Strongly correlated superconductivity in cuprates and layered organics: results and some algorithmic details

A.-M. Tremblay

Charles-David Hébert, Giovanni Sordi, Patrick Sémon, Kristjan Haule, David Sénéchal, Alexandre Day, Vincent Bouliane

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Bâton Rouge, 14 February 2015

VERITATEM IN CHARITATE

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BCS Superconductivity

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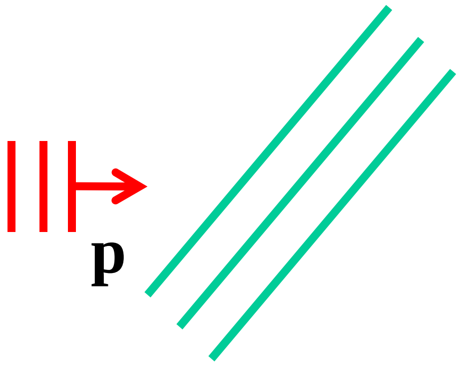
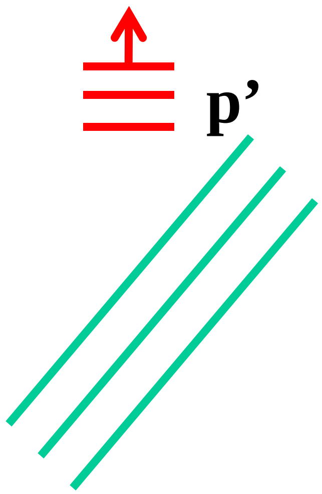
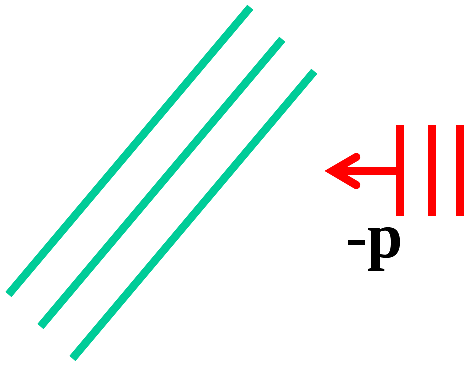
Attraction mechanism in the metallic state



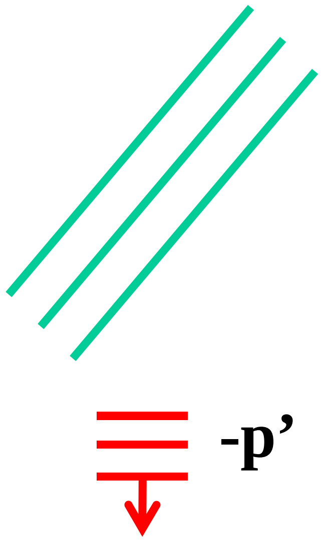
Attraction mechanism in the metallic state



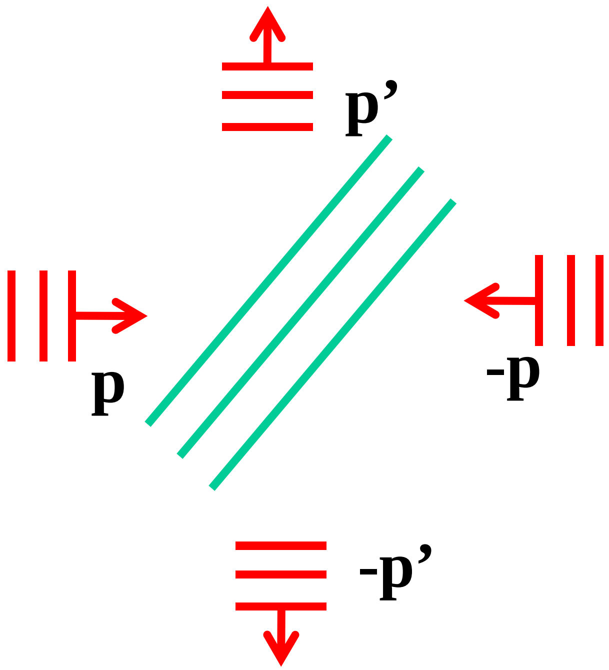
Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



#1 Cooper pair, #2 Phase coherence

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

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

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

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Breakdown of band theory
Half-filled band is metallic?

Half-filled band: Not always a metal

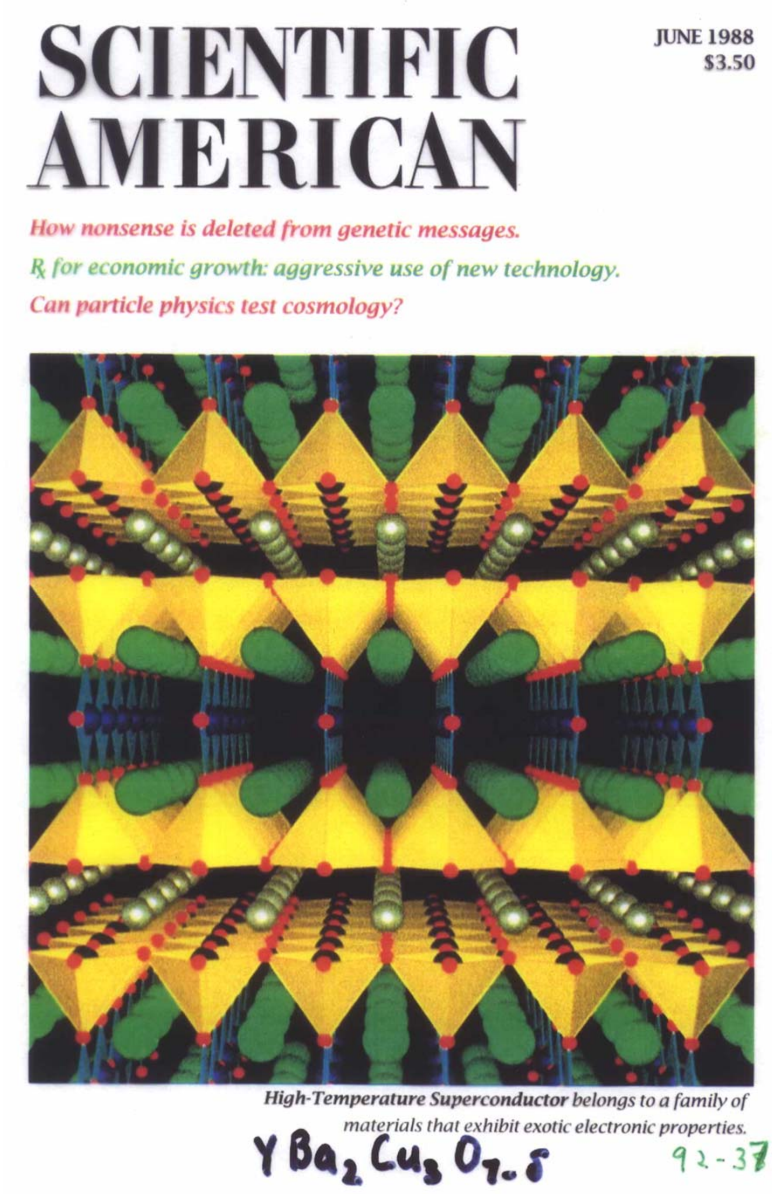
NiO, Boer and Verway

Peierls, 1937

Mott, 1949

Two materials,
two routes to breakdown of band theory
and of BCS superconductivity

Cuprates



SCIENTIFIC AMERICAN

JUNE 1988
$3.50

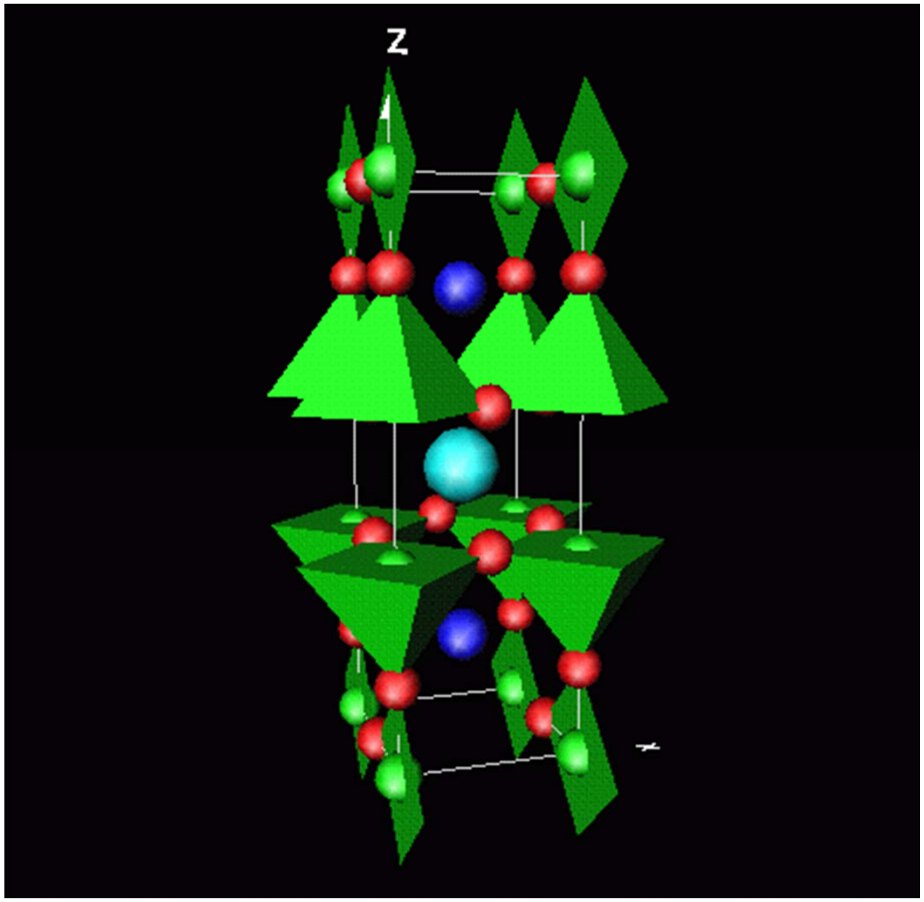
How nonsense is deleted from genetic messages.

℞ for economic growth: aggressive use of new technology.

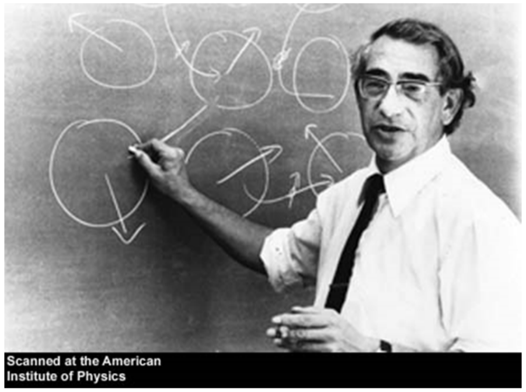
Can particle physics test cosmology?

High-Temperature Superconductor belongs to a family of materials that exhibit exotic electronic properties.

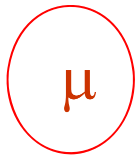
$YBa_2Cu_3O_{7-\delta}$ 92-37

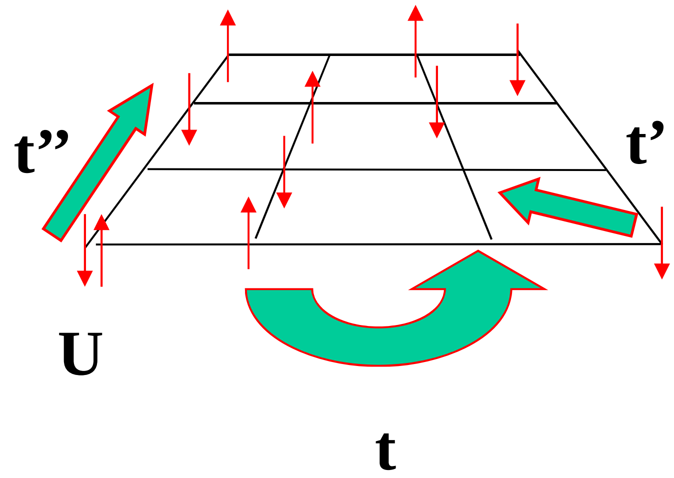


Hubbard model

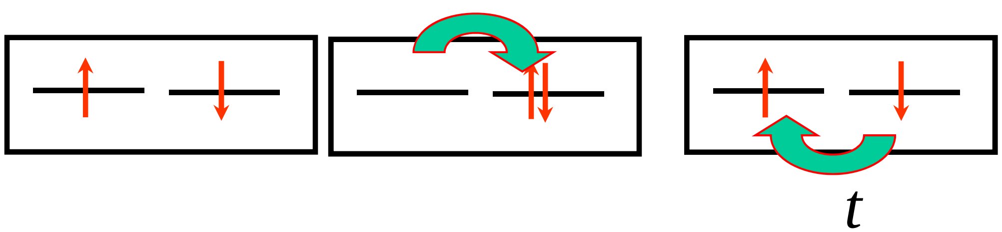


1931-1980





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

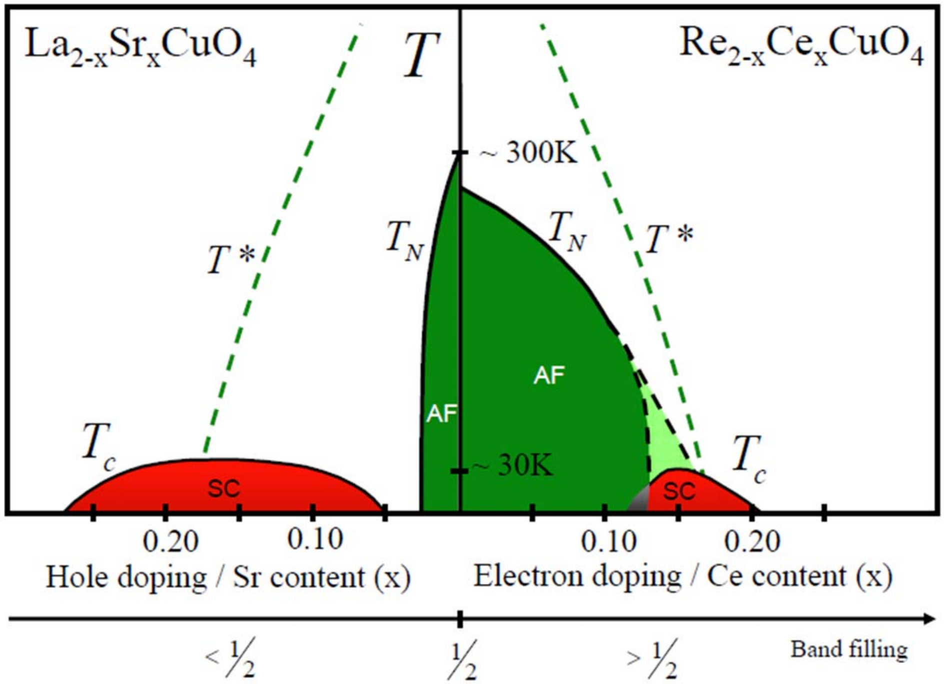


$t = 1$

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

High-temperature superconductors

Armitage, Fournier, Greene, RMP (2009)



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

- Competing order
  - Current loops: Varma, PRB **81,** 064515 (2010)
  - Stripes or nematic: Kivelson et al. RMP 75 1201(2003); J.C.Davis
  - d-density wave : Chakravarty, Nayak, Phys. Rev. B **63**, 094503 (2001); Affleck et al. flux phase
  - SDW: Sachdev PRB **80**, 155129 (2009) ...
- Or Mott Physics?
  - RVB: P.A. Lee Rep. Prog. Phys. **71,** 012501 (2008)

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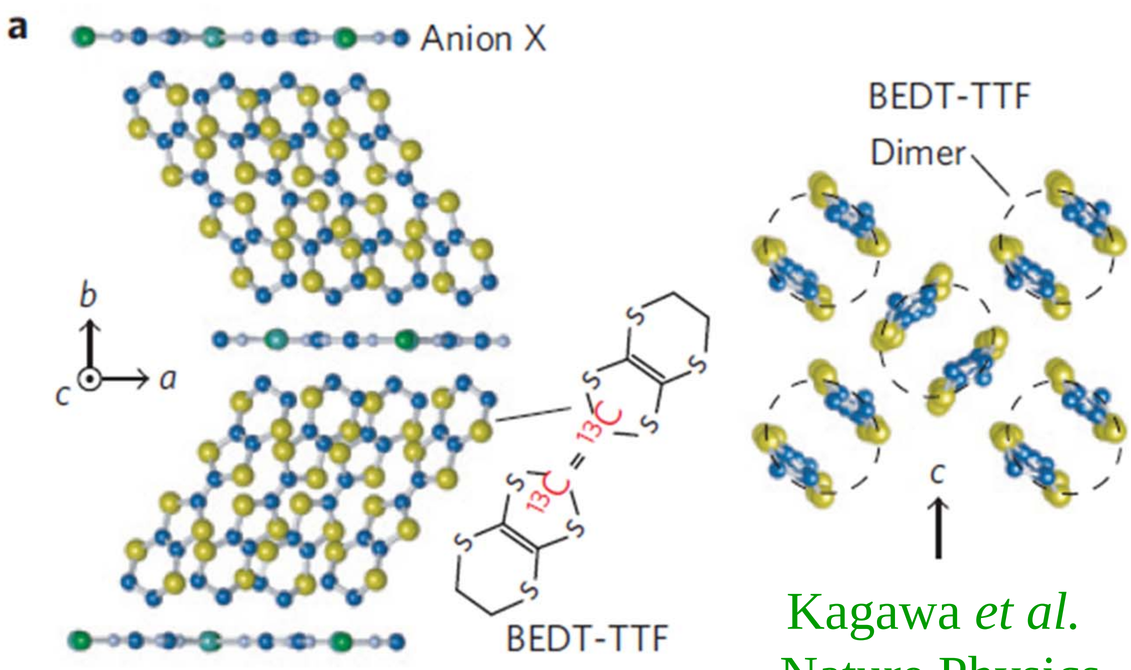
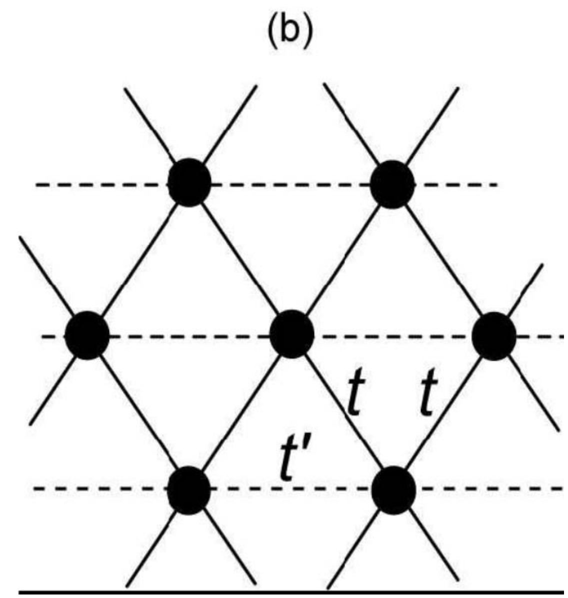
Hubbard on anisotropic triangular lattice

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)



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

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

$t'/t \sim 0.6 - 1.1$

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

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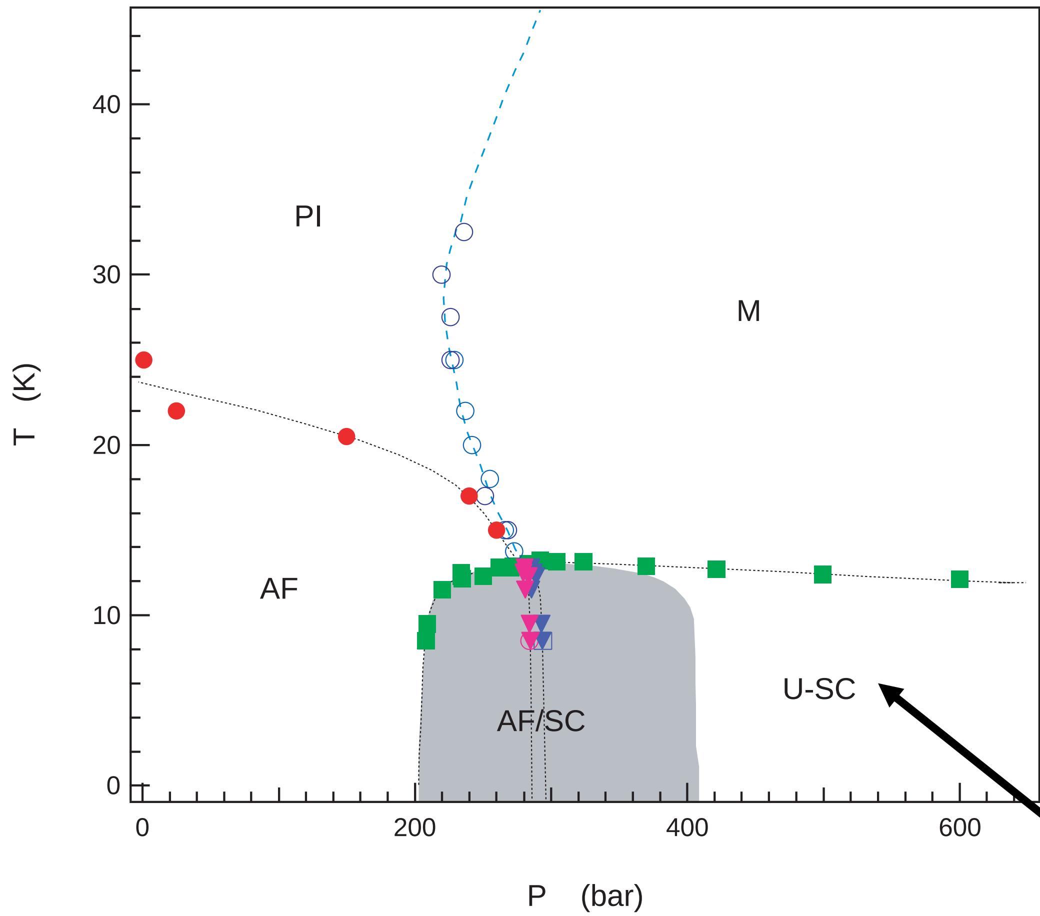
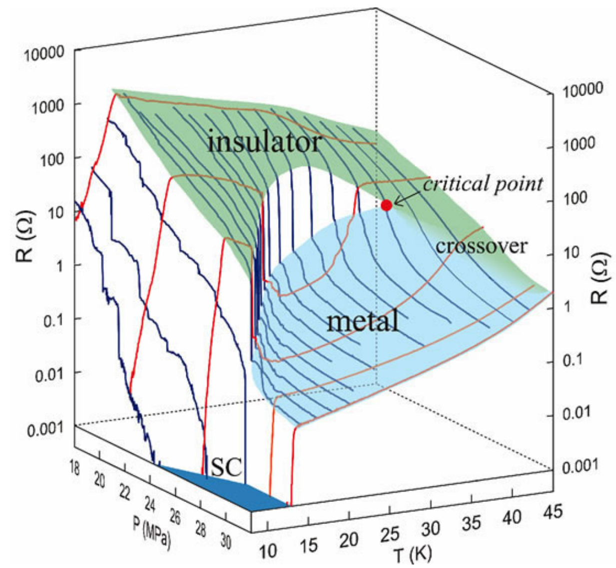
Phase diagram for organics





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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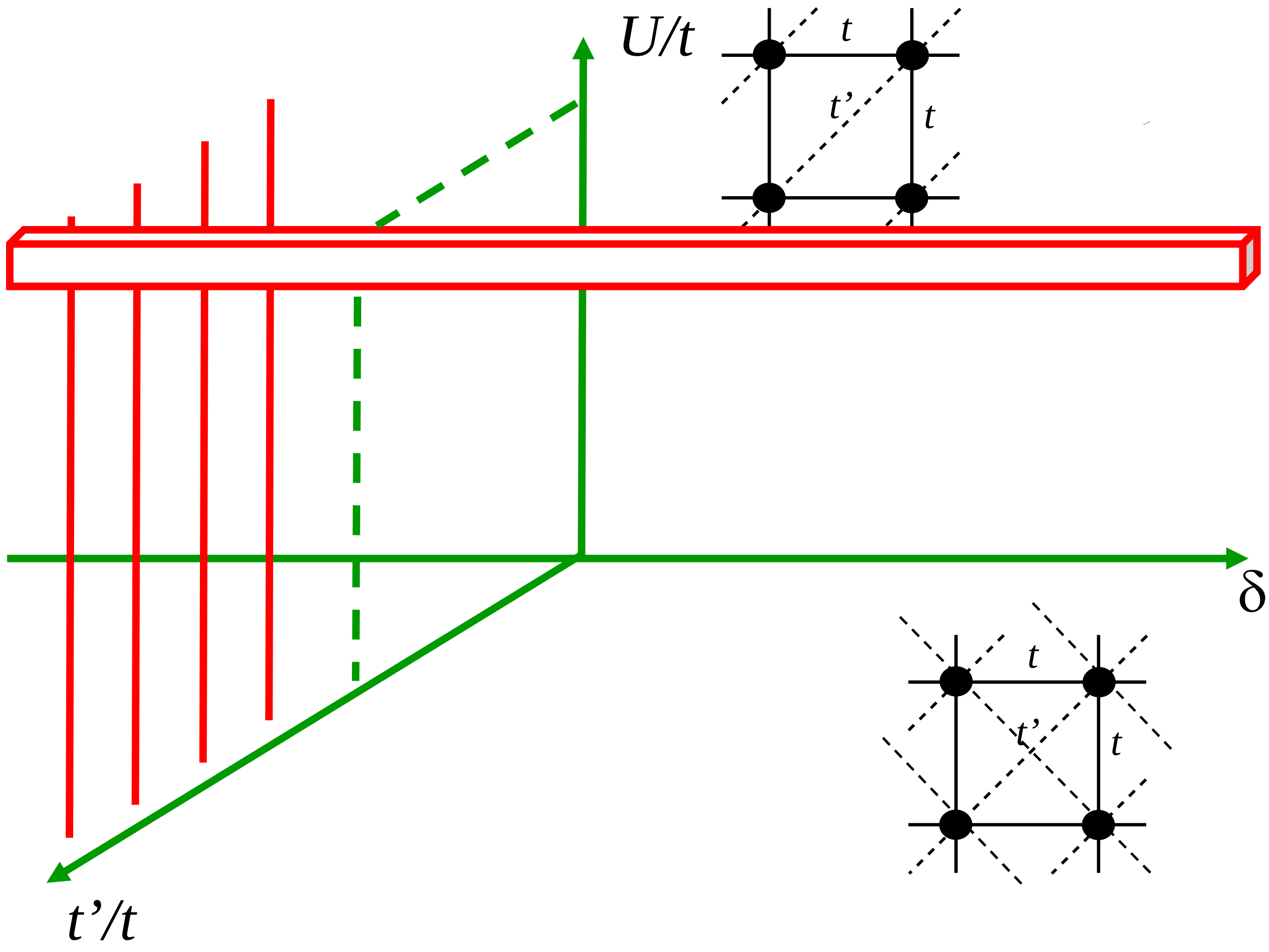
Perspective



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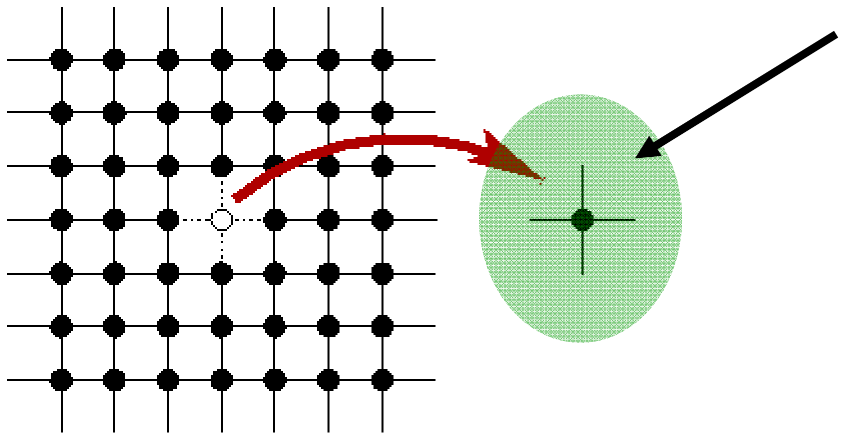
Methods

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

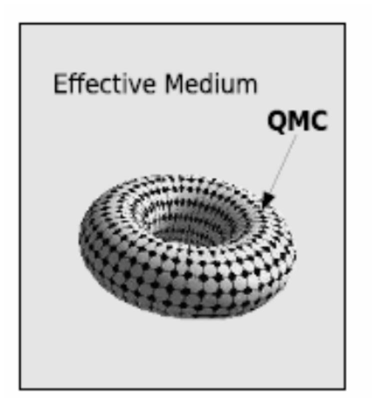
- Compute scattering rate (self-energy) of impurity problem.
- Use that self-energy (ω dependent) for lattice.
- Project lattice on single-site and adjust bath so that single-site DOS obtained both ways be equal.



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

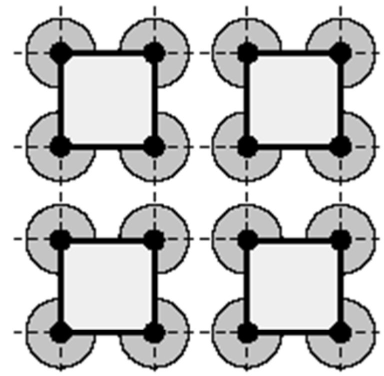
DMFT, (*d = 3)*

2d Hubbard: Quantum cluster method

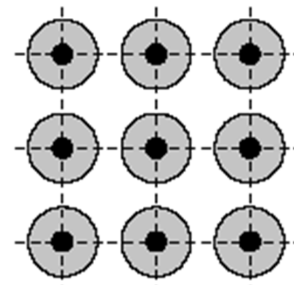


DCA

C-DMFT



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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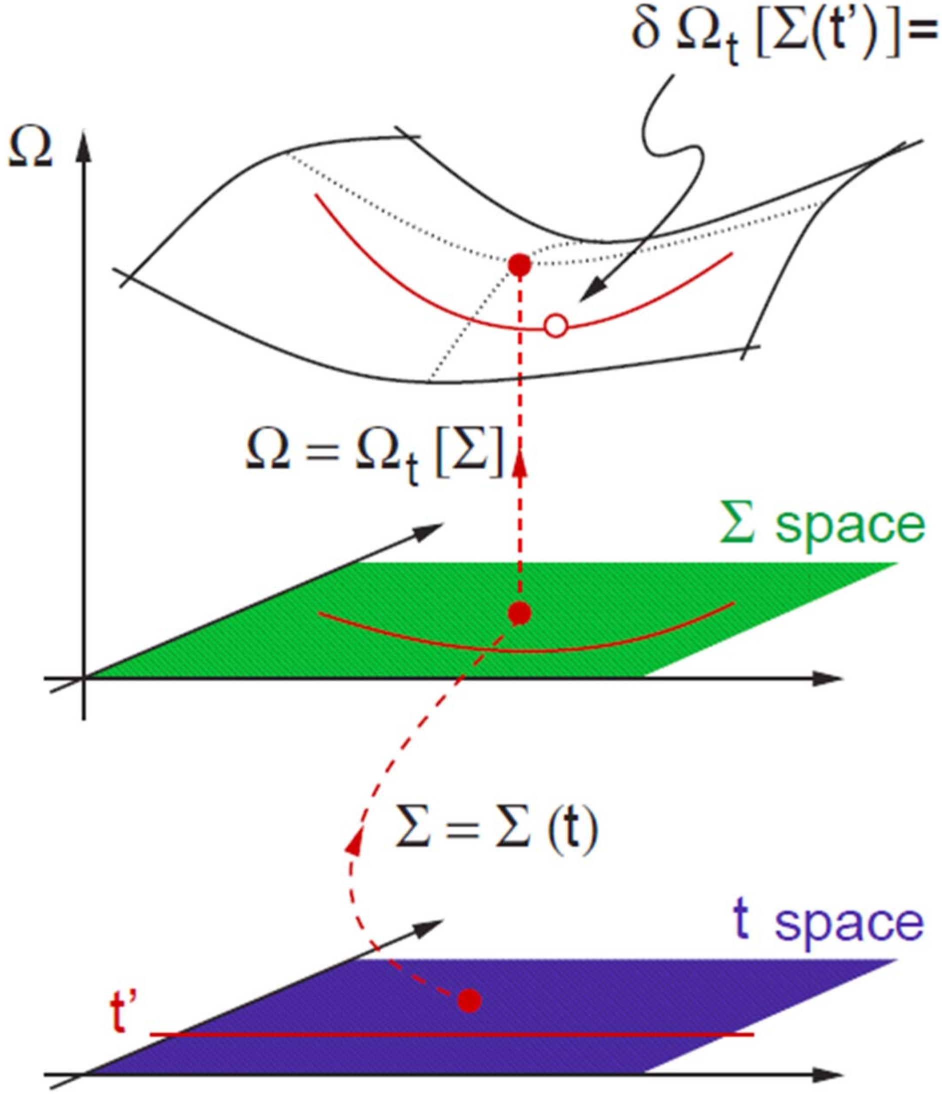
DMFT as a stationnary point

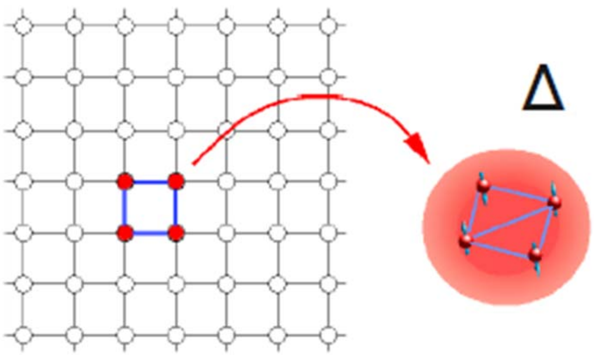


M. Potthoff, Eur. Phys. J. B 32, 429 (2003).

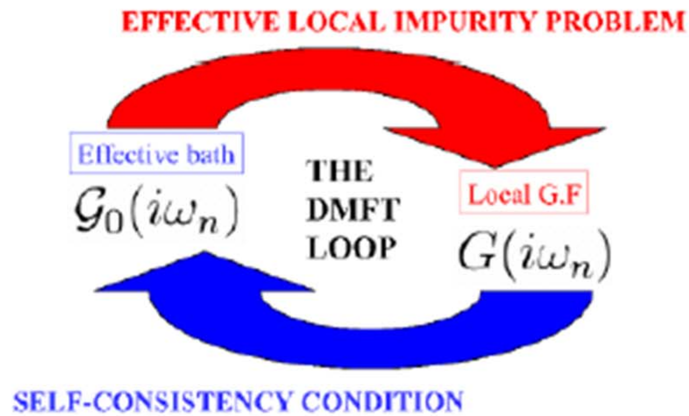
+ and -

- 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

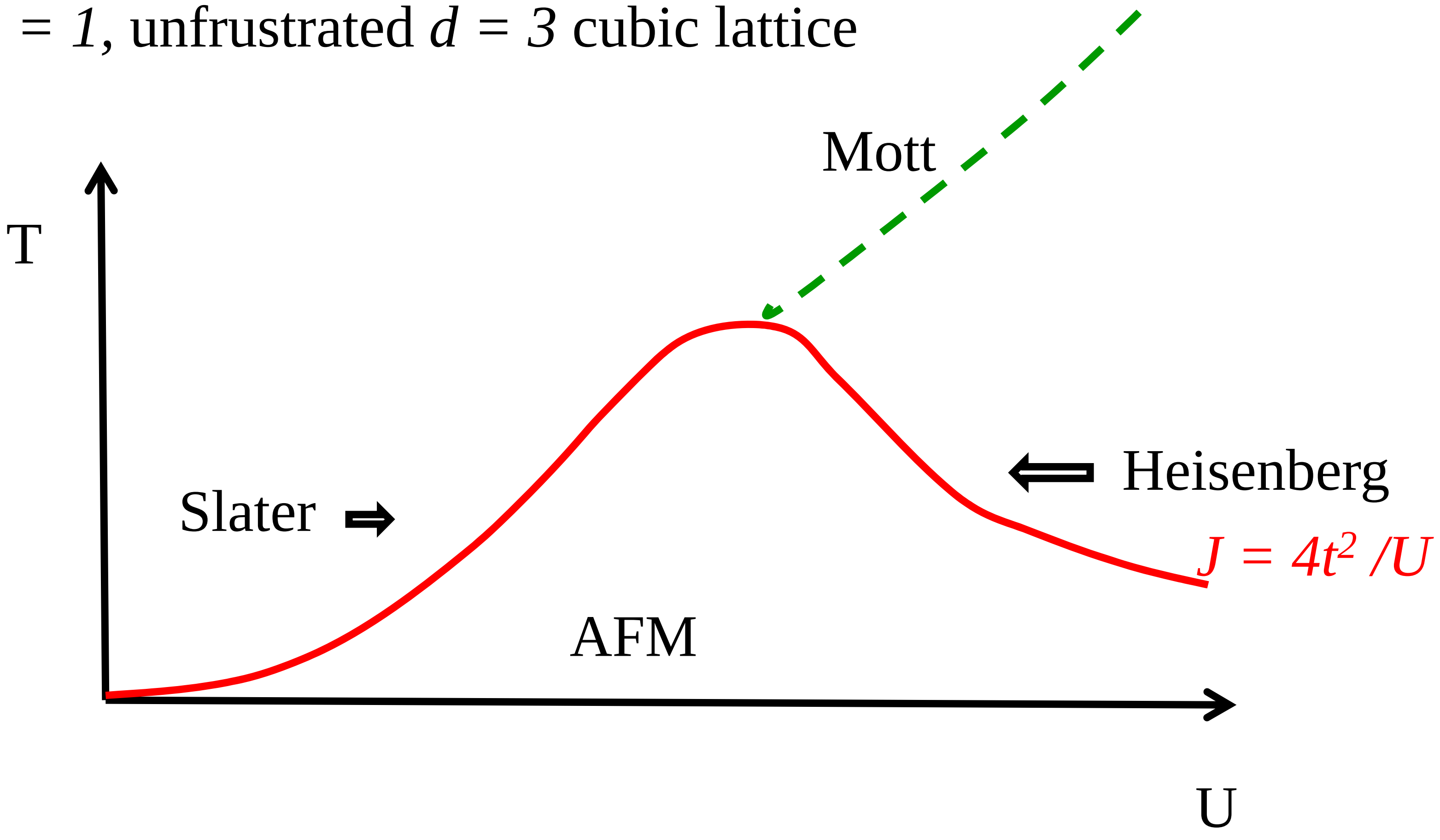
P. Werner, PRL 2006
P. Werner, PRB 2007
K. Haule, PRB 2007

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

Mott transition

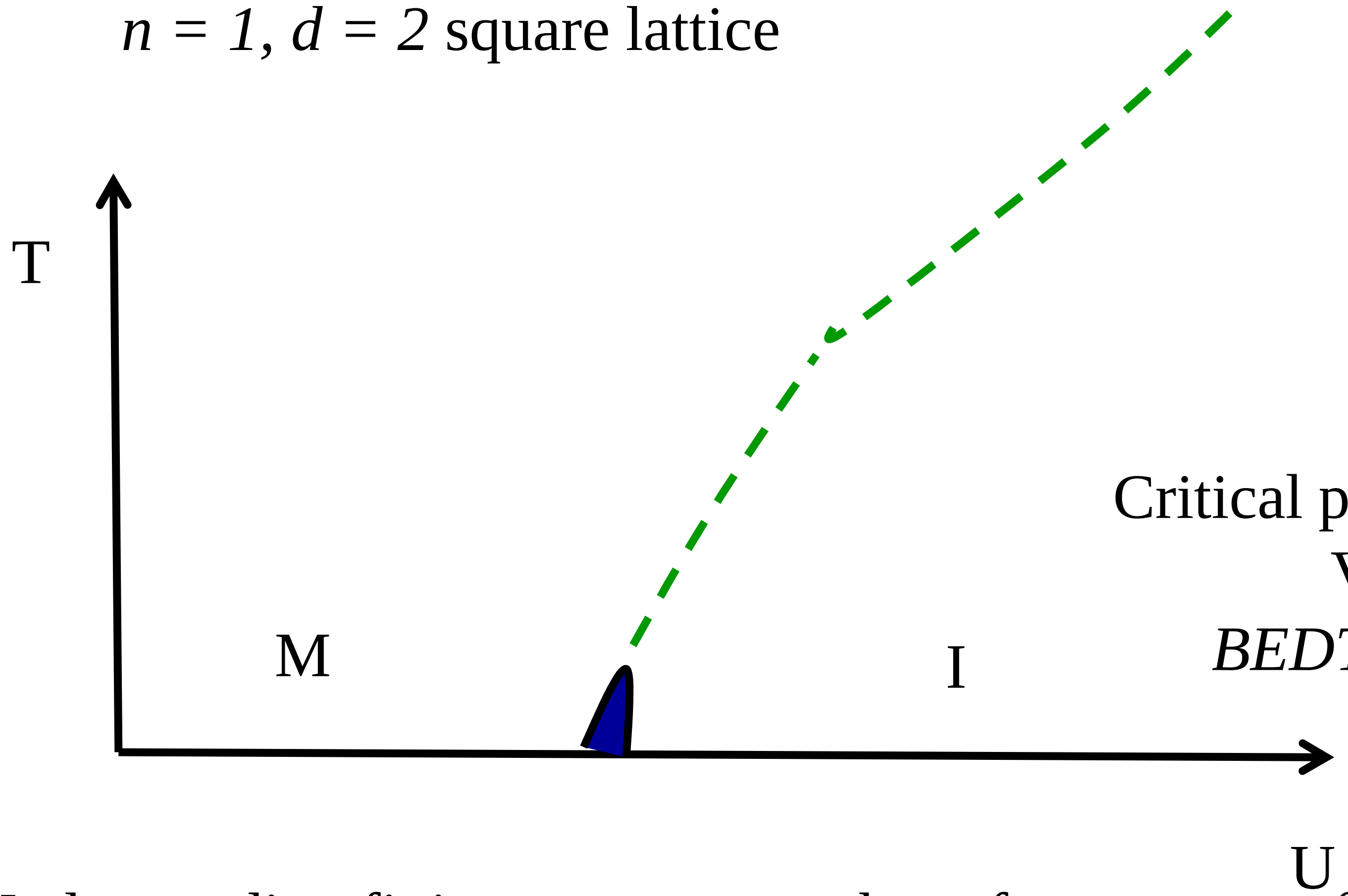
Weak vs Strong correlations

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



Local moment and Mott transition

n = 1, *d = 2* square lattice

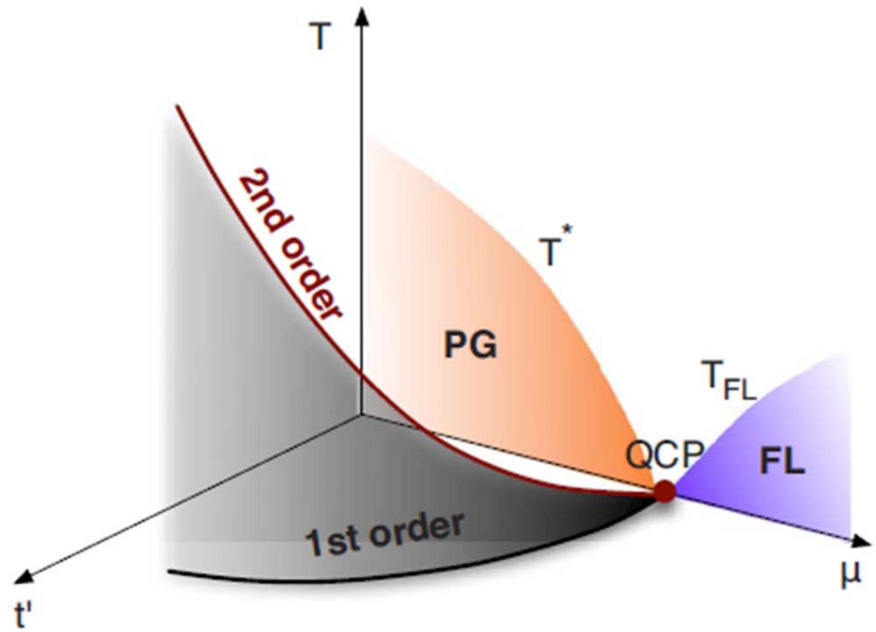


Critical point visible in V_2O_3, *BEDT* organics

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

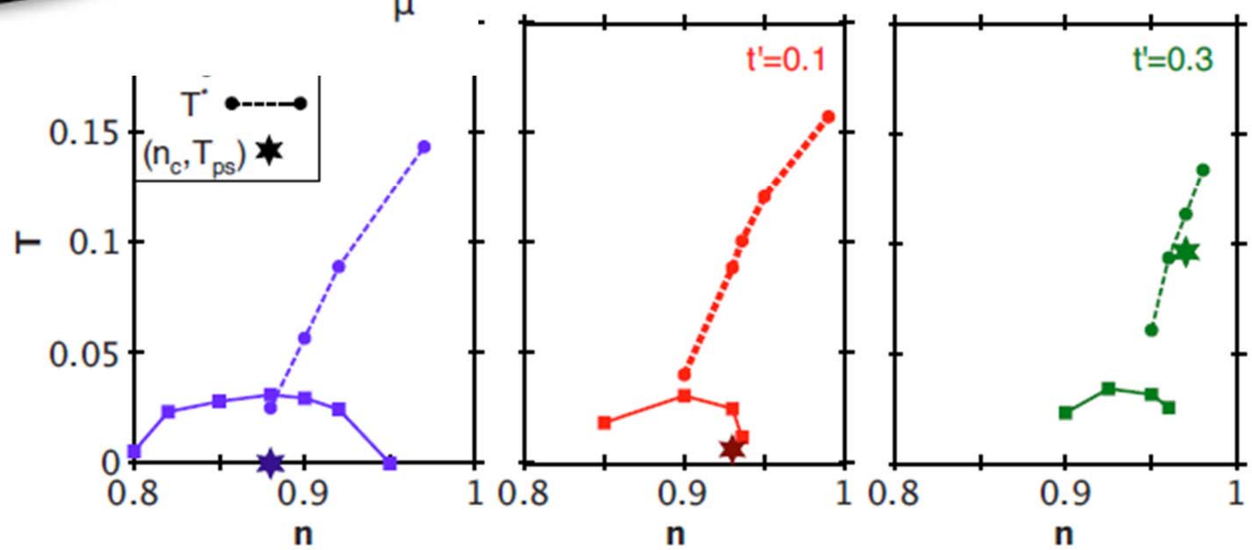
Doping

Phase separation on electron-doped side

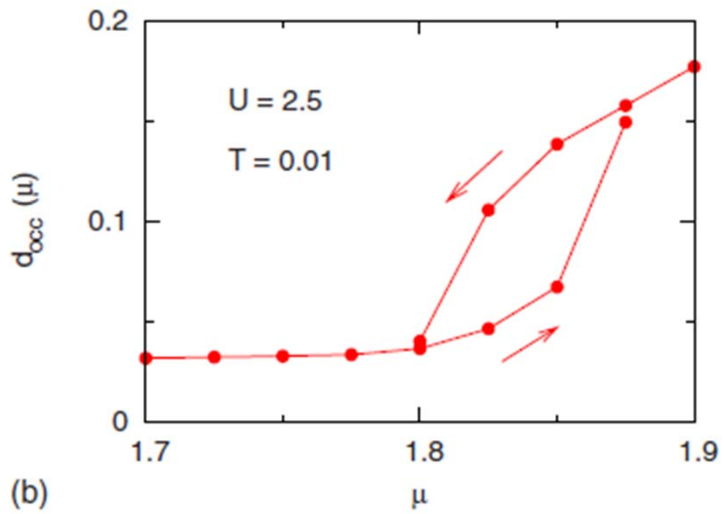


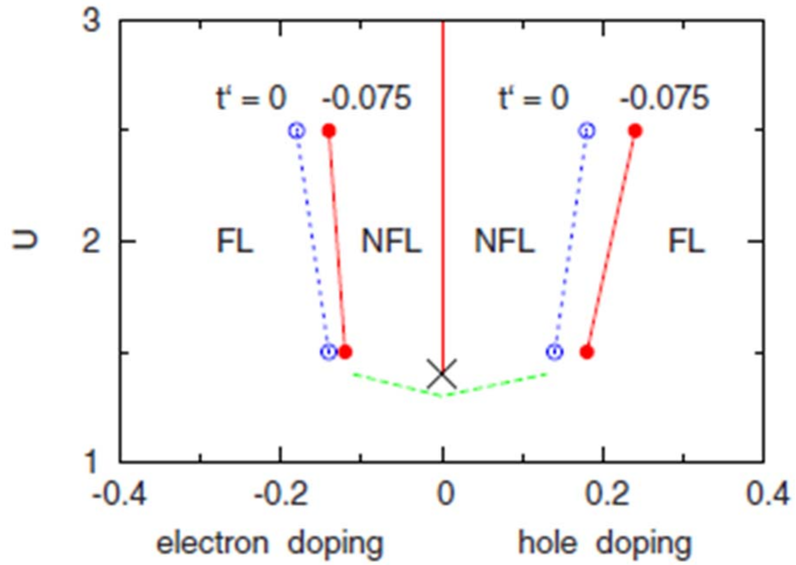
U=8, N_c *= 8, DCA*

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



Crossovers and transition

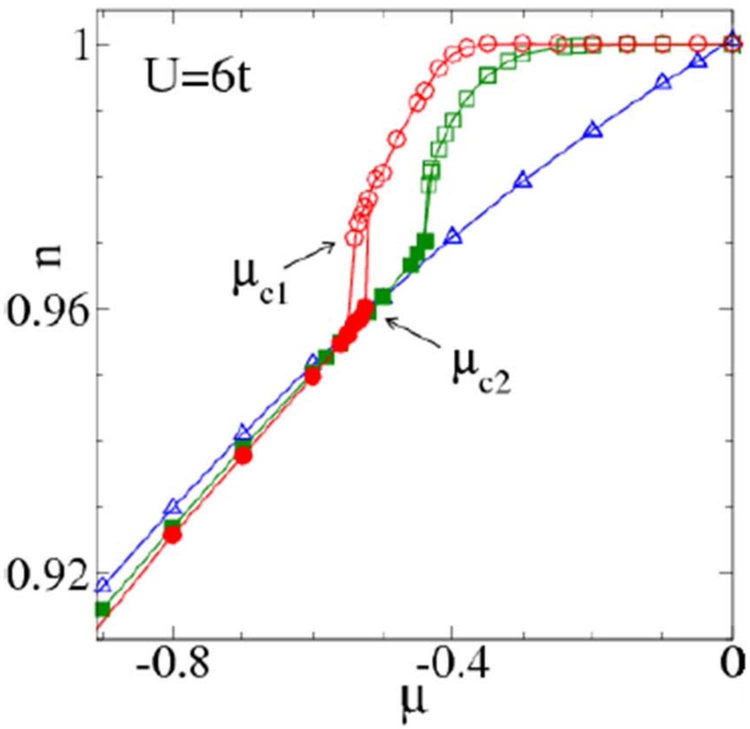




A. Liebsch, N.H. Tong, PRB **80**, 165126 (2009)

First order transition at finite doping

t' = 0

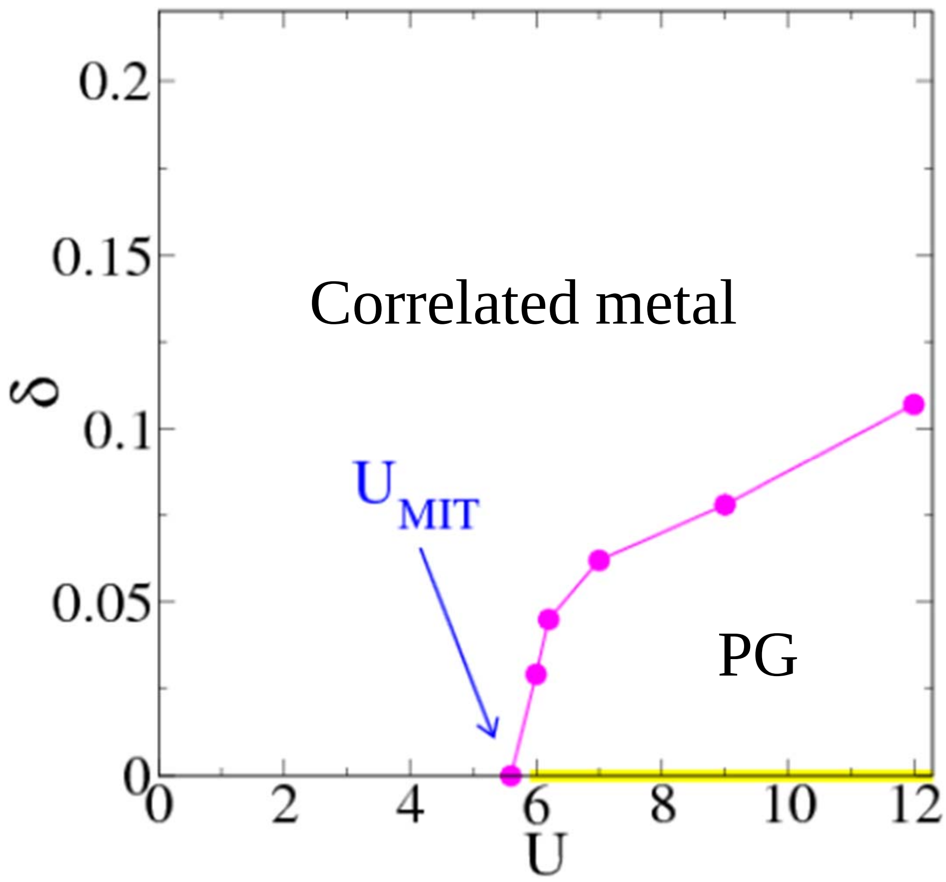


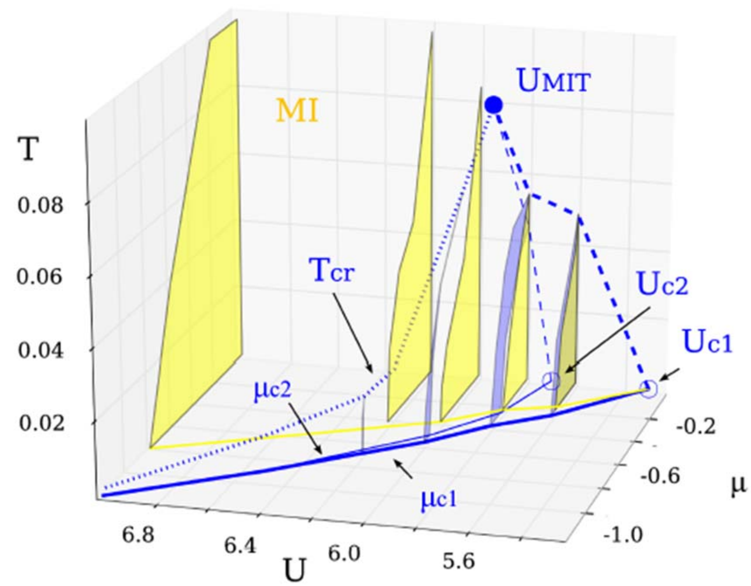
$n(\mu)$ for several temperatures:
$T/t = 1/10,\ 1/25,\ 1/50$

Sordi et al. PRL 2010, PRB 2011

A finite-doping first order transition, linked to Mott transition up to optimal doping

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





Sordi et al. PRL 2010, PRB 2011

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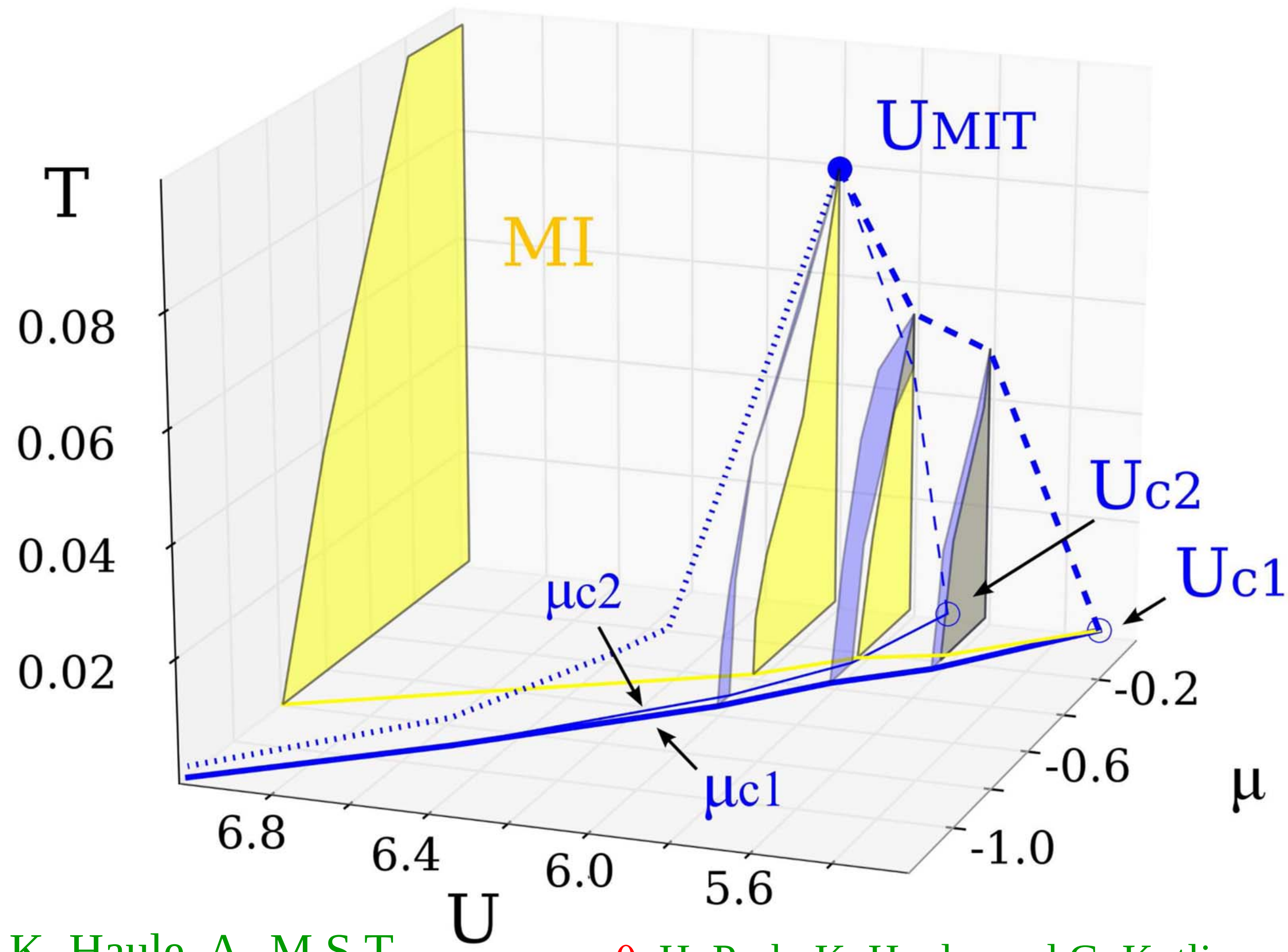
Normal state phase diagram



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

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

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Giovanni Sordi

Patrick Sémon

Kristjan Haule

The Widom line

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

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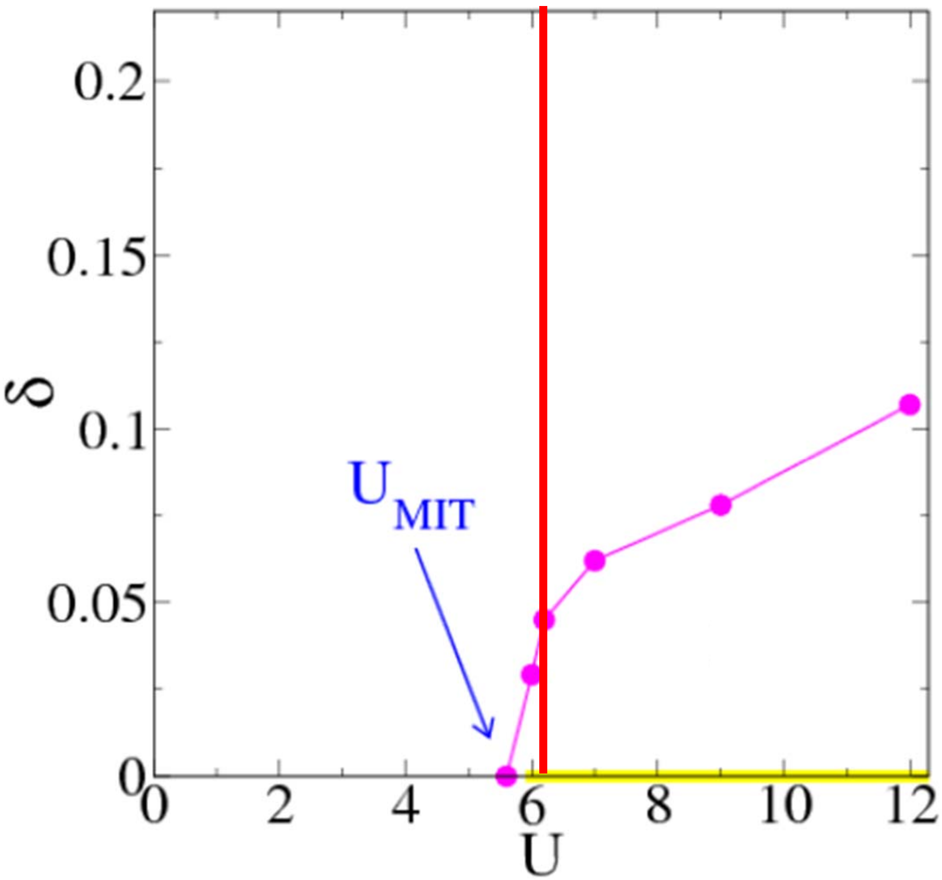
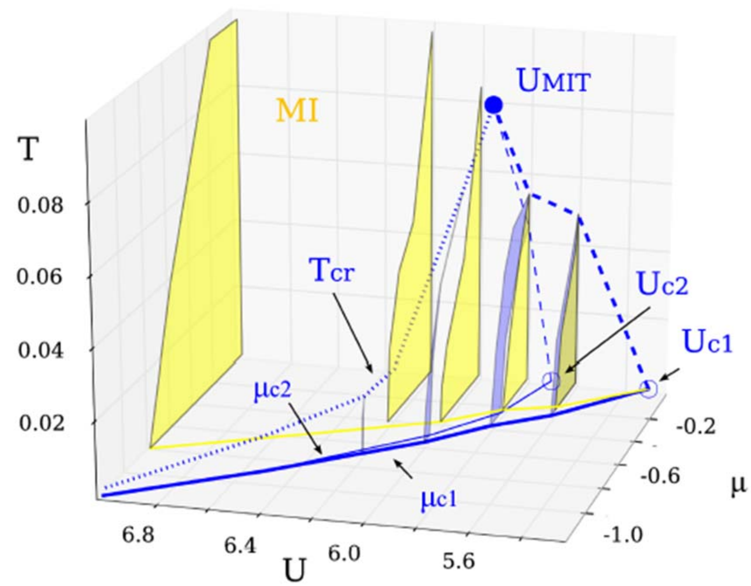
Link to Mott transition up to optimal doping

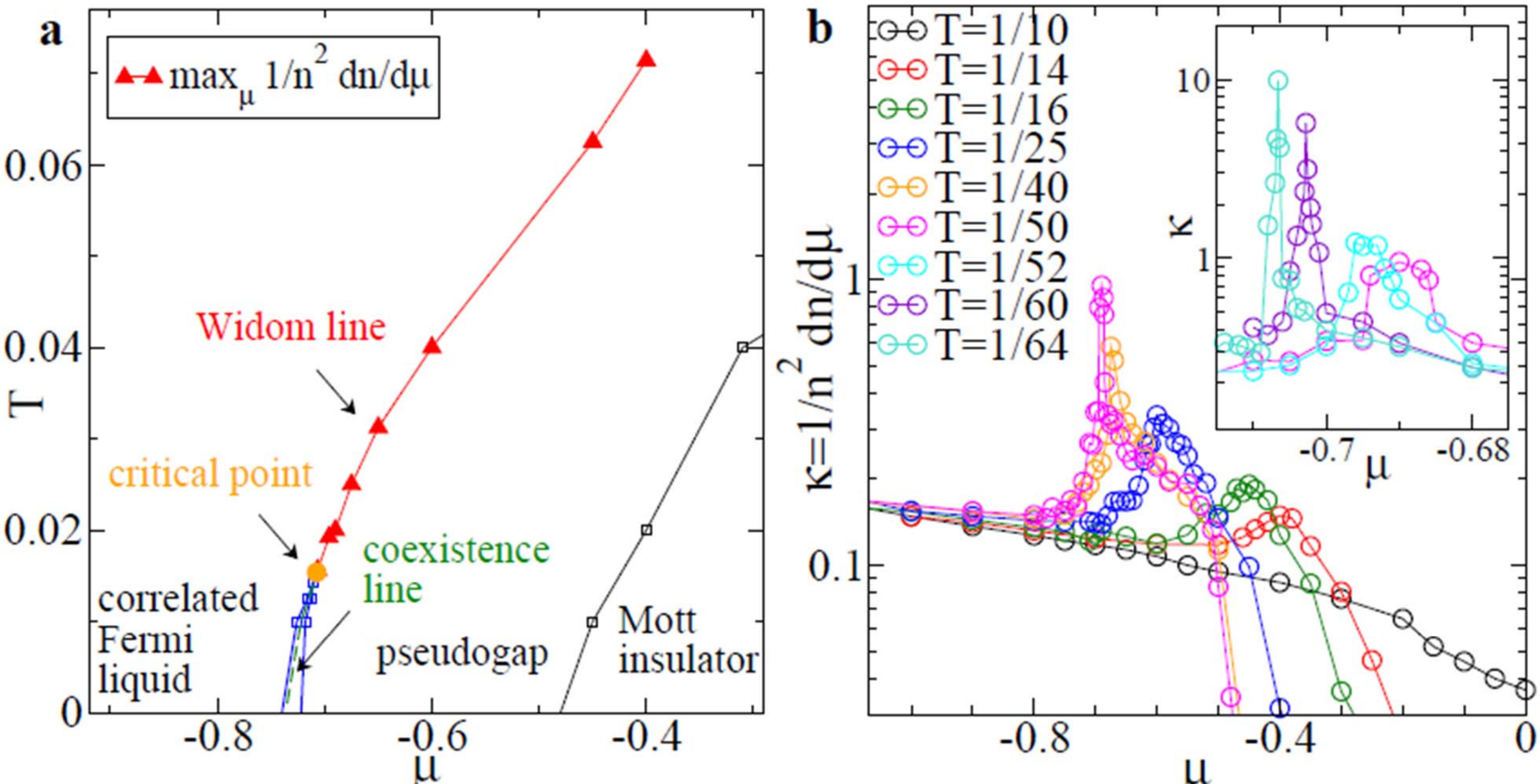
Doping dependence of critical point as a function of *U*





Smaller *D* and *S*

Pseudogap *T** along the Widom line

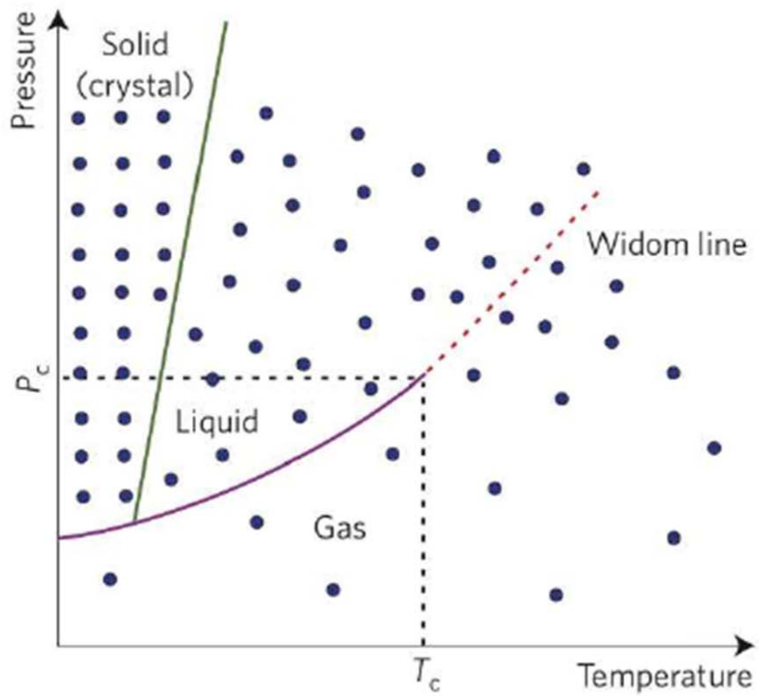


Widom line: defined from maxima of charge compressibility

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

divergence of κ at the (classical) critical point!

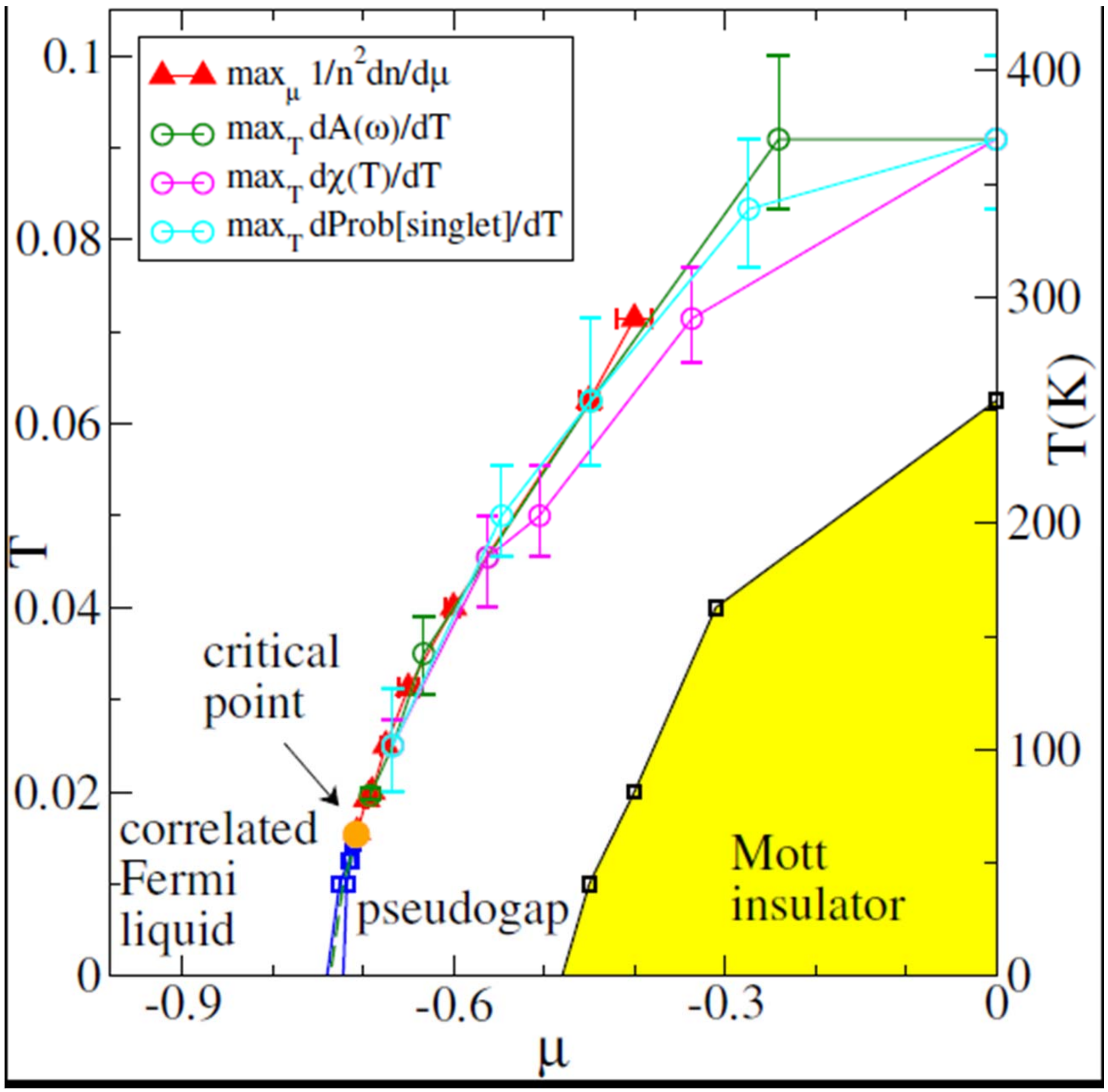
What is the Widom line?



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

Rapid change also in dynamical quantities



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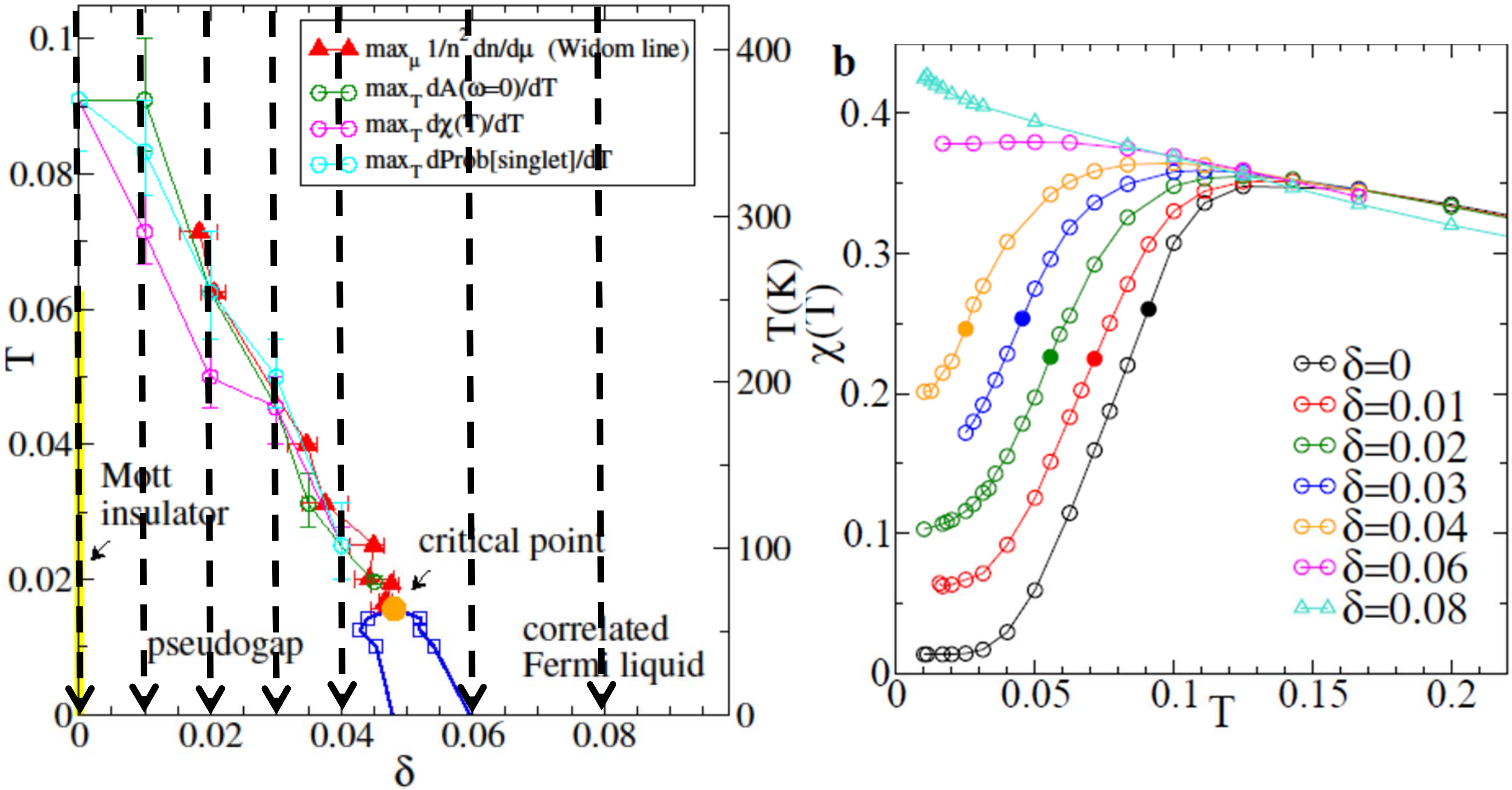
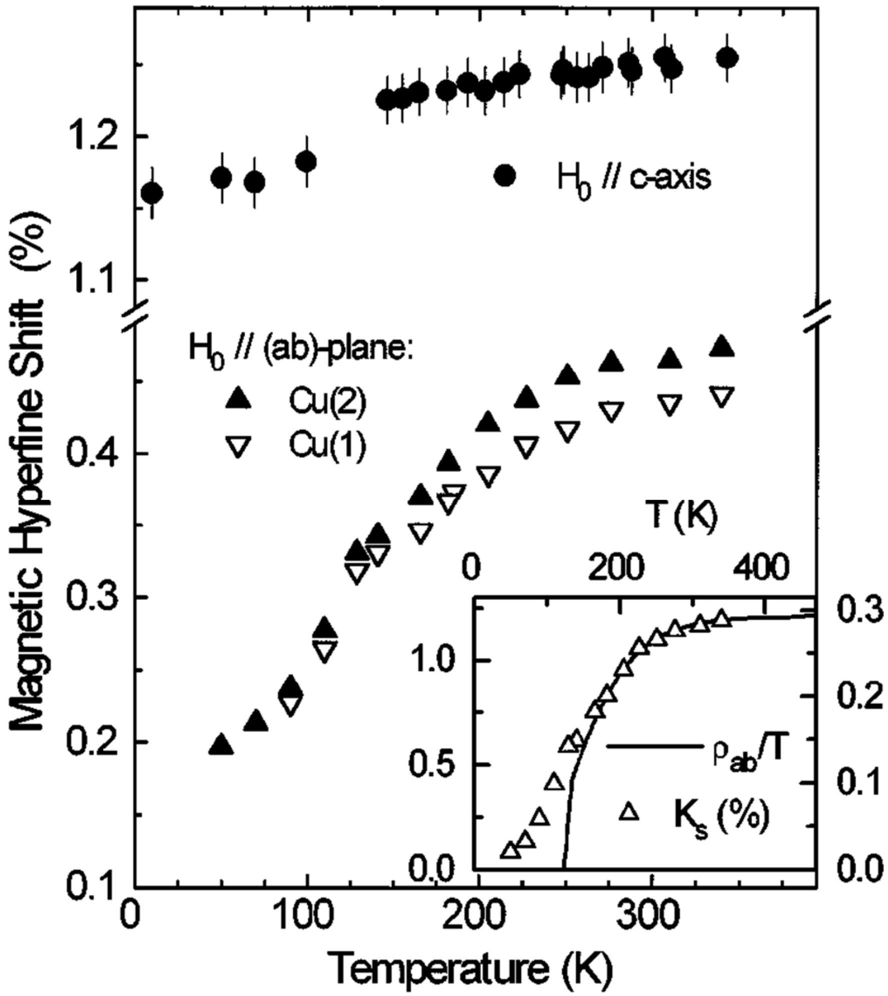
Compare a few results for cuprates

Spin susceptibility

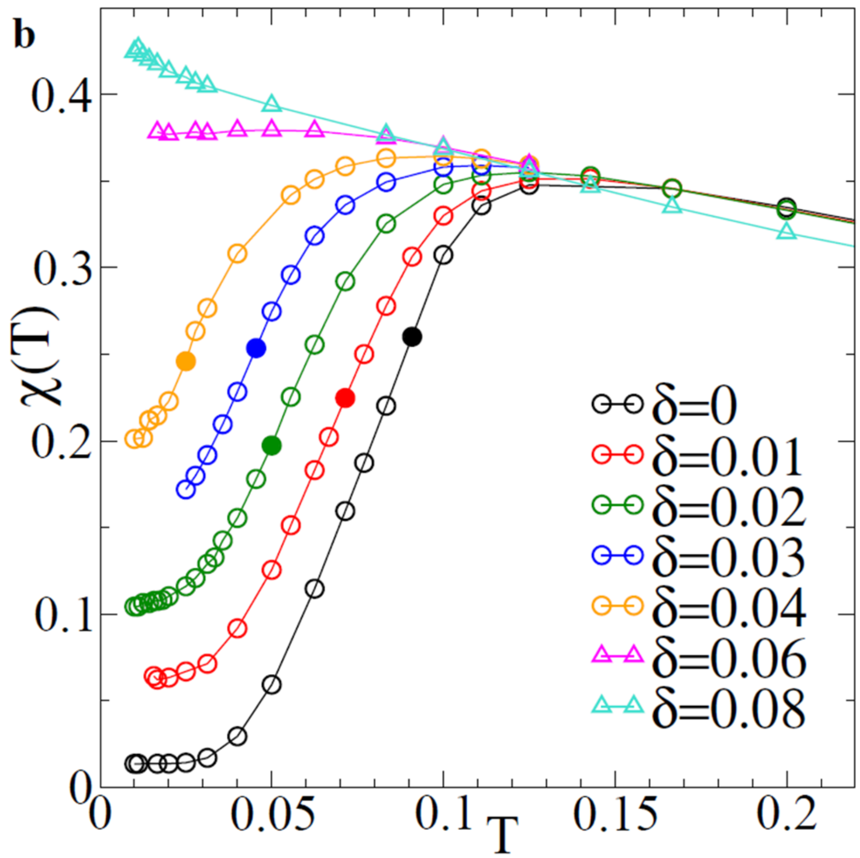


Spin susceptibility



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)

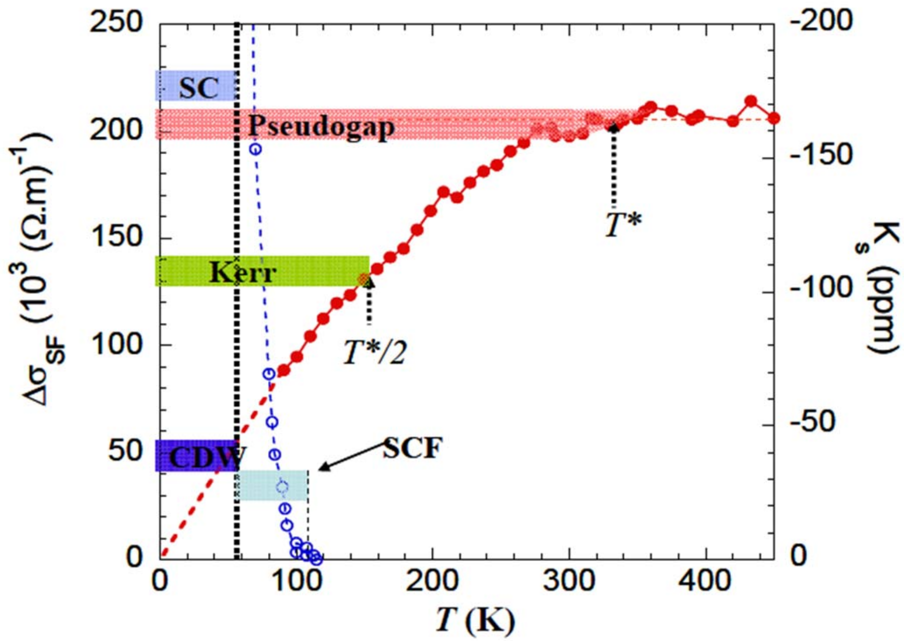
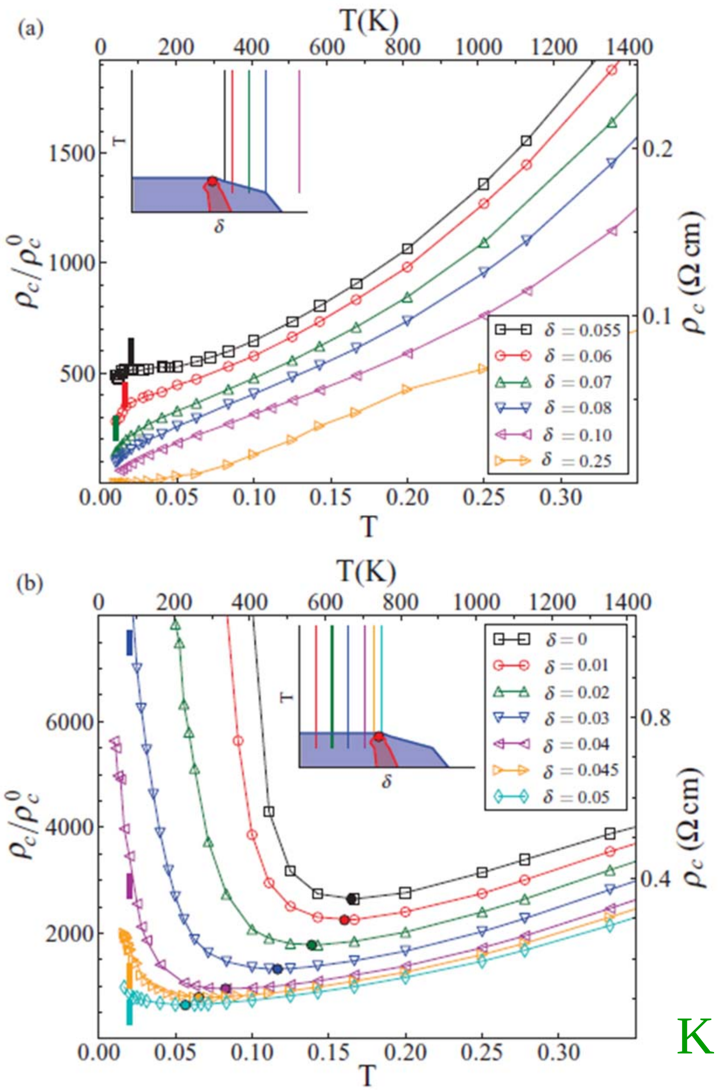
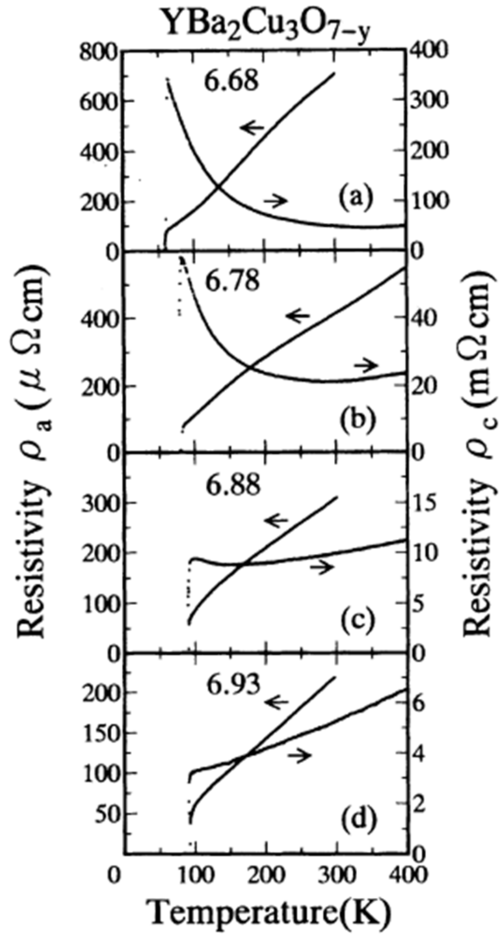


Fig 1 Spin contribution K_s to the ^{89}Y NMR Knight shift [11] for $YBCO_{6.6}$ permit to define the PG onset T^*. Here K_s is reduced by a factor two at $T \sim T^*/2$. The sharp drop of the SC fluctuation conductivity (SCF) is illustrated (left scale) [23]. We report as well the range over which a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

C-axis resistivity





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

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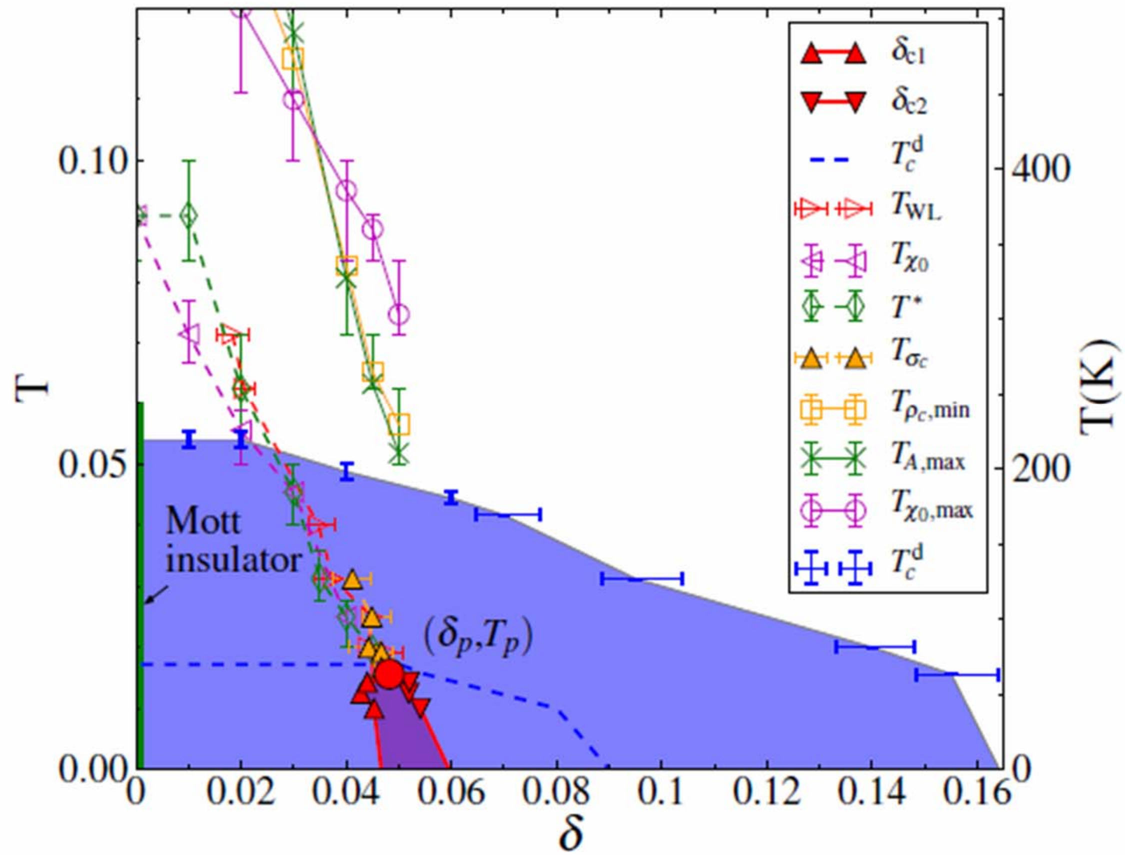
Giovanni Sordi

Two crossover lines

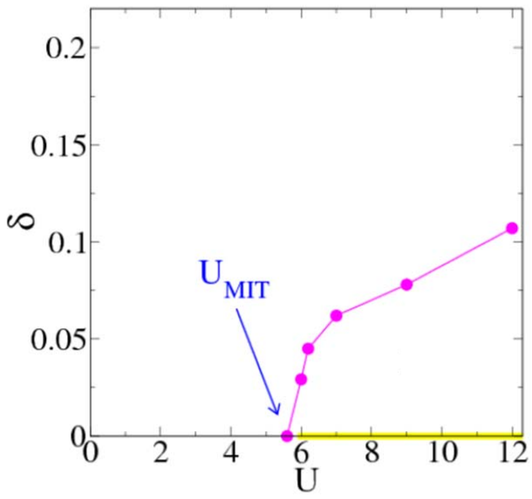
Patrick Sémon

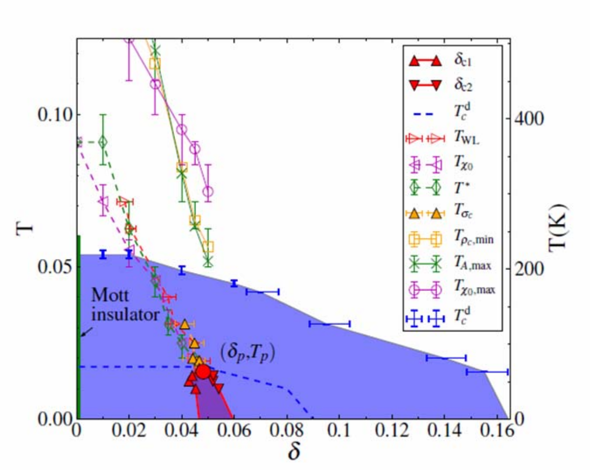


G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)

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

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?)

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Patrick Sémon

Kristjan Haule

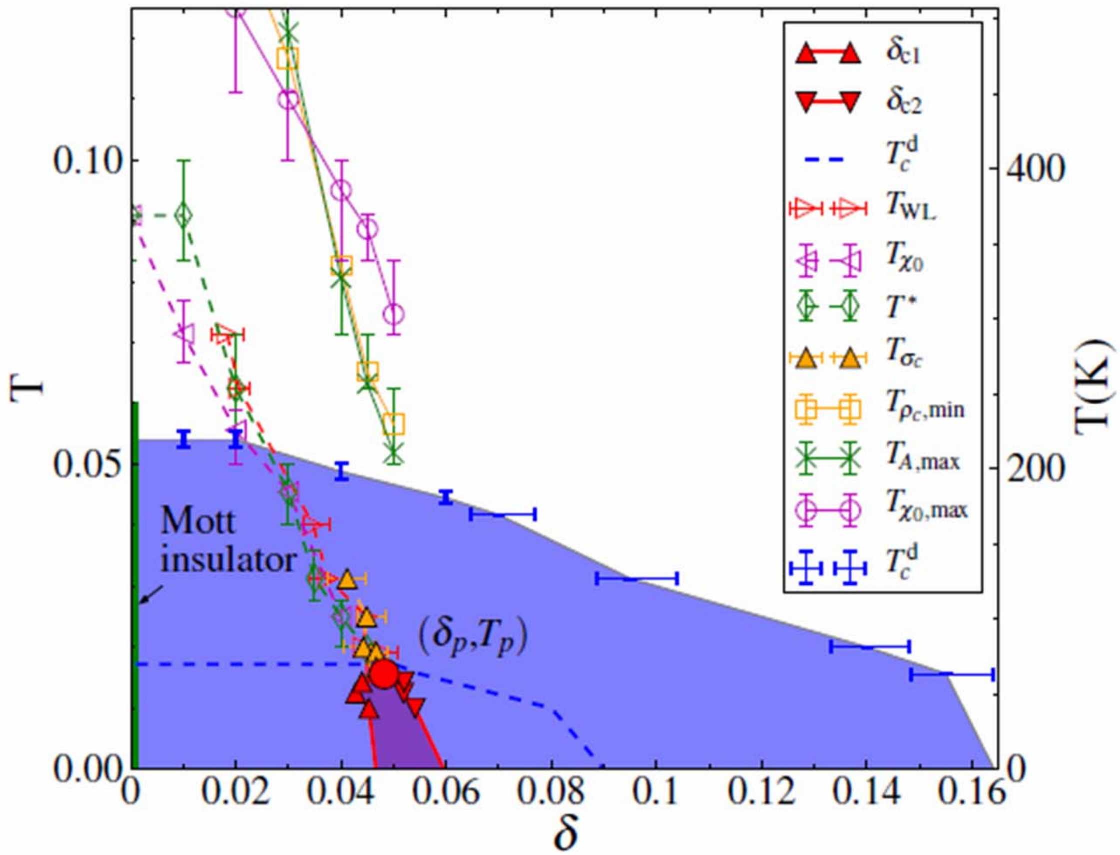
Finite T phase diagram
Superconductivity

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

Phase diagram for $U = 6.2\,t$

Giovanni Sordi

Patrick Sémon



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

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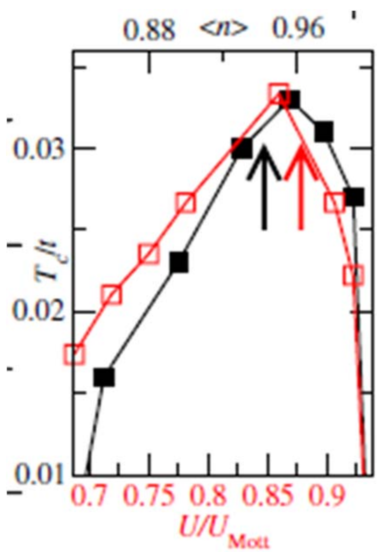
Actual T_c in underdoped

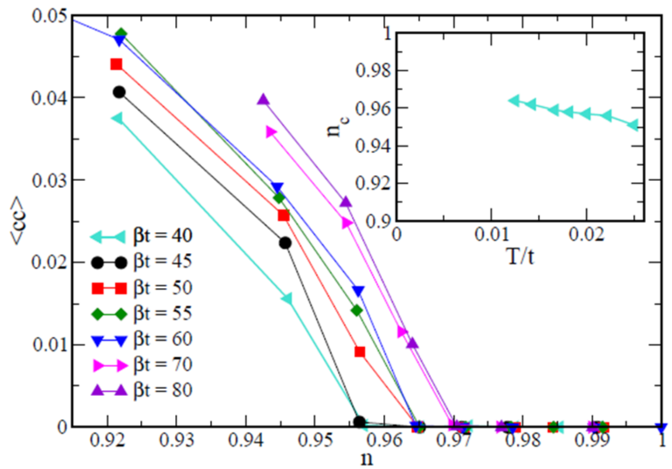
- Quantum and classical phase fluctuations
  - V. J. Emery and S. A. Kivelson, Phys. Rev. Lett. **74**, 3253 (1995).
  - V. J. Emery and S. A. Kivelson, Nature **374**, 474 (1995).
  - D. Podolsky, S. Raghu, and A. Vishwanath, Phys. Rev. Lett. **99**, 117004 (2007).
  - Z. Tesanovic, Nat Phys **4**,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

Larger clusters

- 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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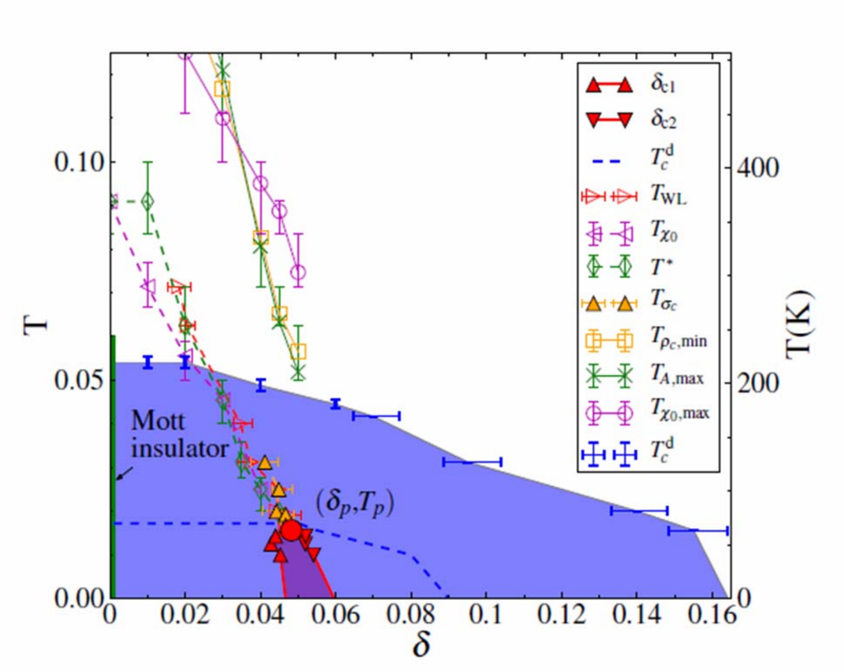
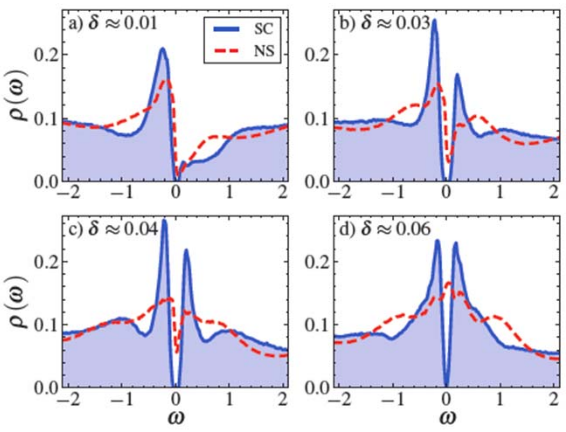
Summary





- Below the dome, not QCP (but Mott)
- Maximum at Widom line
- T^* different from T_c^d
- First-order transition destroyed but traces in the dynamics
- Actual T_c in underdoped
  - Competing order
  - Long wavelength fluctuations (see O.P.)
  - Disorder

Bandwidth control and doping control of the Mott transition in organics

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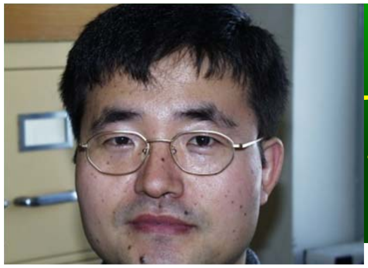
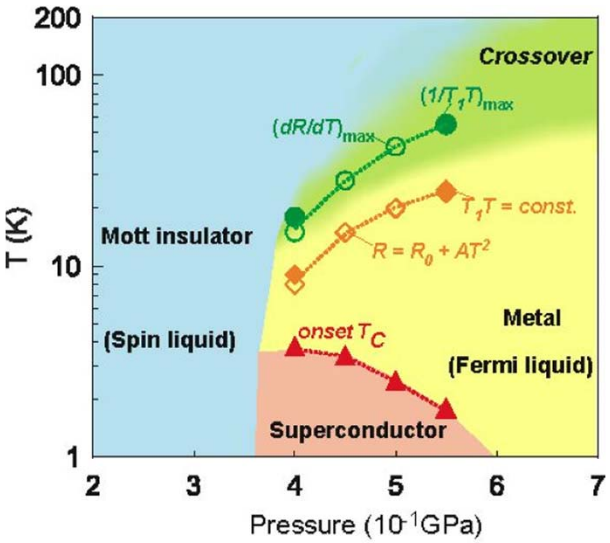
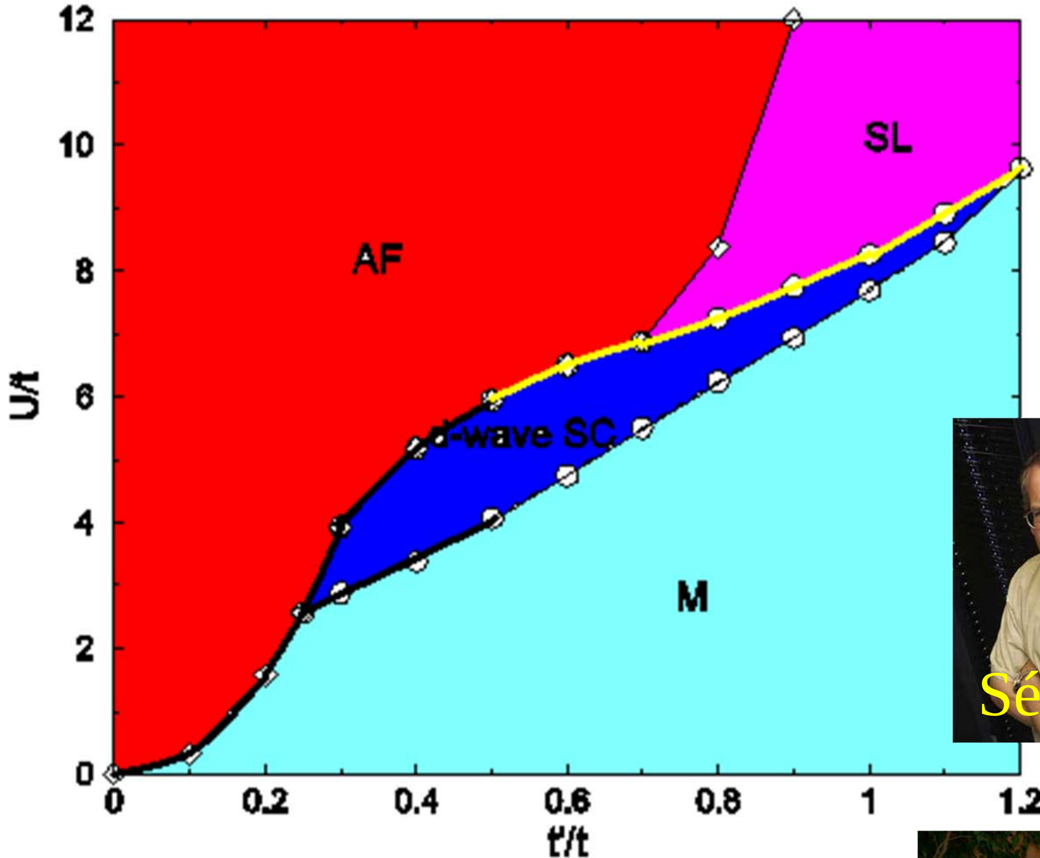
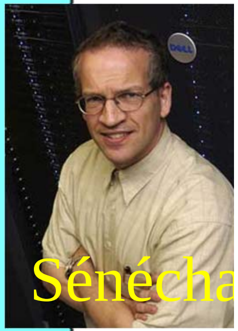


Theoretical phase diagram BEDT

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







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

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

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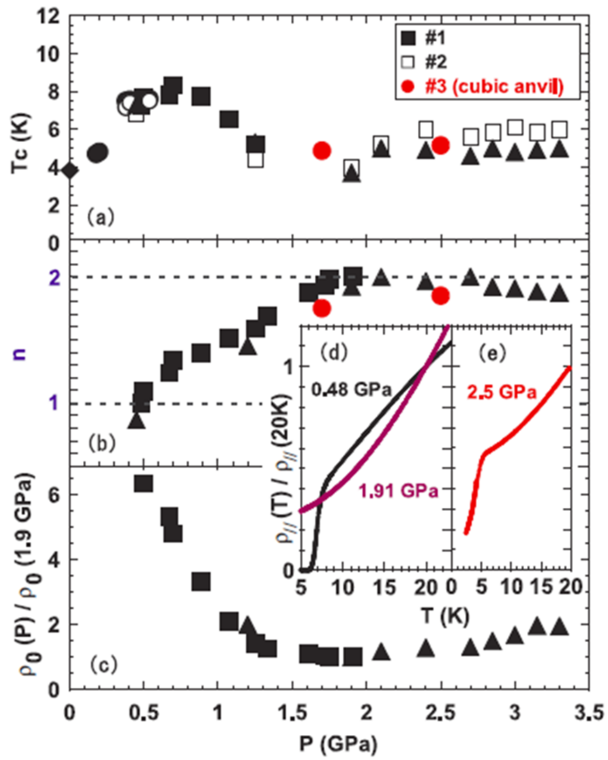
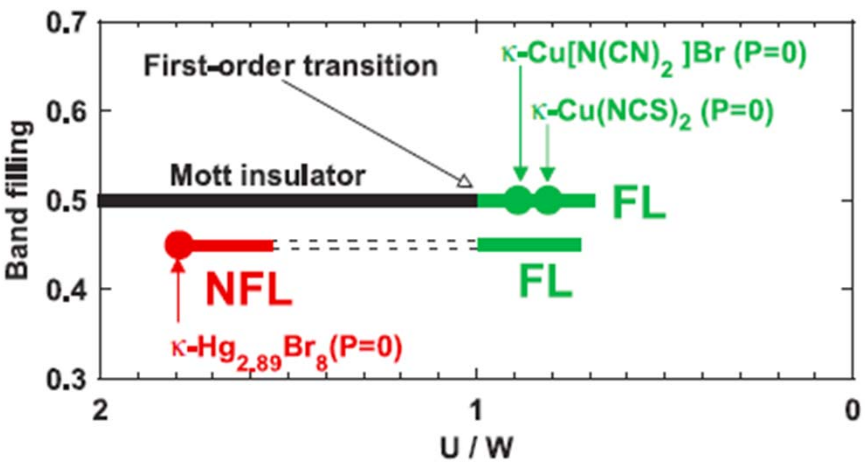
A doped BEDT organic



	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



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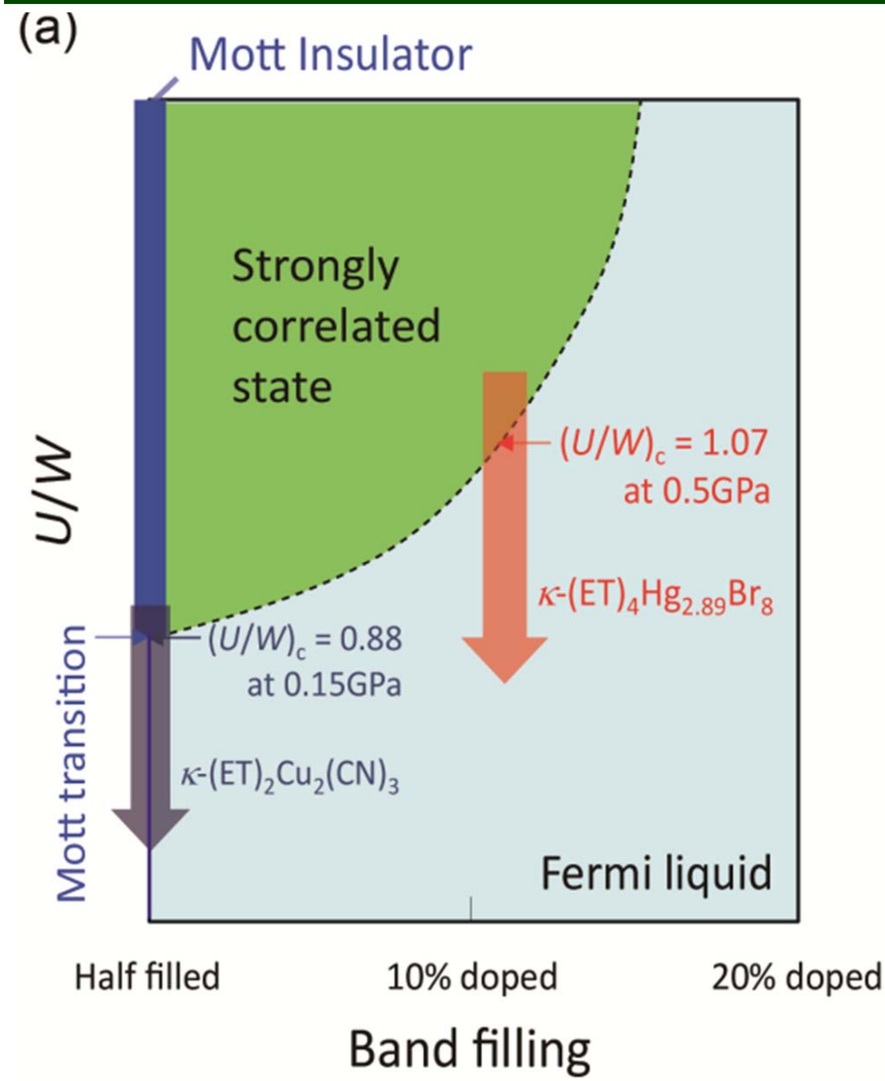
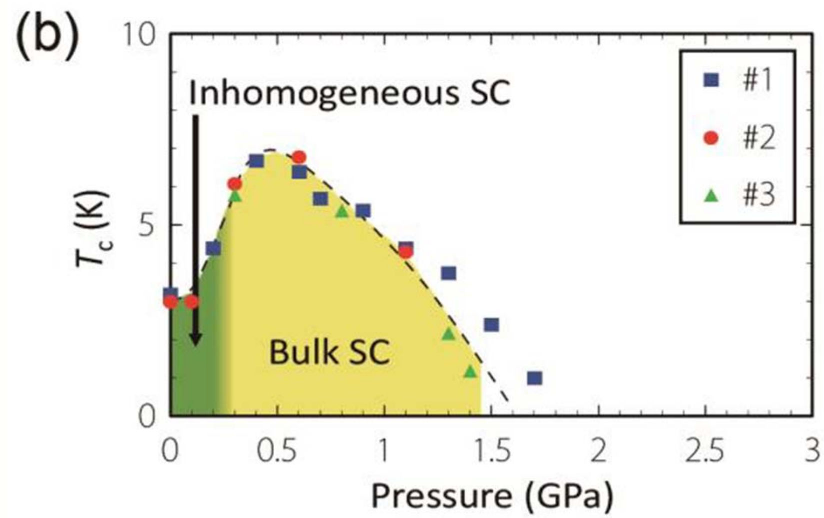
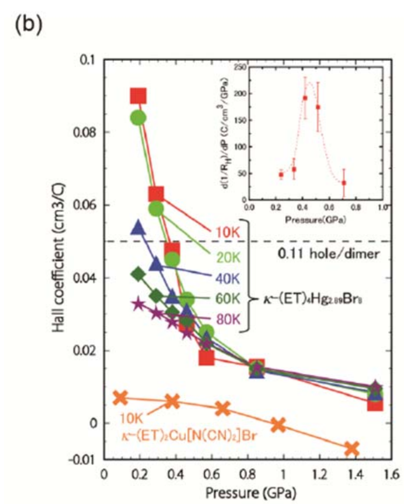
R. N. Lyubovskaya et al. JETP Lett. **45,** 530 (1987)

Doped BEDT







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

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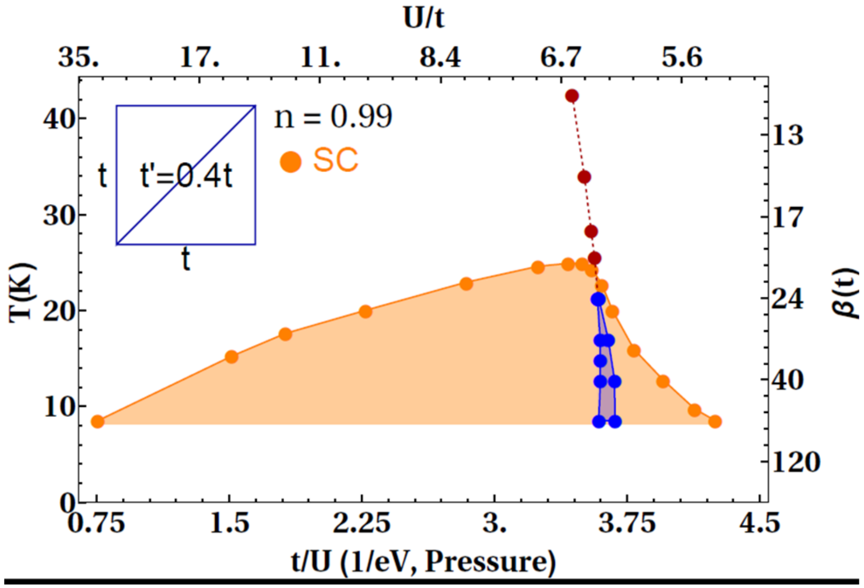
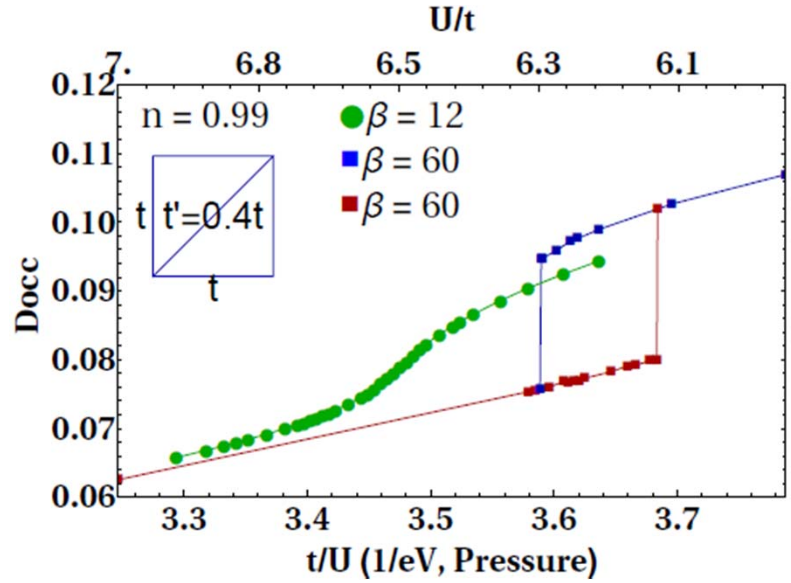
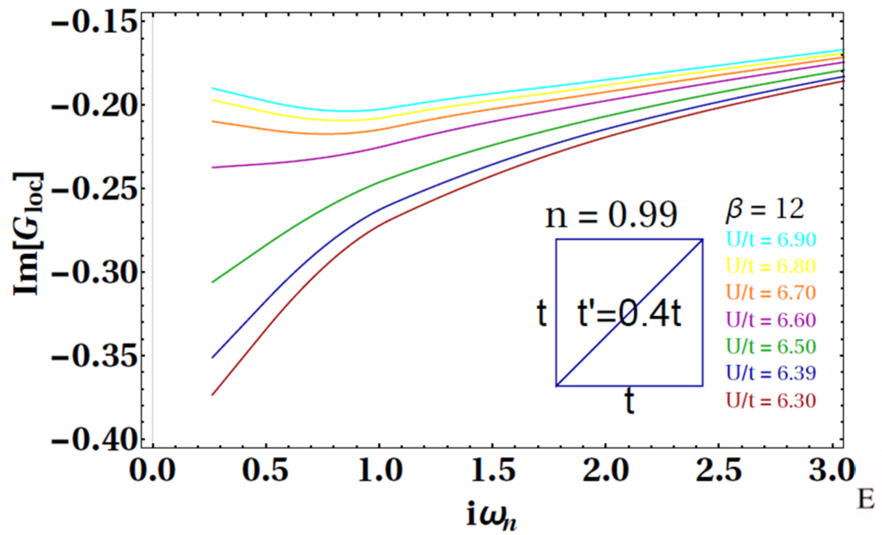
Widom line in organics

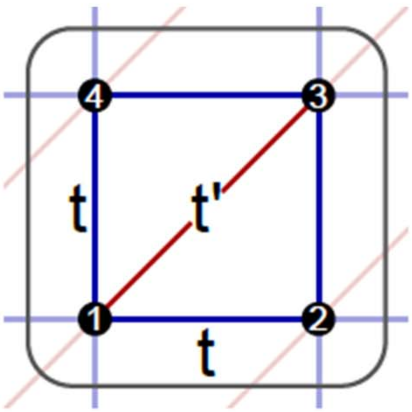




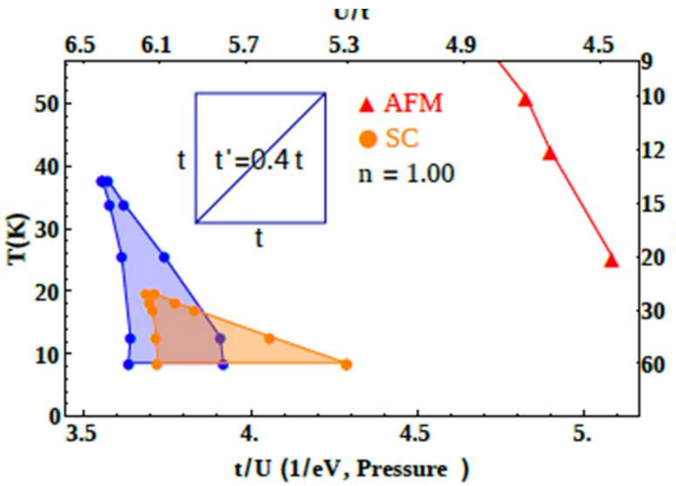


Charles-David Hébert, Patrick Sémon , AMT

t'=0.4t

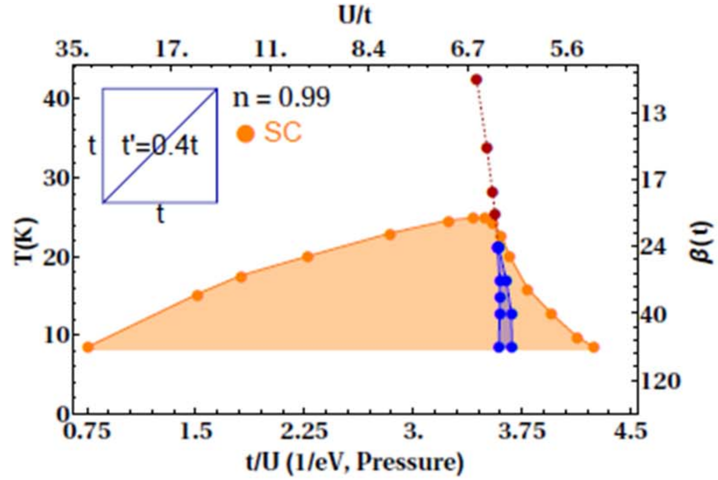


t
t'
t
1
2
3
4



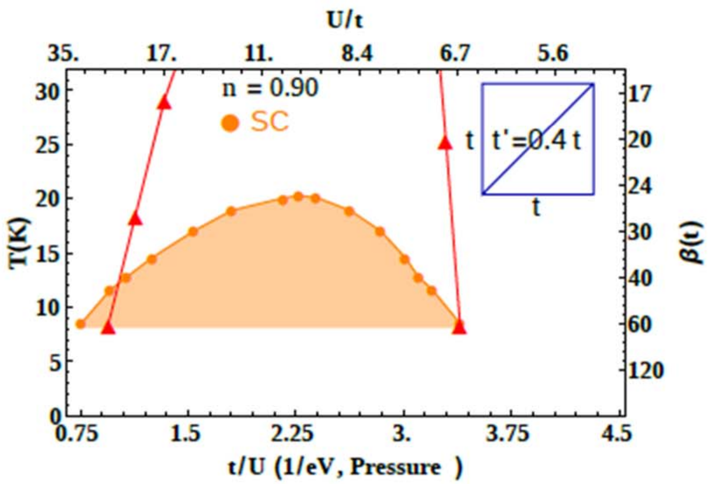
U/t
AFM
SC
n = 1.00
t'=0.4 t
T(K)
β(t)
t/U (1/eV, Pressure)

(a)

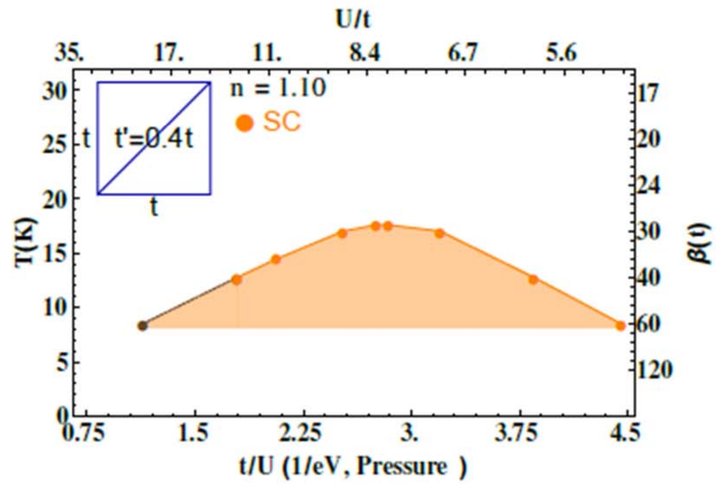


U/t
n = 0.99
SC
t'=0.4t
T(K)
β(t)
t/U (1/eV, Pressure)

(b)

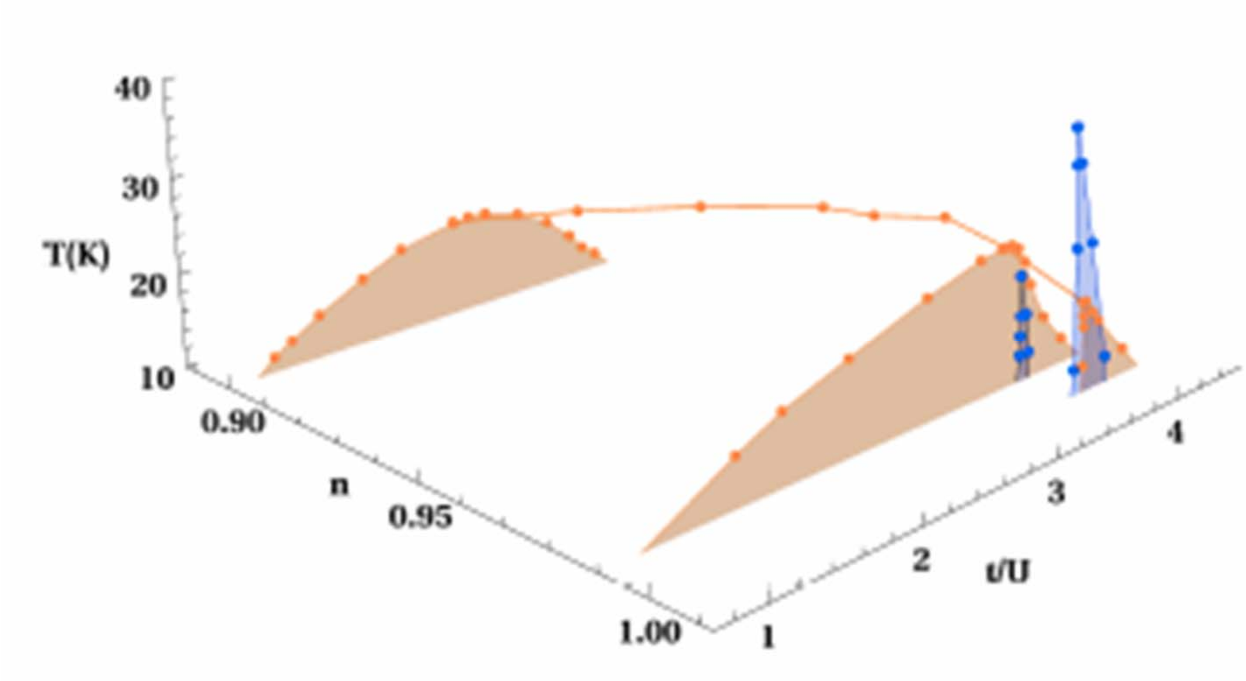


U/t
n = 0.90
SC
t'=0.4 t
T(K)
β(t)
t/U (1/eV, Pressure)



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

t’ = 0.4t overview



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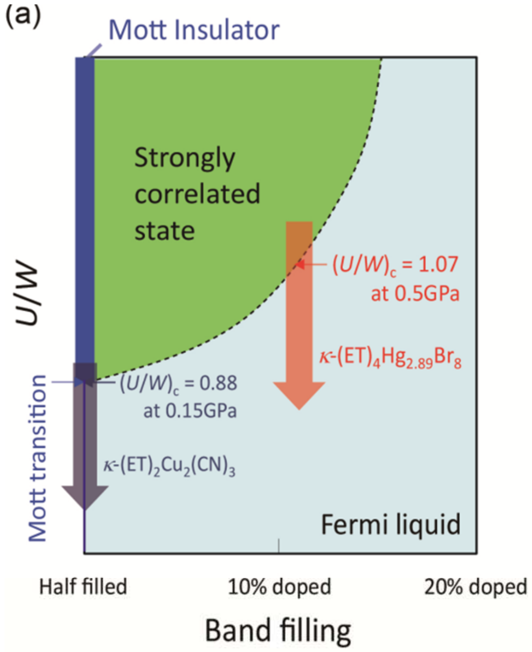
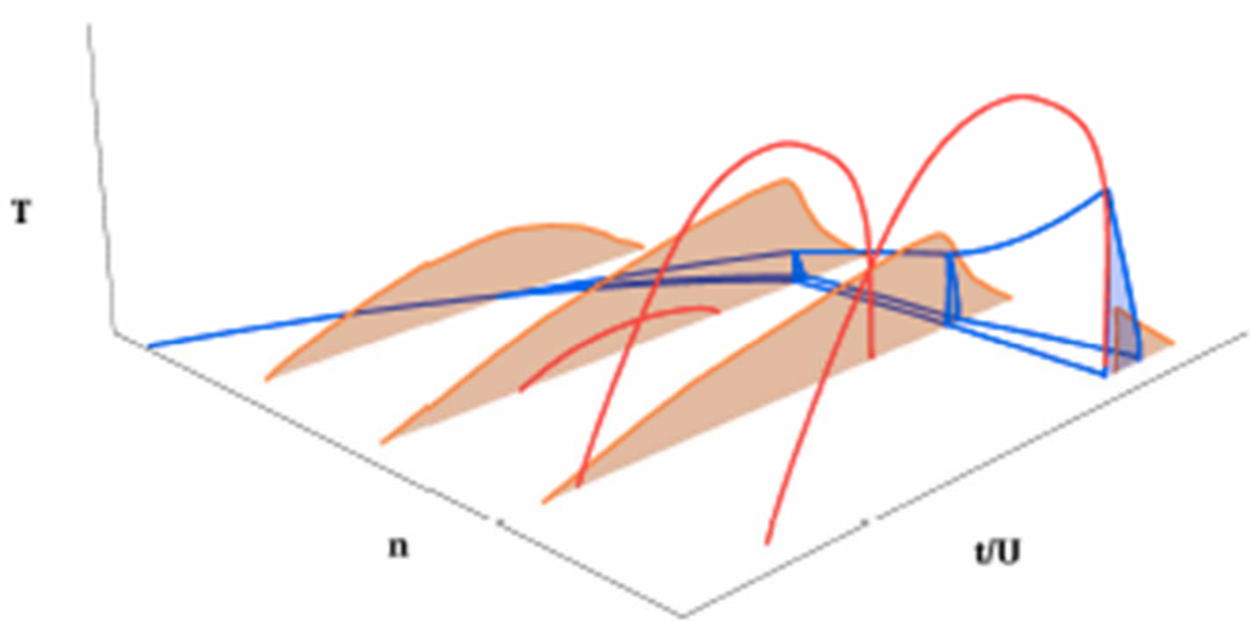
Generic case





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 QCP. Follows first-order.
  - SC from short range *J*.
  - *Tc* decreases at Widom line

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Some Algorithmic details:
3 improvements

Continuous-time QMC : CT-HYB

$$H_{\text{imp}} = H_{\text{loc}}(d_i^\dagger, d_i) + \sum_{i\mu}(V_{\mu i} a_\mu^\dagger d_i + V_{\mu i}^* d_i^\dagger a_\mu) + \sum_\mu \epsilon_\mu a_\mu^\dagger a_\mu,$$

$$Z = \text{Tr}\text{T}_\tau e^{-\beta H_0} e^{-\int_0^\beta d\tau (H_{\text{hyb}}(\tau) + H_{\text{hyb}}^\dagger(\tau))}$$

$$= \sum_{k\geq 0} \frac{1}{k!^2} \int_0^\beta d\tau_1 \cdots d\tau_k \int_0^\beta d\tau_1' \cdots d\tau_k' \text{Tr}\text{T}_\tau e^{-\beta H_0} \times H_{\text{hyb}}(\tau_1) H_{\text{hyb}}^\dagger(\tau_1') \cdots H_{\text{hyb}}(\tau_k) H_{\text{hyb}}^\dagger(\tau_k').$$

$$= \sum_{k\geqslant 0} \sum_{i_1\cdots i_k} \sum_{i_1'\cdots i_k'} \frac{1}{k!^2} \int_0^\beta d\tau_1 \cdots d\tau_k \int_0^\beta d\tau_1' \cdots d\tau_k' \times \text{Tr}\text{T}_\tau e^{-\beta H_{\text{loc}}} d_{i_1}(\tau_1) d_{i_1'}^\dagger(\tau_1') \cdots d_{i_k}(\tau_k) d_{i_k'}^\dagger(\tau_k') \times Z_{\text{bath}} \langle \hat{V}_{i_1}^\dagger(\tau_1) \hat{V}_{i_1'}(\tau_1') \cdots \hat{V}_{i_k}^\dagger(\tau_k) \hat{V}_{i_k'}(\tau_k') \rangle, \qquad \hat{V}_i = \sum_\mu V_{\mu i}^* a_\mu$$

P. Sémon, G. Sordi, A.-M.S. Tremblay, Phys. Rev. B **89**, 165113 (2014)

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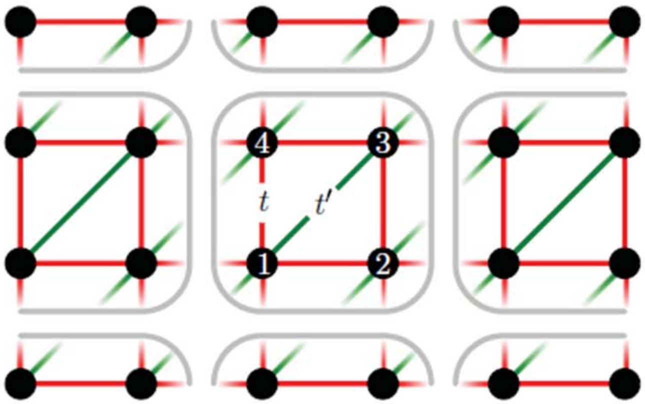
Reducing the sign problem

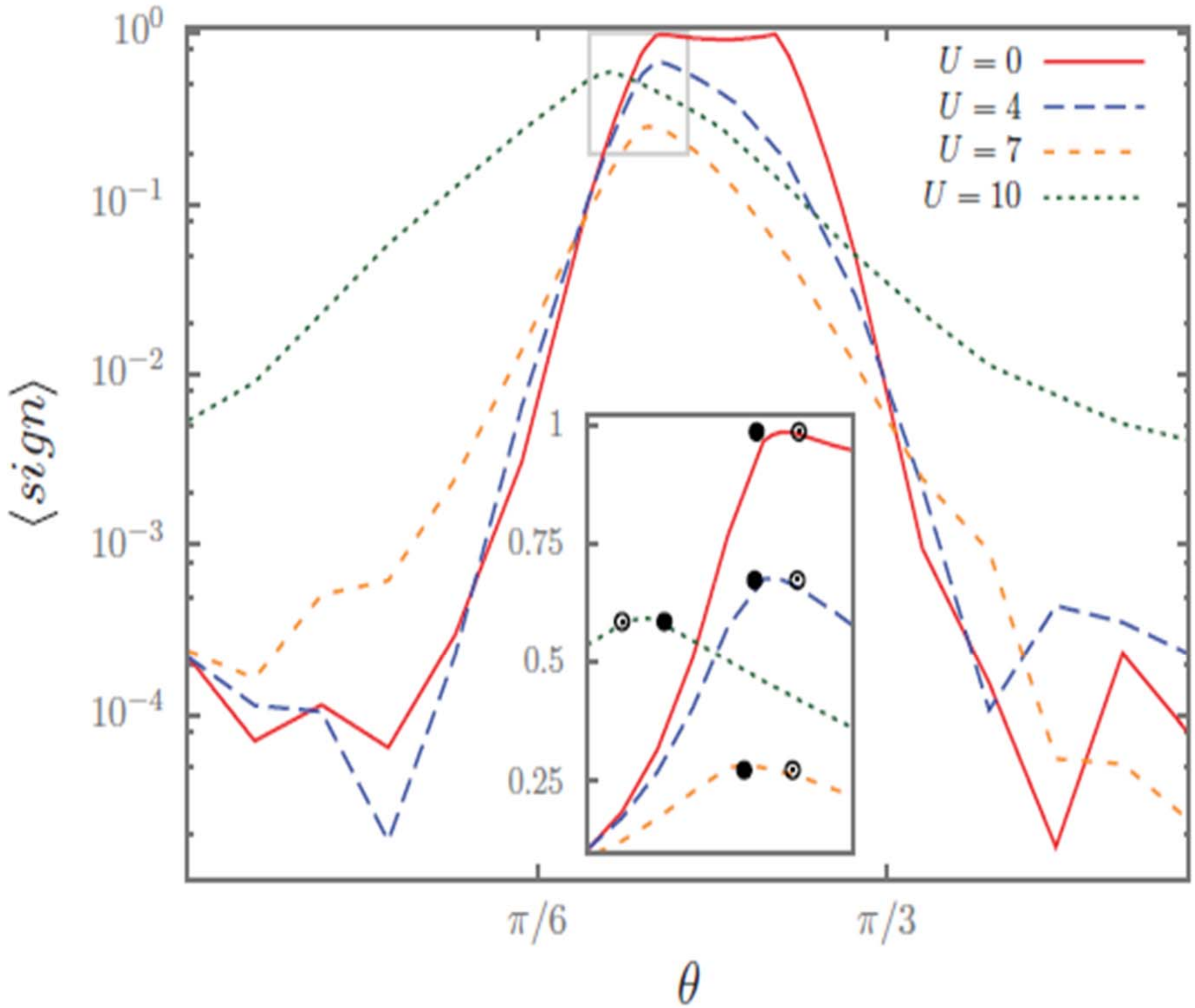
$$\cos\theta c'_{A_1\sigma} - \sin\theta c_{A_1\sigma}, \quad \sin\theta c'_{A_1\sigma} + \cos\theta c_{A_1\sigma}$$



$t'/t = 0.8$

C_{2v}

$2A_1, B_1, B_2$



Ergodicity of the hybridization expansion with two operator updates and broken symmetry

$$H_{\rm imp} = H_{\rm loc}(d_i^\dagger, d_i) + \sum_{i\mu}(V_{\mu i} a_\mu^\dagger d_i + V_{\mu i}^* d_i^\dagger a_\mu) + \sum_\mu \epsilon_\mu a_\mu^\dagger a_\mu,$$

Patrick Sémon

$$Z = {\rm Tr T}_\tau e^{-\beta H_0} e^{-\int_0^\beta d\tau (H_{\rm hyb}(\tau) + H_{\rm hyb}^\dagger(\tau))}$$

$$= \sum_{k\geq 0} \frac{1}{k!^2} \int_0^\beta d\tau_1 \cdots d\tau_k \int_0^\beta d\tau_1' \cdots d\tau_k' {\rm Tr T}_\tau e^{-\beta H_0} \times H_{\rm hyb}(\tau_1) H_{\rm hyb}^\dagger(\tau_1') \cdots H_{\rm hyb}(\tau_k) H_{\rm hyb}^\dagger(\tau_k').$$

$${\rm Tr}[d_{\uparrow(0,\pi)} d_{\downarrow(0,\pi)} d^\dagger_{\downarrow(\pi,0)} d^\dagger_{\uparrow(\pi,0)}] \times \Delta_{a\uparrow(0,\pi),\downarrow(0,\pi)} \Delta_{a\uparrow(\pi,0),\downarrow(\pi,0)}$$

P. Sémon, G. Sordi, A.-M.S. Tremblay, Phys. Rev. B **89**, 165113 (2014)

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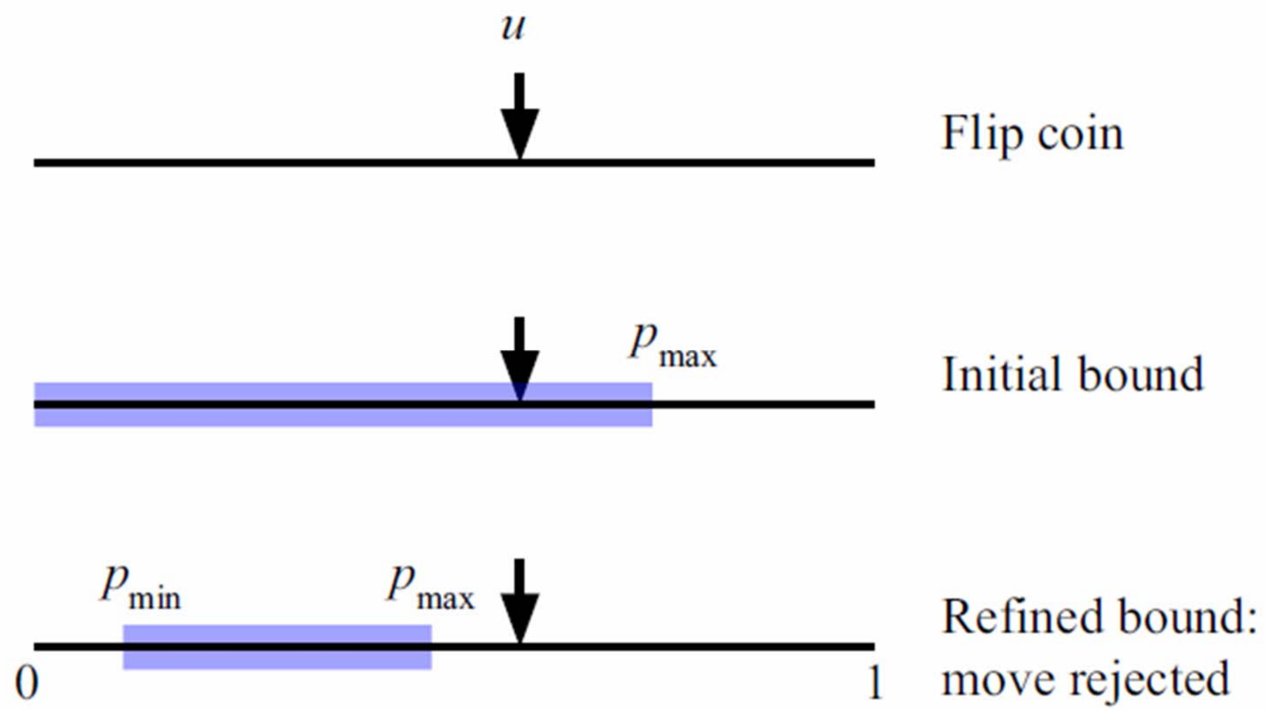
Lazy Skip-List : 1 Lazy

Fast rejection algorithm : the lazy part



P. Sémon, Chuck-Hou Yee, K. Haule, A.-M.S. Tremblay, Phys. Rev. B **90**, 075149 (2014)

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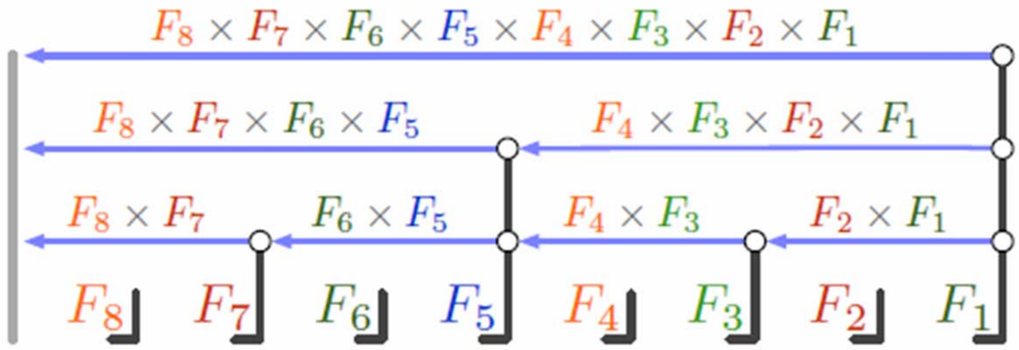
MC weights in CT-HYB some notation

$$w\{(i_1,\tau_1)\cdots(i'_k,\tau'_k)\} = \mathrm{Det}\,\boldsymbol{\Delta}\,\mathrm{Tr}_{\mathrm{loc}}\left[\mathrm{T}_\tau e^{-\beta H_{\mathrm{loc}}} \times d_{i_k}(\tau_k)d^\dagger_{i'_k}(\tau'_k)\cdots d_{i_1}(\tau_1)d^\dagger_{i'_1}(\tau'_1)\right]$$

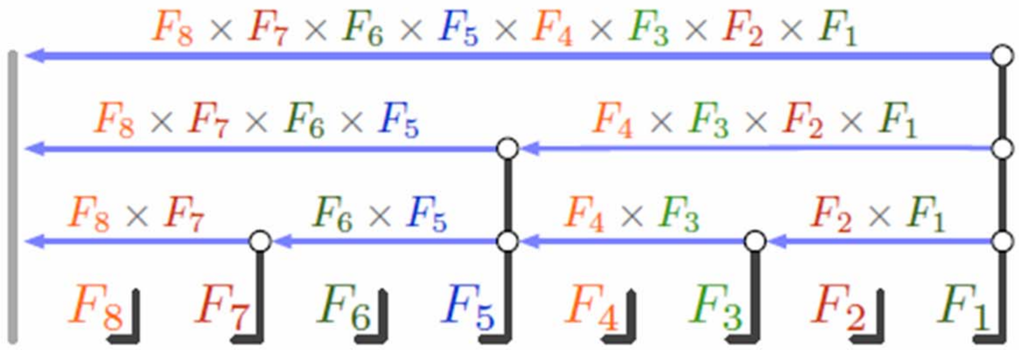
$$\mathrm{Tr}_{\mathrm{loc}}\, P_{\beta-\tau_k} F_{i_k} P_{\tau_k-\tau'_k} F^\dagger_{i'_k} \cdots F_{i_1} P_{\tau_1-\tau'_1} F^\dagger_{i'_1} P_{\tau'_1}$$

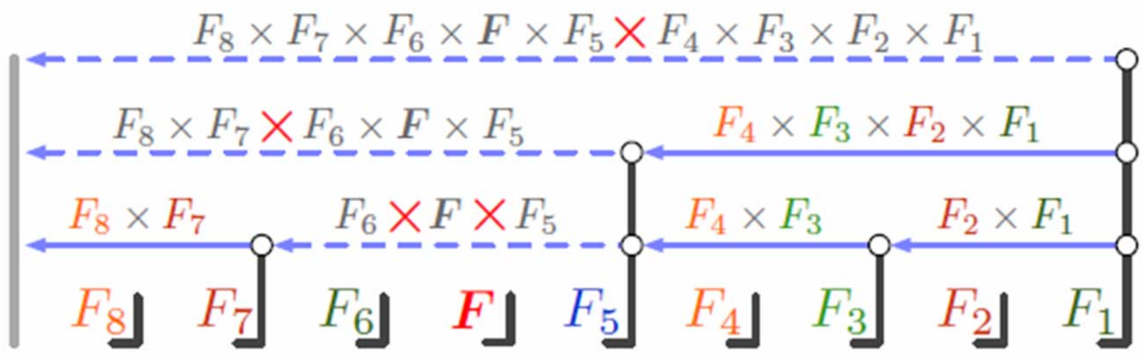
Lazy Skip List : Skip List



Tree structure : E. Gull, ETH thesis

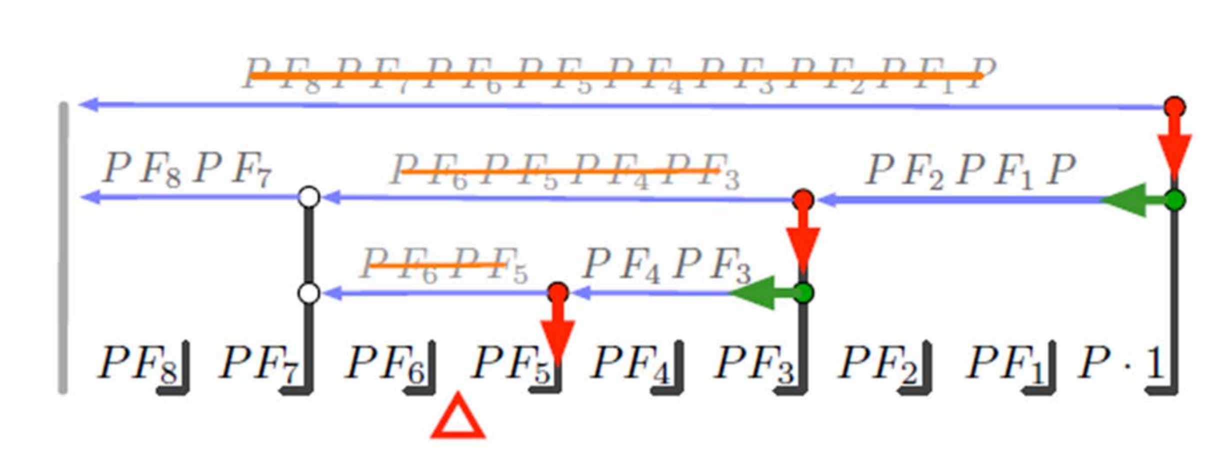
Lazy Skip List : Skip List





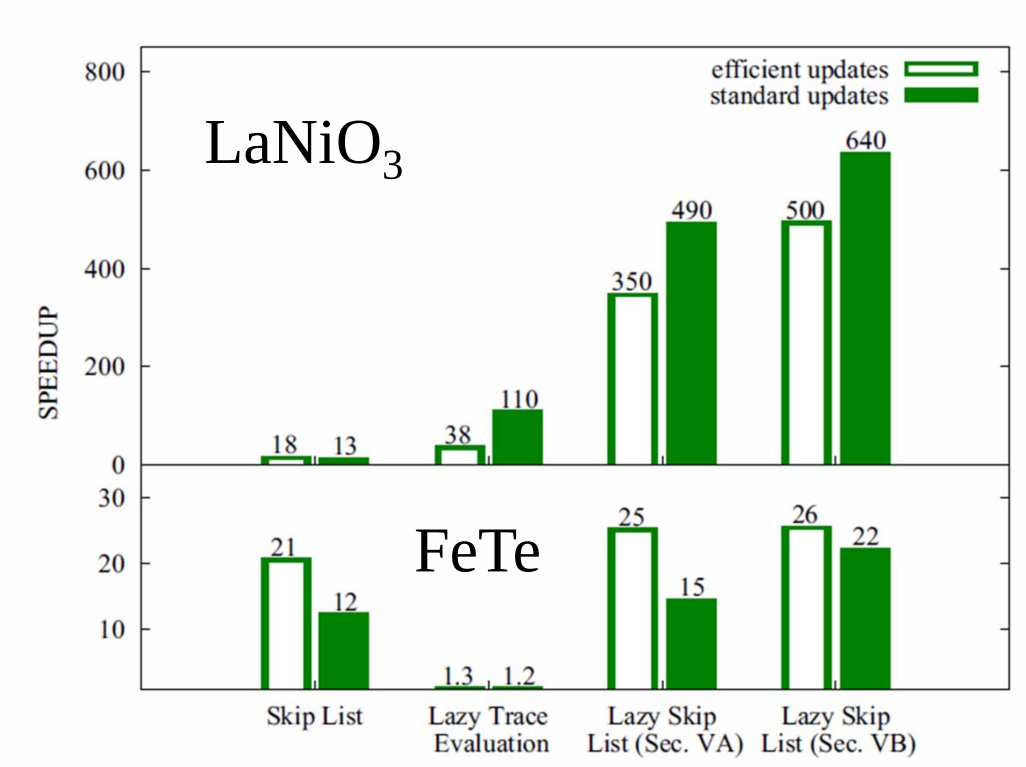
Tree structure : E. Gull, ETH thesis

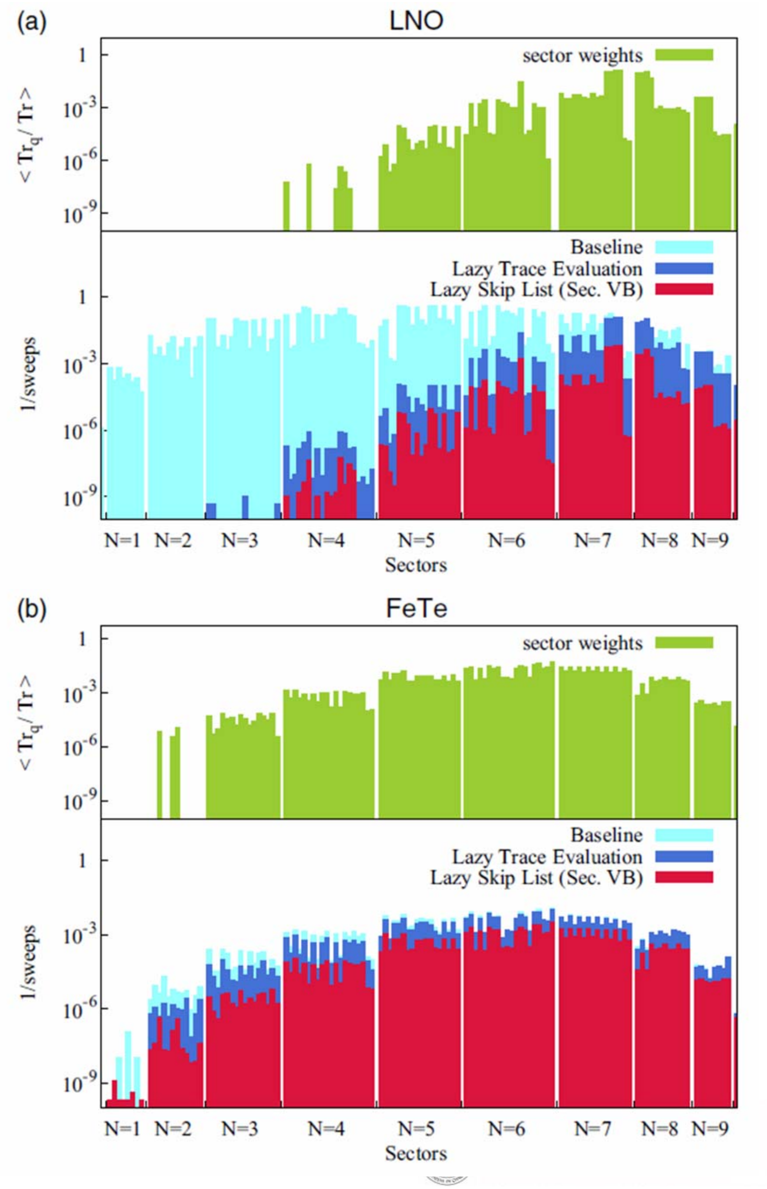
Some more details



Subproducts stored in blue arrows are emptied if tail coincides with red arrow

Lazy Skip-List: Speedup (beat Moore)





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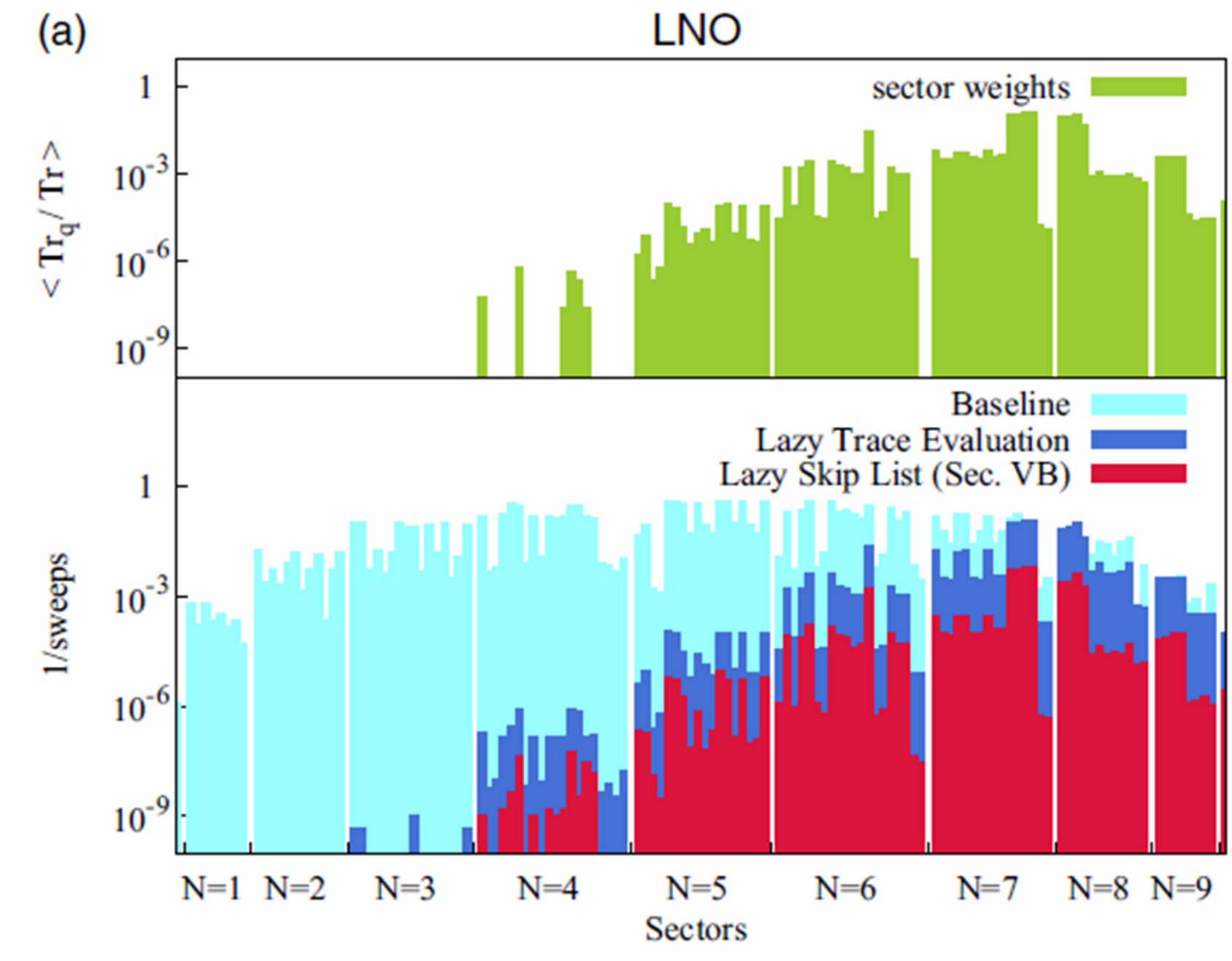

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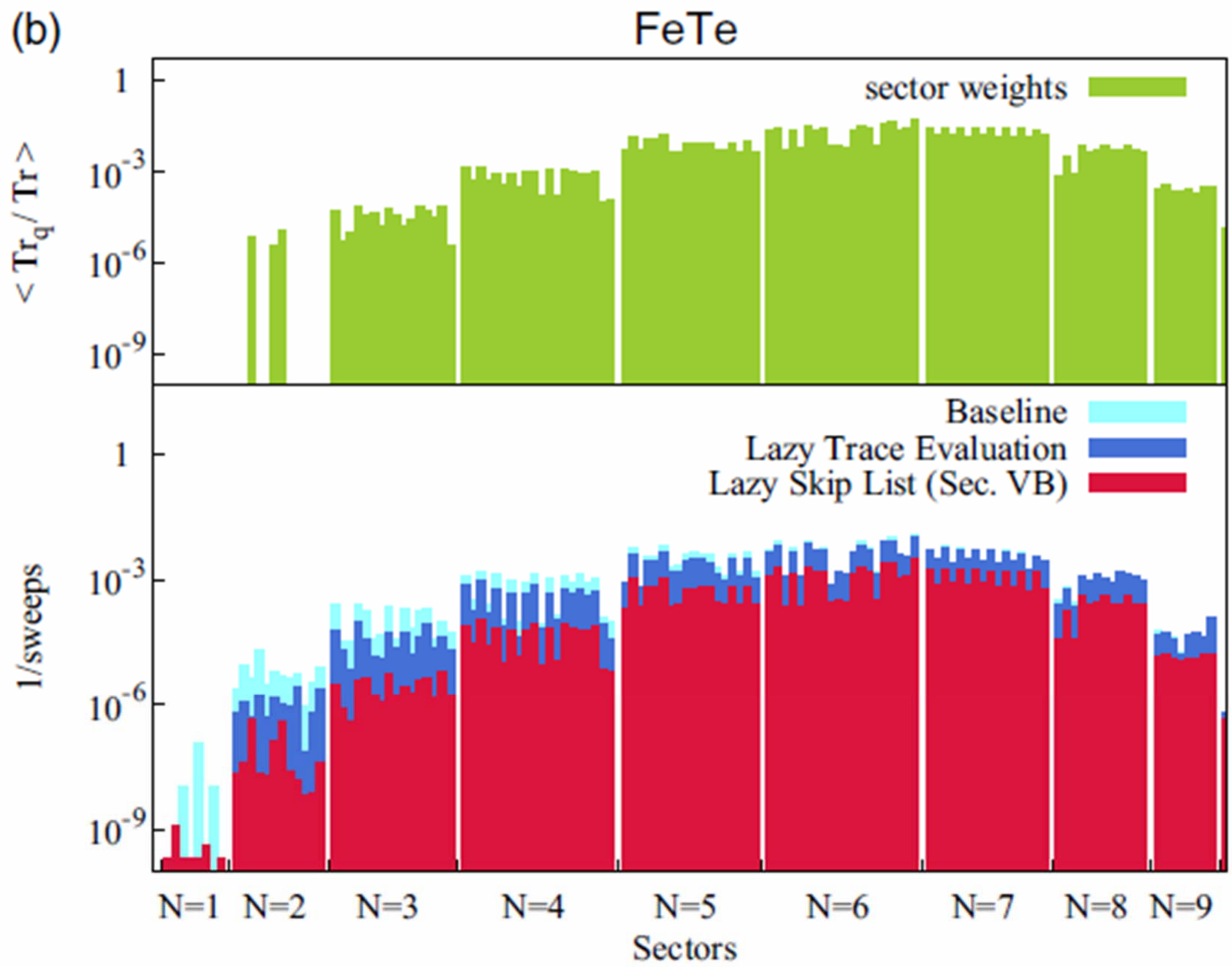

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Collaborators

Giovanni Sordi

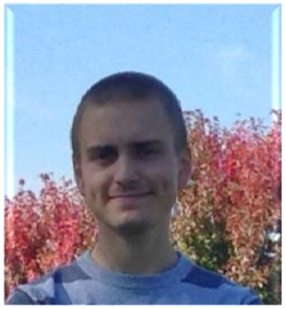
David Sénéchal

Alexandre Day

Vincent Bouliane

Patrick Sémon

Kristjan Haule



Charles-David Hébert

Chuck-Hou Yee

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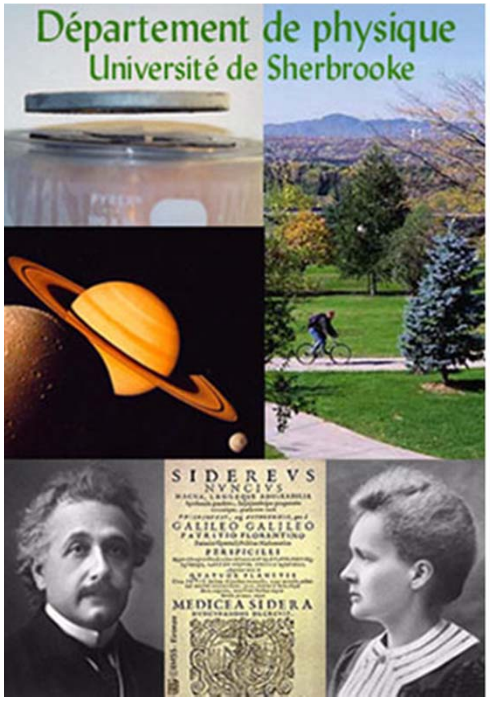

André-Marie Tremblay

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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