Et pourtant ils s'attirent: le cas de la supraconductivité à haute température

A.-M. Tremblay

Sherbrooke, 8 juillet 2015

Half-filled band is metallic?

Half-filled band: Not always a metal

NiO, Boer and Verway

Peierls, 1937

Mott, 1949

BCS Superconductivity

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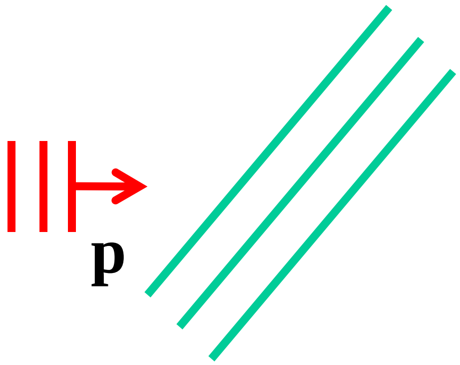
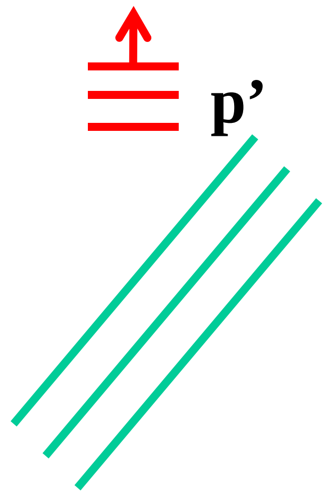
Superconductivity

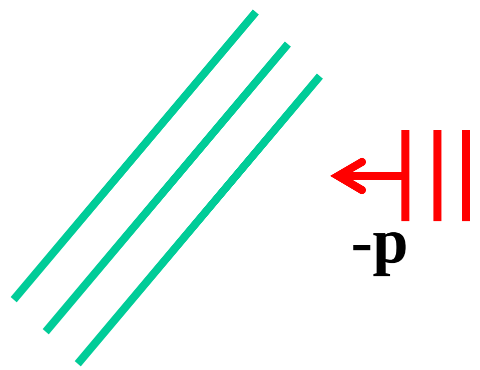
Attraction mechanism in the metallic state



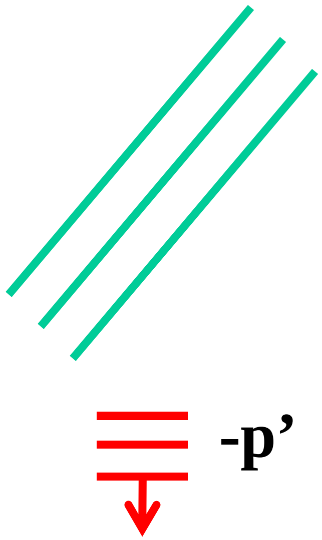
Attraction mechanism in the metallic state



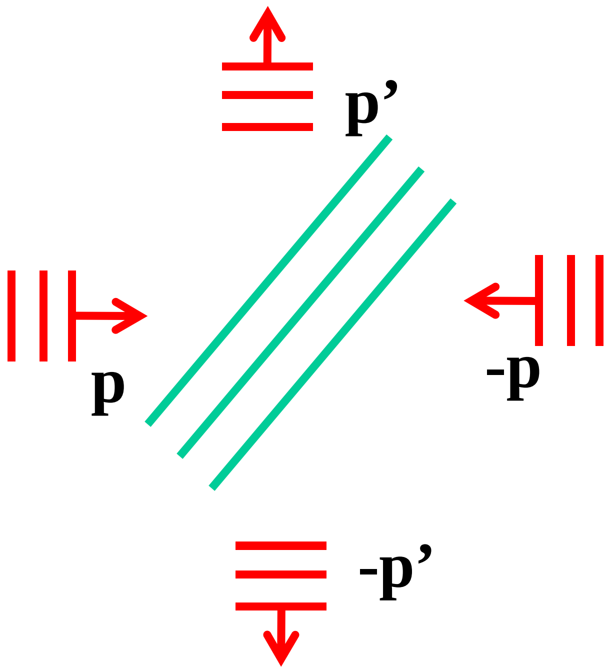
Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



#1 Cooper pair, #2 Phase coherence

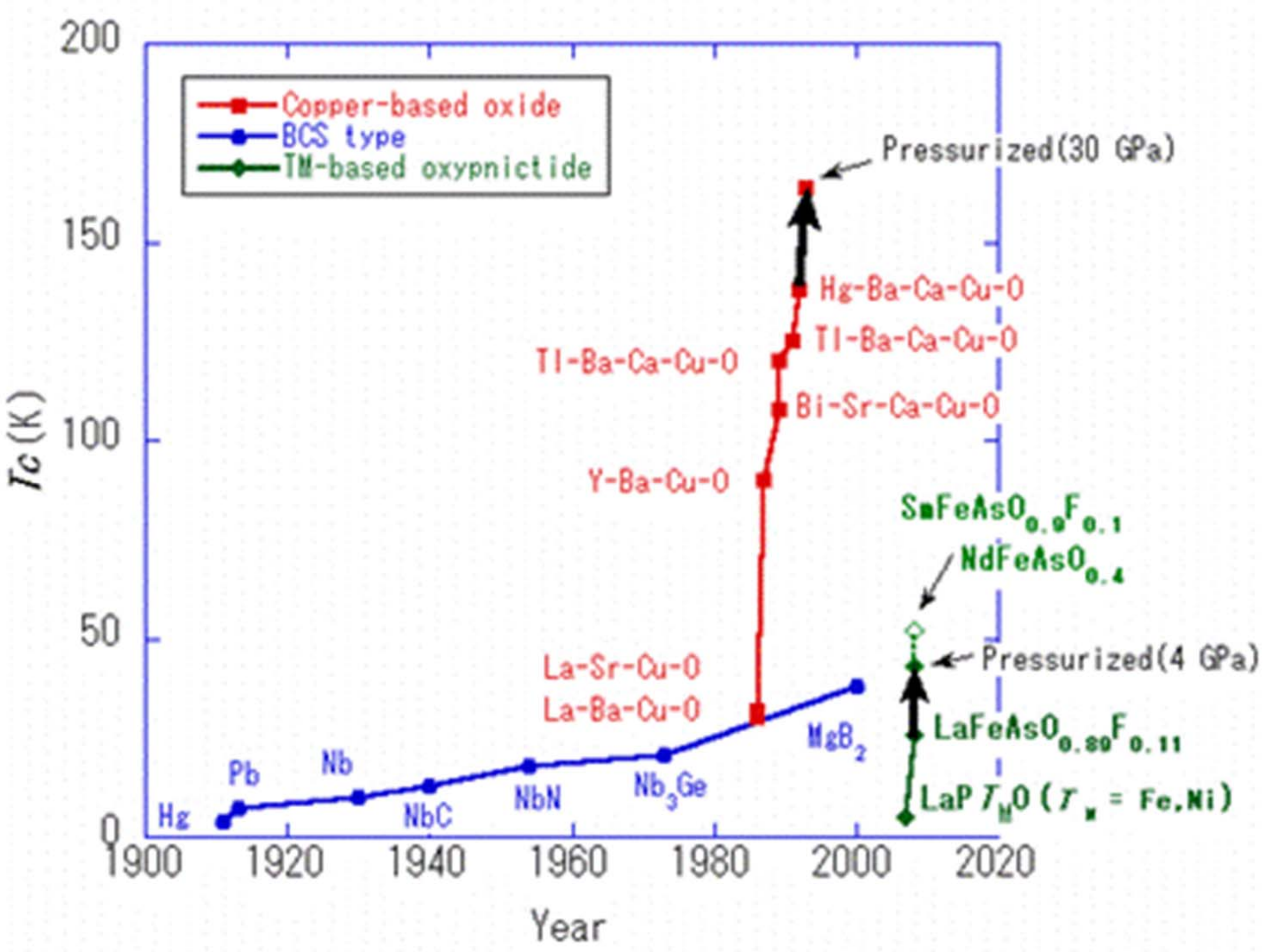
$$E_P = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow} \psi^*_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow}$$

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

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

Kinetic energy increases

New and old superconductors



H. Takahashi: JPSJ Online—News and Comments [June 10, 2008]

March meeting APS, 1987

- New York Times headlines
"The Woodstock of Physics"

"They began lining up outside the New York Hilton Sutton Ballroom at 5:30PM for an evening session that would last until 3:00 AM"

15-18 Aug. 1969
500,000 participants

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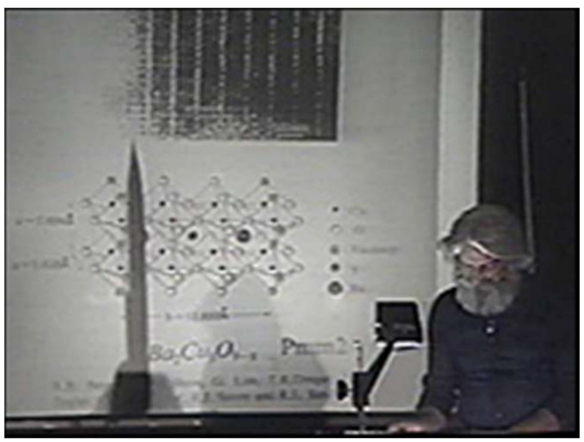

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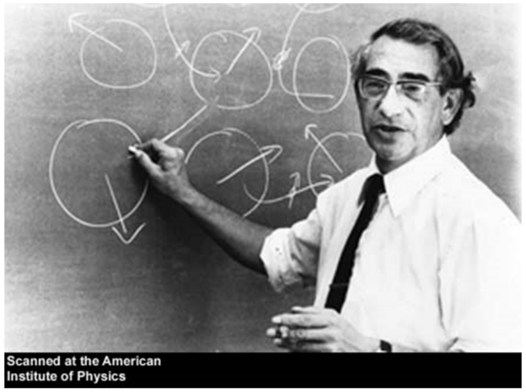
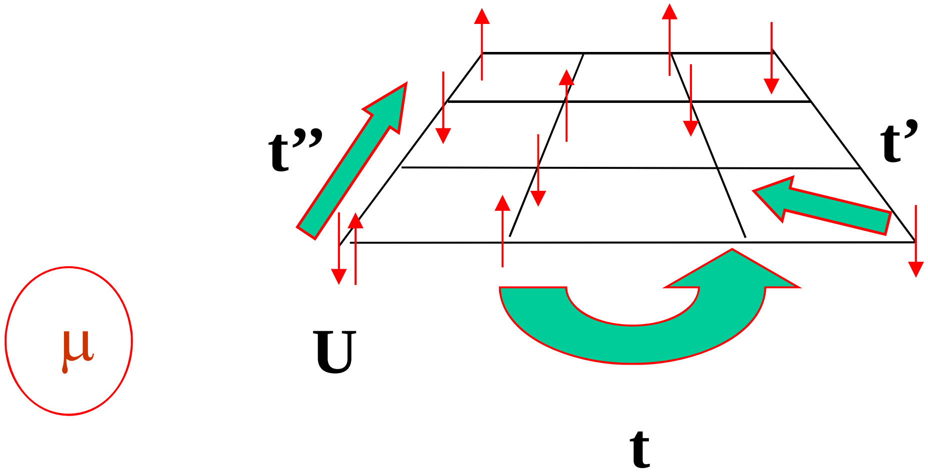
Simplest Model for Mott insulator

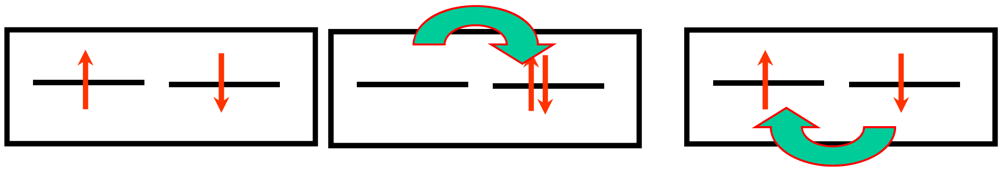
Hubbard model



1931-1980



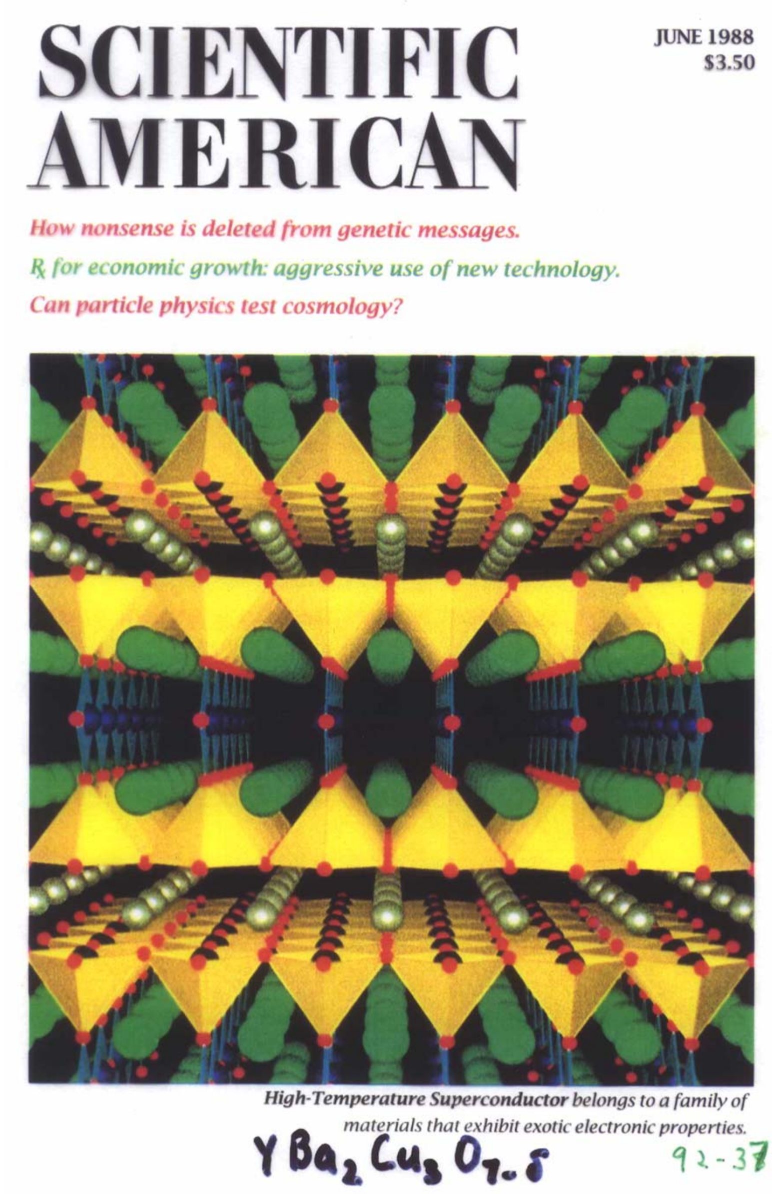
$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}\right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

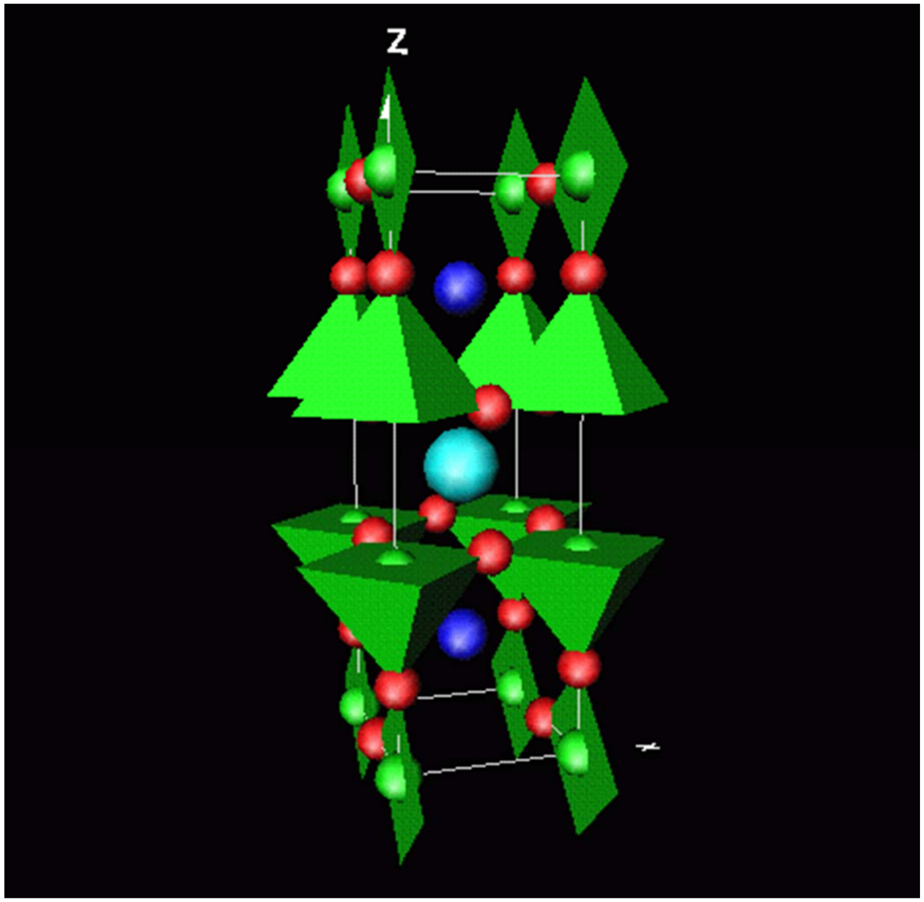


Effective model, Heisenberg: $J = 4t^2/U$

Superconductivity and attraction?

Cuprates





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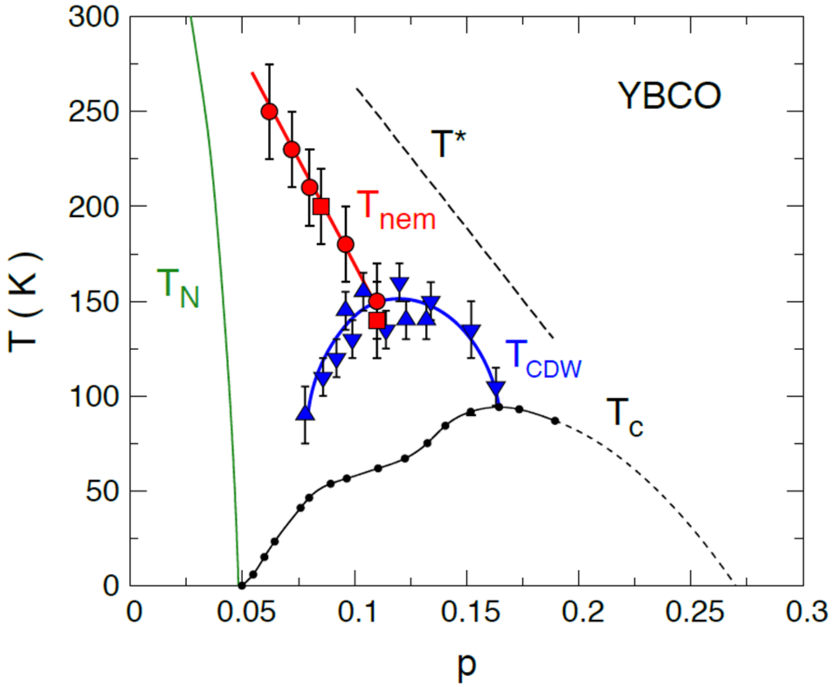
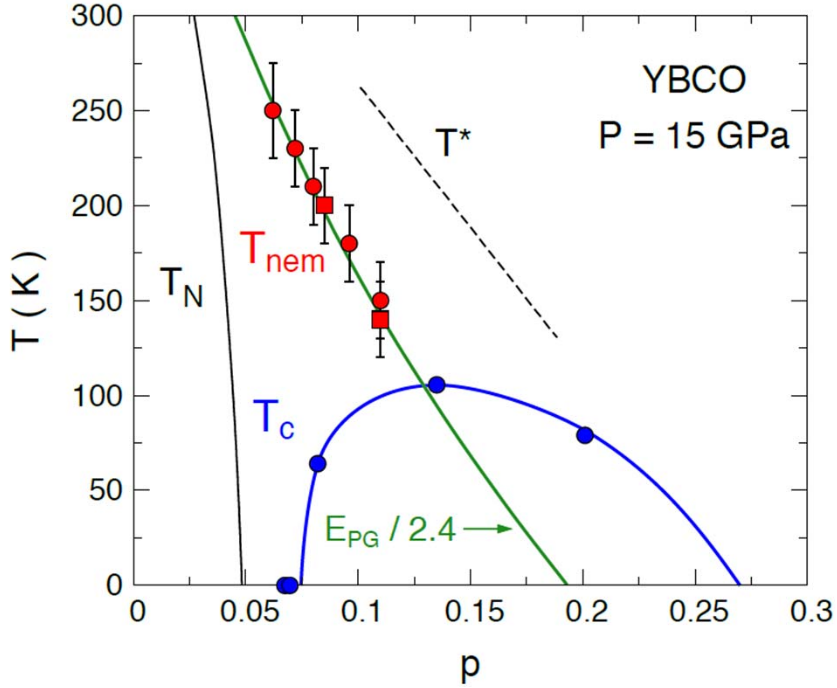
Phase diagram

The central line – $T_x = T_{nem}$

$T_{nem} = E_{PG} / 2.4$



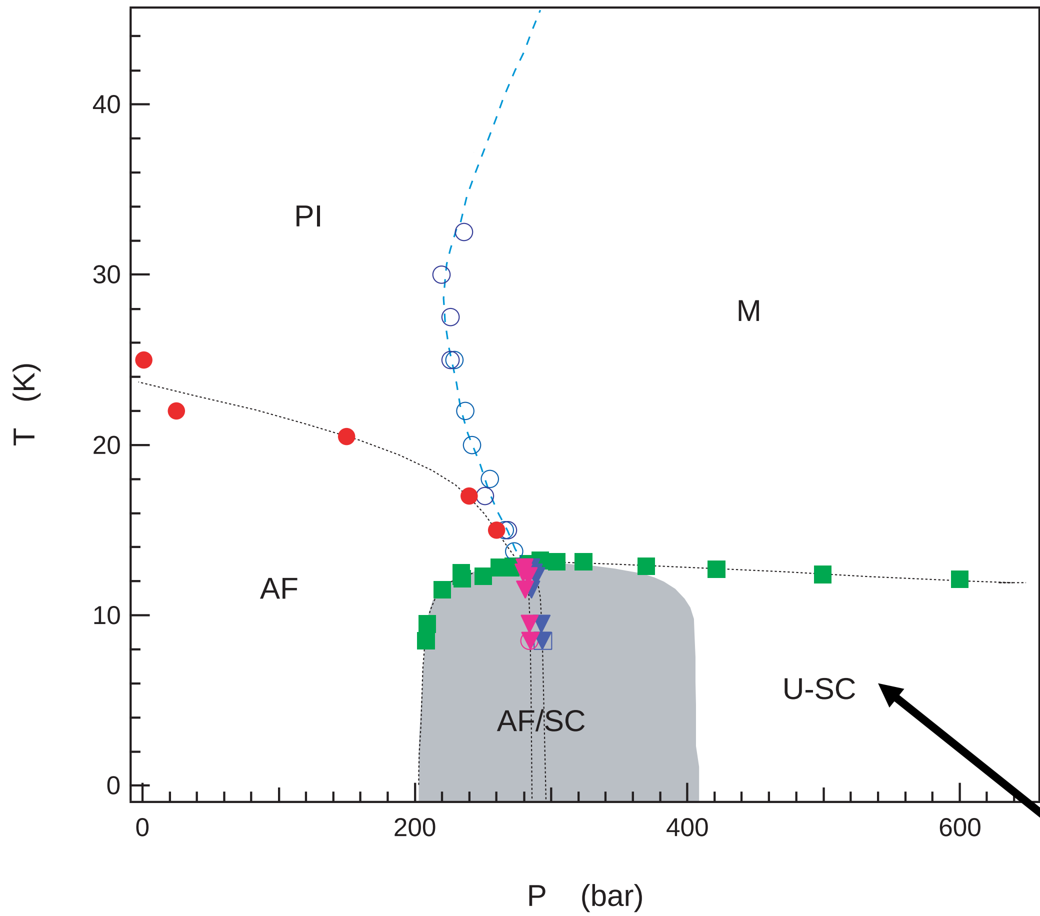


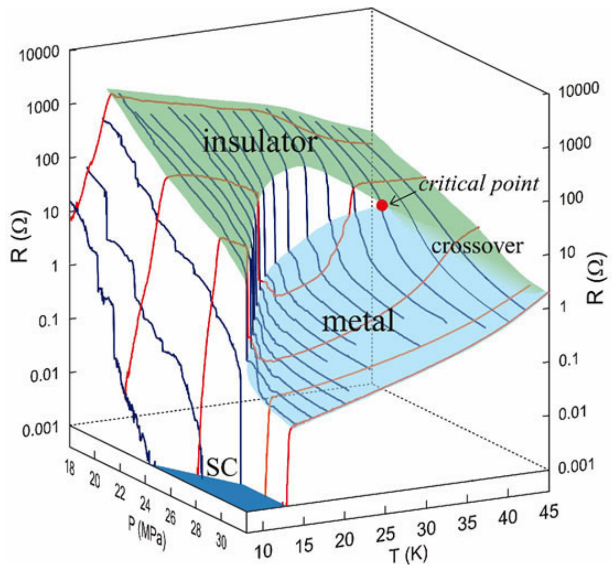
T_{nem} hits T_{CDW} dome at peak

T_{nem} hits T_c dome at peak

Cyr-Choinière *et al*. arXiv:1503.02033

Phase diagram for organics





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

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

Powell, McKenzie cond-mat/0607078

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

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

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Outline

- Method
- *T=0* phase diagram
- Finite *T* phase diagram
  - Normal state
    - First order transition
    - Widom line and pseudogap
  - Superconductivity
    - Condensation energy
    - Superfluid density

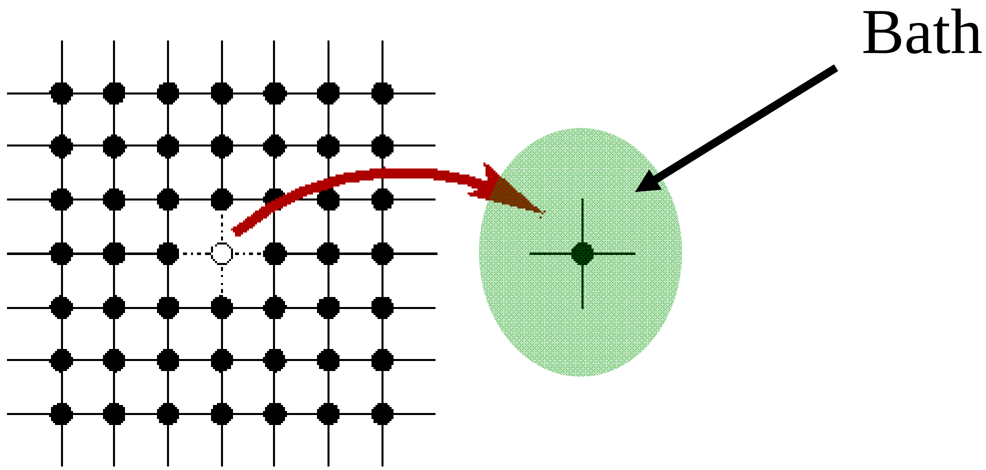
Method

"The effect of concept-driven revolution is to explain old things in new ways. The effect of tool-driven revolution is to discover new things that have to be explained."

Freeman Dyson *Imagined Worlds*

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

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

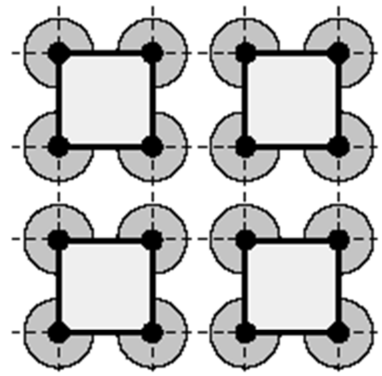


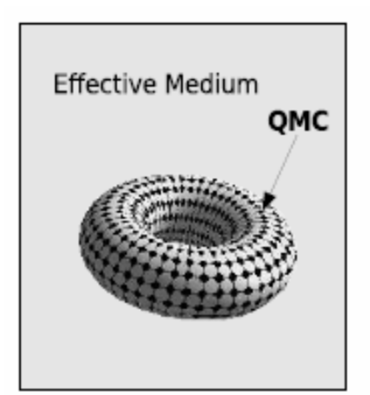
W. Metzner and D. Vollhardt, PRL (1989)
A. Georges and G. Kotliar, PRB (1992)
M. Jarrell PRB (1992)

DMFT, ($d = 3$)

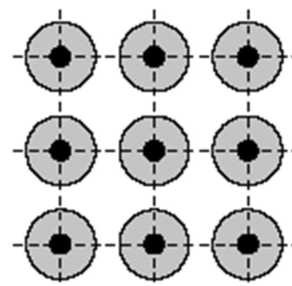
2d Hubbard: Quantum cluster method

C-DMFT





DCA



DMFT

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

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

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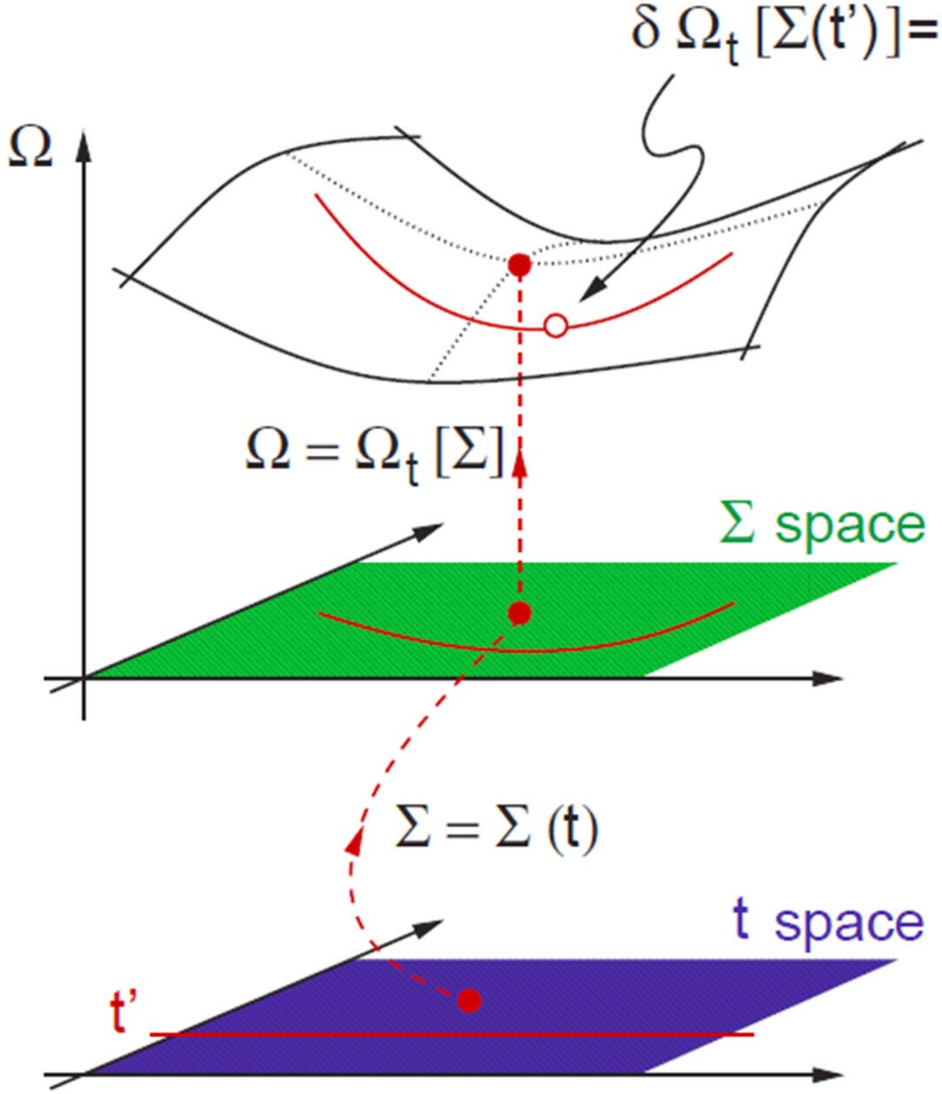
DMFT as a stationnary point



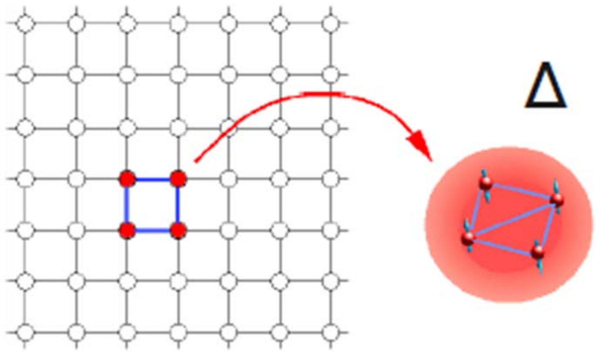
M. Potthoff, Eur. Phys. J. B 32, 429 (2003).

+ and -

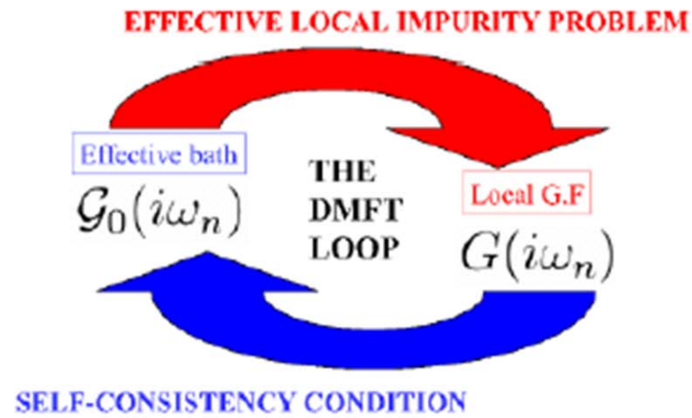
- Long range order:
  - Allow symmetry breaking in the bath (mean-field)
- Included:
  - Short-range dynamical and spatial correlations
- Missing:
  - Long wavelength p-h and p-p fluctuations

Tools: Impurity solver

CTQMC impurity solver (tool) (T finite)



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



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

Here: continuous time QMC

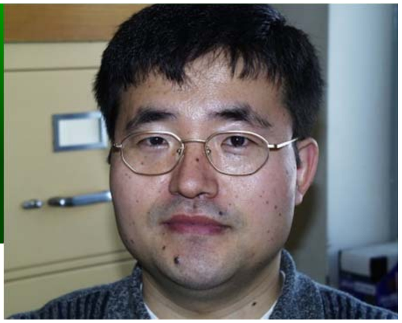
P. Werner, PRL 2006
P. Werner, PRB 2007
K. Haule, PRB 2007

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

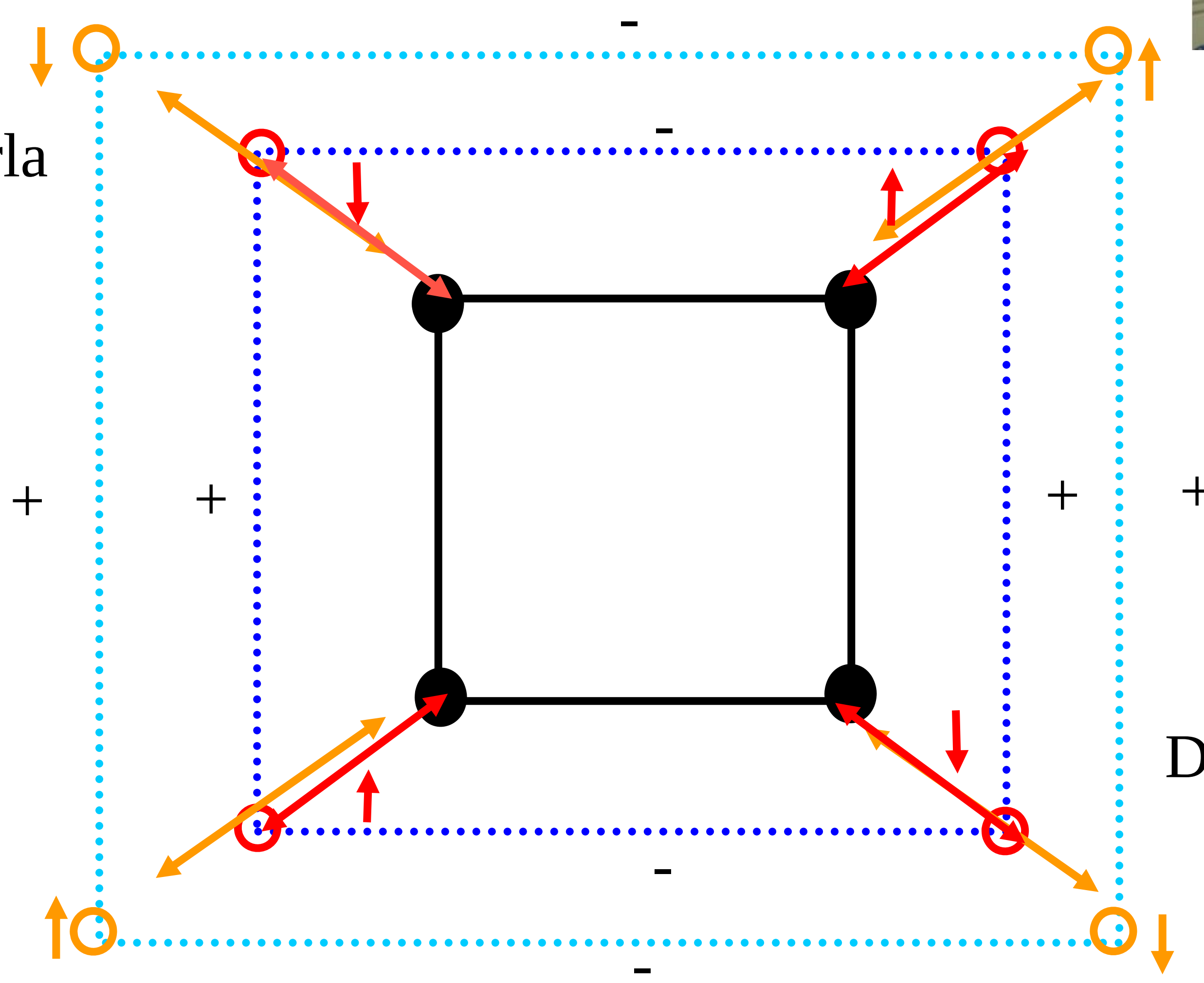
P. Sémon *et al.* PRB **90** 075149 (2014);
and PRB **89**, 165113 (2014)

ED impurity solver ($T = 0$)

S. Kancharla



B. Kyung

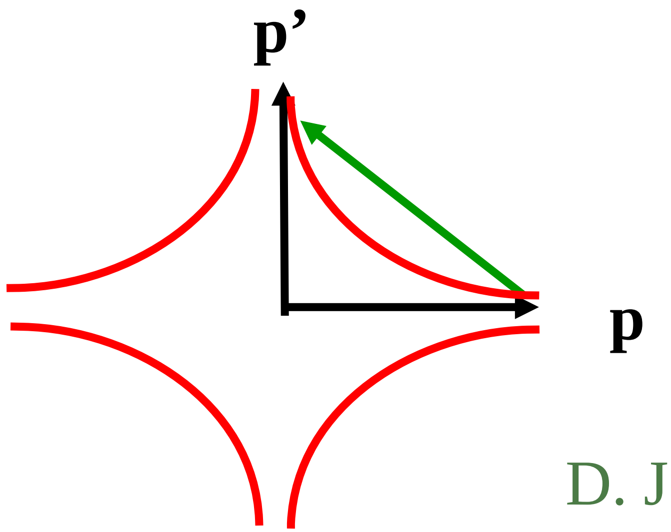


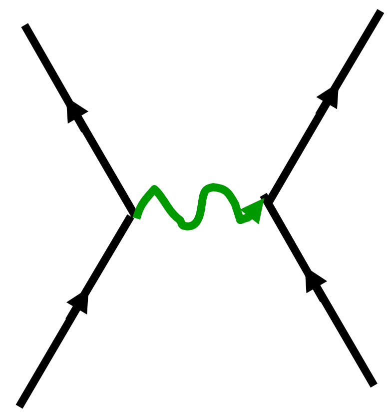
David Sénéchal

A bit of physics: superconductivity and repulsion

Cartoon « BCS » weak-correlation picture (d-wave)

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



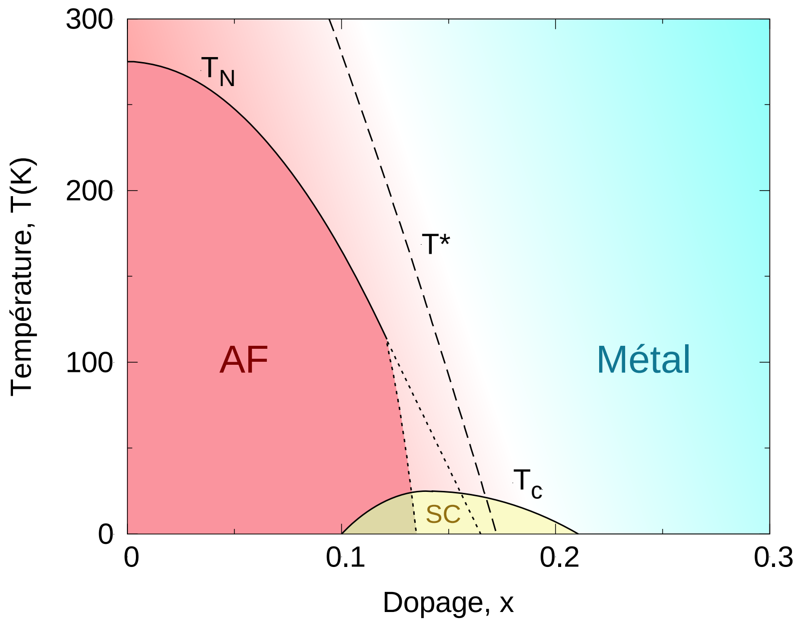


Exchange of spin waves?
Kohn-Luttinger
T_c with pressure

D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch P.R. B **34**, 8190-8192 (1986).
Béal–Monod, Bourbonnais, Emery P.R. B. **34**, 7716 (1986).
Kohn, Luttinger, P.R.L. **15**, 524 (1965).

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

AFM Quantum critical point



A cartoon strong correlation 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

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

Miyake, Schmitt–Rink, and Varma

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

T = 0 phase diagram: cuprates

Phase diagram

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

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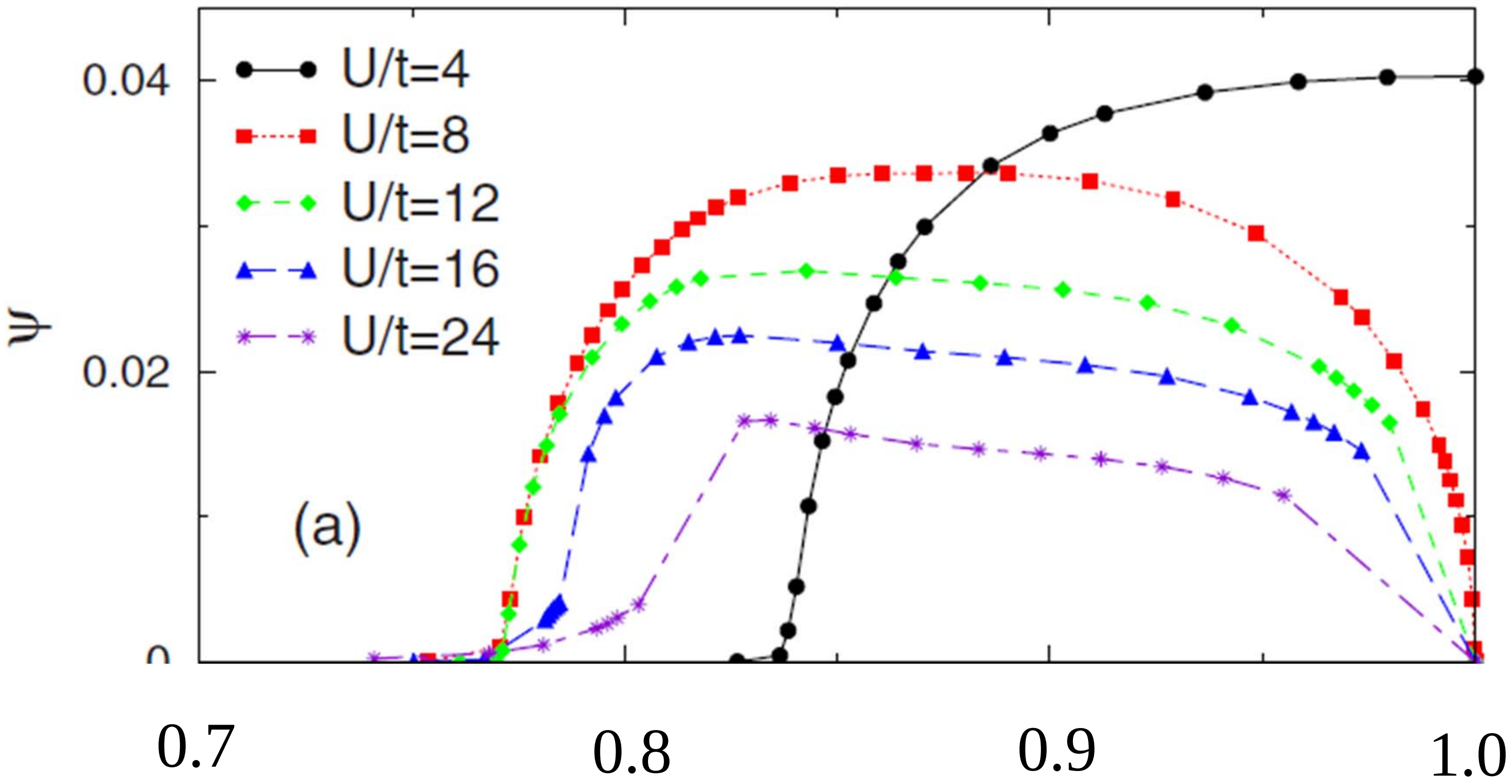
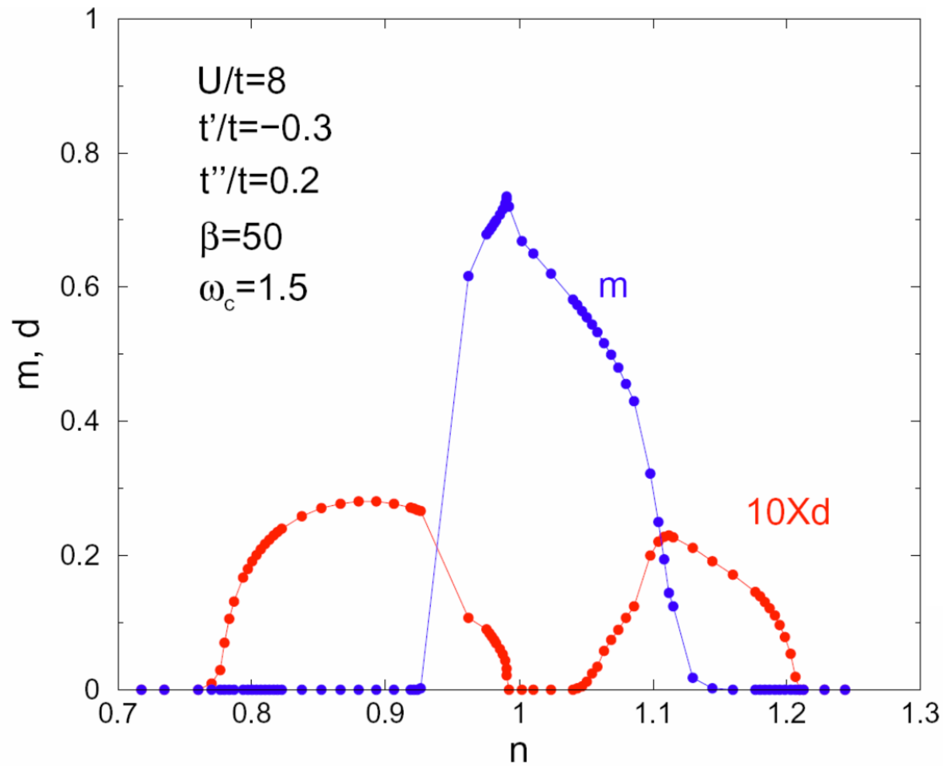
Theory: T_c down vs Mott



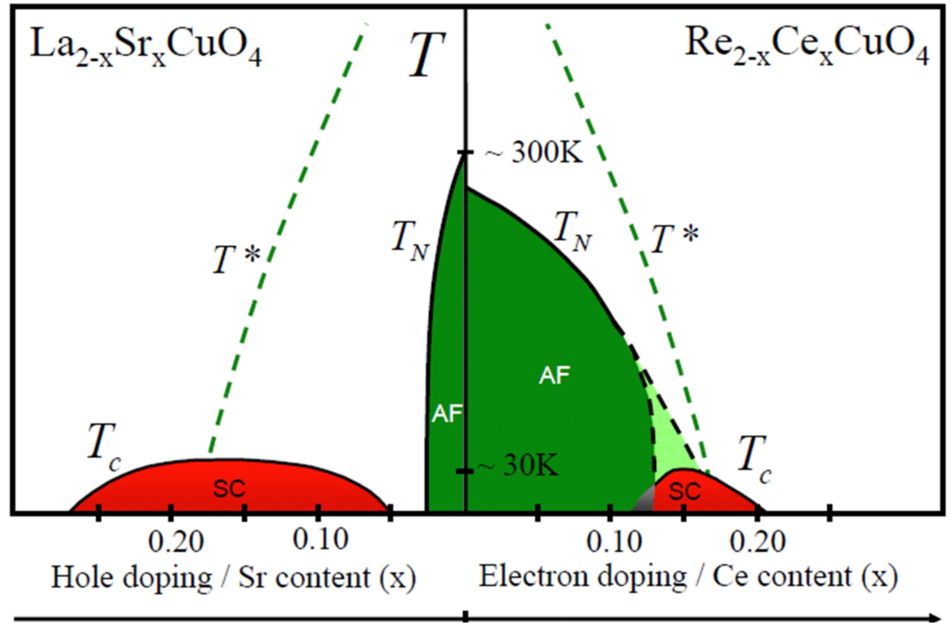
S. Kancharla *et al.* Phys. Rev. B (2008)

CDMFT global phase diagram

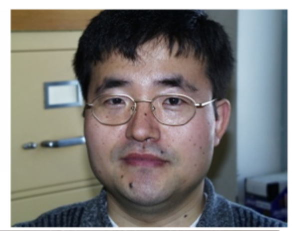
Simon Verret, MSc



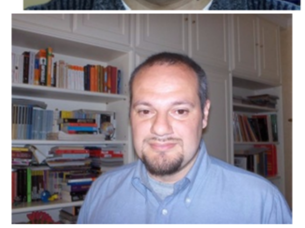
Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008)
AND Capone, Kotliar PRL (2006)



Armitage, Fournier, Greene, RMP (2009)








Outline

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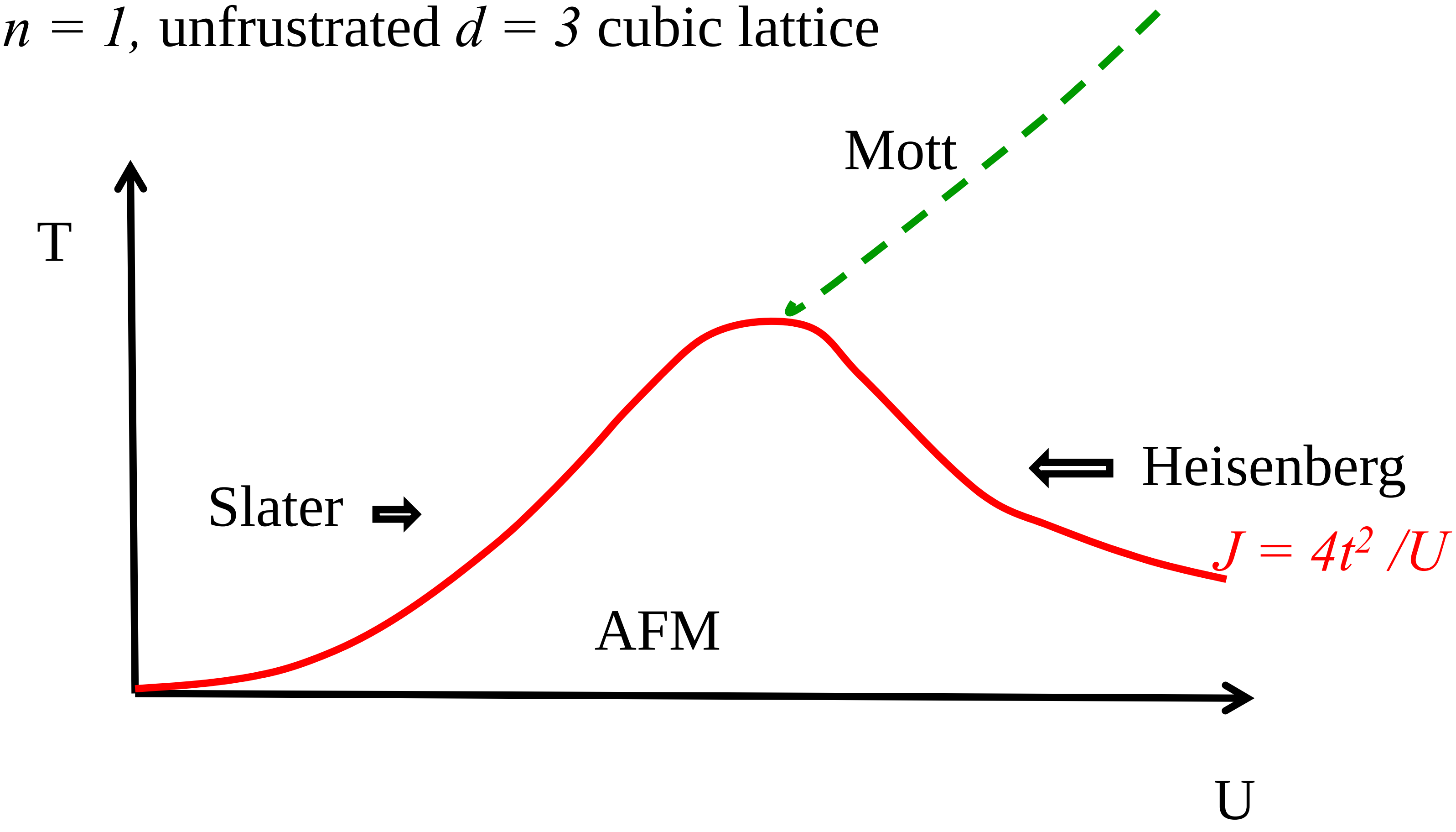
  - Superconductivity
    - Condensation energy
    - Superfluid density

Finite T phase diagram

Normal state of the cuprates

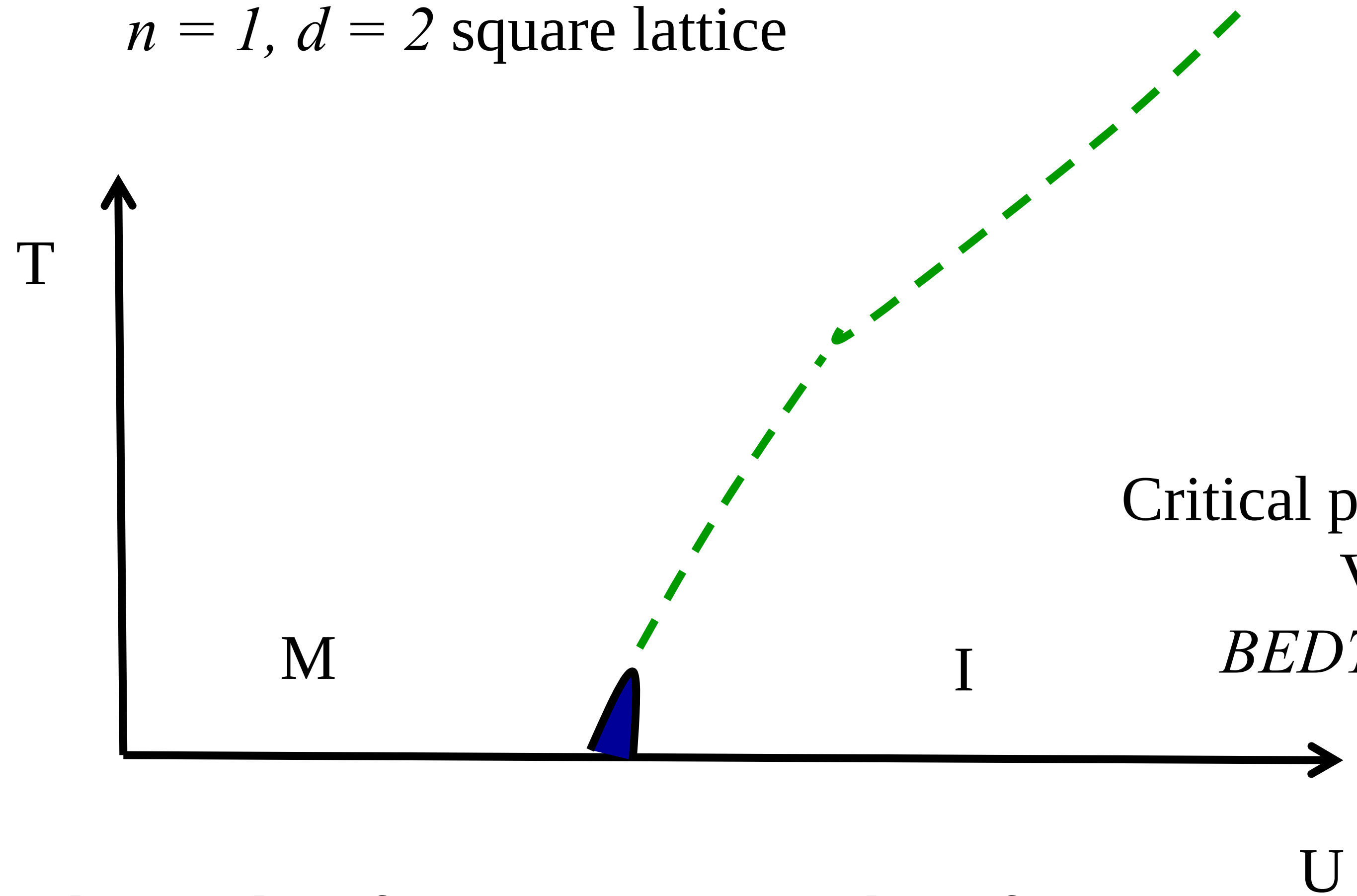
Weak vs Strong correlations

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



Local moment and Mott transition

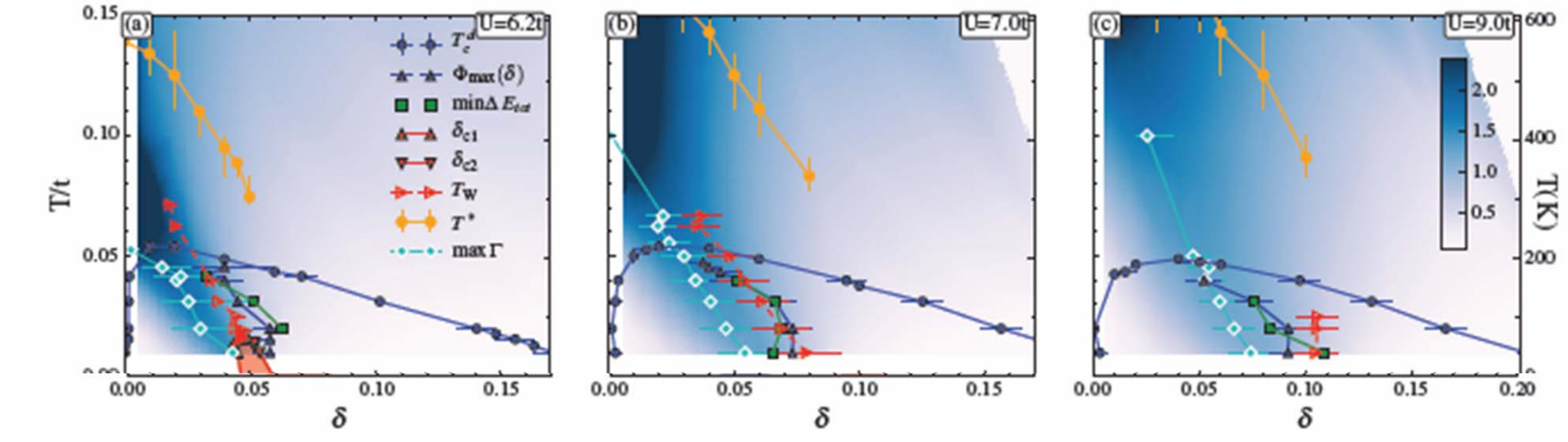
n = 1, d = 2 square lattice

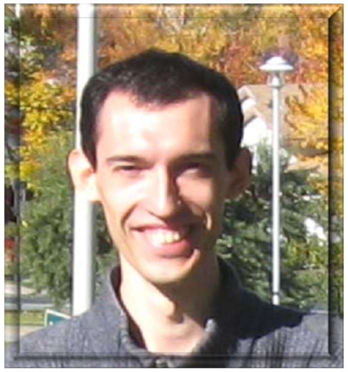


Critical point visible in
V_2O_3,
BEDT organics

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

Finite-doping first-order transition

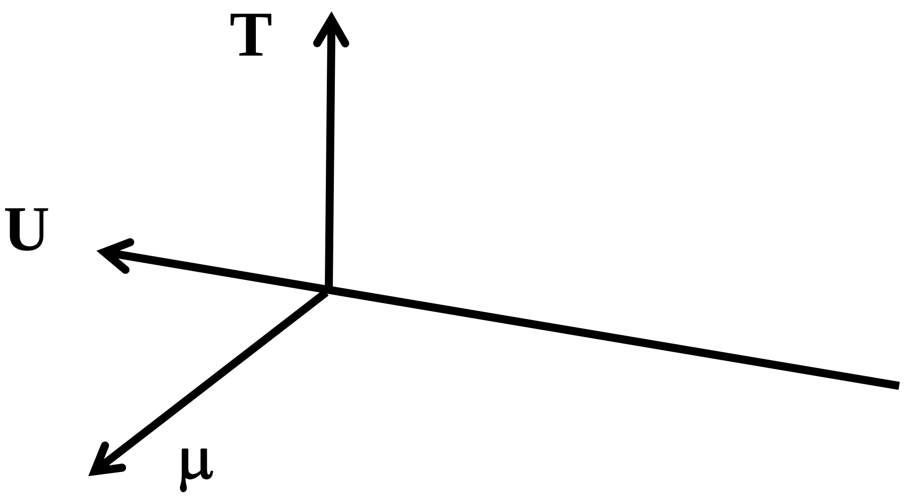




Giovanni Sordi

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

Lesson from DMFT, first order transition + critical point governs phase diagram

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A first order transition at finite doping?

At positive *t'*

A. Macridin, M. Jarrell, and T. Maier,
Phys. Rev. B **74**, 085104 (2006)

E. Khatami, K. Mikelsons, D. Galanakis, A. Macridin, J. Moreno,
R. T. Scalettar, and M. Jarrell
PRB **81**, 201101(R) 2010

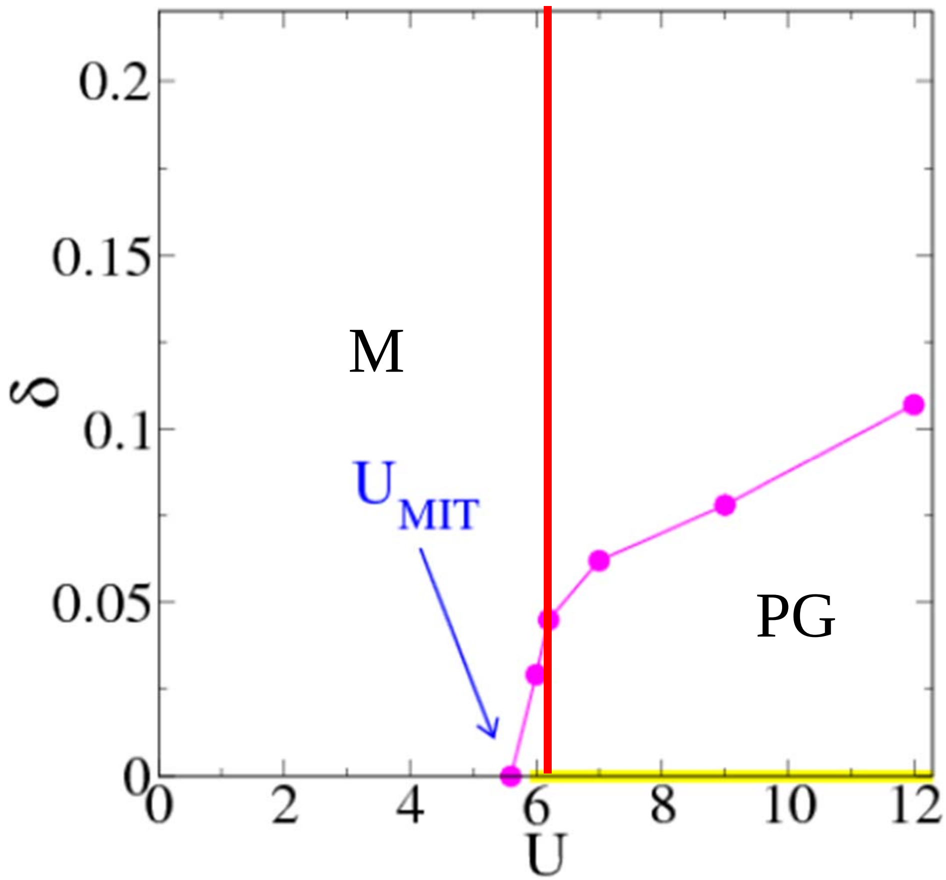
A. Liebsch, N.H. Tong, PRB **80**, 165126 (2009)

Here $t'=0$

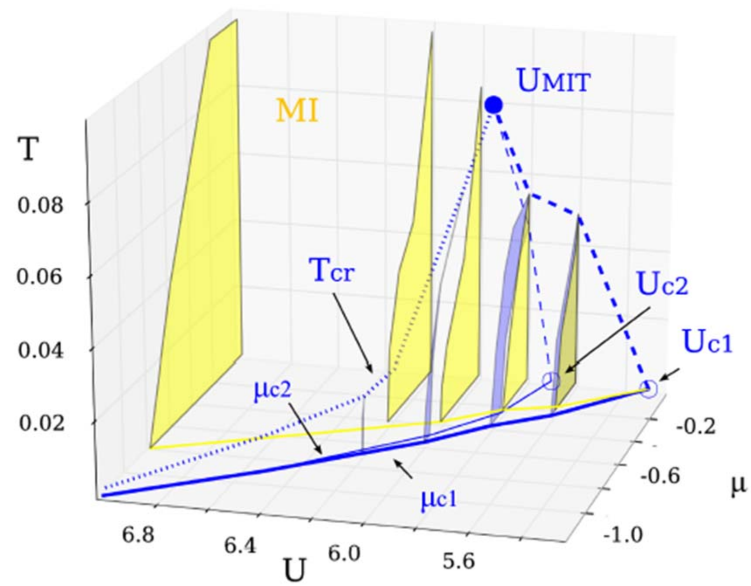
Link to Mott transition up to optimal doping

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

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



Smaller *D* and *S*



$\mu = 0$, H. Park, K. Haule, and`G. Kotliar,
Phys. Rev. Lett. 101, 186403 (2008).

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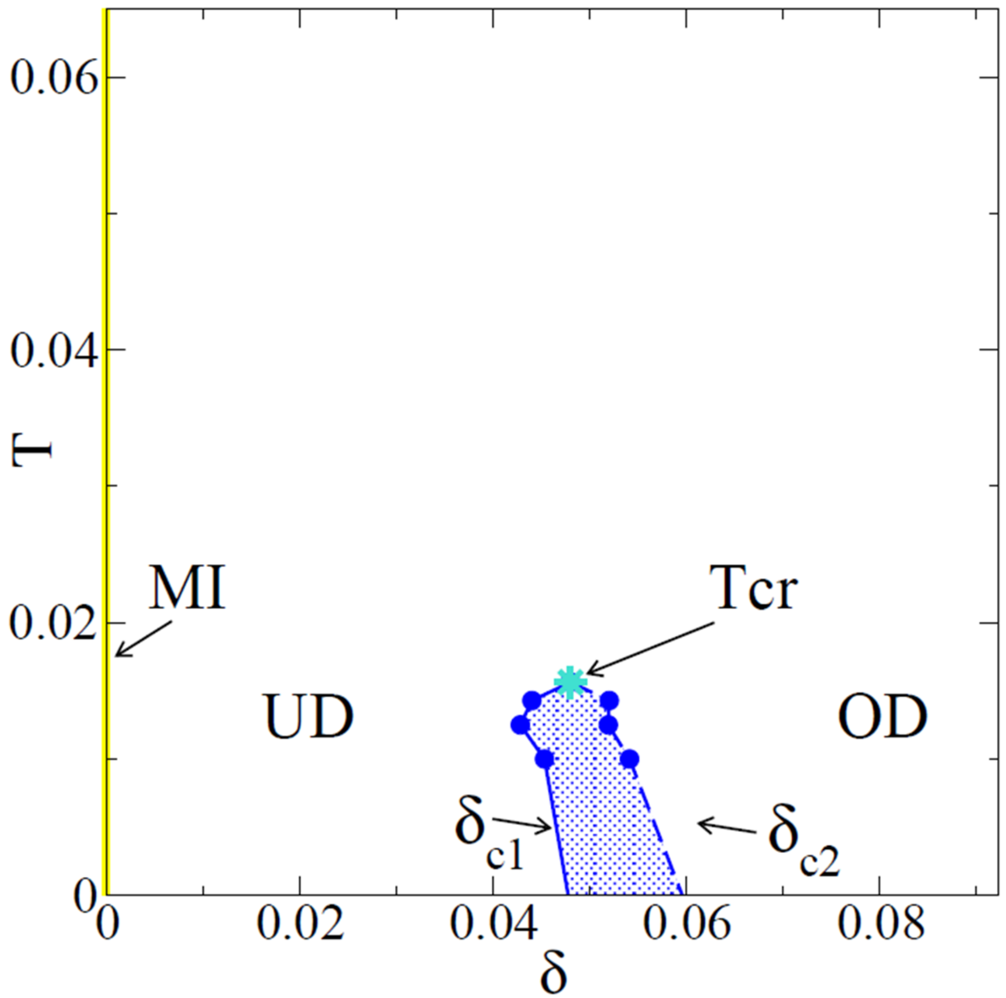
Characterisation of the phases (*U*=6.2*t*)



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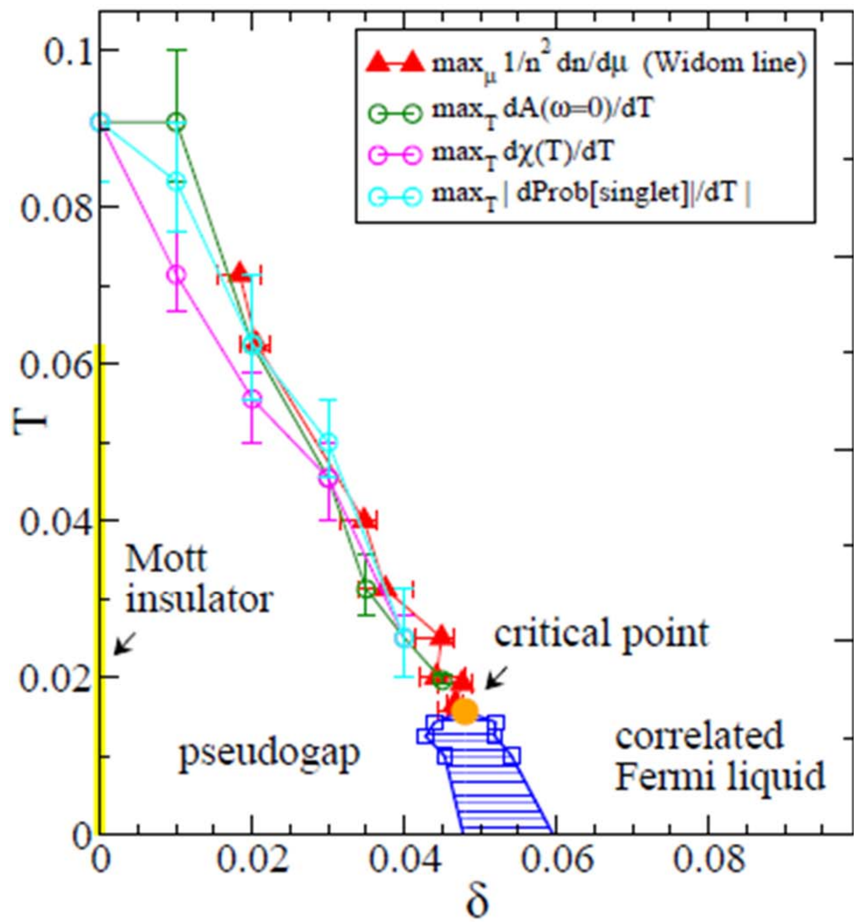
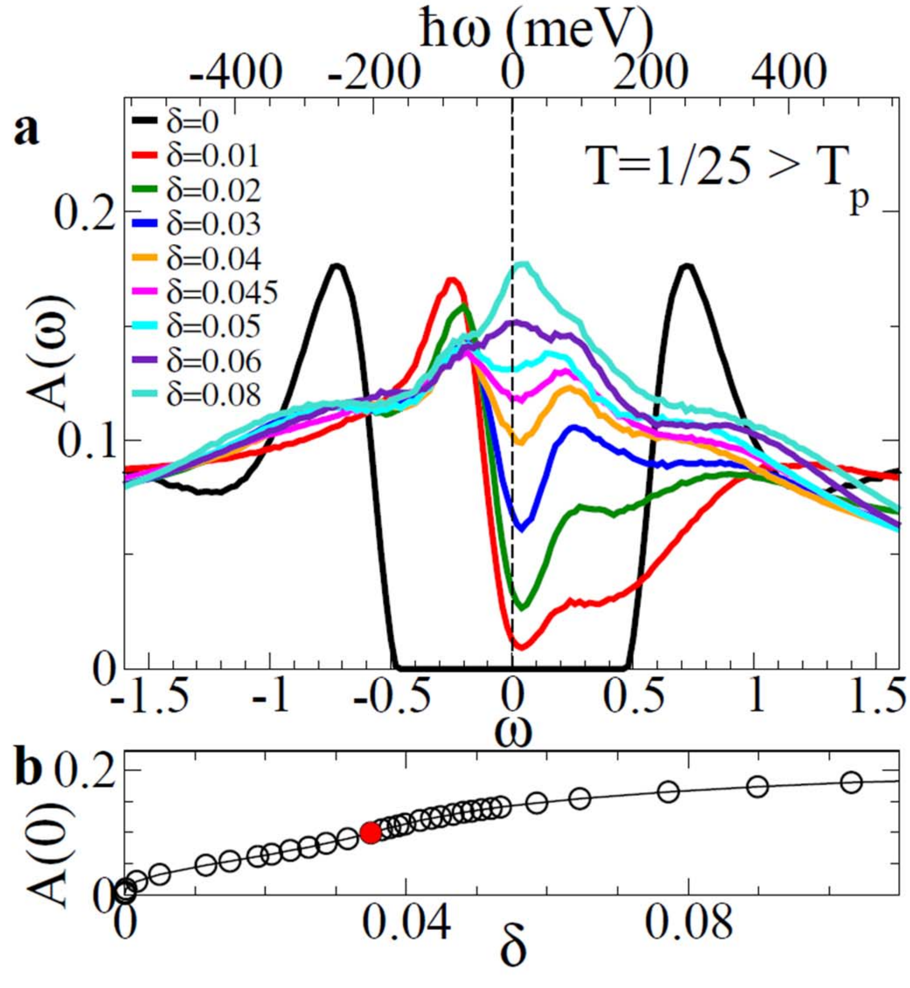
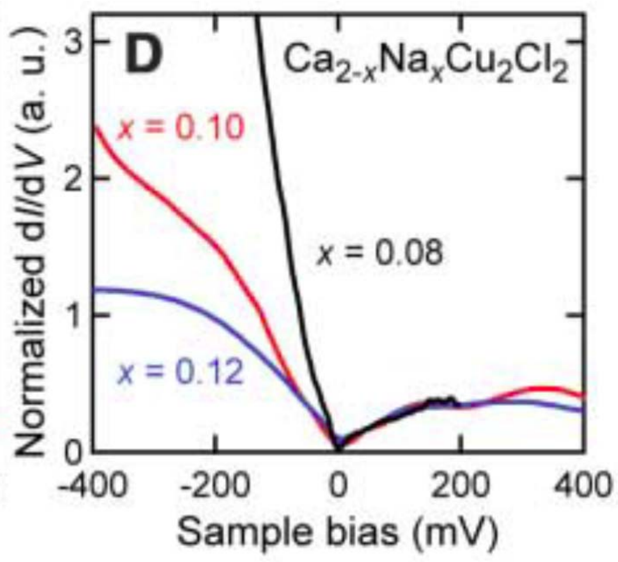
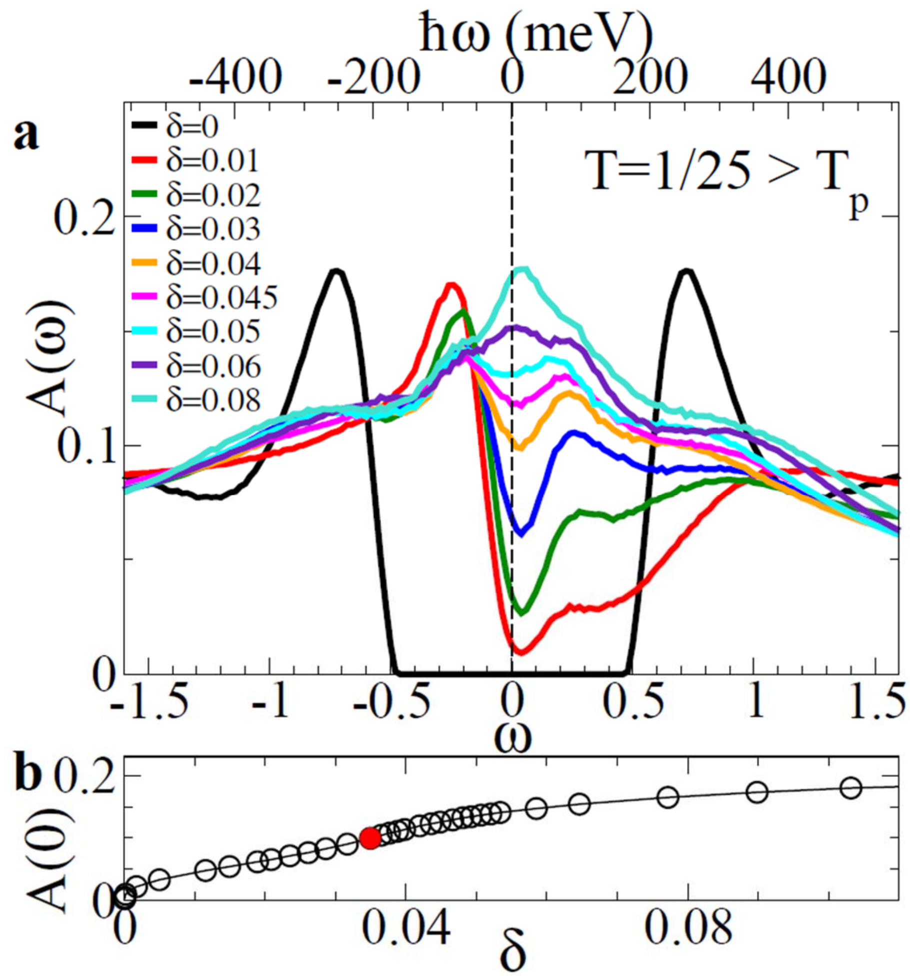
Density of states





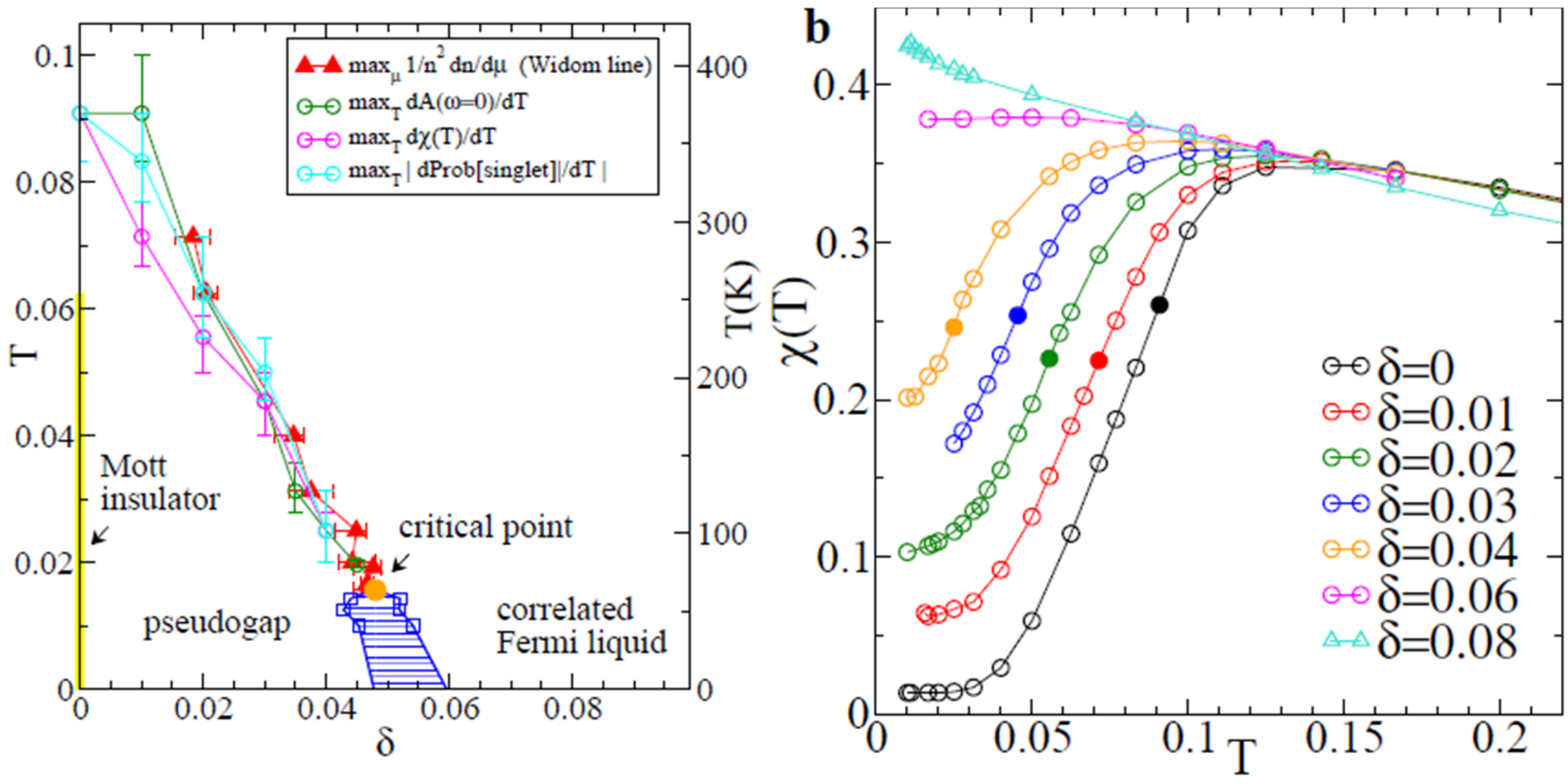
Density of states



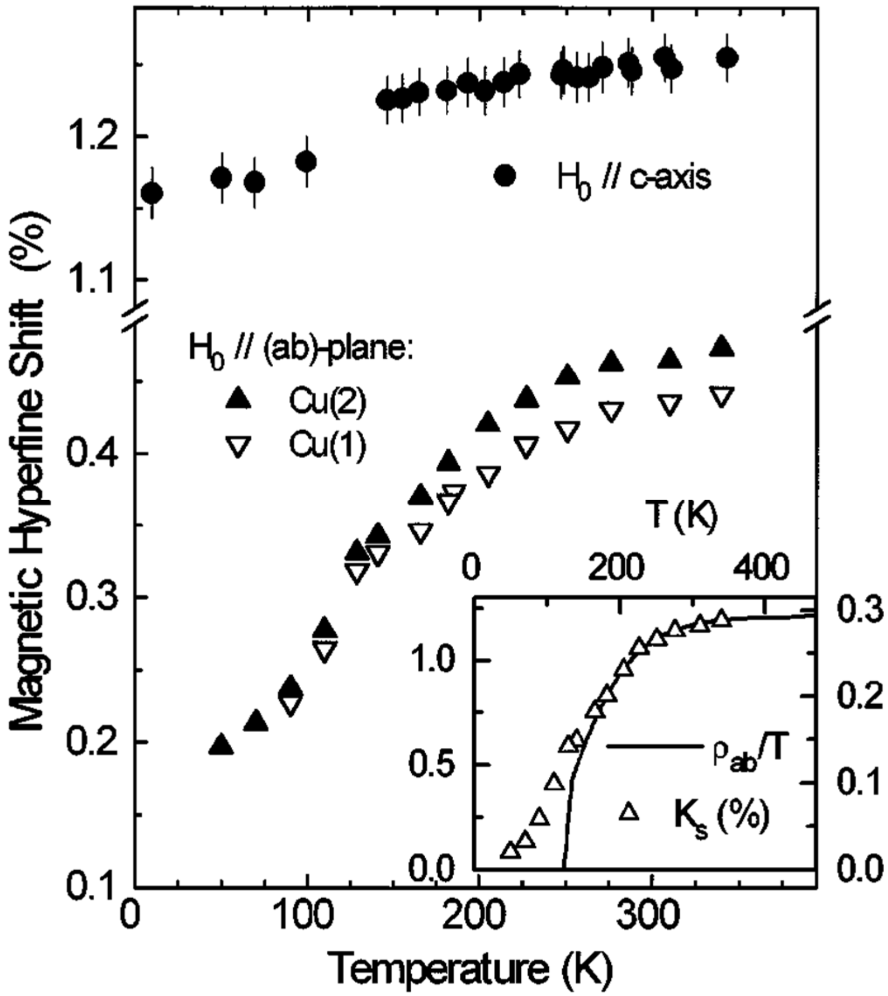


Khosaka et al. *Science* **315**, 1380 (2007);

Spin susceptibility

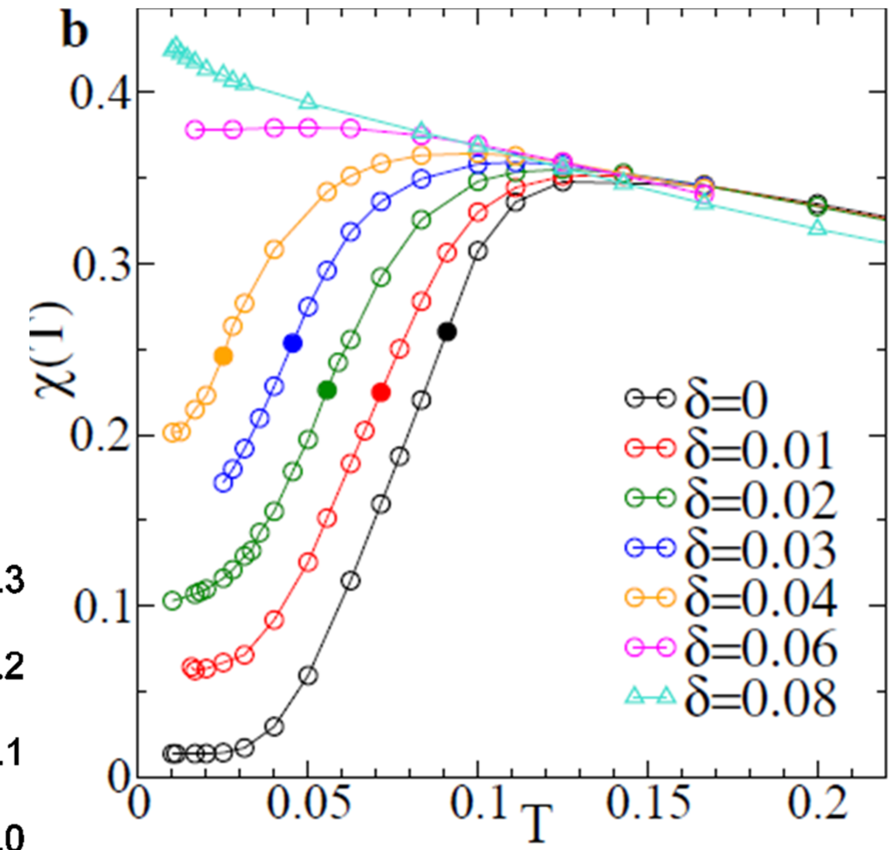


Spin susceptibility



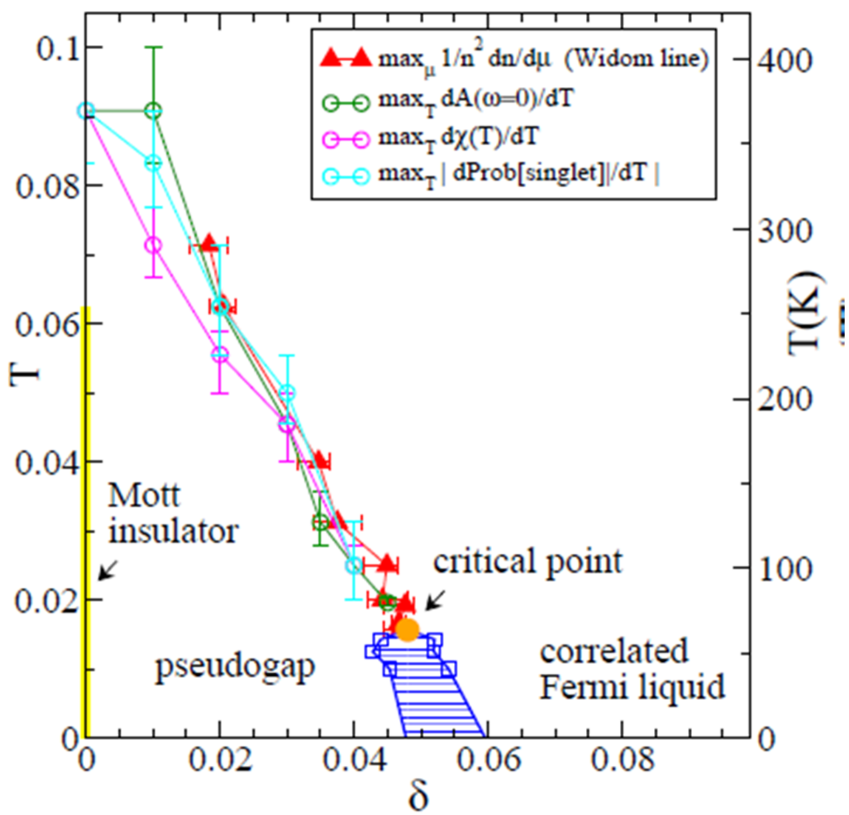
Underdoped Hg1223

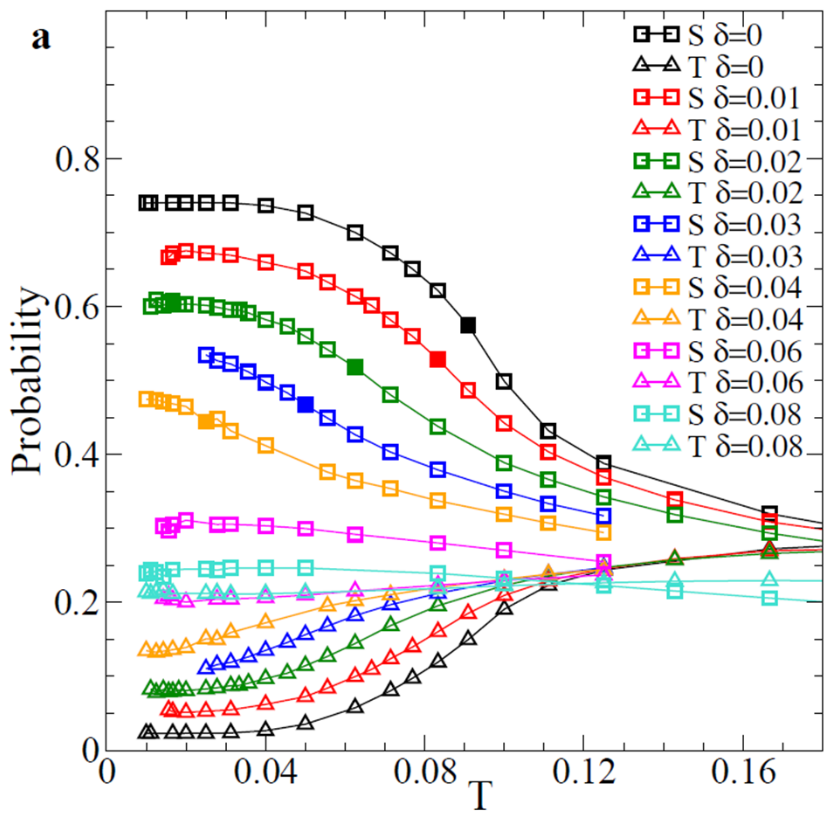
Julien et al. PRL **76,** 4238 (1996)



Physics

Plaquette eigenstates





See also:

Michel Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, A. Georges

PRB **80**, 064501 (2009)

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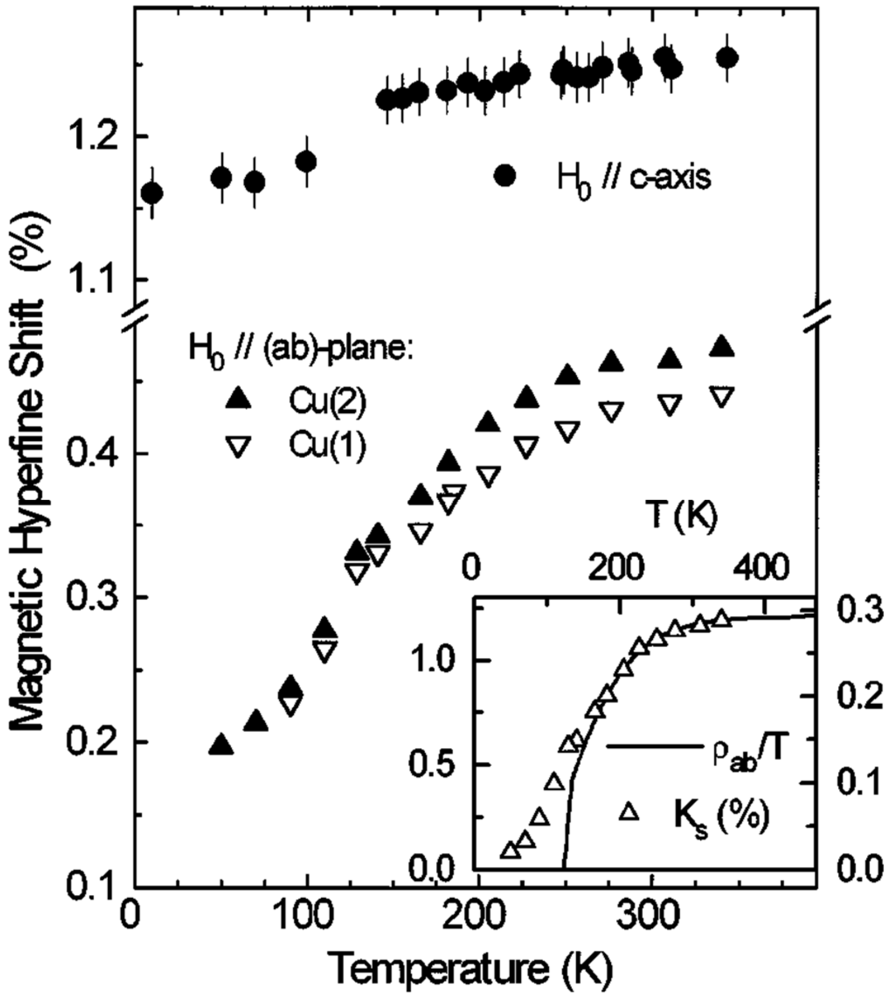
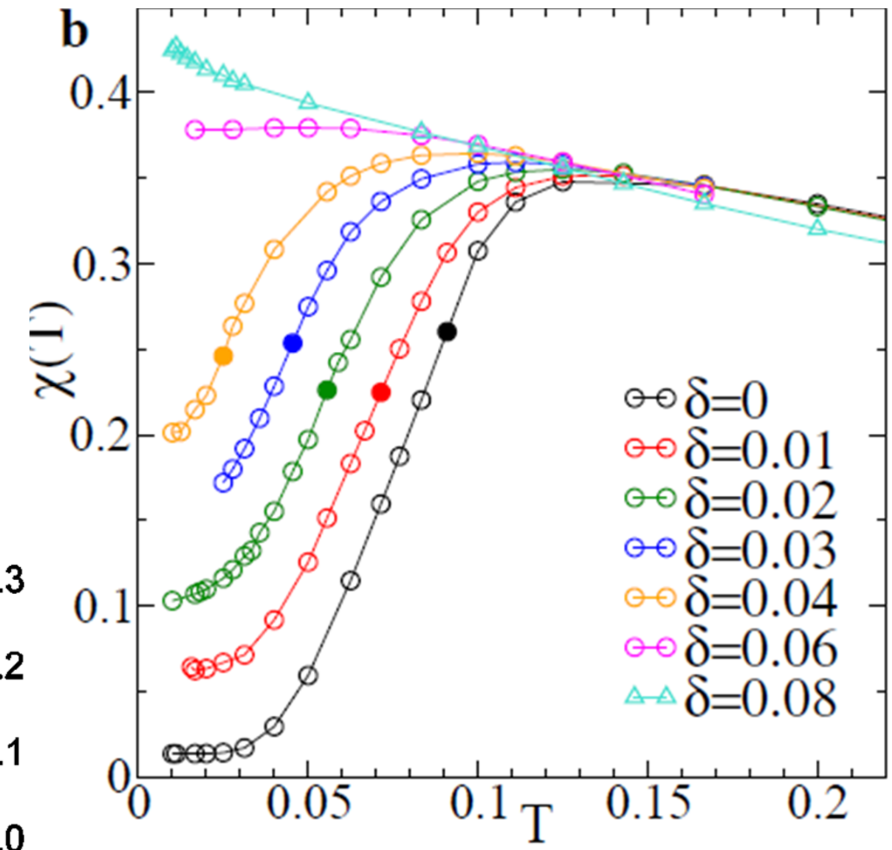
Different definitions for broad crossovers

Spin susceptibility





Underdoped Hg1223

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

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What is the minimal model?

H. Alloul arXiv:1302.3473
C.R. Académie des Sciences, (2014)

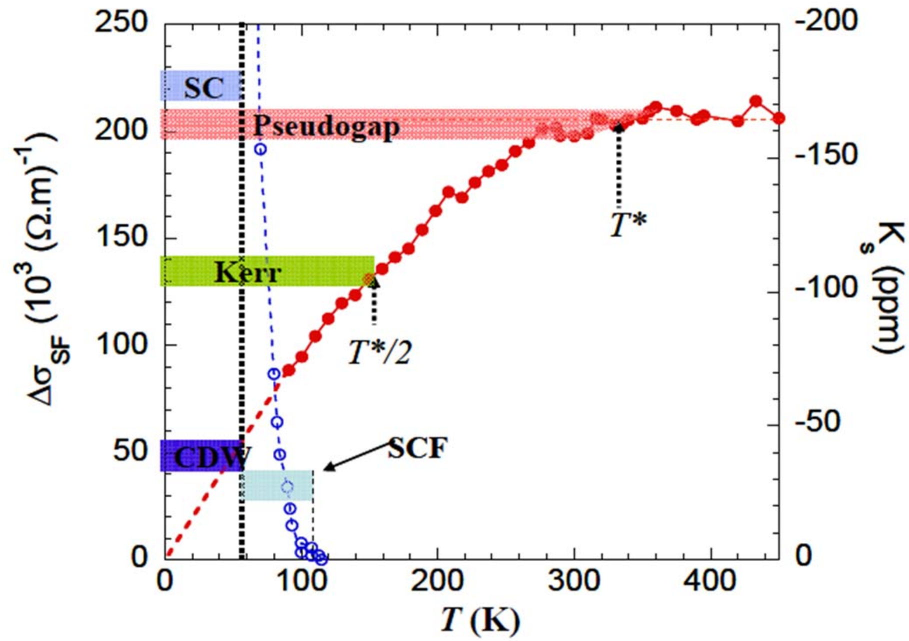
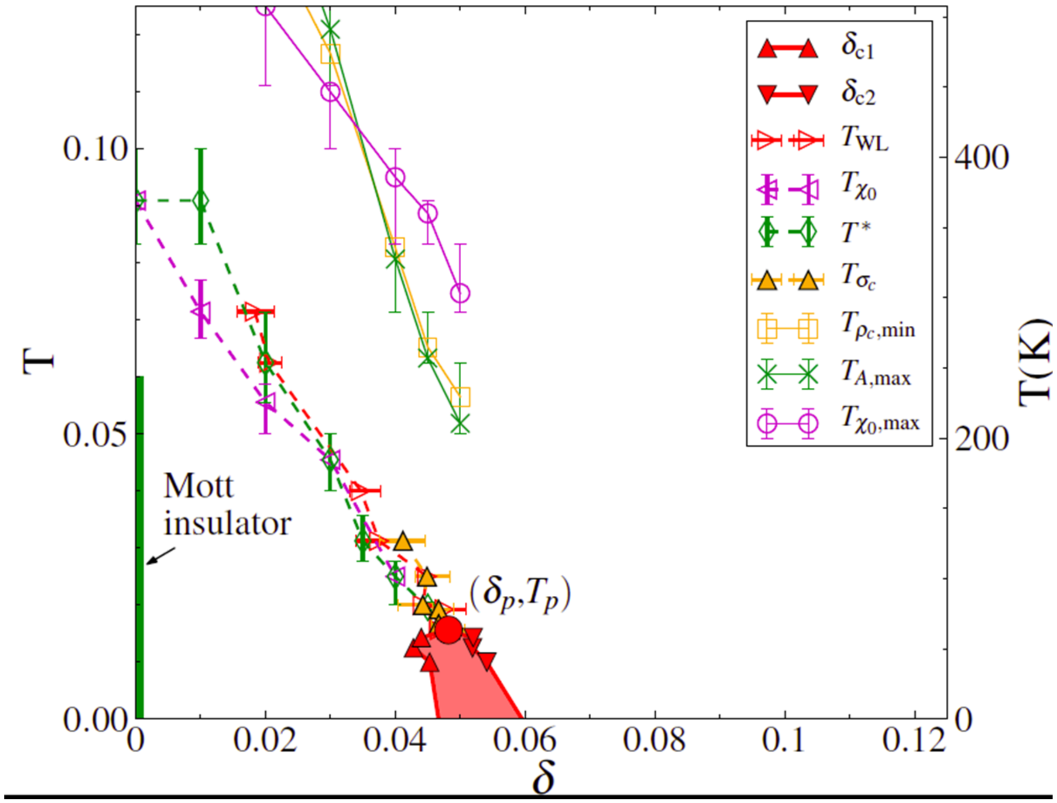


Fig 1 Spin contribution K_s to the ^{89}Y NMR Knight shift [11] for $YBCO_{6.6}$ permit to define the PG onset T^*. Here K_s is reduced by a factor two at $T \sim T^*/2$. The sharp drop of the SC fluctuation conductivity (SCF) is illustrated (left scale) [23]. We report as well the range over which a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

Two crossover lines

Giovanni Sordi

Patrick Sémon



G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)

P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B **89**, 165113/1-6 (2014)

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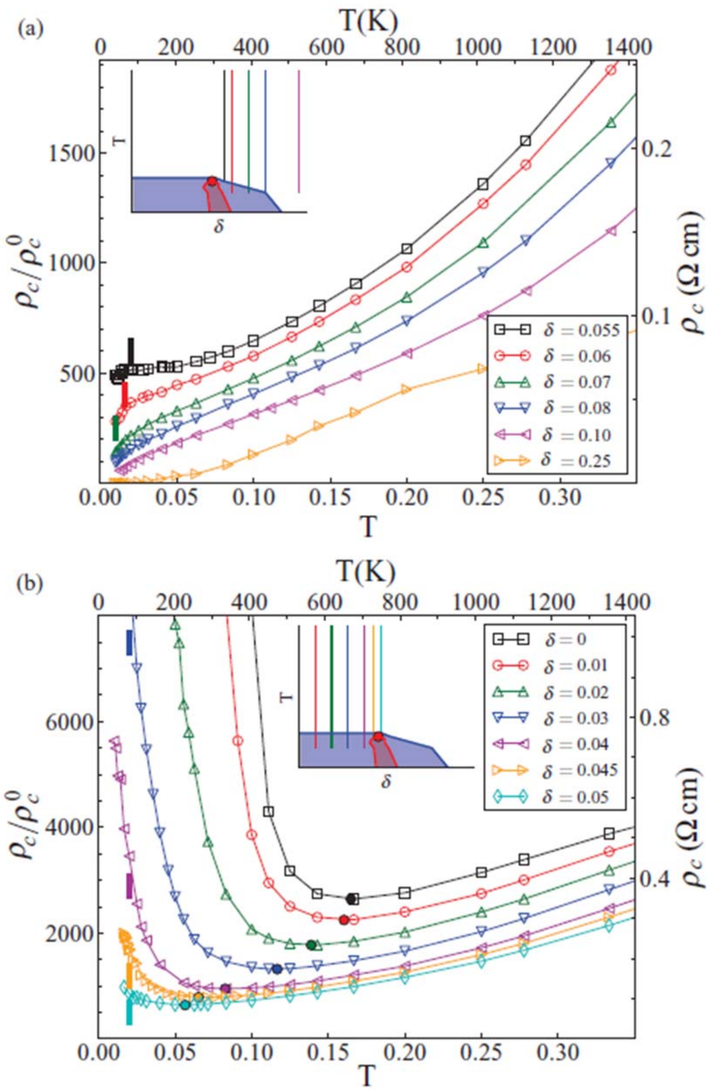
c-axis resistivity



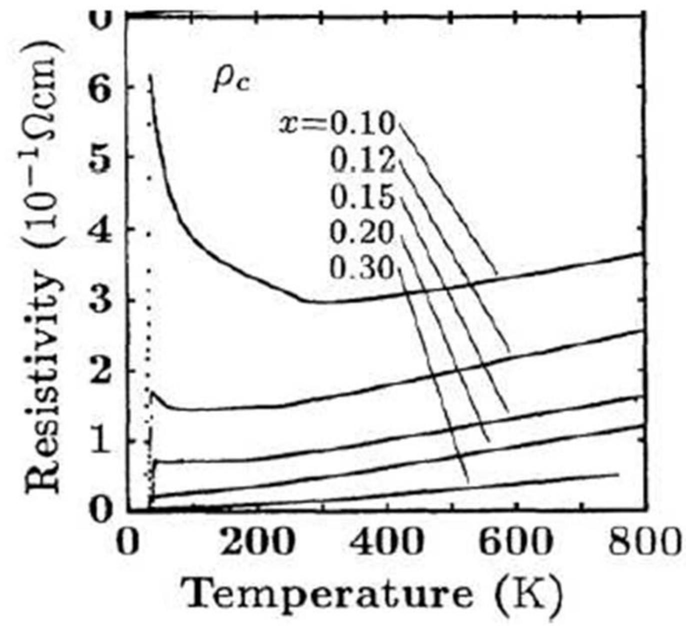


Figure : $La_{2-x}Sr_xCuO_4$ Nakamura et al., PRB 1993

Also K. Takenaka, *et al.*
Phys. Rev.B 50, 6534 (1994).

P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B **89**, 165113/1-6 (2014) UNIVERSITÉ DE SHERBROOKE

Two crossover lines

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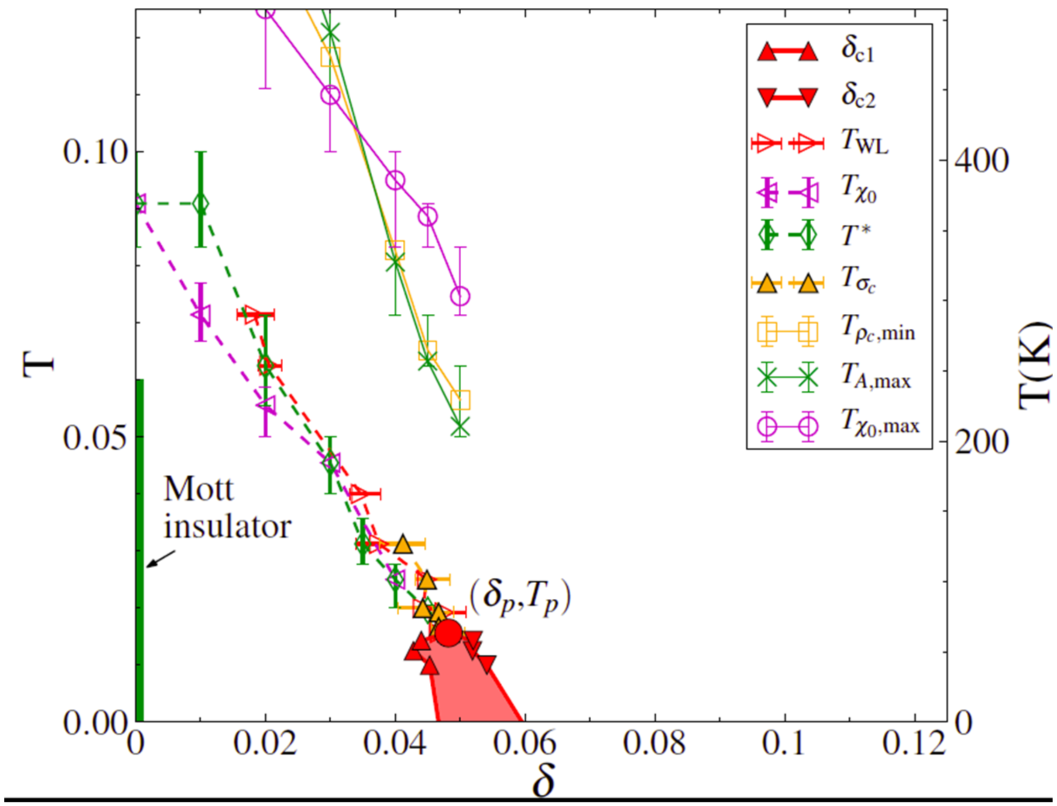

G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)
P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B **89**, 165113/1-6 (2014)

Giovanni Sordi

Patrick Sémon

Kristjan Haul

Widom line *(t' = 0)*

Pseudogap in the normal state and the Widom line

G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)

P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B **89**, 165113/1-6 (2014)

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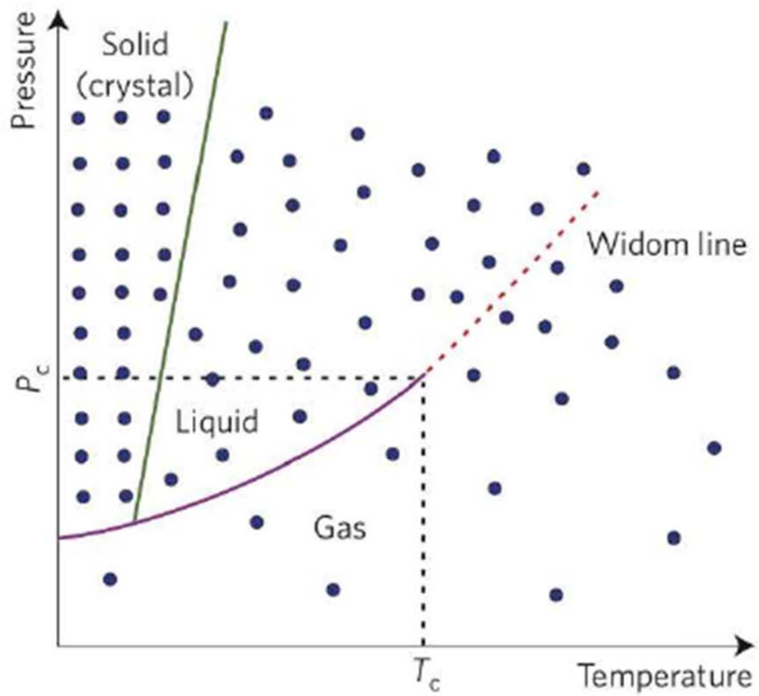
What is the Widom line?



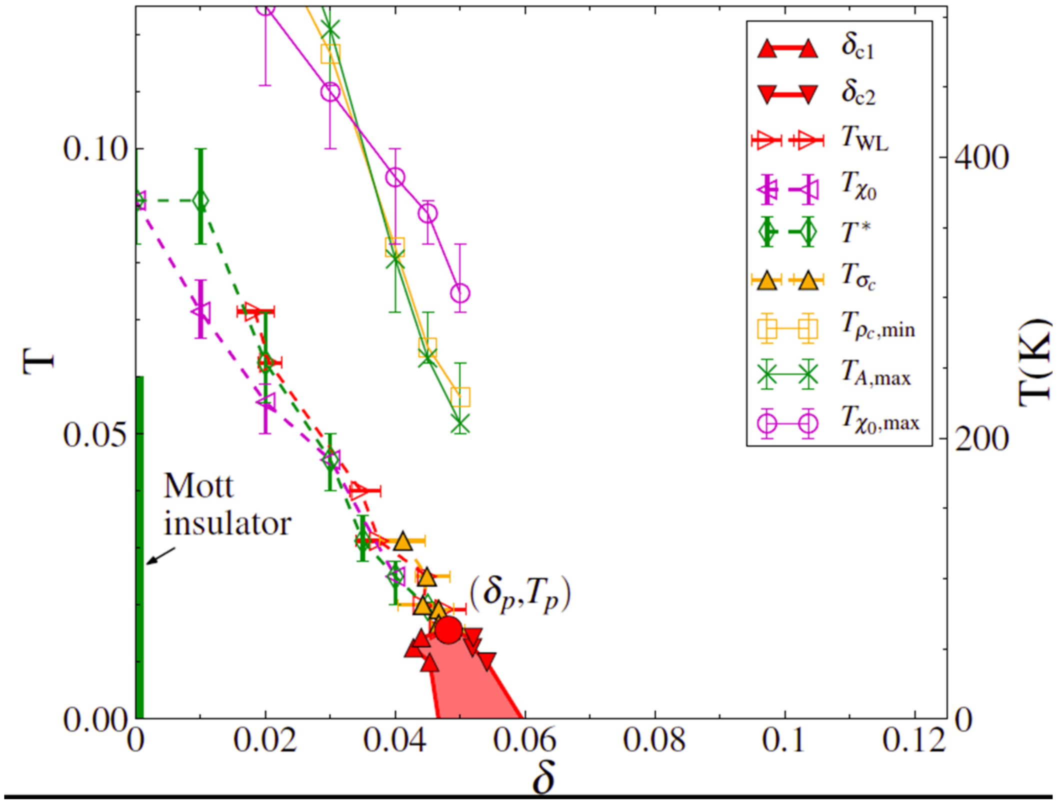
McMillan and Stanley, Nat Phys 2010

- 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

Crossovers and Widom line

Giovanni Sordi

Patrick Sémon



G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)

P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B **89**, 165113/1-6 (2014)

Satoshi Okamoto

David Sénéchal

Marcello Civelli

Maxime Charlebois

Anisotropy (nematicity)

Normal state and large anisotropy

in an *orthorhombic* crystal

ED solver

$t' = -0.3t$

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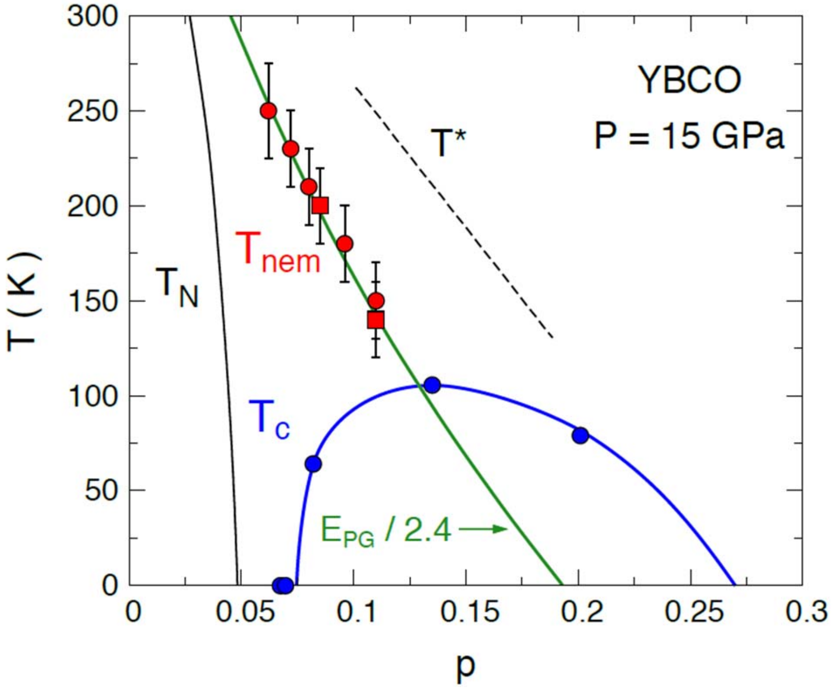
Phase diagram

The central line – $T_x = T_{nem}$

$T_{nem} = E_{PG} / 2.4$



T_{nem} hits T_c dome at peak

Cyr-Choinière *et al*. arXiv:1503.02033

Underdoped metal very sensitive to anisotropy

$$\delta_\sigma = \frac{\sigma_x - \sigma_y}{(\sigma_x + \sigma_y)/2} \qquad t_{x,y} = t(1 \pm \delta_0/2)$$

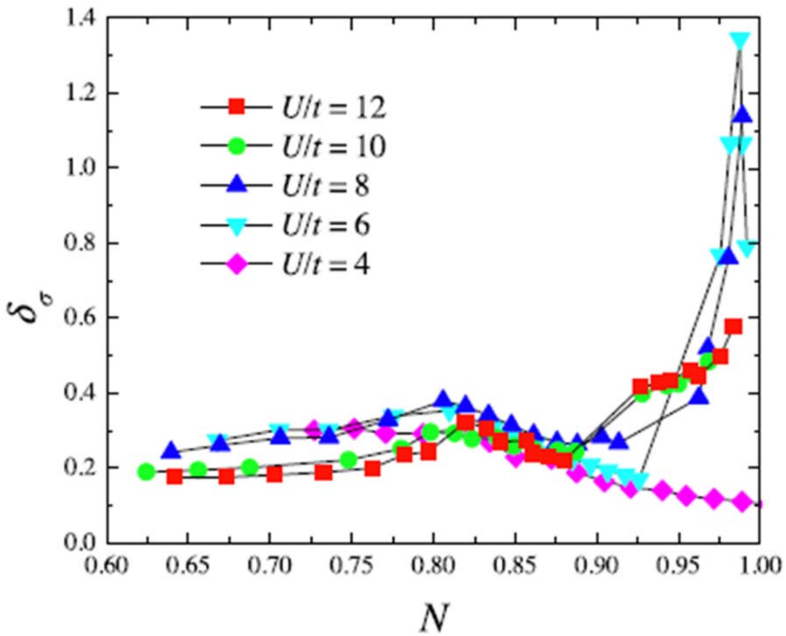
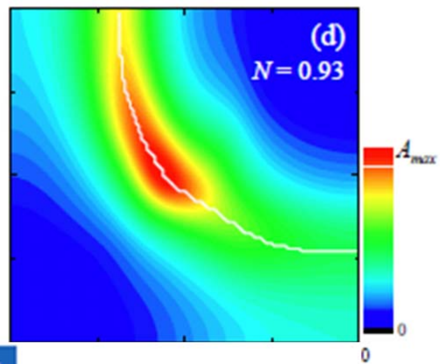
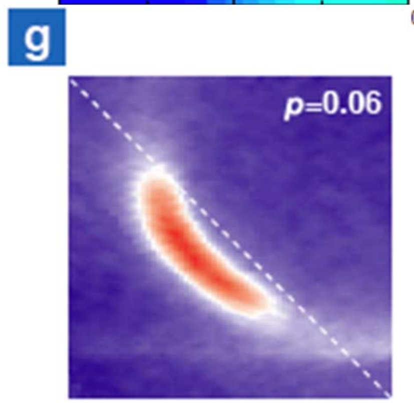


FIG. 3: (Color online) Anisotropy in the CDMFT conductivity $\delta_\sigma = 2\,[\sigma_x(0) - \sigma_y(0)]\,/\,[\sigma_x(0) + \sigma_y(0)]$ as a function of filling N for various values of U and $\eta = 0.1$, $\delta_0 = 0.04$.

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

Dynamical electronic nematicity





D. Fournier *et al.* Nature Physics (2010)

At finite temperature, anisotropy in *Z*

U = 6t,
t'=0
DCA, QMC-Trotter
4x4

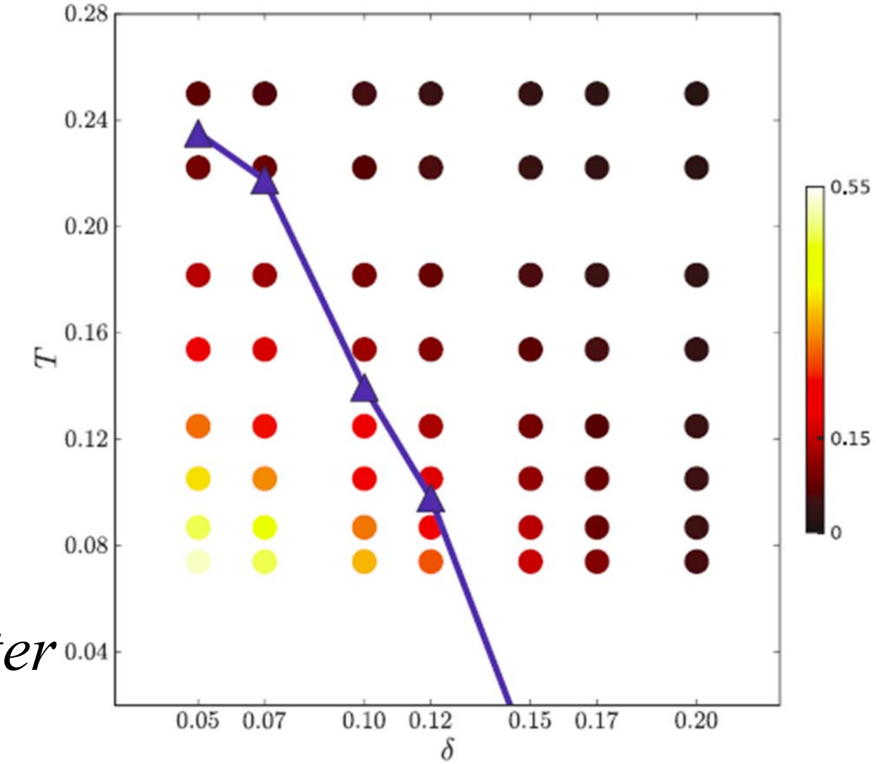


FIG. 3. (Color online) Color map of the anisotropic ratio of the quasiparticle weight σ_Z over the temperature-doping plane, for $U = 6t$. The solid blue curve indicates the pseudogap temperature $T^*(\delta)$ which is obtained as the temperature at which the uniform magnetic susceptibility $\chi_m[q = (0,0), T]$ has a maximum.

Su, Maier, PRB **84**, 220506(R) (2011)

Superconductivity not much influenced by anisotropy in hopping

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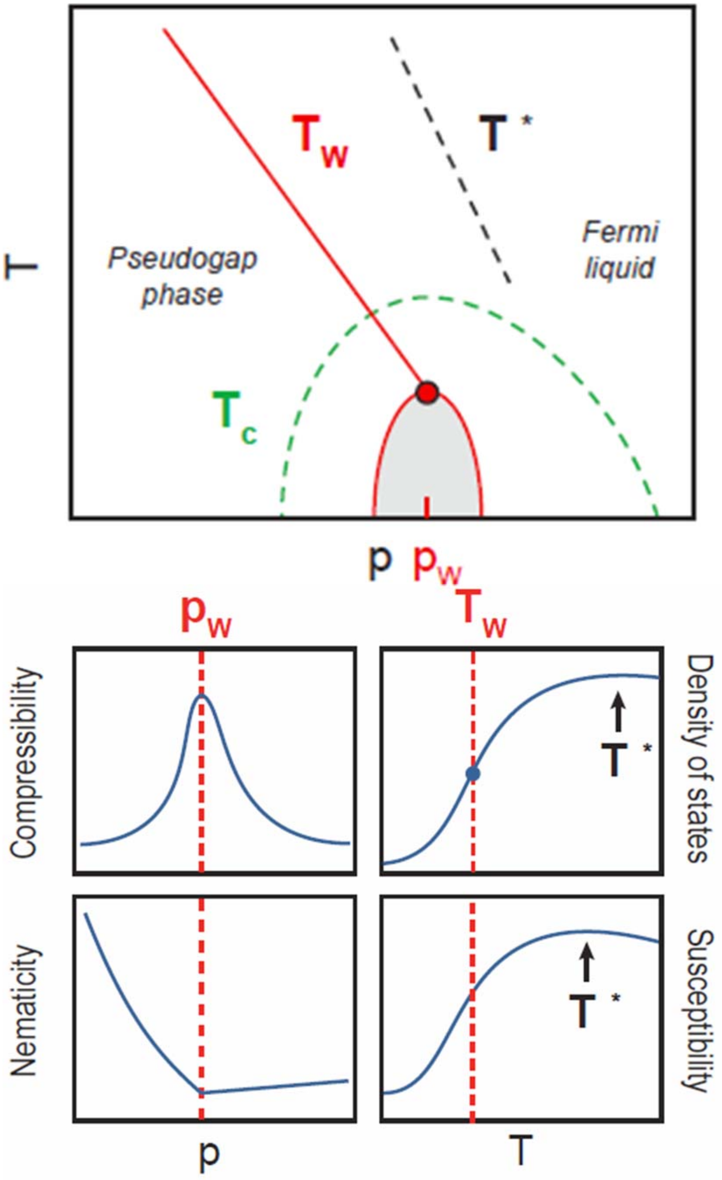
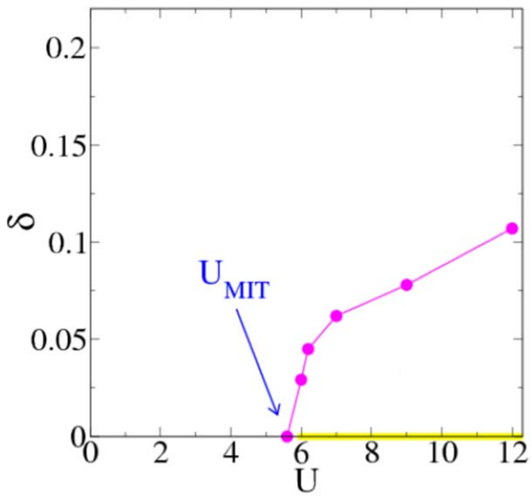
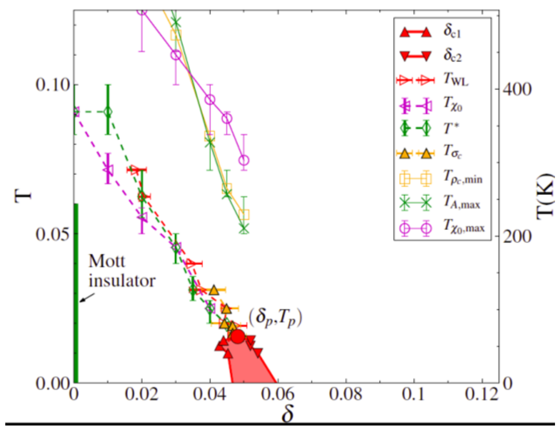
CDMFT: Emergent first-order transition



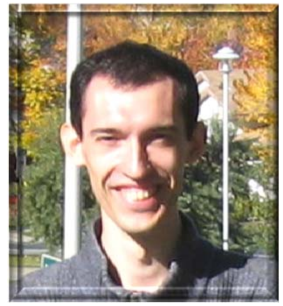
Summary: normal state





- Signatures of Mott physics extend way beyond half-filling
- Pseudogap is a phase
- Pseudogap *T** controlled by a Widom line and its precursor
- High compressibility (stripes?)
- Widom line
  - Thermodynamics (Susceptibility)
  - Transport (c-axis resistivity)
  - DOS

Lorenzo Fratino



Giovanni Sordi

Patrick Sémon

Superconductivity

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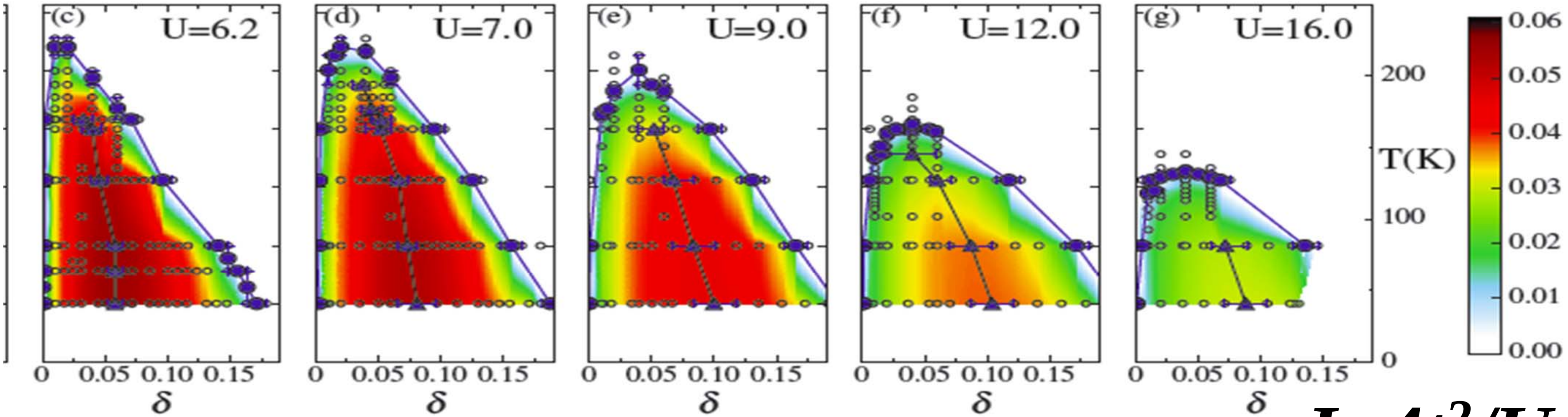
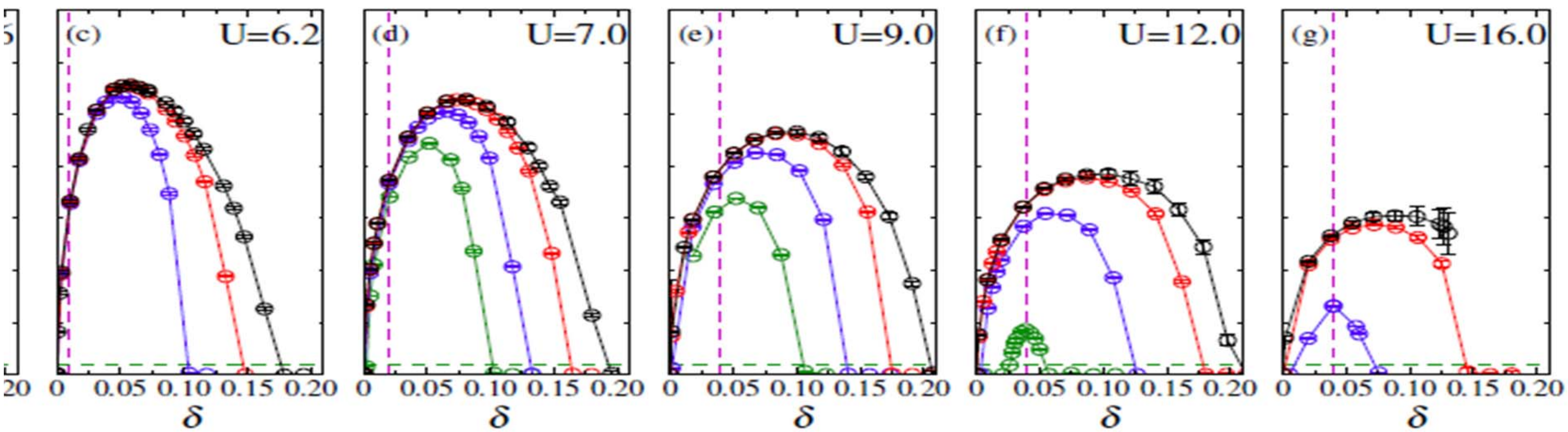
T_c and order parameter, plaquette

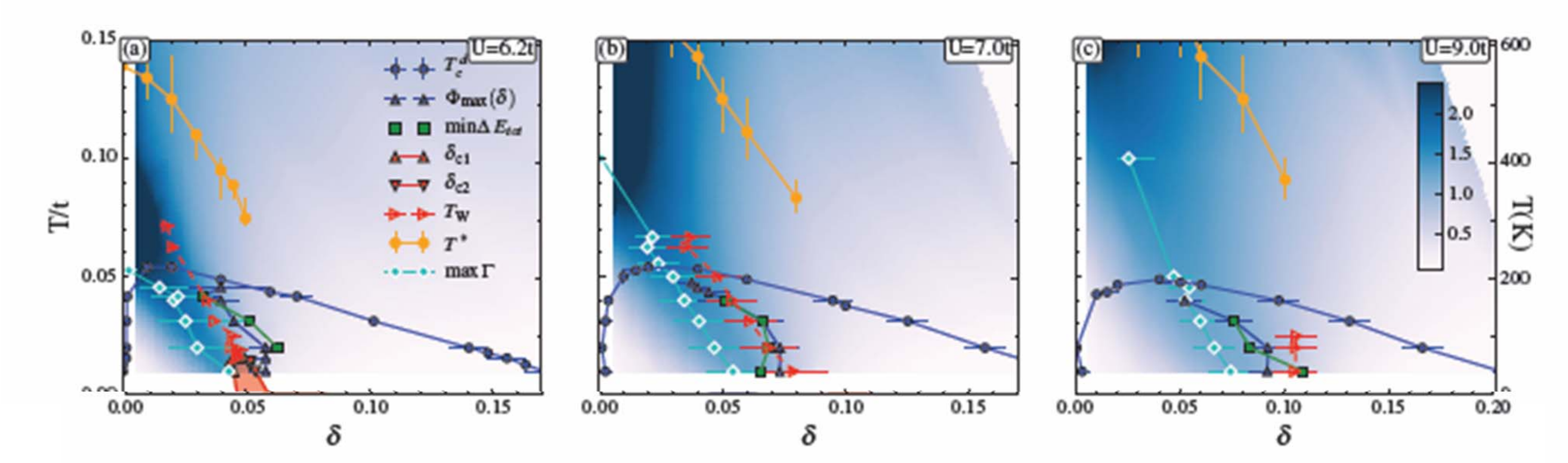


J=4t²/U



L. Fratino, P. Sémon, G. Sordi A.-M.S. T. (unpublished)

Finite-doping first-order transition vs maximum of order parameter



D. J. Scalapino and S. R. White
Phys. Rev. B **58**, 8222 (1998)

Neutron

J.E. Hirsch, F. Marsiglio Physica C **331** 150 (2000)

Condensation energy: mechanism

M. R. Norman, M. Randeria, B. Janko´, and J.C. Campuzano, Phys. Rev. B **61**, 14 742 (2000).

ARPES

H. J. A. Molegraaf, C. Presura, D. van der Marel, P. H. Kes, and M. Li, Science **295**, 2239 (2002).

Optical sum rule

A. F. Santander-Syro, R. P. S.M. Lobo, N. Bontemps,
Z. Konstantinovic, Z. Z. Li, and H. Raffy, Europhys. Lett. **62** 568 (2003)

Optical sum rule

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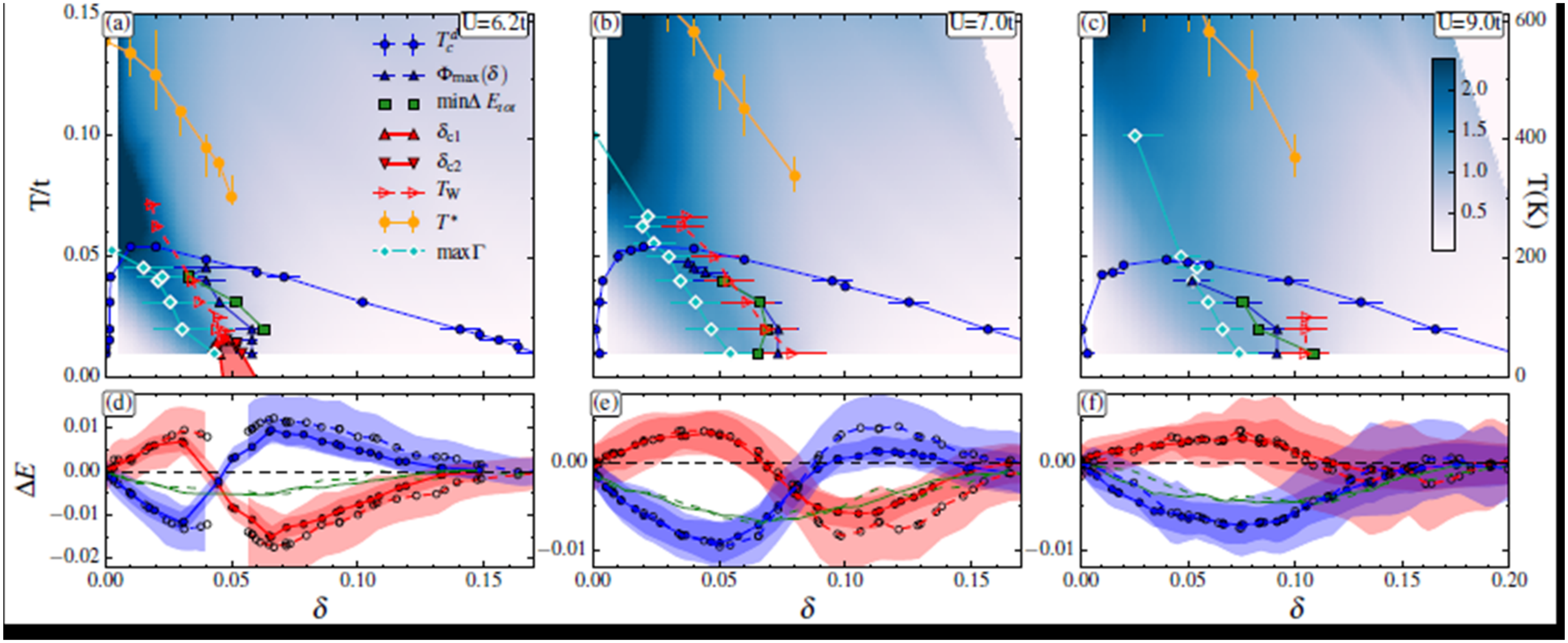
Condensation energy

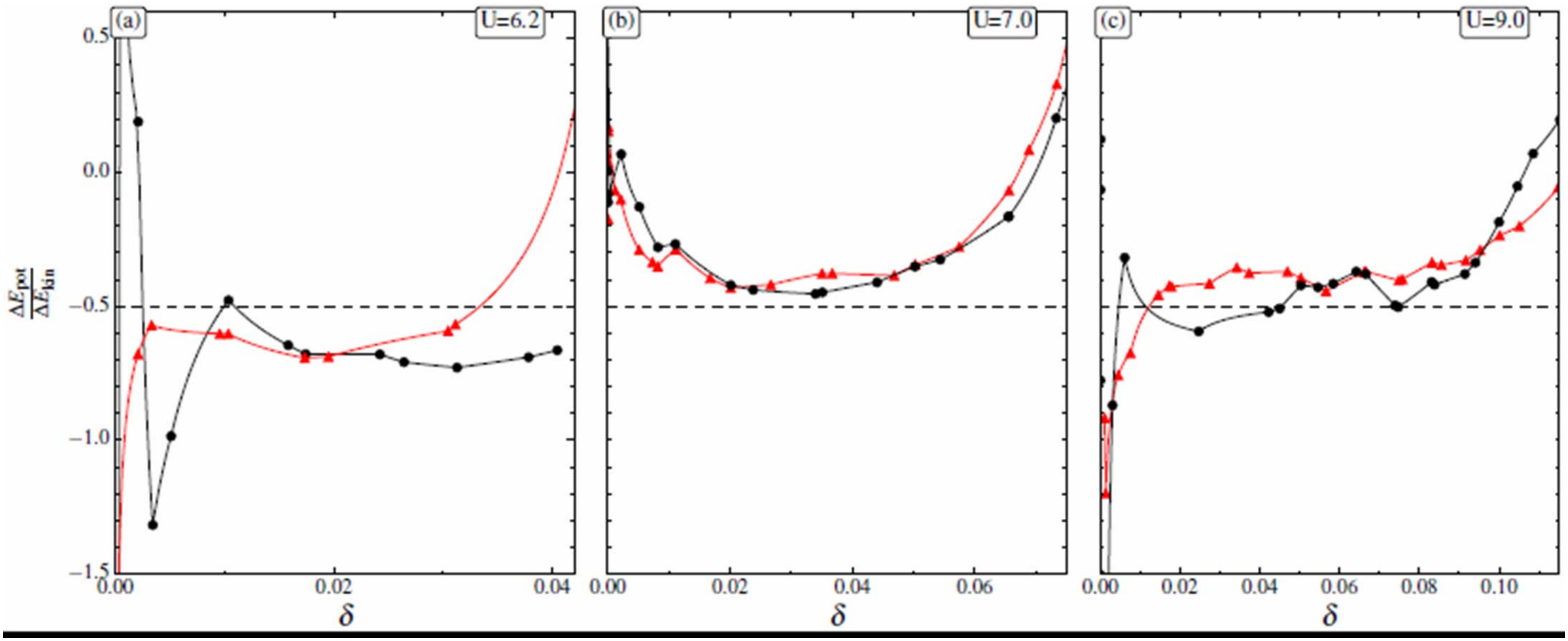


E. Gull, A. Millis, PRB **86**, 241106(R) (2012)

Th. A. Maier, M. Jarrell, et al. PRL **92,** 027005 (2004)

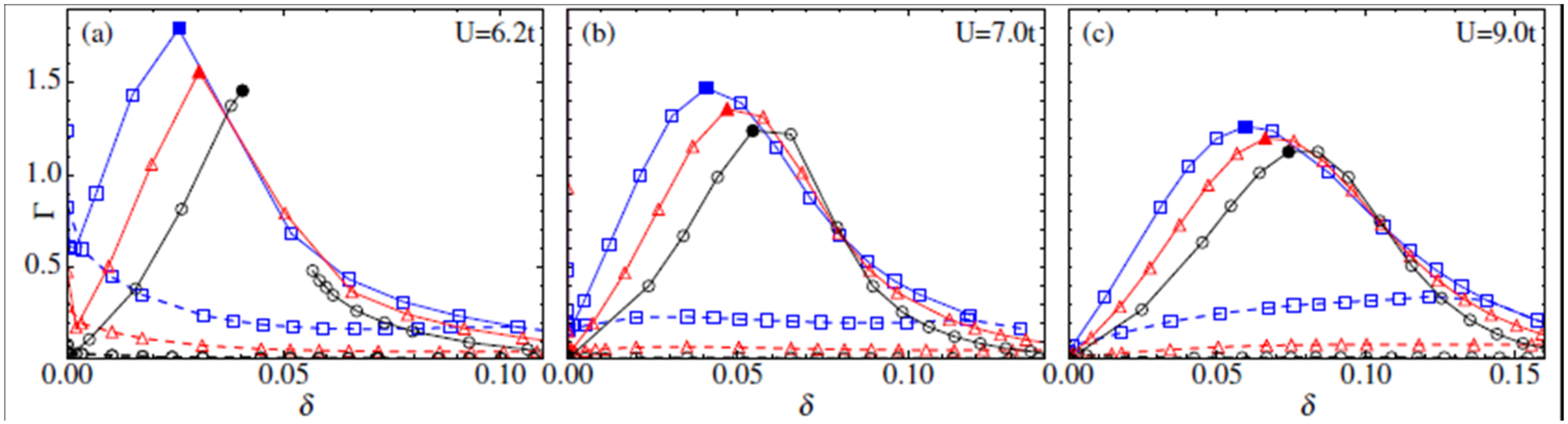
D. J. Scalapino and S. R. White Phys. Rev. B 58, 8222 (1998)

Role of J

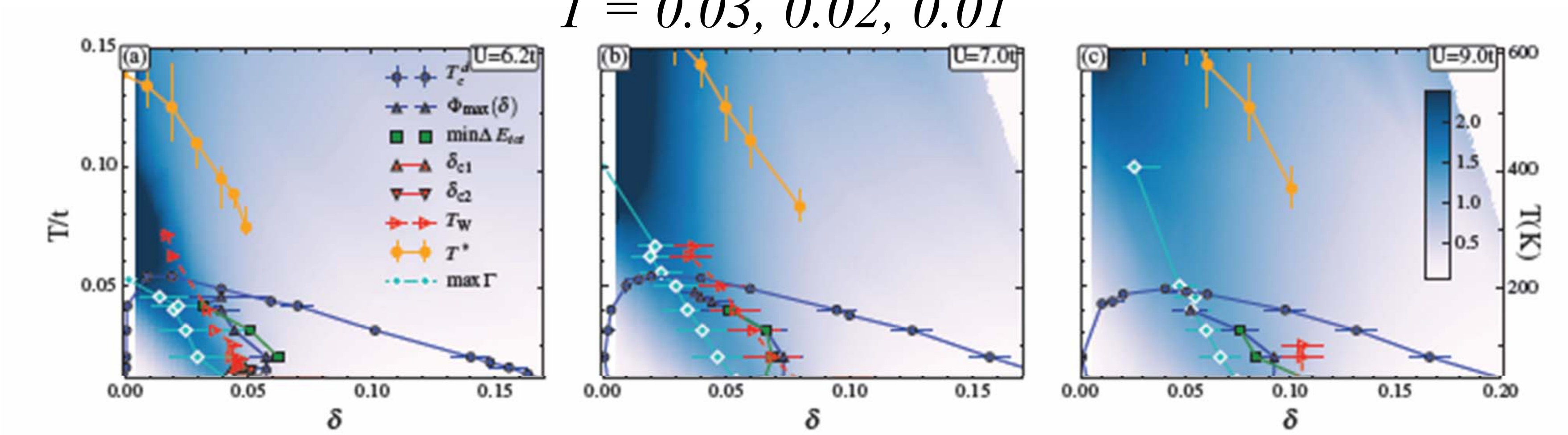


(a)
U=6.2
(b)
U=7.0
(c)
U=9.0
$\frac{\Delta E_{\text{pot}}}{\Delta E_{\text{kin}}}$
0.5
0.0
−0.5
−1.0
−1.5
0.00
0.02
0.04
0.06
0.08
0.10
δ

Kinetic energy gain

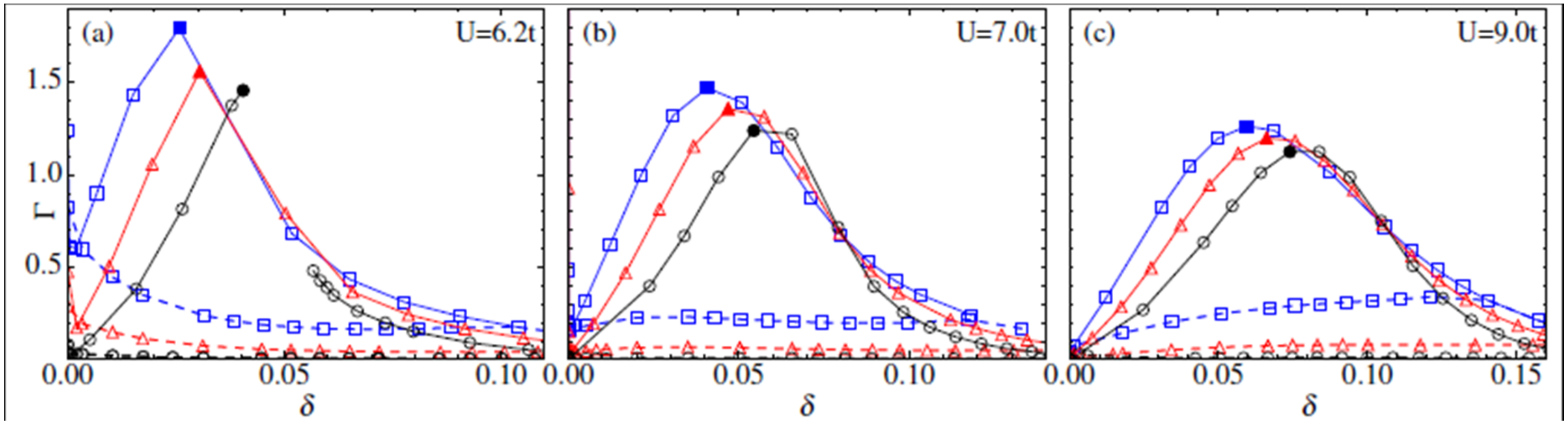


T = 0.03, 0.02, 0.01

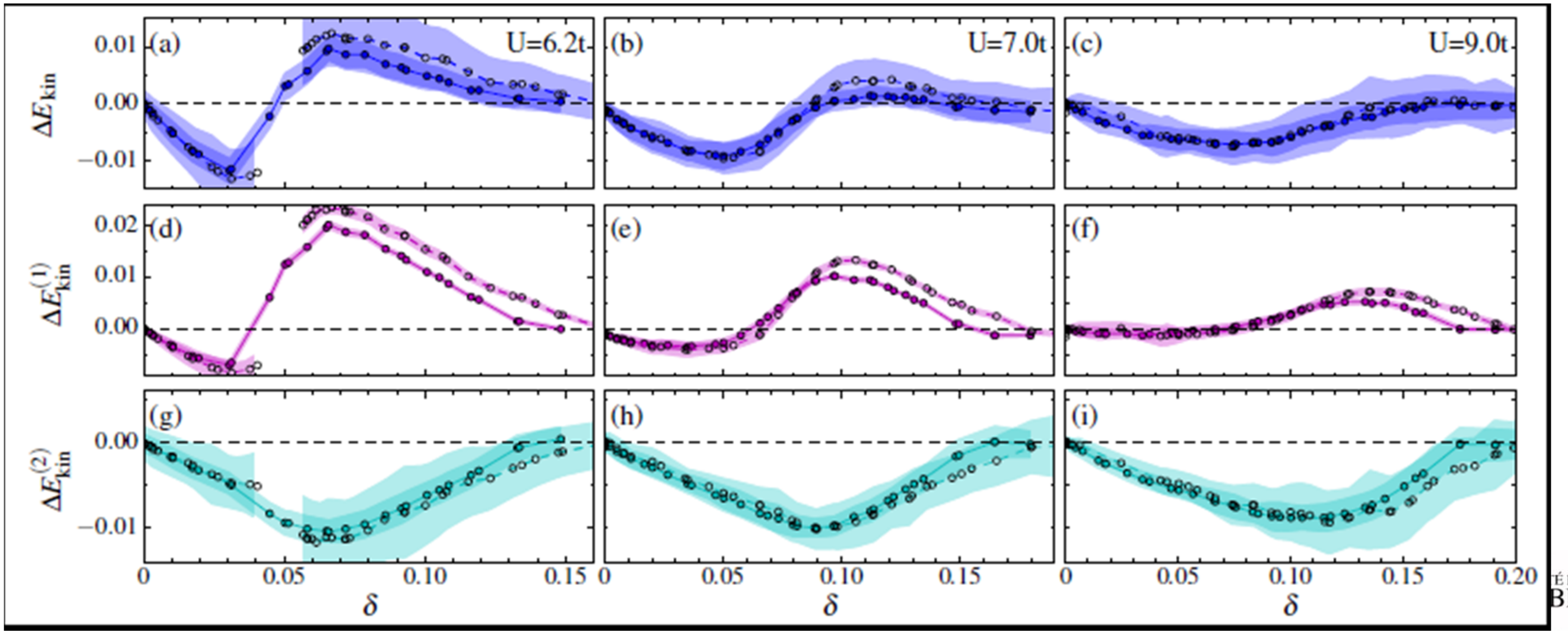


E

Kinetic energy gain



T = 0.03, 0.02, 0.01



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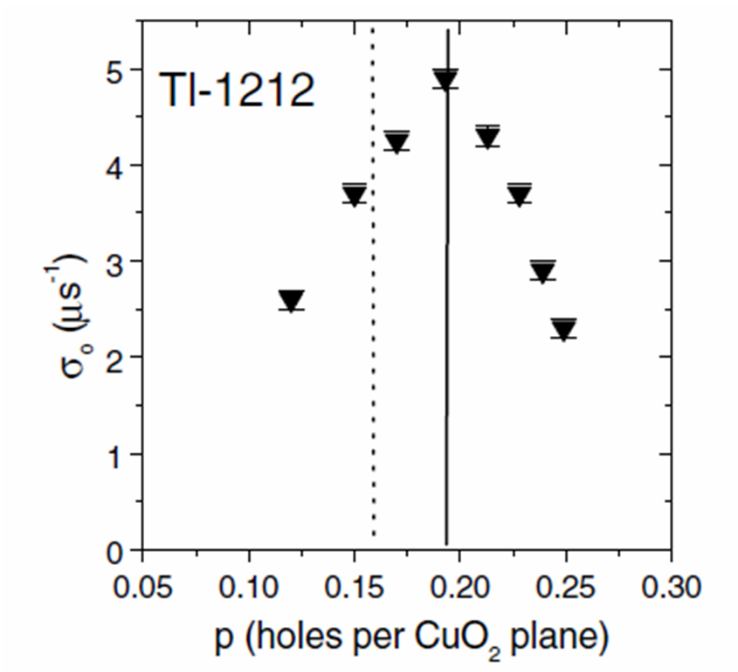
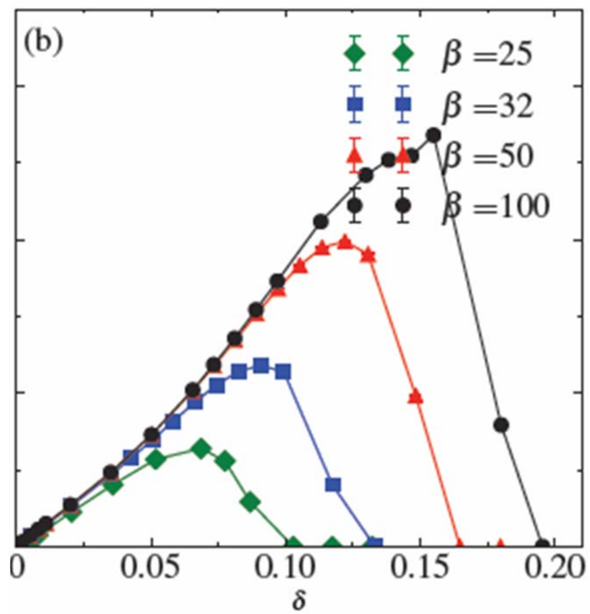
c-axis superfluid stiffness

Experiment – theory ($T \rightarrow 0$)





$U = 7$

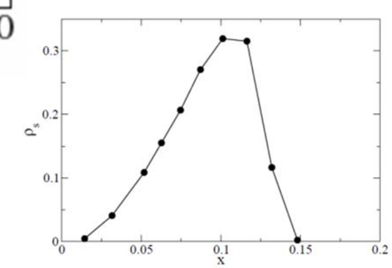
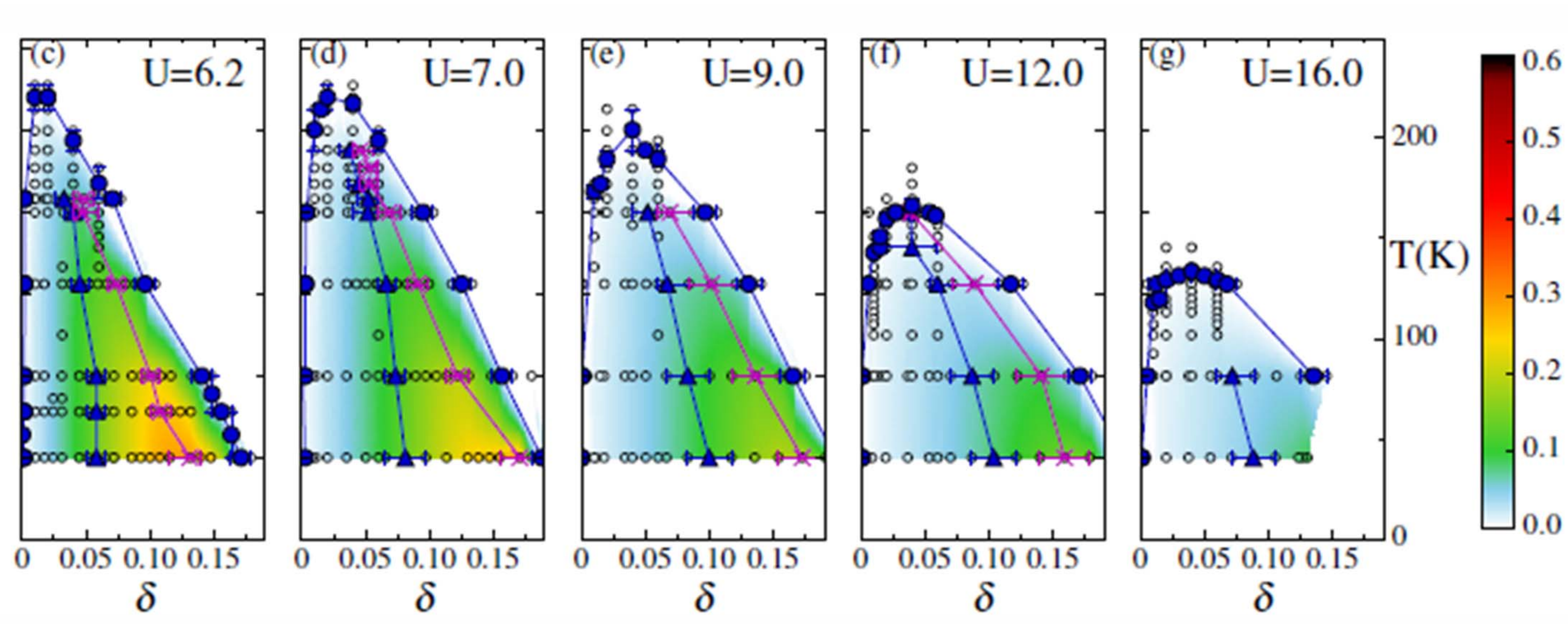


FIG. 8. Superfluid stiffness ρ_s determined in the superconducting state at $T = t/60$ from Eq. 15, as a function of doping.

C. Bernhard, J. L. Tallon, *et al.* PRL (2001)

E. Gull, A.J. Millis,
Phys. Rev. B **88**, 075127 (2013)

Maximum $T \rightarrow 0$ superfluid stiffness does not correspond to maximum T_c



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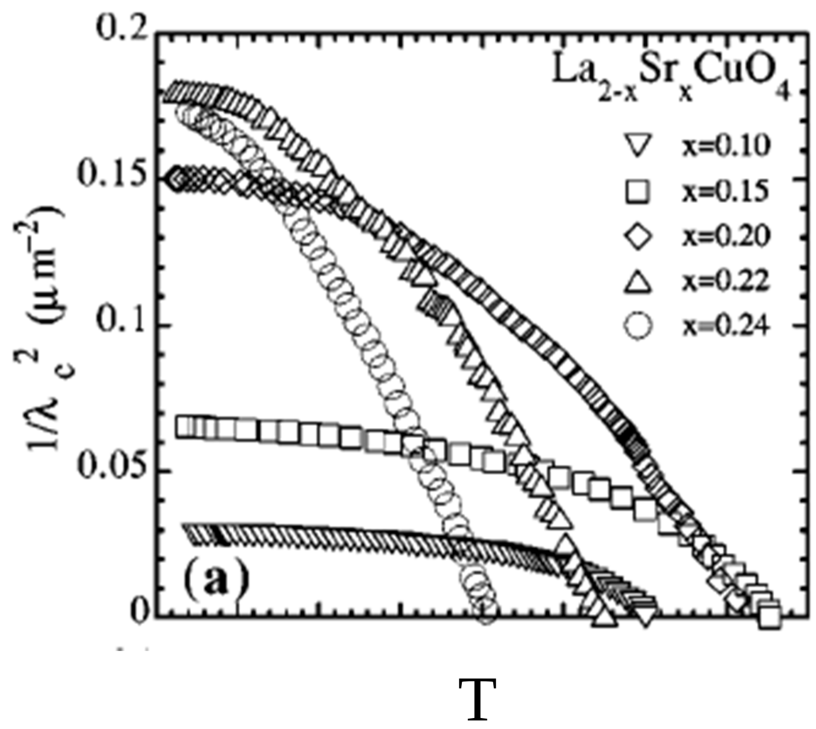
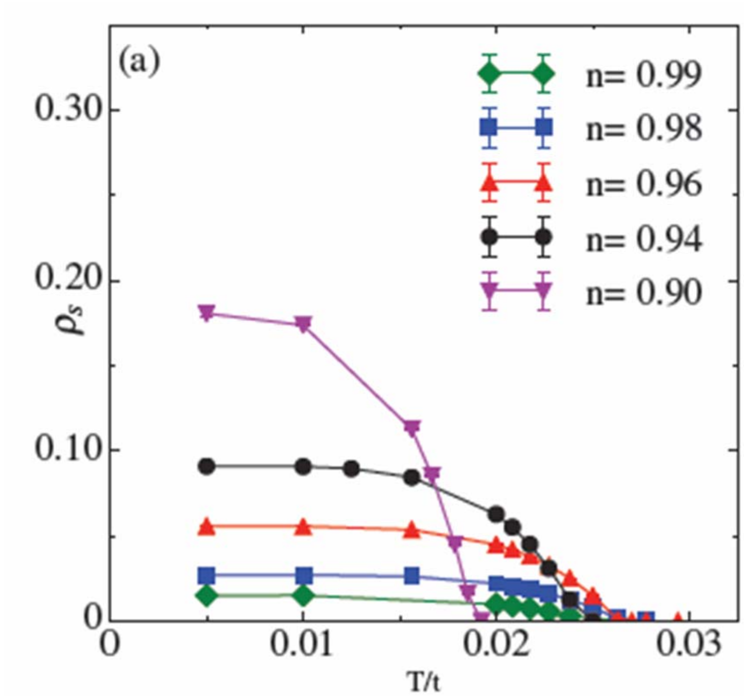
Experiment – theory *T* dependence

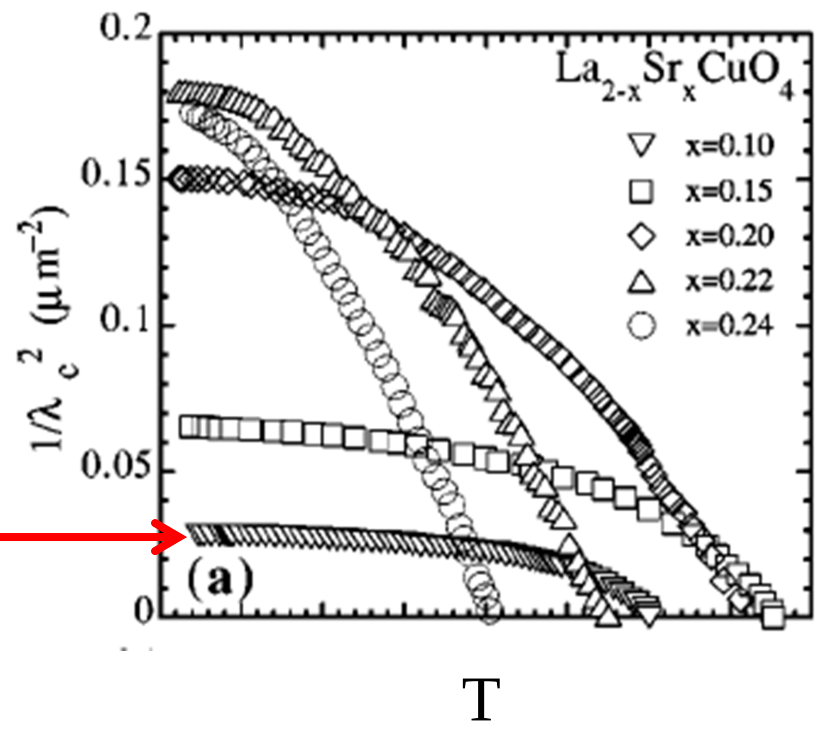
U = 7

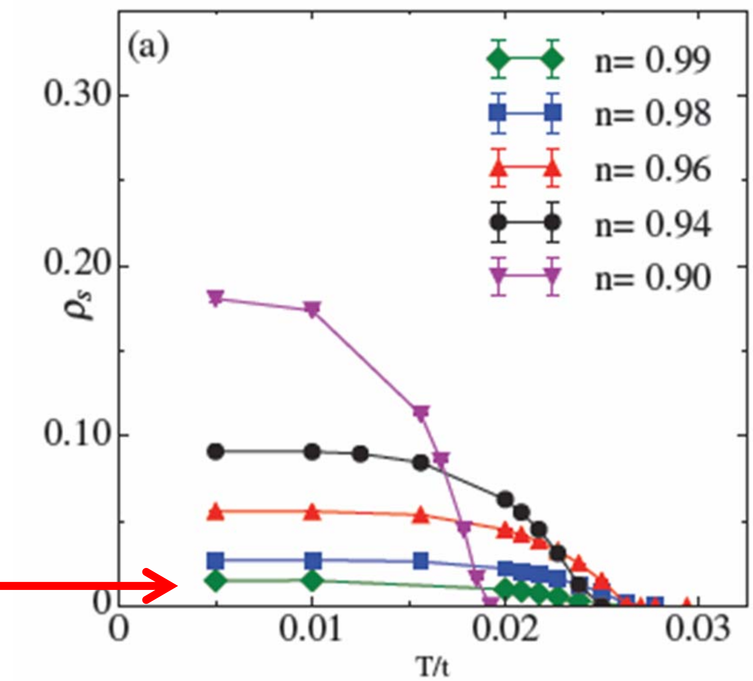




Panagopoulos et al. PRB 2000

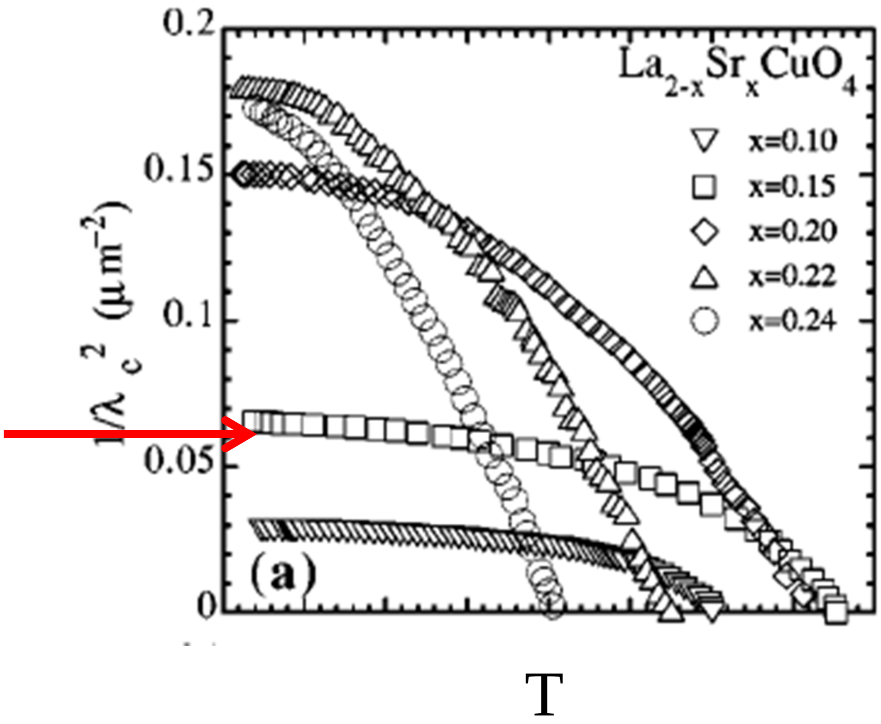
Experiment – theory *T* dependence

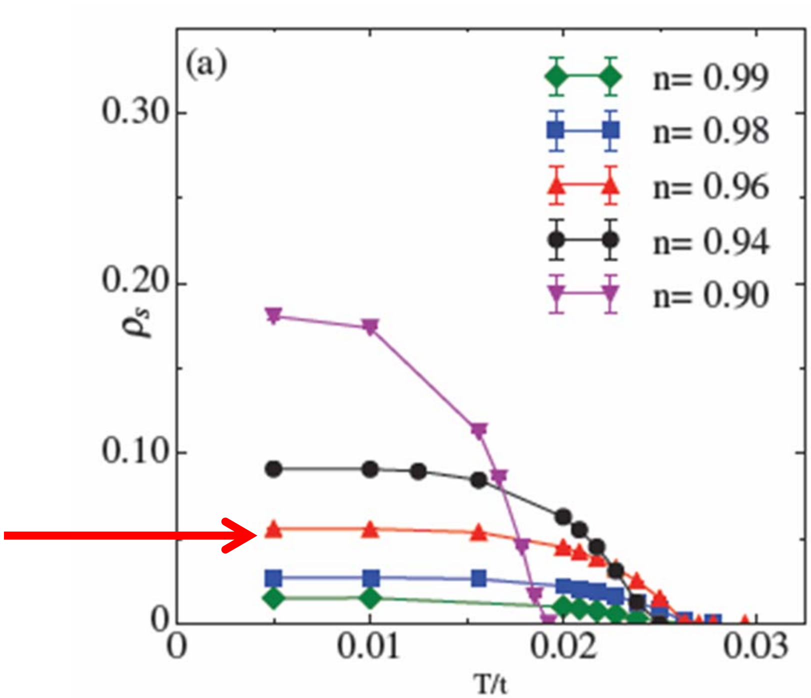




Panagopoulos et al. PRB 2000

Experiment – theory *T* dependence





Panagopoulos et al. PRB 2000

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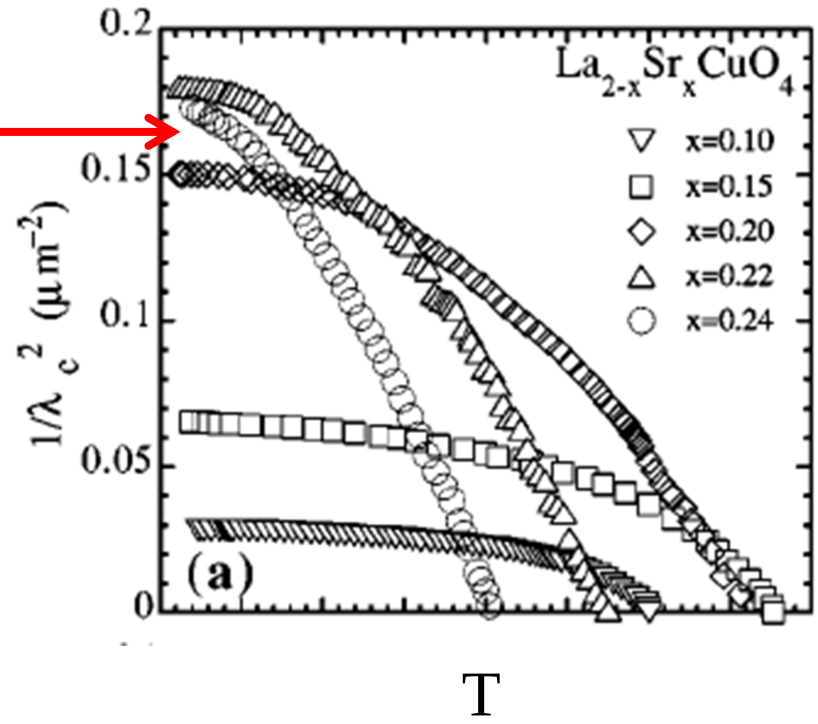
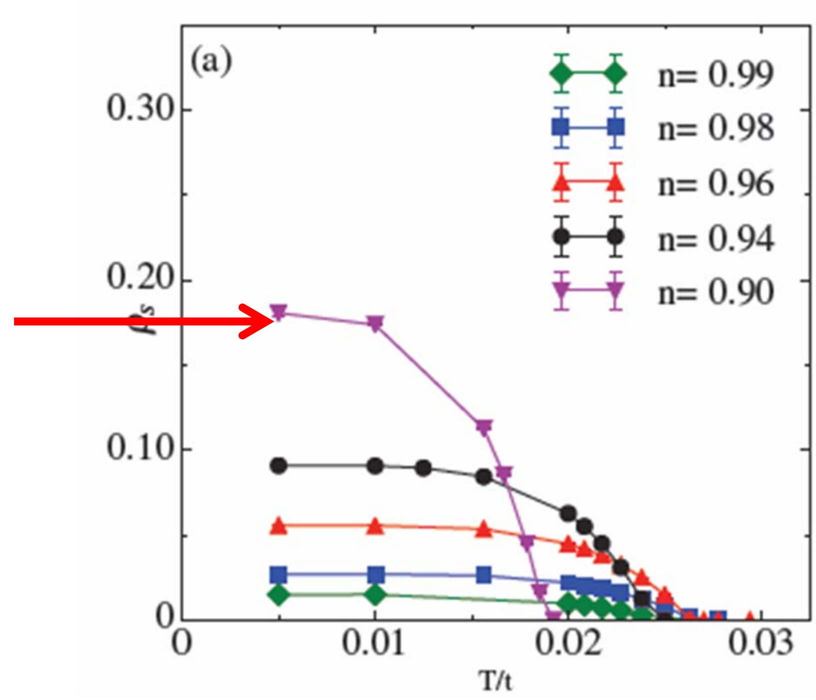
Experiment – theory T dependence





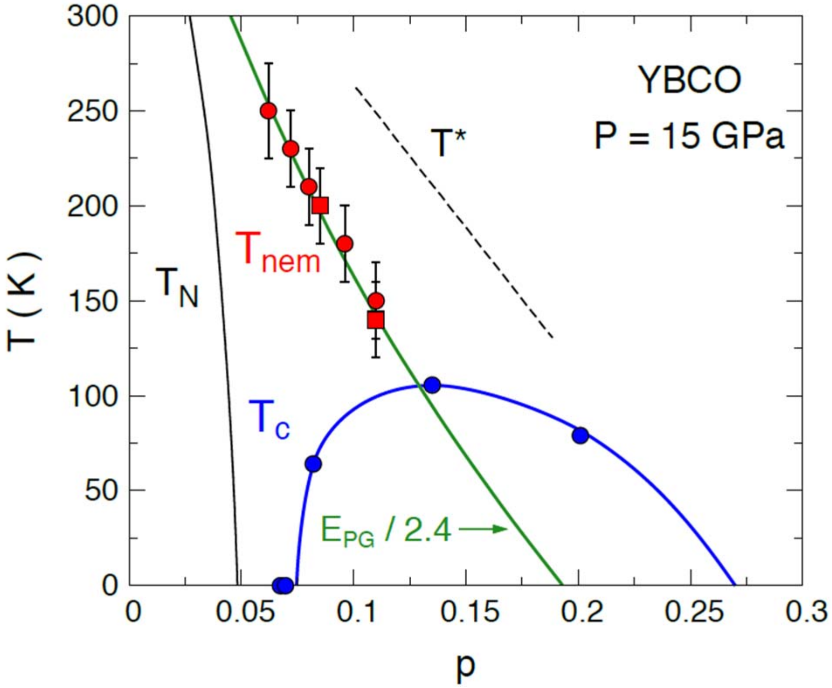
Panagopoulos et al. PRB 2000

Summary

Summary

The central line – T_x = T_{nem}

$T_{nem} = E_{PG} / 2.4$



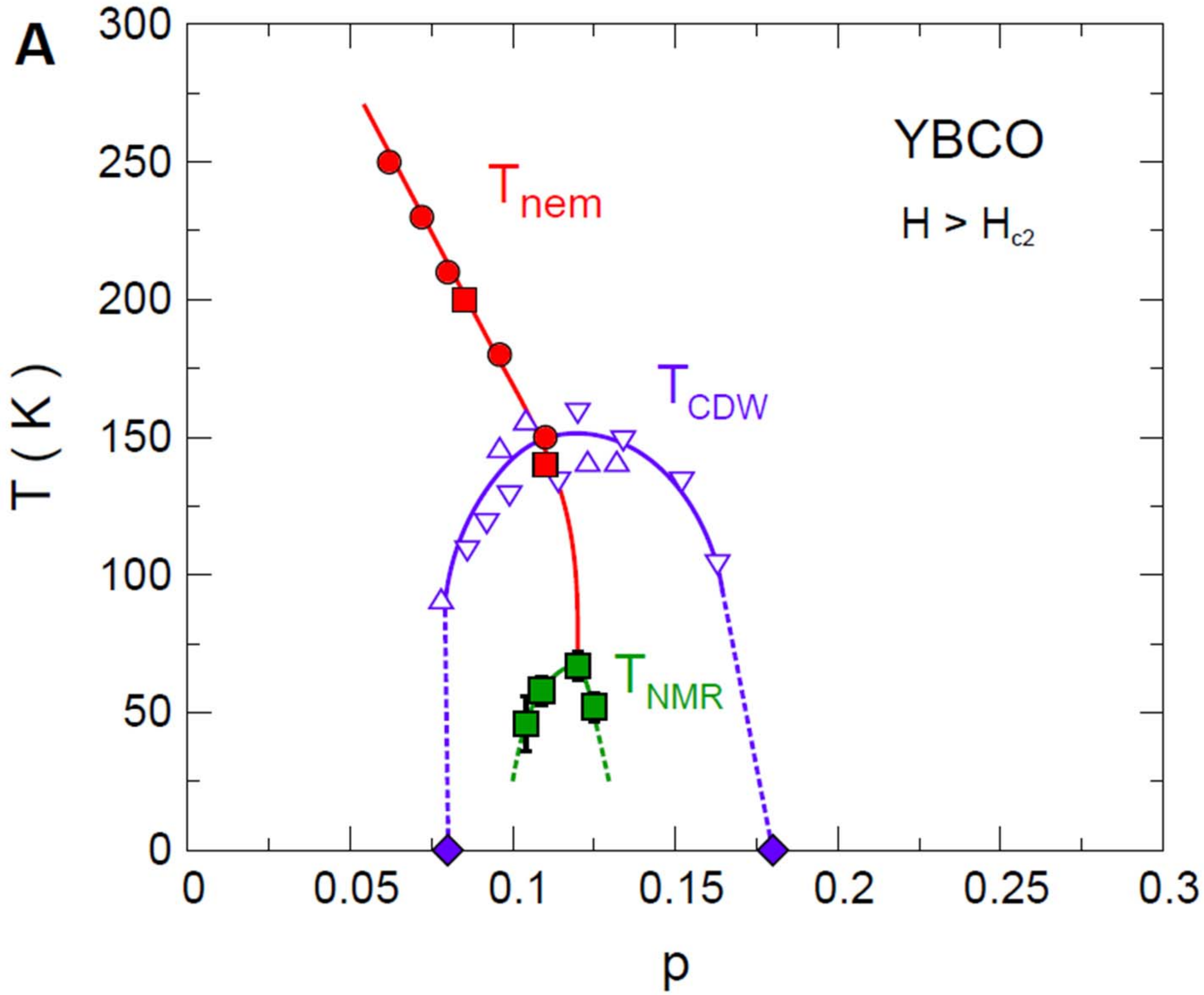
T_{nem} hits T_c dome at peak

Cyr-Choinière *et al*. arXiv:1503.02033

Summary

- With a single theoretical framework,
- Essential physics is described by the one-band Hubbard model
  - Mott + short-range superexchange leads to an emergent phase transition that is an organizing principle for both
    - normal state properties, including pseudogap
    - non BCS features of the normal state (Potential vs Kinietic energy driven…)

Two speculations



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To do

- Effect of *t'* (Sordi, Fratino, Sémon)
- Three-band model (Sordi, Fratino, Sémon)
- Nematicity at finite T
- Nematicity CDW at $T = 0$ (Maxime Charlebois)
- STM at $T = 0$ (Simon Verret)
- Transport properties (Anne-Marie Gagnon)
- Effect of V on pairing (Alexis Reymbaut, Marco Fellous Asiani)
- Iron oxides (Reza Nourafkan)

Main collaborators

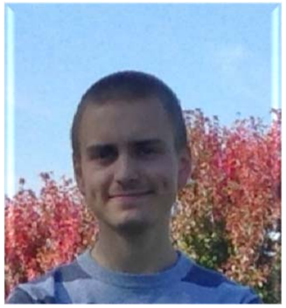
Giovanni Sordi

Patrick Sémon

Kristjan Haule

David Sénéchal

Lorenzo Fratino



Charles-David Hébert

Bumsoo Kyung

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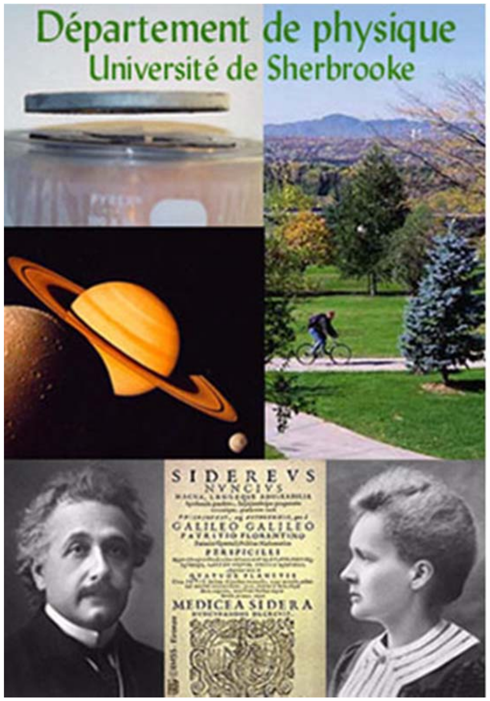
Team

Tremblay, Reymbaut, Gagnon, Verret, Hébert, Charlebois, Nourafkan



André-Marie Tremblay

CANADA RESEARCH CHAIRS
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Calcul Québec

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Review: A.-M.S.T. arXiv: 1310.1481

Merci

Thank you

A.-M.S. Tremblay

"Strongly correlated superconductivity"

Chapt. 10 : *Emergent Phenomena in Correlated Matter Modeling and Simulation, Vol. 3,* E. Pavarini, E. Koch, and U. Schollwöck (eds.)
Verlag des Forschungszentrum Jülich, 2013