Repelled, yet attracted: the case of strongly correlated superconductivity

A.-M. Tremblay

G. Sordi, K. Haule, D. Sénéchal, C.-D. Hébert

P. Sémon, B. Kyung, G. Kotliar

CIFAR
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McGill, 26 February, 2015

VERITATEM IN CHARITATE

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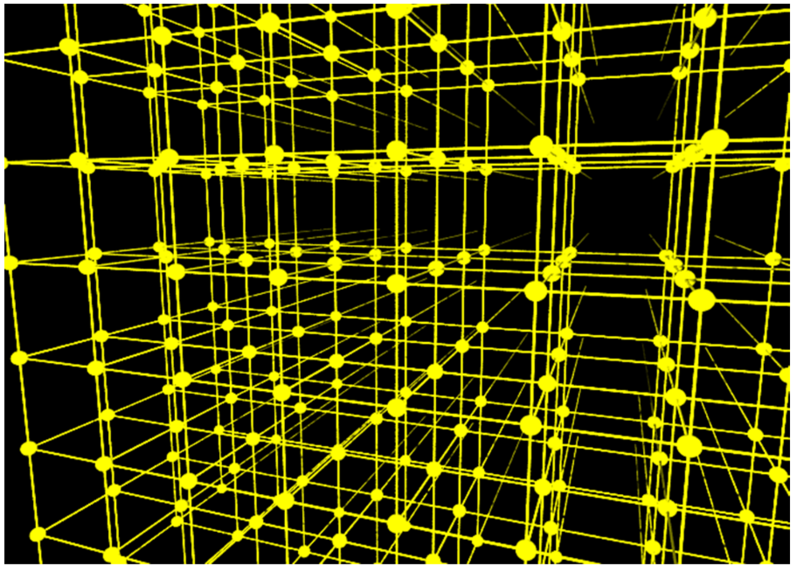
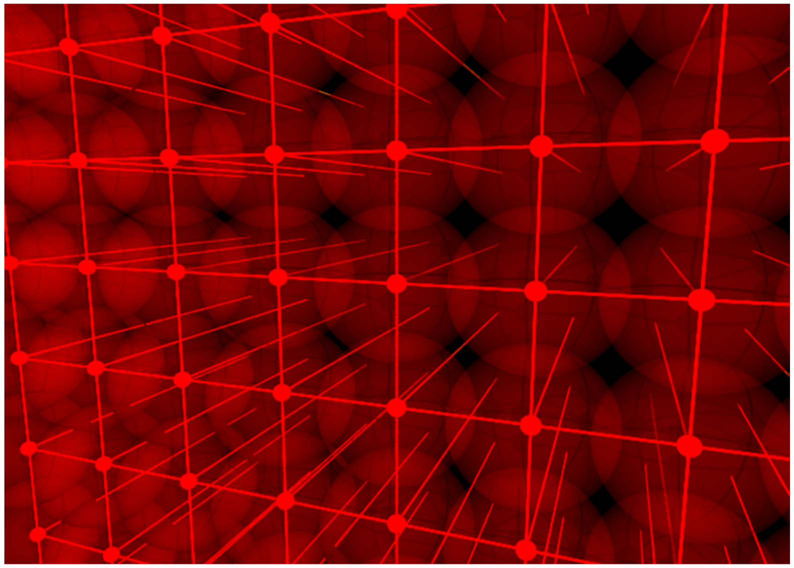
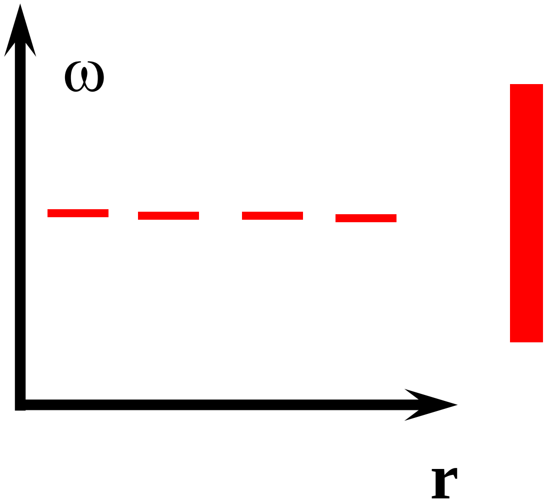
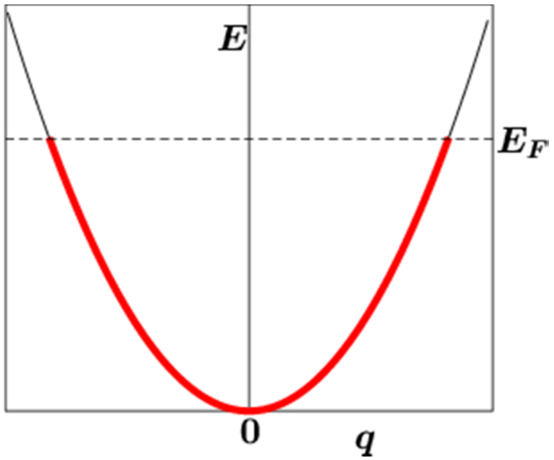
How to make a metal







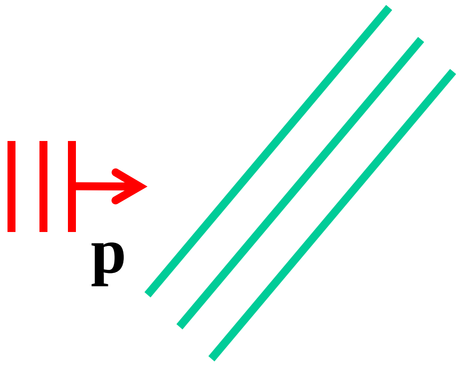


Courtesy, S. Julian

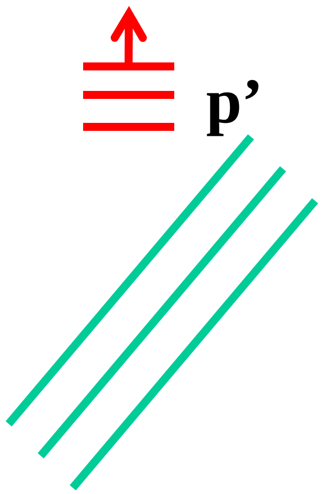
Superconductivity

Superconductivity

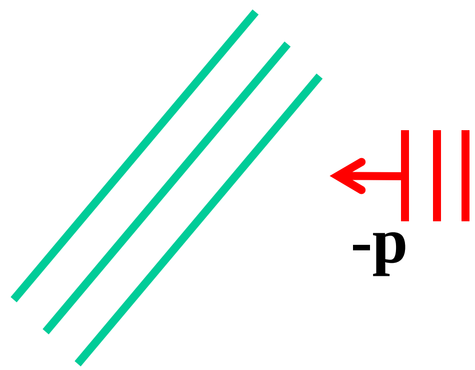
Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



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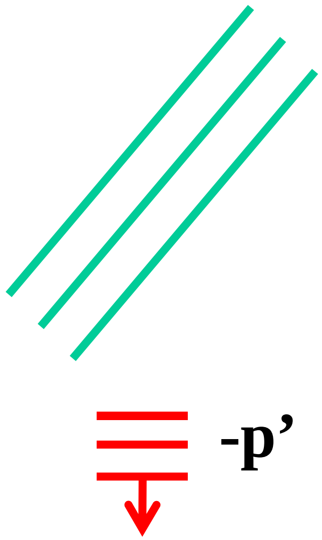
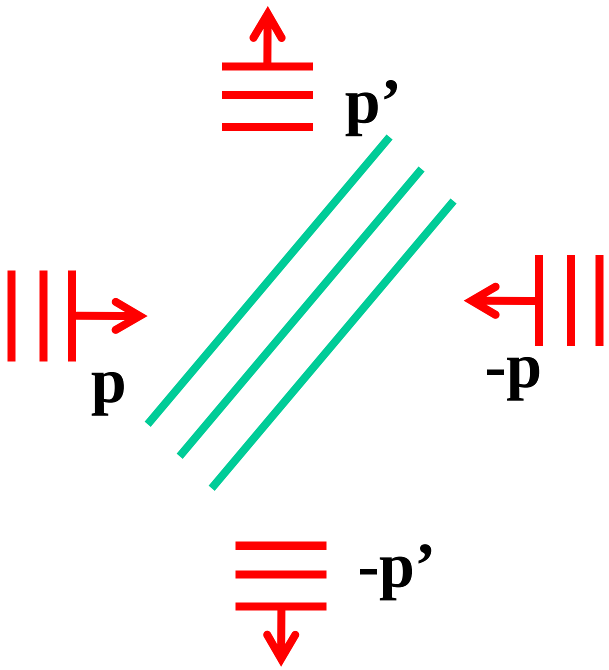
Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



#1 Cooper pair, #2 Phase coherence

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

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

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

Half-filled band is metallic?

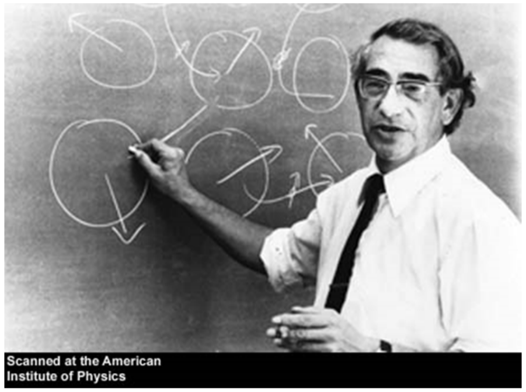
Half-filled band: Not always a metal

NiO, Boer and Verway

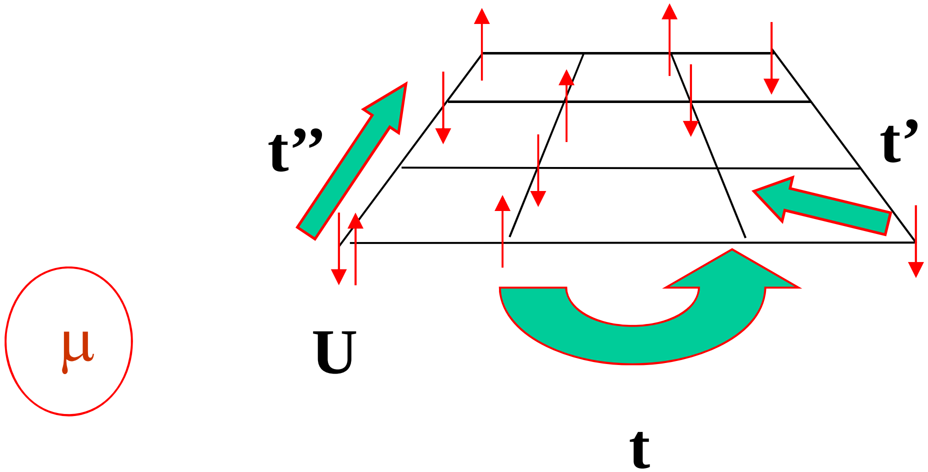
Peierls, 1937

Mott, 1949

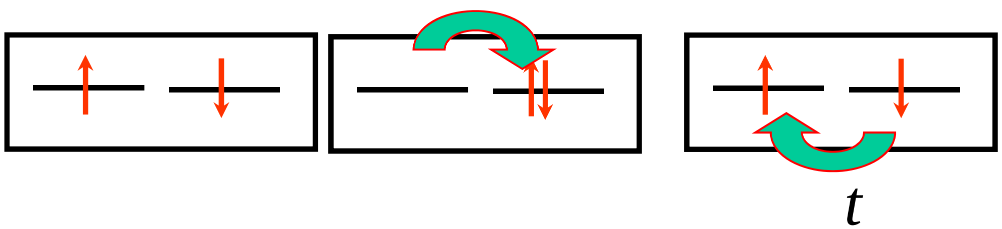
Hubbard model



1931-1980



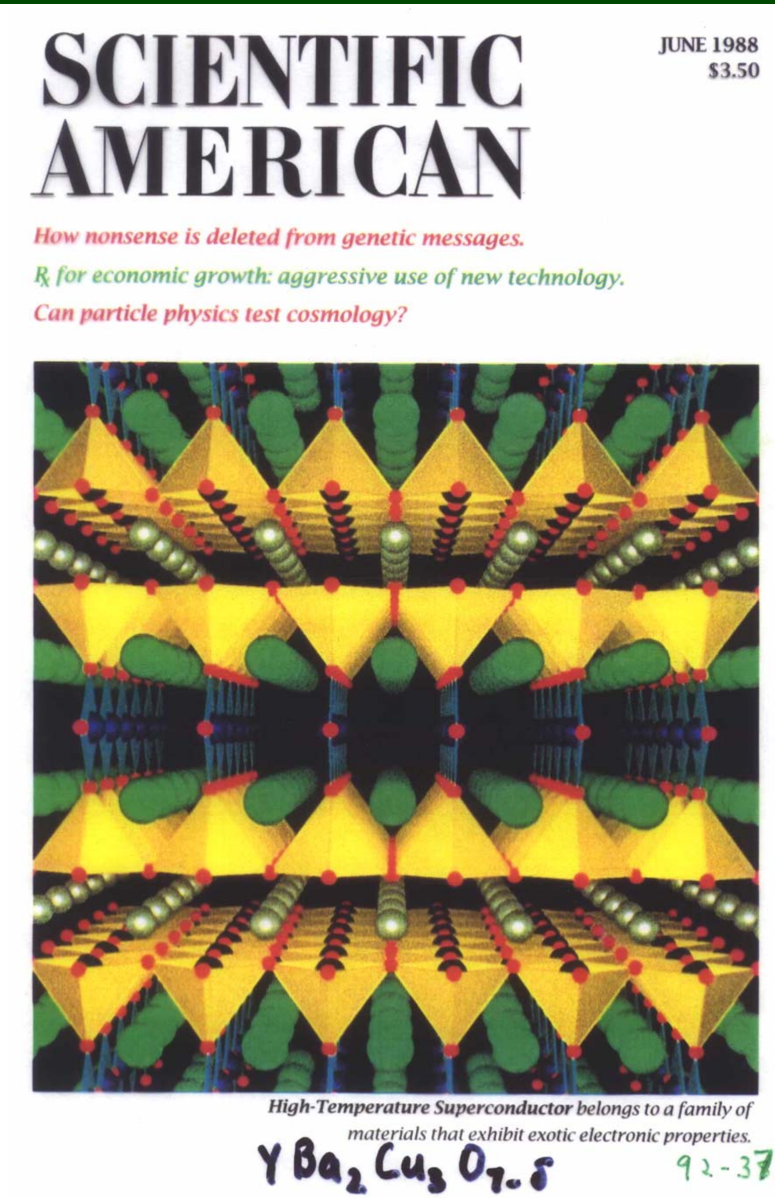
$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c_{i\sigma}^{\dagger}c_{j\sigma} + c_{j\sigma}^{\dagger}c_{i\sigma}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

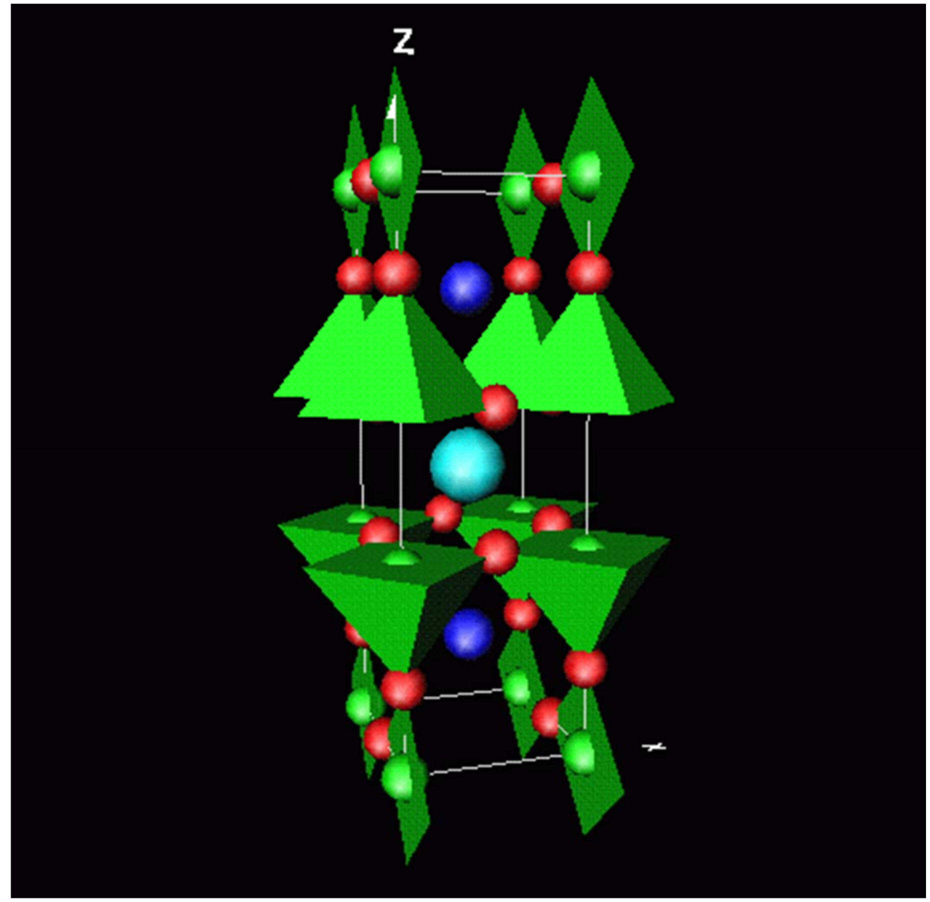


Effective model, Heisenberg: $J = 4t^2/U$

Superconductivity and attraction?

Cuprates





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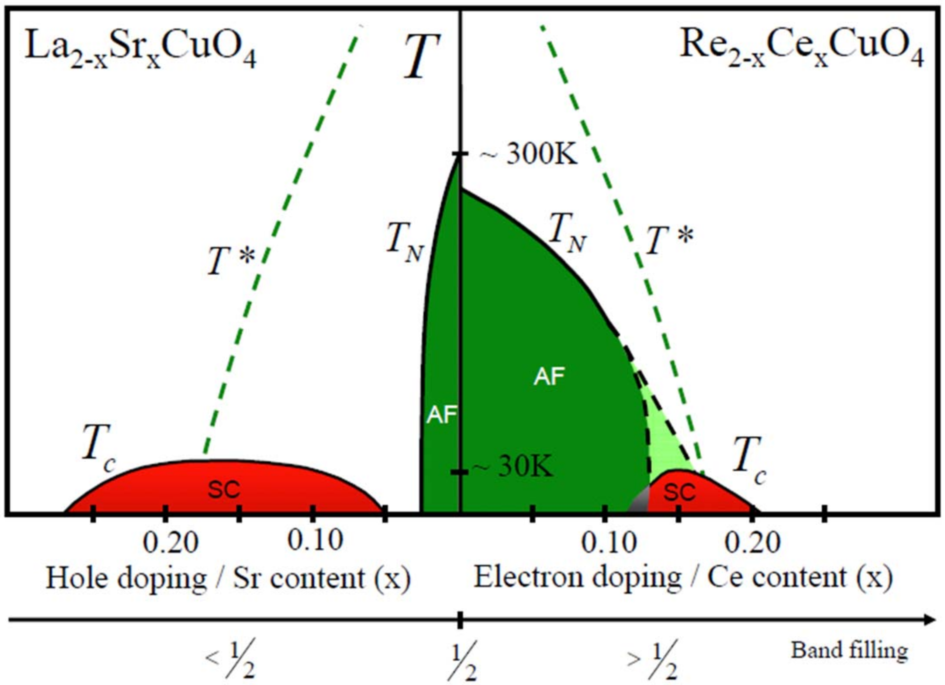
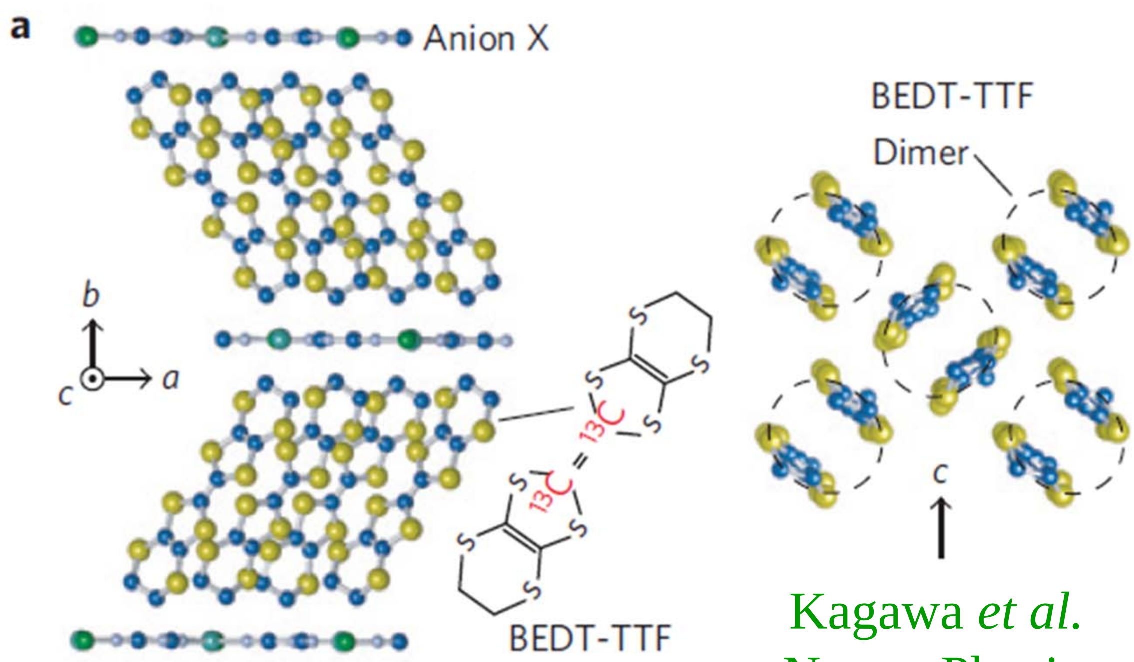
High-temperature superconductors

Armitage, Fournier, Greene, RMP (2009)

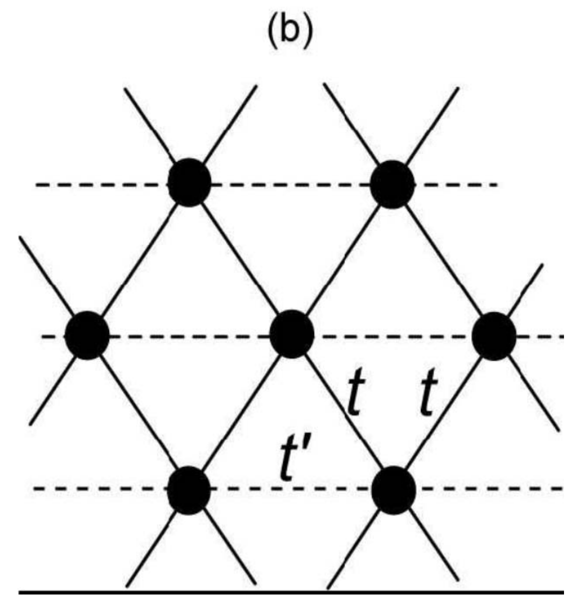


Hubbard on anisotropic triangular lattice

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



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



n=1, varying *t'/t*

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

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

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

$t'/t \sim 0.6 - 1.1$

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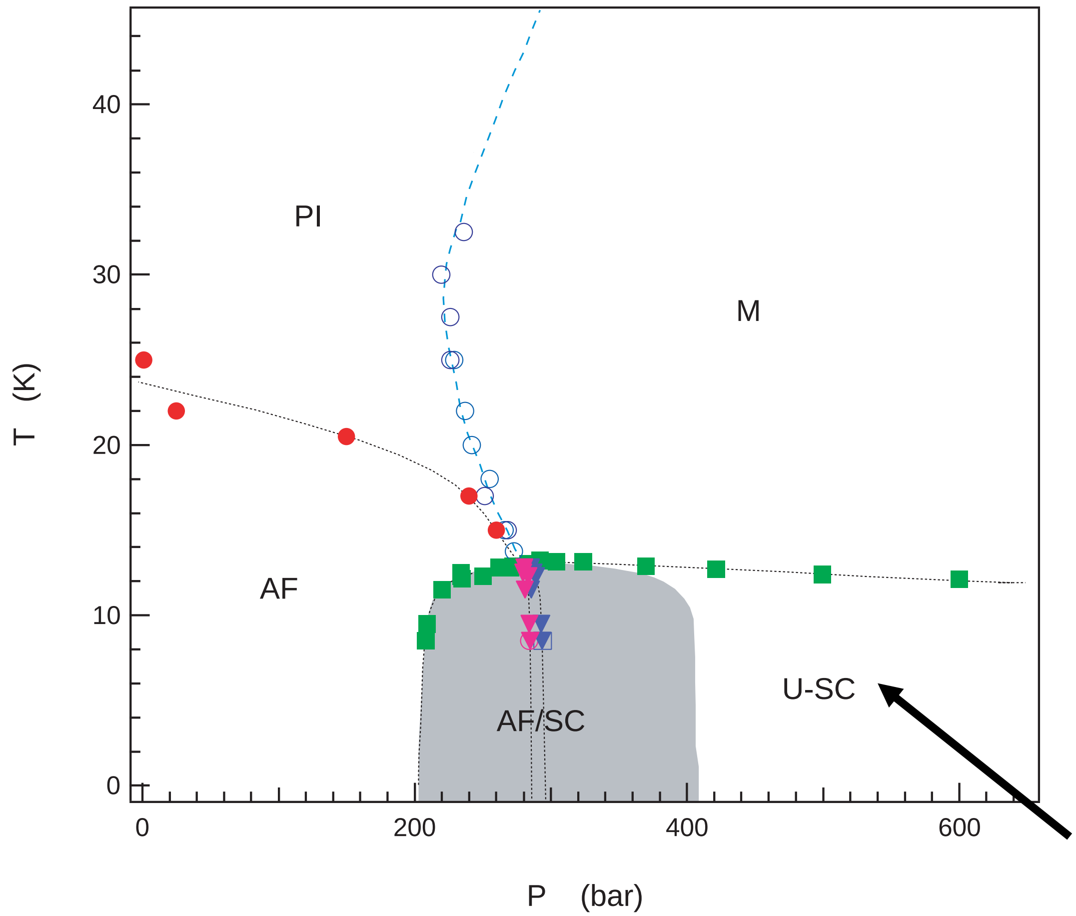
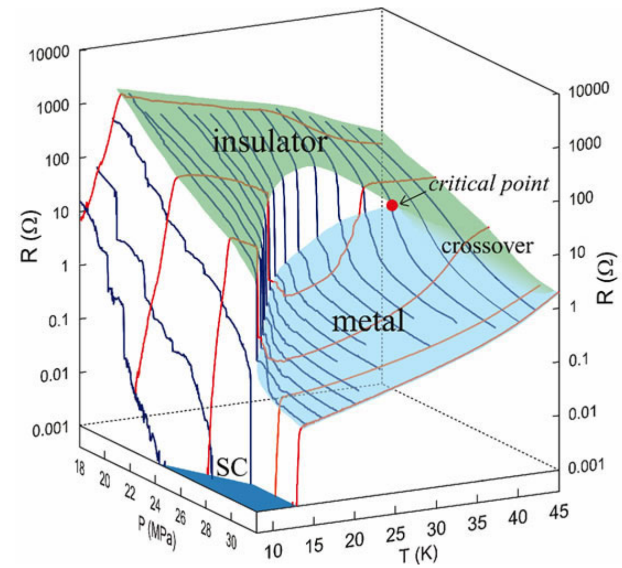
Phase diagram for organics





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

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

Powell, McKenzie cond-mat/0607078

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

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

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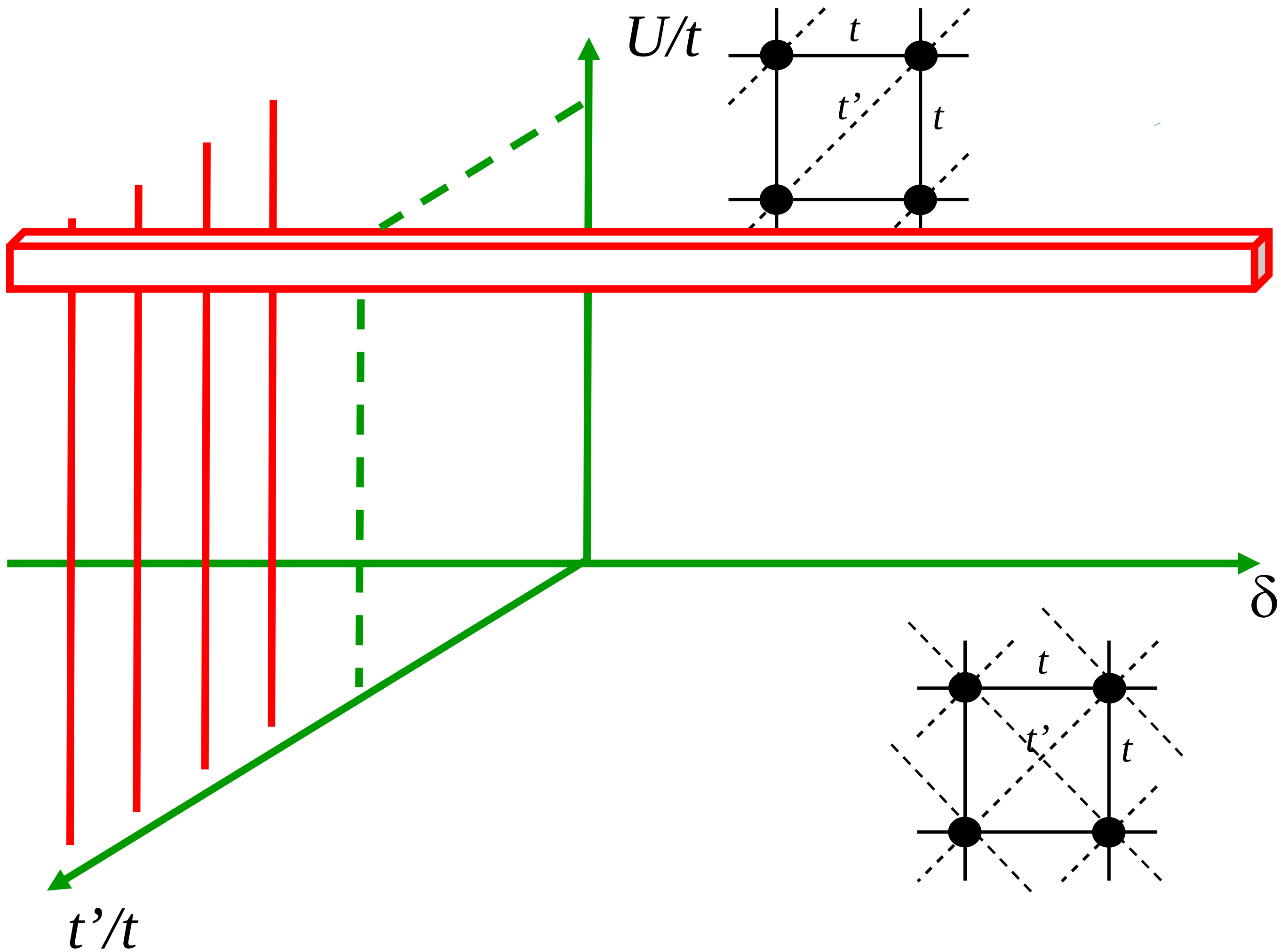
Perspective



Outline

- Method
- $T=0$ phase diagram
  - The « glue »
- Finite T phase diagram
  - Normal state
    - First order transition
    - Widom line and pseudogap
  - Superconductivity

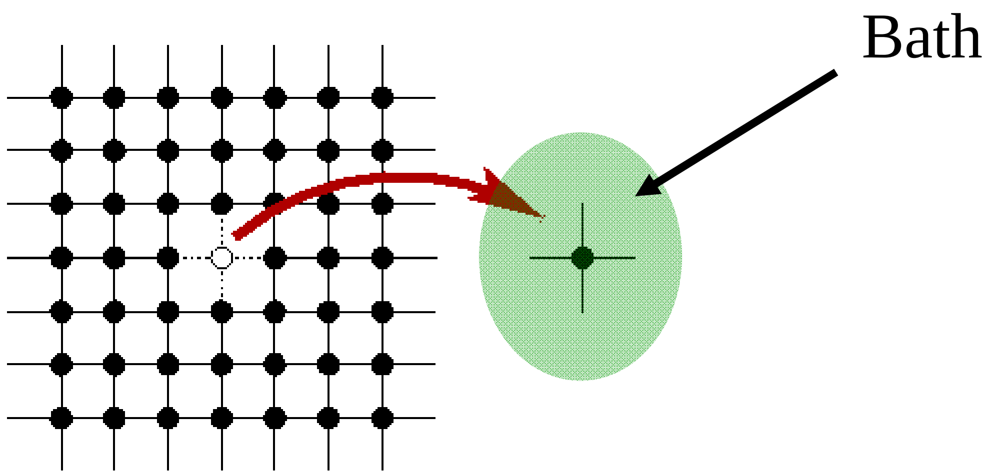
Method

"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)

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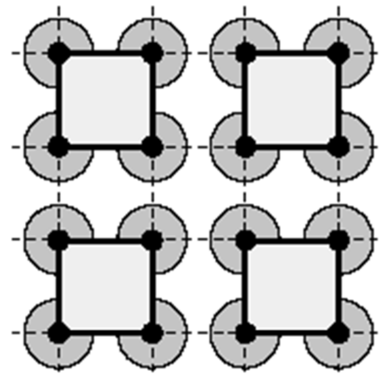
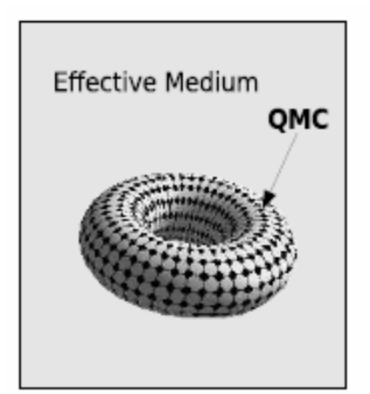
2d Hubbard: Quantum cluster method

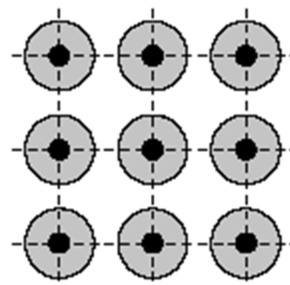
C-DMFT





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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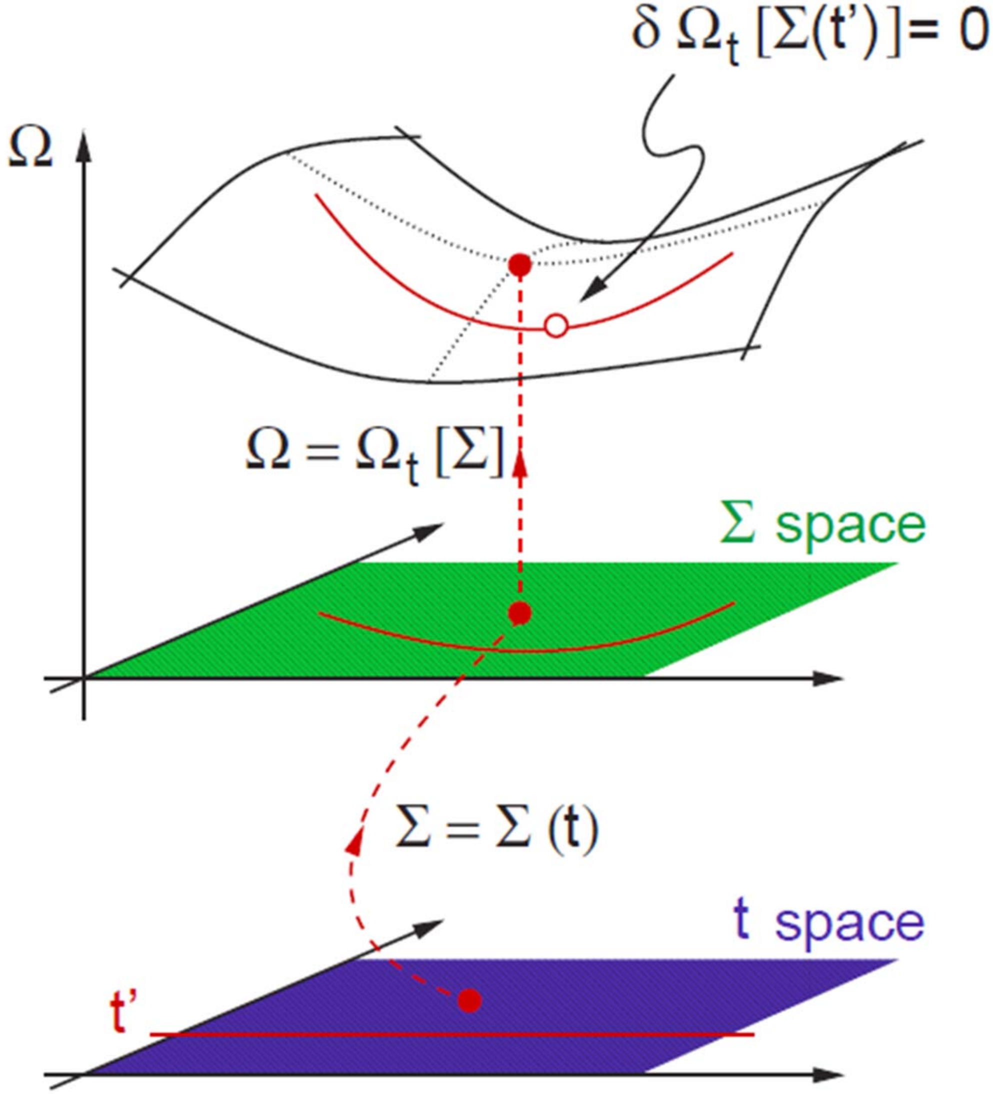
DMFT as a stationnary point



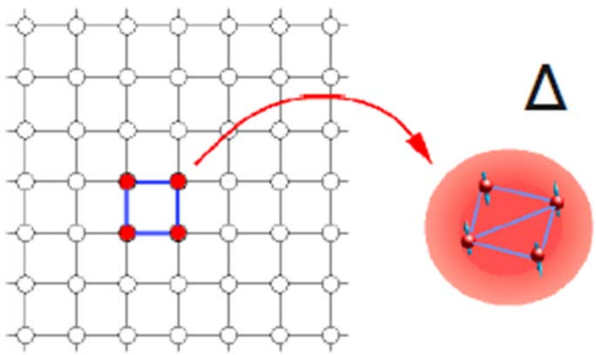
M. Potthoff, Eur. Phys. J. B 32, 429 (2003).

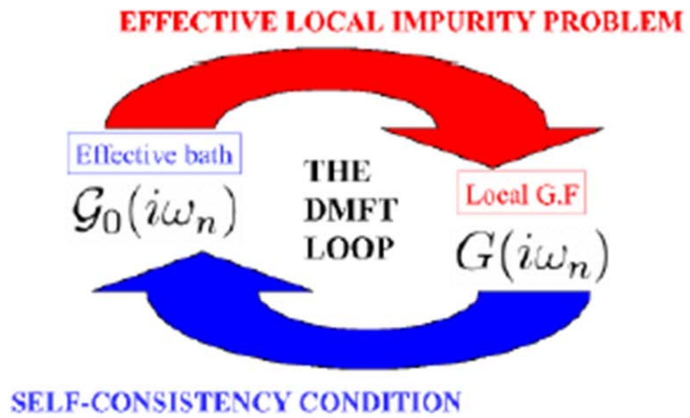
+ and -

- 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

C-DMFT

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





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

Here: continuous time QMC

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

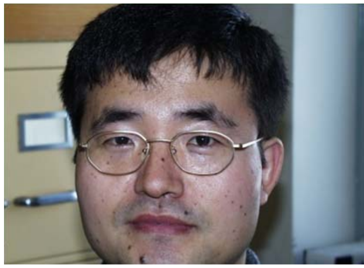
Why important

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

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

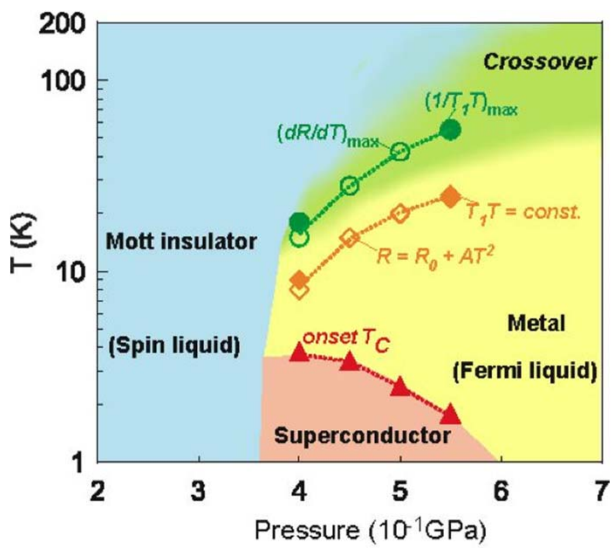
Phase diagram

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



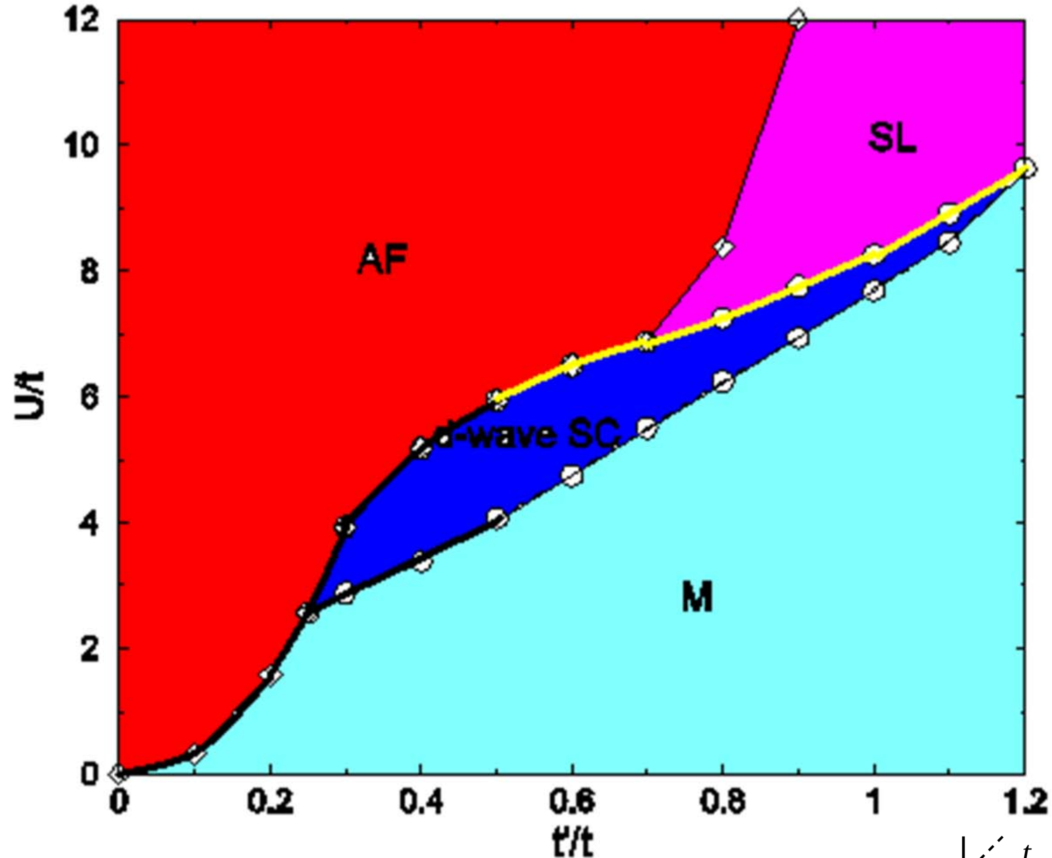
Theoretical phase diagram BEDT

X= $Cu_2(CN)_3$ (t'~ t)

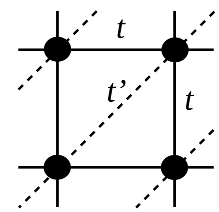


Y. Kurisaki, et al.

Phys. Rev. Lett. **95**, 177001(2005)



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



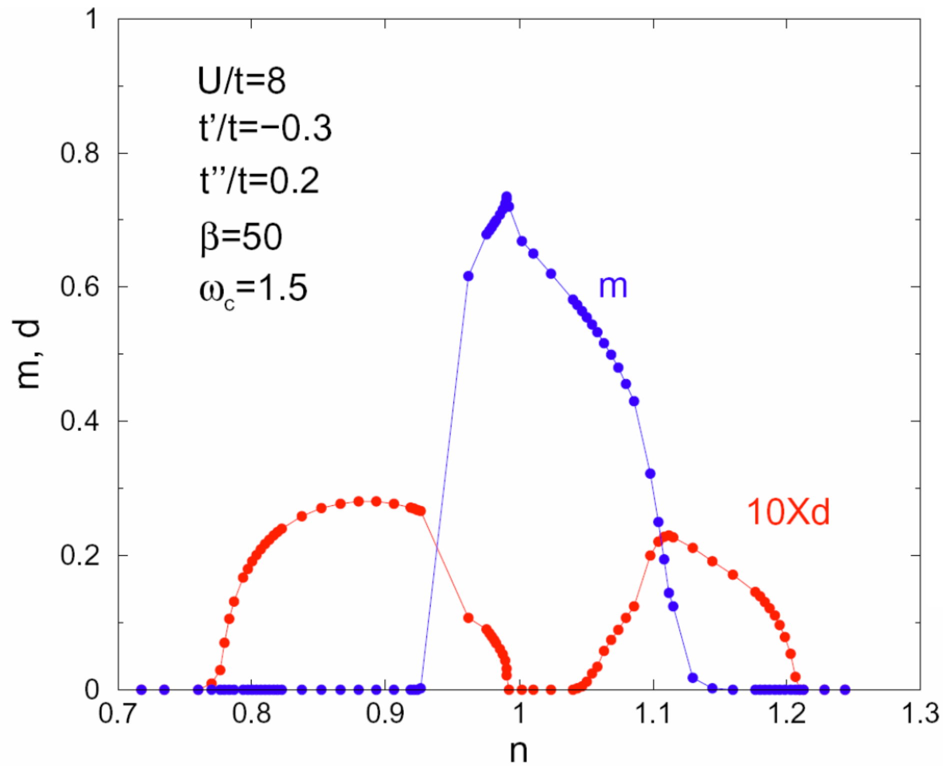
Y. Shimizu, et al. Phys. Rev. Lett. **91**, (2003)

T = 0 phase diagram: cuprates

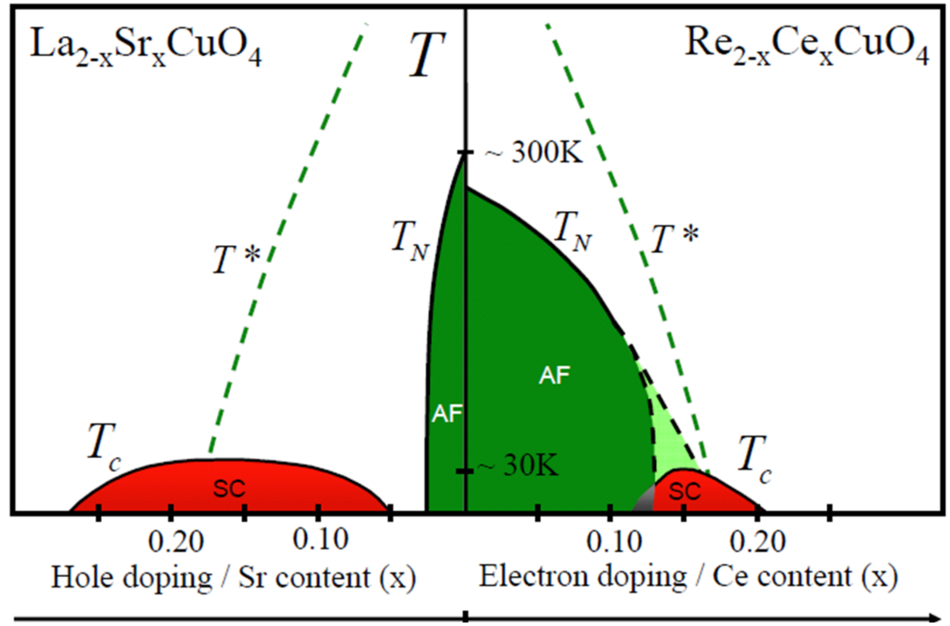
Phase diagram

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

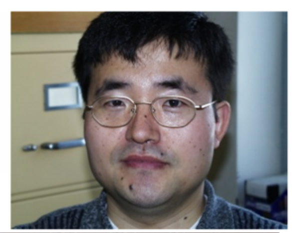
CDMFT global phase diagram



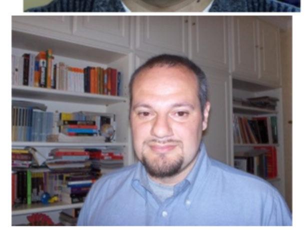
Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008)
AND Capone, Kotliar PRL (2006)



Armitage, Fournier, Greene, RMP (2009)





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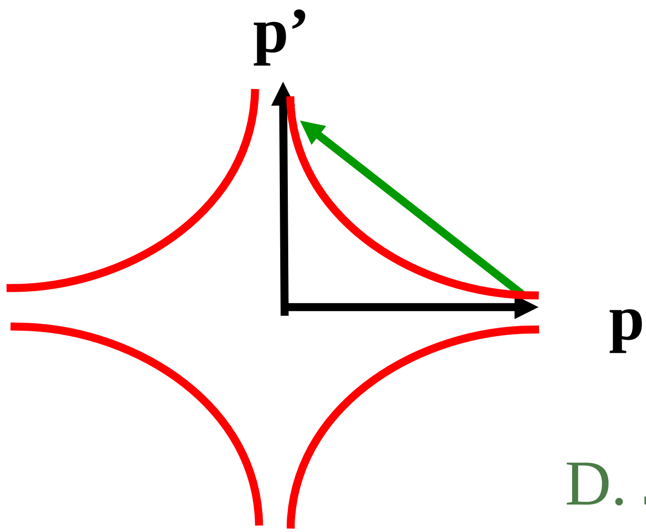
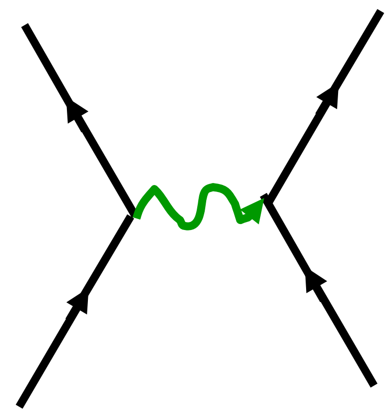
A bit of physics: superconductivity and repulsion

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

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





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).

Exchange of spin waves?
Kohn-Luttinger
T_c with pressure

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

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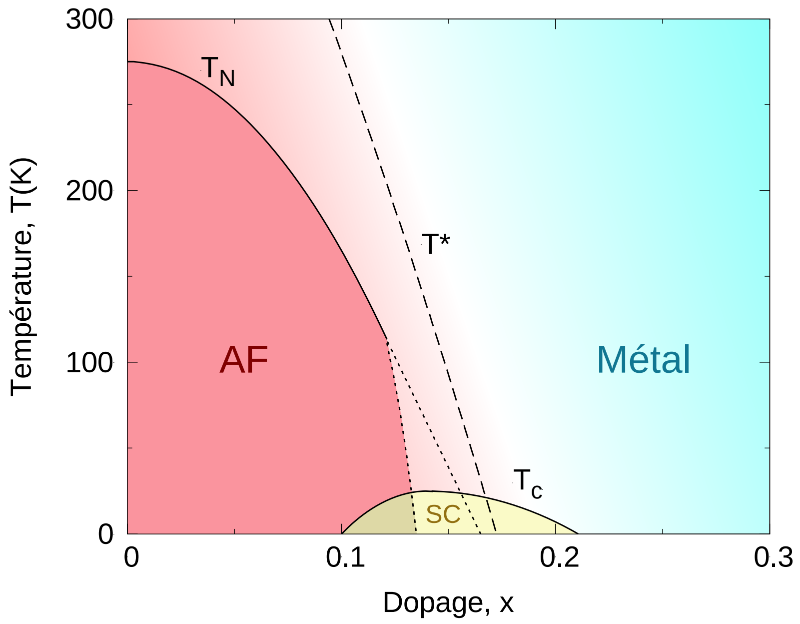
AFM Quantum critical point



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)

The glue

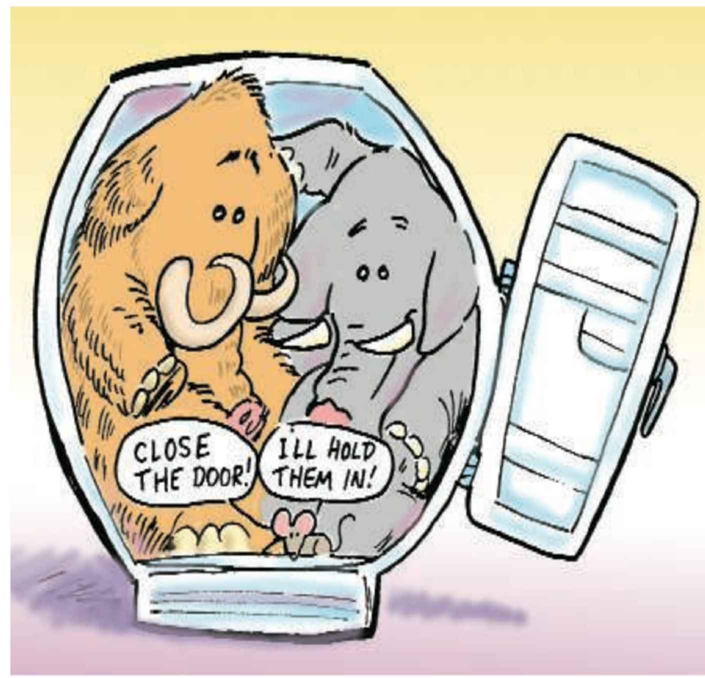
Raising the question

Is There Glue in Cuprate Superconductors?
Philip W. Anderson
Science **316**, 1705 (2007);
DOI: 10.1126/science.1140970

Is There Glue in Cuprate Superconductors?

Philip W. Anderson

Many theories about electron pairing in cuprate superconductors may be on the wrong track.



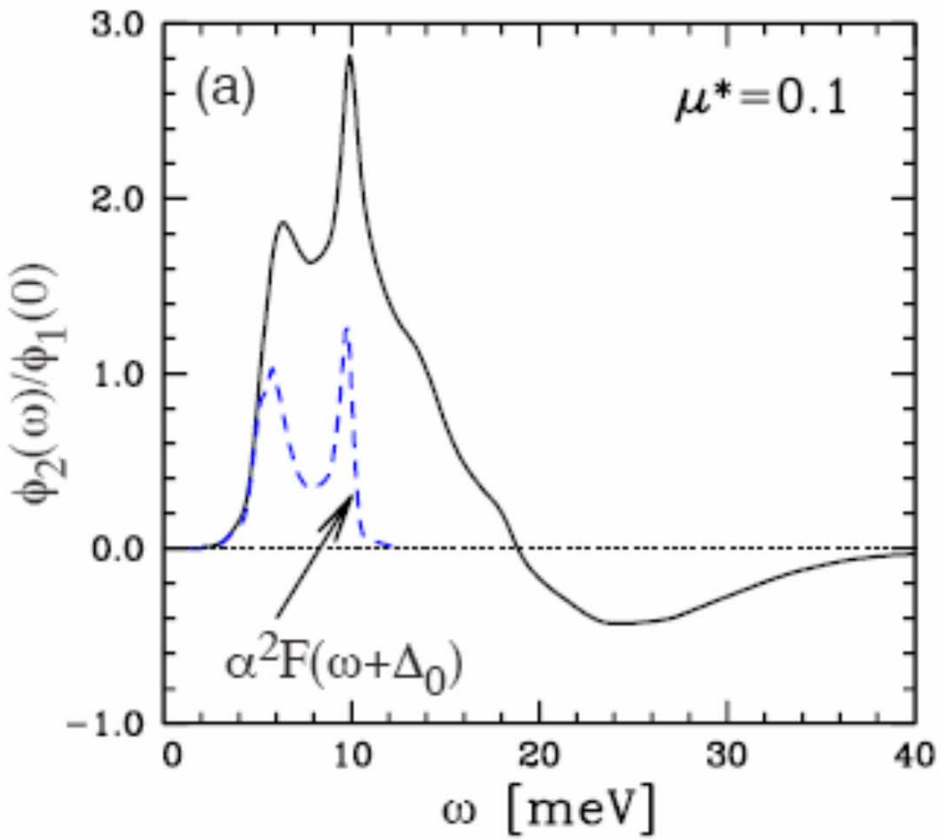
"We have a mammoth and an elephant in our refrigerator—do we care much if there is also a mouse?"

Retardation

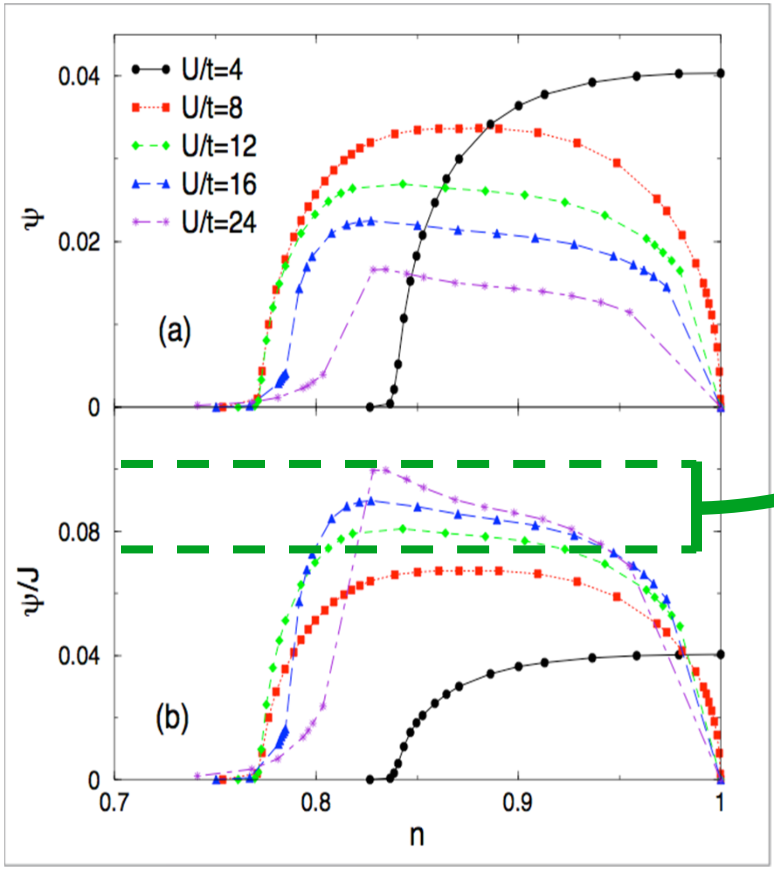
$$V^{eff}_{él-ph}(\vec{q},\omega) = \frac{e^2}{4\pi\varepsilon_0(q^2+k_{TF}^2)}\left[1+\frac{\omega_{ph}^2(\vec{q})}{\omega^2-\omega_{ph}^2(\vec{q})}\right]$$

Im Σ_{an} and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)



Strength of pairing: cuprates

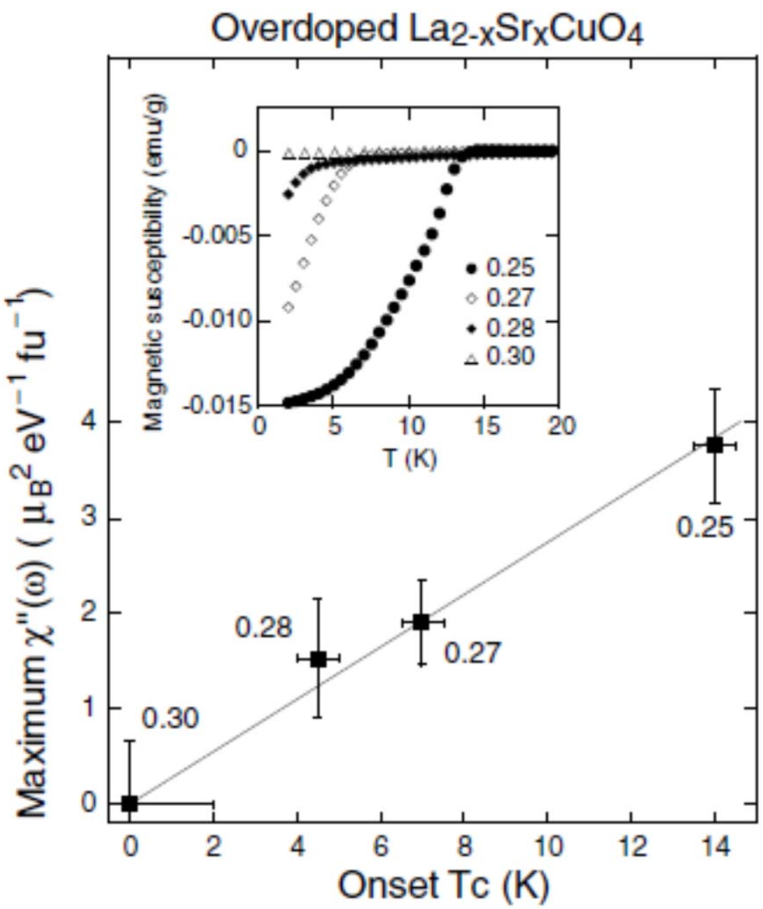


$$J = \frac{4t^2}{U}$$

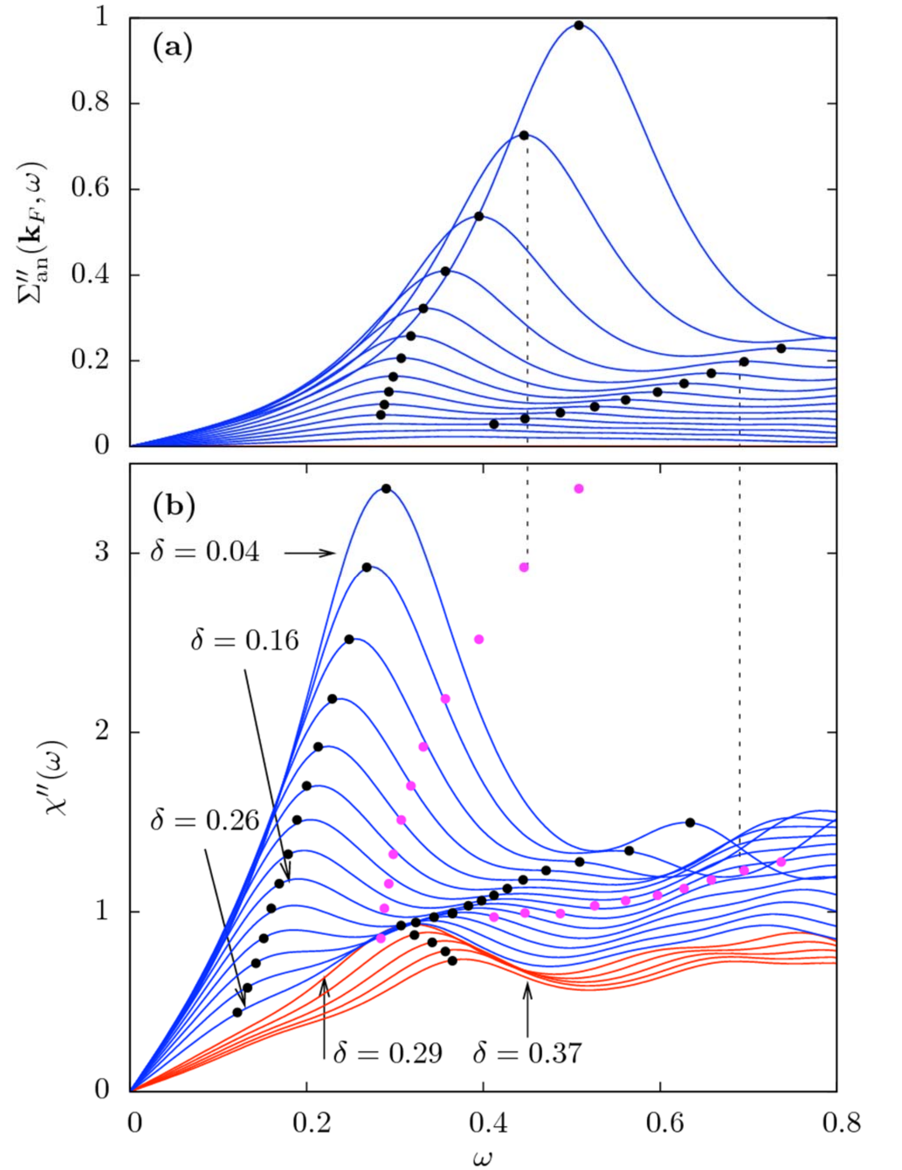
The superconducting order parameter scales like *J*

The glue

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



Wakimoto … Birgeneau PRL (2004)



The glue and neutrons

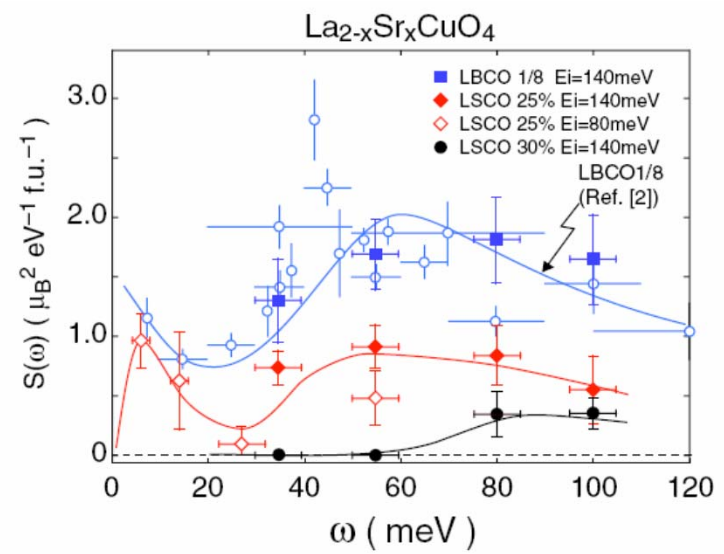
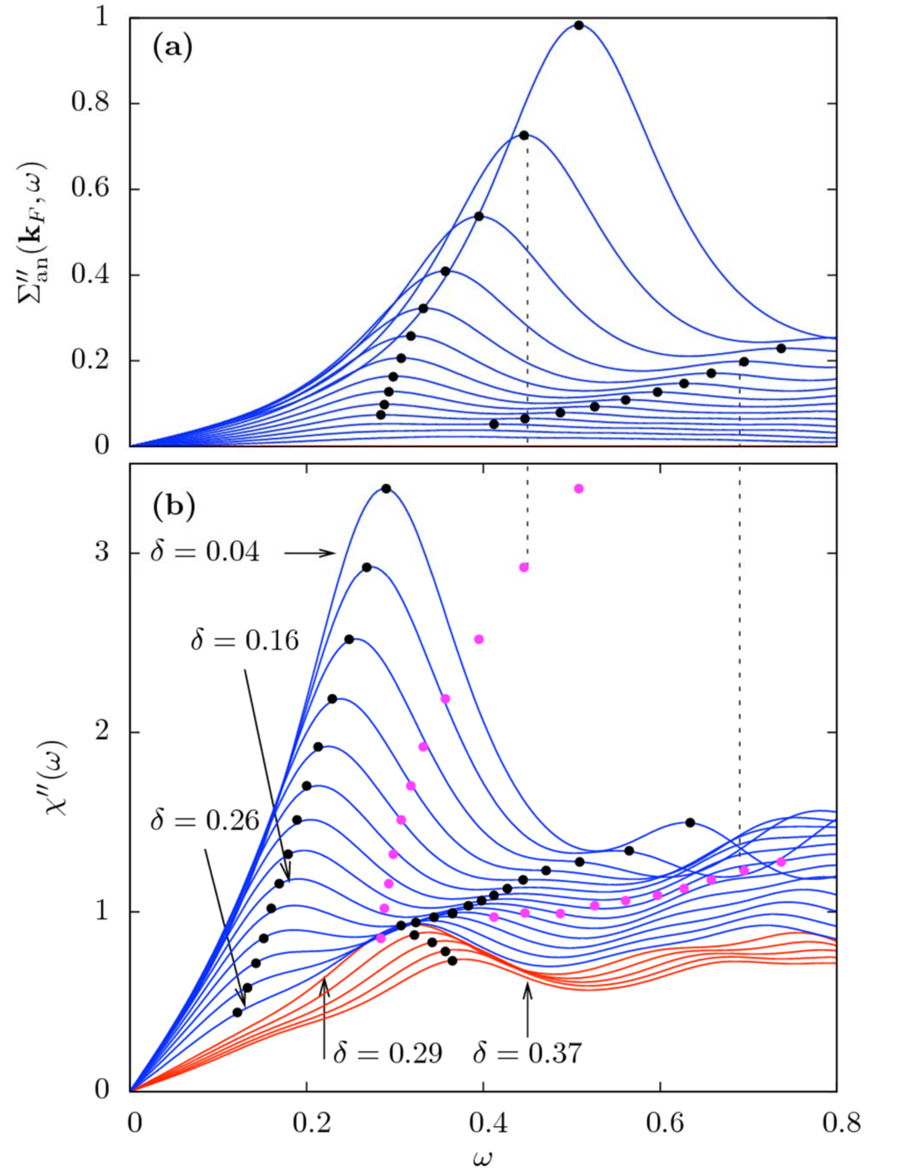


FIG. 3 (color online). **Q**-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i = 140$ meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO 1/8 (open circles) from [2]. The solid lines following data of LSCO $x = 0.25$ and 0.30 are guides to the eyes.

Wakimoto … Birgeneau PRL (2007);
PRL (2004)



Resilience to near-neighbor repulsion V

$$\hat{\mathcal{H}}_{Hubbard} = -\sum_{\langle i,j\rangle_{1,2,3}\ \sigma}\left(t_{ij}\,\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + c.h\right) + U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + V\sum_{\langle i,j\rangle}\hat{n}_{i}\hat{n}_{j} - \mu\sum_{i\ \sigma}\hat{n}_{i\sigma}$$

$YBa_2Cu_3O_7$: $t = 1$ $t' = -0.3$ $t'' = 0.2$

We expect superconductivity to disappear when:

$V > \frac{U^2}{W}$ **In weakly correlated case U/W < 1**

$V > J$ **In mean-field strongly correlated case**

In cuprates:

$V = 400\,\mathrm{meV}$

$J = 130\,\mathrm{meV}$

$$U_c = V_c/[1 + N(0)V_c \ln(E_F/\omega_c)]$$

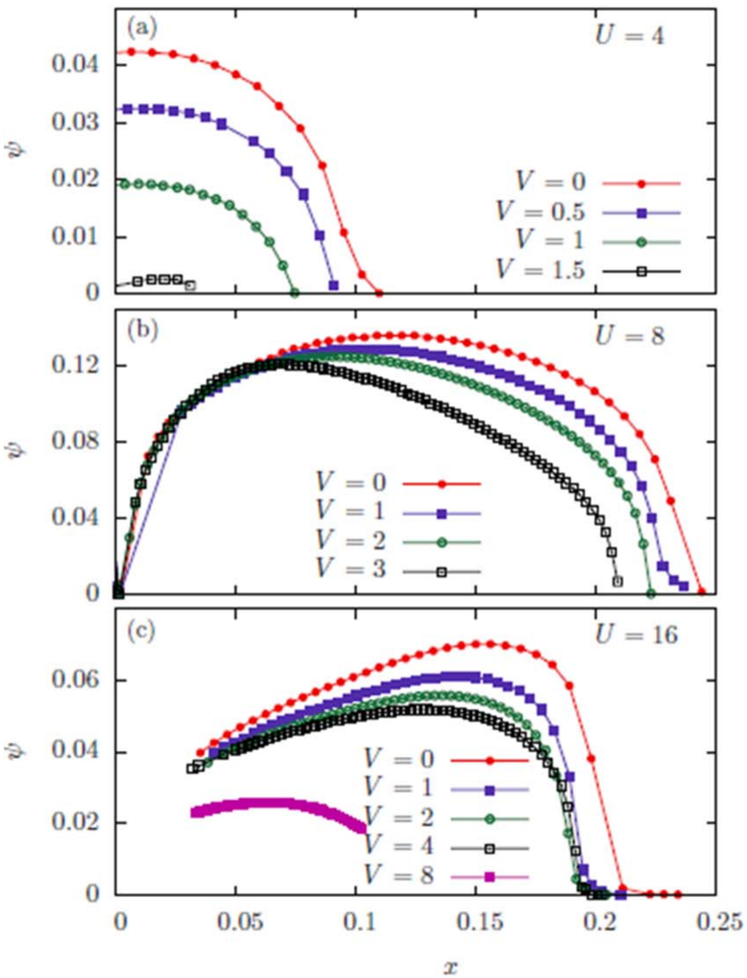
S. Onari, R. Arita, K. Kuroki et H. Aoki, PRB **70**, 094523 (2004)
S. Raghu, E. Berg, A. V. Chubukov et S. A. Kivelson, PRB **85**, 024516 (2012)
S. Sorella, et al. Phys. Rev. Lett. 88, 117002 (2002)

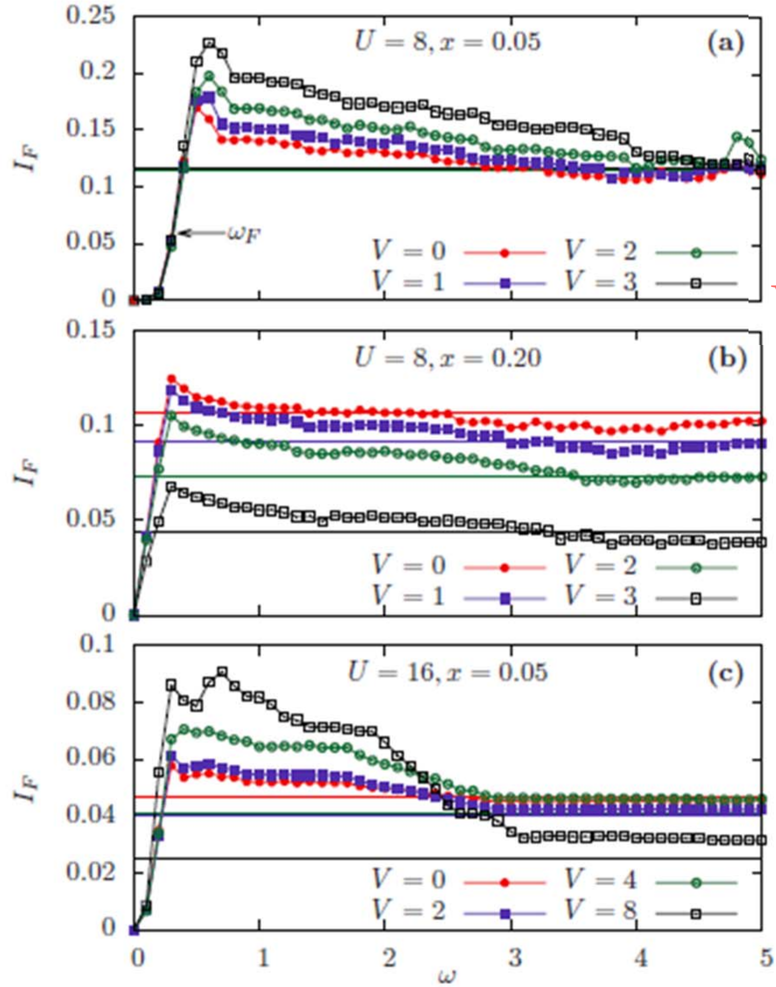
Resilience to near-neighbor repulsion

David Sénéchal

Alexandre Day

Vincent Bouliane





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

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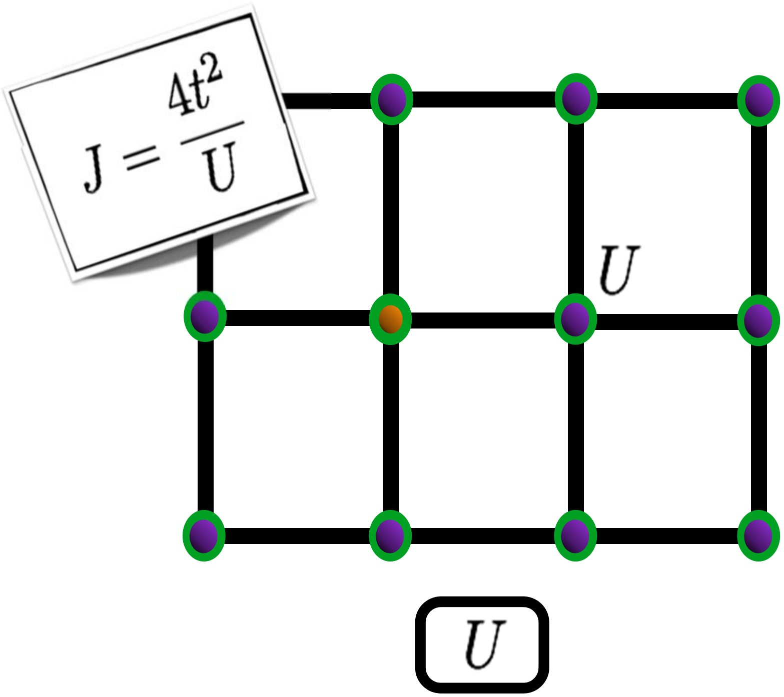
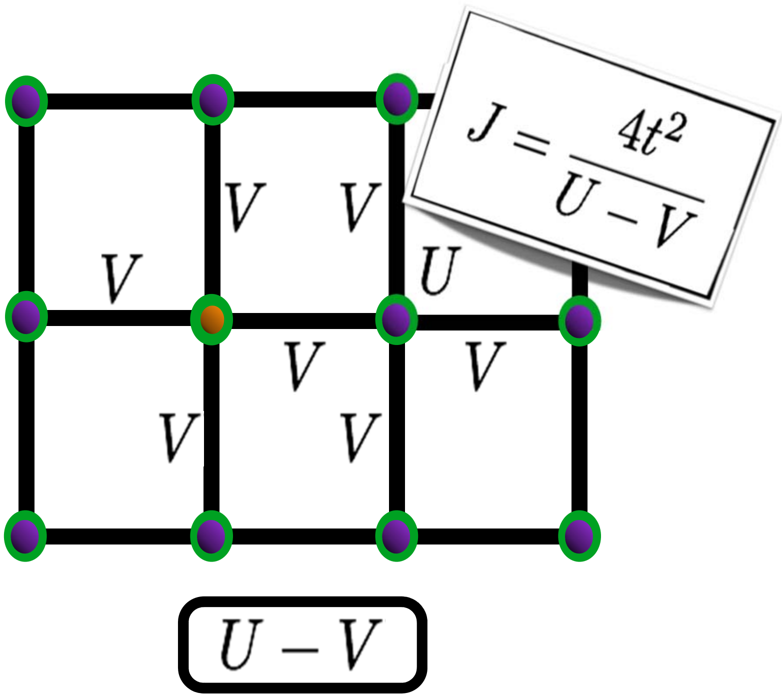
V also increases J



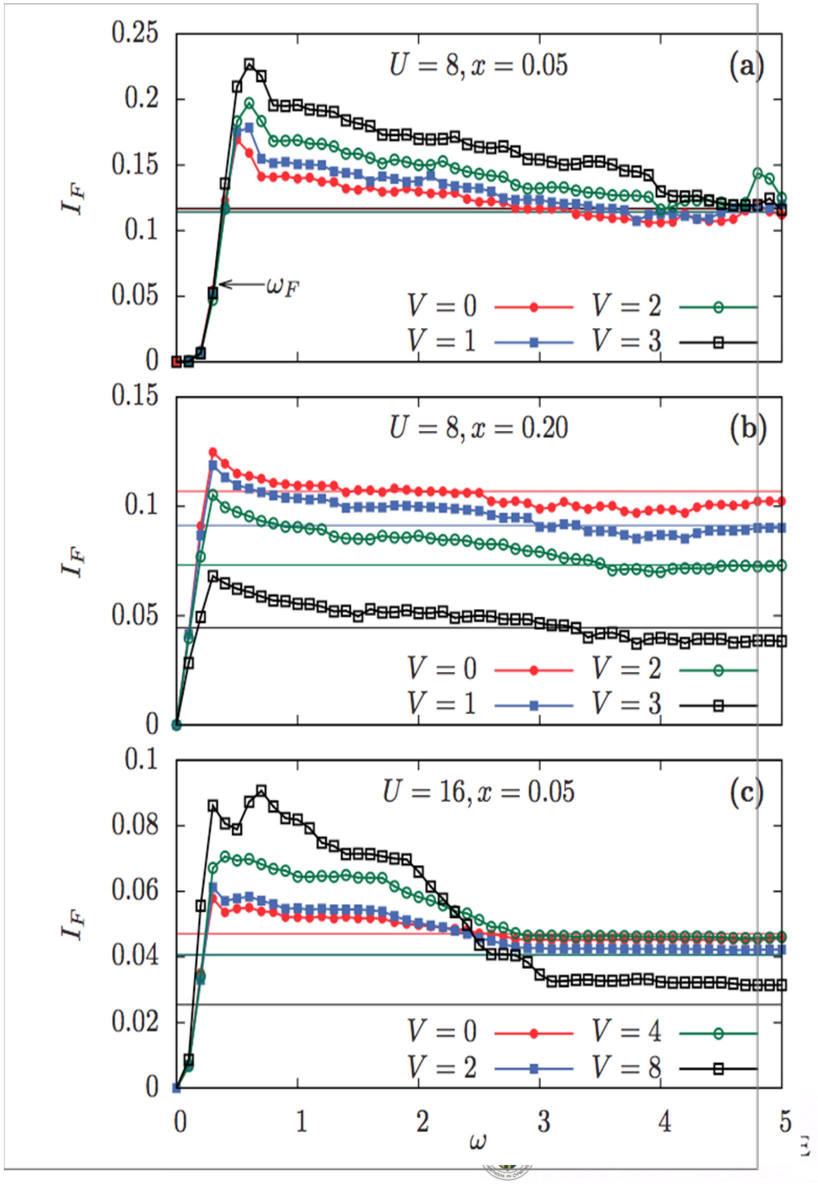


Binding aspects of V

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

J **increases with** ***V*** **explaining better pairing at low frequency**

But V also induces more repulsion at high frequency, explaining the negative impact at high frequency on binding



Outline

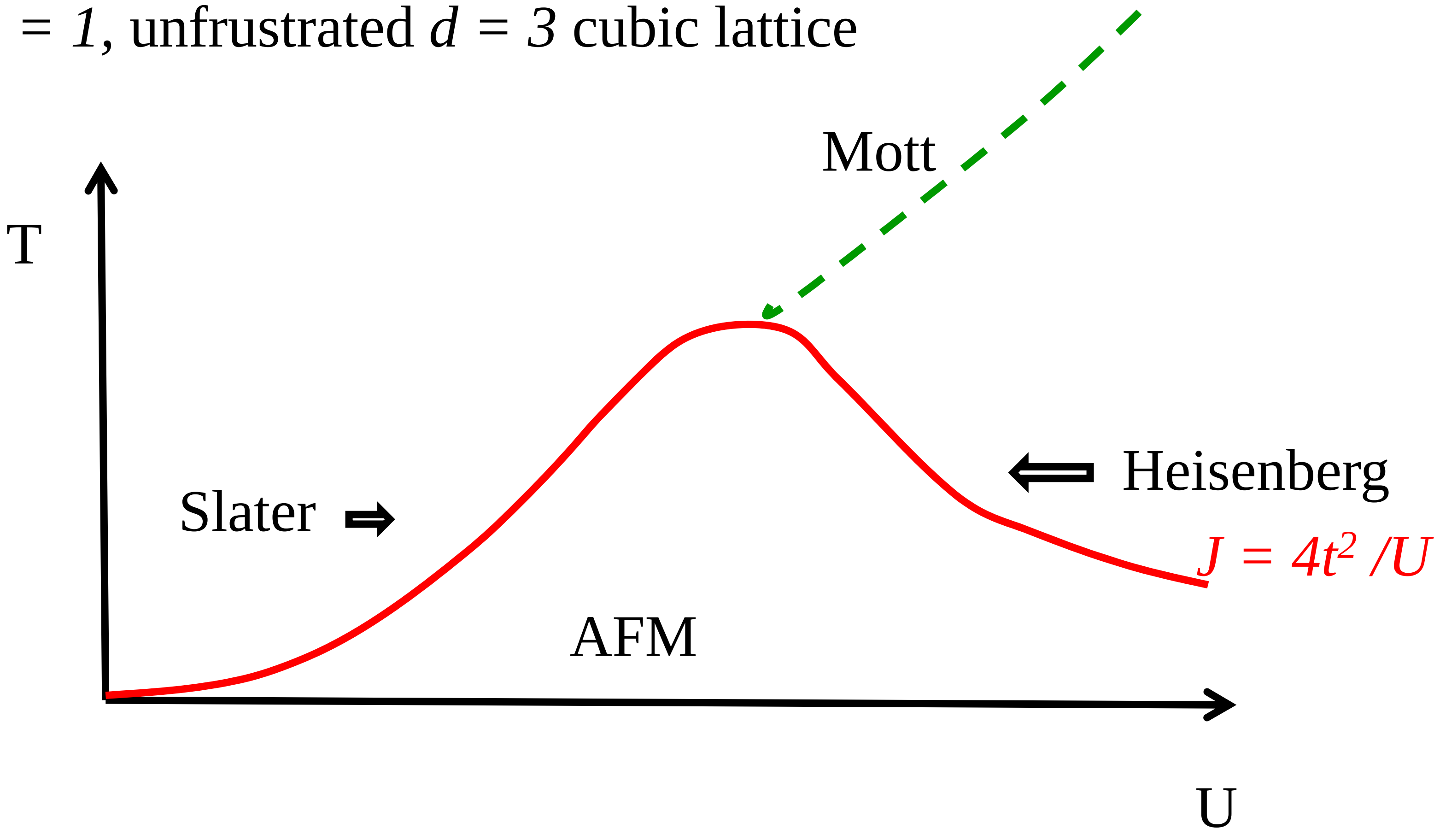
- Method
- *T=0* phase diagram
  - The « glue »
- Finite *T* phase diagram
  - Normal state
    - First order transition
    - Widom line and pseudogap
  - Superconductivity

Finite *T* phase diagram

Normal state of the cuprates

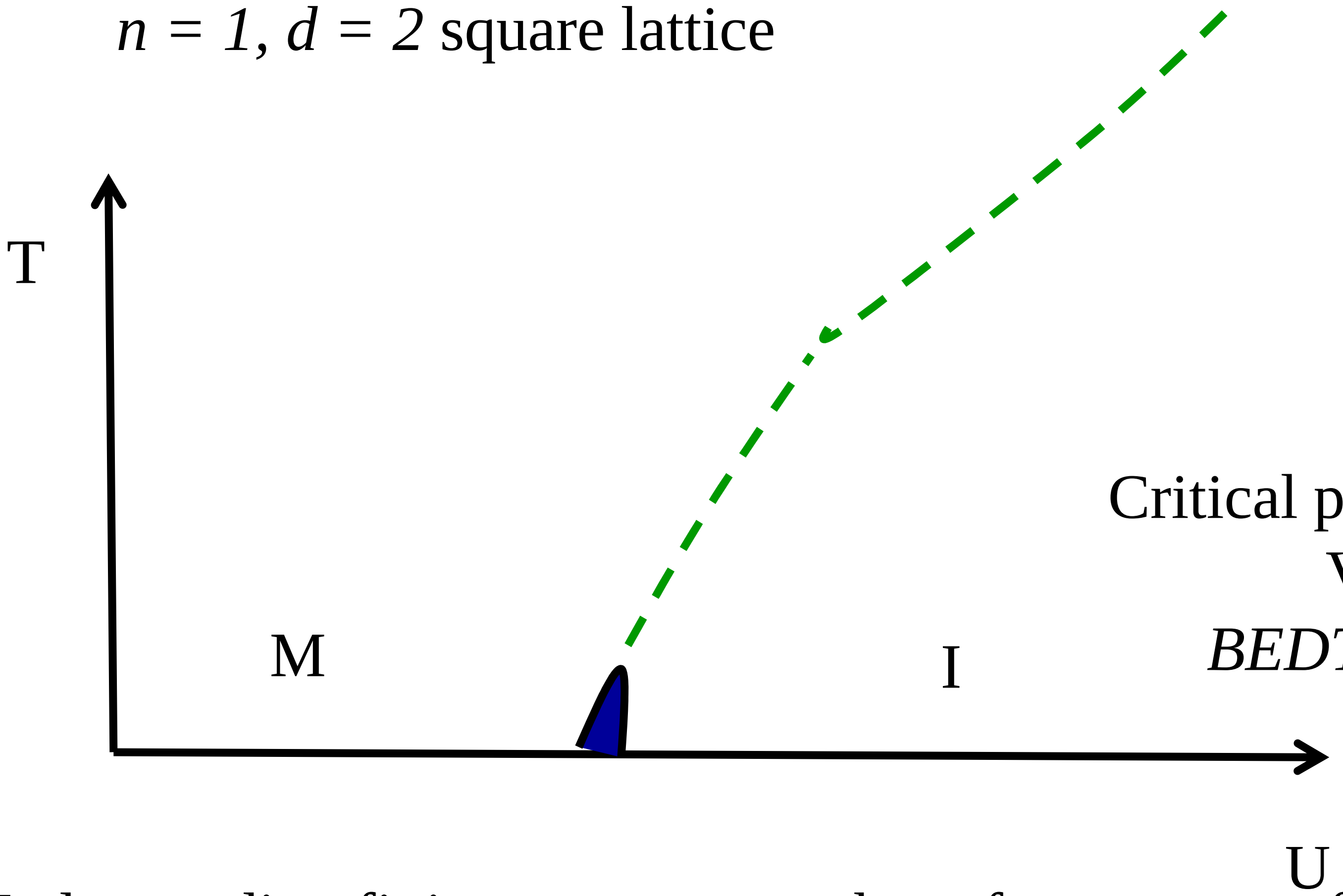
Weak vs Strong correlations

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



Local moment and Mott transition

n = 1, d = 2 square lattice

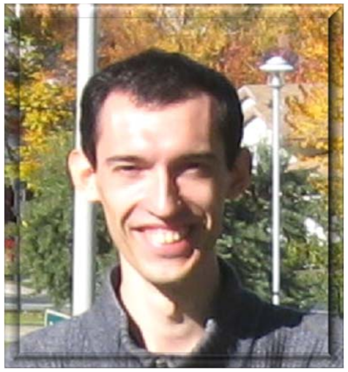


Critical point visible in V_2O_3, *BEDT* organics

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

Finite *T* phase diagram

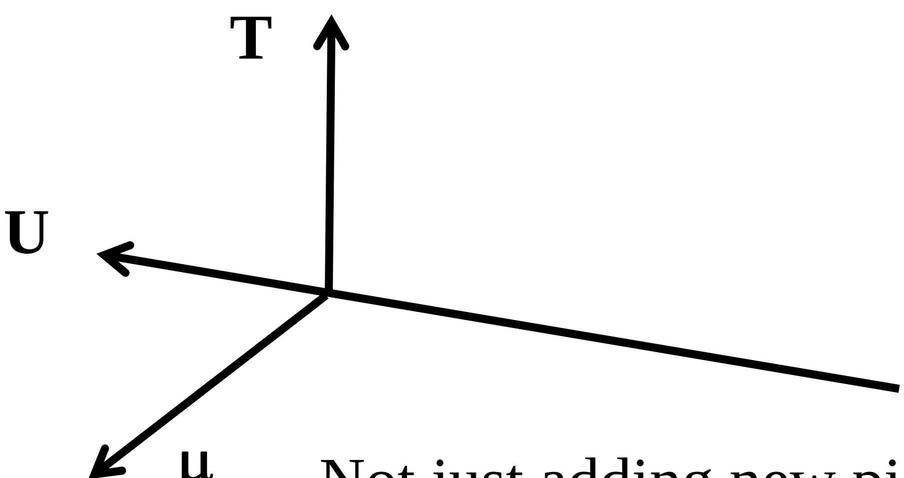
Normal state of the cuprates



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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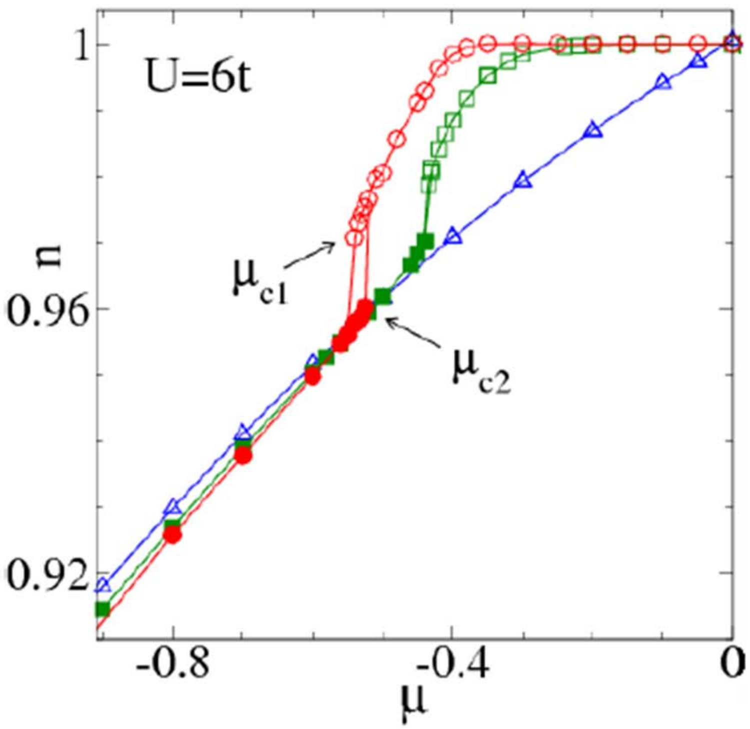
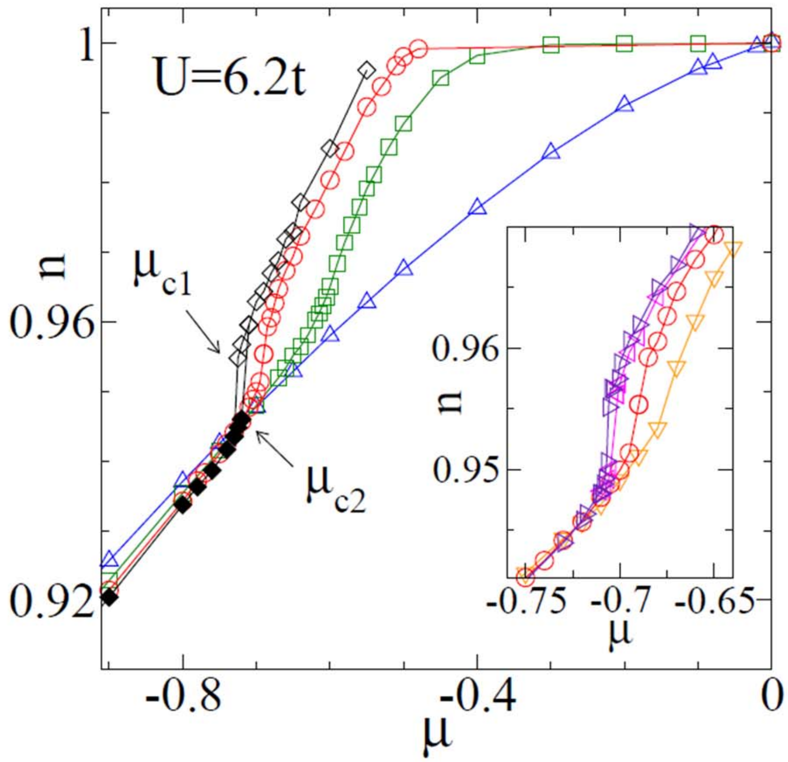
First order transition at finite doping

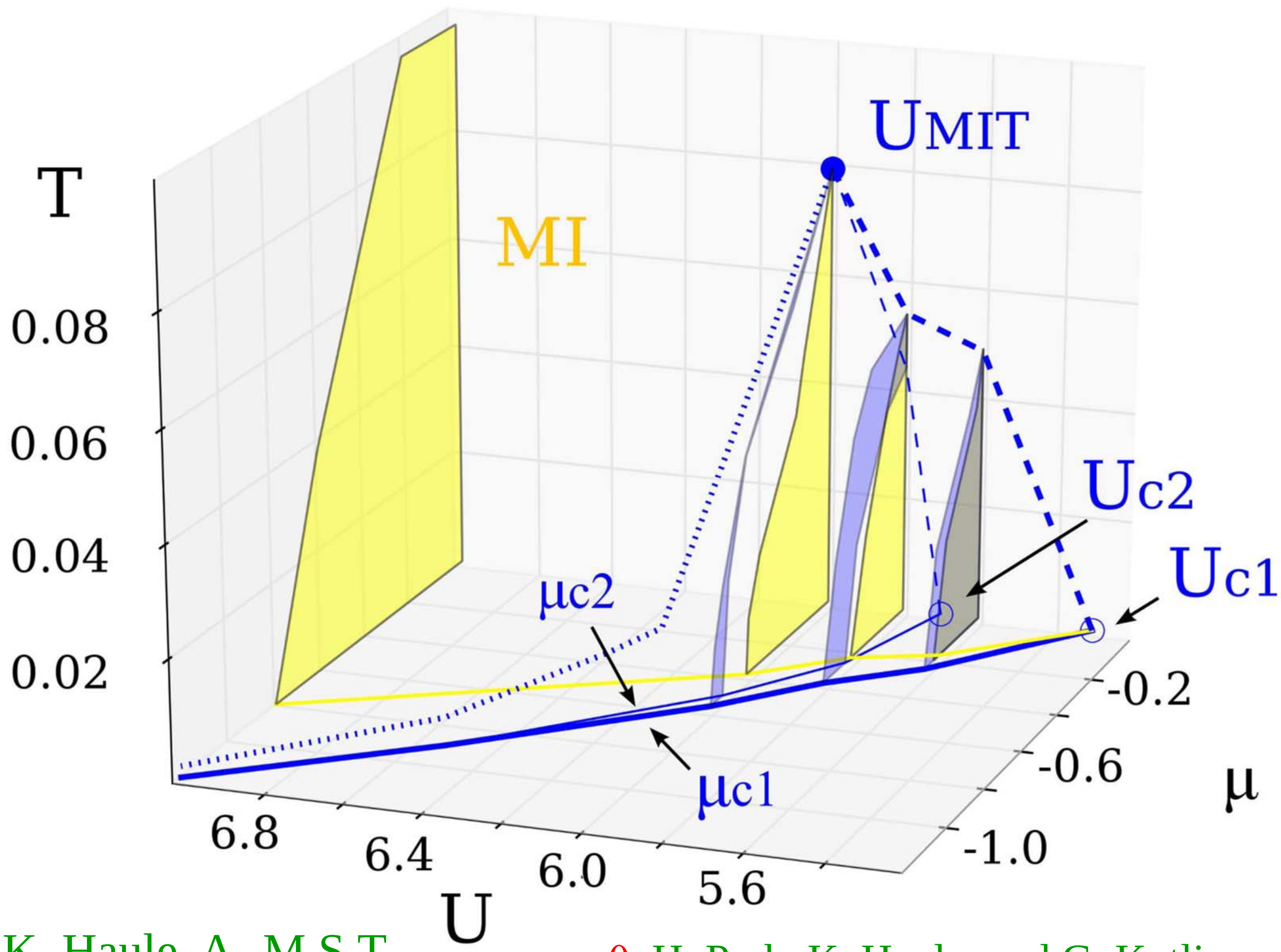


$n(\mu)$ for several temperatures:
$T/t =$ 1/10, 1/25, 1/50

The critical point



Normal state phase diagram



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

μ = 0, H. Park, K. Haule, and G. Kotliar,
Phys. Rev. Lett. 101, 186403 (2008)

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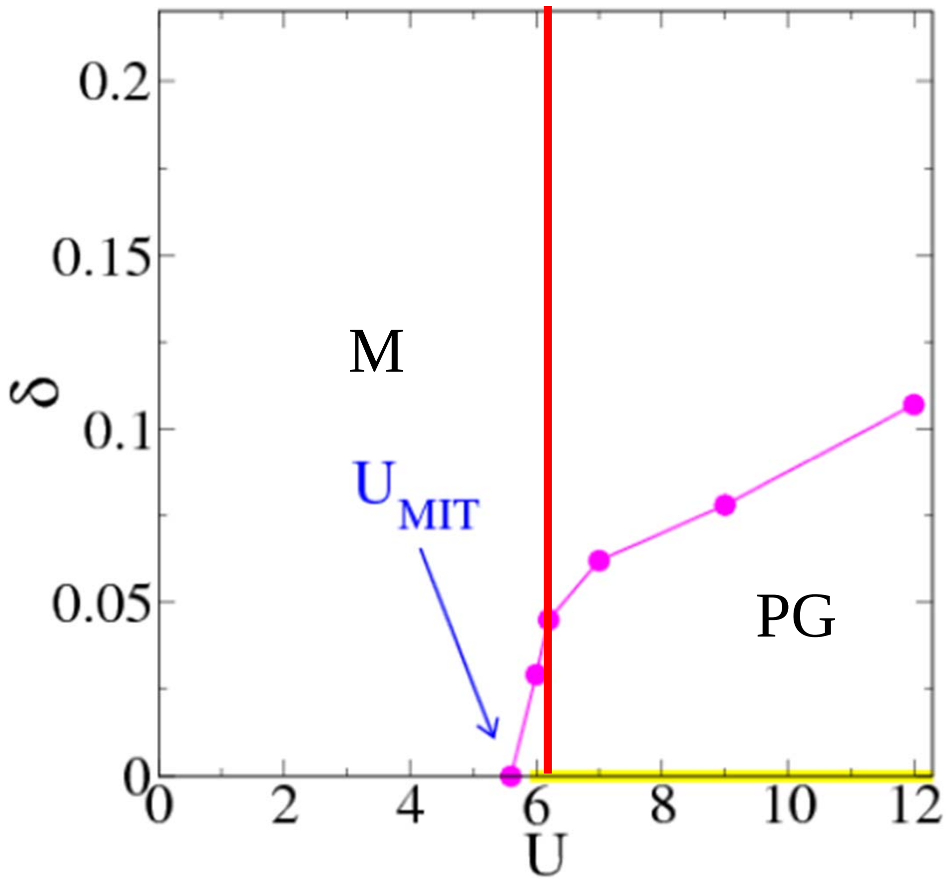
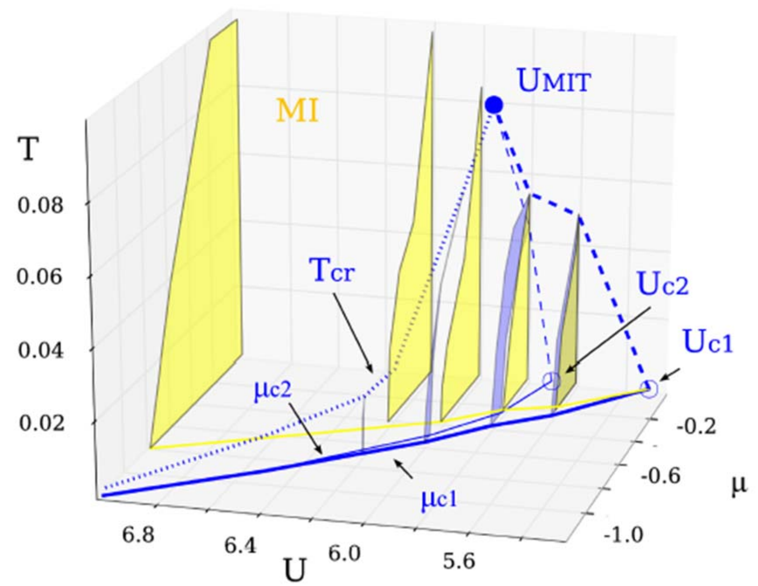
Link to Mott transition up to optimal doping

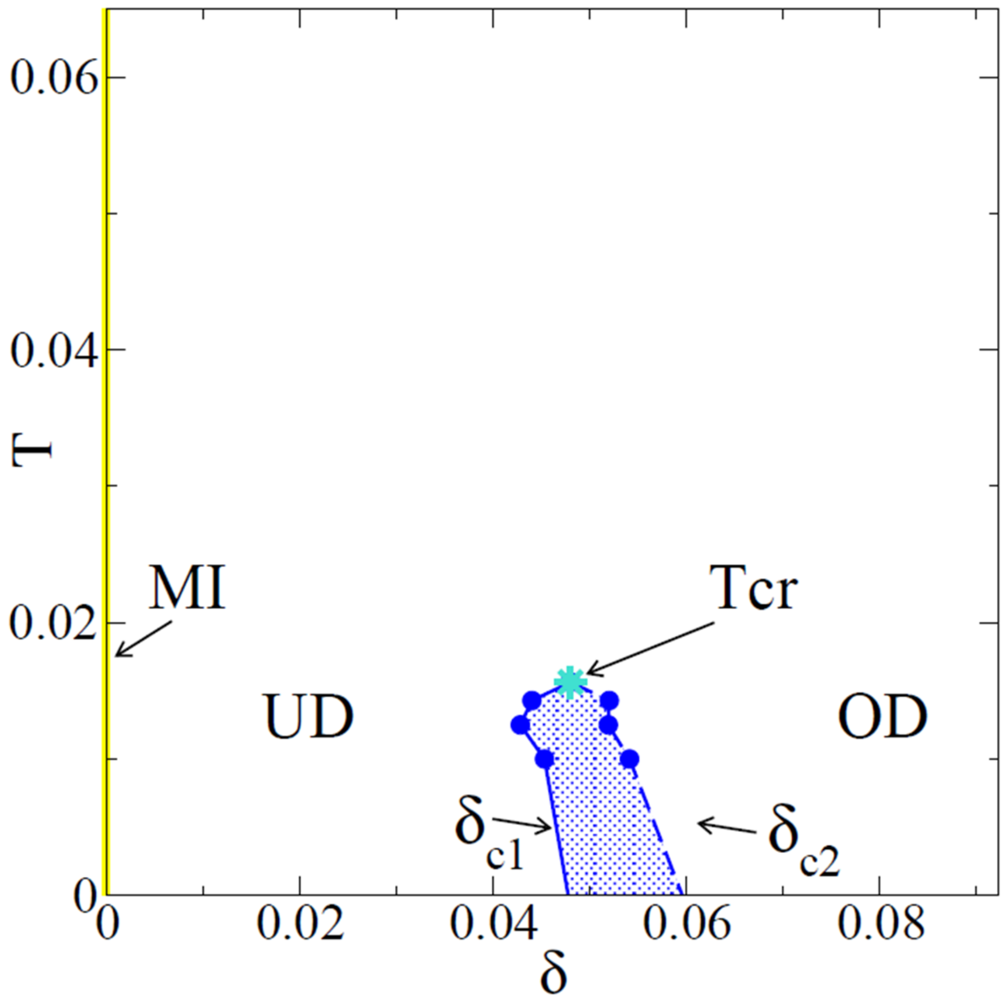
Doping dependence of critical point as a function of *U*



Smaller *D* and *S*



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



$U > U_{\mathrm{MIT}}$:

1. Mott insulator (MI)
2. Underdoped phase (UD): $\delta < \delta_c$
3. Overdoped phase (OD): $\delta > \delta_c$
4. Coexistence/forbidden region

Here "optimal doping" δ_c = doping at which the 1st order transition occurs

How does the UD phase differ from the OD phase?

Giovanni Sordi

Patrick Sémon

Kristjan Haul

Finite *T* phase diagram

Pseudogap in the normal state and the Widom line

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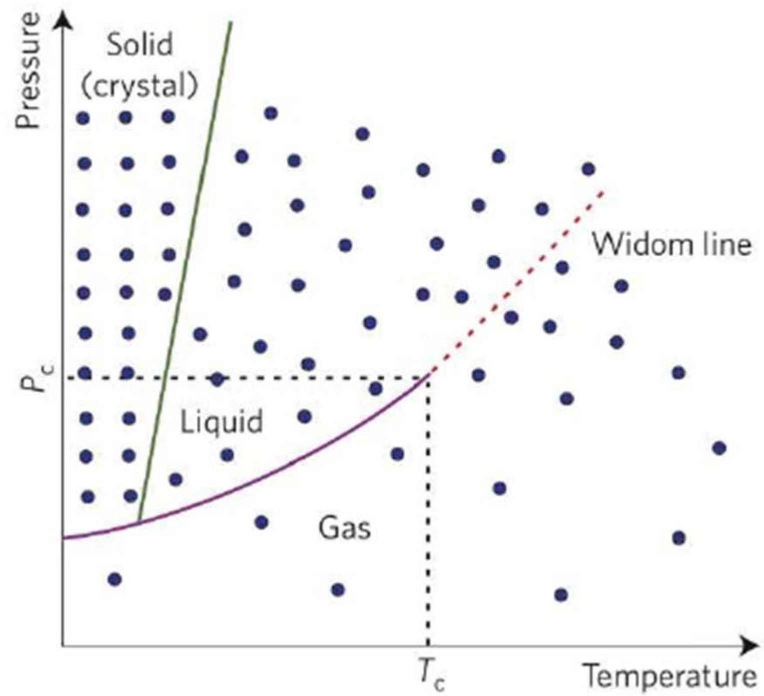
What is the Widom line?



McMillan and Stanley, Nat Phys 2010

- it is the continuation of the coexistence line in the supercritical region
- line where the maxima of different response functions touch each other asymptotically as $T \to T_p$
- liquid-gas transition in water: max in isobaric heat capacity C_p, isothermal compressibility, isobaric heat expansion, etc

- DYNAMIC crossover arises from crossing the Widom line!
  water: Xu et al, PNAS 2005, Simeoni et al Nat Phys 2010

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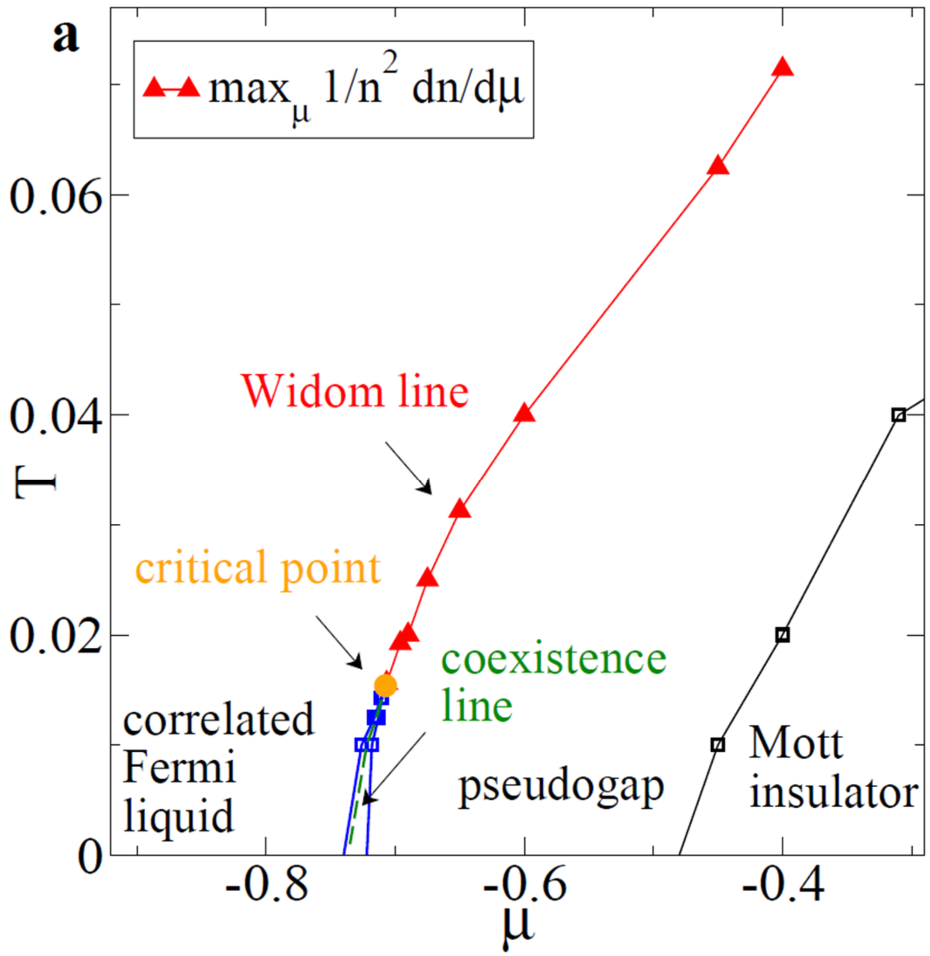
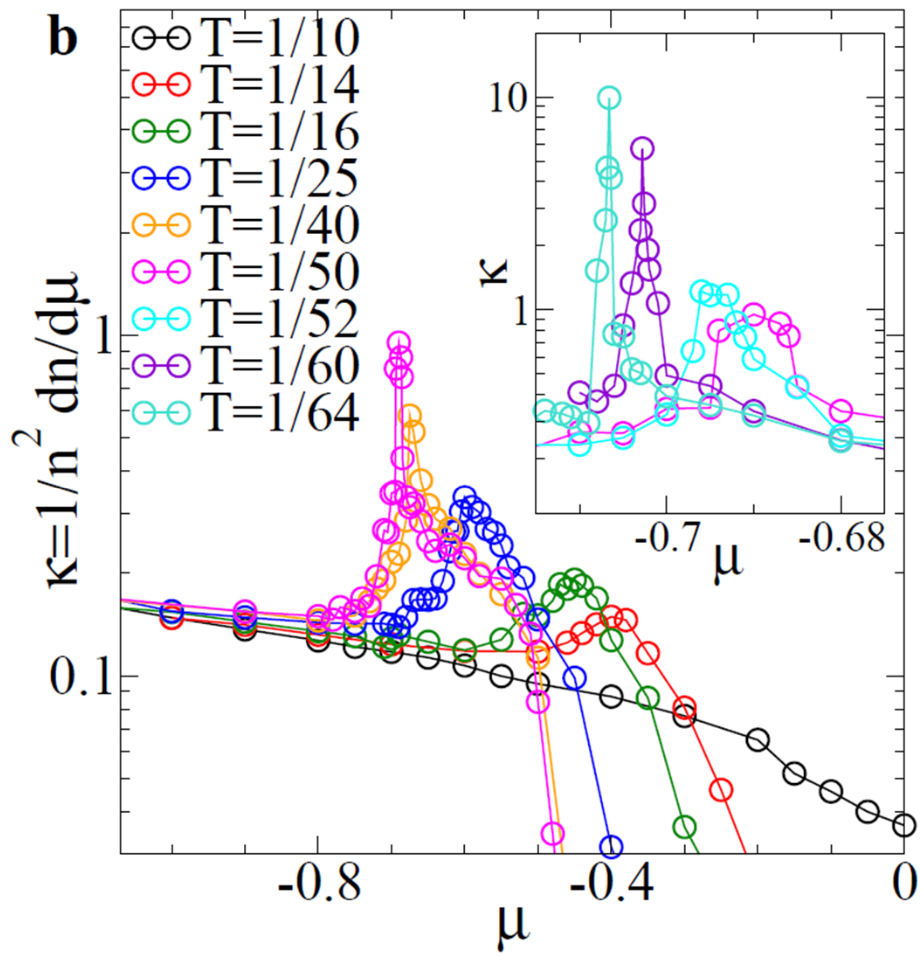
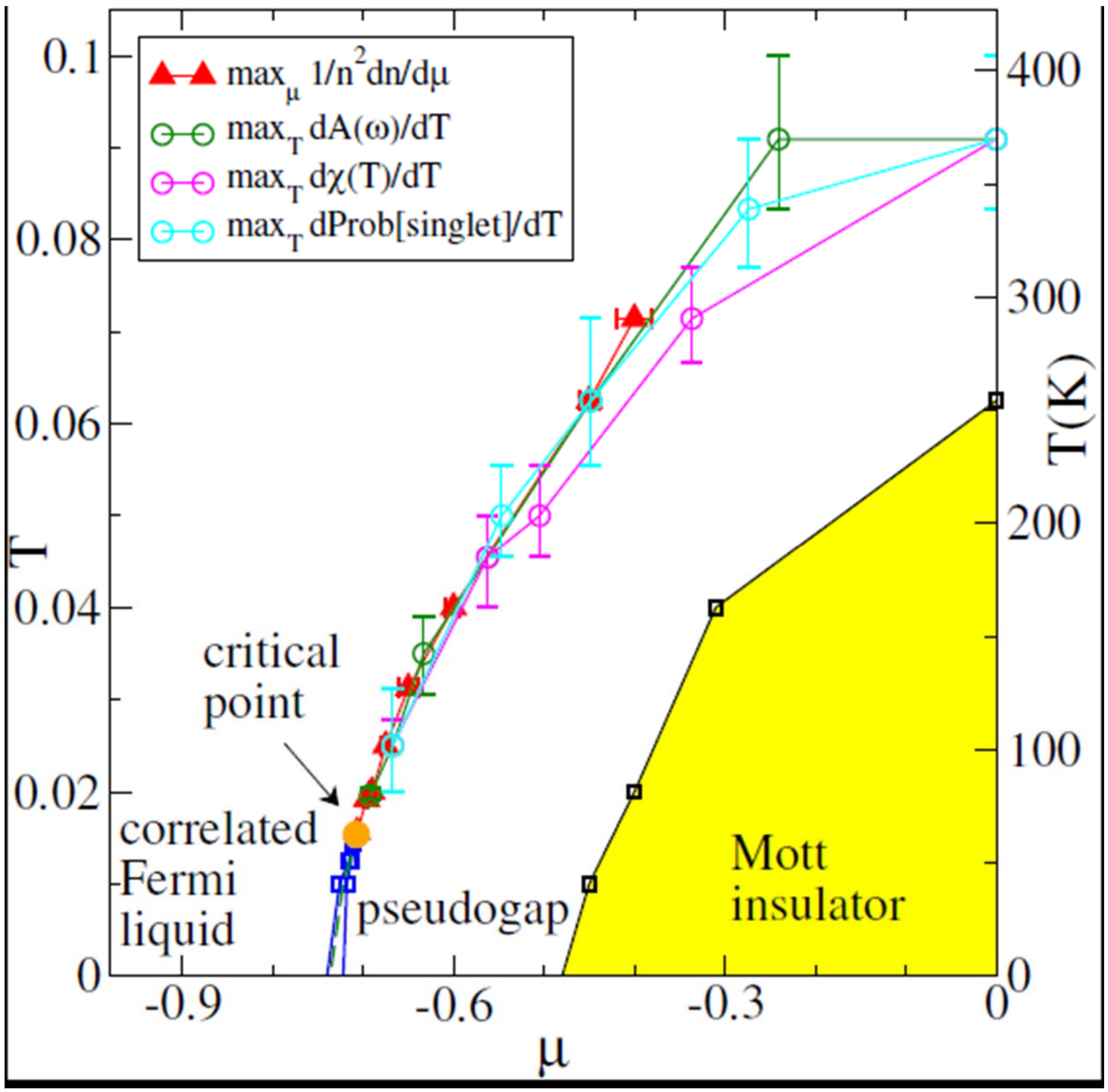
The Widom line





Rapid change also in dynamical quantities



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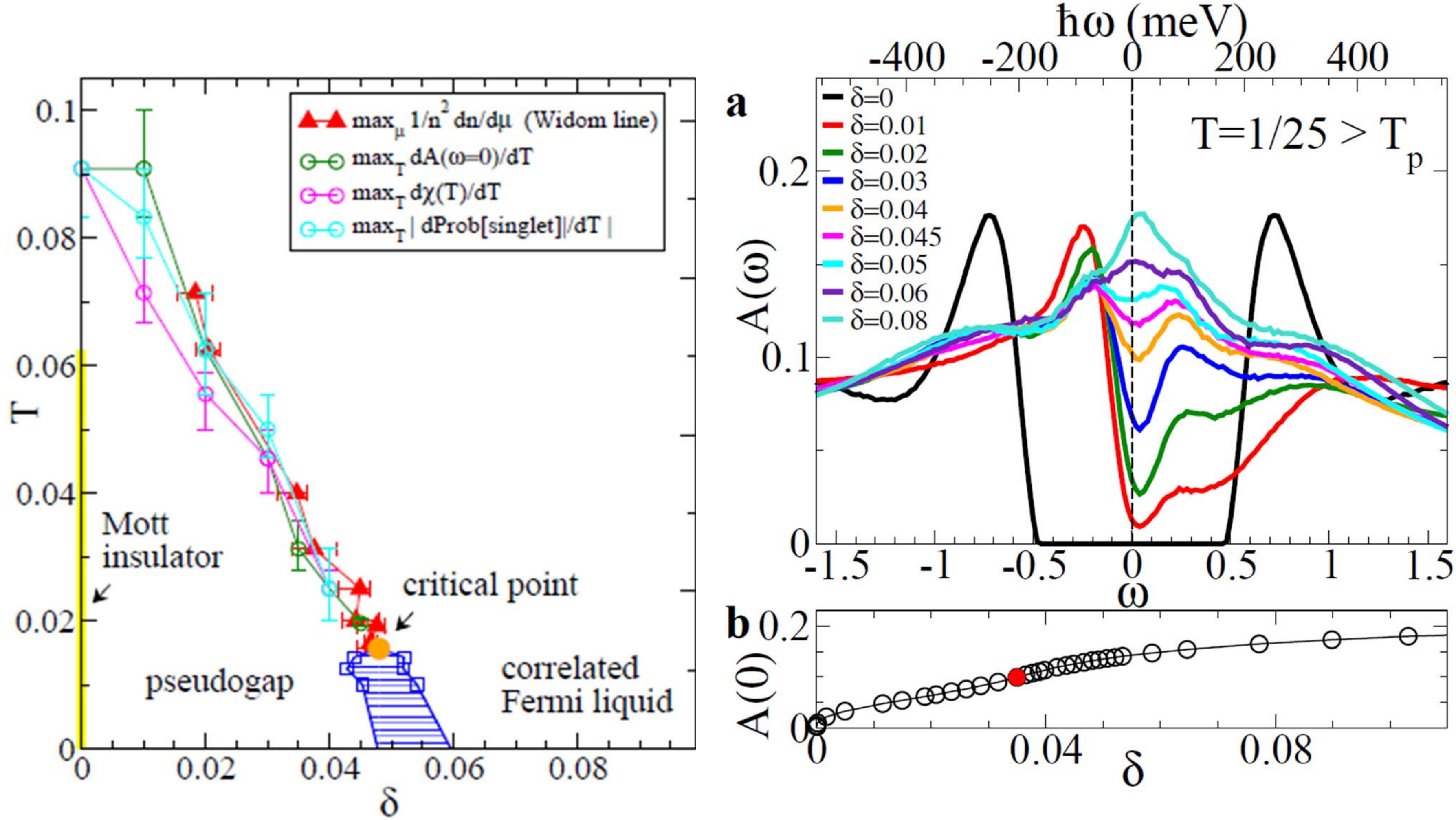
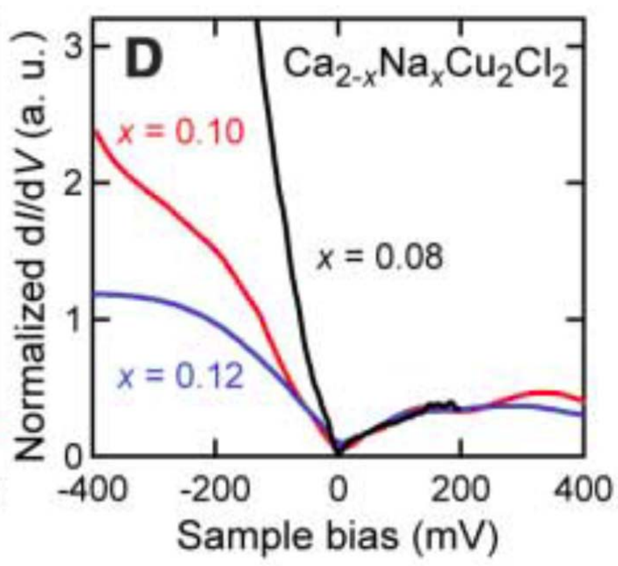
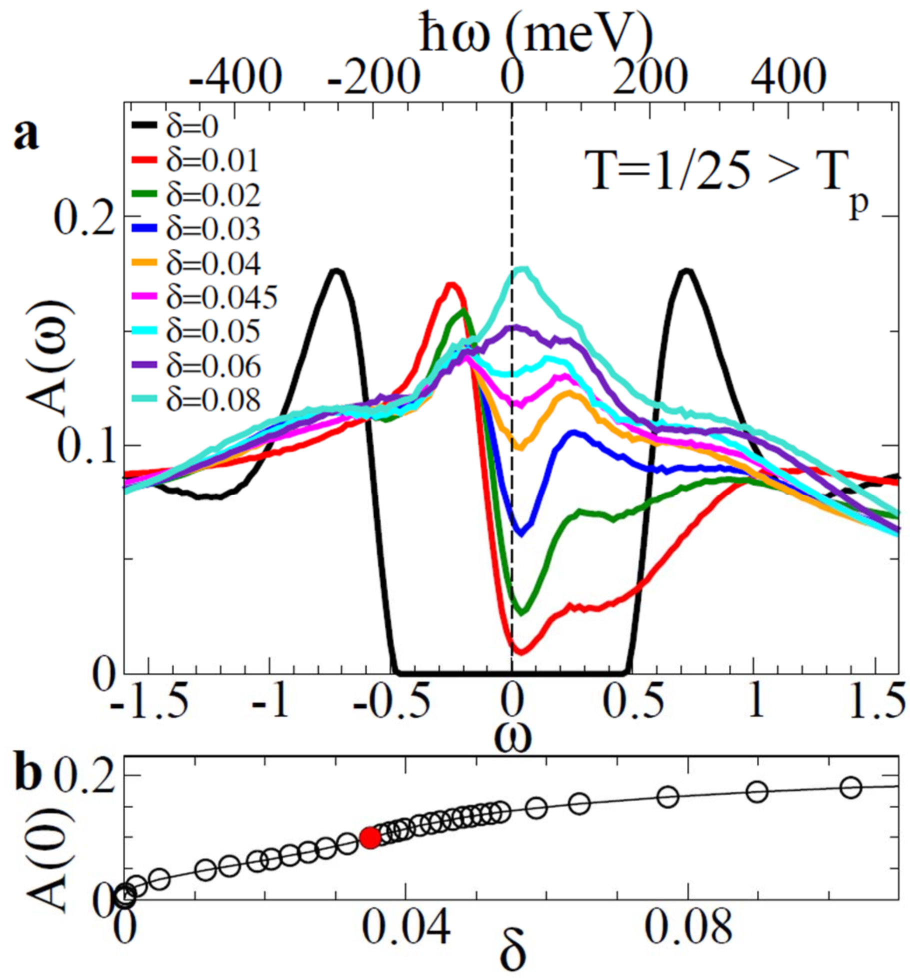
Density of states



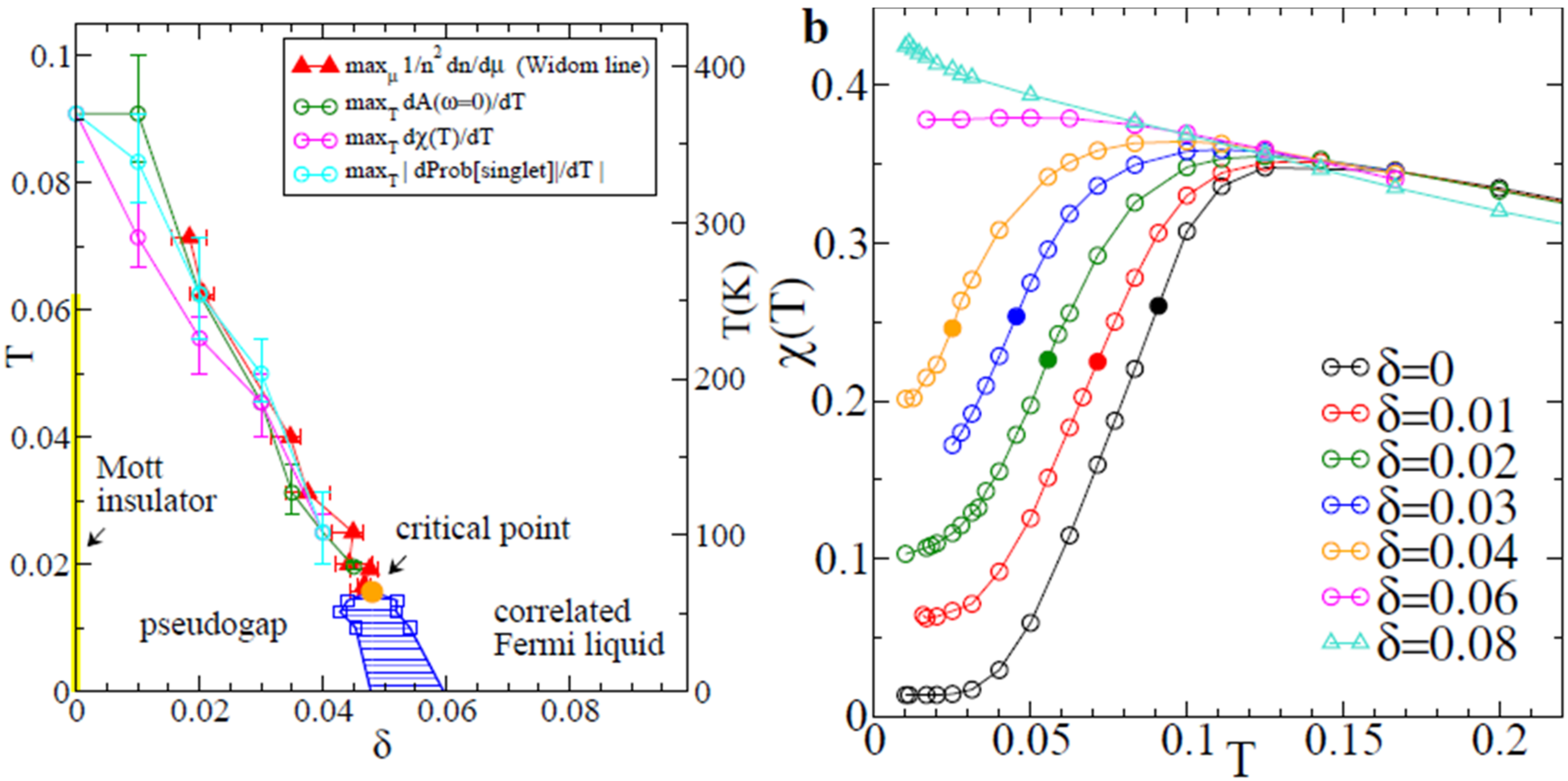
Density of states



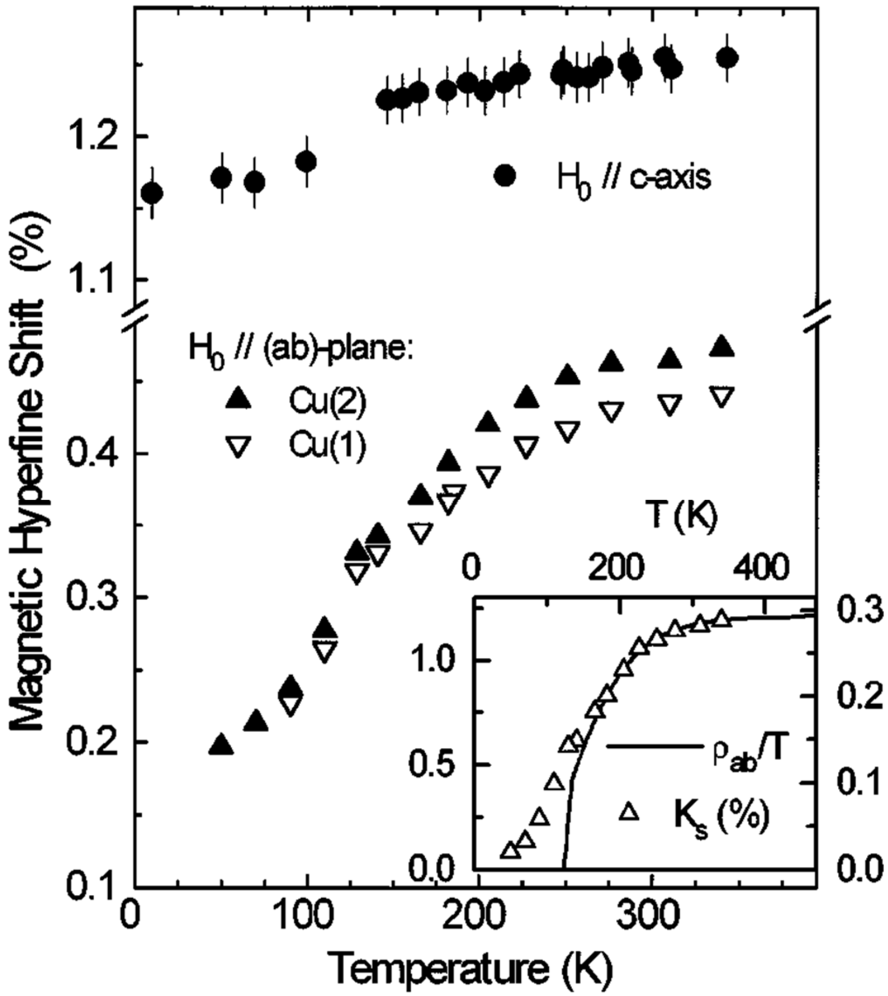


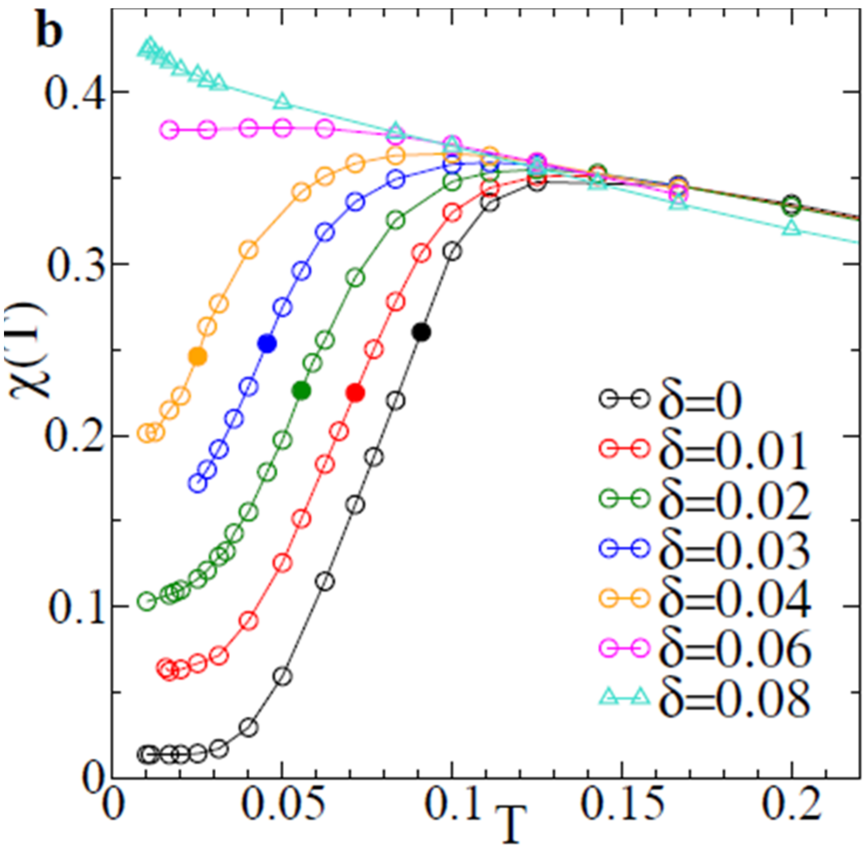
Khosaka et al. *Science* **315**, 1380 (2007);

Spin susceptibility



Spin susceptibility

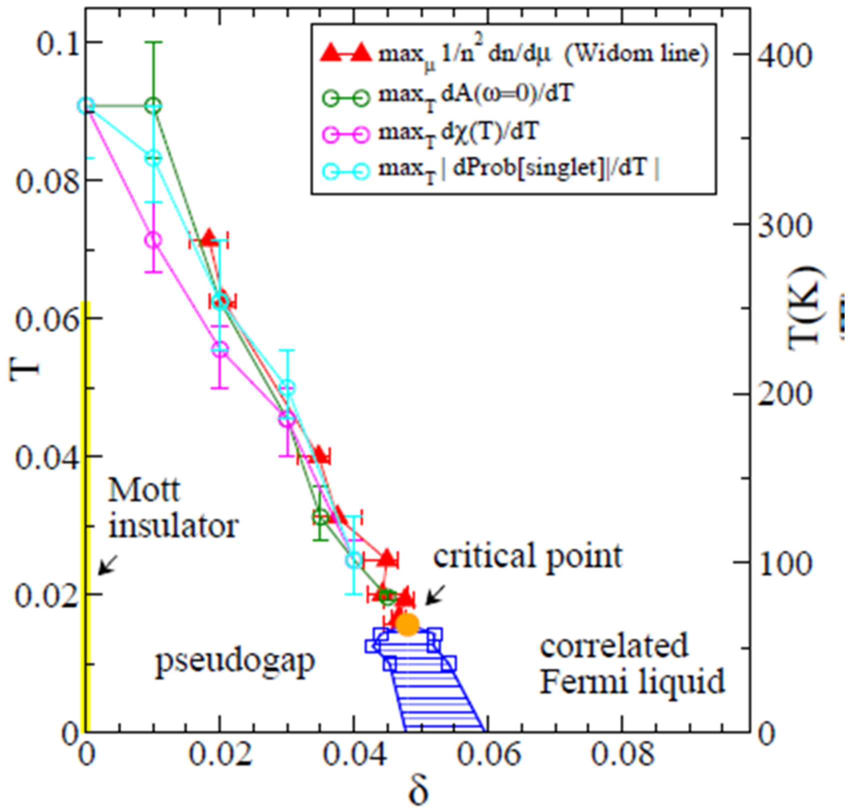


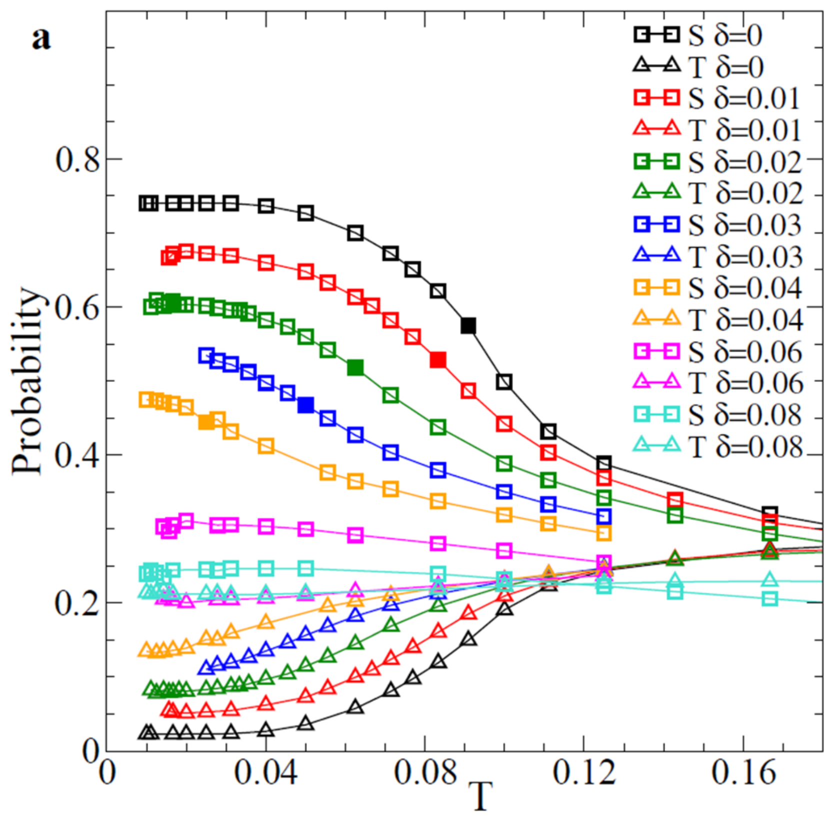


Underdoped Hg1223

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

Plaquette eigenstates





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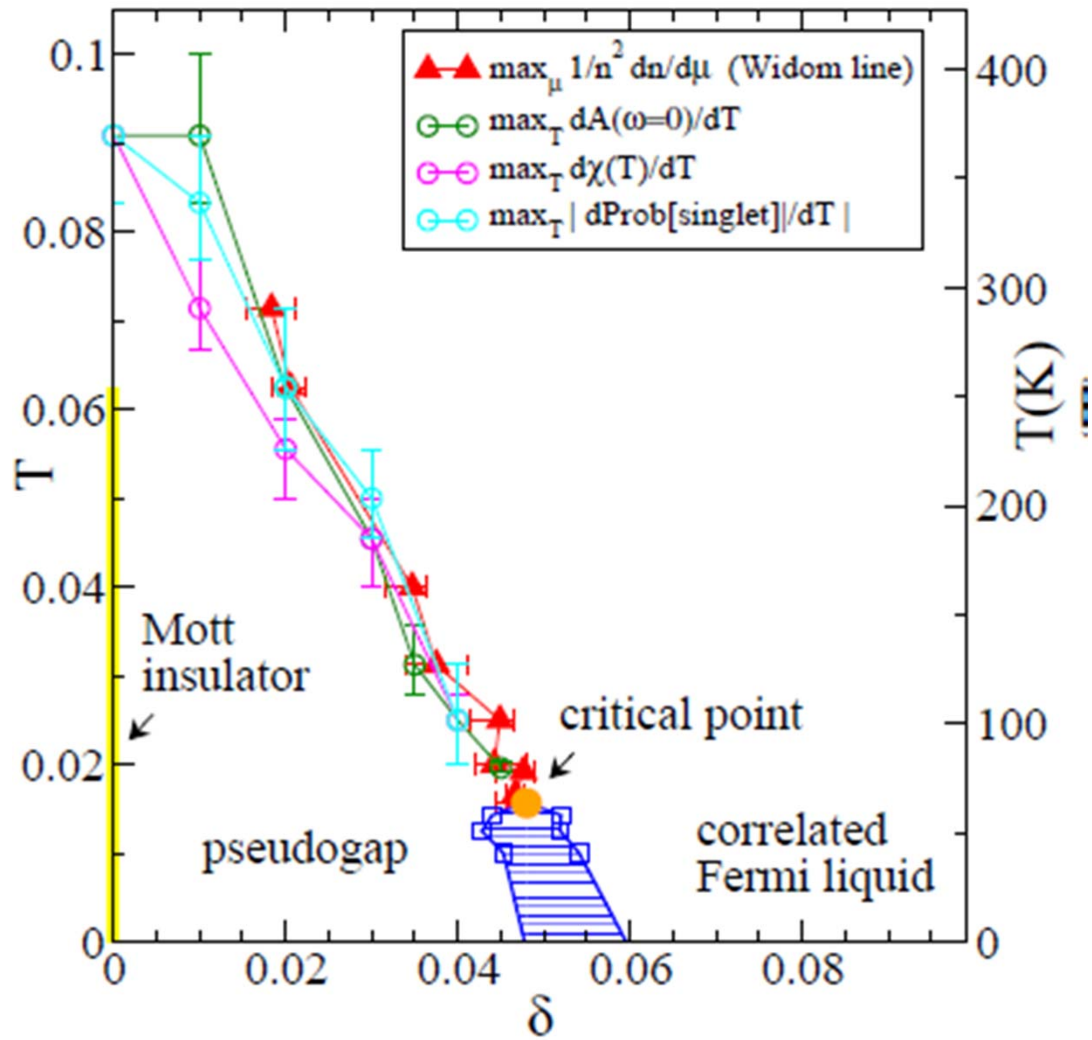
Pseudogap *T** along the Widom line



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What is the minimal model?

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

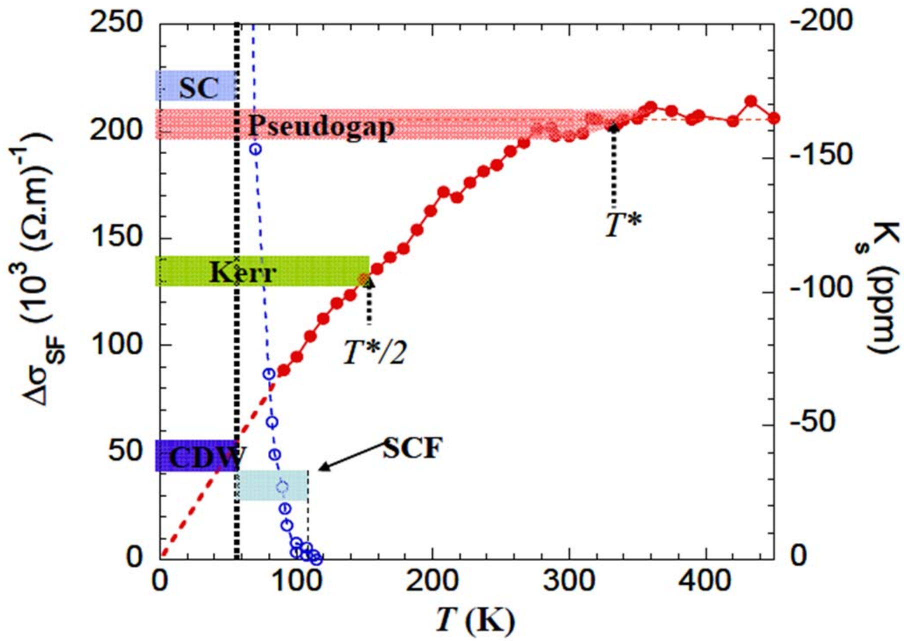

Fig 1 Spin contribution K_s to the ^{89}Y NMR Knight shift [11] for $YBCO_{6.6}$ permit to define the PG onset T^*. Here K_s is reduced by a factor two at $T \sim T^*/2$. The sharp drop of the SC fluctuation conductivity (SCF) is illustrated (left scale) [23]. We report as well the range over which a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

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Two crossover lines

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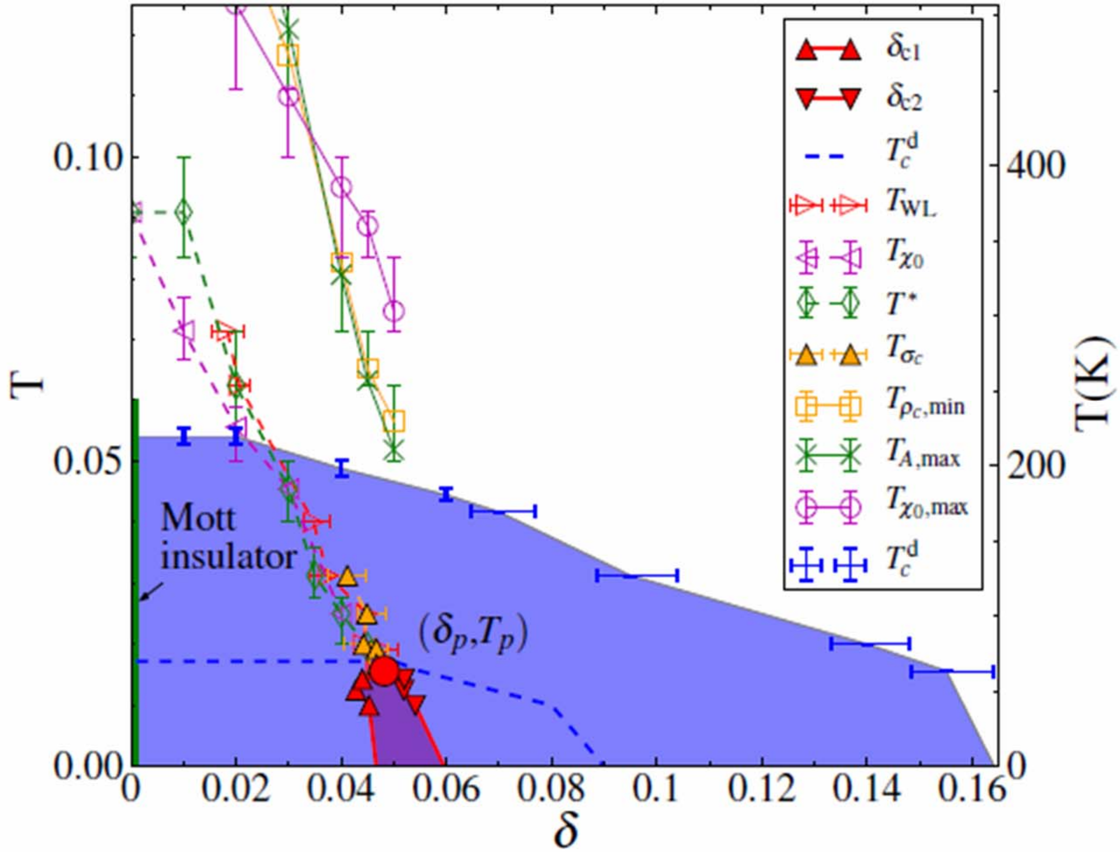
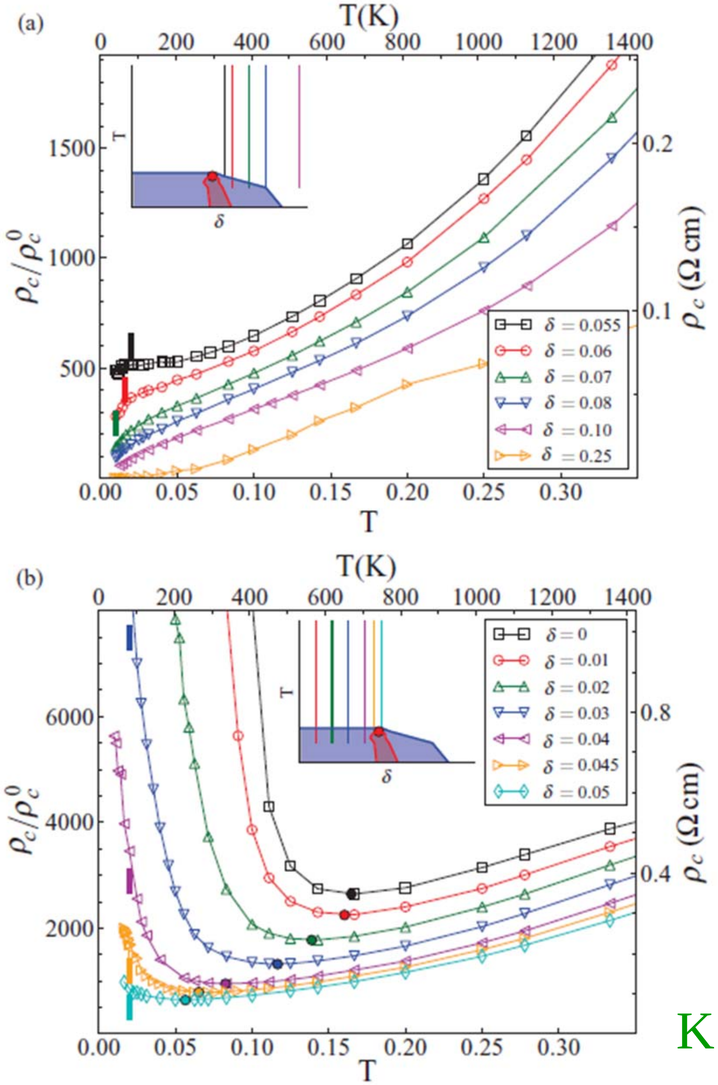
Patrick Sémon

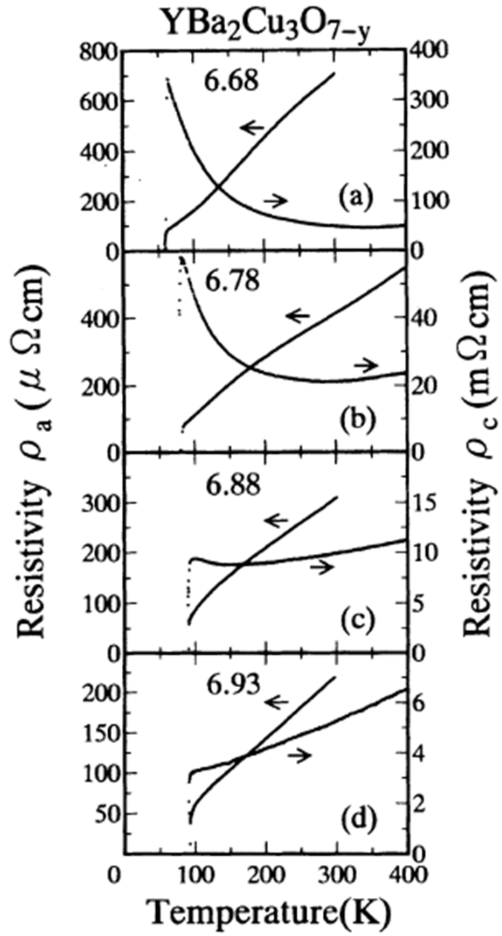


G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)

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

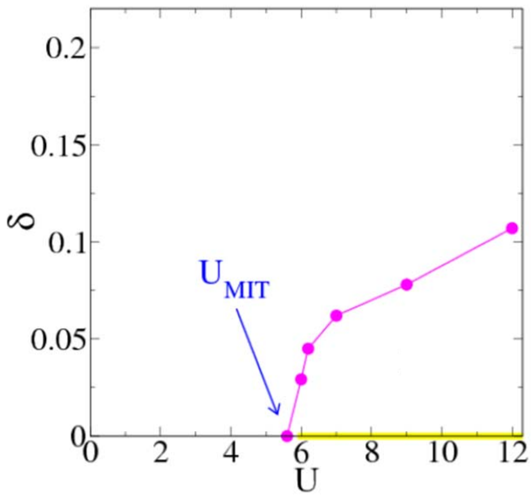
C-axis resistivity

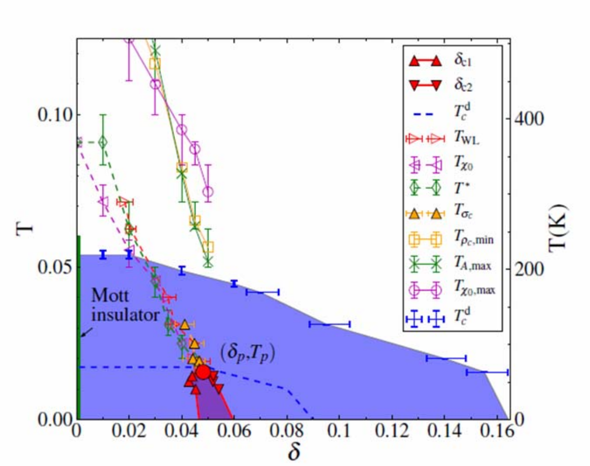




K. Takenaka, K. Mizuhashi, H. Takagi, and S. Uchida, Phys. Rev.B 50, 6534 (1994).

Summary: normal state





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

Giovanni Sordi

Patrick Sémon

Kristjan Haul

Finite *T* phase diagram

Superconductivity

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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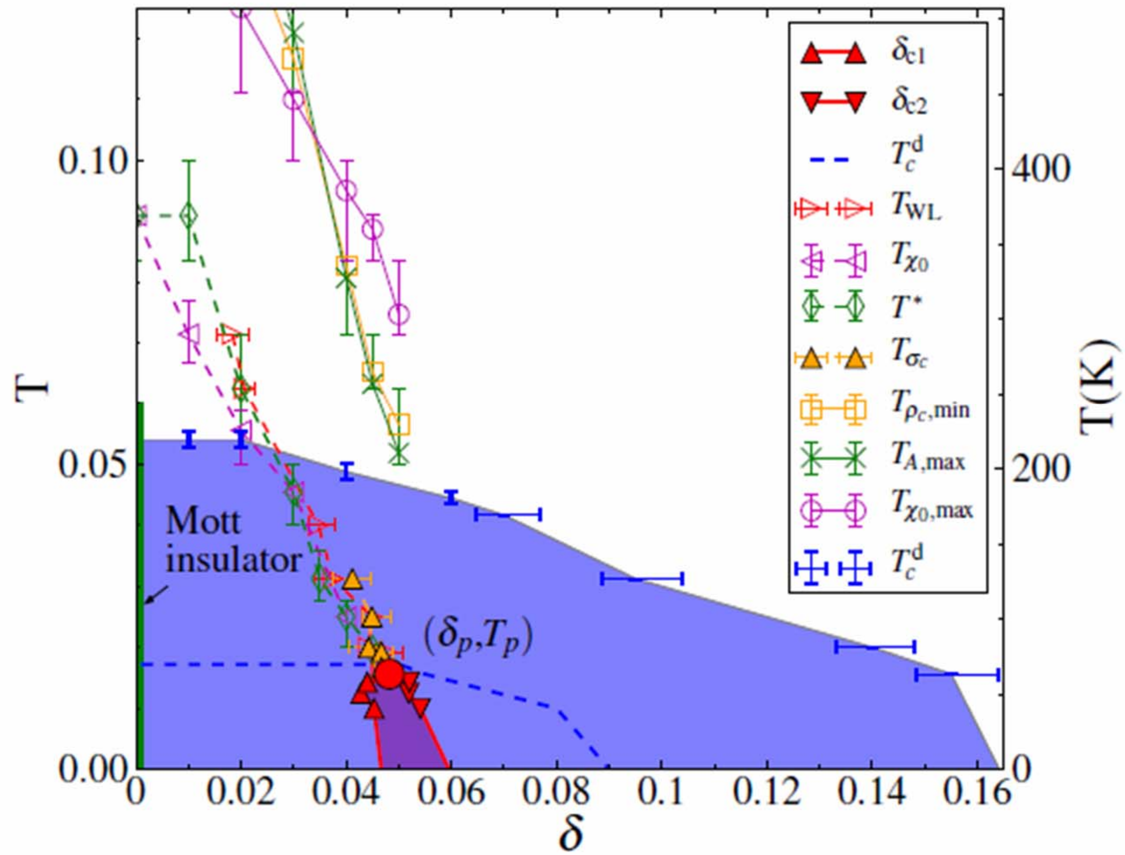
Dôme?

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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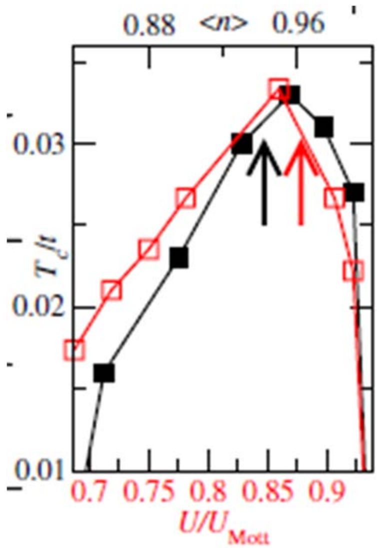
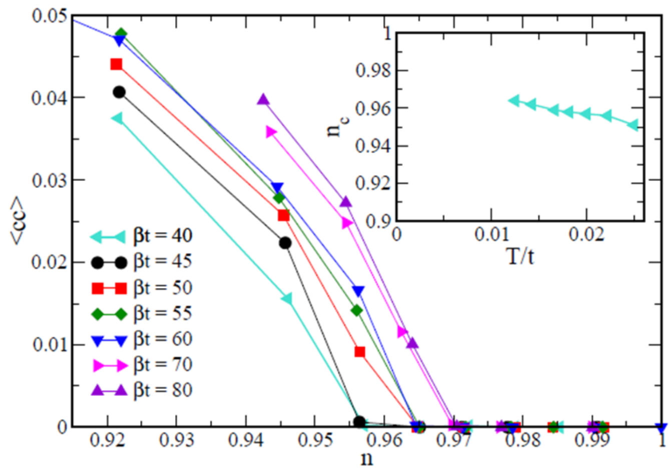
Larger clusters

- In 2x2 T_c vanishes extremely close to half-filling. In larger cluster, earlier.
- Local pairs in underdoped (2x2)



8 site DCA, $U=6t$



8 site DCA, $U=6.5t$

Gull Parcollet Millis,
PRL **110**, 216405 (2013)

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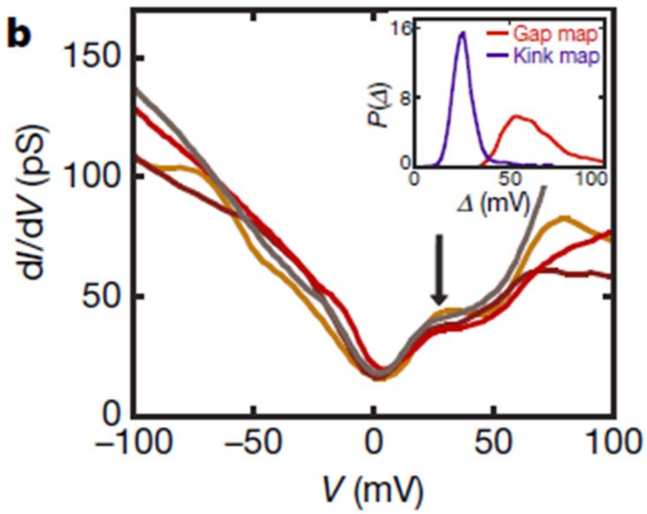
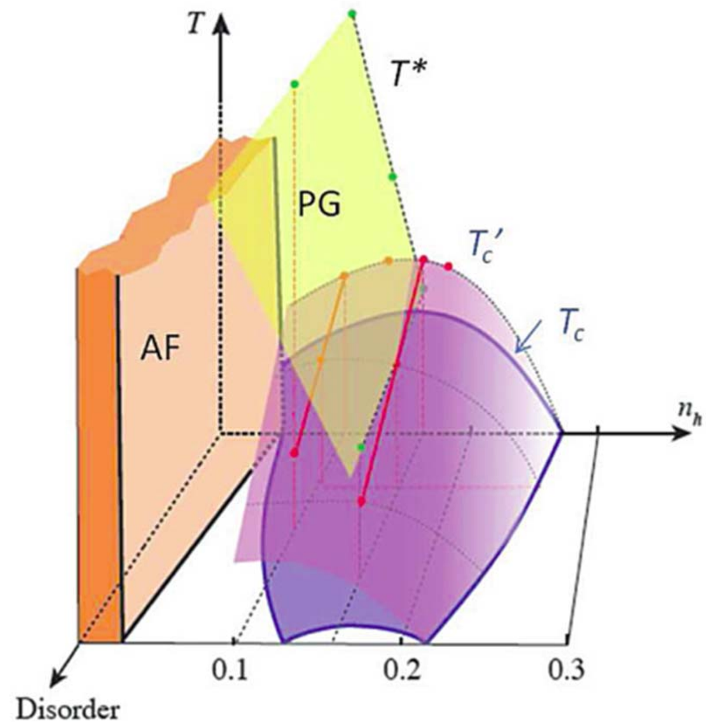
Meaning of T_c^d

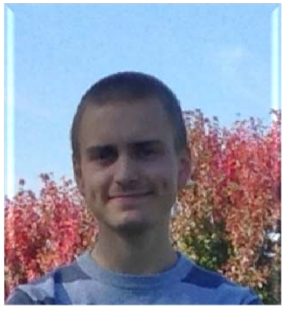
- Local pair formation



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



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



Charles-David Hébert

Patrick Sémon

Bandwidth control and doping control of the Mott transition in organics

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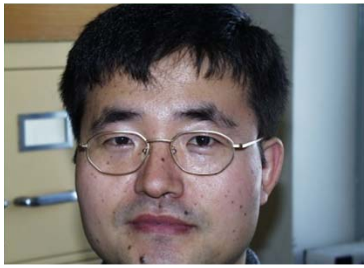
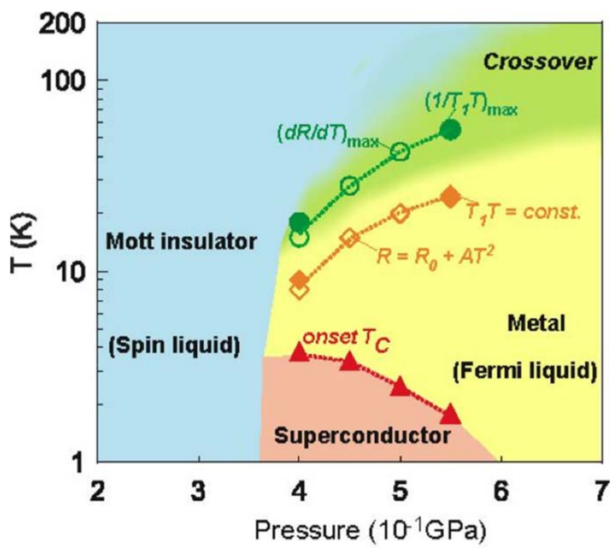
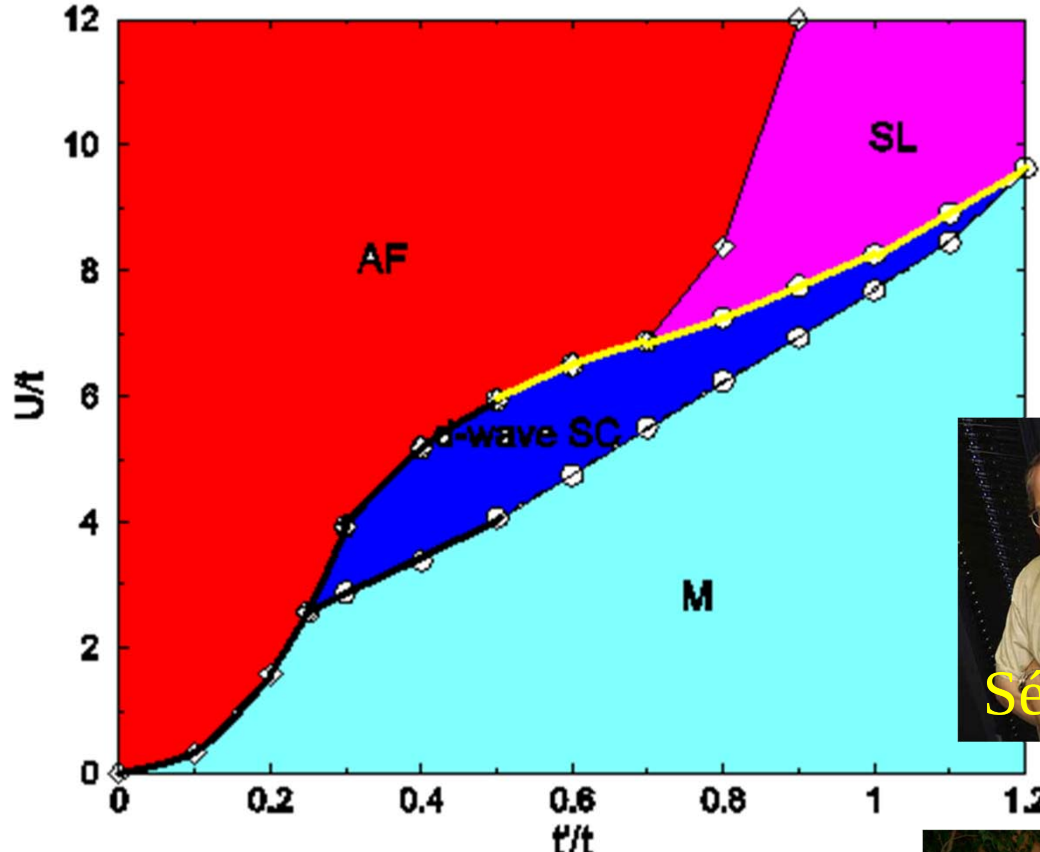


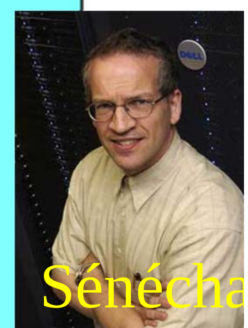
Theoretical phase diagram BEDT

X= $Cu_2(CN)_3$ (t'~ t)



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



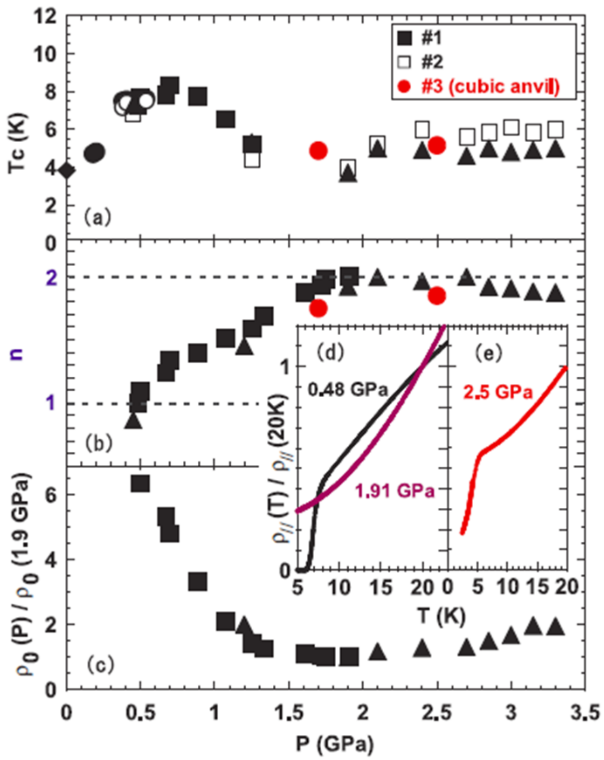


Kyung, A.-M.S.T. PRL 97, 046402 (2006)

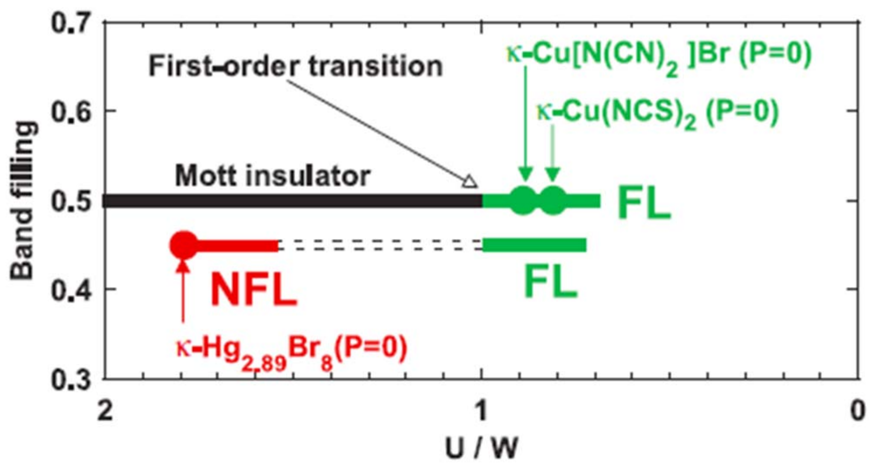
Sénéchal, Sahebsara, Phys. Rev. Lett. **97**, 257004

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

A doped BEDT organic



	W (eV)	U (eV)	U/W	BF	T_c (K)
κ-Cu(NCS)$_2$ [a)]	0.57	0.46	0.81	0.50	10.4
κ-Cu[N(CN)$_2$]Br [a)]	0.55	0.49	0.89	0.50	11.8
κ-Hg$_{2.89}$Br$_8$ [b)]	0.26	0.465	1.79	0.45	4.3



Taniguchi et al. J. Phys. Soc. Japan, **76**, 113709 (2007)

R. N. Lyubovskaya et al. JETP Lett. **45,** 530 (1987)

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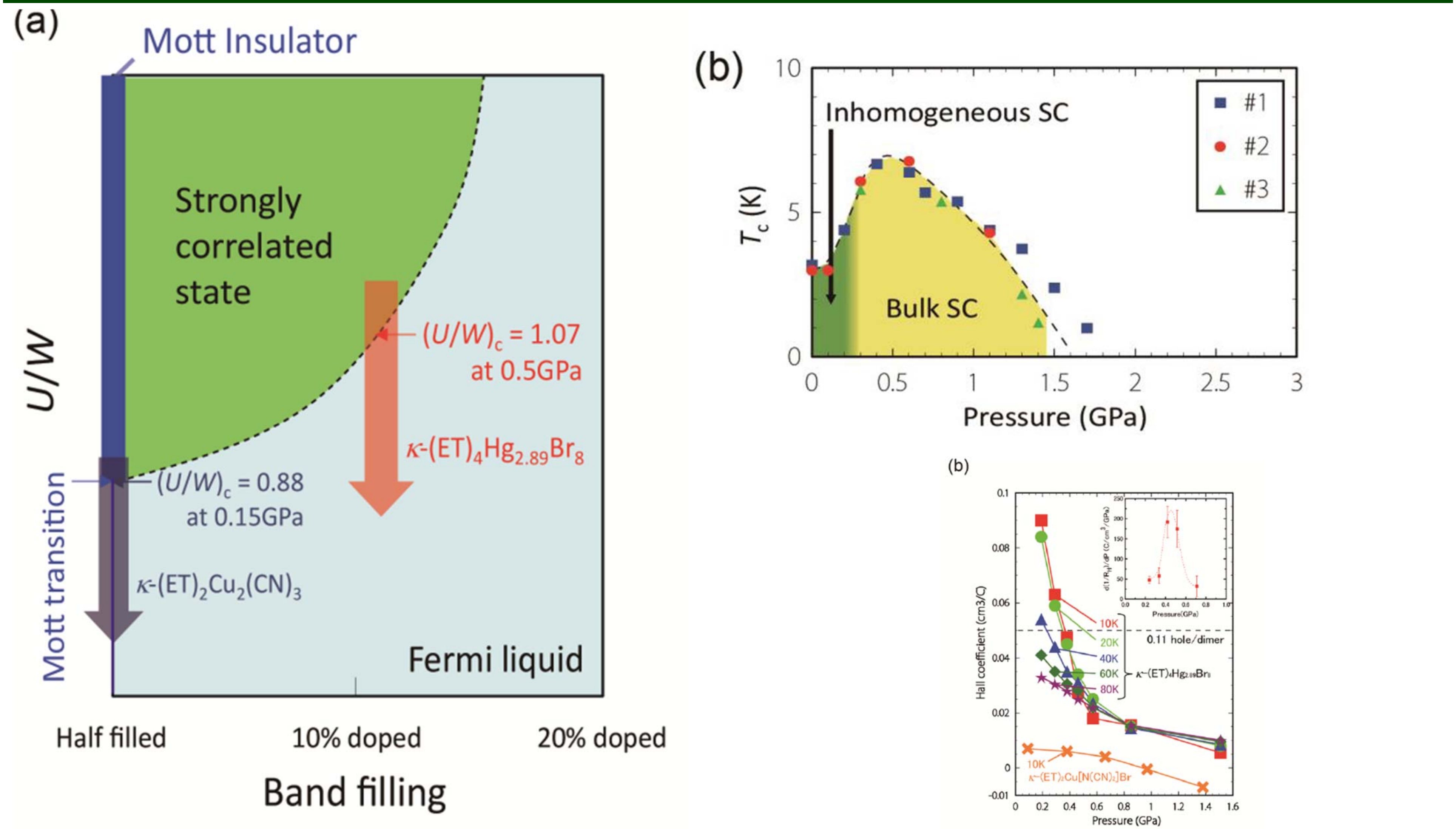
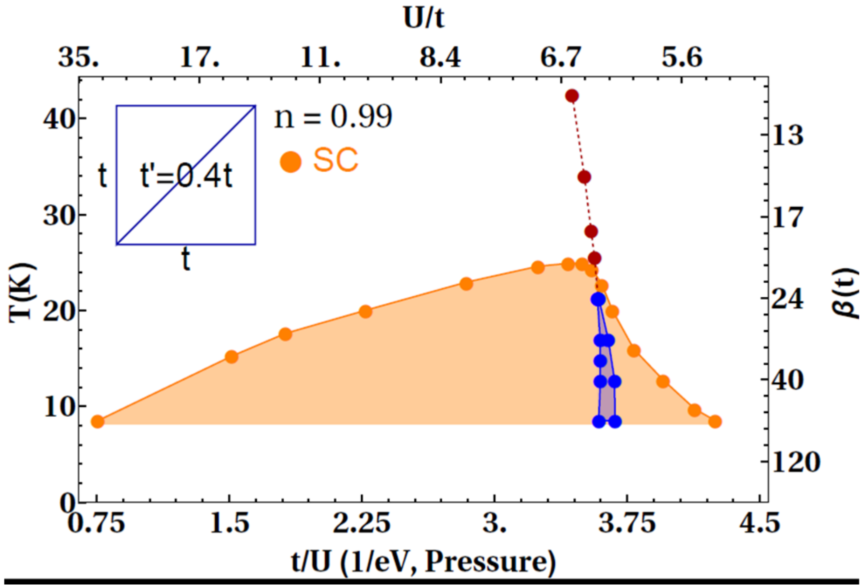
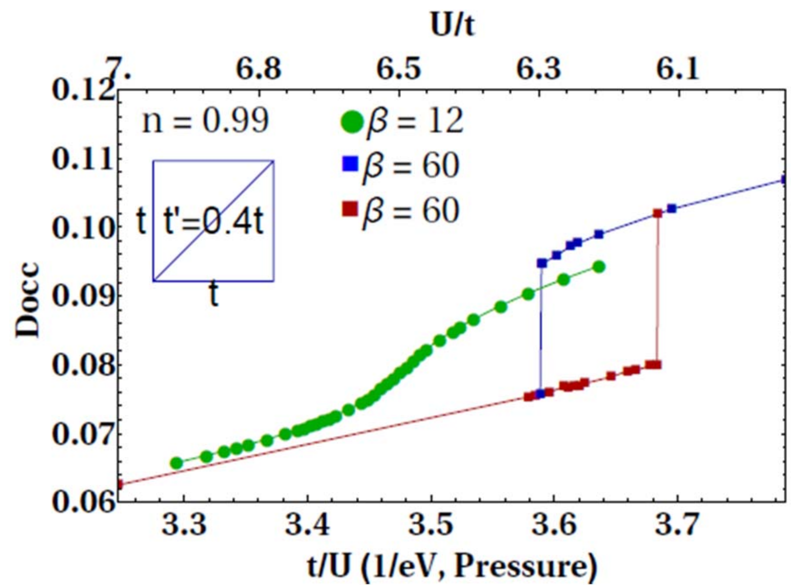
Doped BEDT

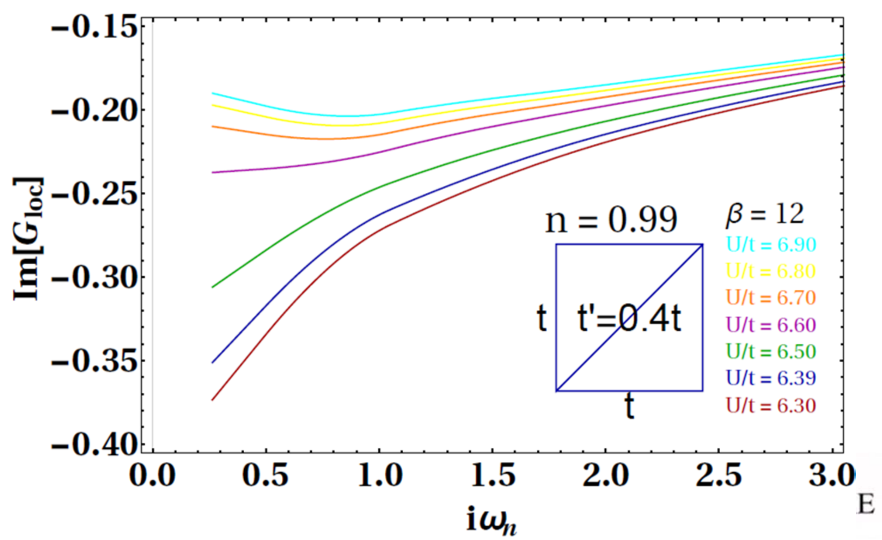


H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

Widom line in organics

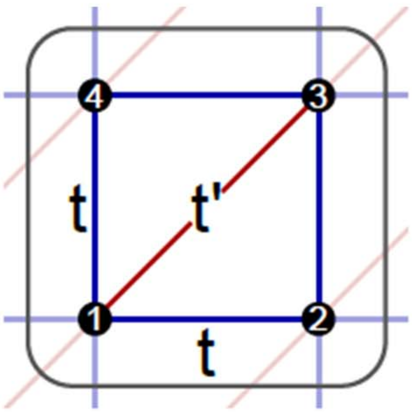




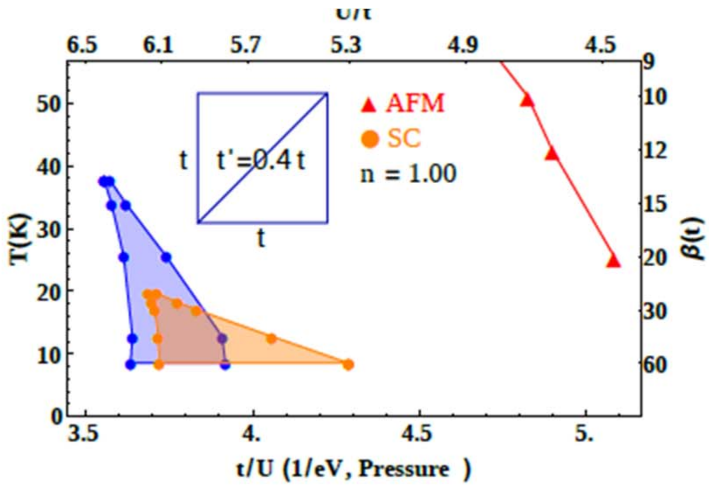


Charles-David Hébert, Patrick Sémon , AMT

t’=0.4t

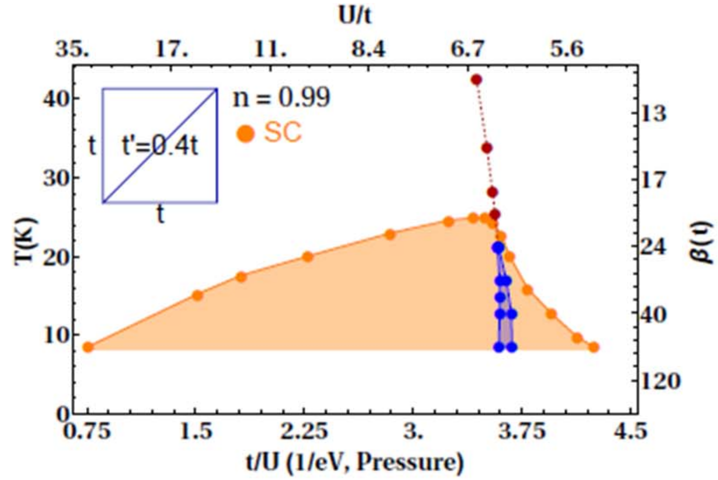


t
t'
t
1
2
3
4



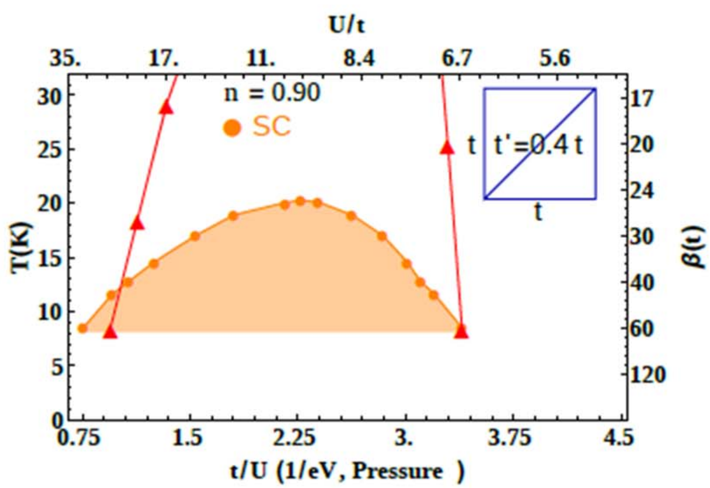
U/t
T(K)
β(t)
t/U (1/eV, Pressure)
AFM
SC
n = 1.00
t'=0.4 t

(a)

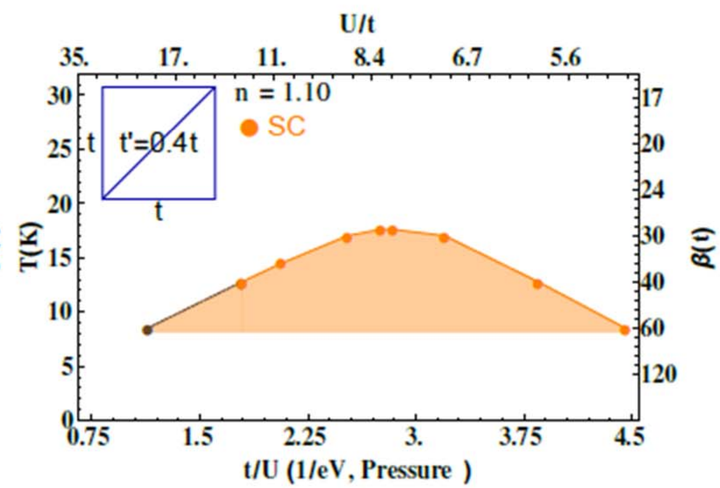


U/t
T(K)
β(t)
t/U (1/eV, Pressure)
n = 0.99
SC
t'=0.4t

(b)

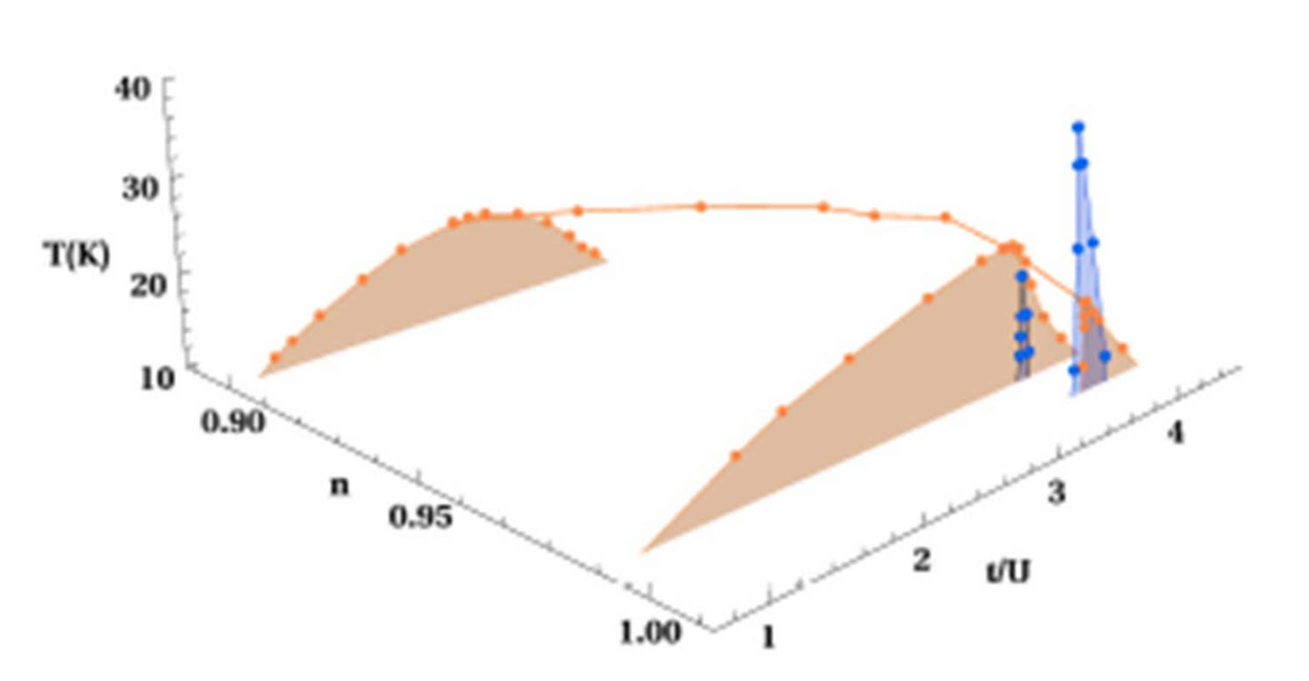


U/t
T(K)
β(t)
t/U (1/eV, Pressure)
n = 0.90
SC
t'=0.4 t

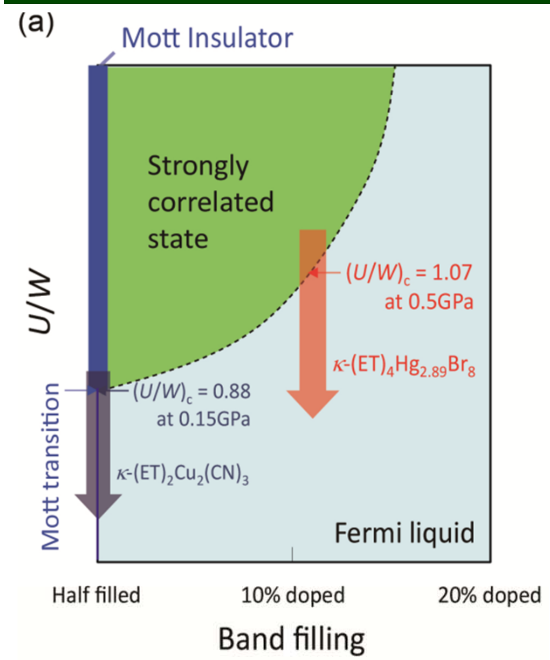


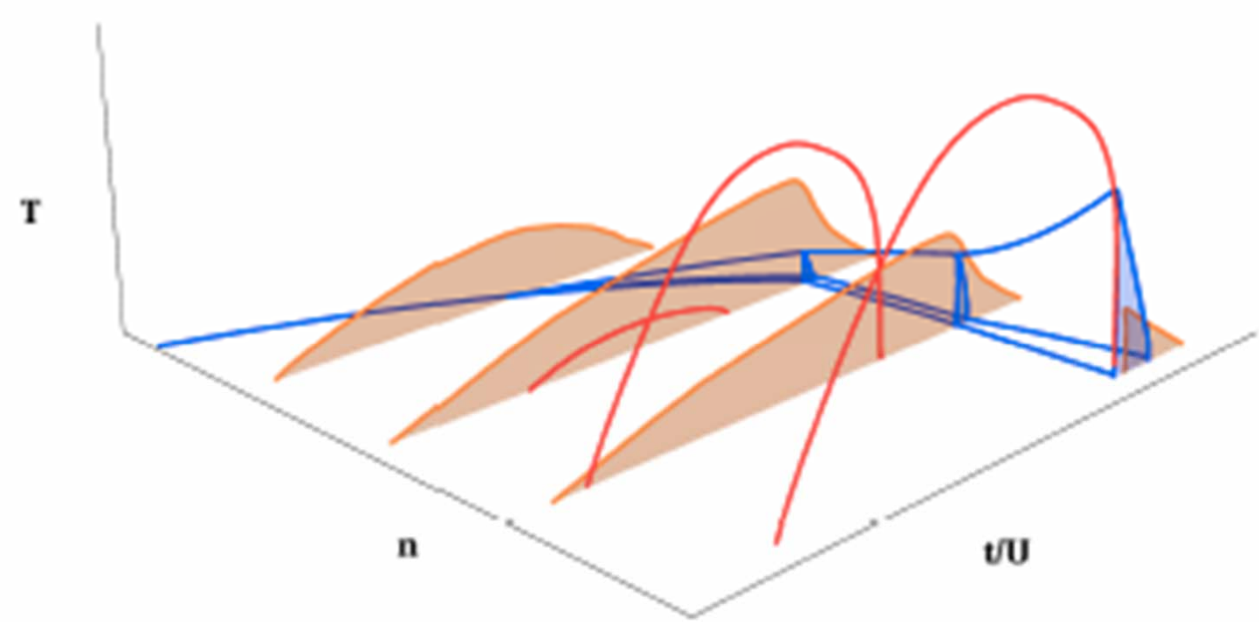
U/t
T(K)
β(t)
t/U (1/eV, Pressure)
n = 1.10
SC
t'=0.4t

t’ = 0.4t overview



Generic case





Summary : organics

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

Main collaborators

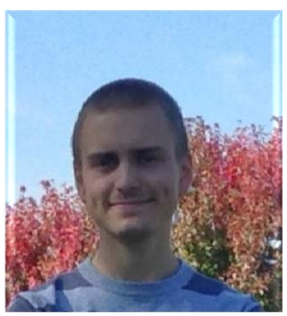
Giovanni Sordi

Kristjan Haule

David Sénéchal

Bumsoo Kyung

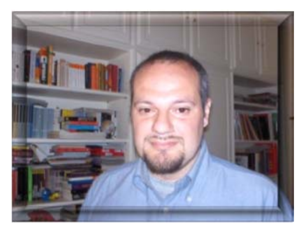
Patrick Sémon



Charles-David Hébert

Sarma Kancharla

Marcello Civelli



Massimo Capone

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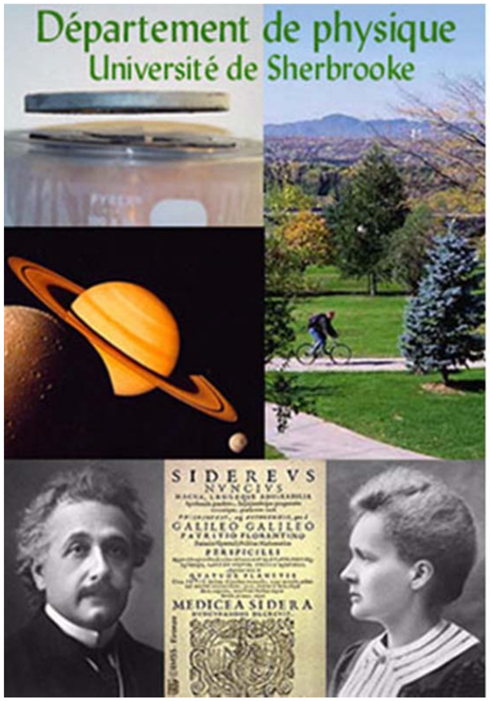

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Merci

Thank you

A.-M.S. Tremblay

"Strongly correlated superconductivity"

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