

Insulators, metals, pseudogaps and cuprate superconductivity

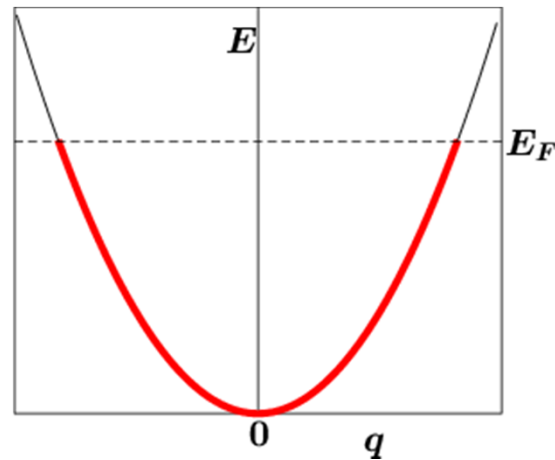
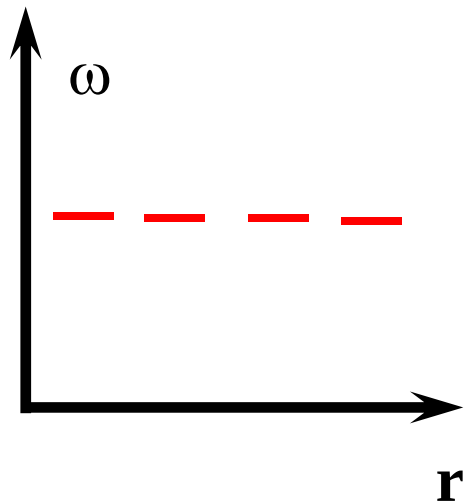
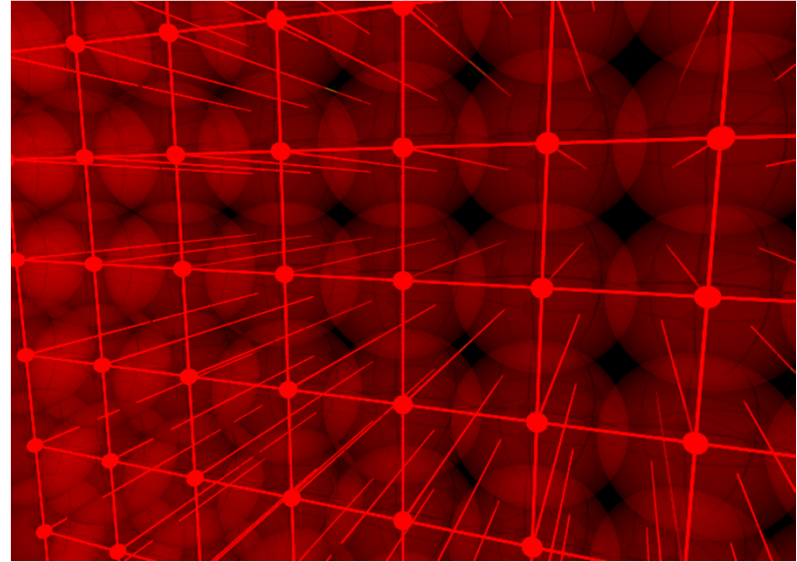
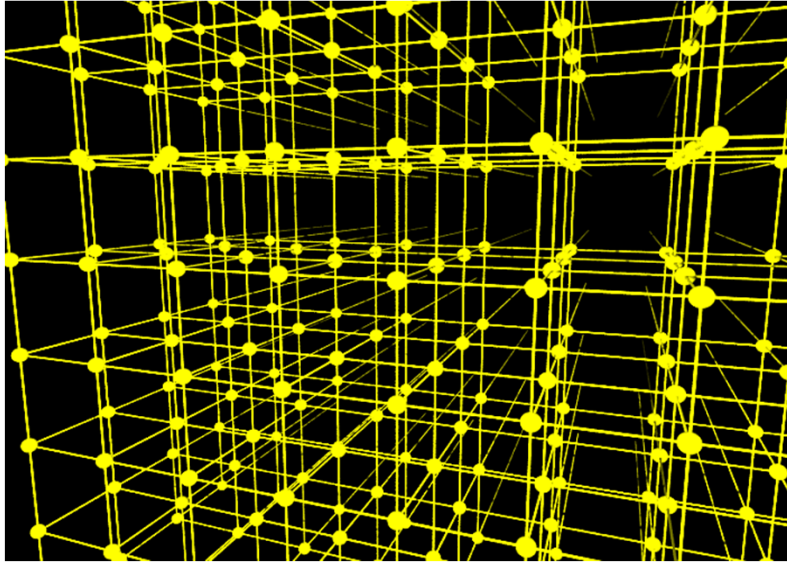
A.-M. Tremblay



Rutherford, June 20th, 2013



How to make a metal



Courtesy, S. Julian



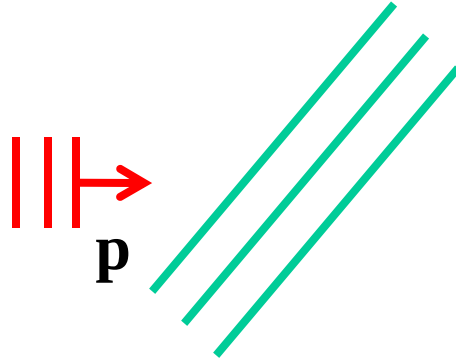
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Superconductivity

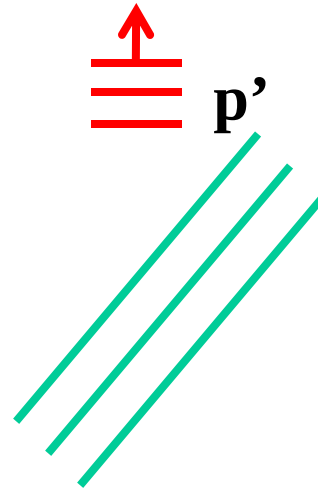


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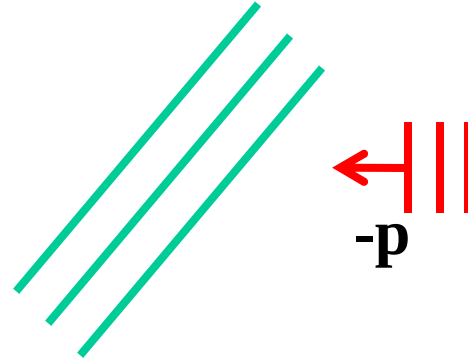
Attraction mechanism in the metallic state



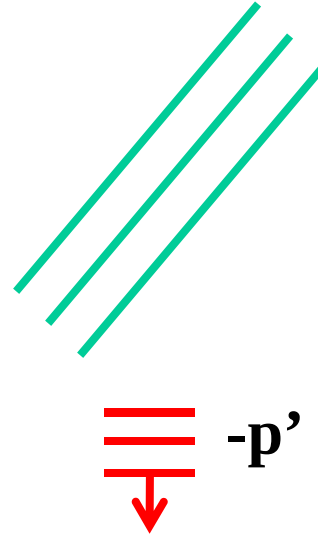
Attraction mechanism in the metallic state



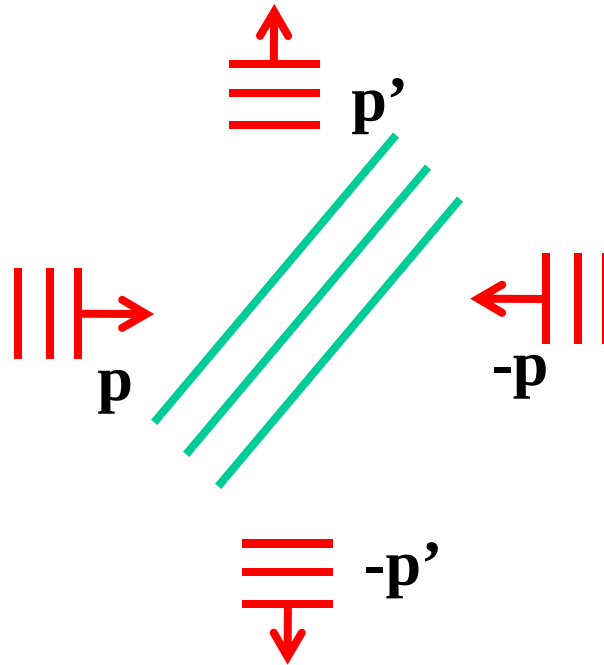
Attraction mechanism in the metallic state



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 Verway



Peierls, 1937



Mott, 1949



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« Conventional » Mott transition

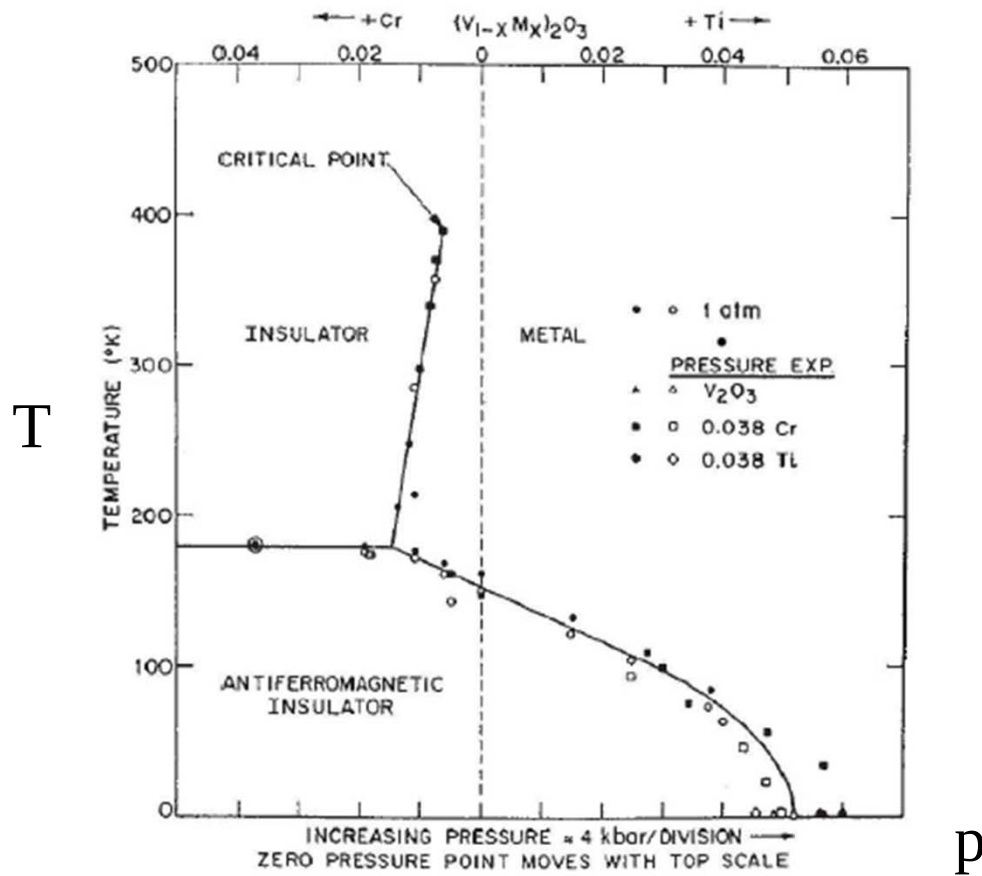


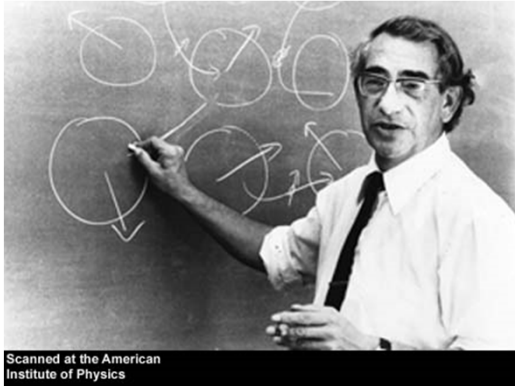
Figure: McWhan, PRB 1970; Limelette, Science 2003

Model

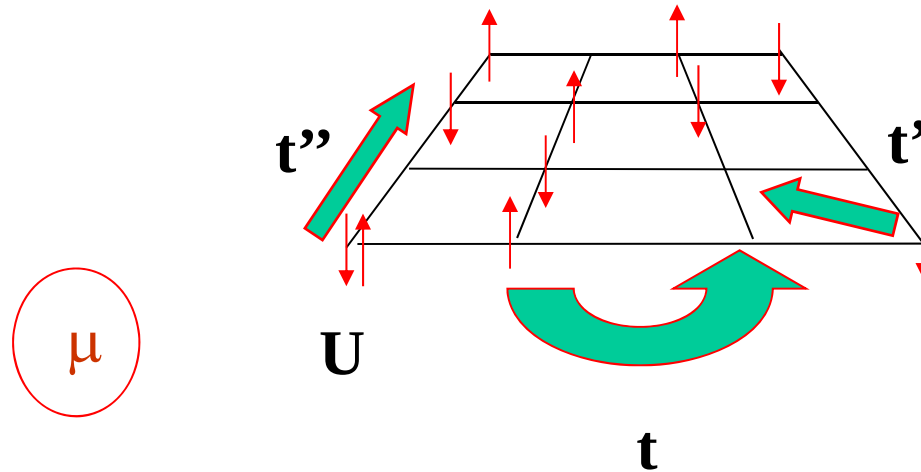
$$H = -\sum_{\langle ij \rangle \sigma} t_{i,j} \left(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



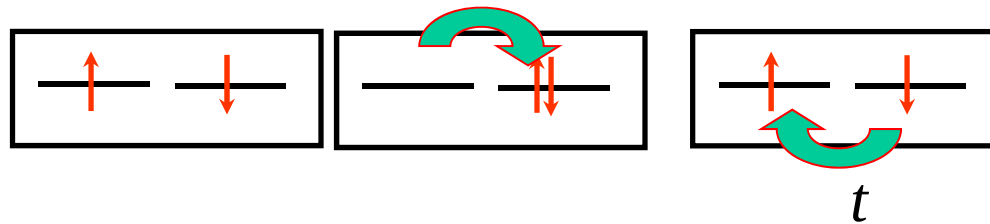
Hubbard model



1931-1980



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



$t = 1$

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



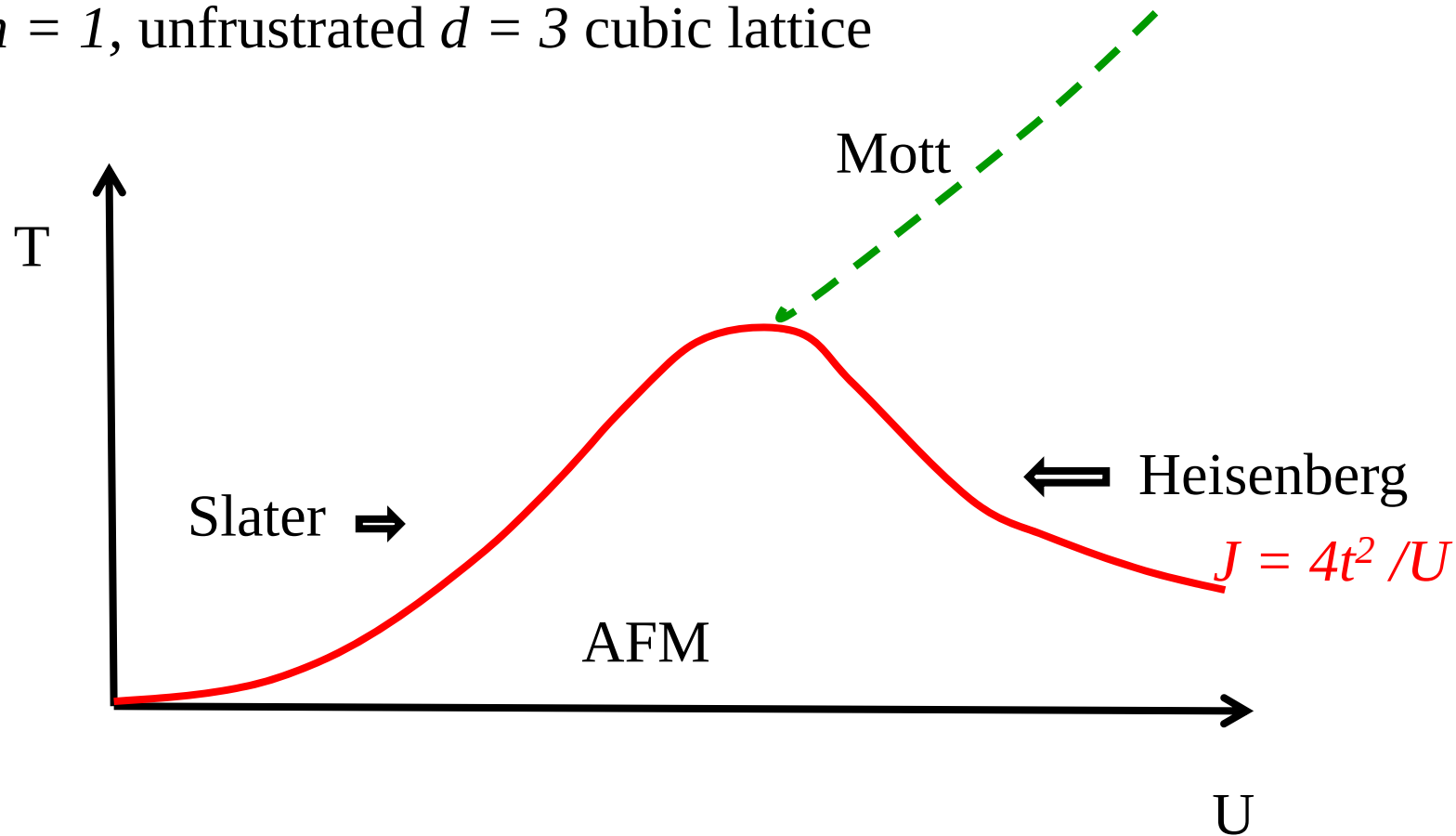
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Strongly vs weakly correlated



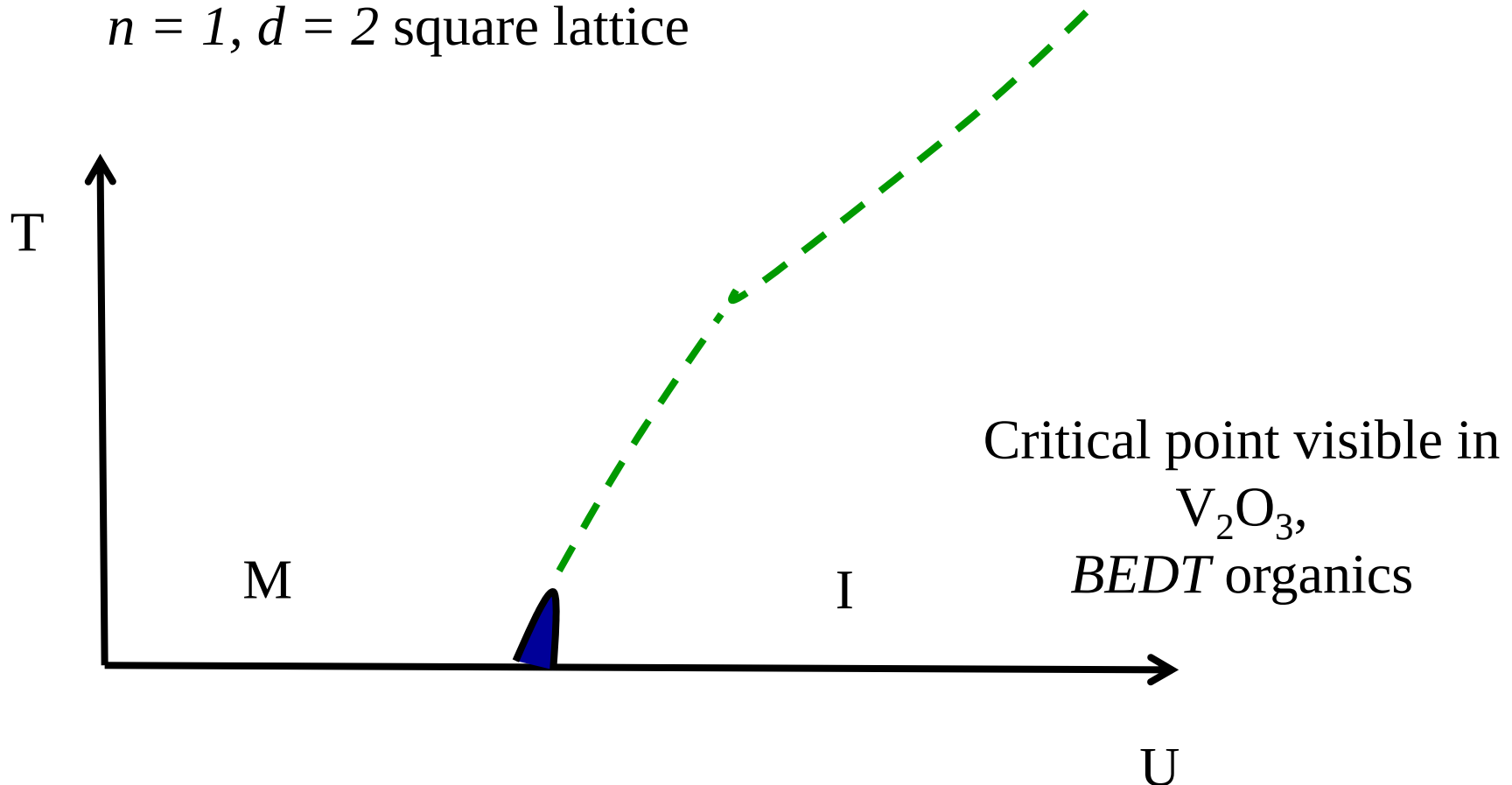
Local moment and Mott transition

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



Local moment and Mott transition

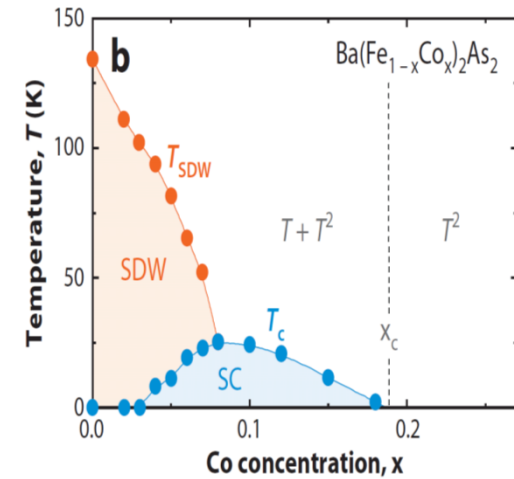
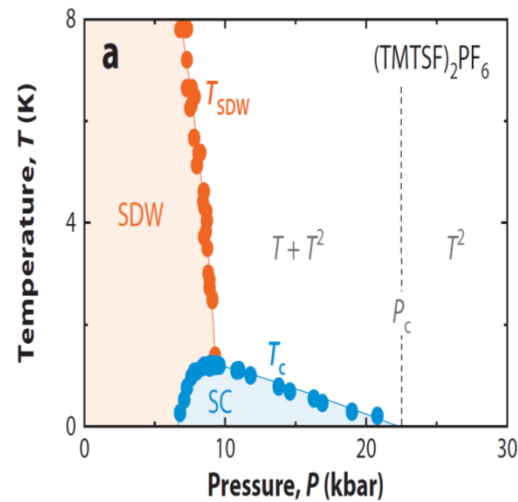
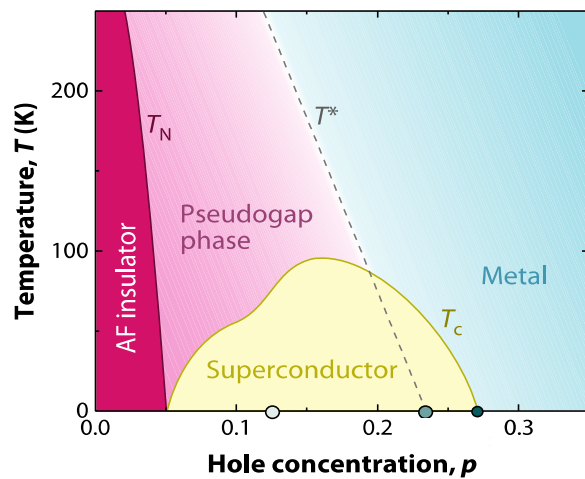
$n = 1, d = 2$ square lattice



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

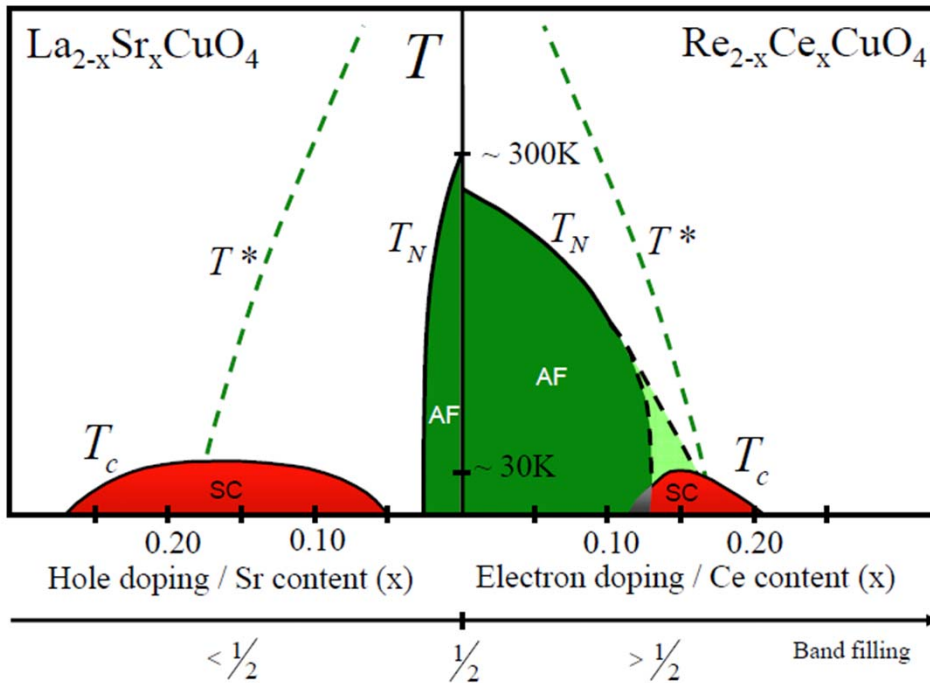


Superconductivity and strong repulsion



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) ...

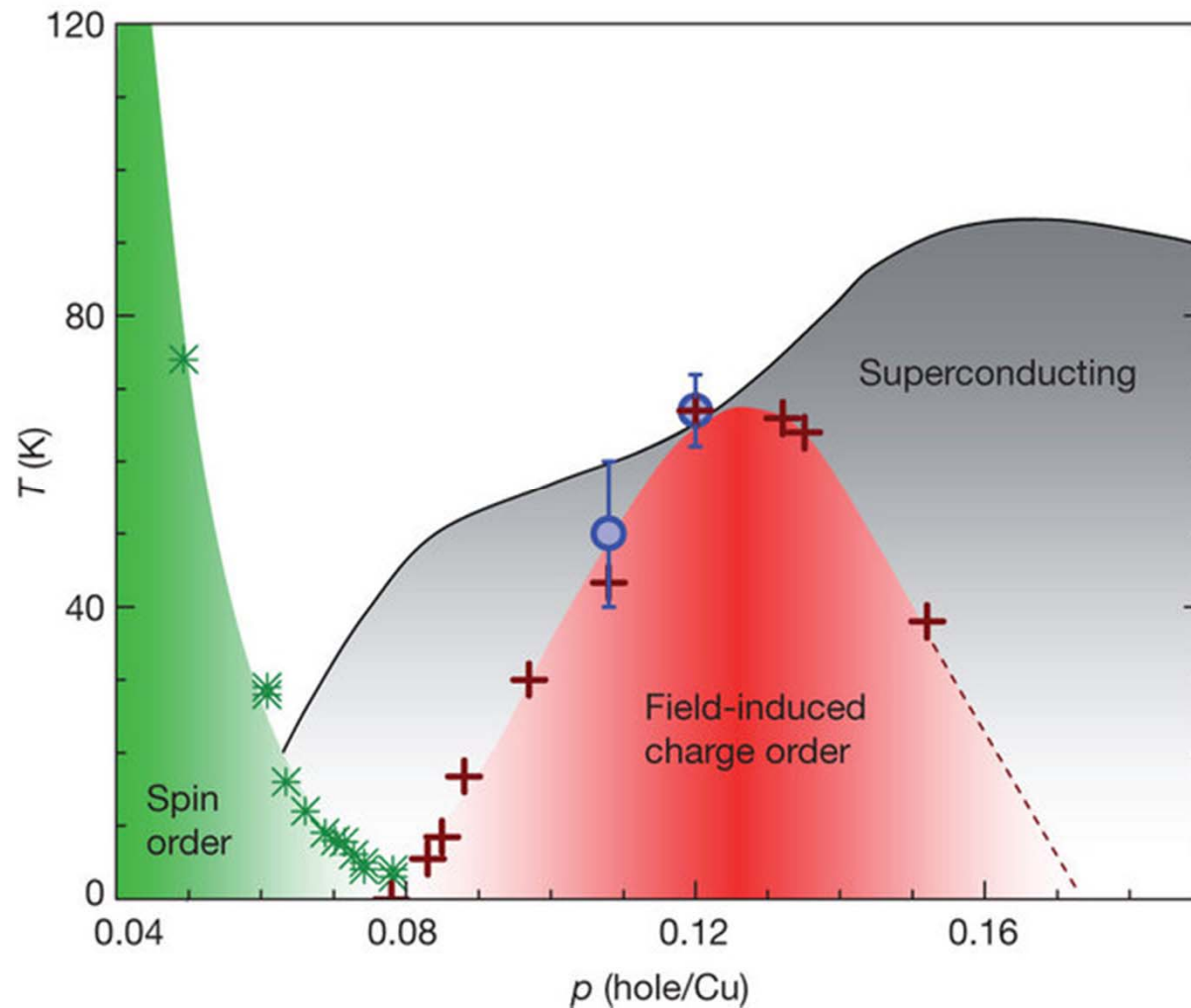
- Or Mott Physics?

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

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



Stripes and reconstructed Fermi surface



Wu et al. Julien, Nature **477**, 191–194 (2011)



Competing CDW order

- Wise, W. D. et al. Charge-density-wave origin of cuprate checkerboard visualized by scanning tunnelling microscopy. *Nature Phys.* 4, 696699 (2008).
- Lawler, M. J. et al. Intra-unit-cell electronic nematicity of the high- T_c copper-oxide pseudogap states. *Nature* 466, 347351 (2010).
- Parker, C. V. et al. Fluctuating stripes at the onset of the pseudogap in the high- T_c superconductor $B2Sr2CaCu2O8C_x$. *Nature* 468, 677680 (2010).
- Chang, J. et al. Direct observation of competition between superconductivity and charge density wave order in $YBa2Cu3O6.67$. *Nature Phys.* 8, 871876 (2012).
- Ghiringhelli, G. et al. Long-range incommensurate charge fluctuations in $(Y;Nd)Ba2Cu3O6C_x$. *Science* 337, 821825 (2012).
- Achkar, A. J. et al. Distinct charge orders in the planes and chains of ortho-III-ordered $YBa2Cu3O6C$ superconductors identified by resonant elastic X-ray scattering. *Phys. Rev. Lett.* 109, 167001 (2012).
- Wu, T. et al. Magnetic-field-induced charge-stripe order in the high-temperature superconductor $YBa2Cu3O_y$. *Nature* 477, 192194 (2011).
- LeBoeuf, D. et al. Thermodynamic phase diagram of static charge order in underdoped $YBa2Cu3O_y$. *Nature Phys.* 9, 7983 (2013).



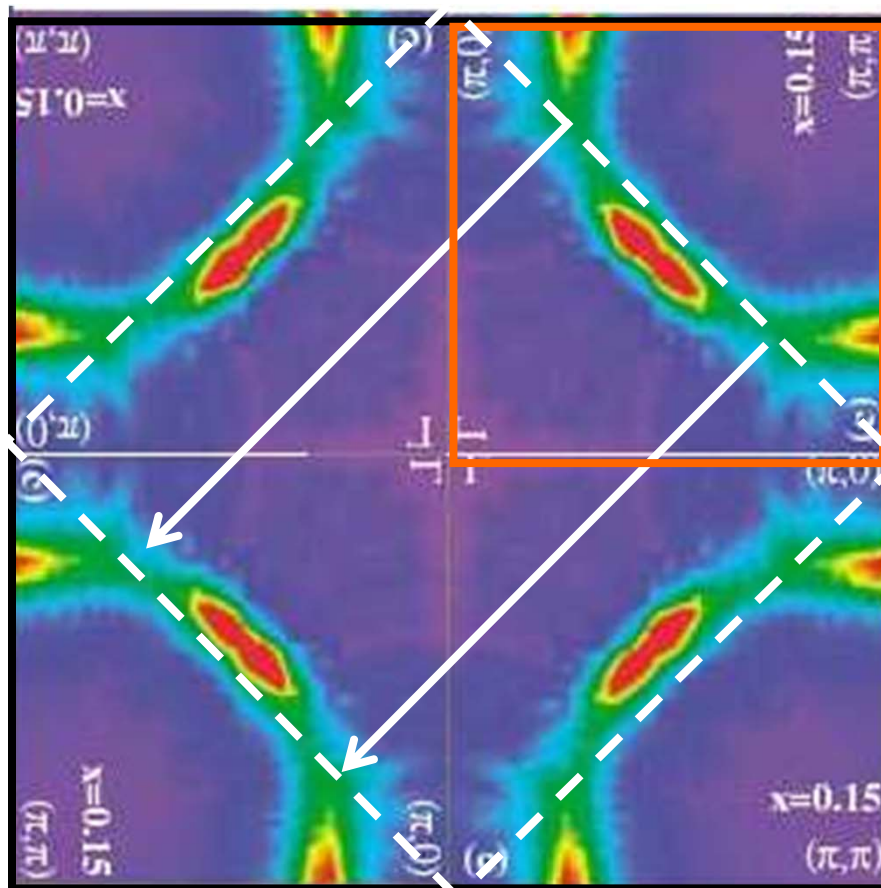
Three broad classes of mechanisms for pseudogap

- 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)



Hot spots from AFM quasi-static scattering

$d = 2$

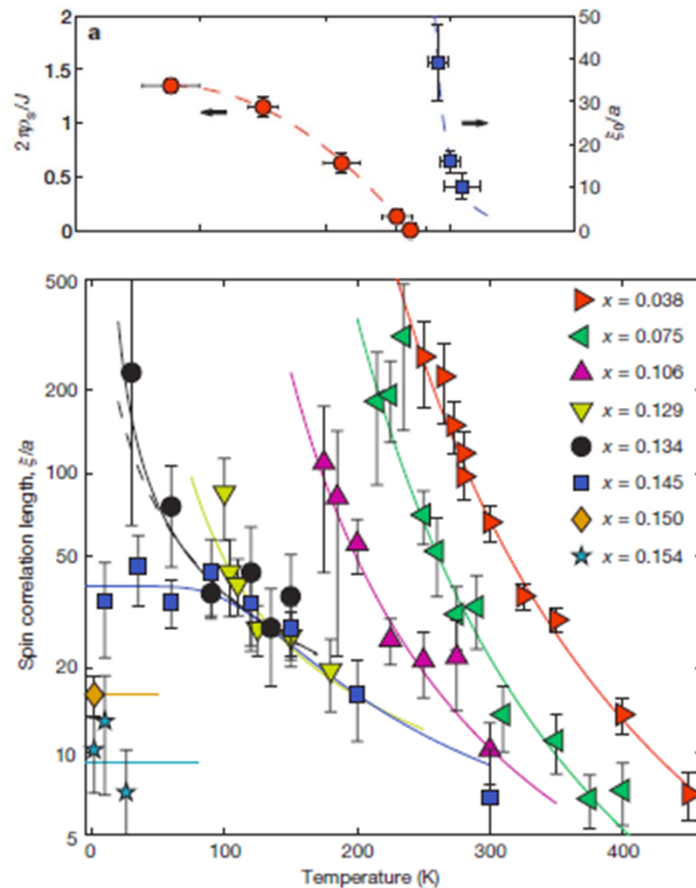


Armitage et al. PRL 2001

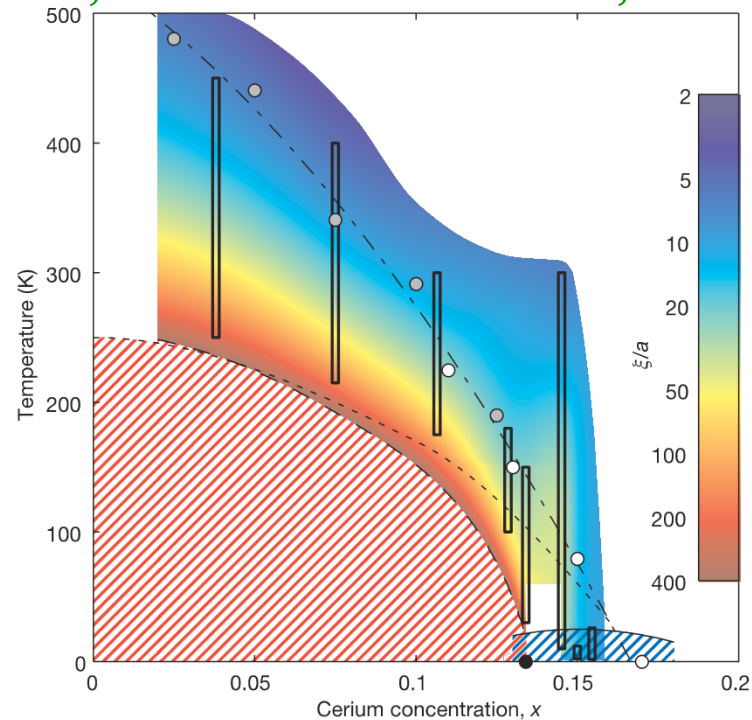
e-doped cuprates: precursors

NCCO

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

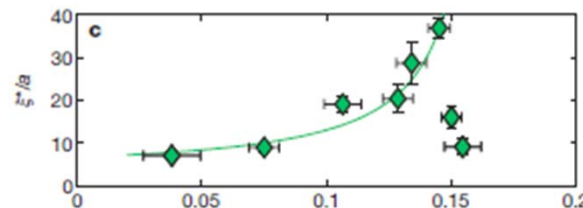


$z = 1$



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

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



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



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Back to hole-doped



What is the minimal model?

H. Alloul arXiv:1302.3473

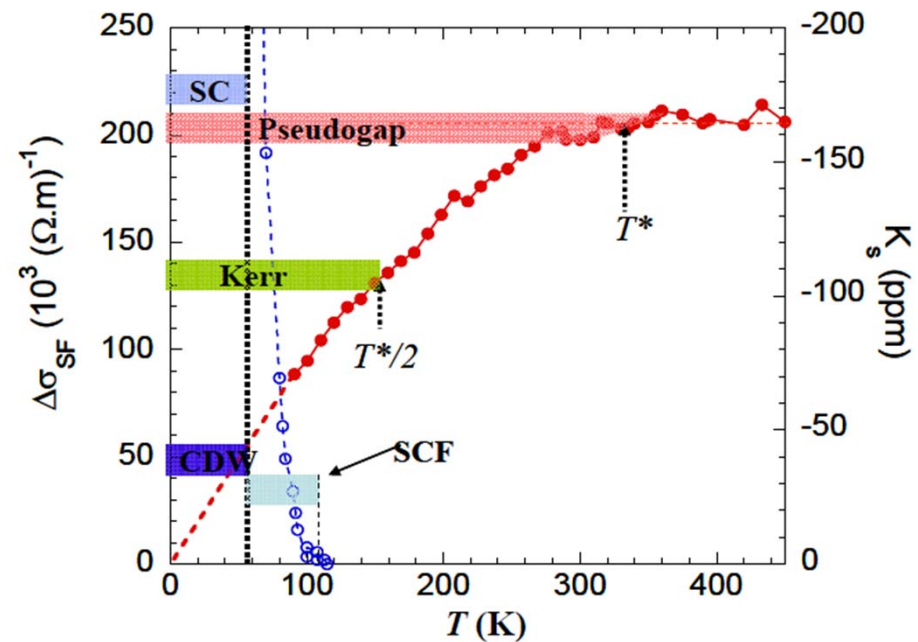
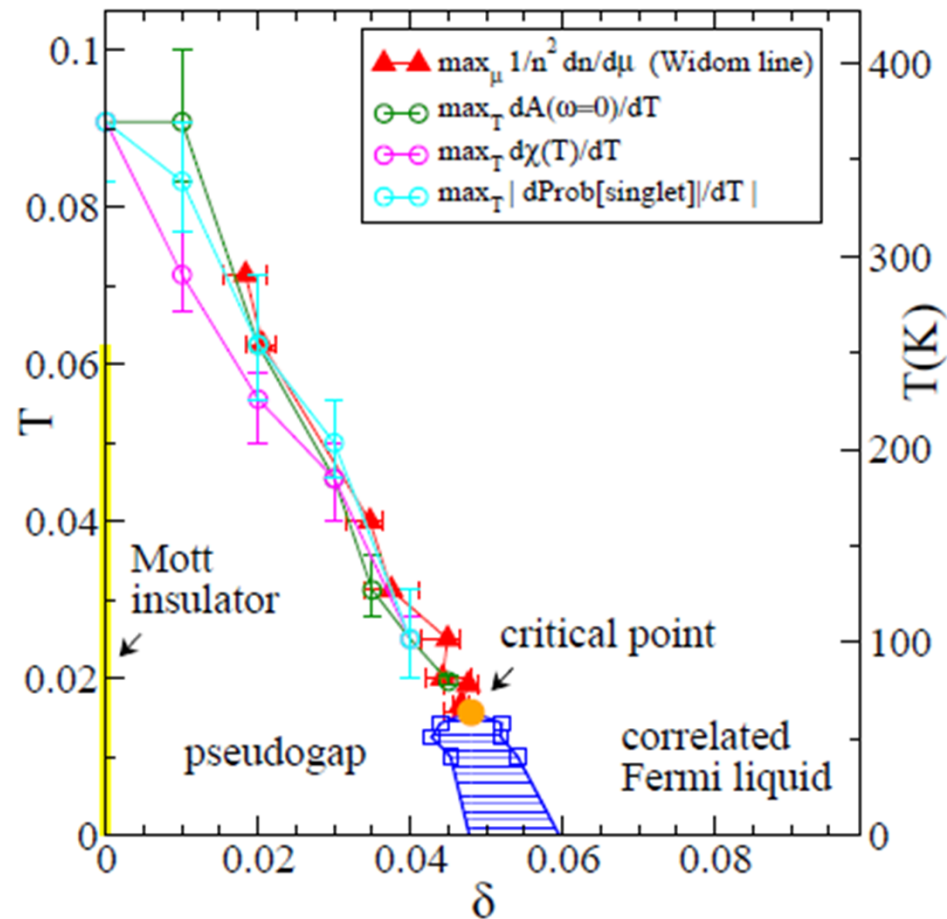


Fig 1 Spin contribution K_s to the ^{89}Y NMR Knight shift [11] for $\text{YBCO}_{6.6}$ permit to define the PG onset T^* . Here K_s is reduced by a factor two at $T \sim T^*/2$. The sharp drop of the SC fluctuation conductivity (SCF) is illustrated (left scale) [23]. We report as well the range over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



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

Competing order is a consequence of the pseudogap, not its cause:

Parker et al. Nature 468, 677 (2010)



Hole-doped cuprates as Mott insulators



Mott-Ioffe-Regel limit

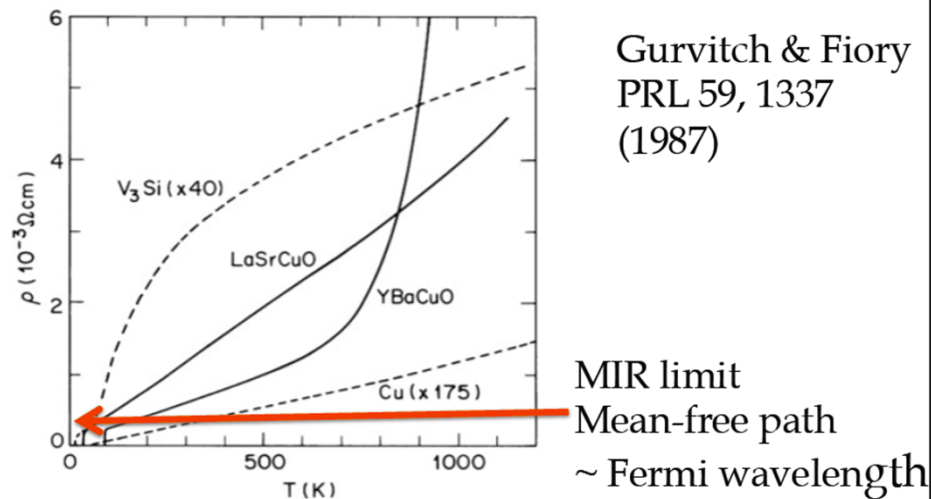
$$\sigma = \frac{ne^2\tau}{m}$$

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

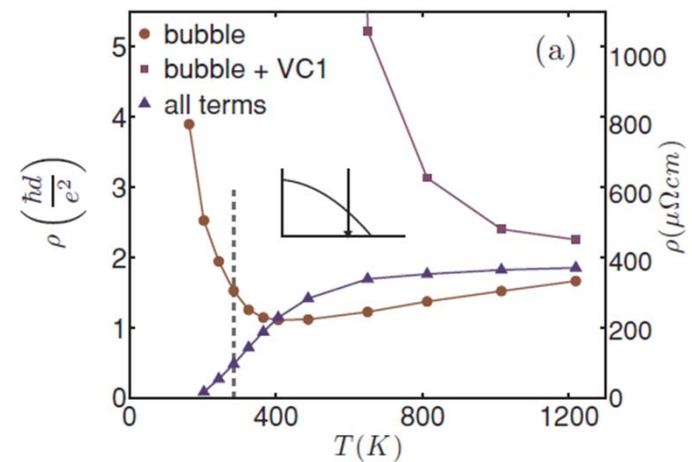
$$\sigma_{MIR} = \frac{e^2}{hd}$$



Hole-doped cuprates and MIR limit



LSCO 17%, YBCO optimal



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

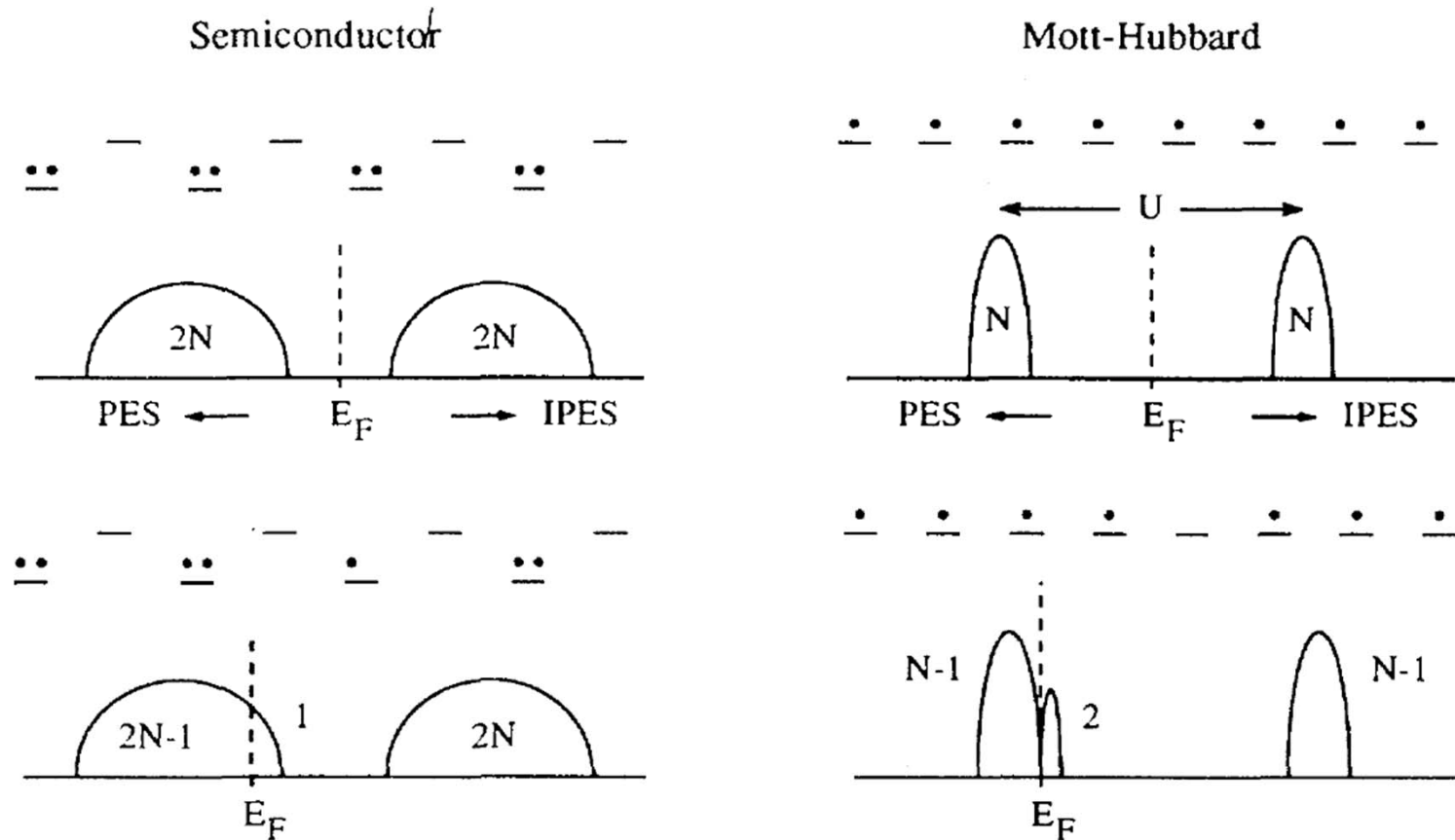
PHYSICAL REVIEW B 84, 085128 (2011)

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



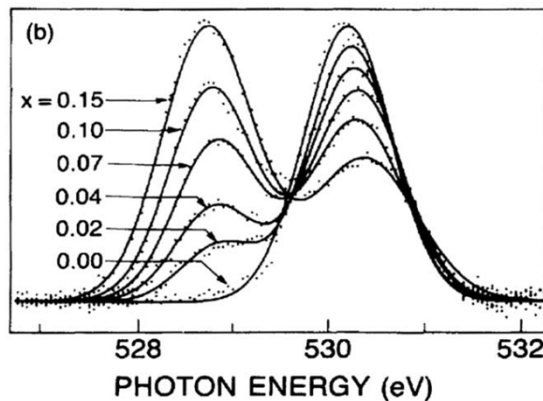
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Spectral weight transfer

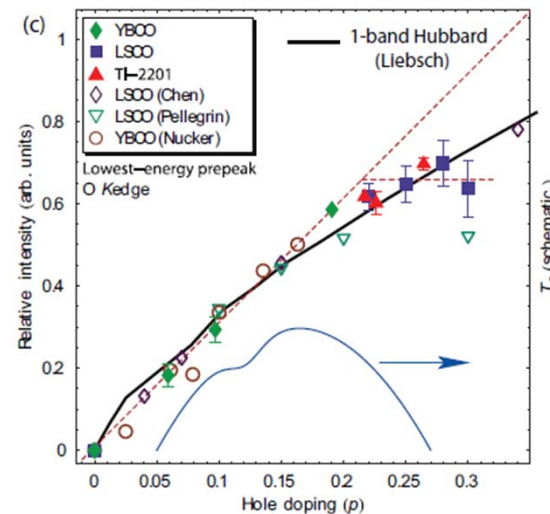


Meinders *et al.* PRB **48**, 3916 (1993)

Experiment: X-Ray absorption



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



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

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

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

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

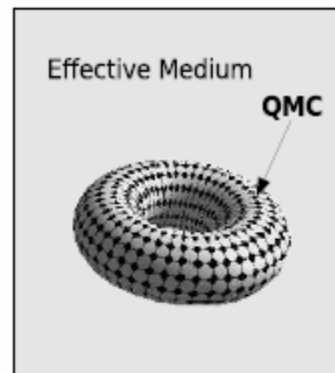
Outline

- Method
- Finite T phase diagram
 - Normal state (no LRO, what is below the dome)
 - First order transition
 - Widom line and pseudogap
 - Superconductivity

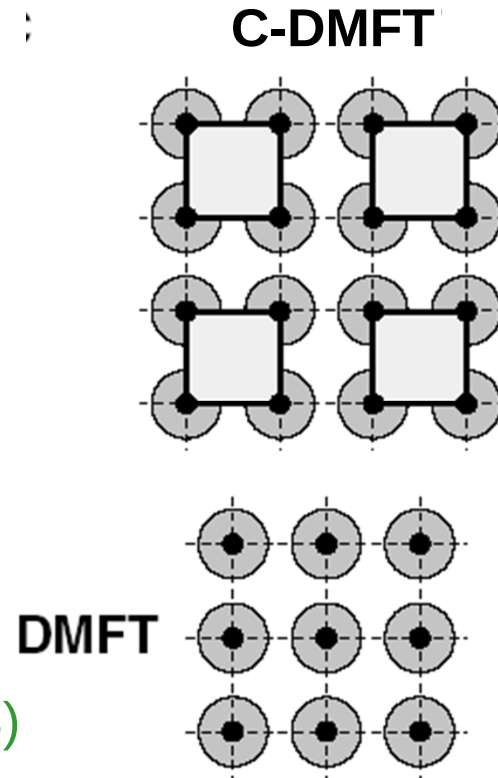


Method

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)



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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 $H_0(\mathbf{t}')$

+ 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



Finite T phase diagram

Normal state of the cuprates





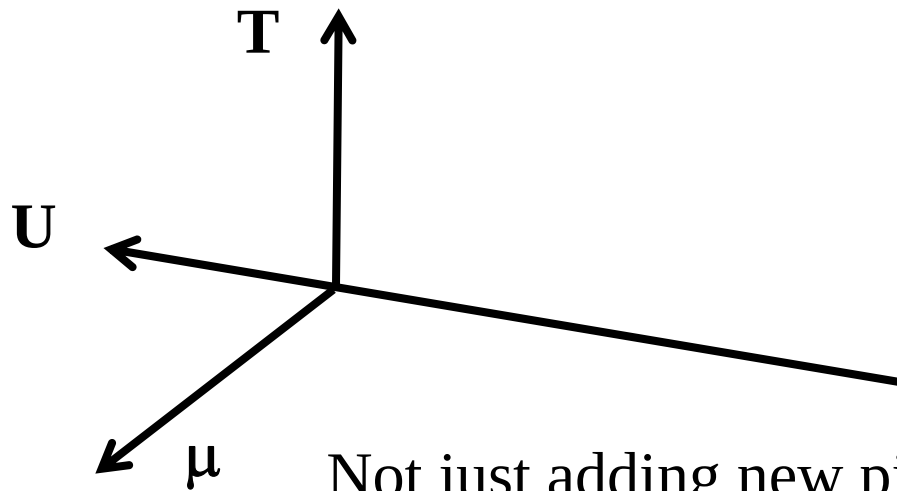
Giovanni Sordi

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

and

Phys. Rev. B. **84**, 075161 (2011)

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



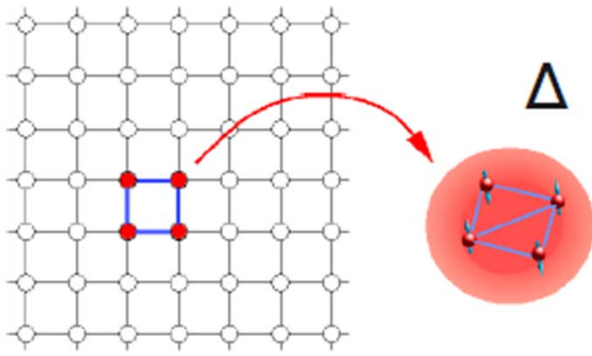
Kristjan Haule

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



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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

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

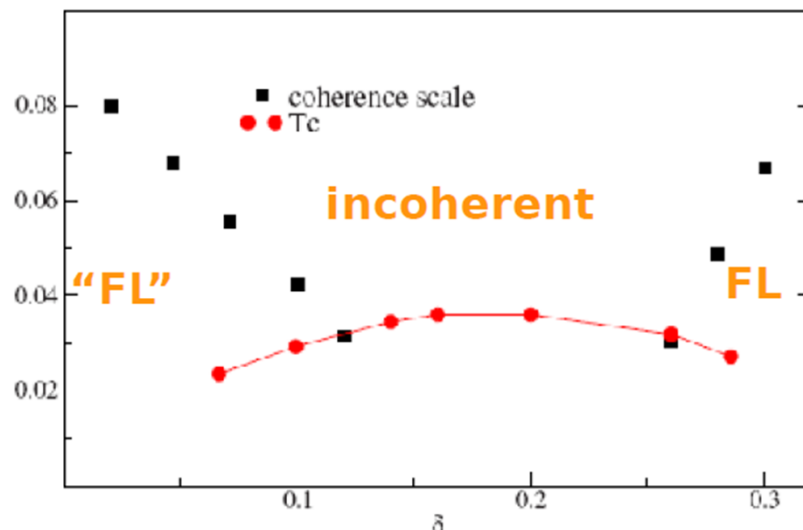
Continuous-time Quantum Monte Carlo calculations to sum all diagrams generated from expansion in powers of hybridization.

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

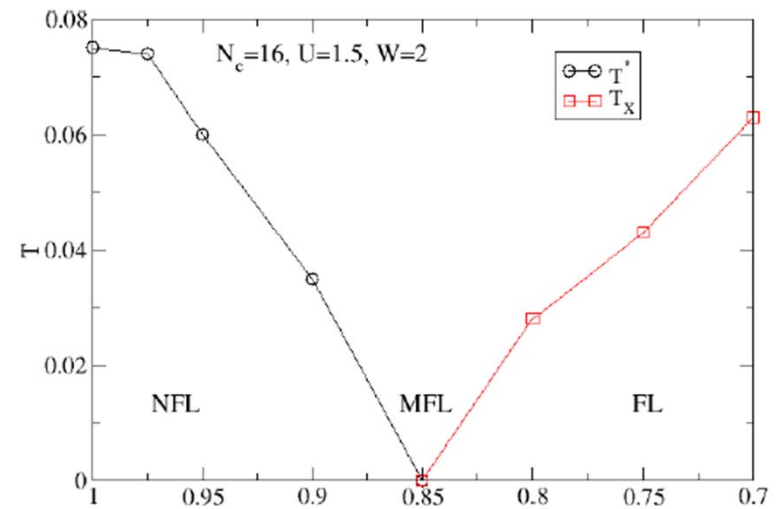
K. Haule, Phys. Rev. B **75**, 155113 (2007).

Doping driven Mott transition, $t' = 0$

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

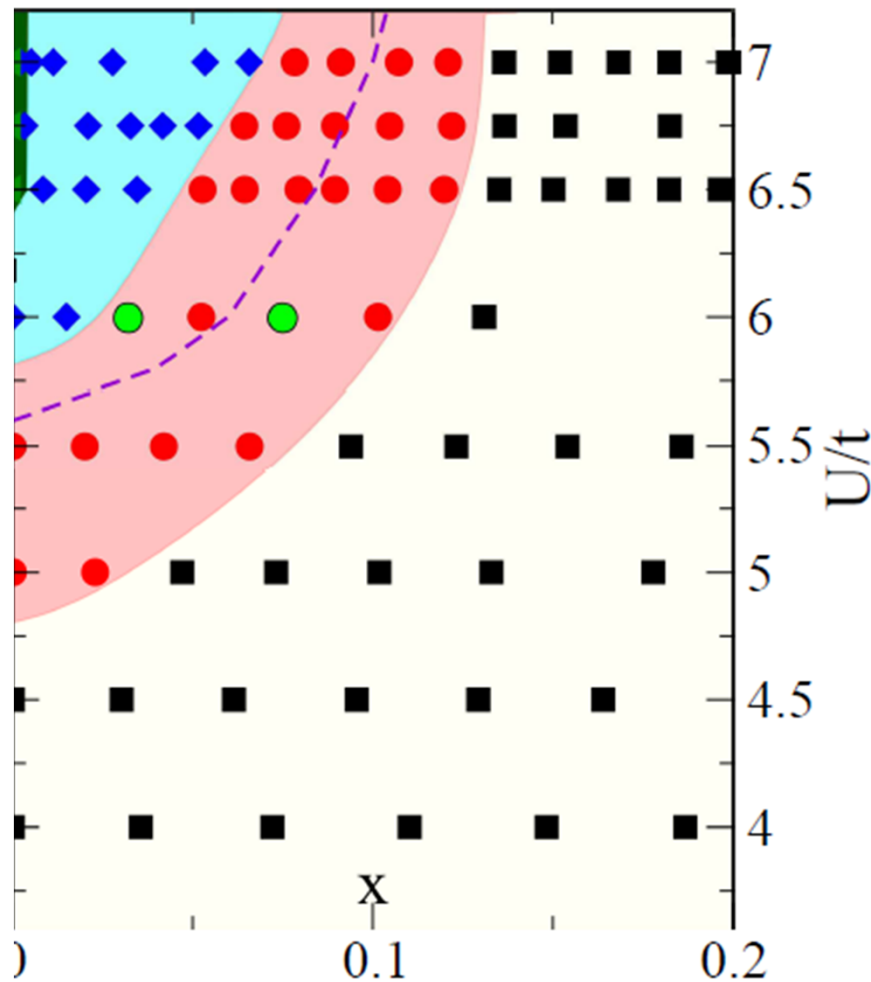


K. Haule, G. Kotliar, PRB (2007)



Vildhyadhiraja, PRL (2009)

Doping driven Mott transition



$$T = 0.25 t$$

Gull, Parcollet, Millis
arXiv:1207.2490v1

Gull, Werner, Millis, (2009)

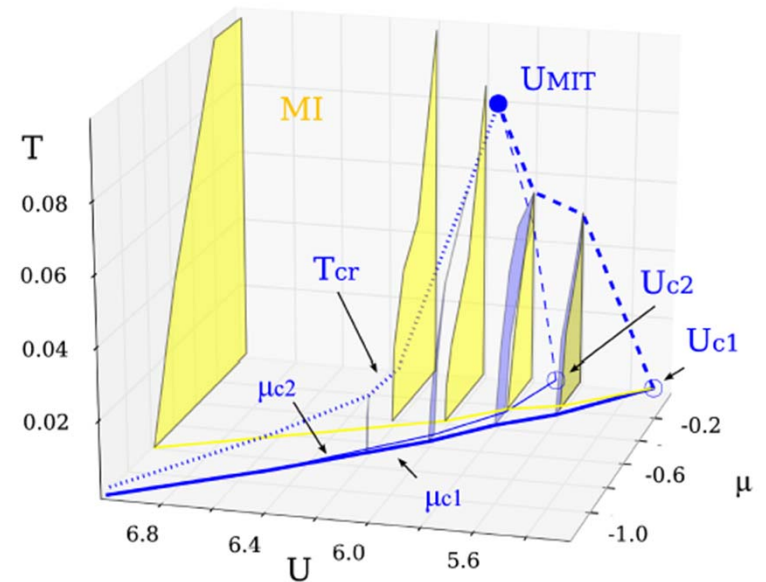
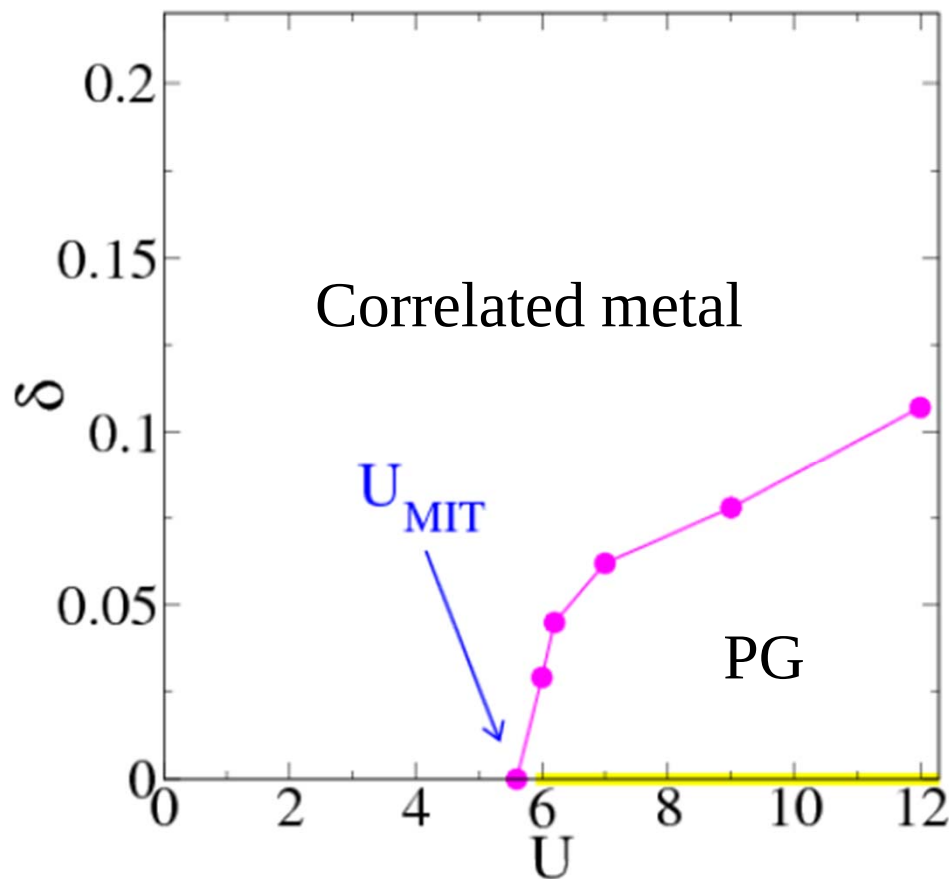
E. Gull, M. Ferrero, O. Parcollet, A. Georges, and A. J. Millis (2010)



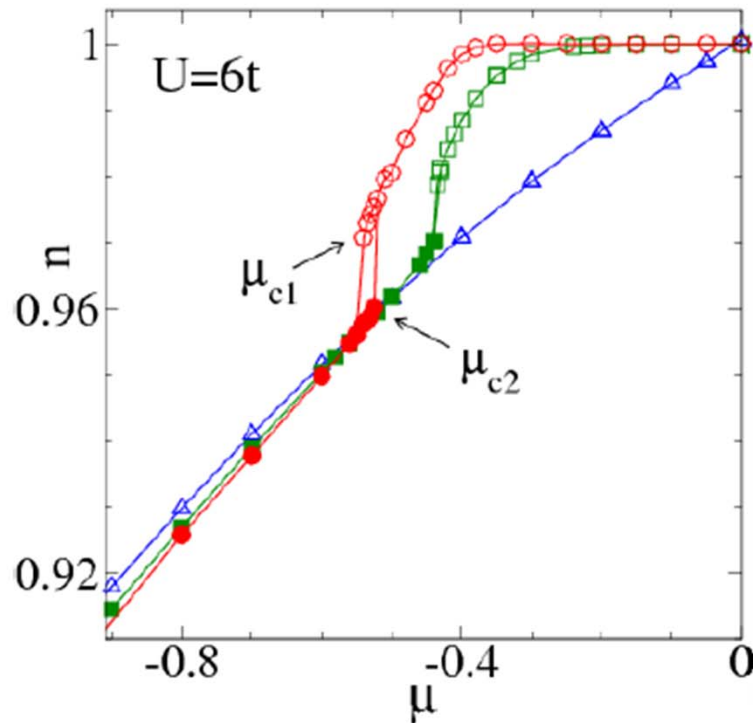
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Link to Mott transition up to optimal doping

Doping dependence of critical point as a function of U



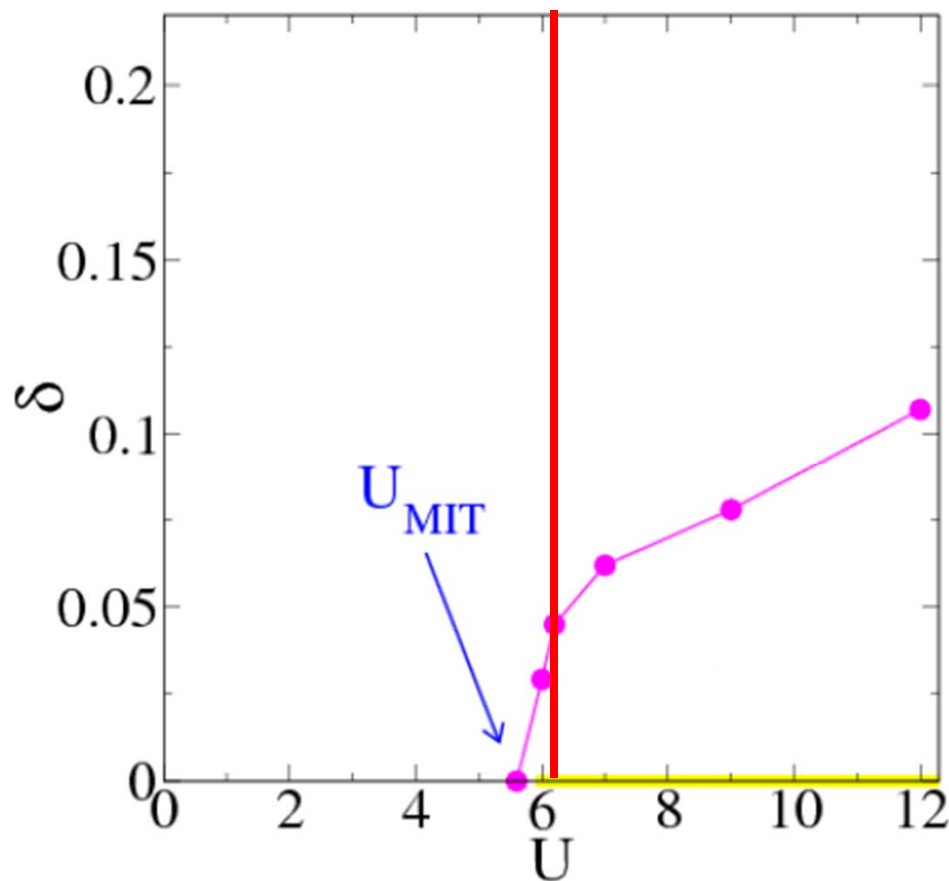
First order transition at finite doping



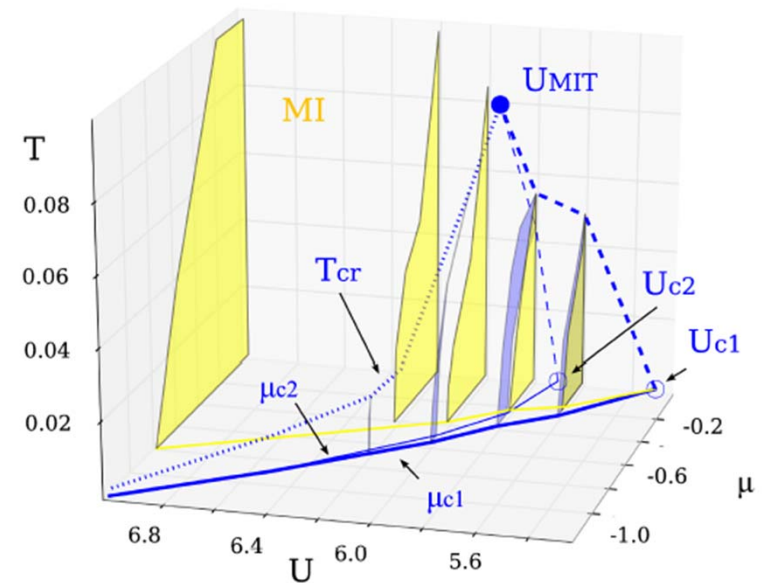
$n(\mu)$ for several temperatures:
 $T/t = 1/10$, $1/25$, $1/50$

Link to Mott transition up to optimal doping

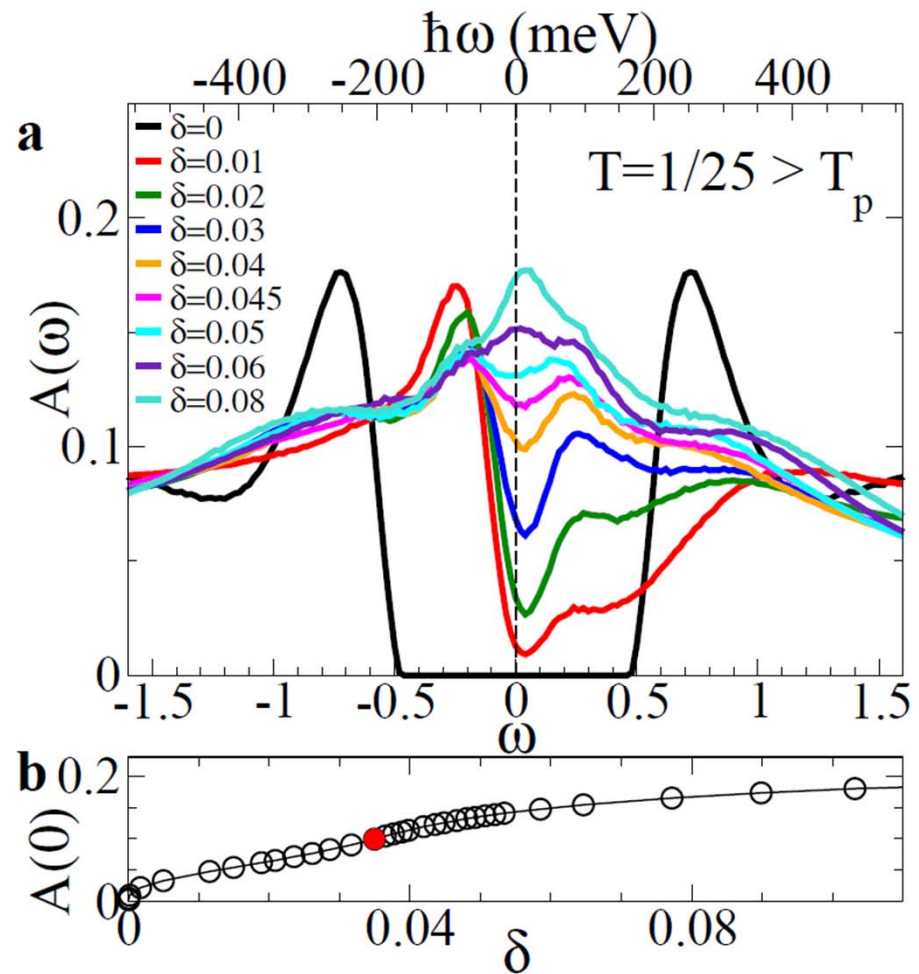
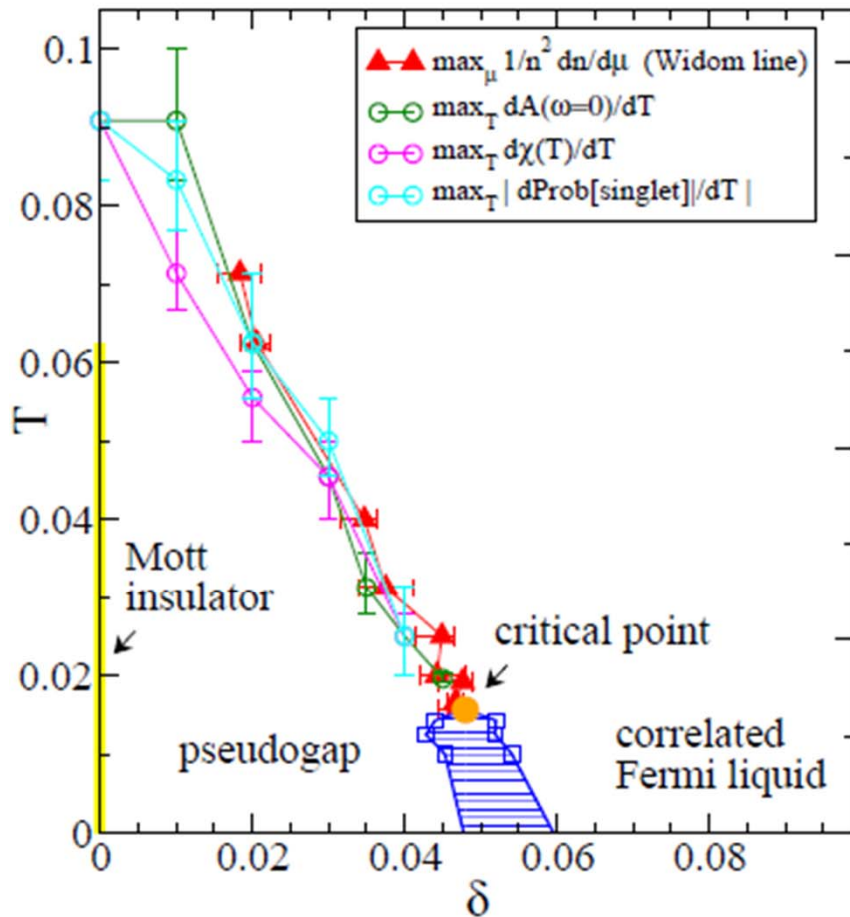
Doping dependence of critical point as a function of U



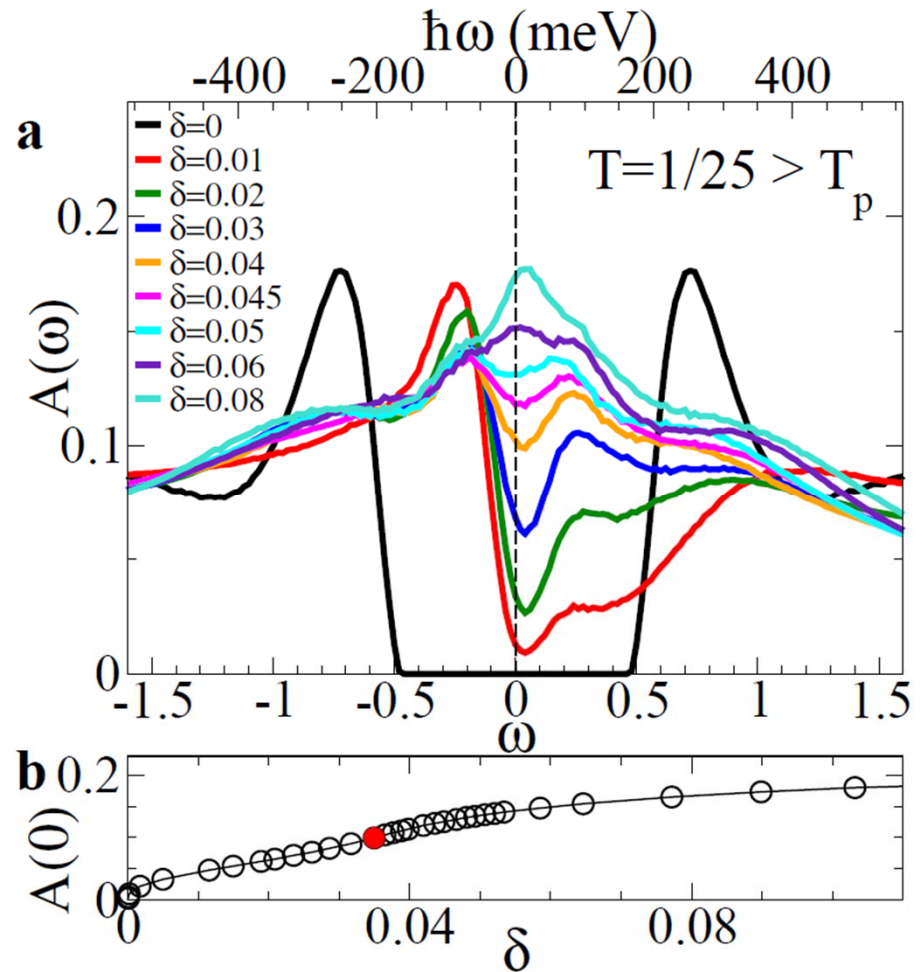
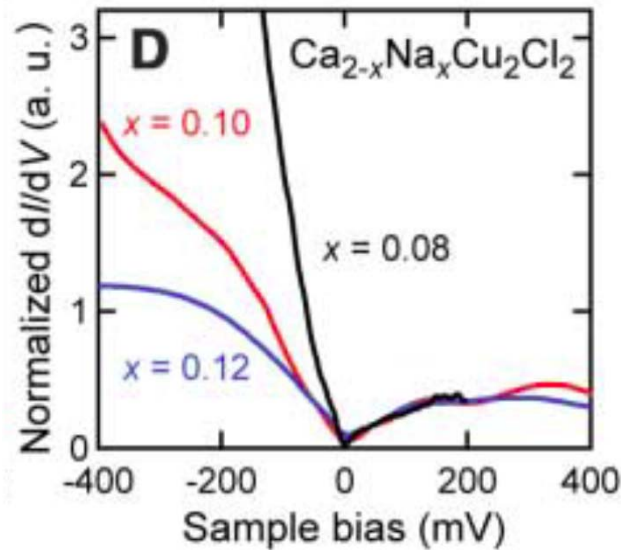
Smaller D and S



Density of states

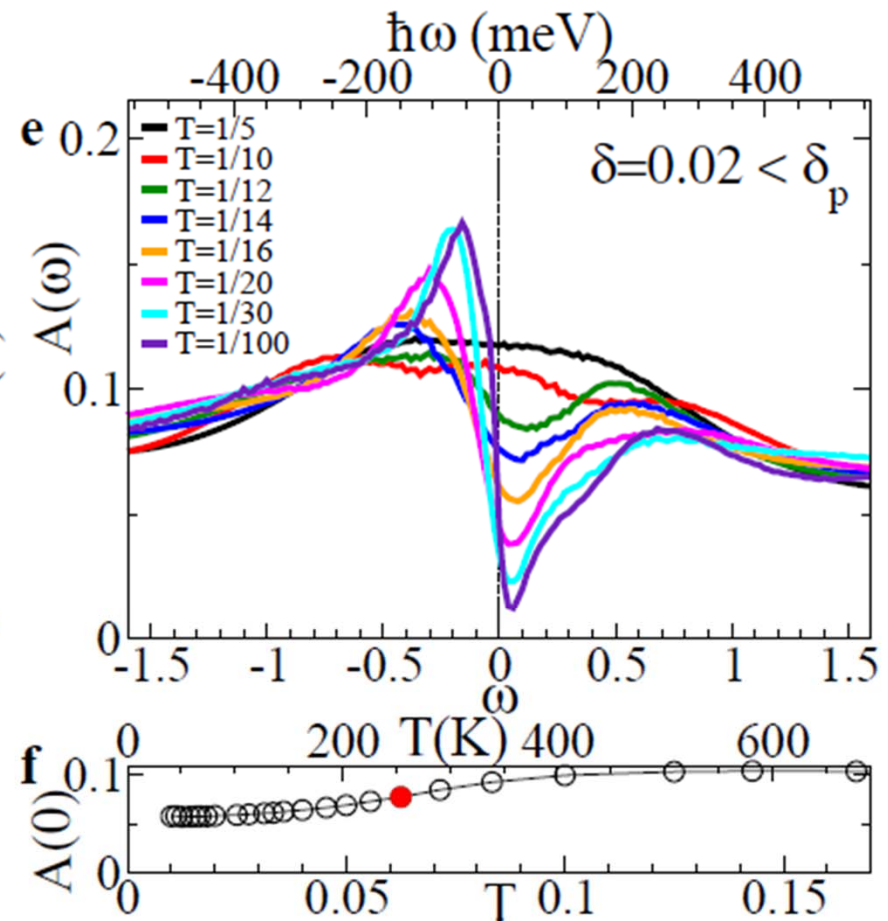
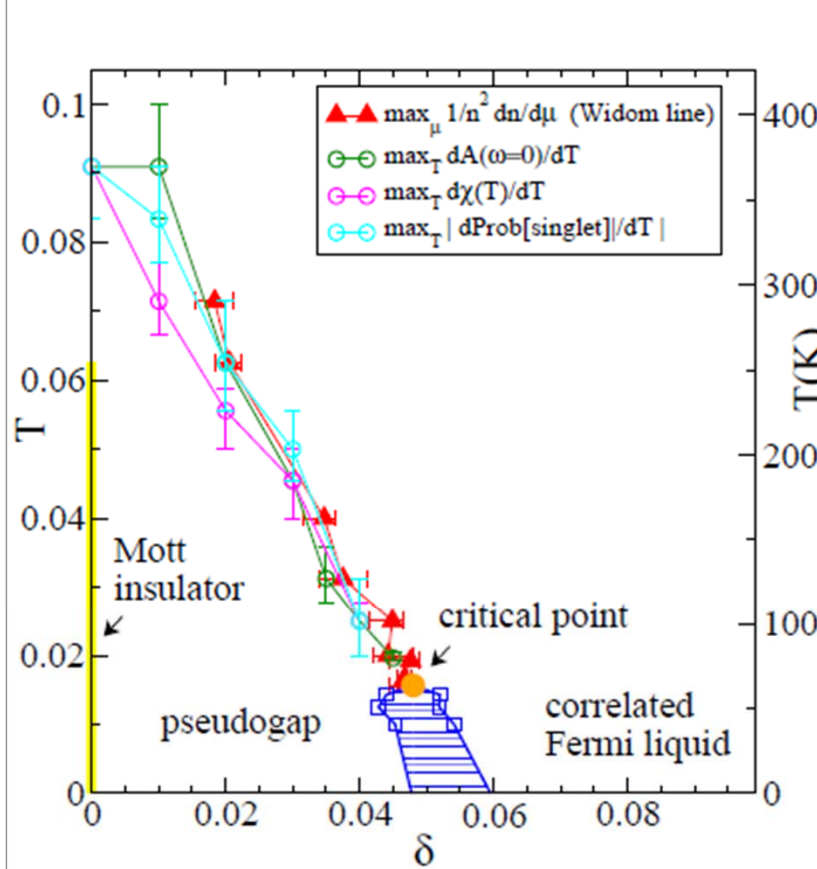


Density of states

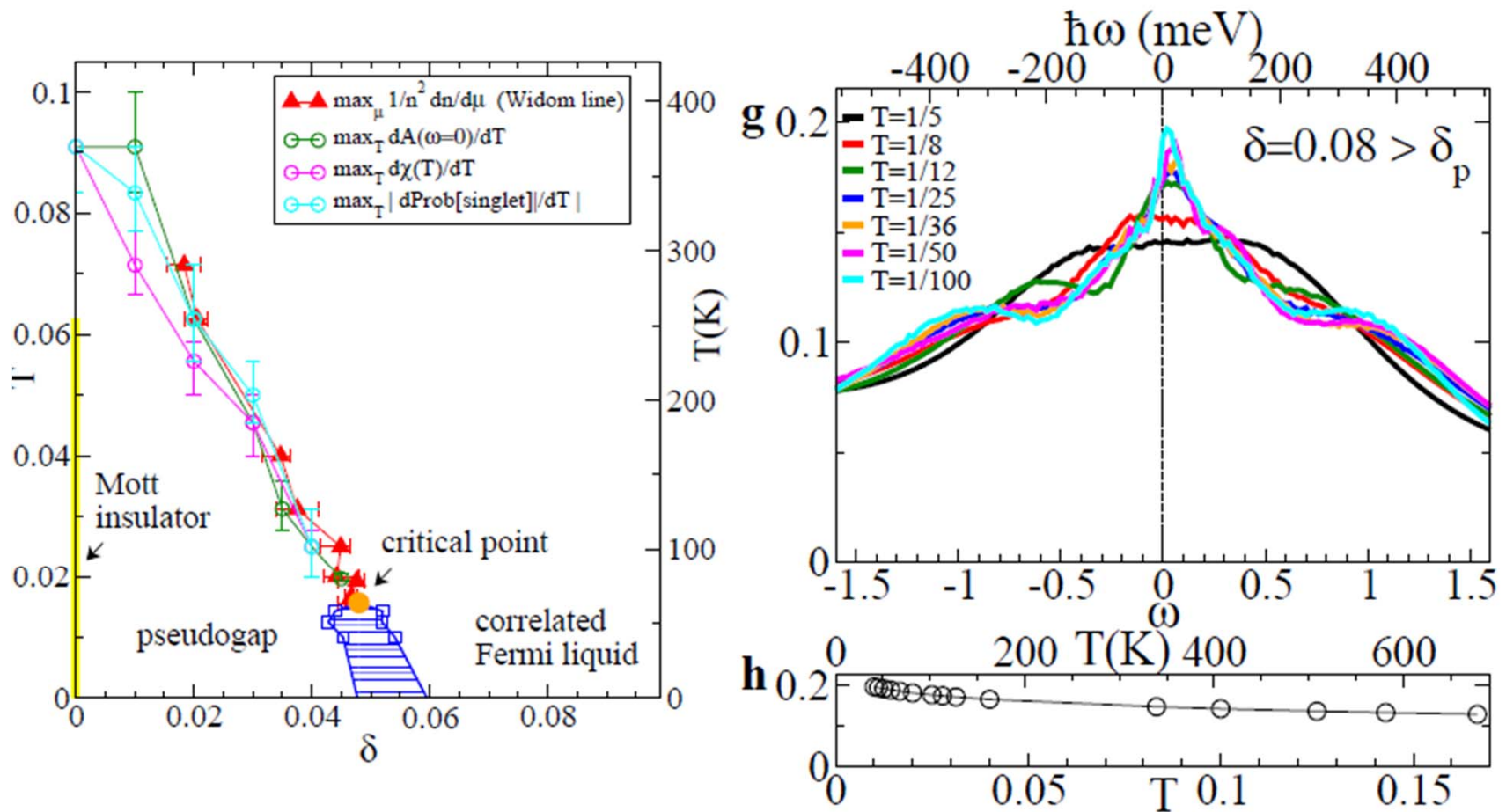


Khosaka et al. *Science* **315**, 1380 (2007);

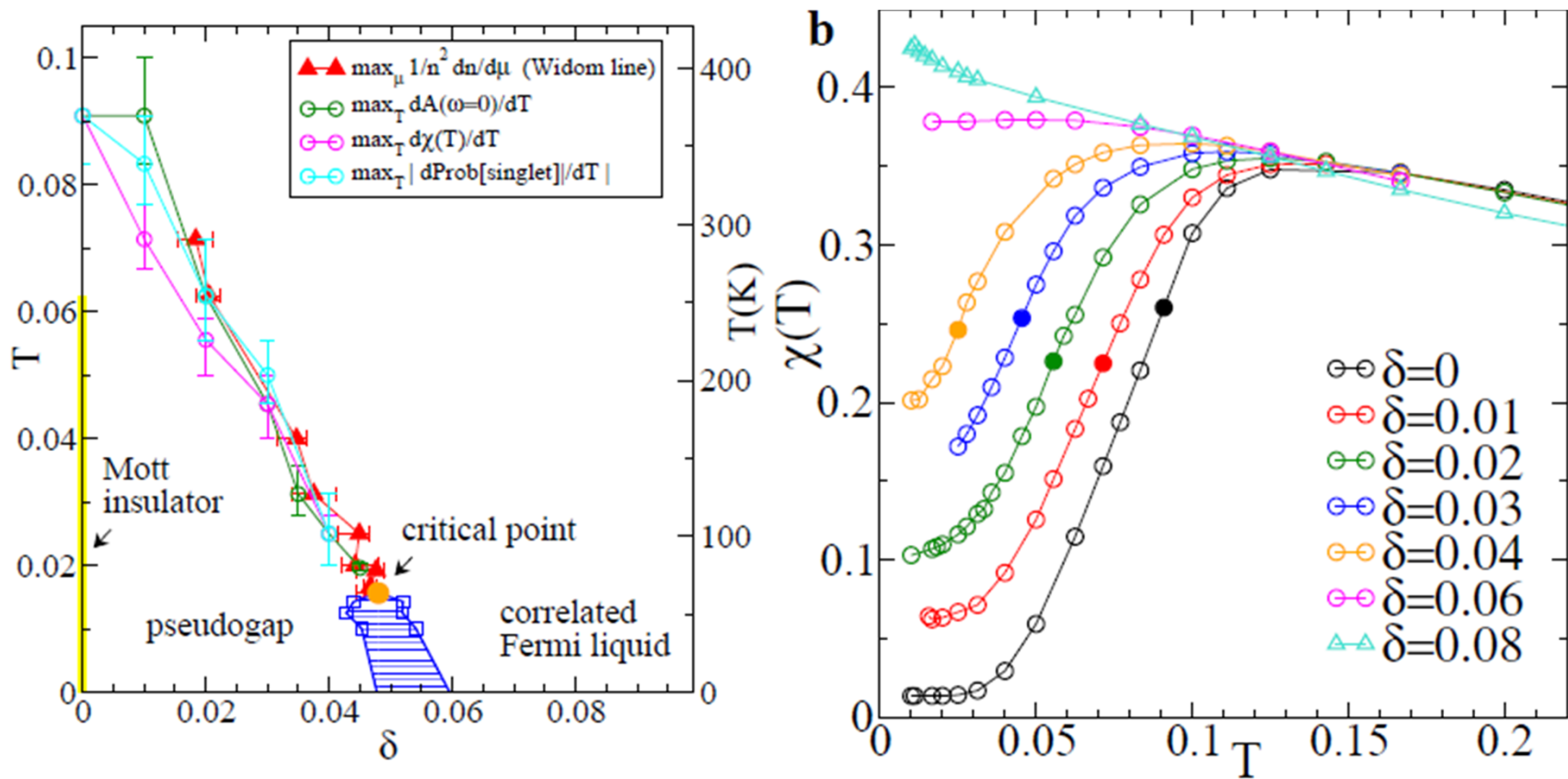
Density of states



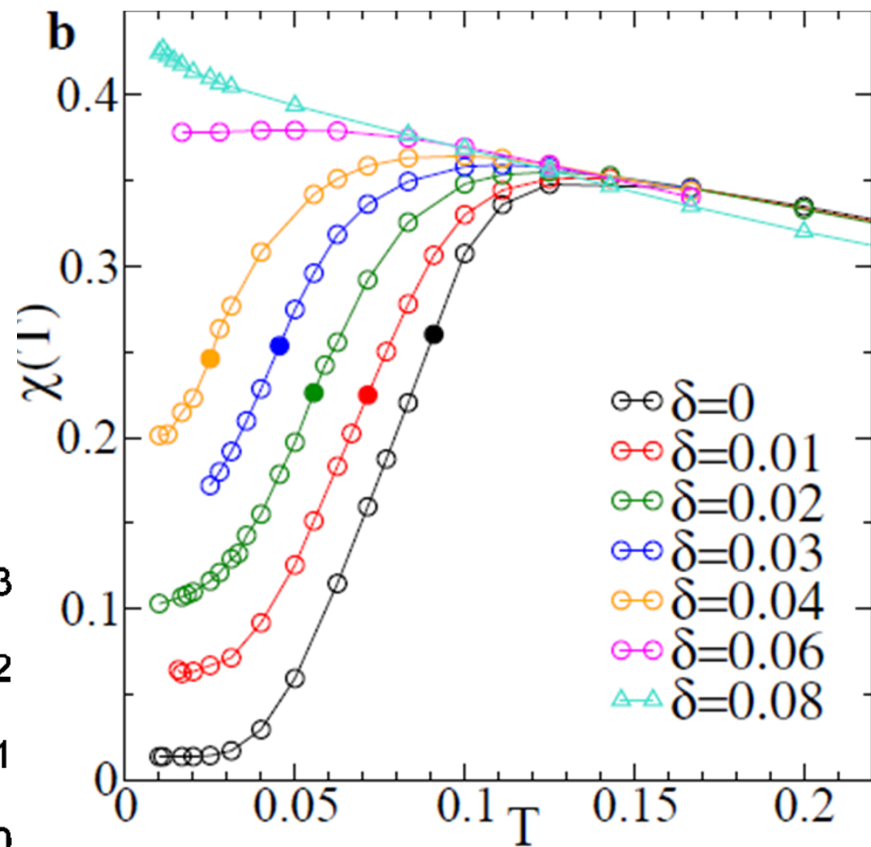
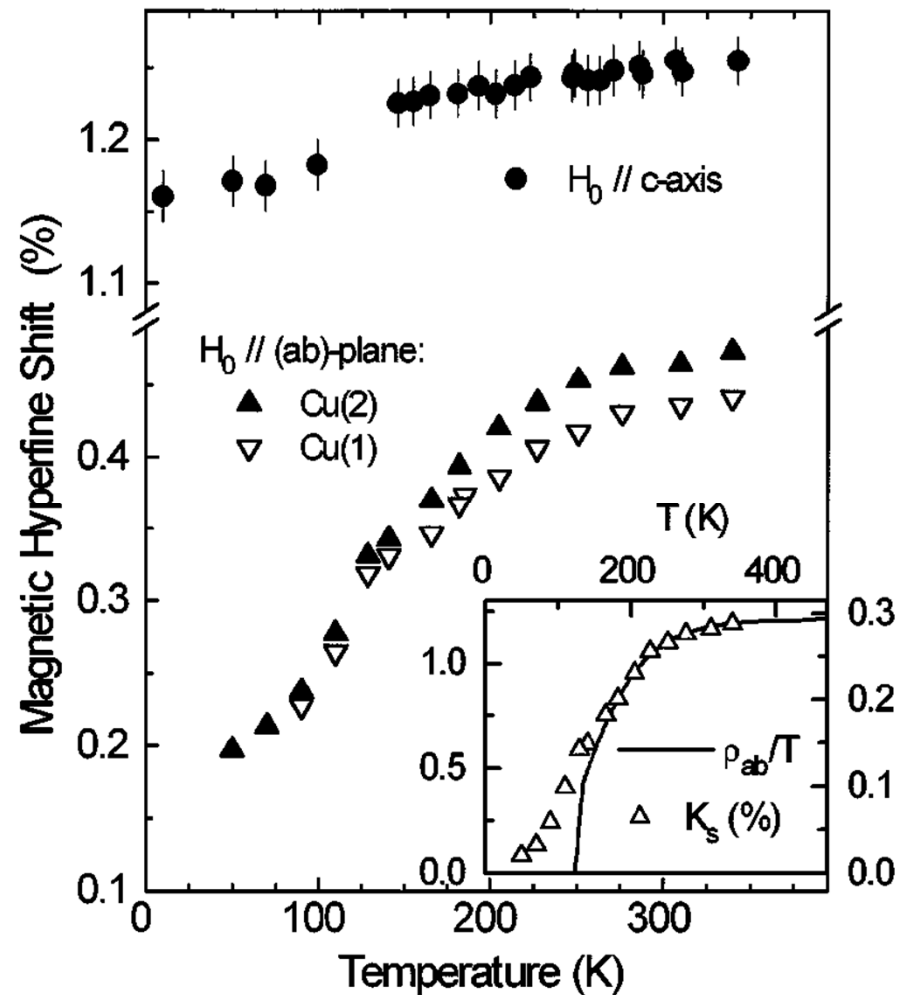
Density of states



Spin susceptibility



Spin susceptibility



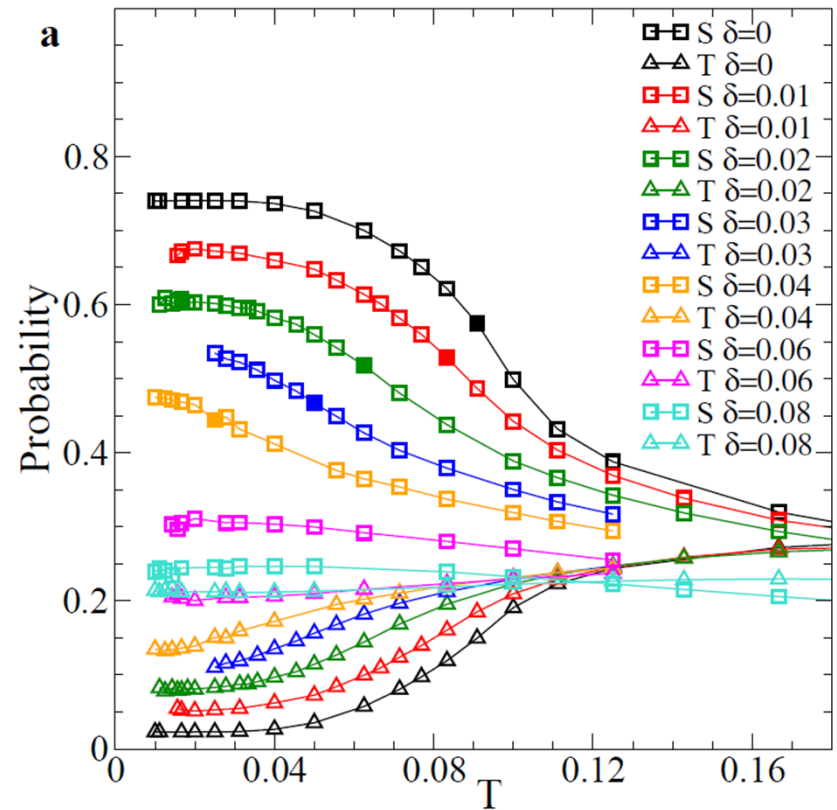
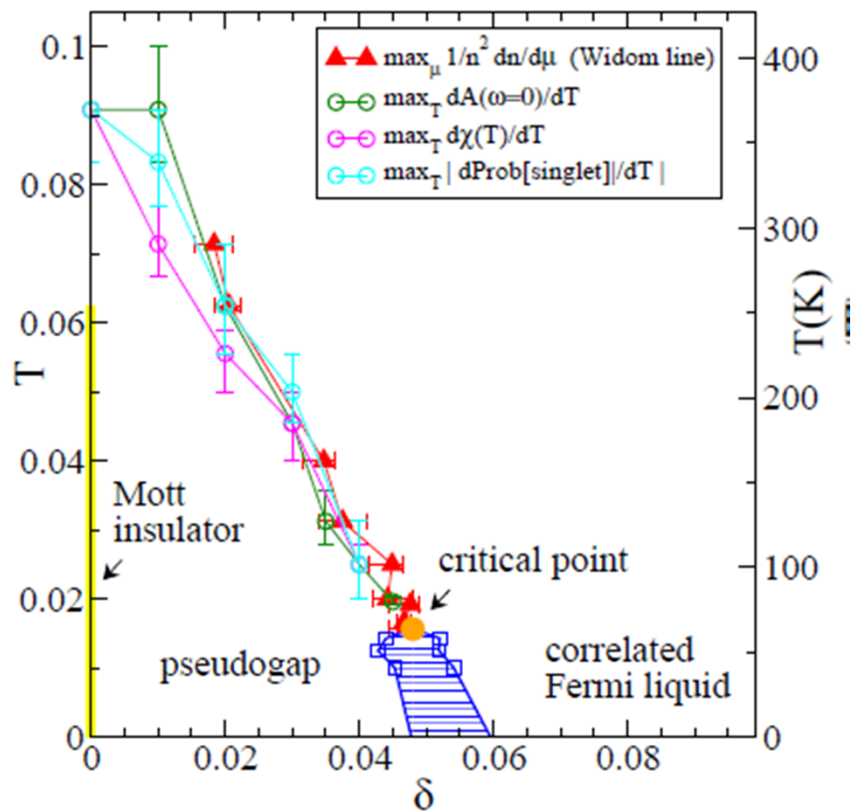
Underdoped Hg1223

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



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Plaquette eigenstates



What is the minimal model?

H. Alloul arXiv:1302.3473

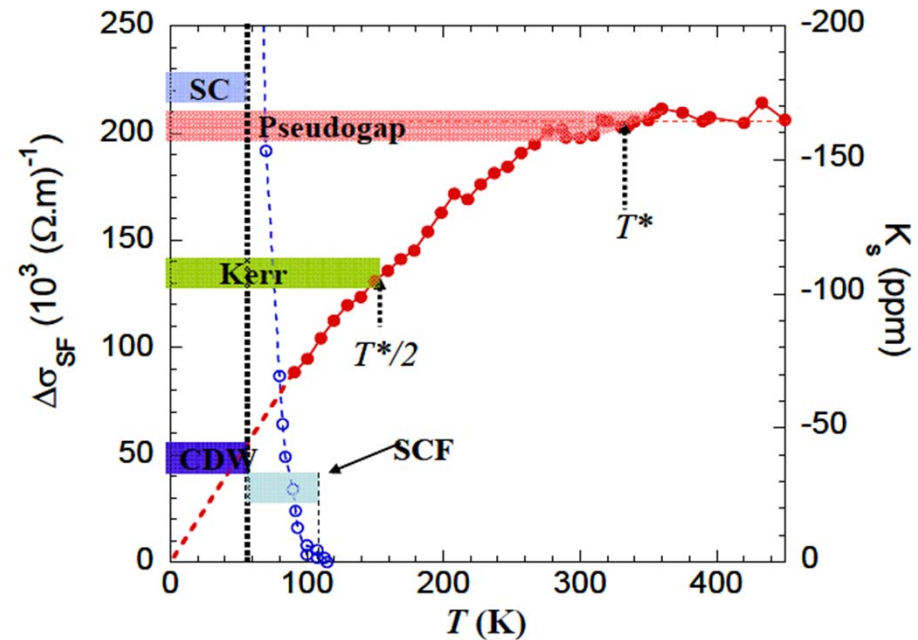
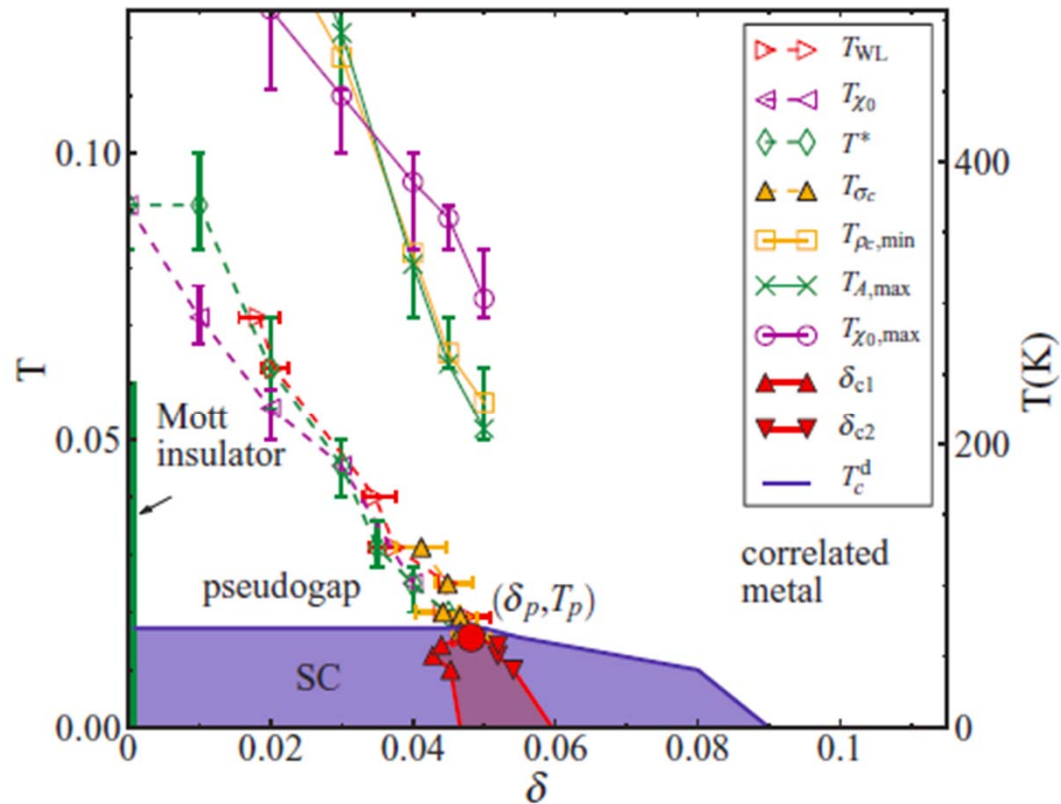


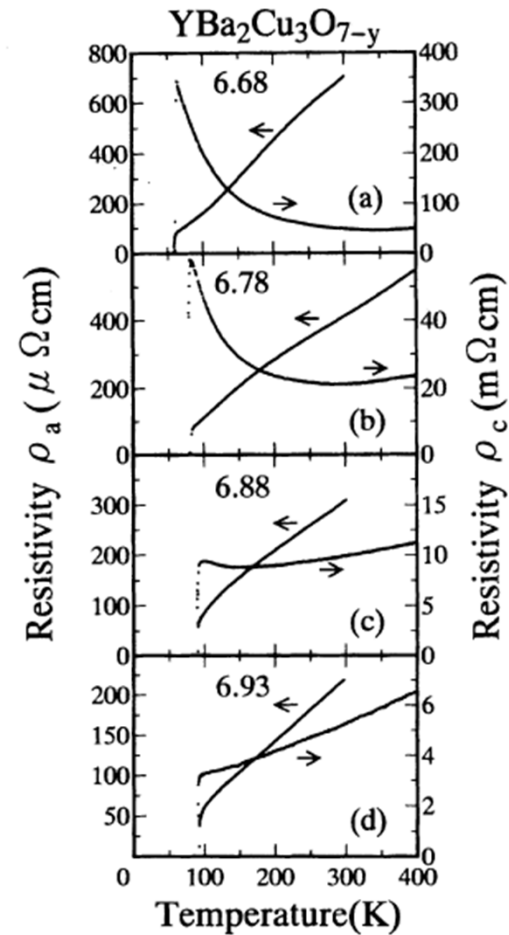
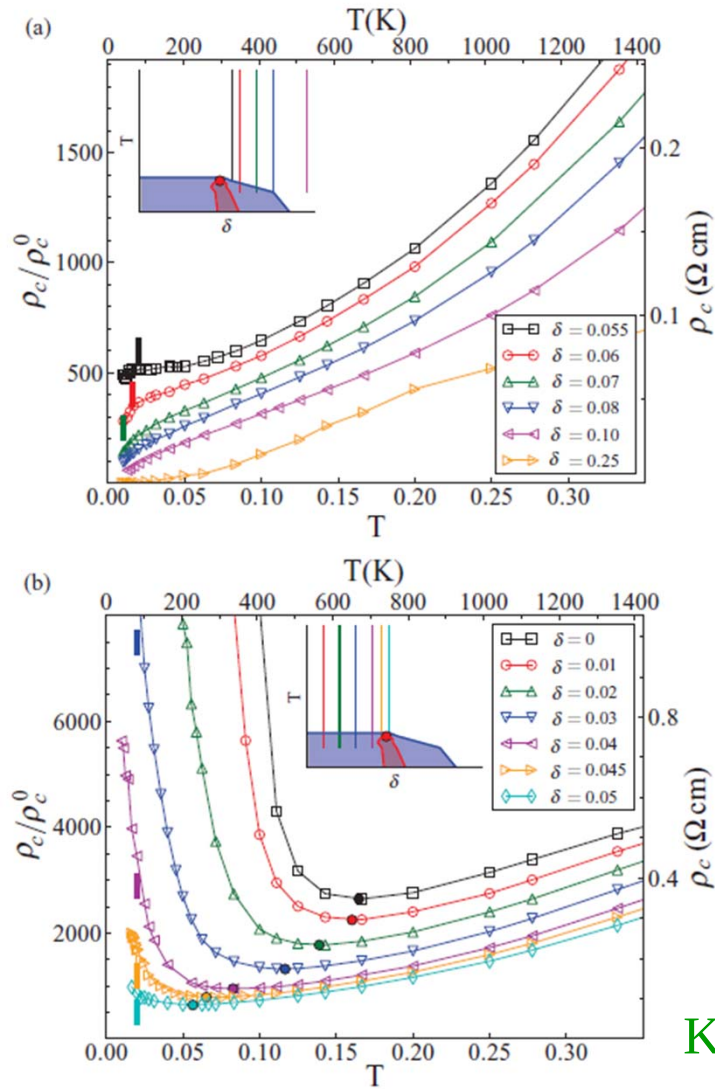
Fig 1 Spin contribution K_s to the ^{89}Y NMR Knight shift [11] for $\text{YBCO}_{6.6}$ permit to define the PG onset T^* . Here K_s is reduced by a factor two at $T \sim T^*/2$. The sharp drop of the SC fluctuation conductivity (SCF) is illustrated (left scale) [23]. We report as well the range over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

Two crossover lines



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

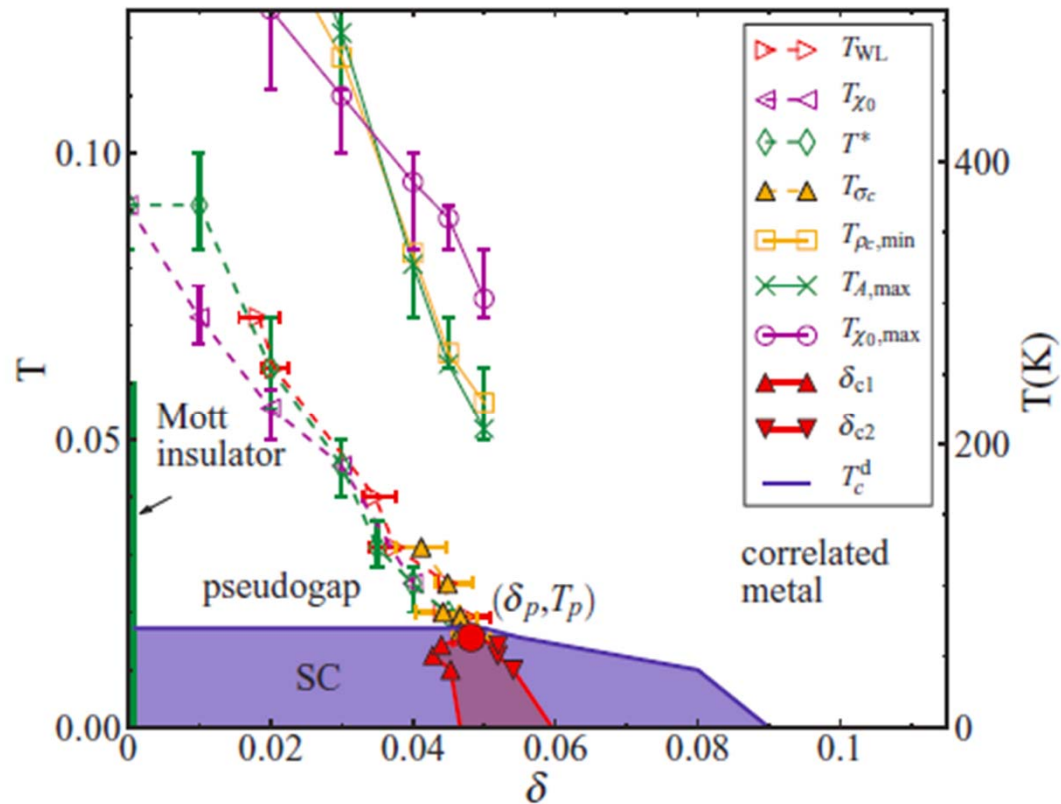
C-axis resistivity



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

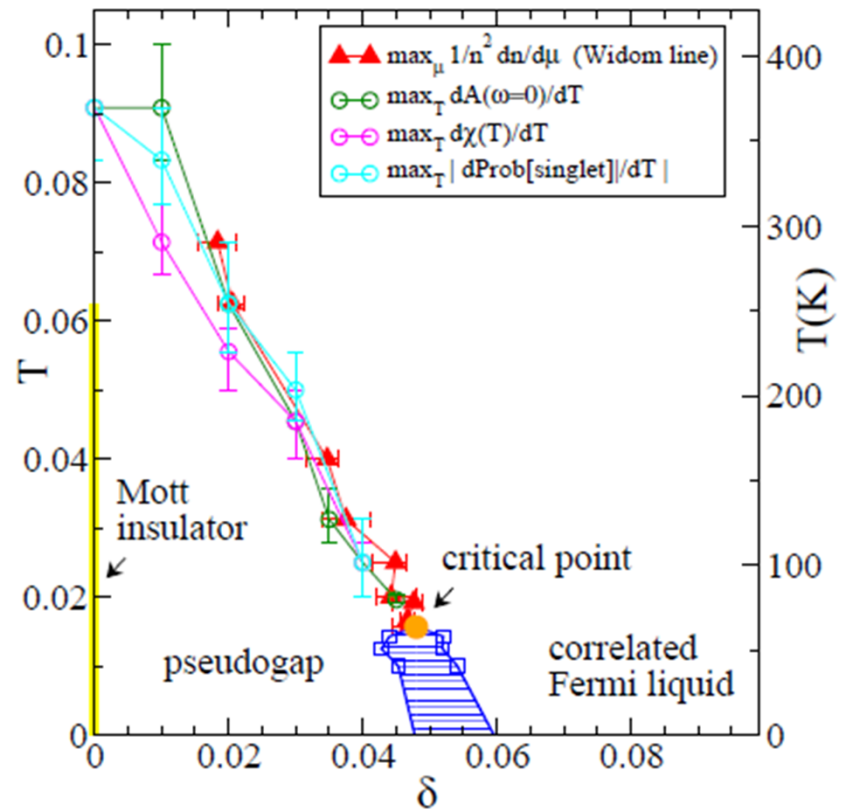


Two crossover lines



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

Pseudogap T^* along the Widom line





Giovanni Sordi



Patrick Sémon



Kristjan Haule

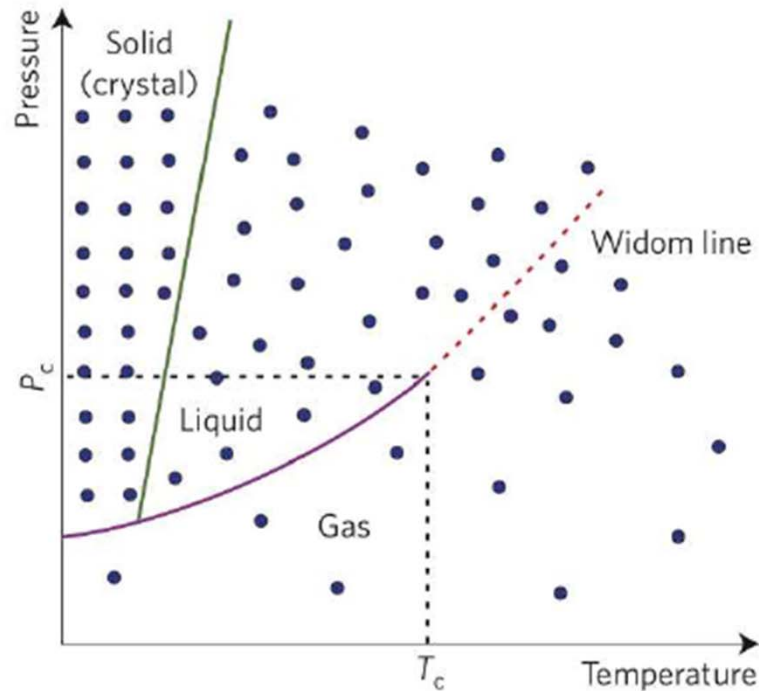
The Wisdom line

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



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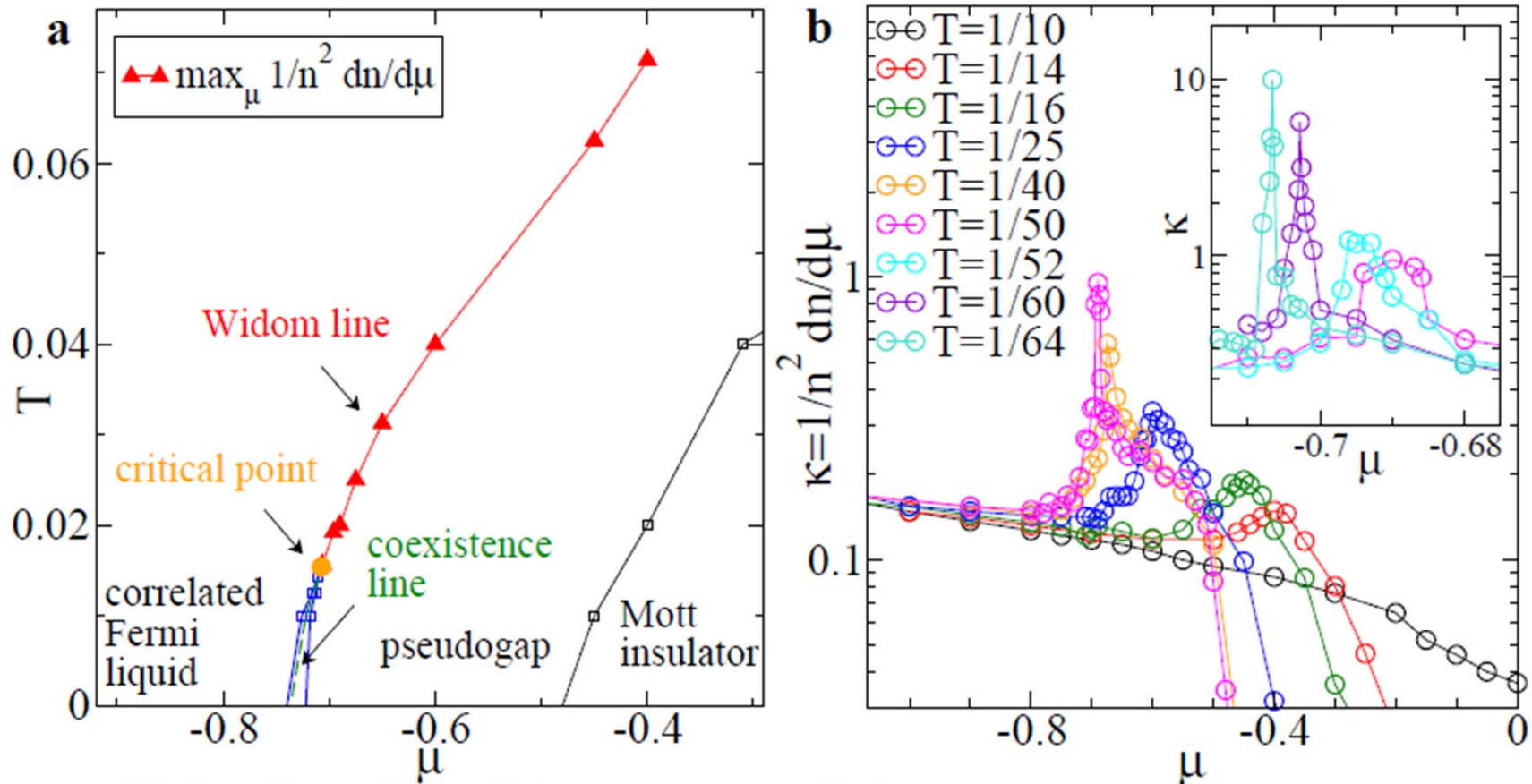
What is the Widom line?



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 $T \rightarrow T_p$
- ▶ 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

Pseudogap T^* along the Widom line

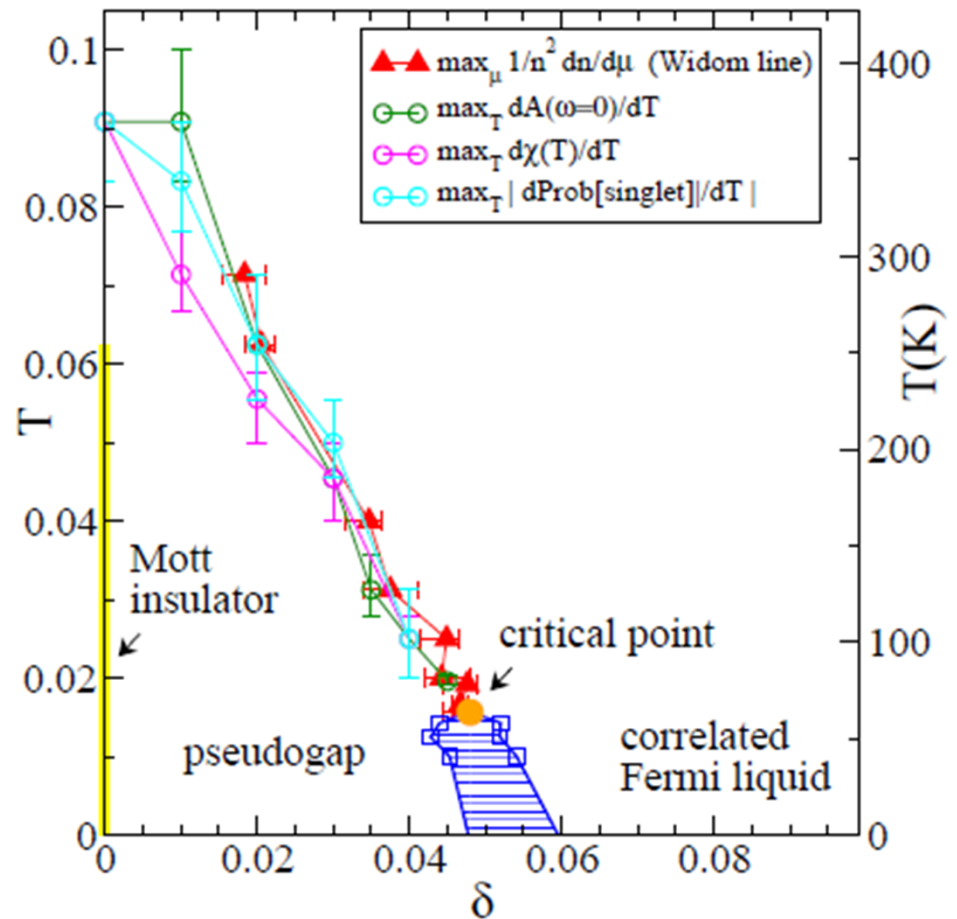


Widom line: defined from maxima of charge compressibility

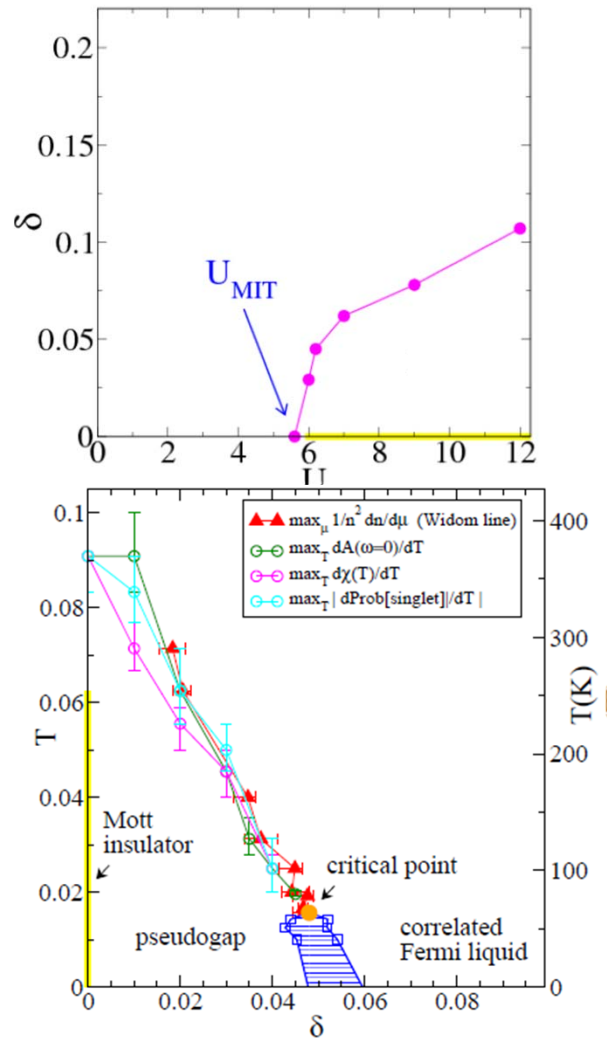
$$\kappa = 1/n^2 (dn/d\mu)_T$$

divergence of κ at the (classical) critical point!

Phase diagram



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

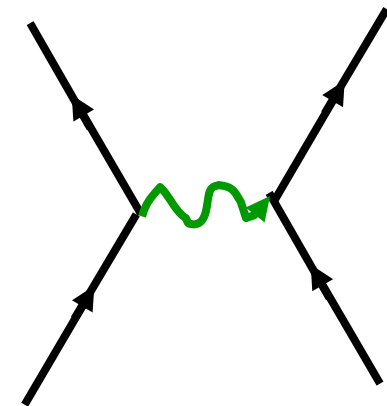
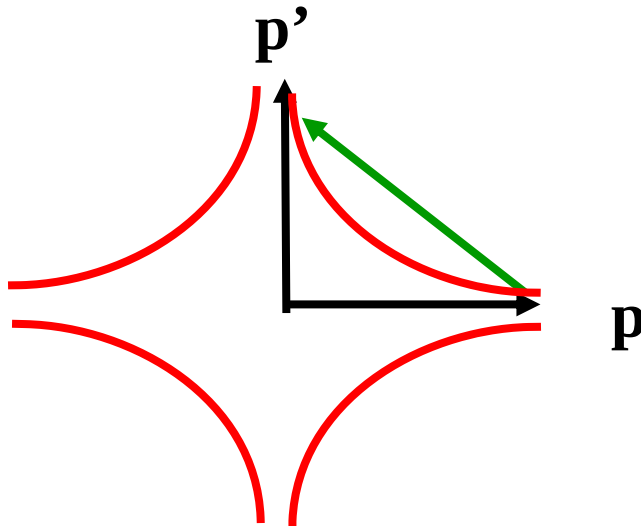
Sordi et al. PRL **108**, 216401 (2012)



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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)



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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

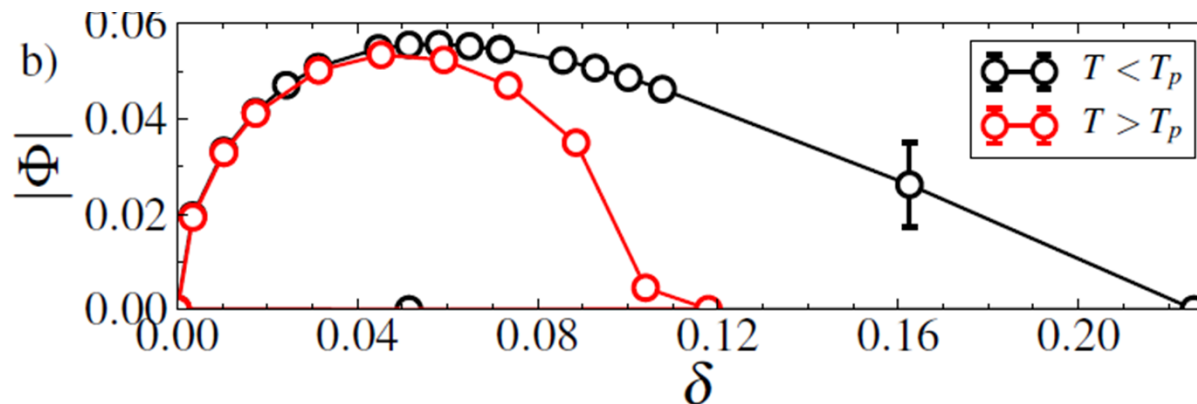
Miyake, Schmitt–Rink, and Varma
P.R. B **34**, 6554-6556 (1986)





Giovanni Sordi

Cuprates (doping driven transition)



Patrick Sémon



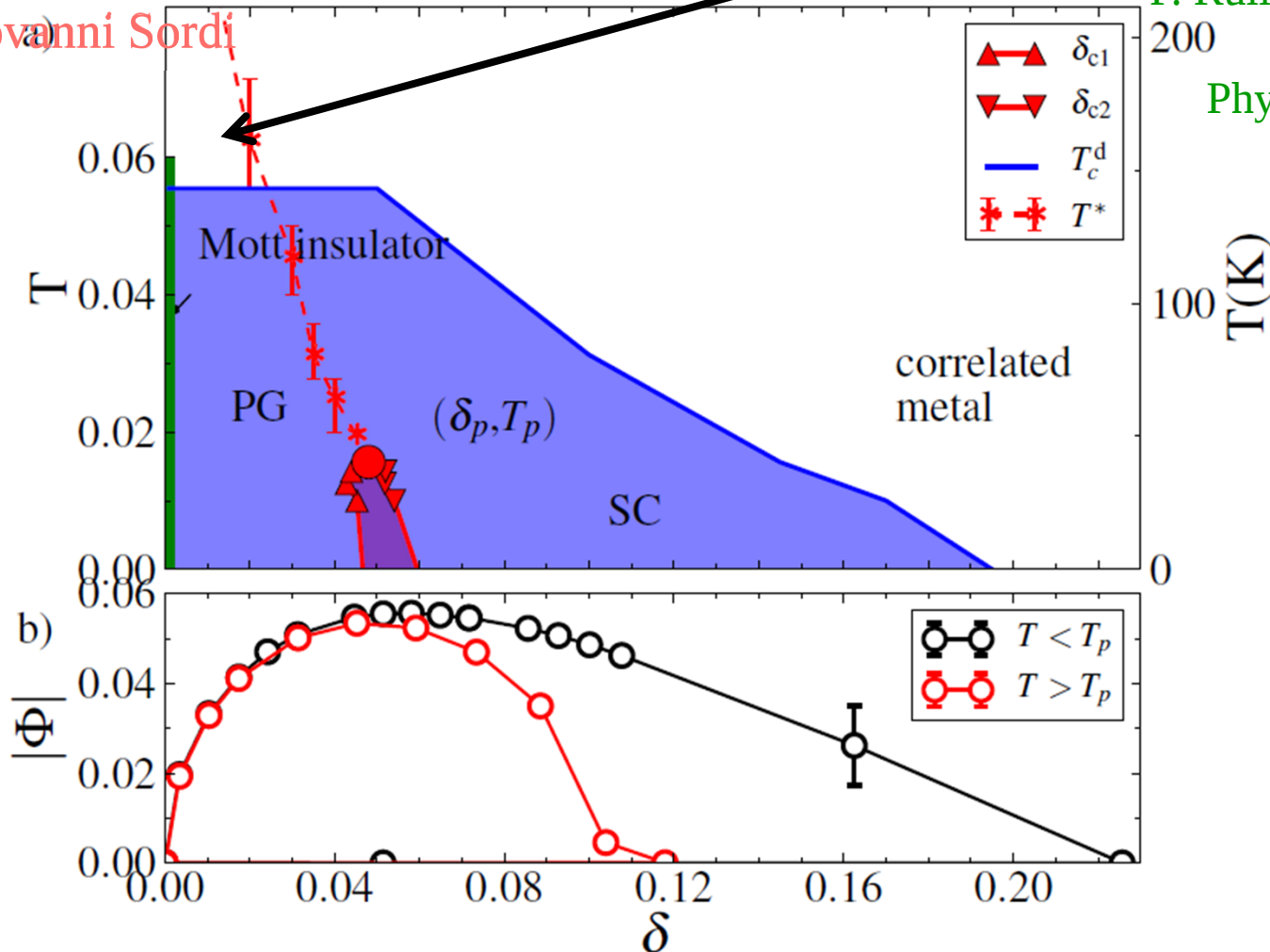


Cuprates (doping driven transition)

Pseudogap vs pair

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

Giovanni Sordi

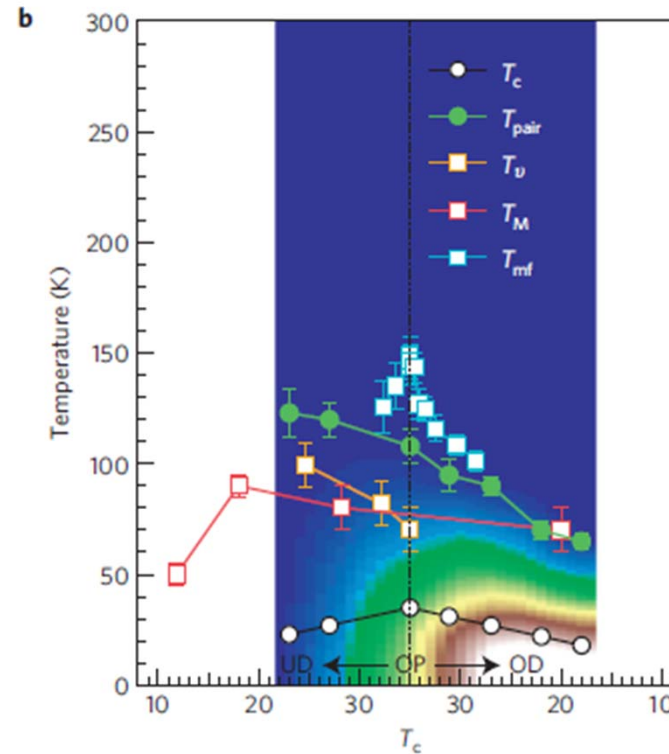


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T_{pair}



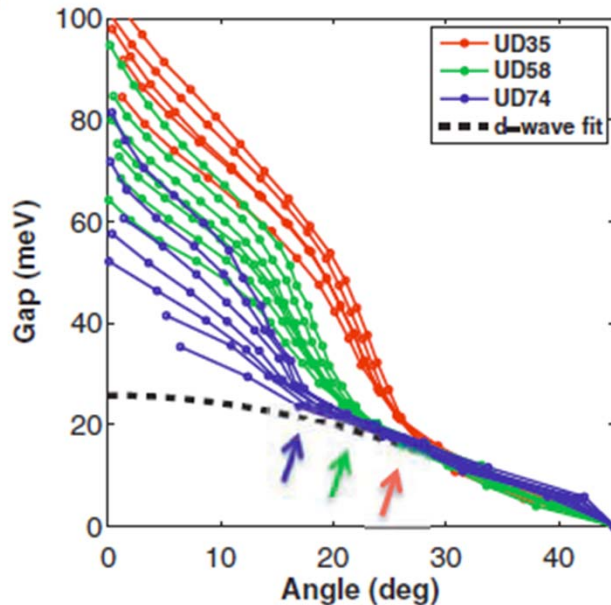
ARPES
Bi2212

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



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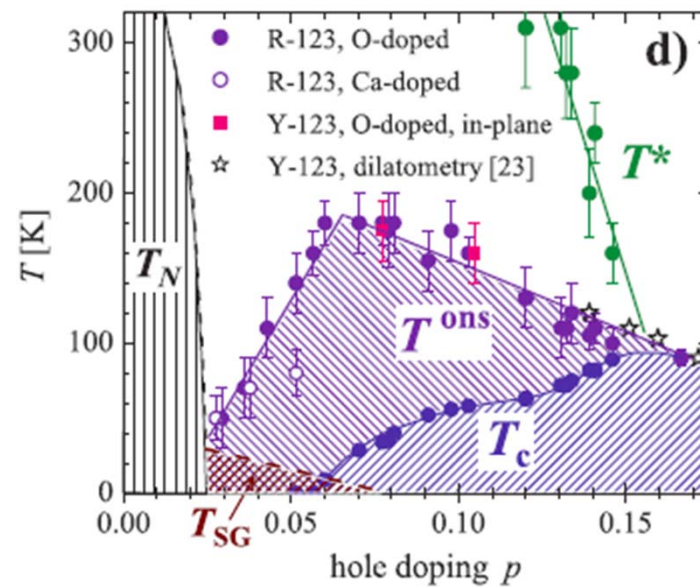
Meaning of T_c^d : Local pair formation



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.

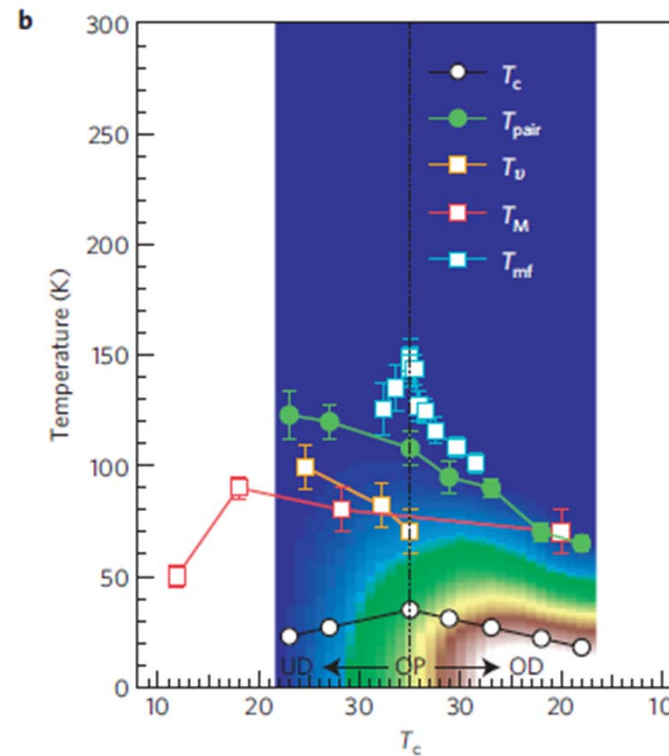
Fluctuating region



Infrared response

Dubroka et al. PRL 106, 047006 (2011)

T_{pair}

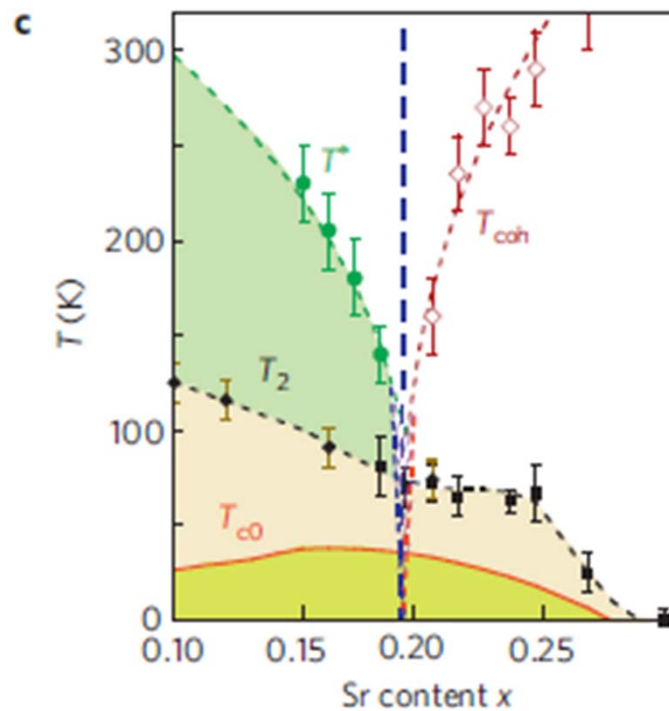


ARPES
Bi2212

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)



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Giant proximity effect

$$T_c = 32 \text{ K}$$
$$T_c < 5 \text{ K}$$

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

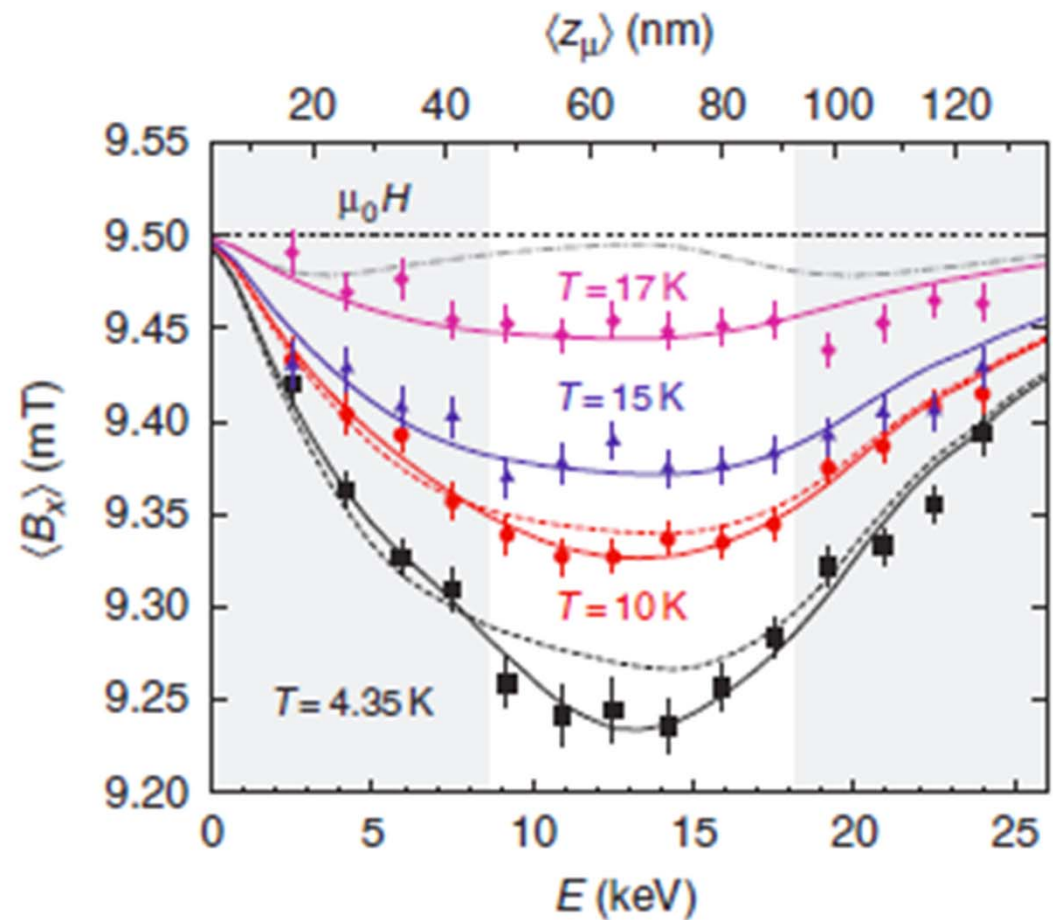


Figure 6 | Depth profile of the local field at different temperatures. The

Actual T_c in underdoped

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



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

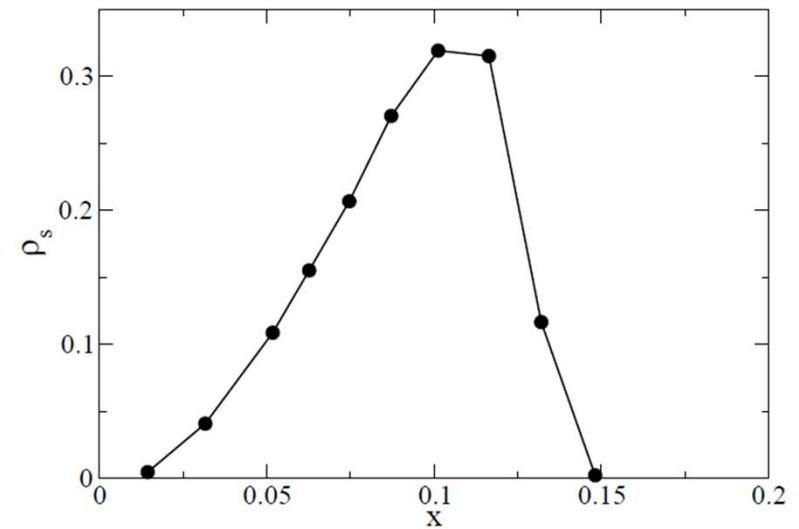
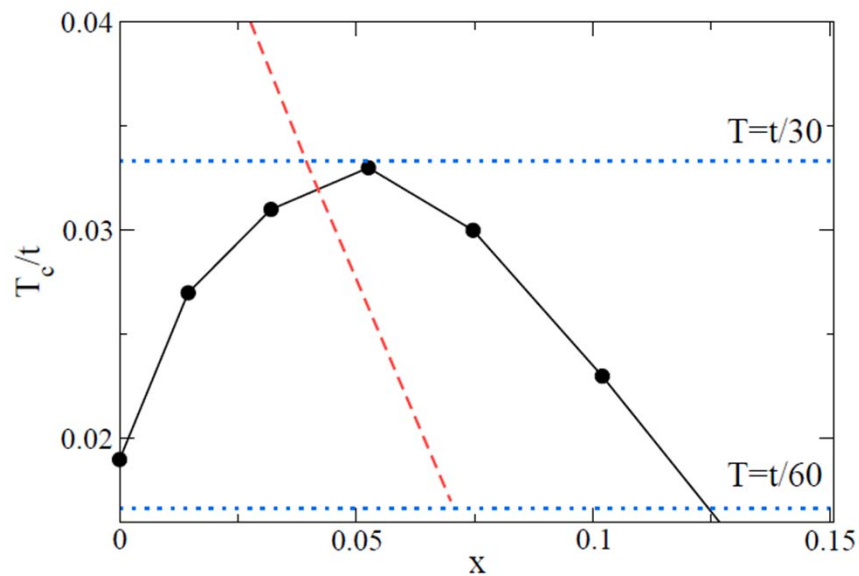
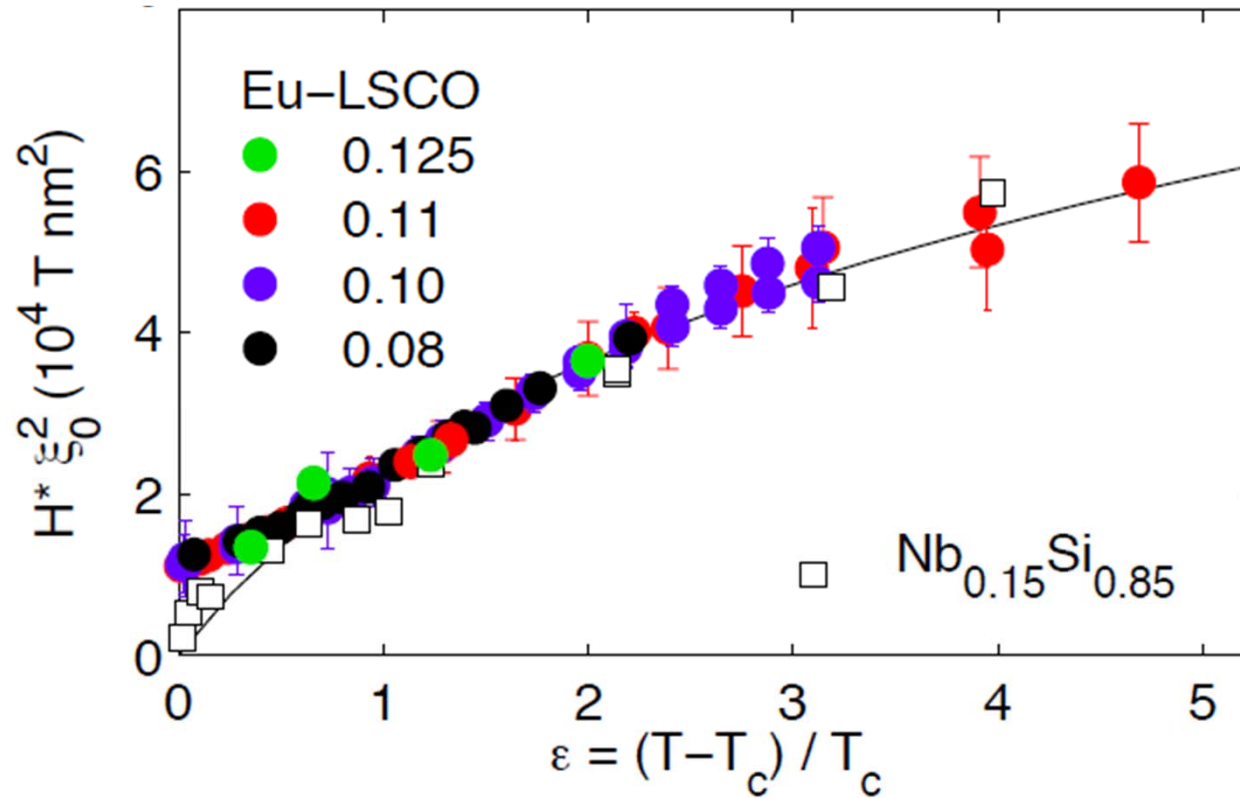


FIG. 8. Superfluid stiffness ρ_s determined in the superconducting state at $T = t/60$ from Eq. 15, as a function of doping.

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

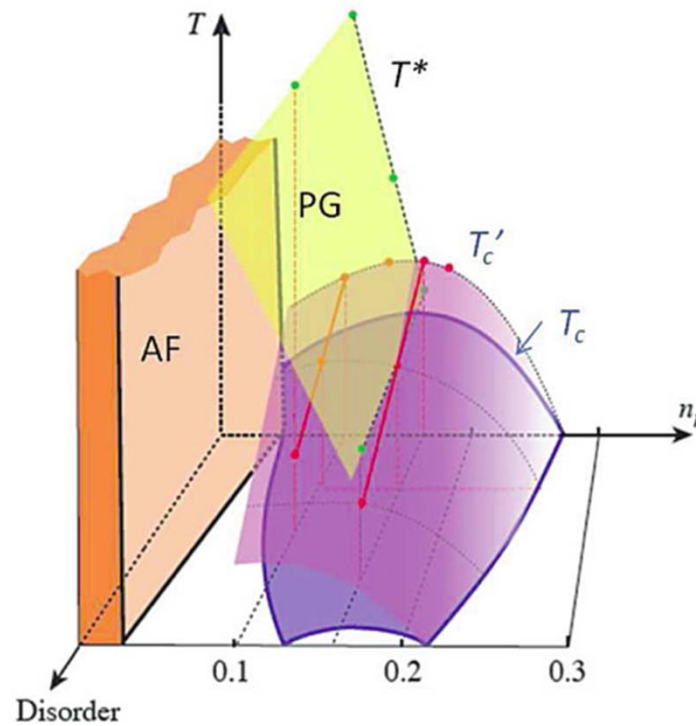


Gaussian amplitude fluctuations in Eu-LSCO



Chang, Doiron-Leyraud et al.

Effect of disorder

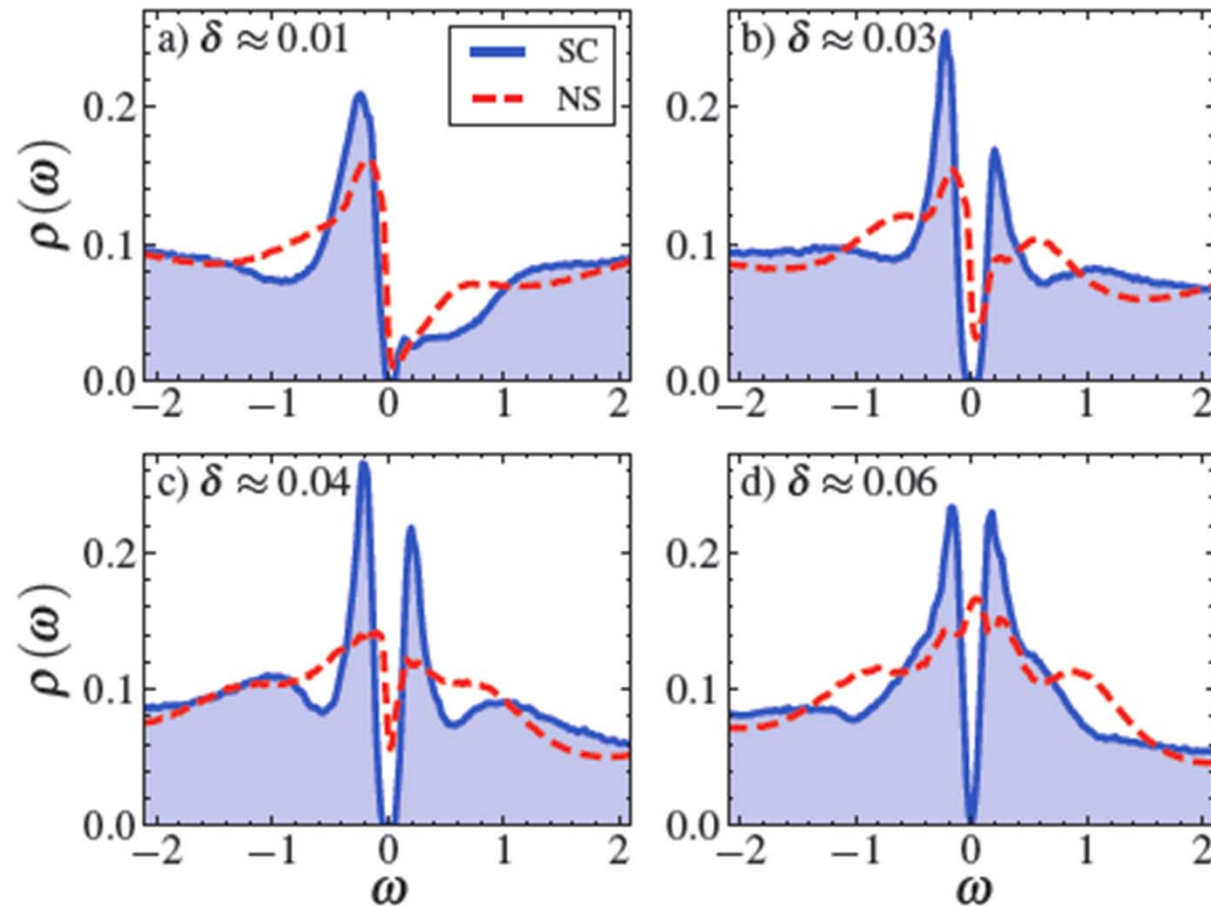


F. Rullier-Albenque, H. Alloul, and G. Rikken,
Phys. Rev. B **84**, 014522 (2011).

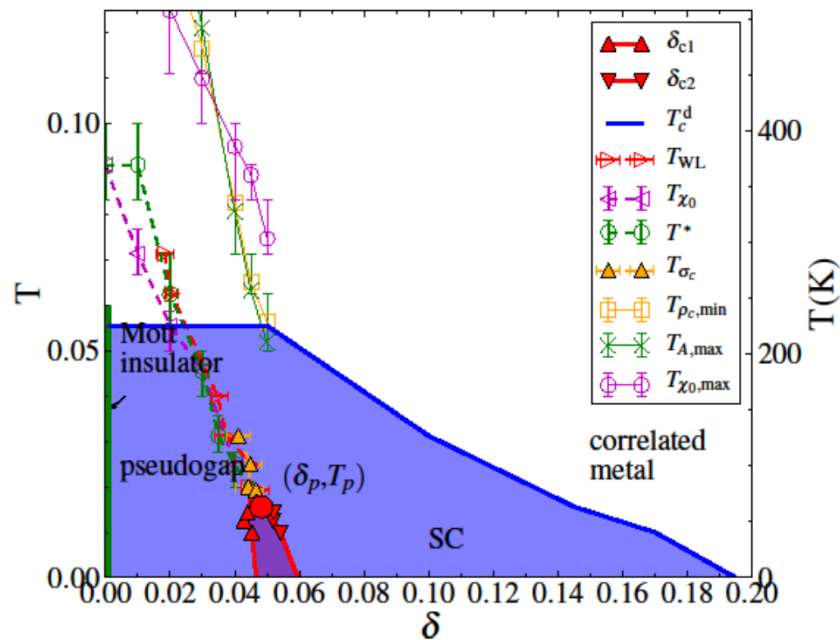
One last remark: Strongly correlated
superconductivity



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

Conclusions

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



Main collaborators



Giovanni Sordi



Kristjan Haule



David Sénéchal



Bumsoo Kyung



Patrick Sémon



Dominic Bergeron



Sarma Kancharla



Marcello Civelli



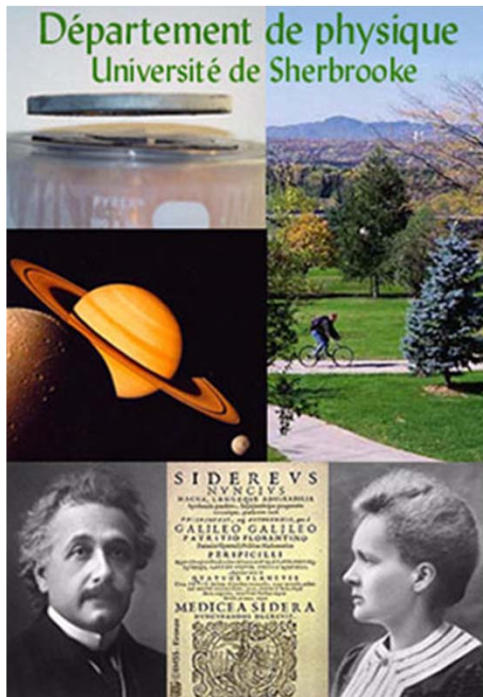
Massimo Capone



Gabriel Kotliar



André-Marie Tremblay



Le regroupement québécois sur les matériaux de pointe



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Merci

Thank you