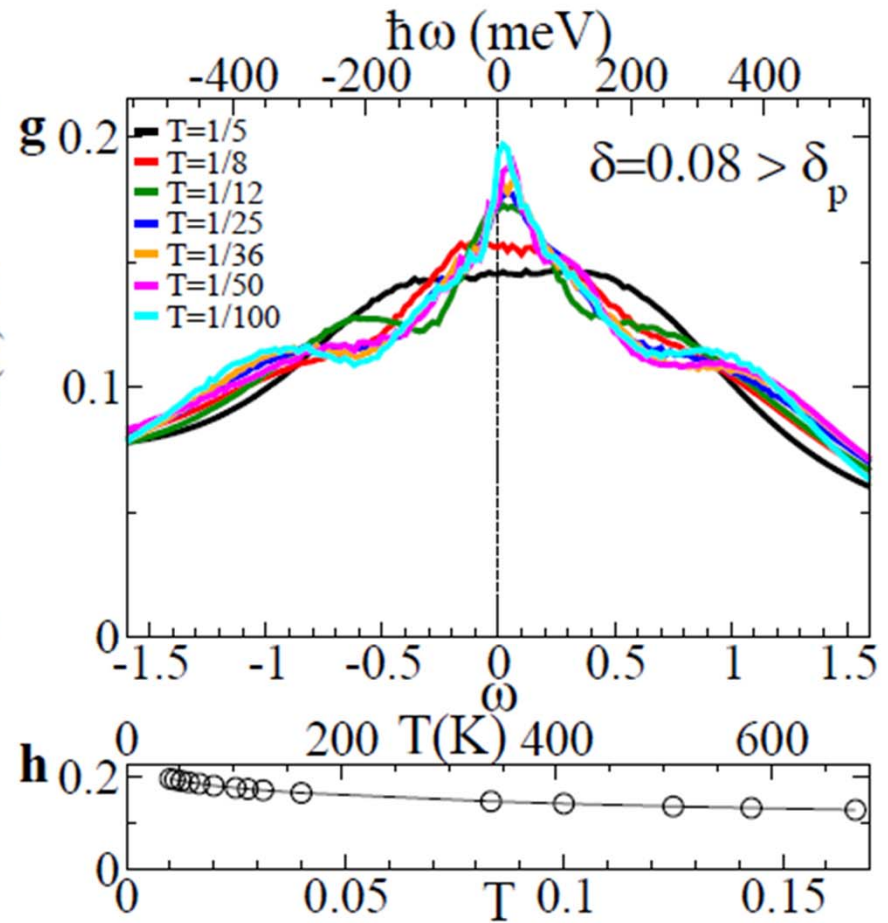
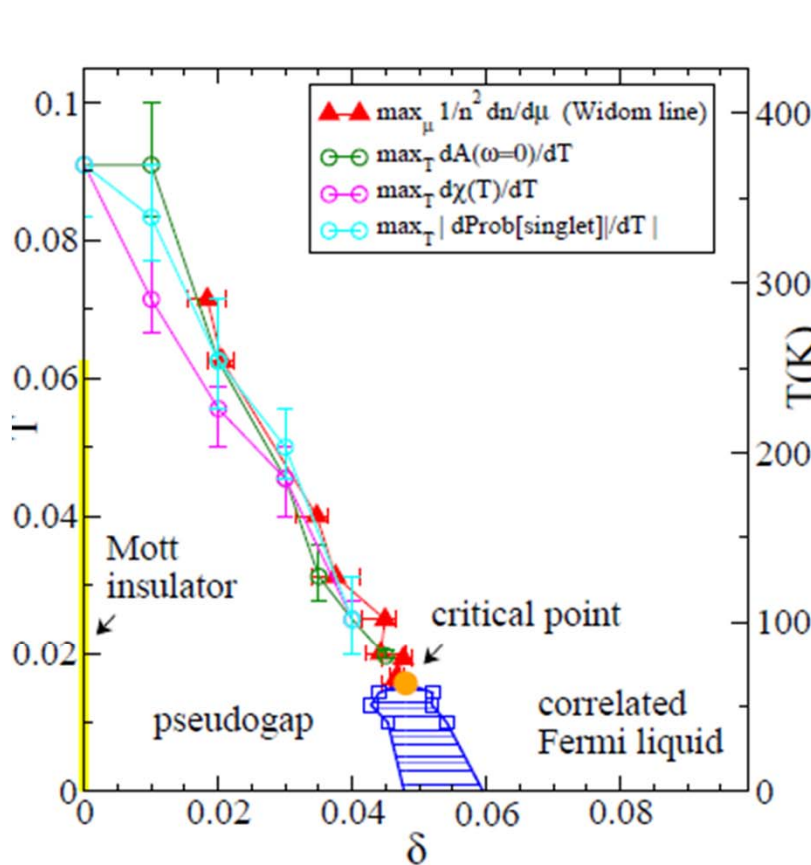
Khosaka et al. *Science* **315**, 1380 (2007);



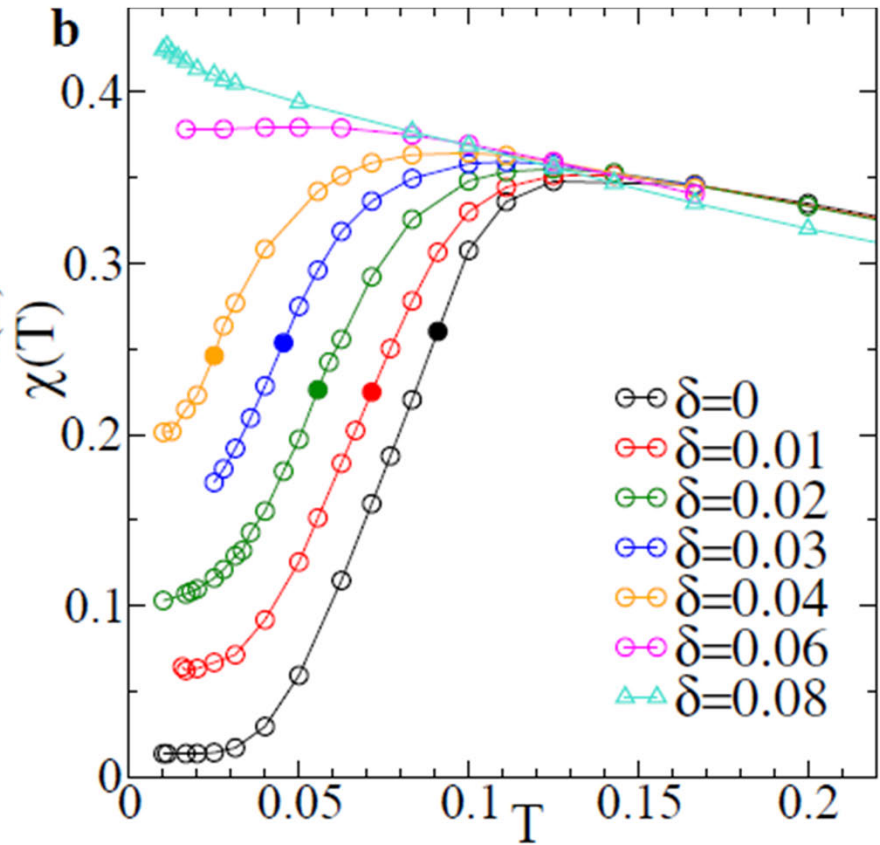
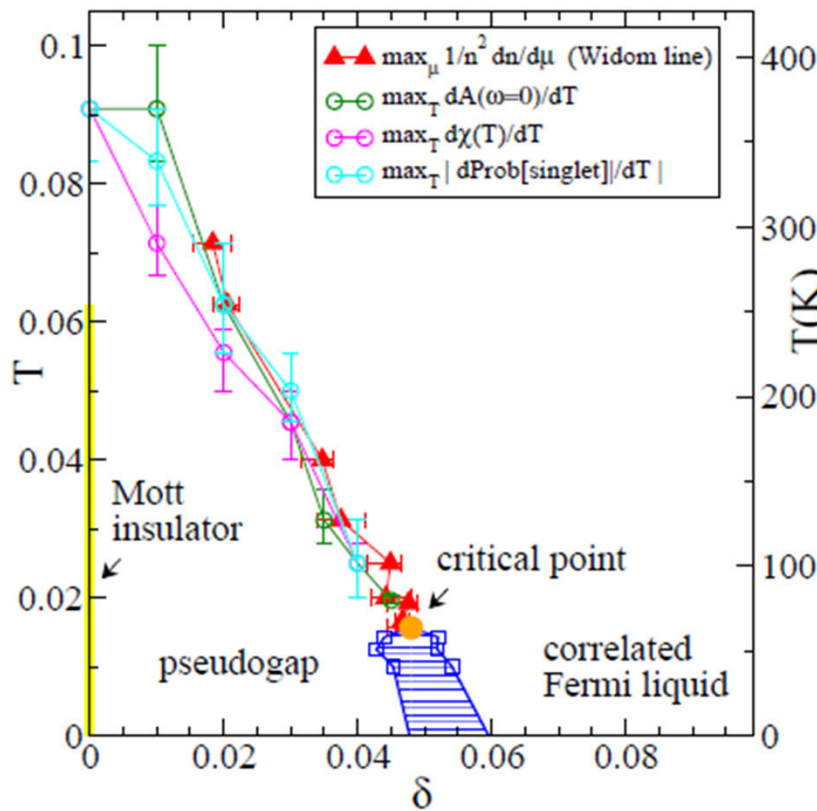
Density of states



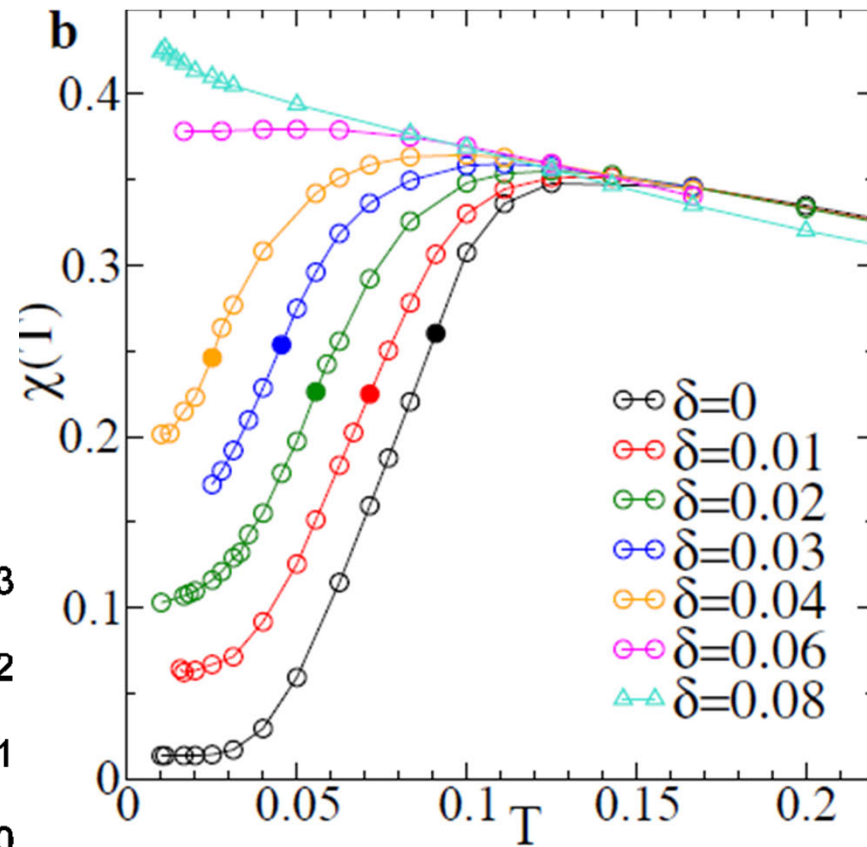
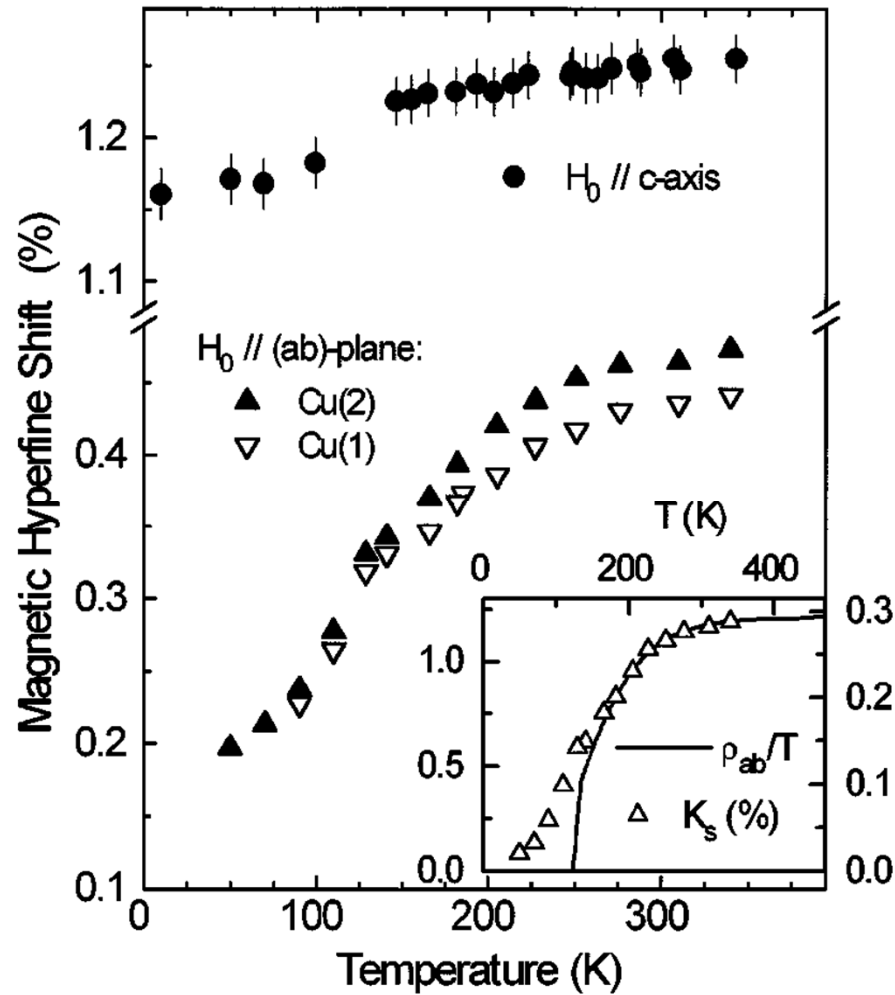
Density of states



Spin susceptibility



Spin susceptibility



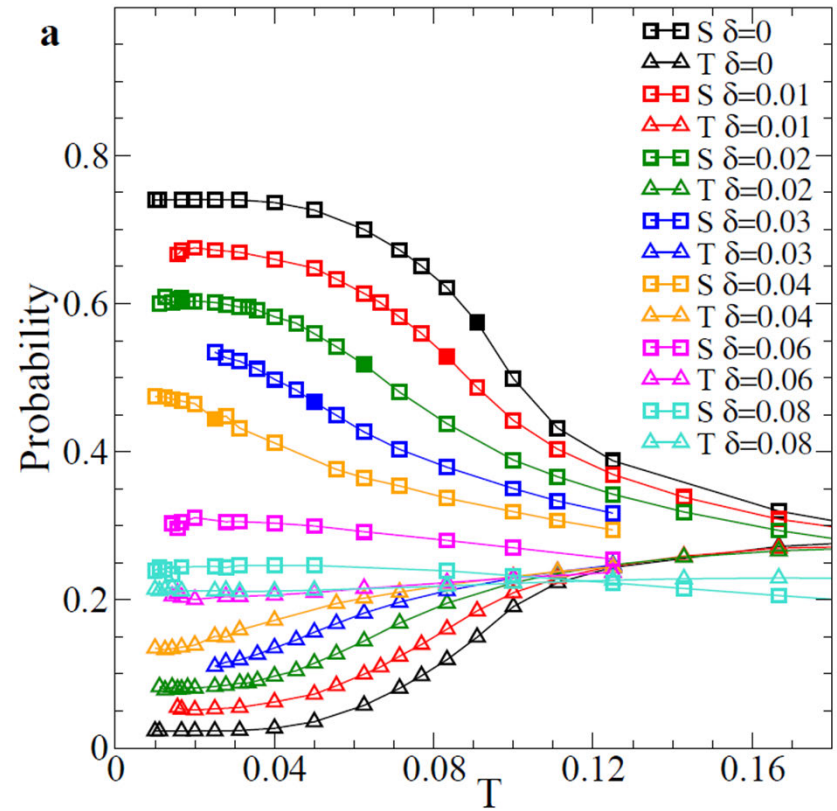
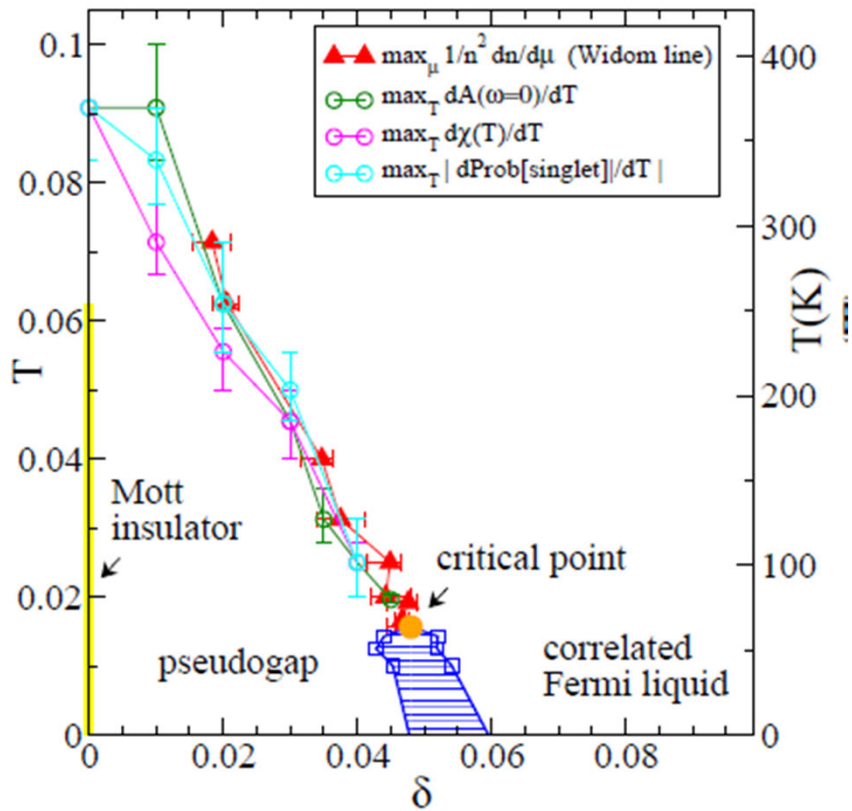
Underdoped Hg1223

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



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Plaquette eigenstates



What is the minimal model?

H. Alloul arXiv:1302.3473

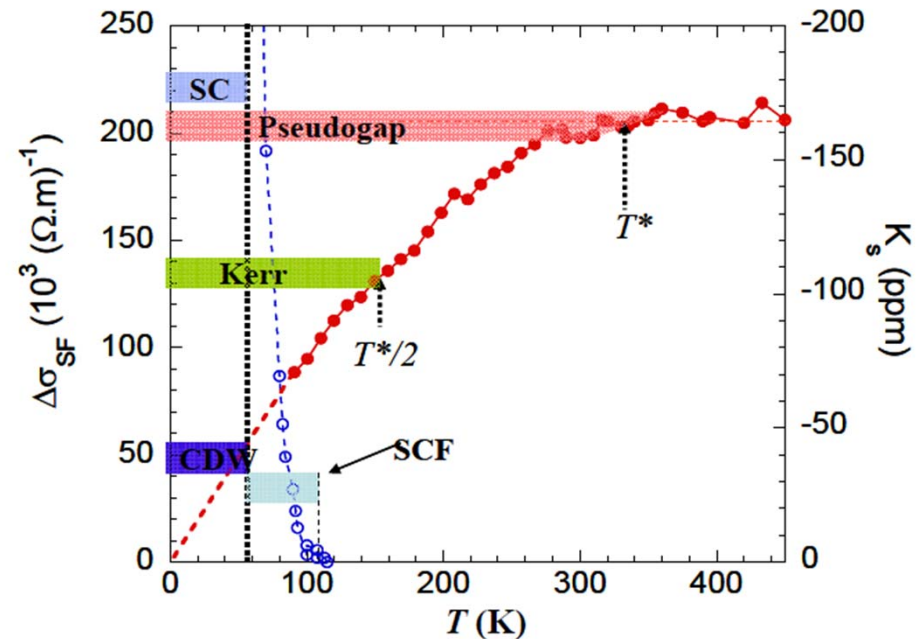
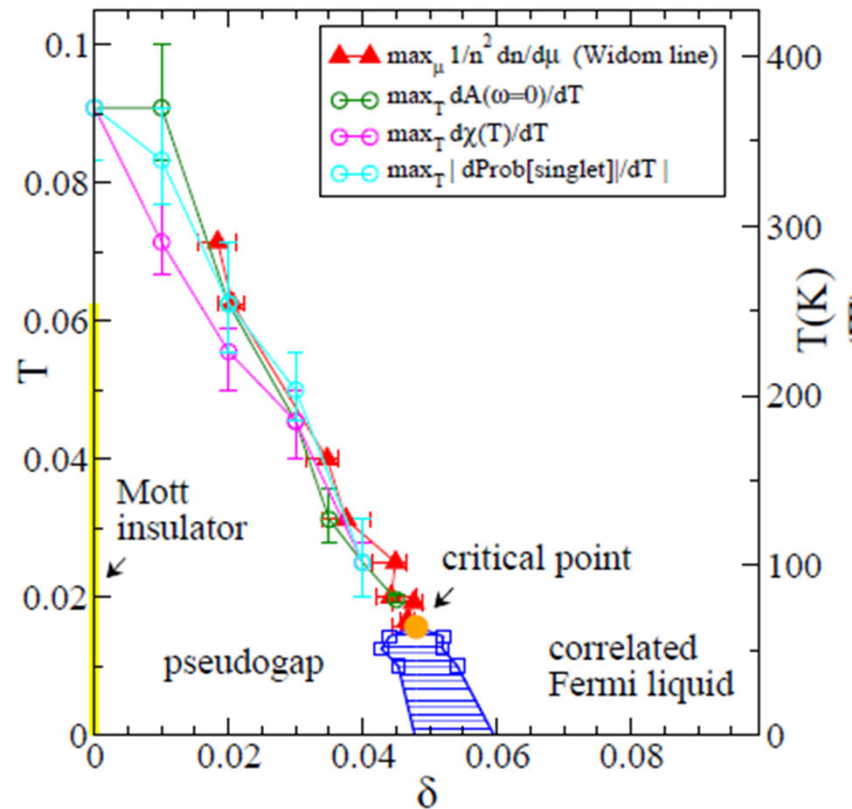


Fig 1 Spin contribution K_s to the ^{89}Y NMR Knight shift [11] for $\text{YBCO}_{6.6}$ permit to define the PG onset T^* . Here K_s is reduced by a factor two at $T \sim T^*/2$. The sharp drop of the SC fluctuation conductivity (SCF) is illustrated (left scale) [23]. We report as well the range over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

Pseudogap T^* along the Widom line





Giovanni Sordi



Patrick Sémon



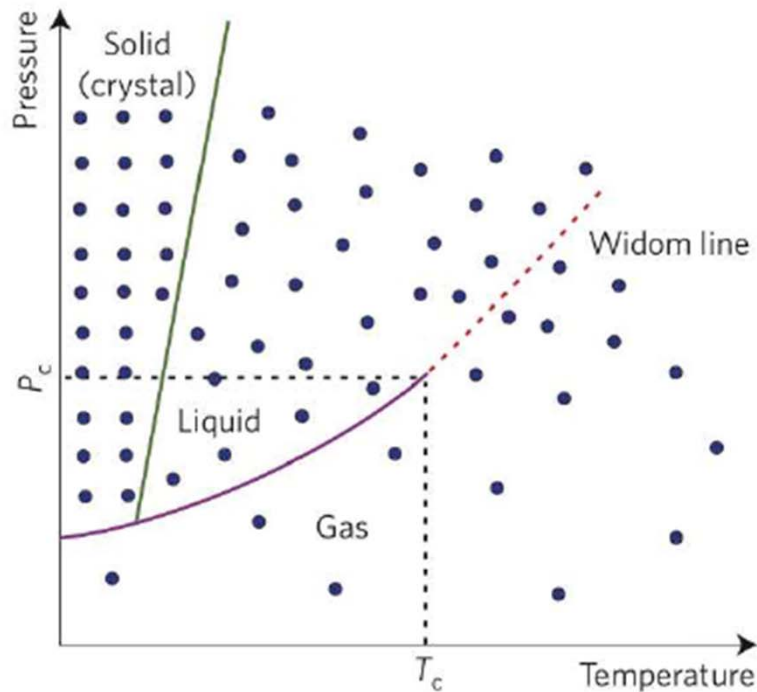
Kristjan Haule

The Wisdom line

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



What is the Widom line?

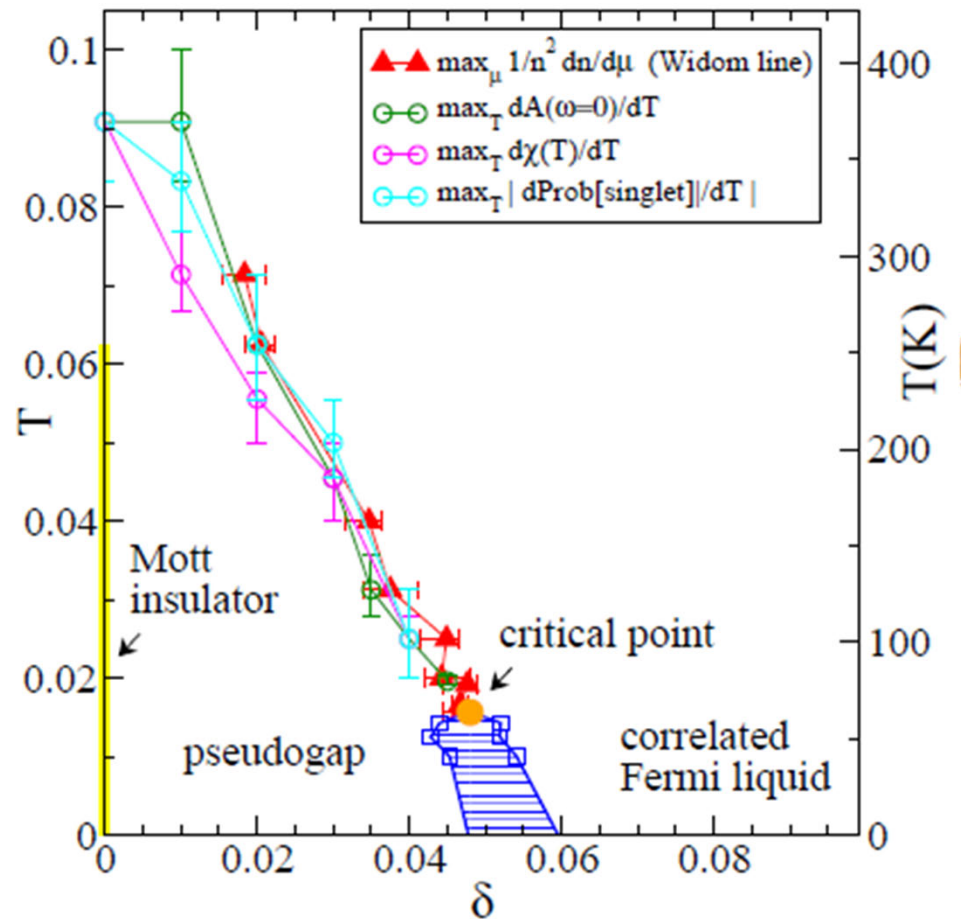


McMillan and Stanley, Nat Phys 2010

- ▶ 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 $T \rightarrow T_p$
- ▶ 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



Phase diagram



What is the minimal model?

H. Alloul arXiv:1302.3473

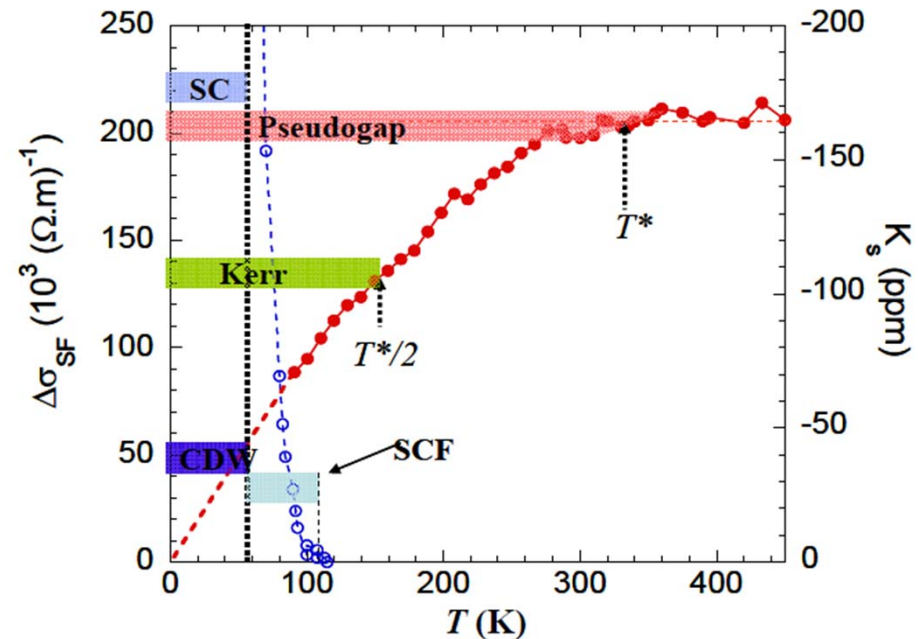
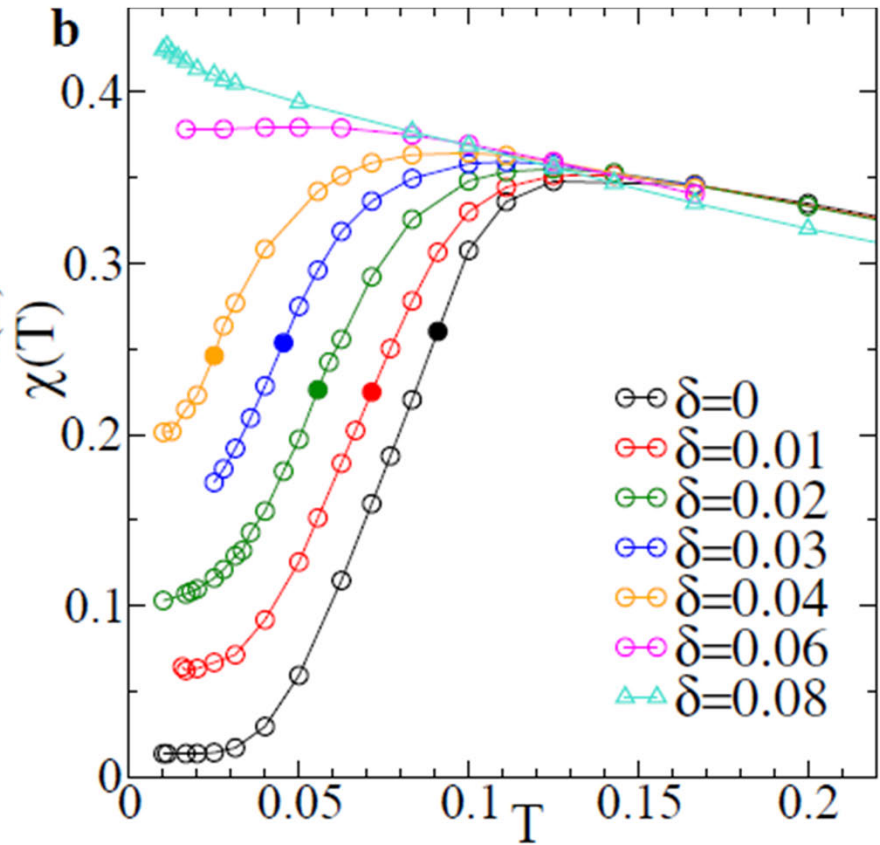
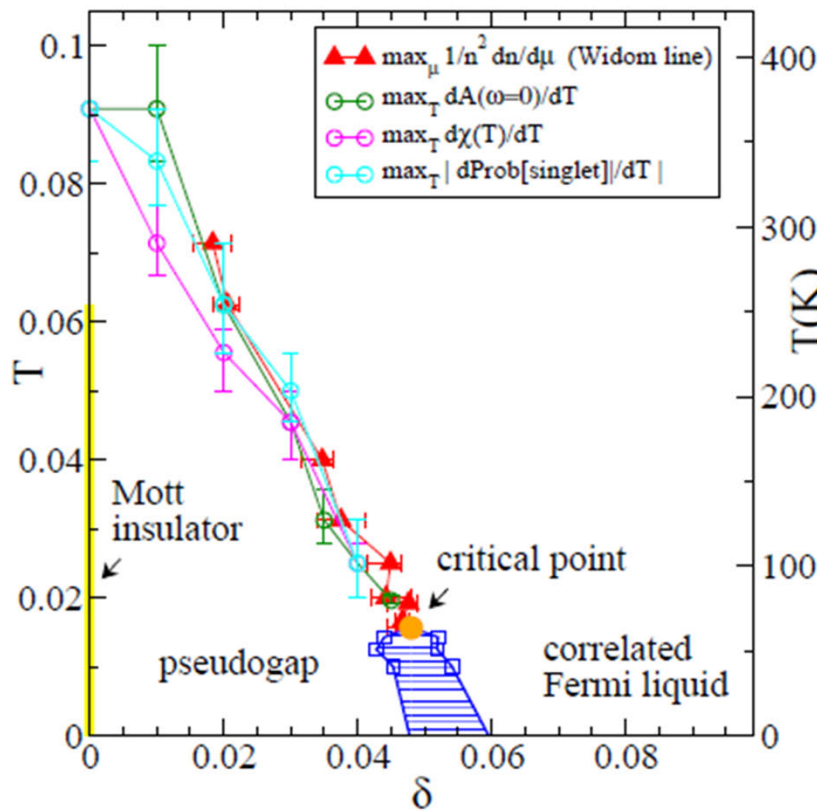
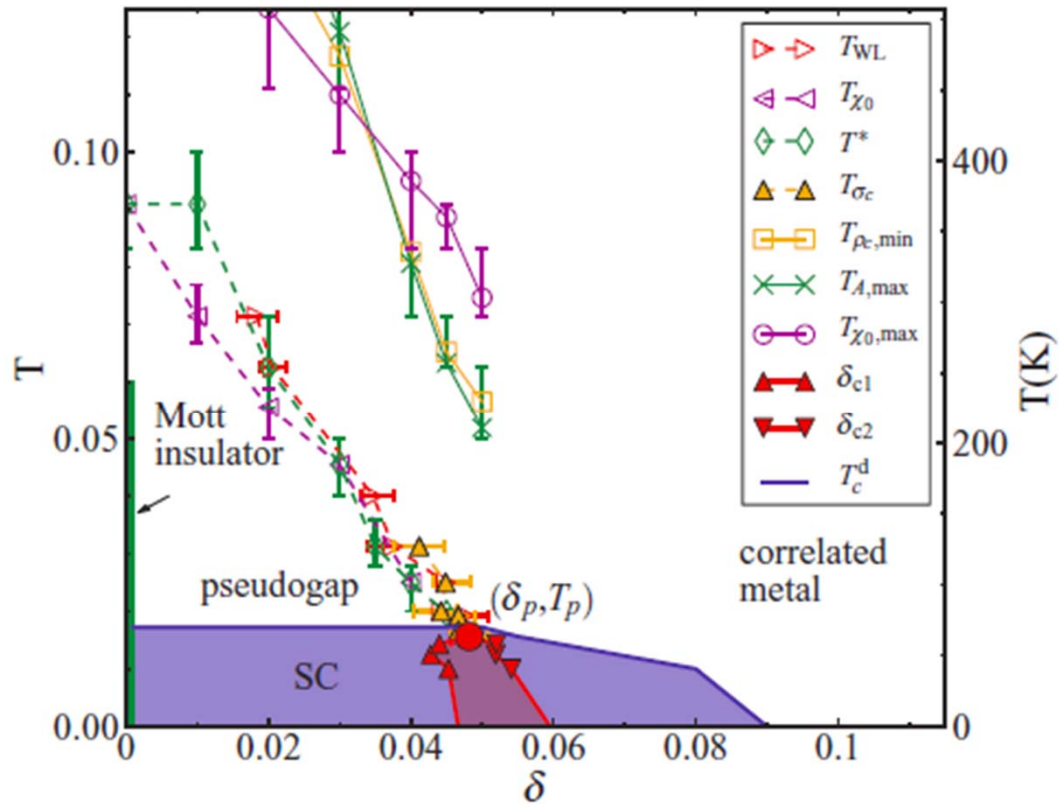


Fig 1 Spin contribution K_s to the ^{89}Y NMR Knight shift [11] for $\text{YBCO}_{6.6}$ permit to define the PG onset T^* . Here K_s is reduced by a factor two at $T \sim T^*/2$. The sharp drop of the SC fluctuation conductivity (SCF) is illustrated (left scale) [23]. We report as well the range over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

Spin susceptibility

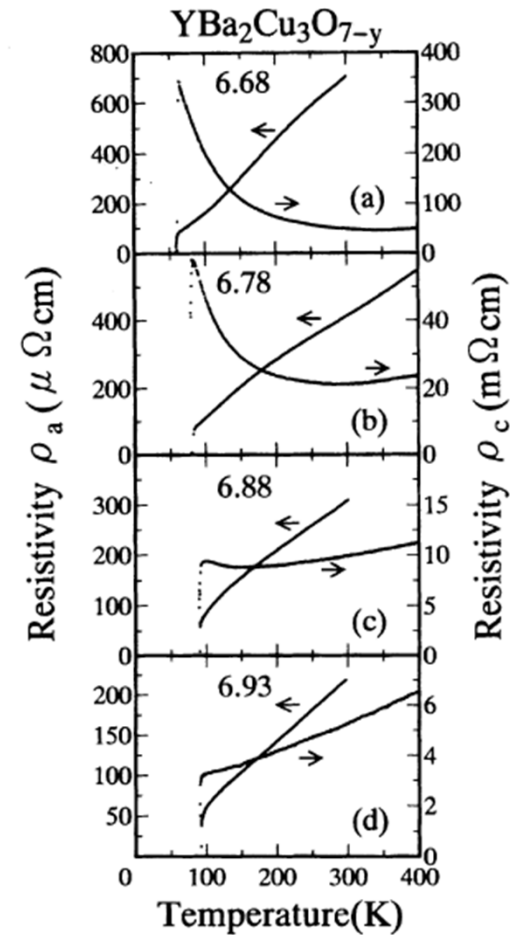
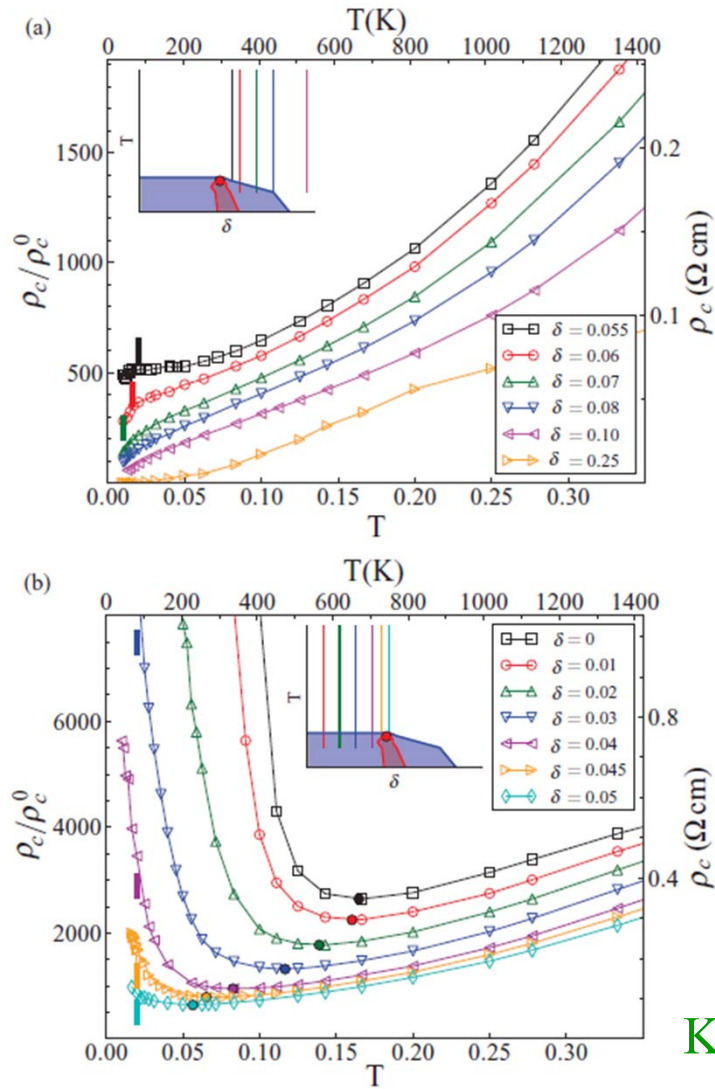


Two crossover lines



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

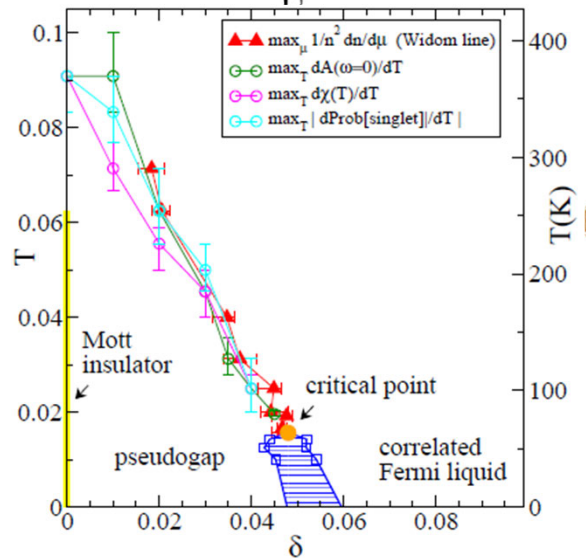
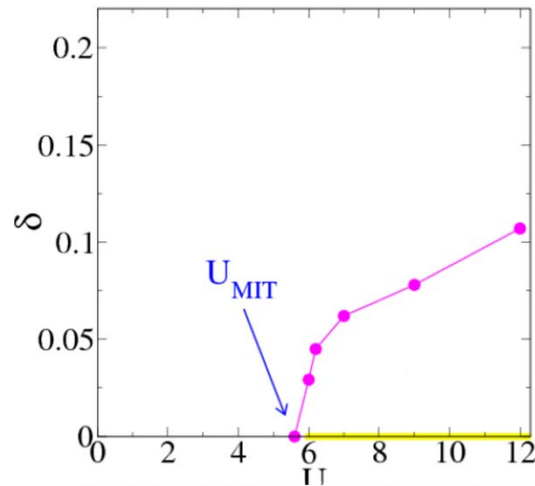
C-axis resistivity



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



Summary: normal state



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





Giovanni Sordi



Patrick Sémon



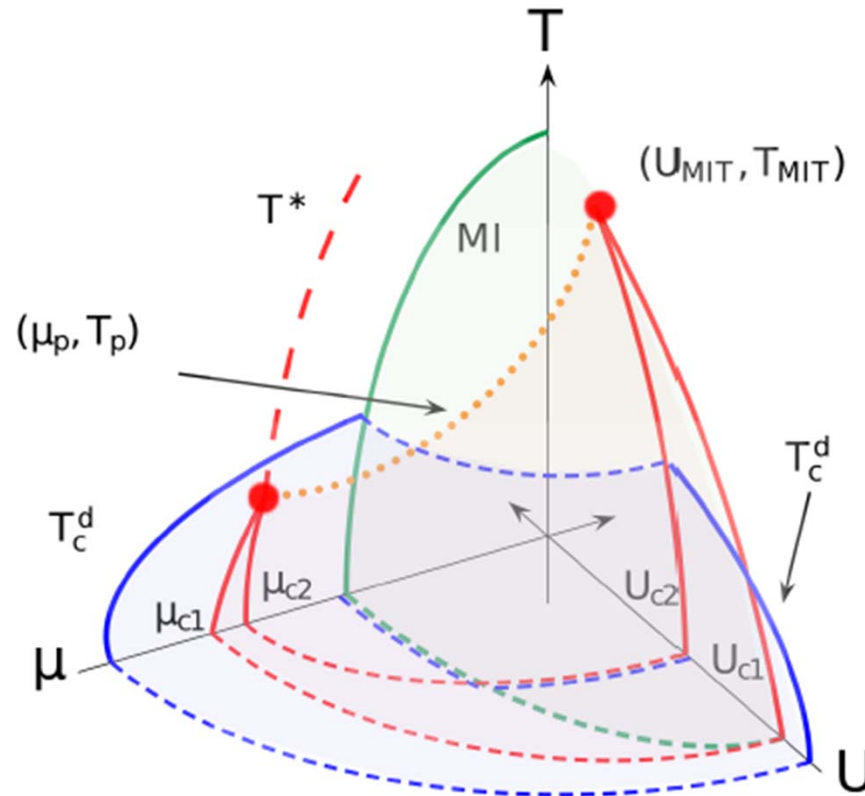
Kristjan Haule

Finite T phase diagram Superconductivity

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



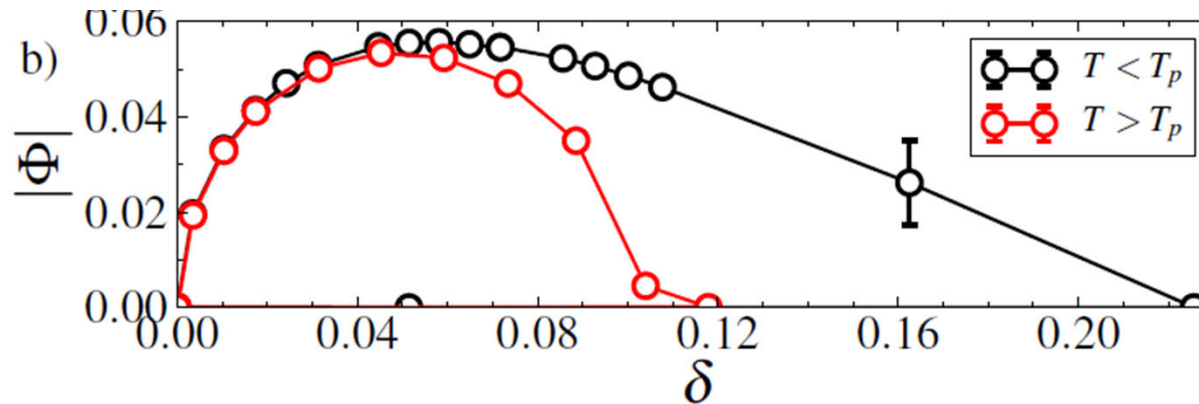
Unified phase diagram





Cuprates (doping driven transition)

Giovanni Sordi



Patrick Sémon



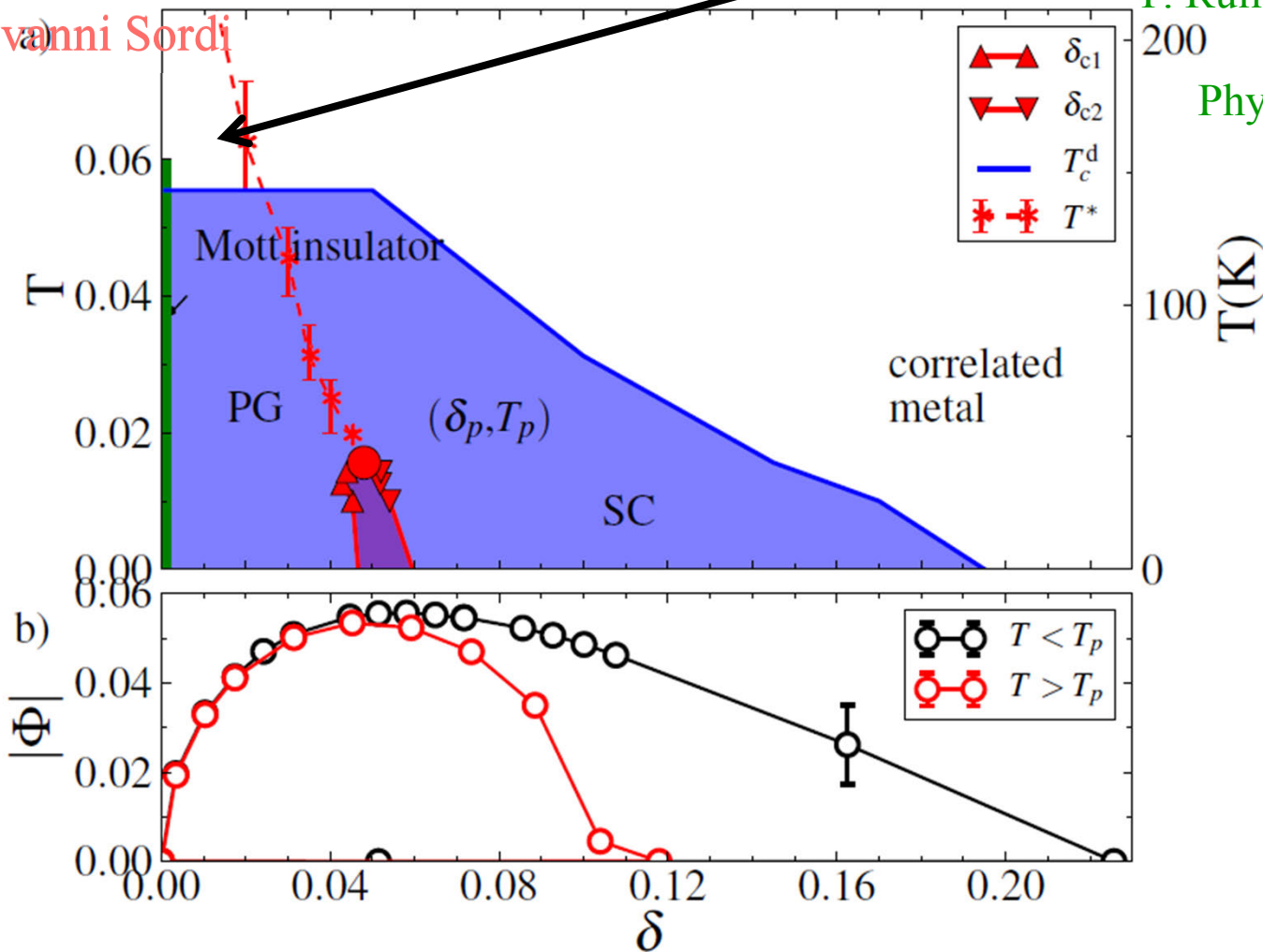


Cuprates (doping driven transition)

Pseudogap vs pair

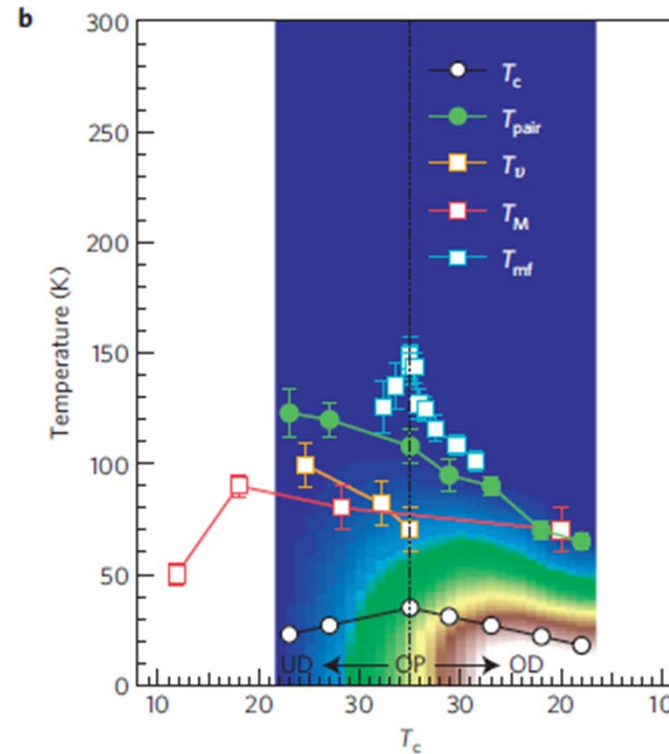
F. Rullier-Albenque, H. Alloul, and G. Rikken, Phys. Rev. B **84**, 014522 (2011).

Giovanni Sordi



Patrick Sémon

T_{pair}

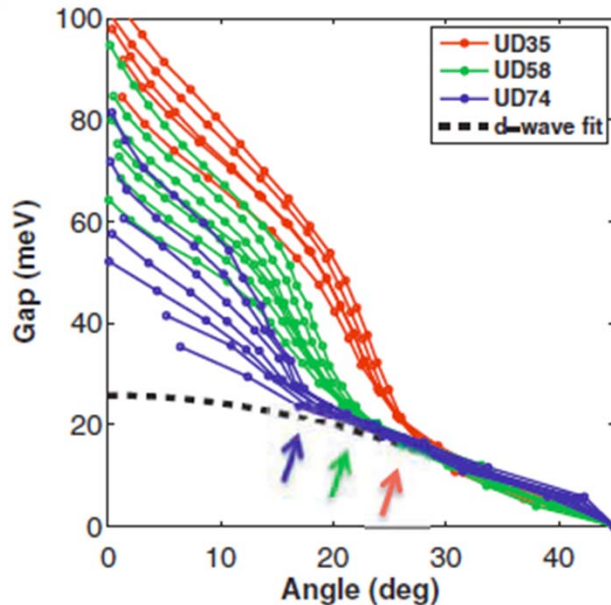


ARPES
Bi2212

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



Meaning of T_c^d : Local pair formation

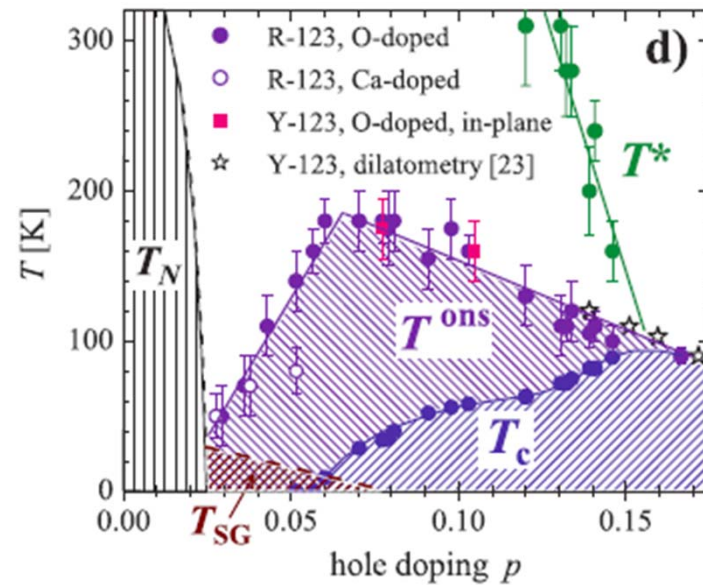


A. Pushp, Parker, ... A. Yazdani,
Science **364**, 1689 (2009)

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.



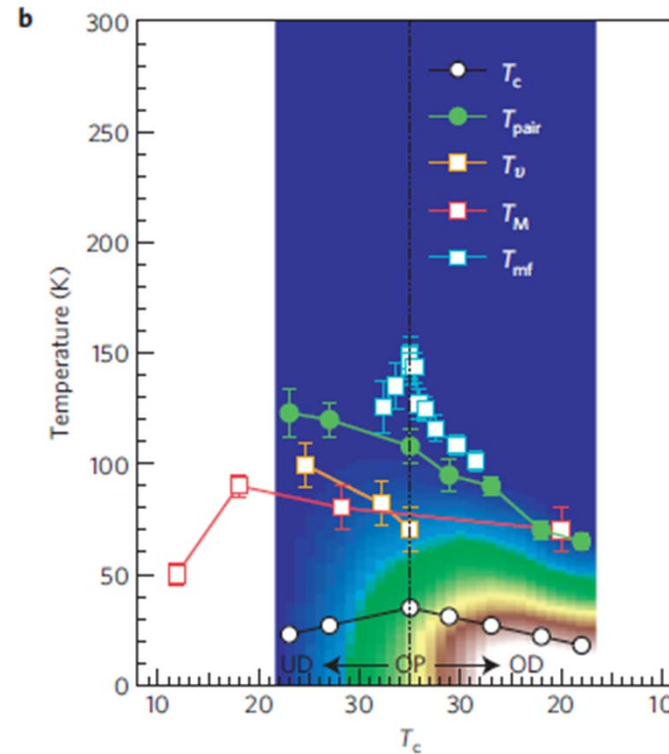
Fluctuating region



Infrared response

Dubroka et al. PRL 106, 047006 (2011)

T_{pair}

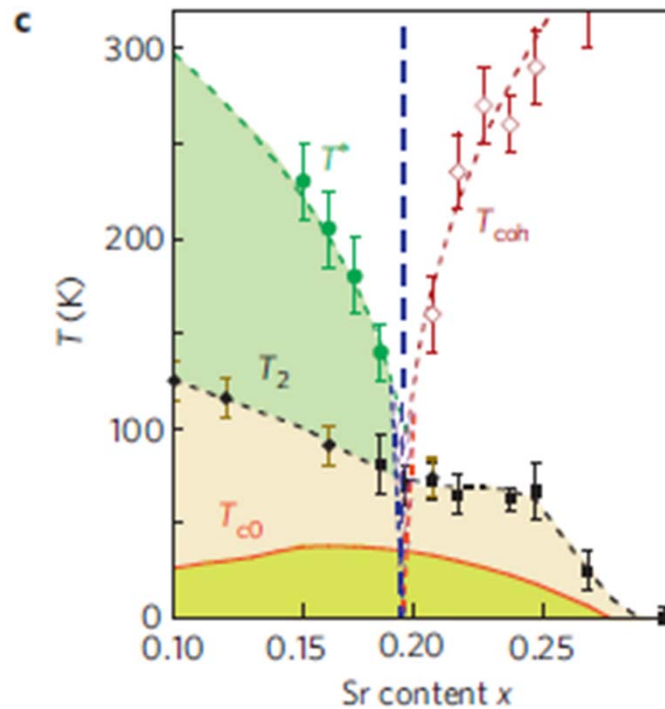


ARPES
Bi2212

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



T_2



Magnetoresistance, LSCO
Fluctuating vortices

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



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

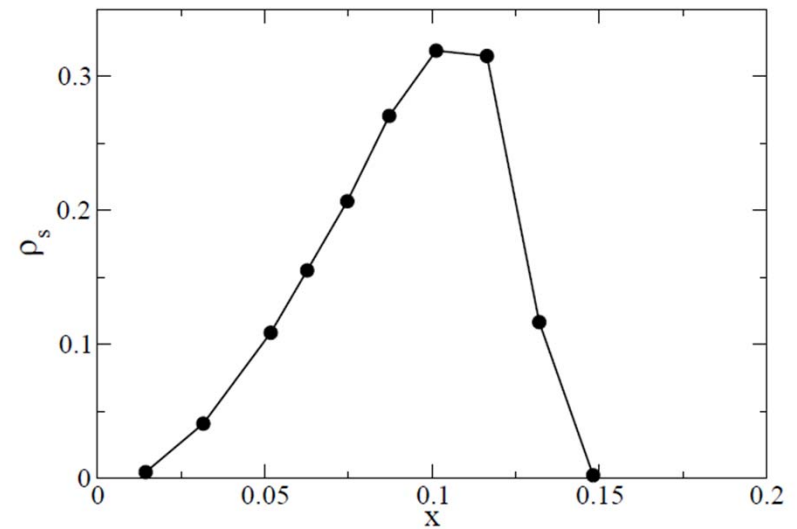
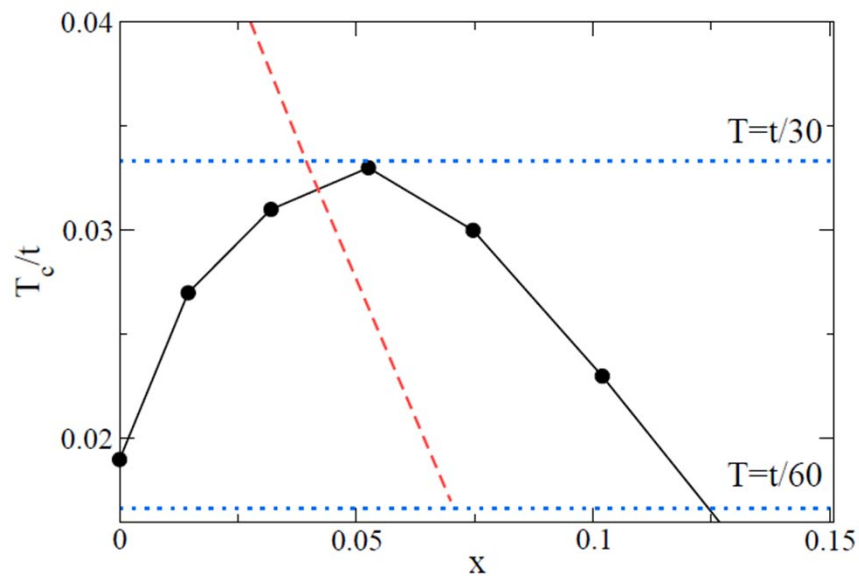
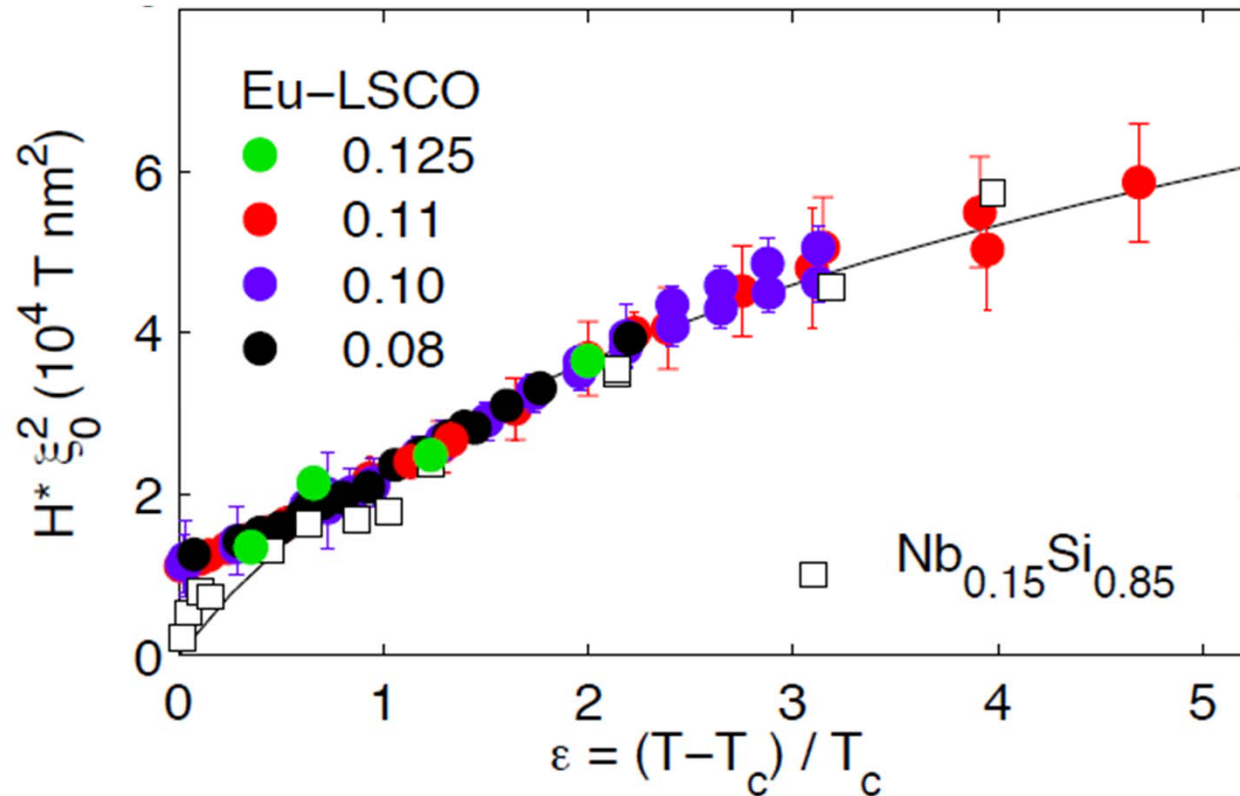


FIG. 8. Superfluid stiffness ρ_s determined in the superconducting state at $T = t/60$ from Eq. 15, as a function of doping.

Gull, Millis, [arxiv.org:304.6406](https://arxiv.org/abs/304.6406)



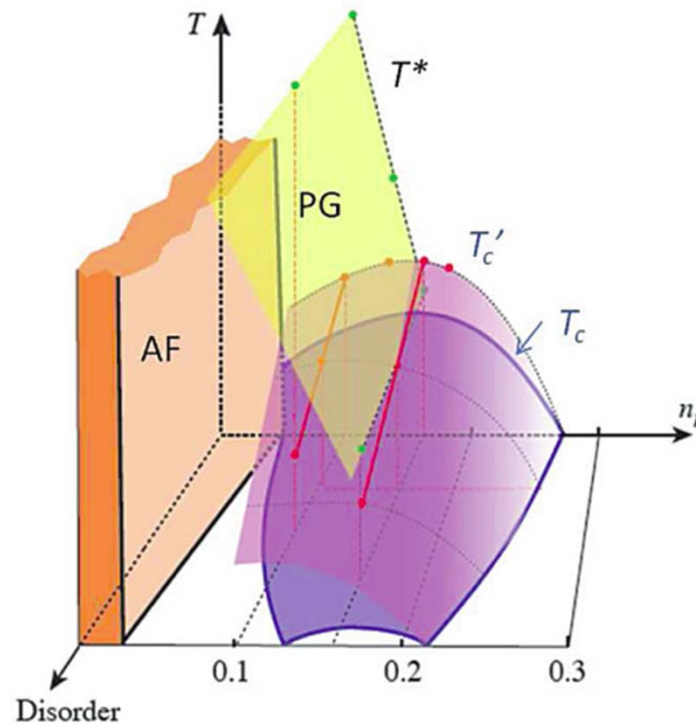
Gaussian amplitude fluctuations in Eu-LSCO



Chang, Doiron-Leyraud et al.



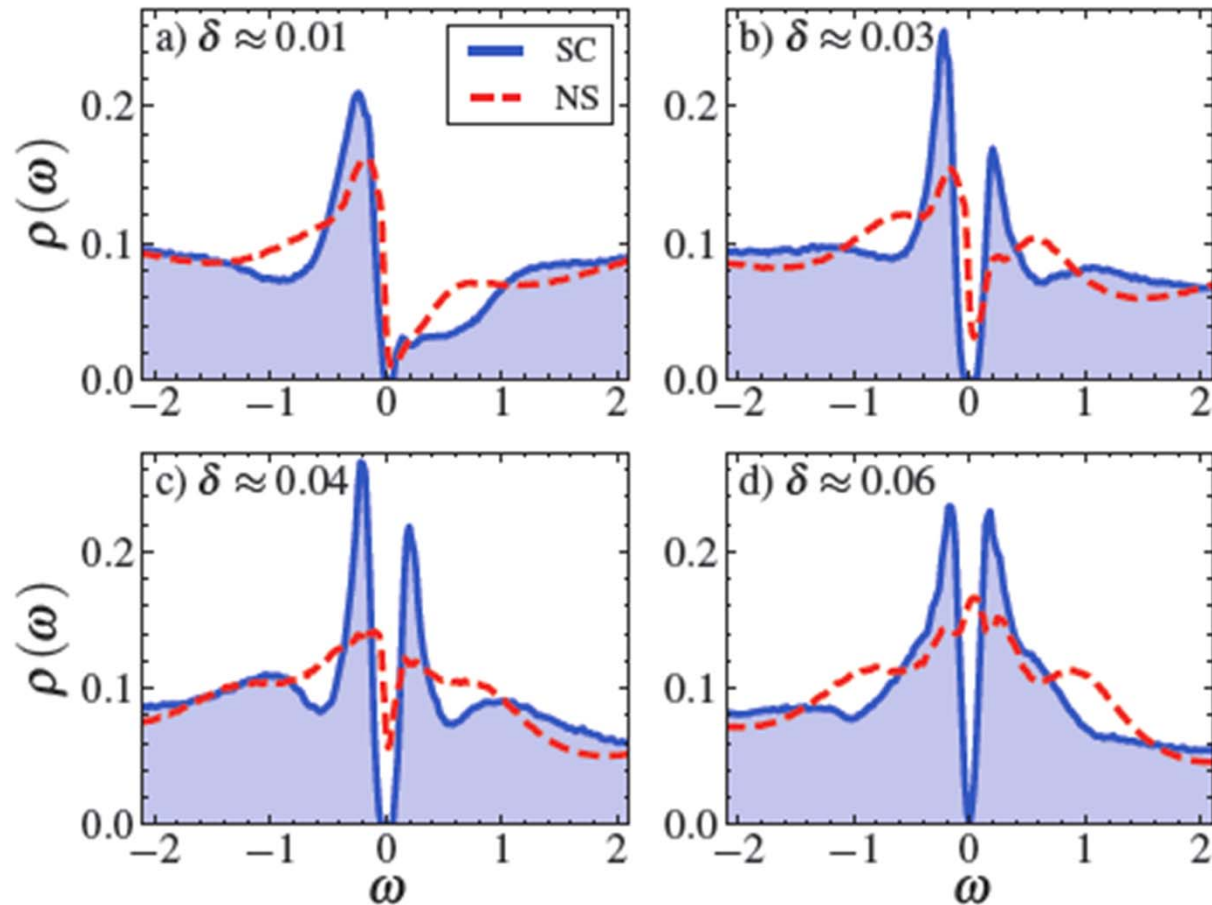
Effect of disorder



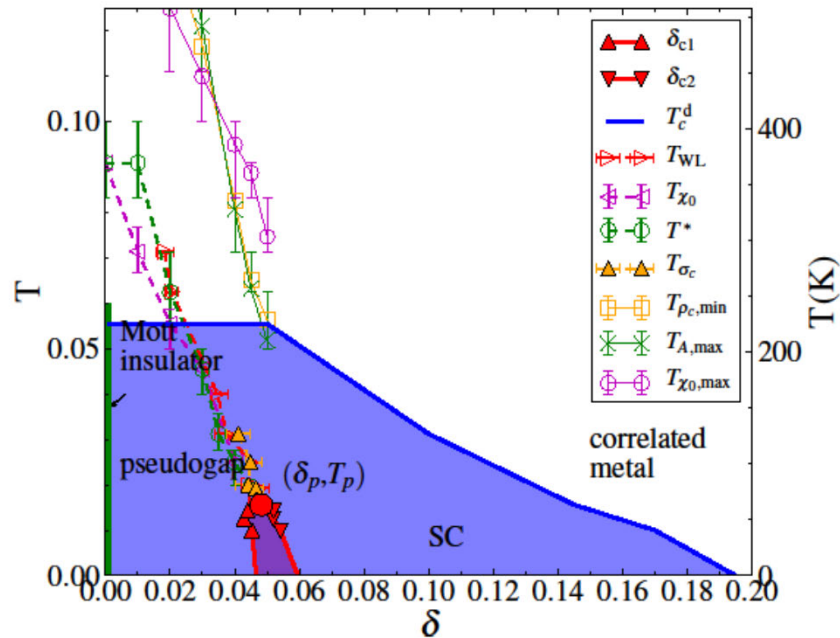
F. Rullier-Albenque, H. Alloul, and G. Rikken,
Phys. Rev. B **84**, 014522 (2011).



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
- T^* different from T_c^d
- Actual T_c in underdoped
 - Competing order
 - Long wavelength fluctuations (see O.P.)
 - Disorder

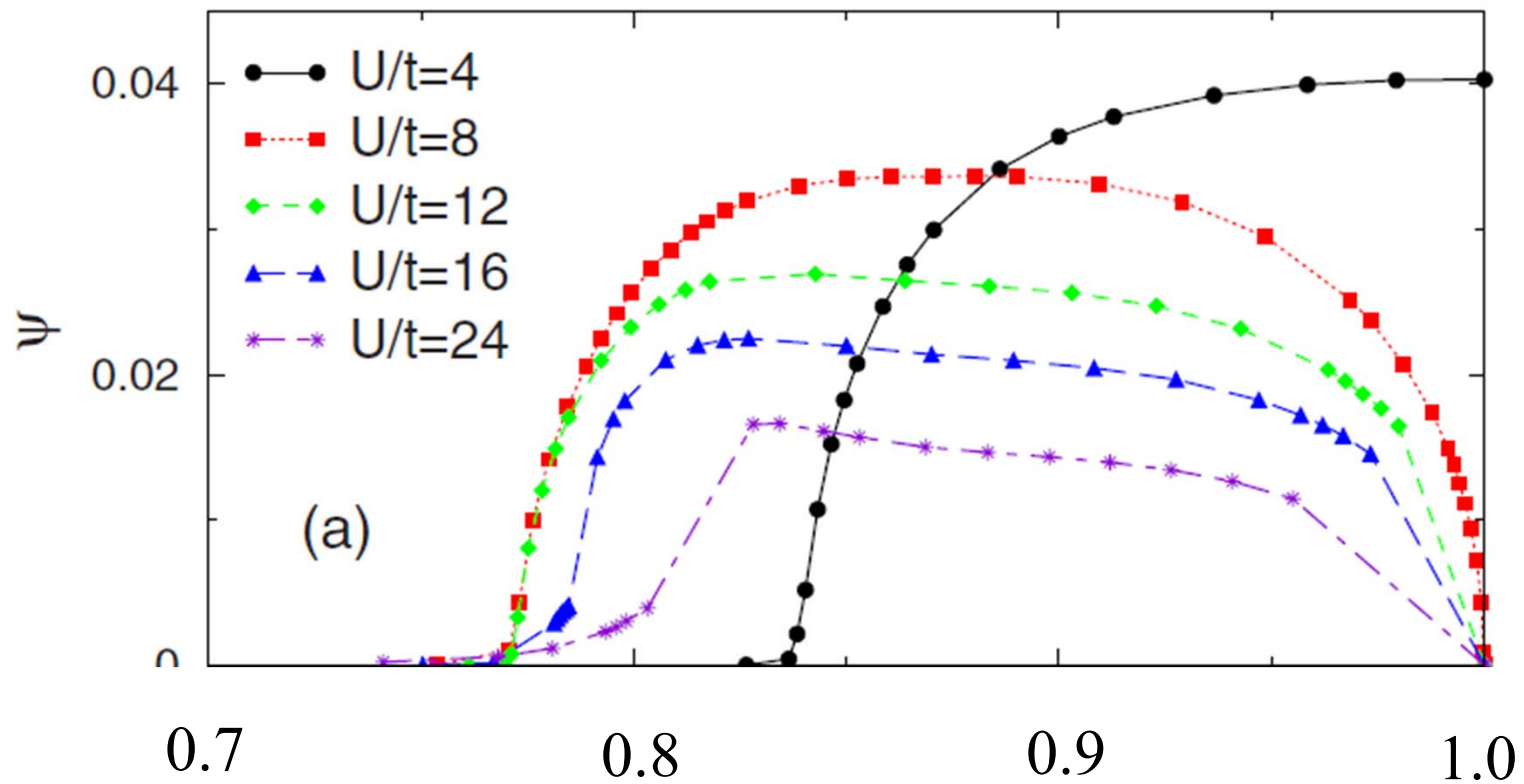


$T = 0$ phase diagram: superconductivity

Mechanism at strong coupling

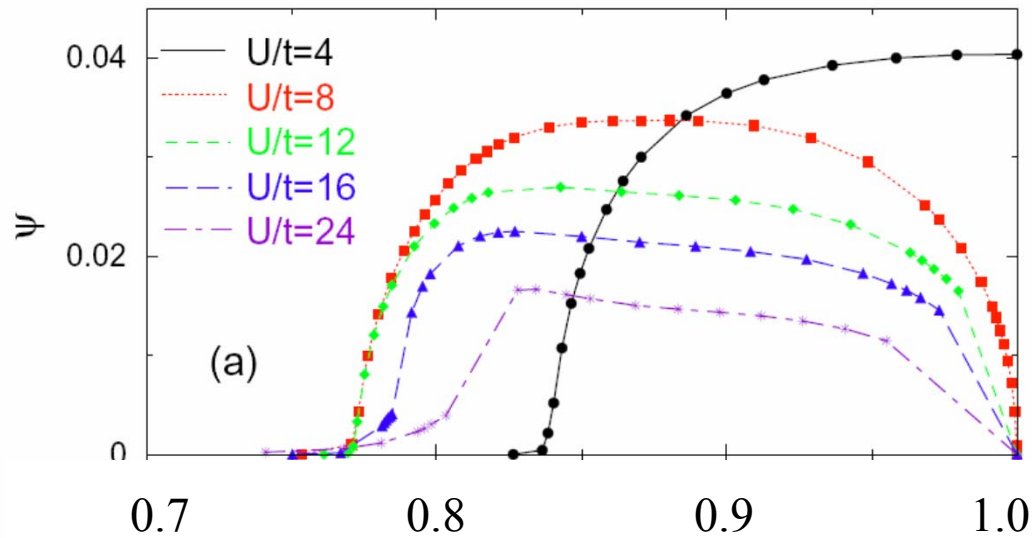


Theory: T_c down vs Mott



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

Dome vs Mott (CDMFT)

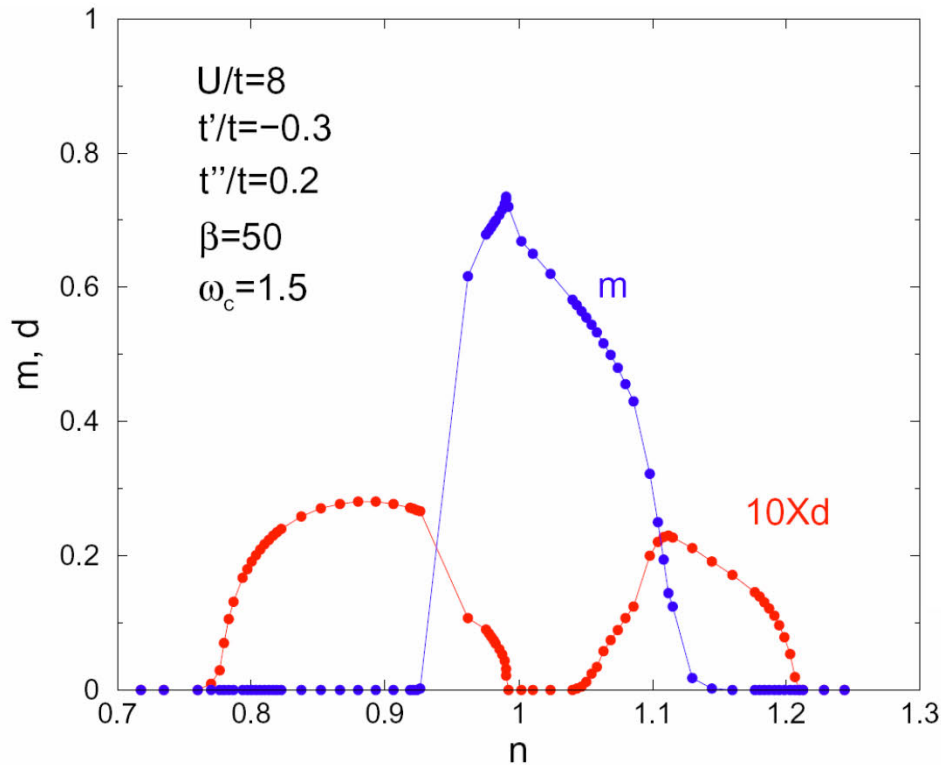


Kancharla, Kyung, Civelli,
Sénéchal, Kotliar AMST
Phys. Rev. B (2008)

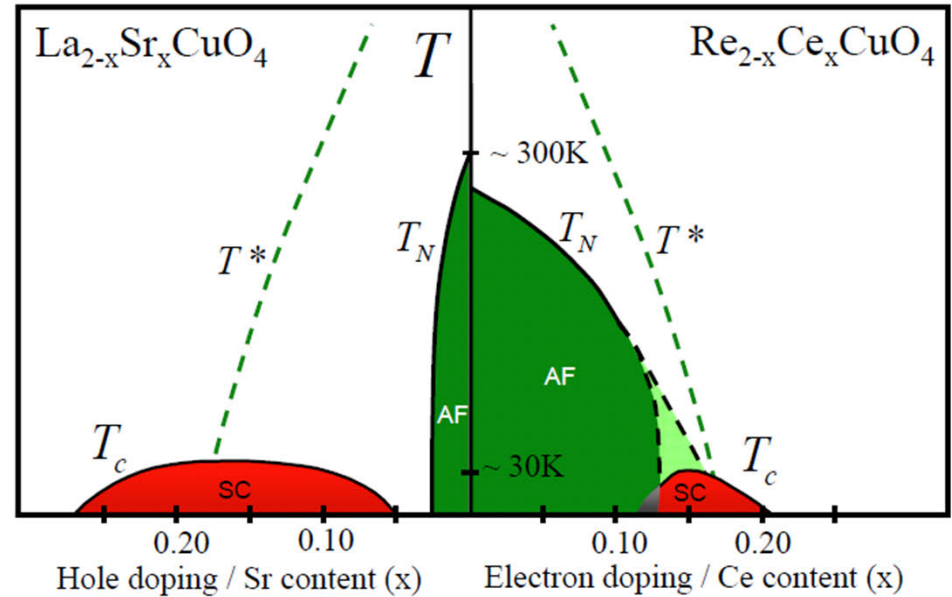


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CDMFT global phase diagram



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



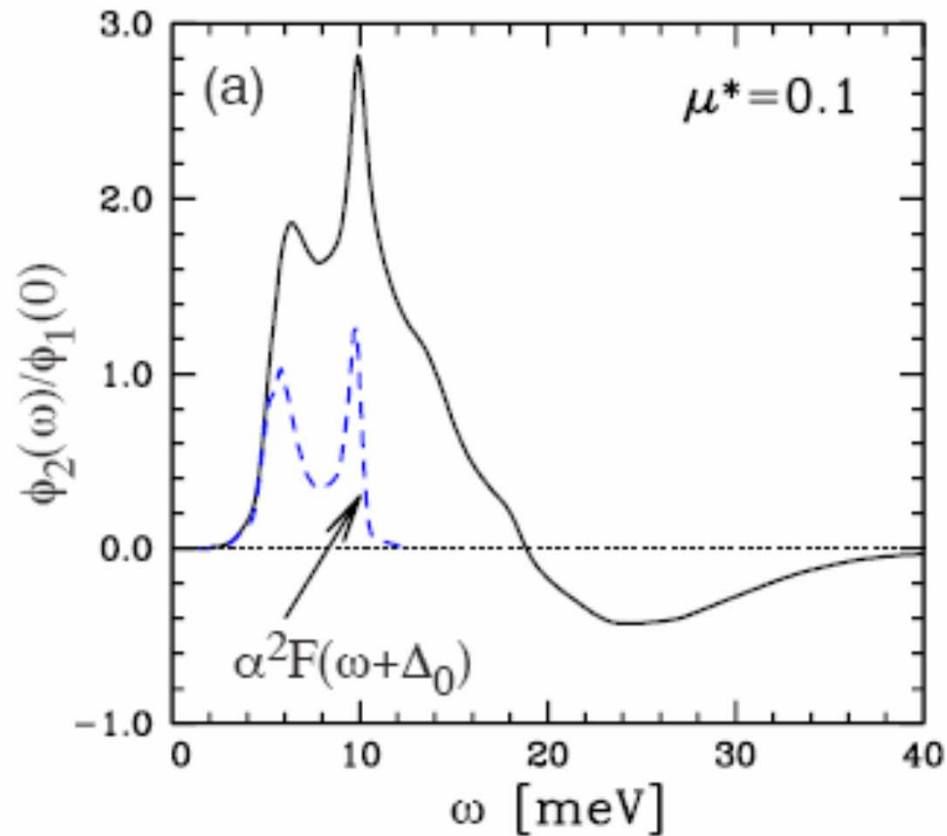
Armitage, Fournier, Greene, RMP (2009)



The glue

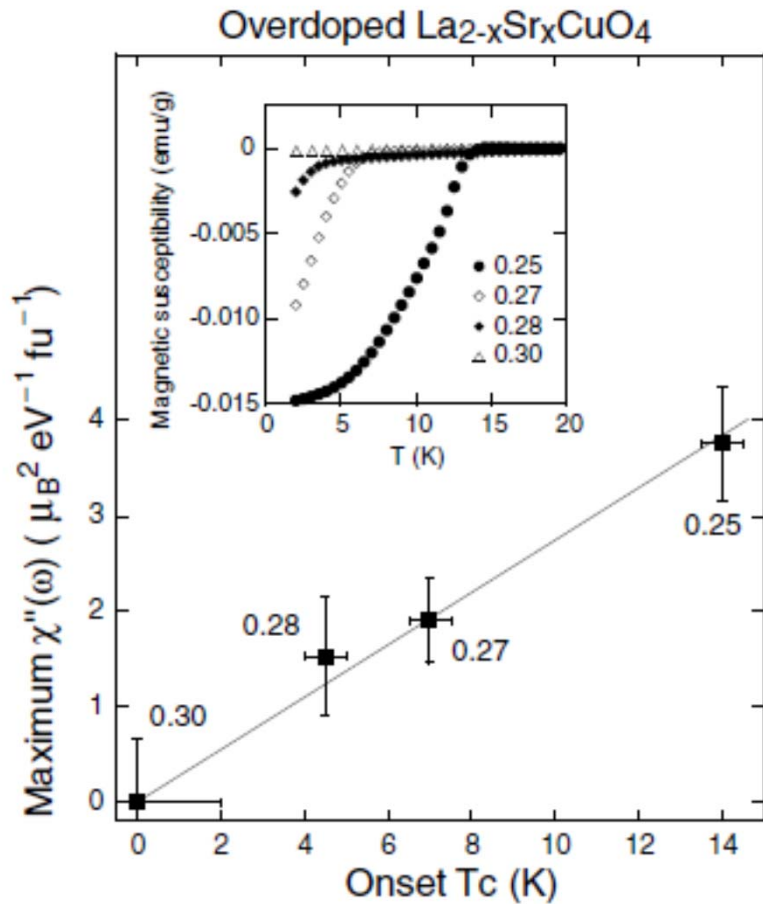
$\text{Im } \Sigma_{an}$ and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

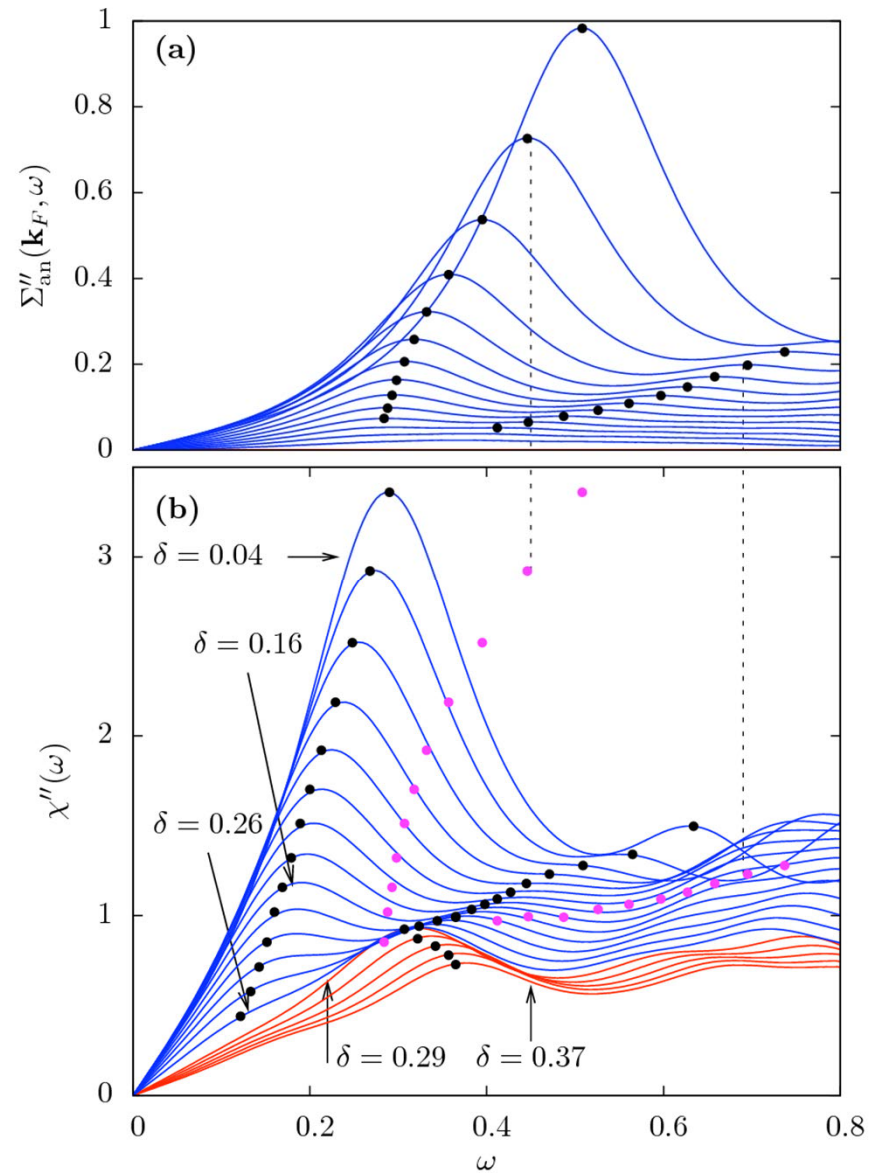


The glue

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



Wakimoto ... Birgeneau
 PRL (2004)



The glue and neutrons

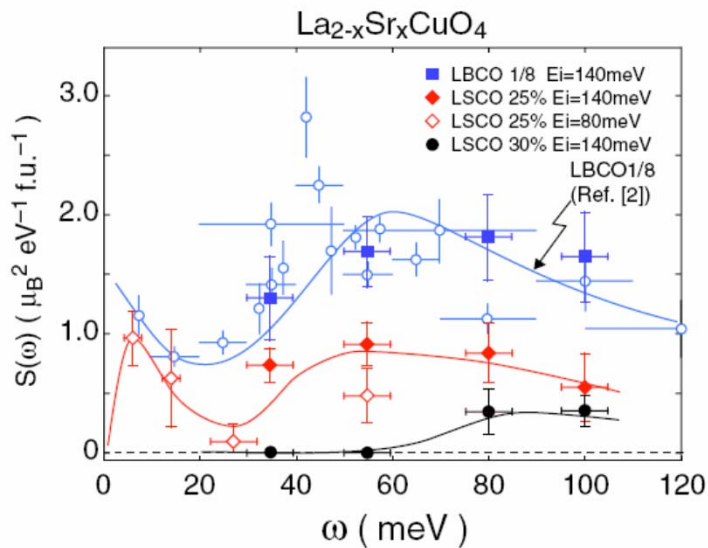
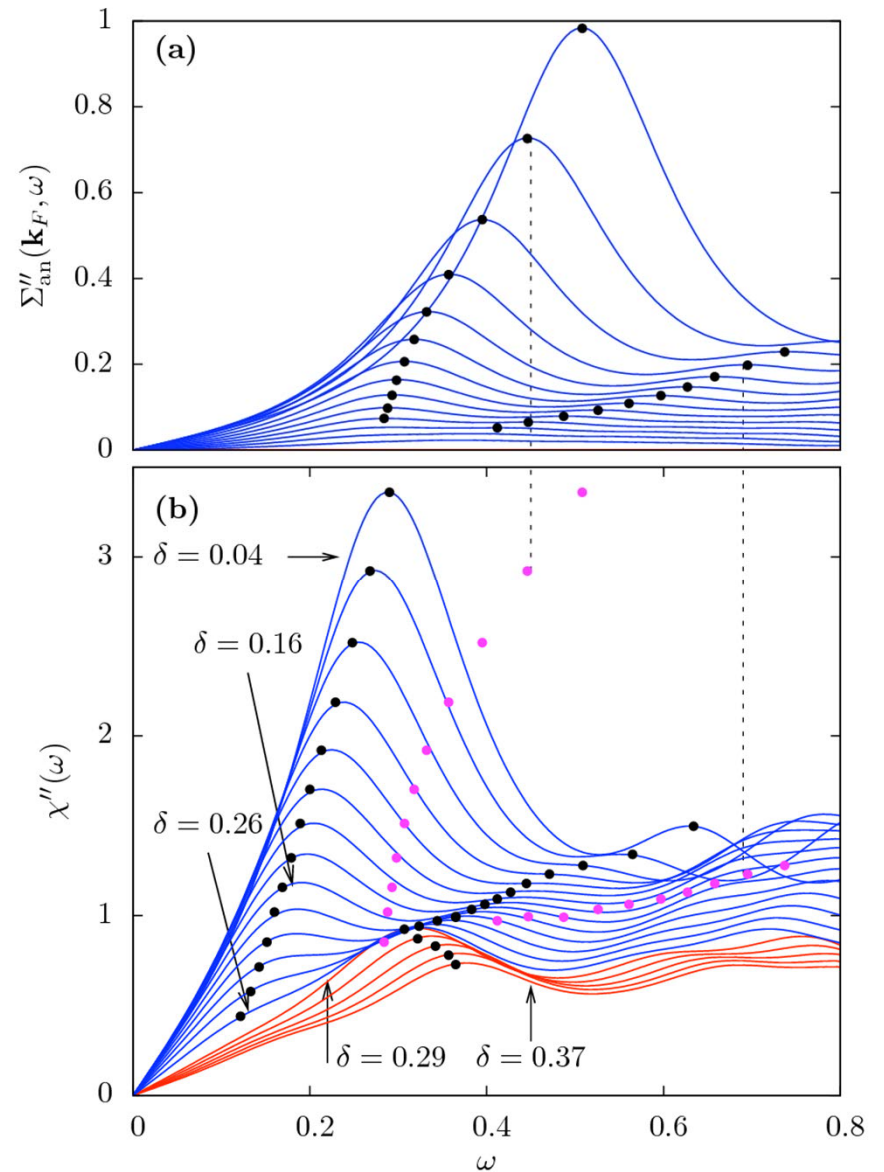


FIG. 3 (color online). \mathbf{Q} -integrated dynamic structure factor $S(\omega)$ which is derived from the wide- H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i = 140$ meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for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

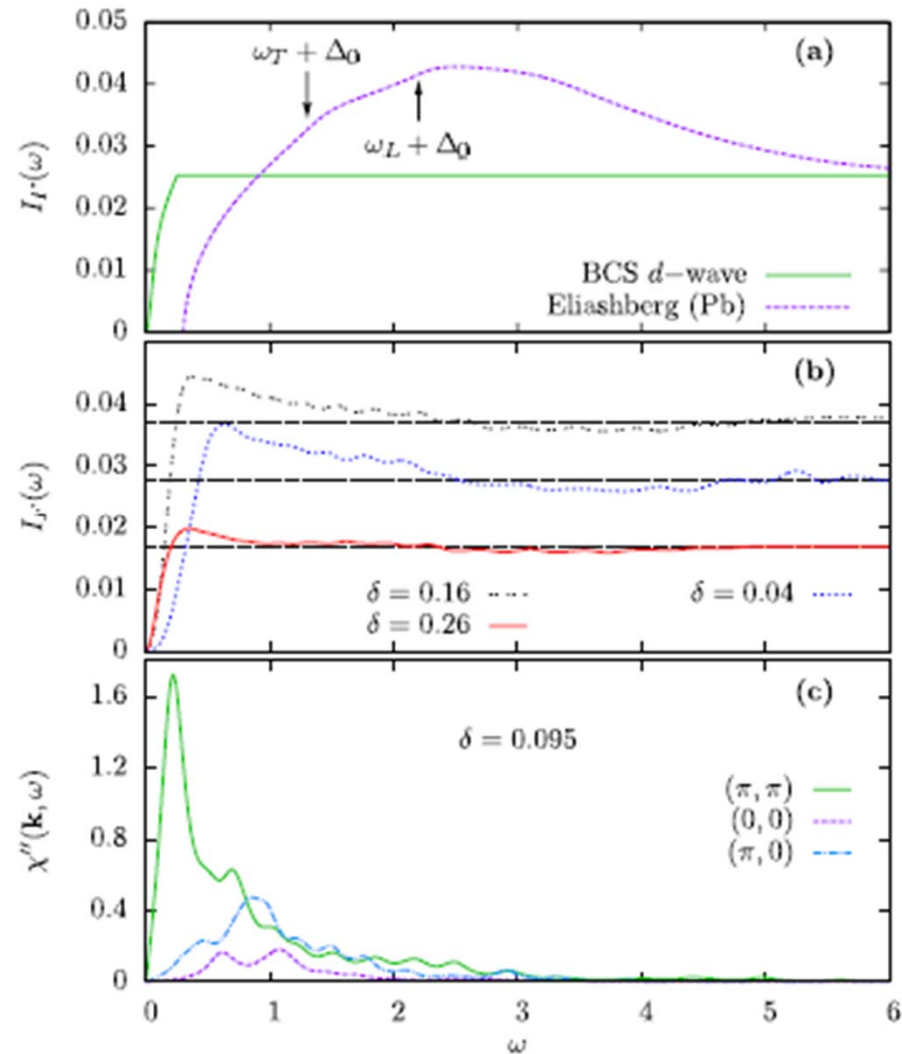


Bumsoo Kyung

David Sénéchal

$$I_F(\omega) \equiv - \int_0^\omega \frac{d\omega'}{\pi} \text{Im} F_{ij}^R(\omega').$$

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



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, $J - V$ $J = 130 \text{ meV}$
 $V = 400 \text{ meV}$

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).

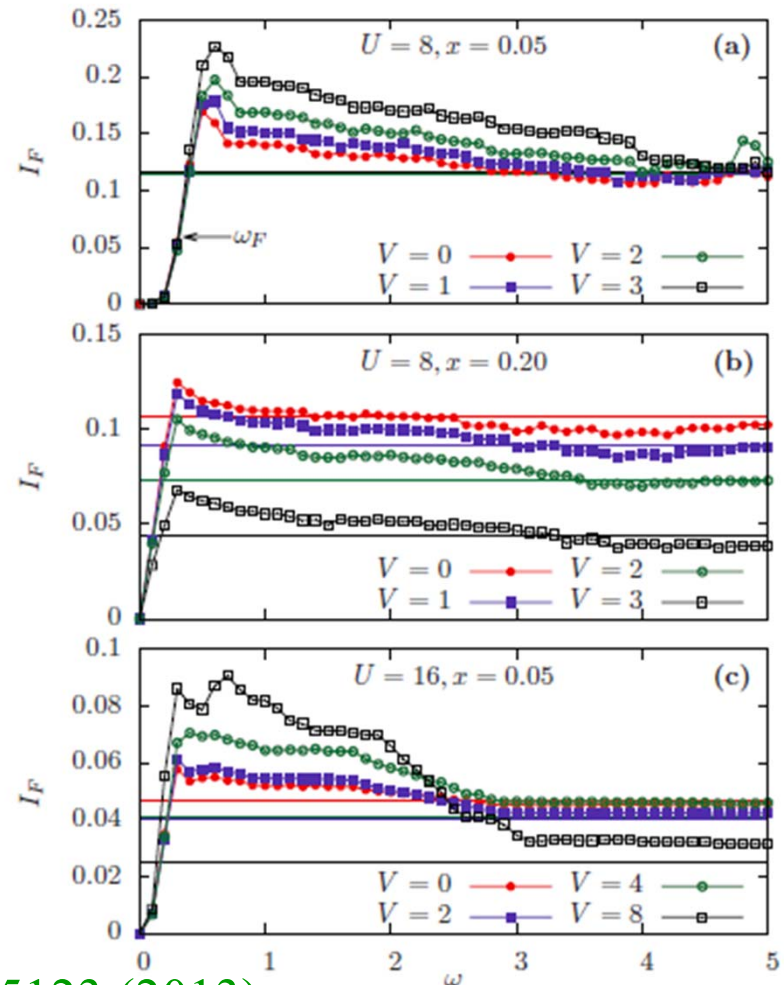
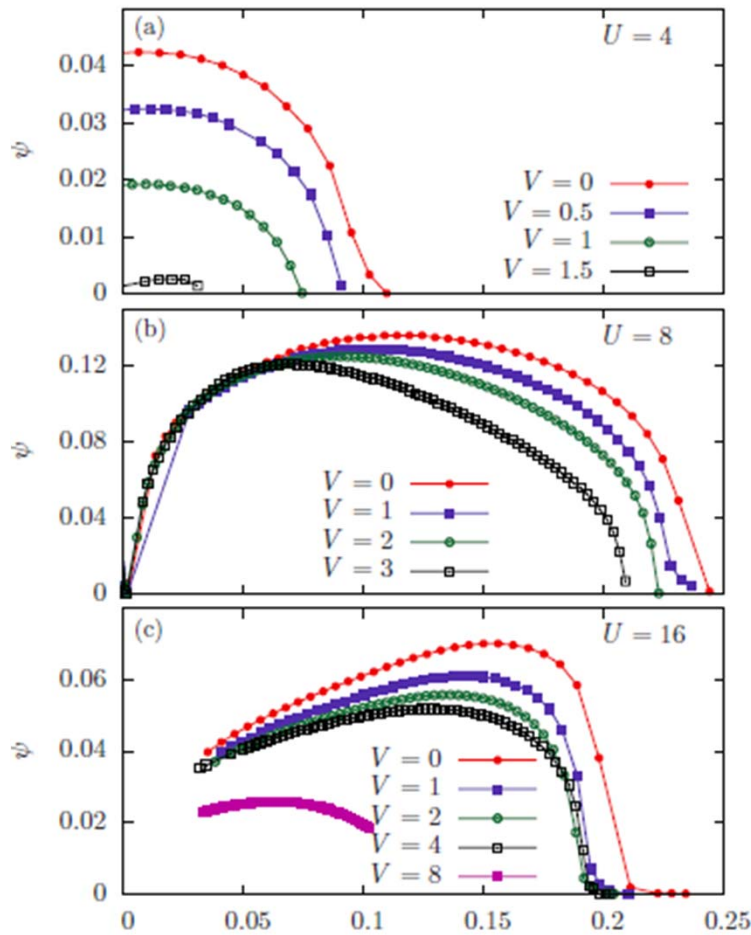




Resilience to near-neighbor repulsion

David Sénéchal

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



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



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$T = 0$ phase diagram

Normal state and large anisotropy



Underdoped metal very sensitive to anisotropy

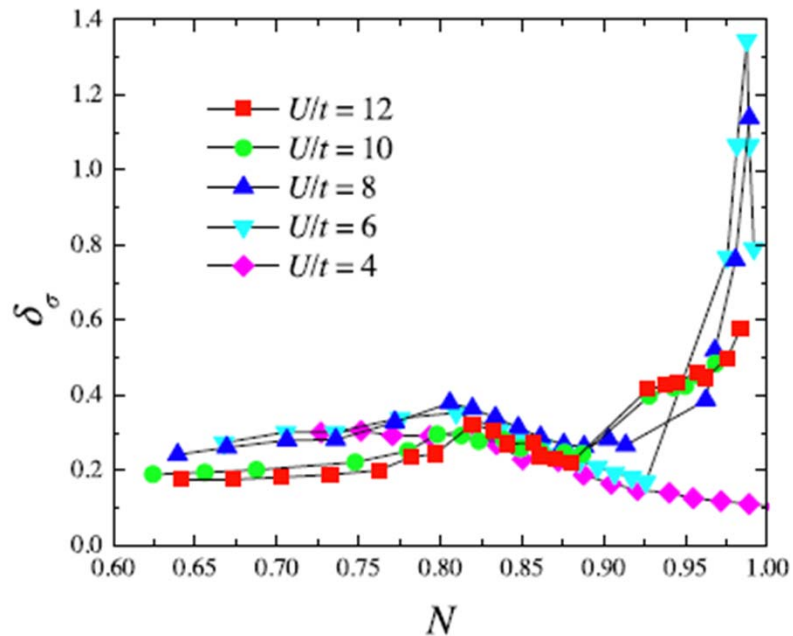
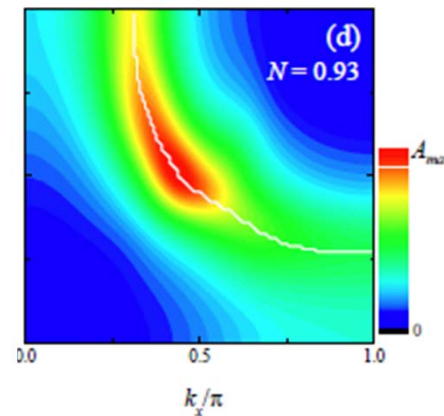
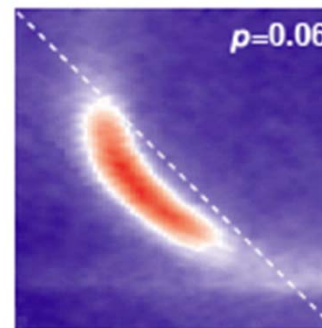


FIG. 3: (Color online) Anisotropy in the CDMFT conductivity $\delta_\sigma = 2[\sigma_x(0) - \sigma_y(0)] / [\sigma_x(0) + \sigma_y(0)]$ as a function of filling N for various values of U and $\eta = 0.1, \delta_0 = 0.04$.

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



g



Satoshi Okamoto



David Sénéchal



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

Methods



Measurable quantities : Green's functions

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

$$\begin{aligned} \mathcal{G}_{\mathbf{k}\sigma}(\tau) &= -\langle T_{\tau}[c_{\mathbf{k}\sigma}(\tau)c_{\mathbf{k}\sigma}^{\dagger}] \rangle \\ &= -\theta(\tau)\langle c_{\mathbf{k}\sigma}(\tau)c_{\mathbf{k}\sigma}^{\dagger} \rangle + \theta(-\tau)\langle c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}\sigma}(\tau) \rangle. \end{aligned}$$

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

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

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



Green's function: free electrons, atomic limit

$$H = -\sum_{\langle ij \rangle \sigma} t_{i,j} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma})$$

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

$$H =$$

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

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



Self-energy and all that

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

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

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

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

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

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



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

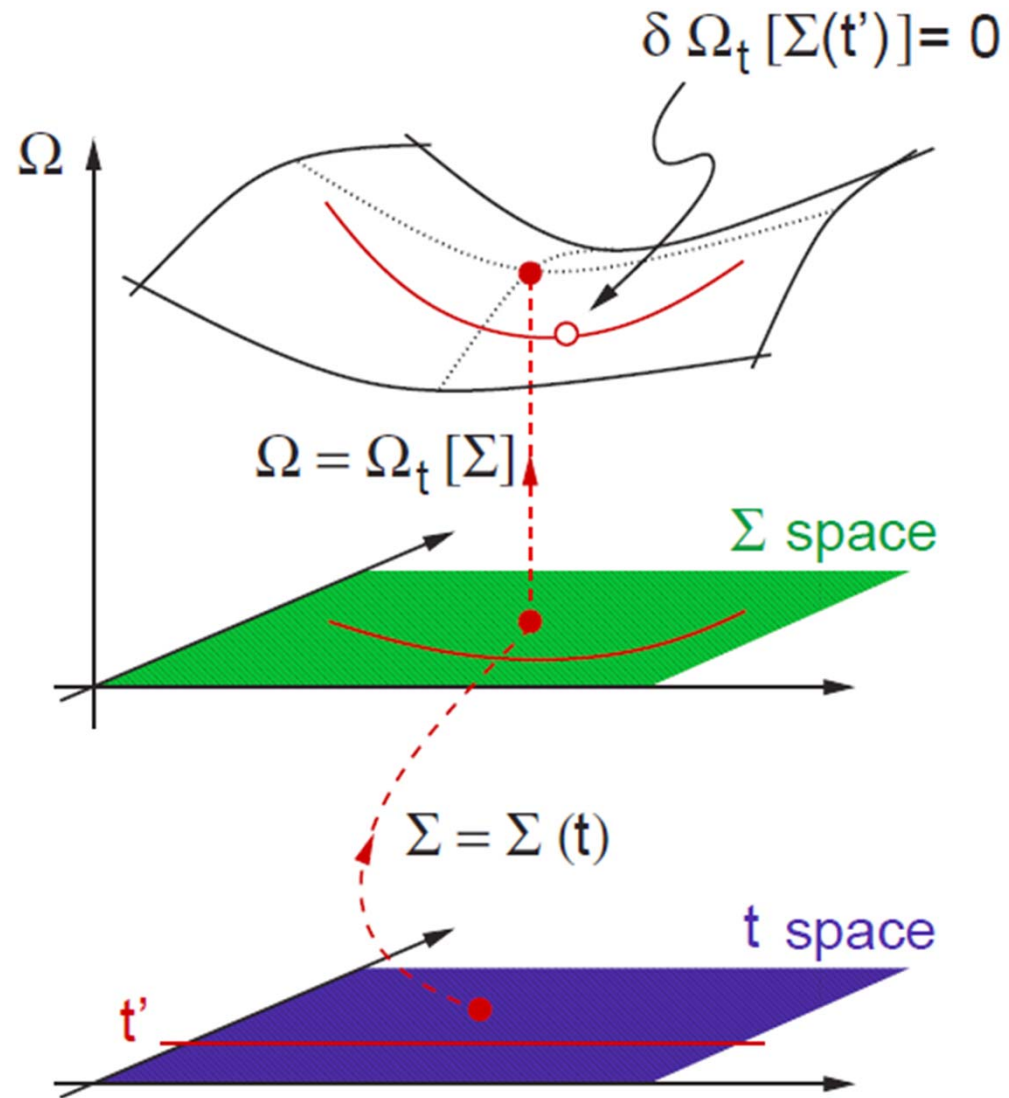
- Cavity method
- Local nature of perturbation theory in infinite dimensions
- Expansion around the atomic limit
- Effective medium theory
- Potthoff self-energy functional

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

A. Georges *et al.*, *Rev. Mod. Phys.* **68**, 13 (1996).



DMFT as a stationary point



Another way to look at this (Potthoff)

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

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

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

Still stationary (chain rule)

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

SFT : Self-energy Functional Theory

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

$$\Omega_t[\Sigma] = F[\Sigma] + \text{Tr} \ln(-(G_0^{-1} - \Sigma)^{-1})$$

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

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

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

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

CT-QMC impurity solver

Monte Carlo method

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

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

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

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

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



Monte Carlo: Markov chain

- Ergodicity
- Detailed balance

$$\frac{W_{\mathbf{xy}}}{W_{\mathbf{yx}}} = \frac{p(\mathbf{y})}{p(\mathbf{x})}$$

$$W_{\mathbf{xy}} = W_{\mathbf{xy}}^{\text{prop}} W_{\mathbf{xy}}^{\text{acc}}$$

$$W_{\mathbf{xy}}^{\text{acc}} = \min[1, R_{\mathbf{xy}}]$$

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



Reminder on perturbation theory

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

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

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



Partition function as sum over configurations

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

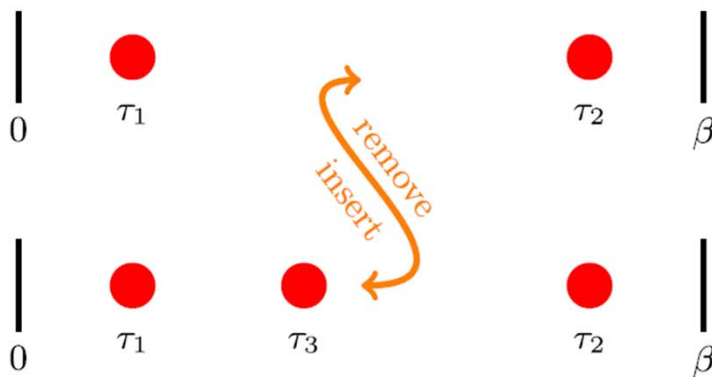
$$= \sum_k (-1)^k \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \text{Tr}[e^{-\beta H_a} H_b(\tau_k) \\ \times H_b(\tau_{k-1}) \cdots H_b(\tau_1)].$$

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

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



Updates



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

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

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

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

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

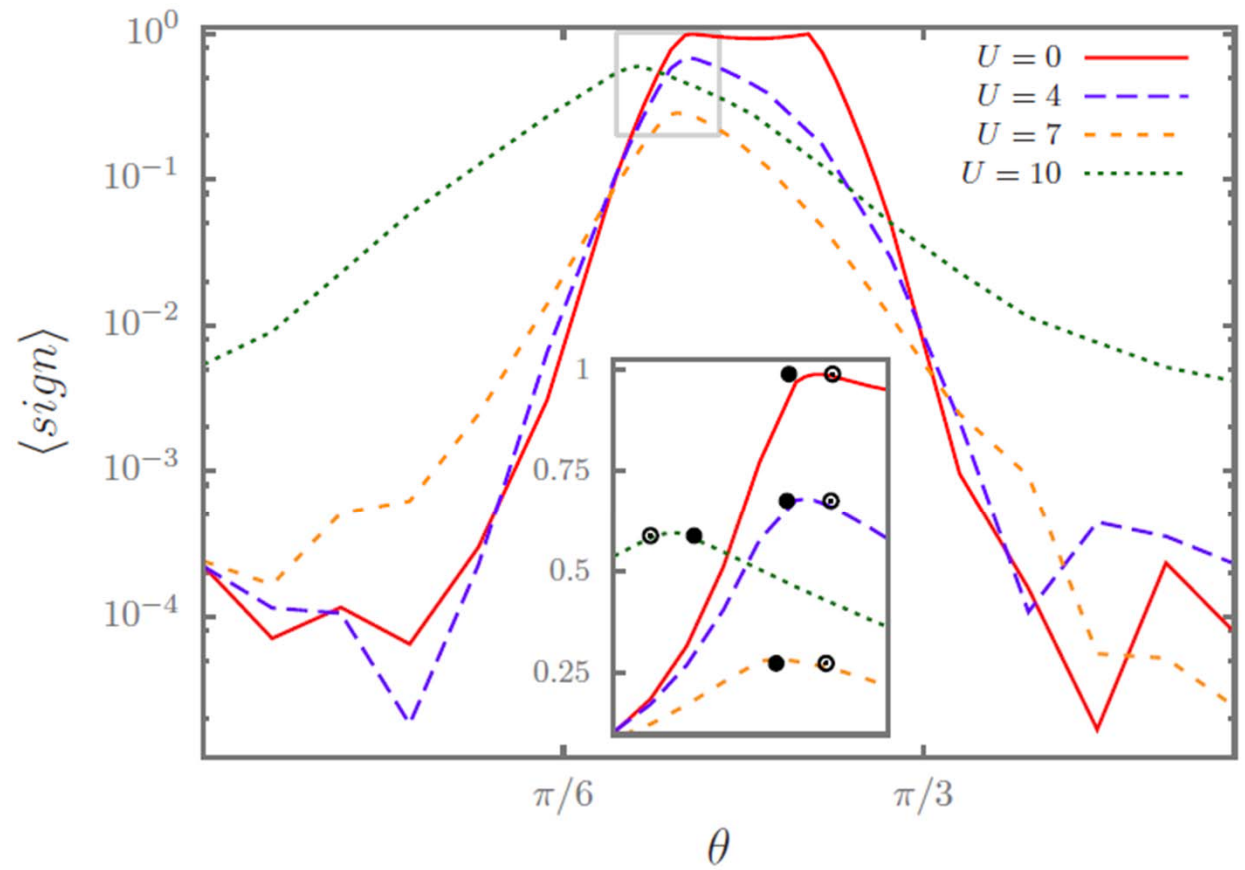
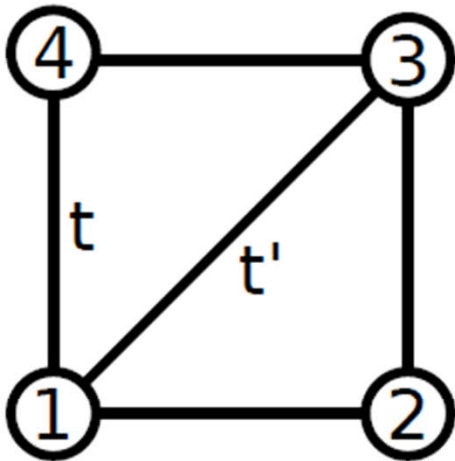
$$\begin{aligned} Z &= \sum_{k=0}^{\infty} \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \int_0^\beta d\tau'_1 \cdots \int_{\tau'_{k-1}}^\beta d\tau'_k \\ &\times \sum_{\substack{j_1, \dots, j_k \\ j'_1, \dots, j'_k}} \sum_{\substack{p_1, \dots, p_k \\ p'_1, \dots, p'_k}} V_{p_1}^{j_1} V_{p'_1}^{j'_1*} \cdots V_{p_k}^{j_k} V_{p'_k}^{j'_k*} \\ &\times \text{Tr}_d [T_\tau e^{-\beta H_{\text{loc}}} d_{j_k}(\tau_k) d_{j'_k}^\dagger(\tau'_k) \cdots d_{j_1}(\tau_1) d_{j'_1}^\dagger(\tau'_1)] \\ &\times \text{Tr}_c [T_\tau e^{-\beta H_{\text{bath}}} c_{p_k}^\dagger(\tau_k) c_{p'_k}(\tau'_k) \cdots c_{p_1}^\dagger(\tau_1) c_{p'_1}(\tau'_1)]. \end{aligned}$$

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



Sign problem

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



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:
$$U_{sp} = \frac{\delta \Sigma_{\uparrow}}{\delta G_{\downarrow}} - \frac{\delta \Sigma_{\downarrow}}{\delta G_{\uparrow}}$$

(b) analog of the Bethe-Salpeter equation:

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

(c) self-energy:

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

2. Factorization



TPSC...

$$U_{sp} = U \frac{\langle n_{\uparrow} n_{\downarrow} \rangle}{\langle n_{\uparrow} \rangle \langle n_{\downarrow} \rangle} \quad \text{Kanamori-Brückner screening}$$

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

3. The F.D. theorem and Pauli principle

$$\langle (n_{\uparrow} - n_{\downarrow})^2 \rangle = \langle n_{\uparrow} \rangle + \langle n_{\downarrow} \rangle - 2\langle n_{\uparrow} n_{\downarrow} \rangle$$

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

II: Improved self-energy

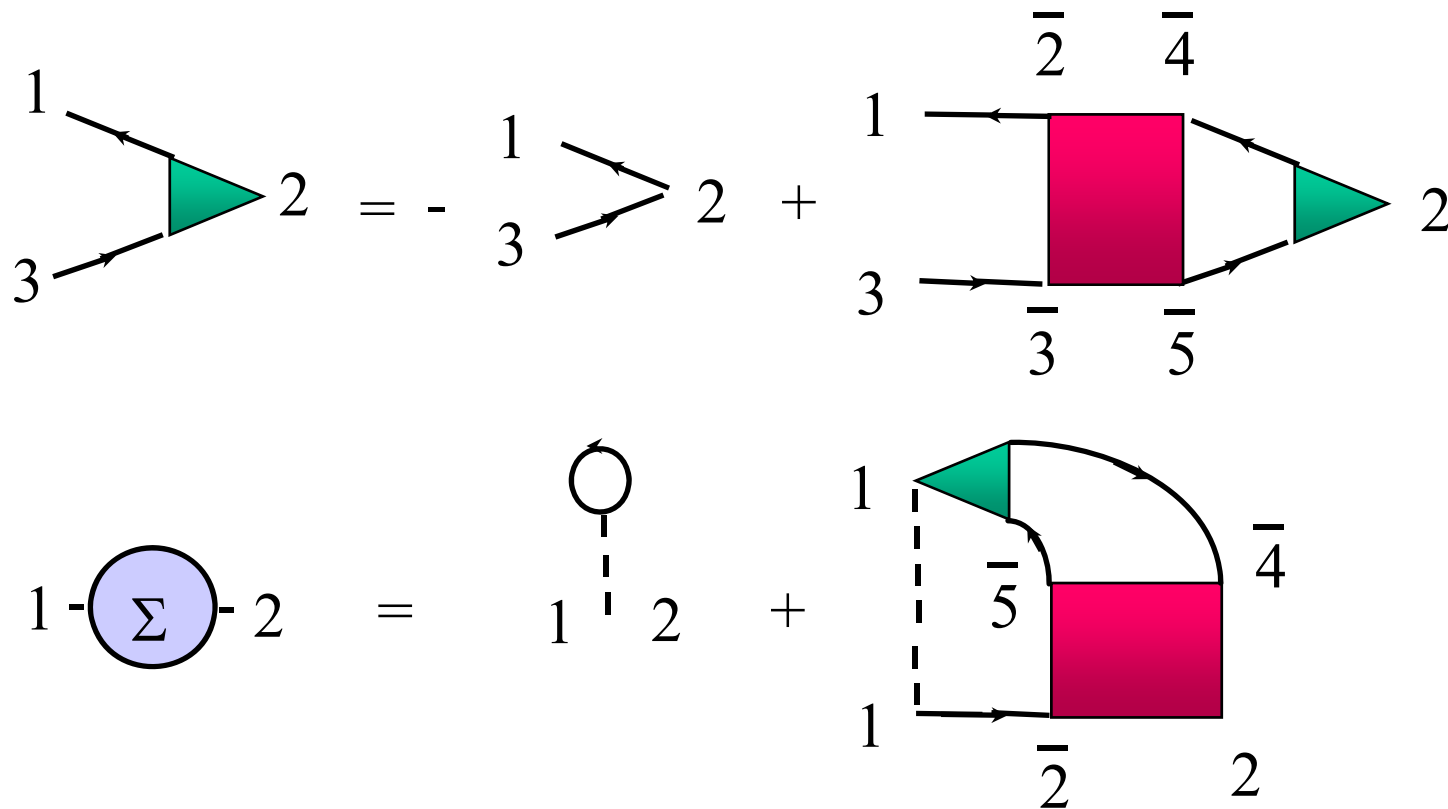
Insert the first step results

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

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



A better approximation for single-particle properties (Ruckenstein)



Y.M. Vil'k and A.-M.S. Tremblay, J. Phys. Chem. Solids **56**, 1769 (1995).

Y.M. Vil'k and A.-M.S. Tremblay, Europhys. Lett. **33**, 159 (1996);

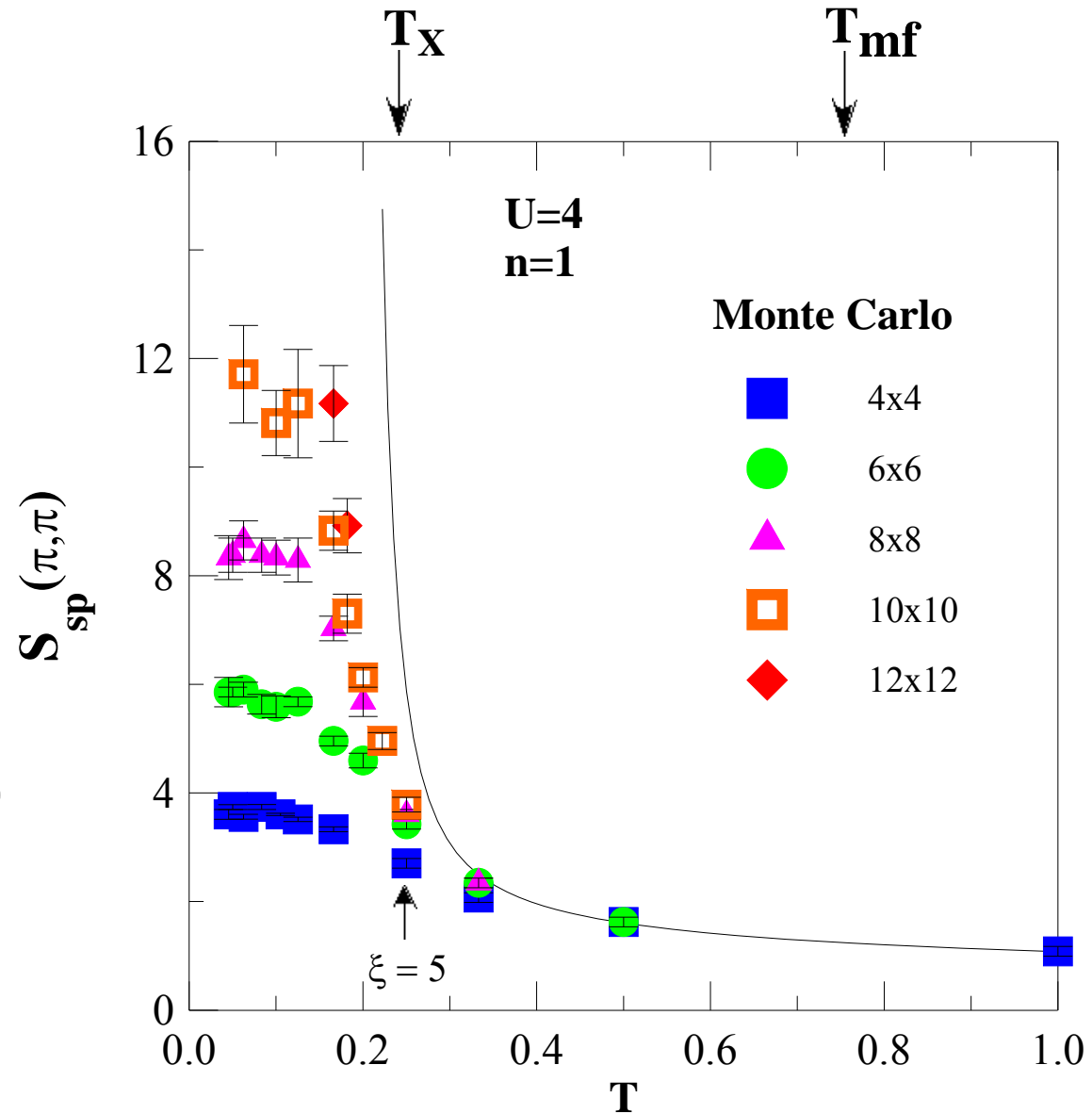
N.B.: No Migdal theorem



Benchmarks for TPSC

$n=1$

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



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

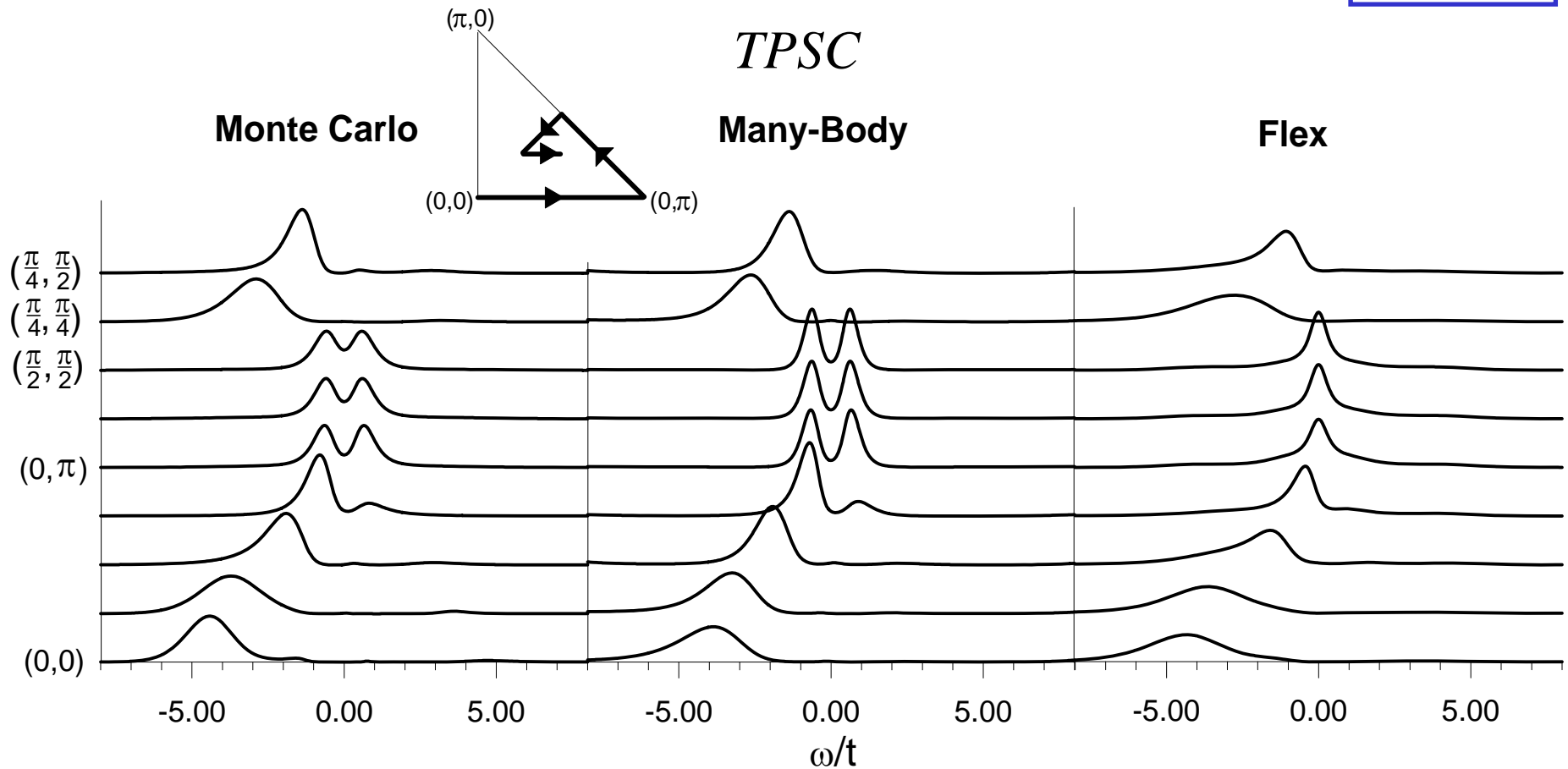
QMC: S. R. White, et al. Phys. Rev. **40**, 506 (1989).

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



Proofs...

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



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



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Sarma Kancharla



Marcello Civelli



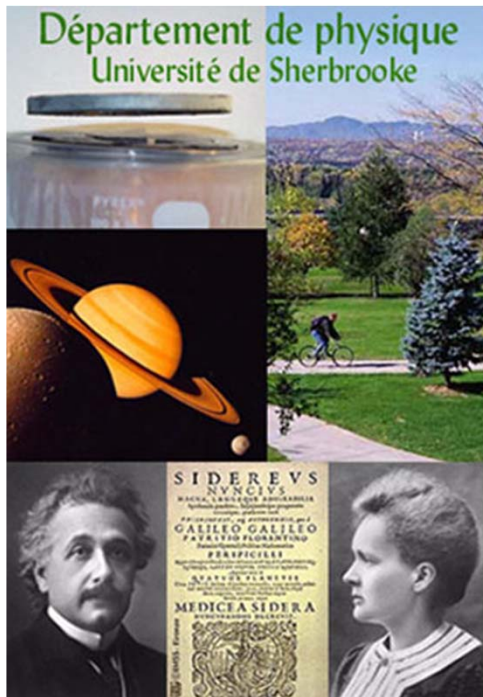
Massimo Capone



Gabriel Kotliar



André-Marie Tremblay



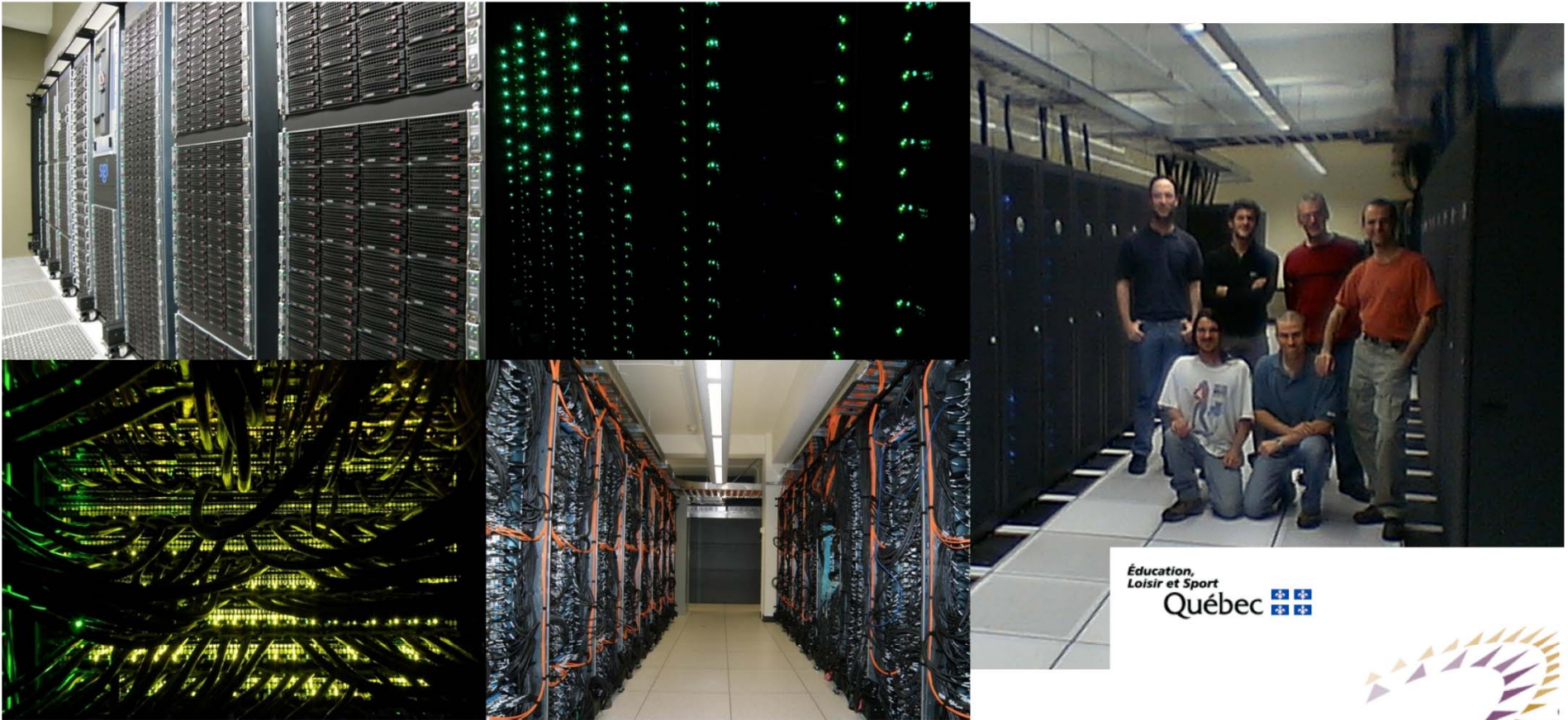
Le regroupement québécois sur les matériaux de pointe



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Merci

Thank you