Superconductivity, antiferromagnetism and Mott critical point in the BEDT family

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P. Sémon, G. Sordi, K. Haule,

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VERITATEM IN CHARITATE

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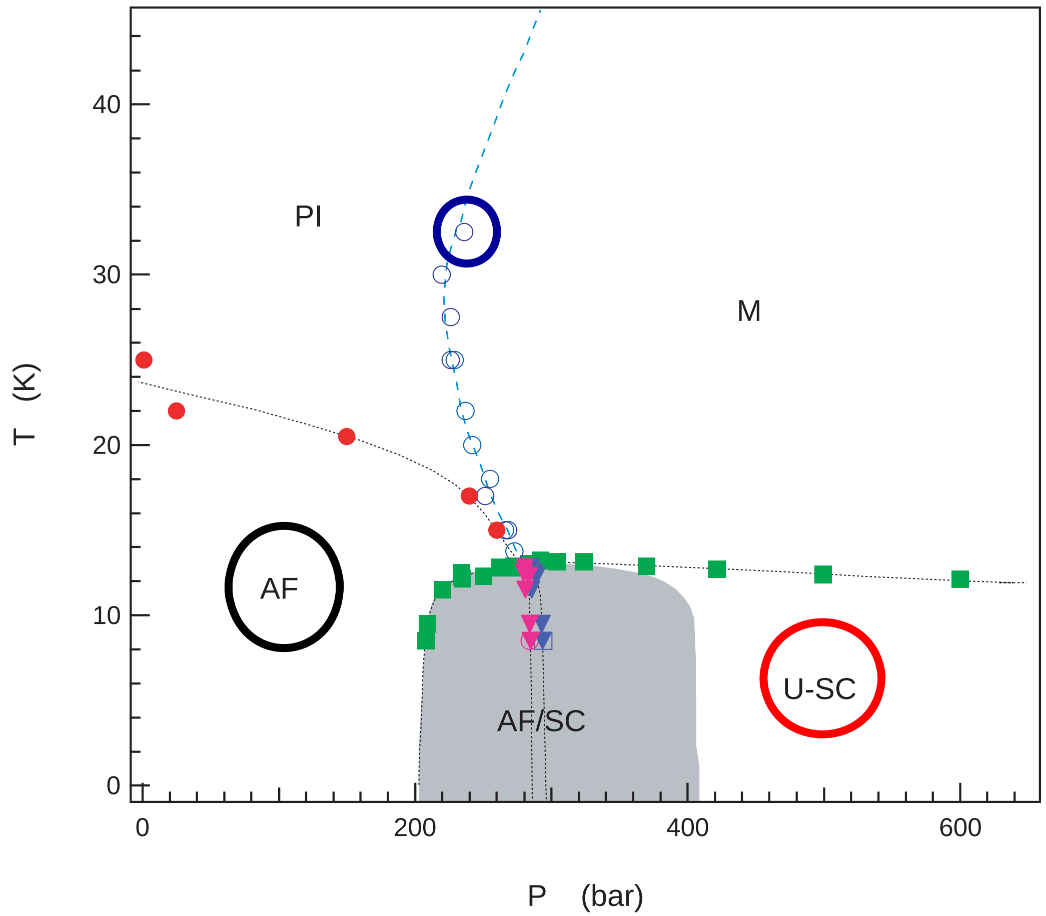
Half-filled band: Not always a metal

NiO, Boer and Verway

Peierls, 1937

Mott, 1949

Mott, antiferromagnetism, superconductivity



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

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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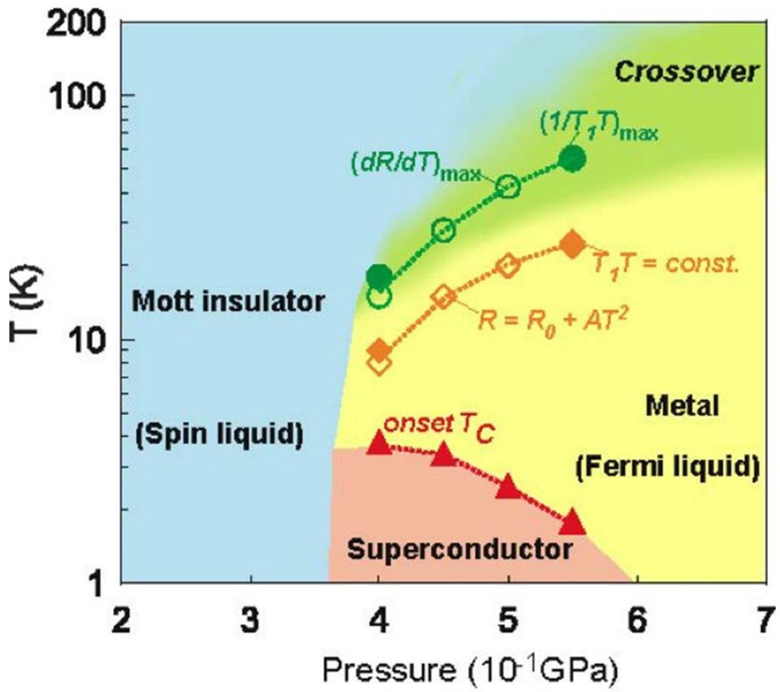
« Spin liquid »

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



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

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

Reviews:

B J Powell and Ross H McKenzie, Rep. Prog. Phys. 74 (2011) 056501

K. Kanoda and R. Kato, Annu. Rev. Condens.Matter Phys. 2011. 2:167–88

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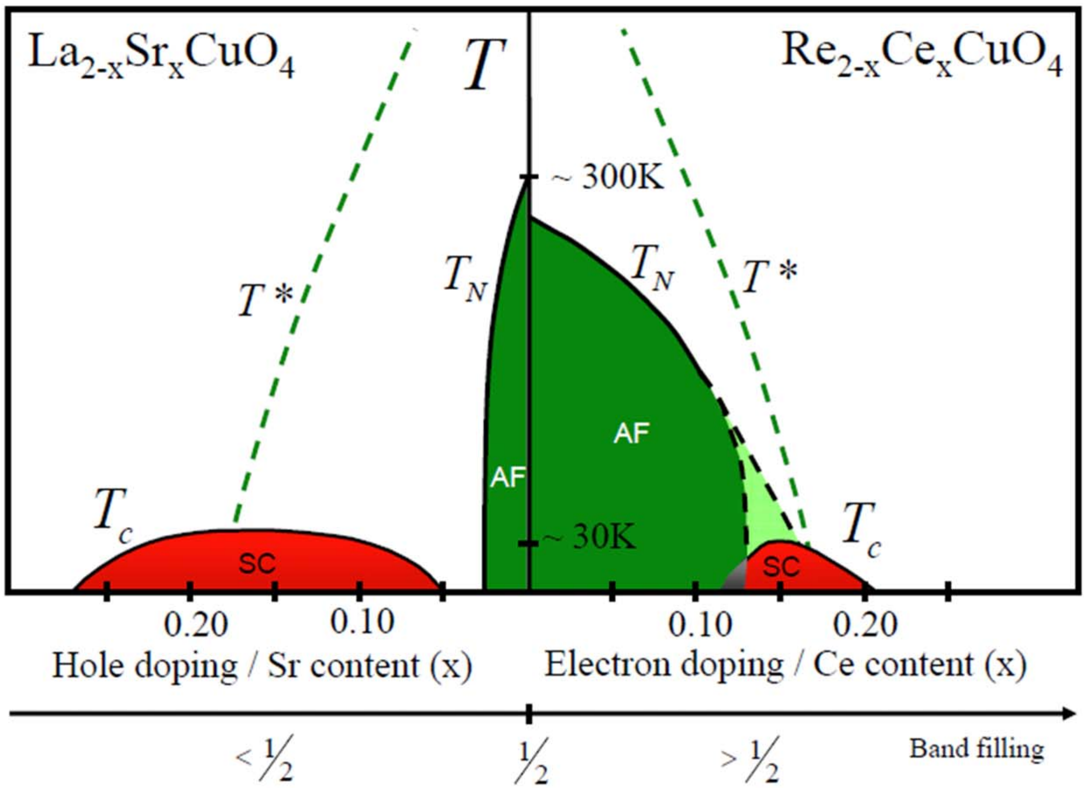
Competing order or Mott Physics ?

Armitage, Fournier, Greene, RMP (2009)



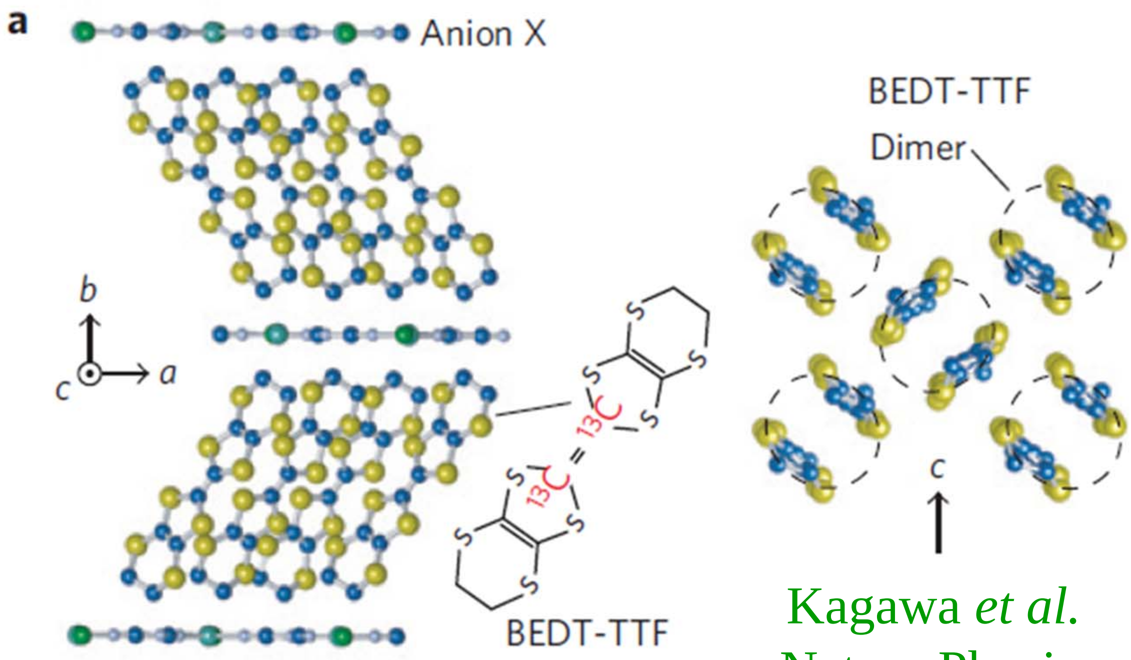
Outline

- Model and method
  - *T=0*
  - Finite *T*
- Phase diagram: Organics and cuprates
  - *T = 0*
  - Finite *T*
- The Mott critical point and critical exponents PII-36

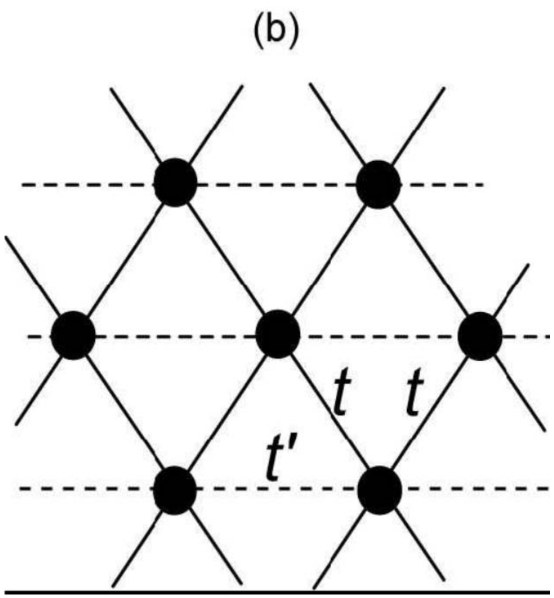
The model

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)



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

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

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

$t'/t \sim 0.6 - 1.1$

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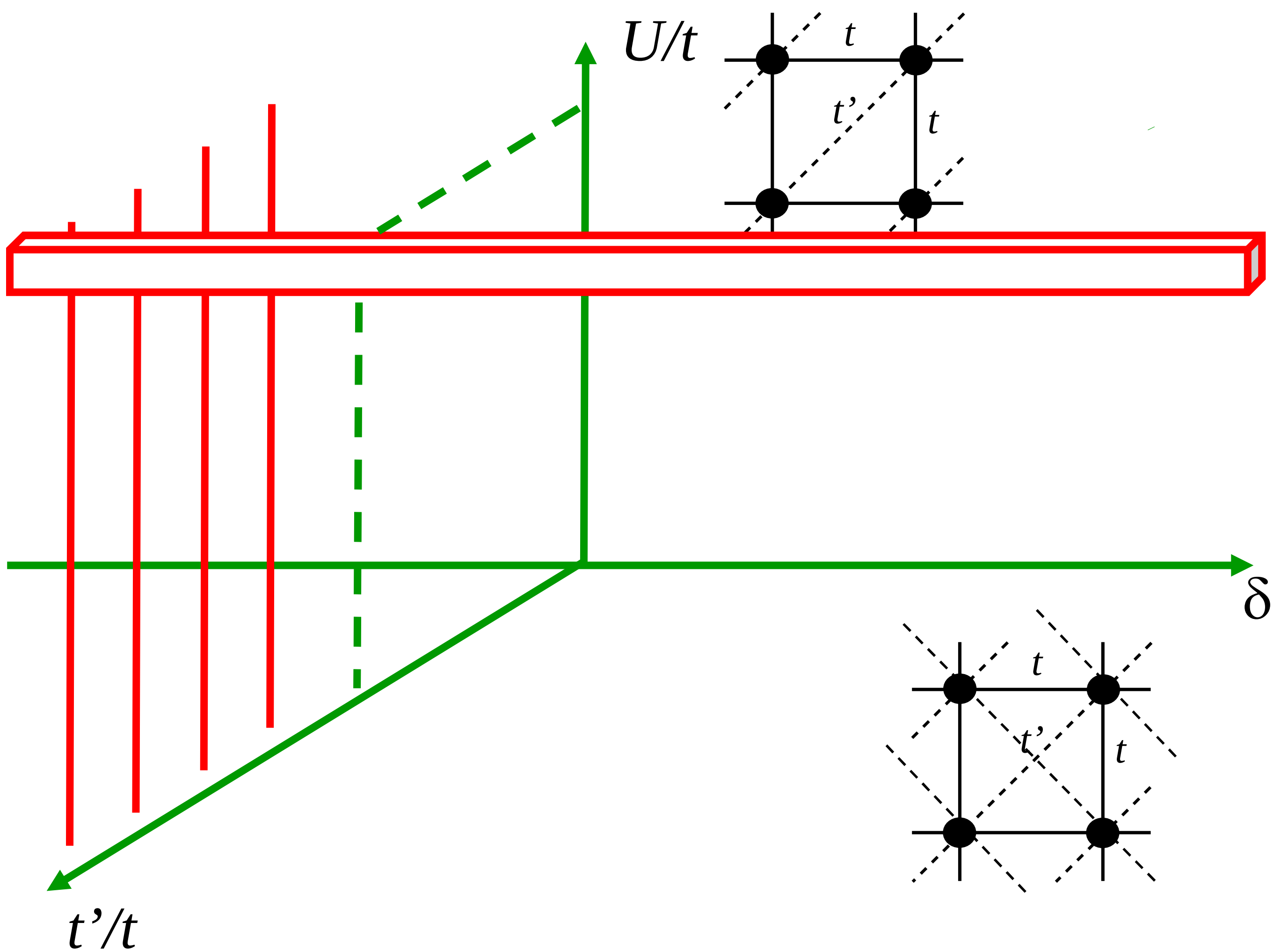
Perspective



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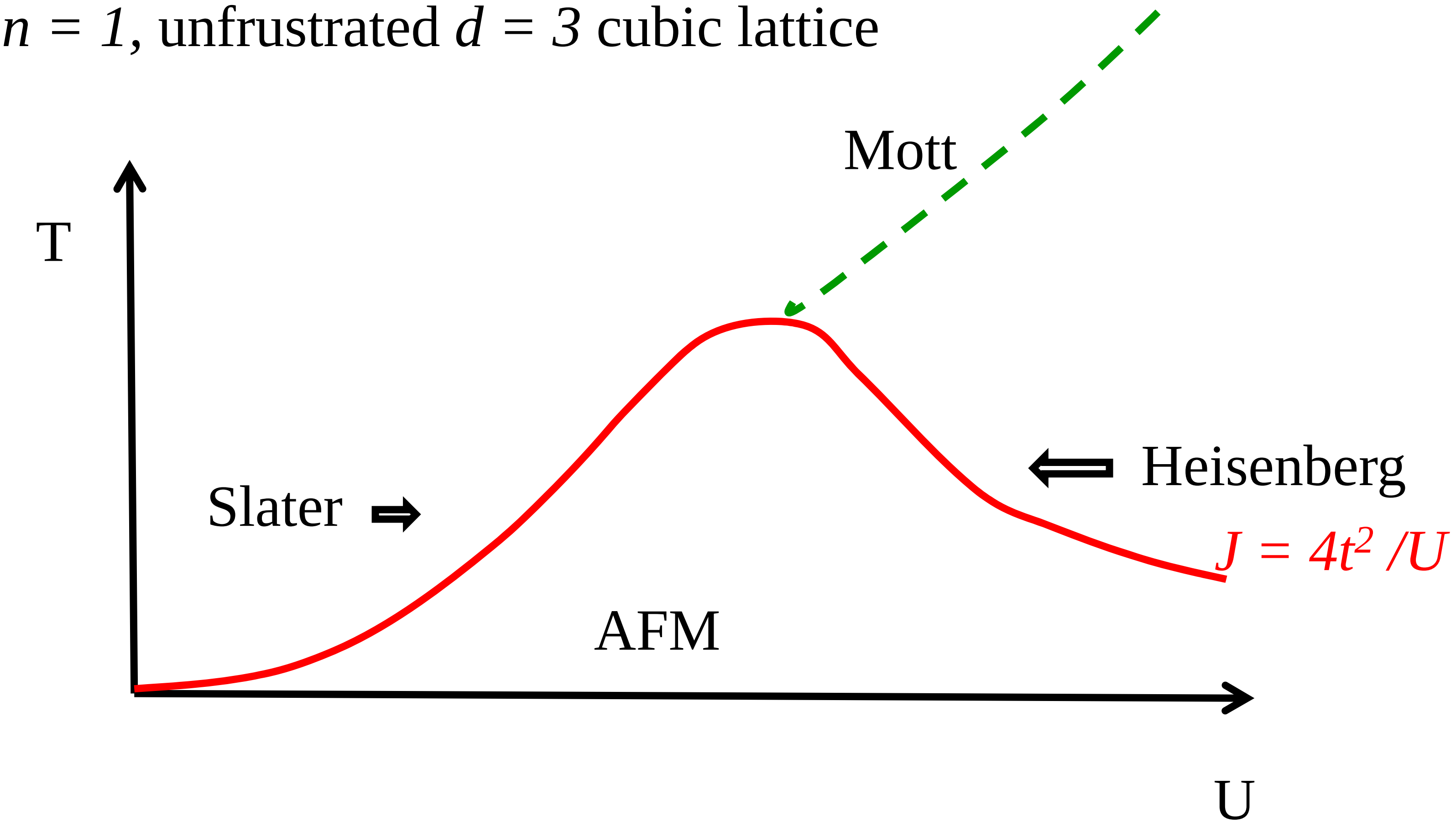
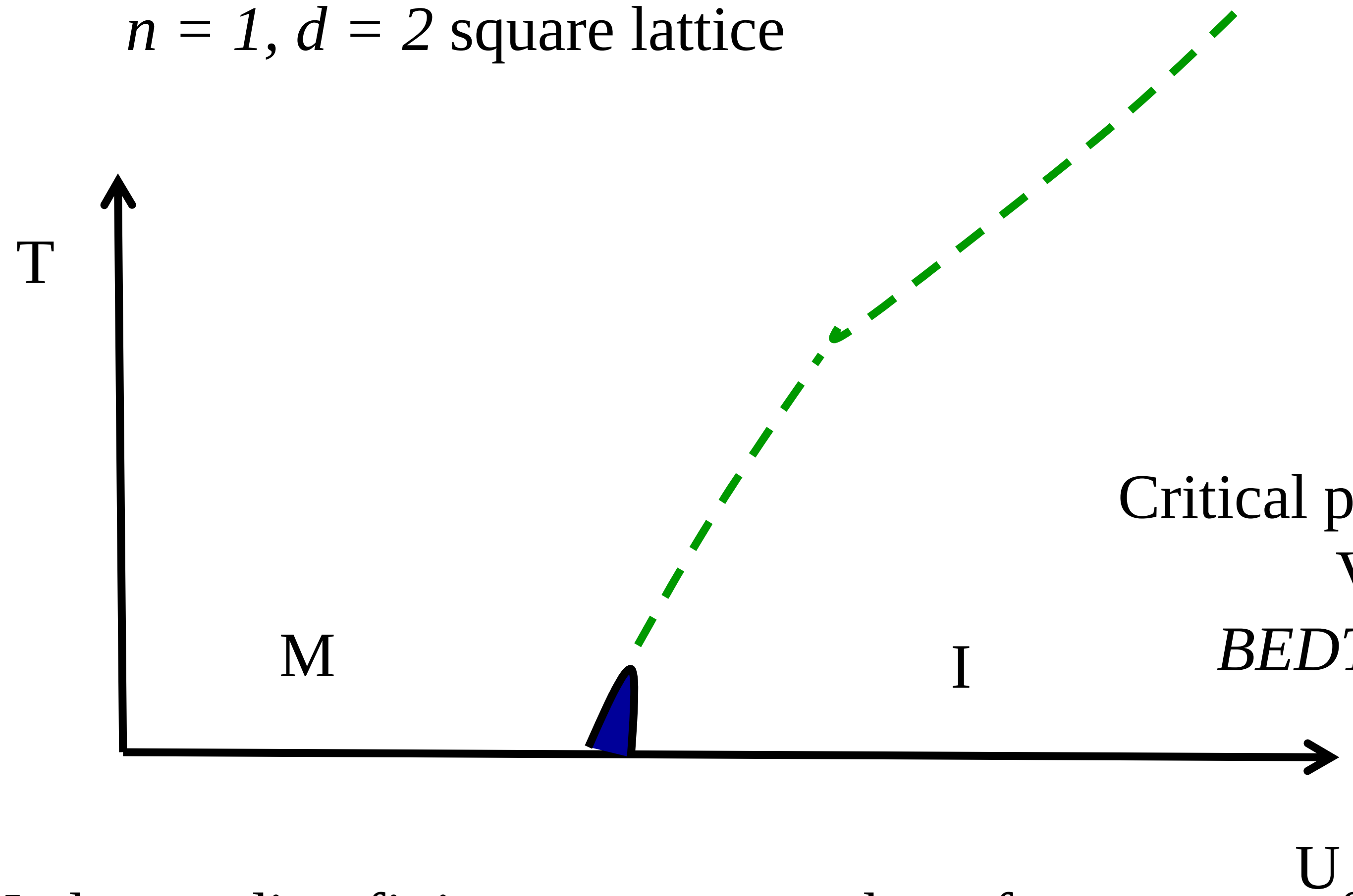
Weak-strong coupling, and Mott transition

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



Local moment and Mott transition

n = 1, d = 2 square lattice

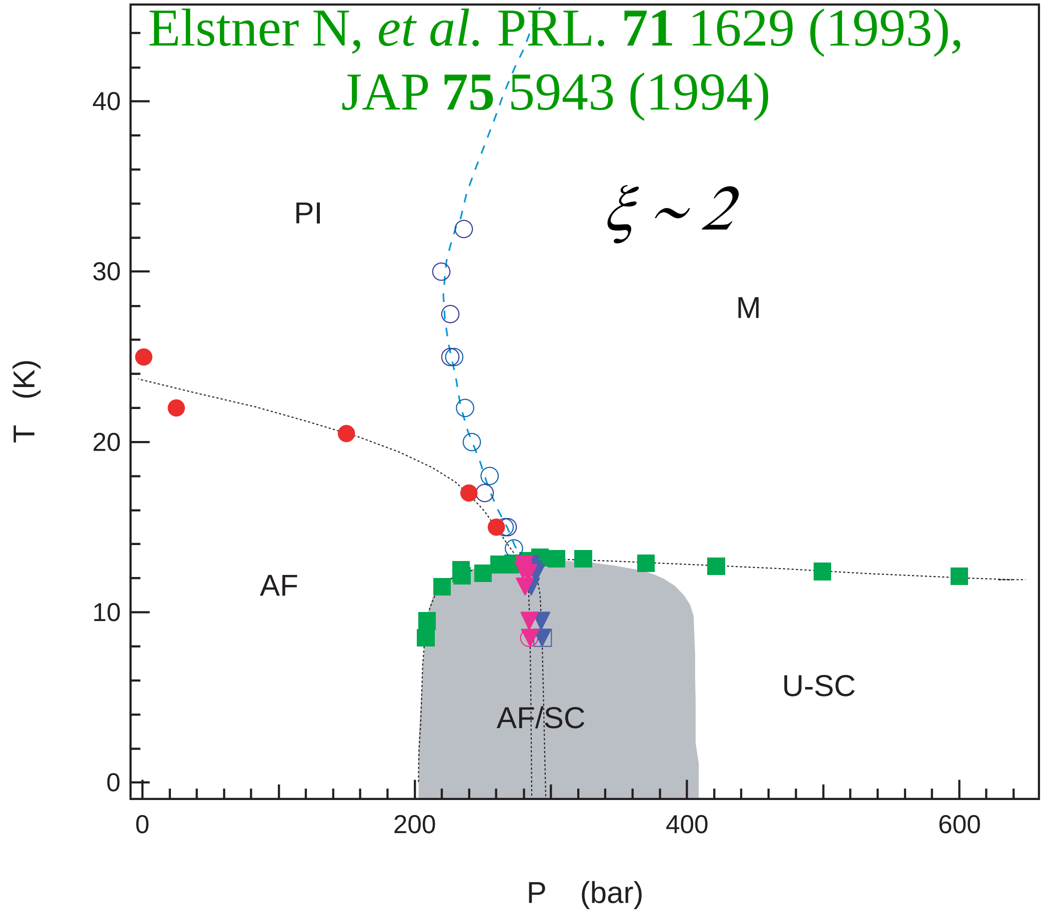


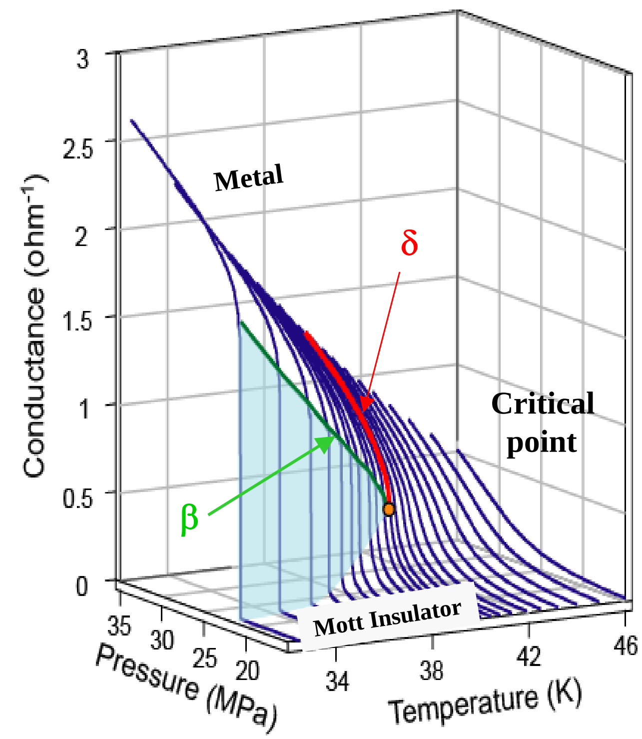
Critical point visible in V_2O_3, *BEDT* organics

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

Bare Mott critical point in organics

Elstner N, *et al.* PRL. **71** 1629 (1993), JAP **75** 5943 (1994)





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

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Sample litterature on the phase diagram

H. Morita et al., J. Phys. Soc. Jpn. **71**, 2109 (2002).

H. Kondo, T. Moriya, J.Phys.Soc.Japan **73,** 812–814 (2004)

J. Liu et al., Phys. Rev. Lett. **94**, 127003 (2005).

S.S. Lee et al., Phys. Rev. Lett. **95**, 036403 (2005).

B. Powell et al., Phys. Rev. Lett. **94**, 047004 (2005). RVB

J.Y. Gan et al., Phys. Rev. Lett. **94**, 067005 (2005).

J. Y. Gan, Yan Chen, and F. C. Zhang Phys. Rev. B **74**, 094515 (2006). RMFT

Watanabe T, *et al.* J. Phys. Soc. Japan **75** 074707 2006

Galitski V and Kim Y B *Phys. Rev. Lett.* **99** 266403 (2007).

Wrobel P and Suleja W *Phys. Rev.* B **76** 214509 (2007).

Powell B J and McKenzie R H *Phys. Rev. Lett.* **98** 027005 (2007).

Hunpyo Lee, Gang Li, and Hartmut Monien, Phys. Rev. B **78**, 205117 (2008).

T. Watanabe et al. Phys. Rev. B **77**, 214505 (2008). Variational WF

Meng, Jarrell, *et al.* triangular lattice DCA cond-mat /1304.7739v1 (2013).

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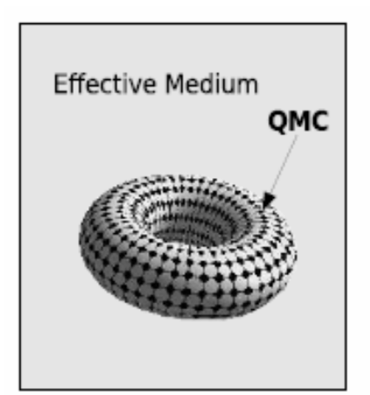
No SC phase

L. F. Tocchio, A. Parola, C. Gros, and F. Becca, Phys. Rev. B 80, 064419 (2009).
T. Kashima and M. Imada, J. Phys. Soc. Jpn. 70, 2287 (2001). (PIRG)
Clay R T, Li H and Mazumdar S Phys. Rev. Lett. **101** 166403 (2008).
S. Dayal, R. T. Clay, and S. Mazumdar, Phys. Rev. B 85, 165141 (2012). (PIRG)
N. Gomes, R. T. Clay, and S. Mazumdar, arXiv:1305.0843

¼ filled model

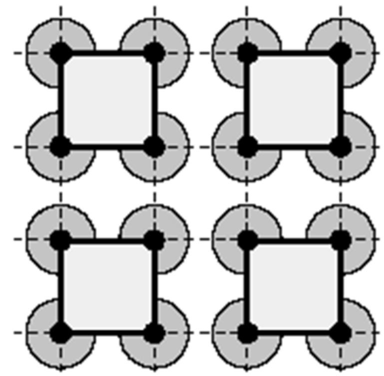
The method

2d Hubbard: Quantum cluster method

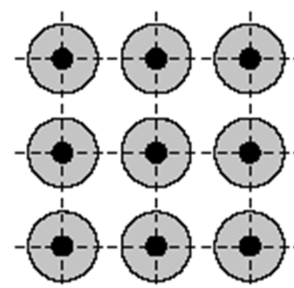


DCA

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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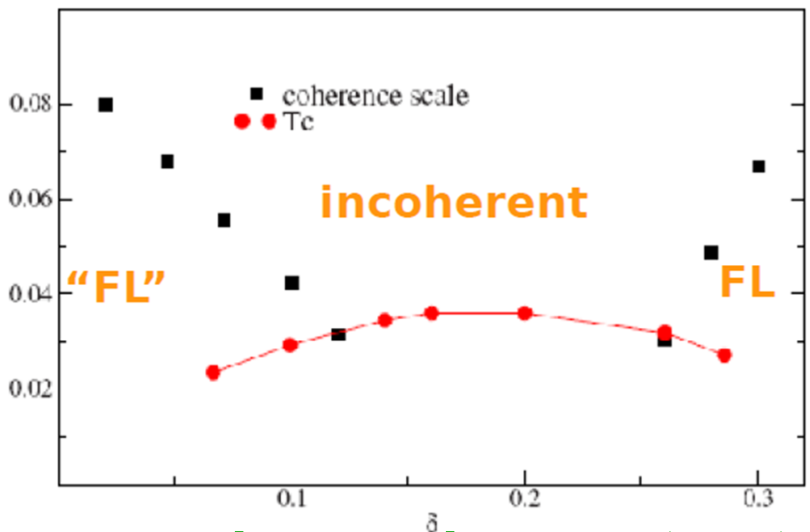
+ and -

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

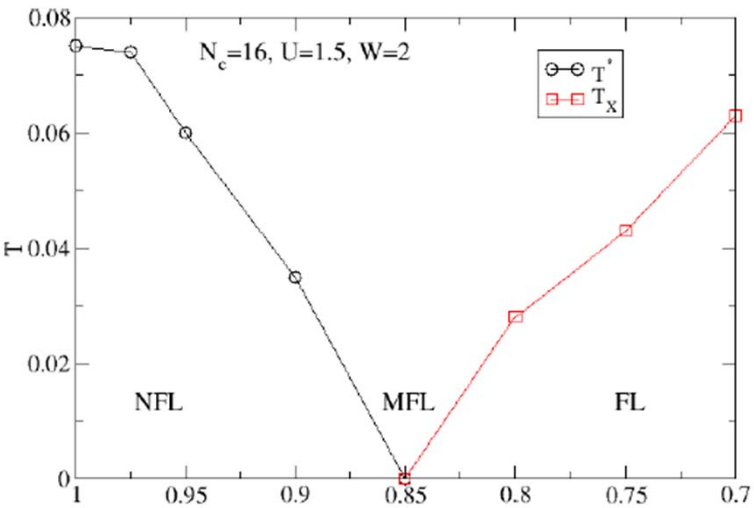
- Missing:
  - Long wavelength p-h and p-p fluctuations

Doping driven Mott transition, *t' = 0*

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

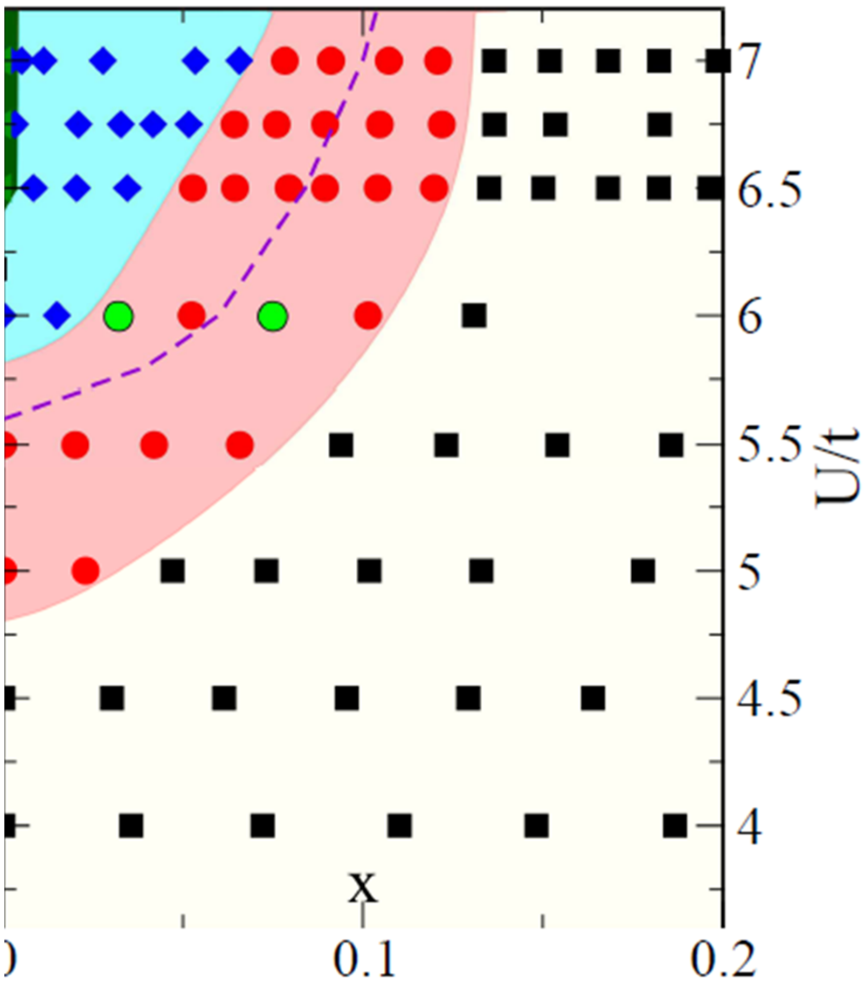


K. Haule, G. Kotliar, PRB (2007)



Vildhyadhiraja, PRL (2009)

Doping driven Mott transition



T = 0.25 t

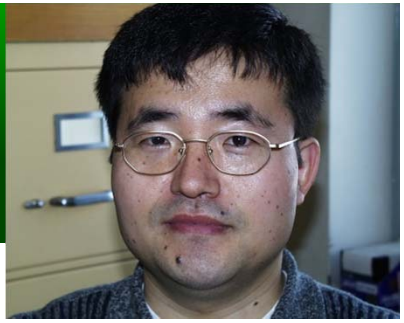
Gull, Parcollet, Millis
arXiv:1207.2490v1

Gull, Werner, Millis, (2009)
E. Gull, M. Ferrero, O. Parcollet, A. Georges, and A. J. Millis (2010)

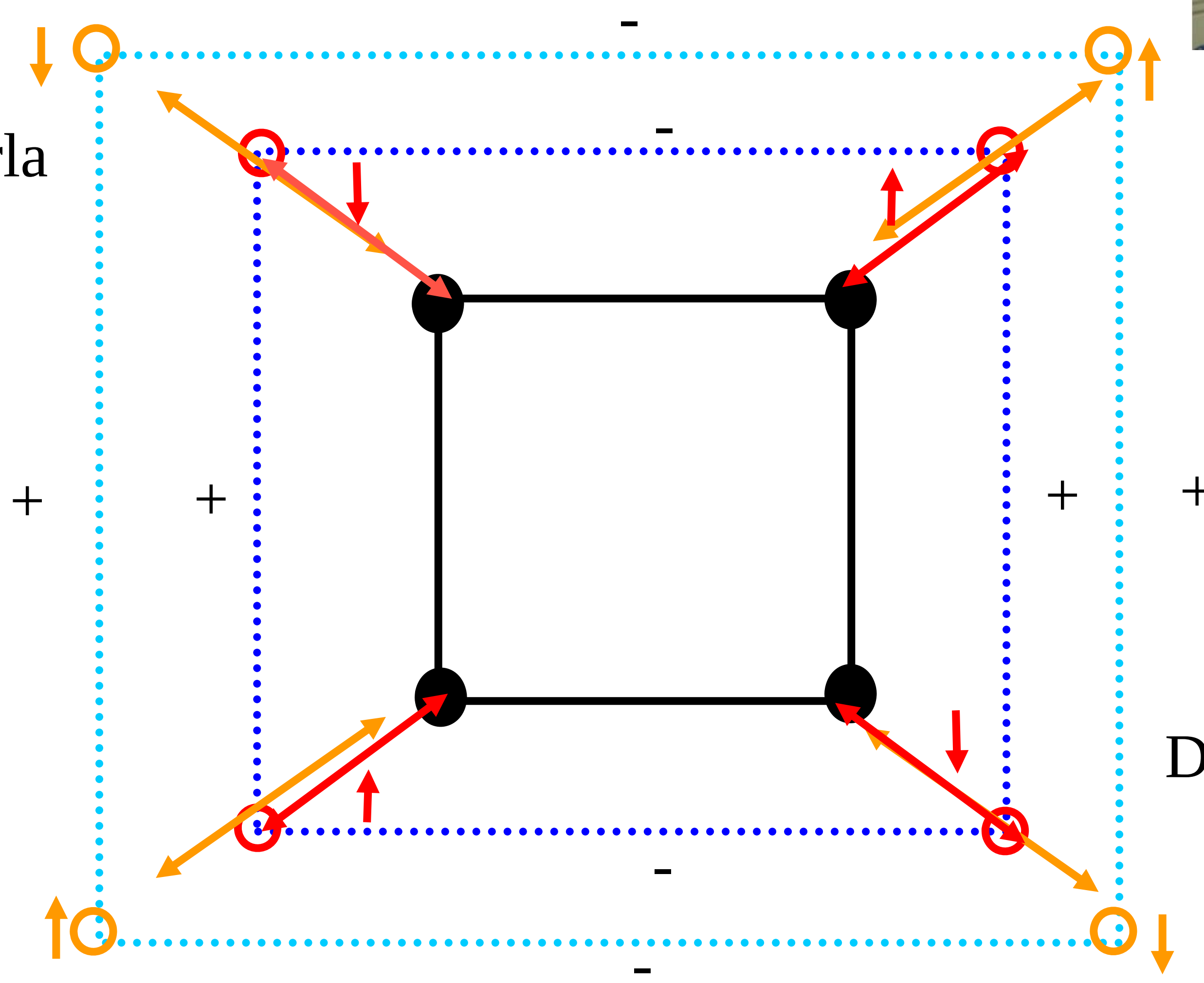
Two solvers for the cluster-in-a-bath problem

Competition AFM-dSC

S. Kancharla



B. Kyung



David Sénéchal

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

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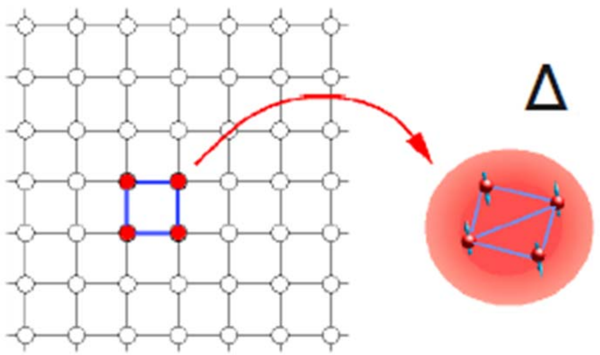
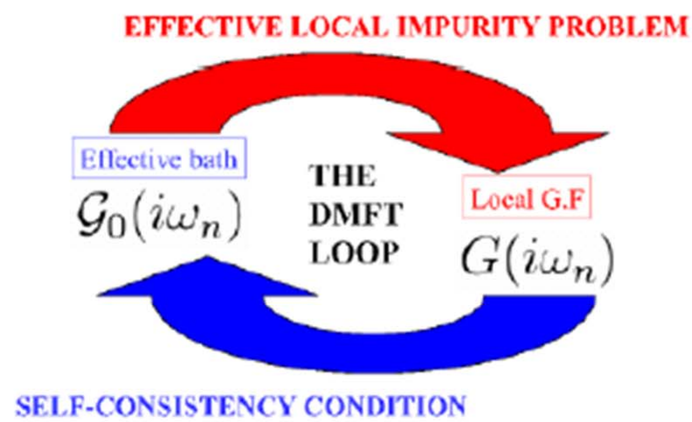
C-DMFT

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





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

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

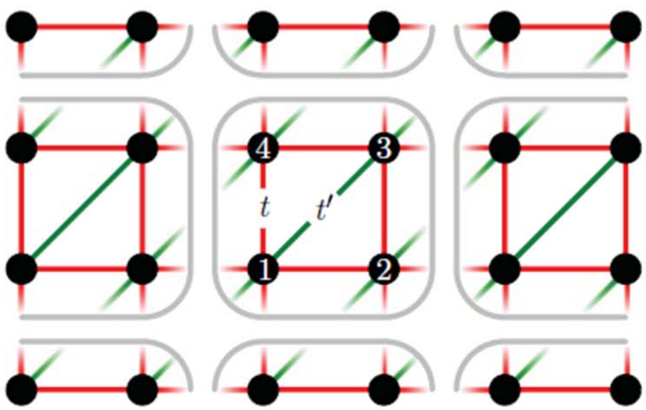
At finite T, solving cluster in a bath problem

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

Reducing the sign problem: PII-36

Patrick Sémc

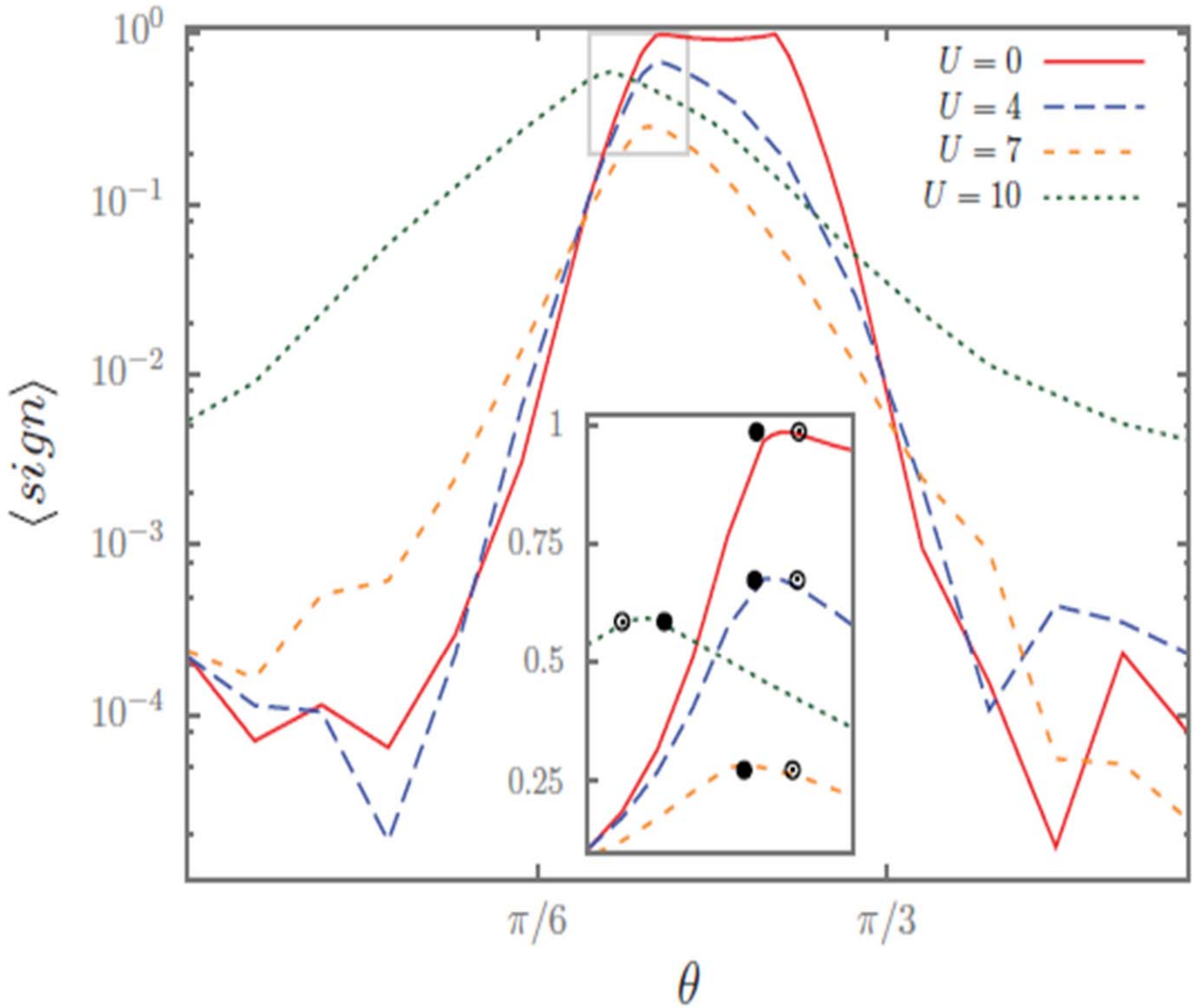
$$\cos\theta c'_{A_1\sigma} - \sin\theta c_{A_1\sigma}, \quad \sin\theta c'_{A_1\sigma} + \cos\theta c_{A_1\sigma}$$



$t'/t = 0.8$

C_{2v}

$2A_1, B_1, B_2$



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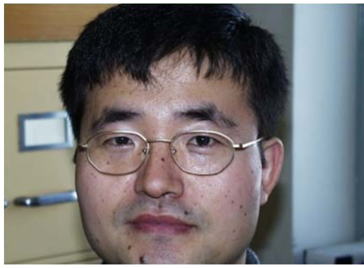
- The Mott critical point and critical exponents PII-36

$\boldsymbol{T = 0}$ phase diagram $n = 1$

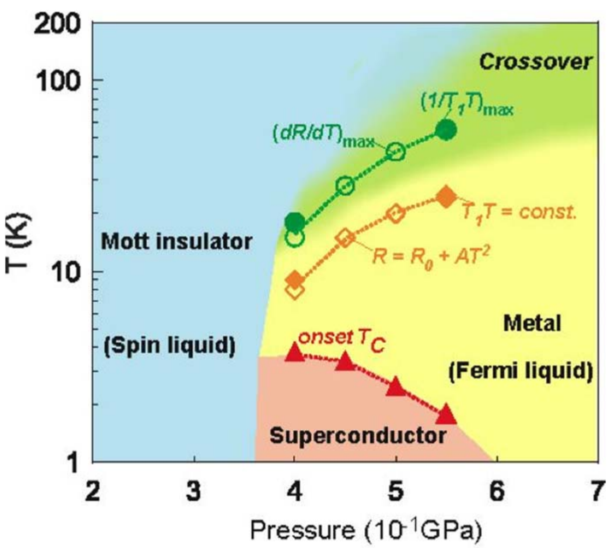
Phase diagram

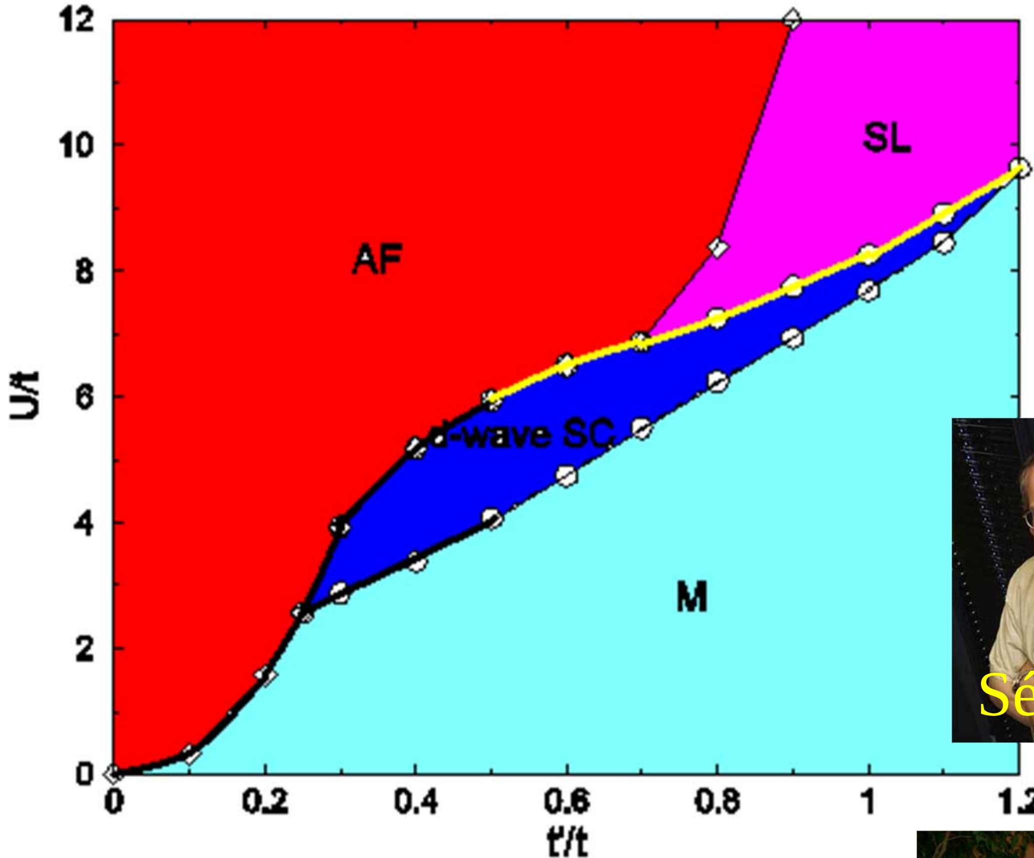
Exact diagonalization as solver for cluster-in-a bath problem ($T=0$).

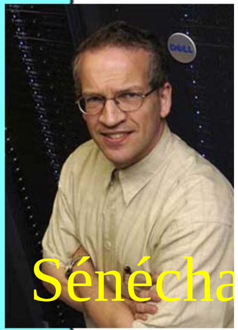


Theoretical phase diagram BEDT

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







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

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

Y. Kurisaki, et al.

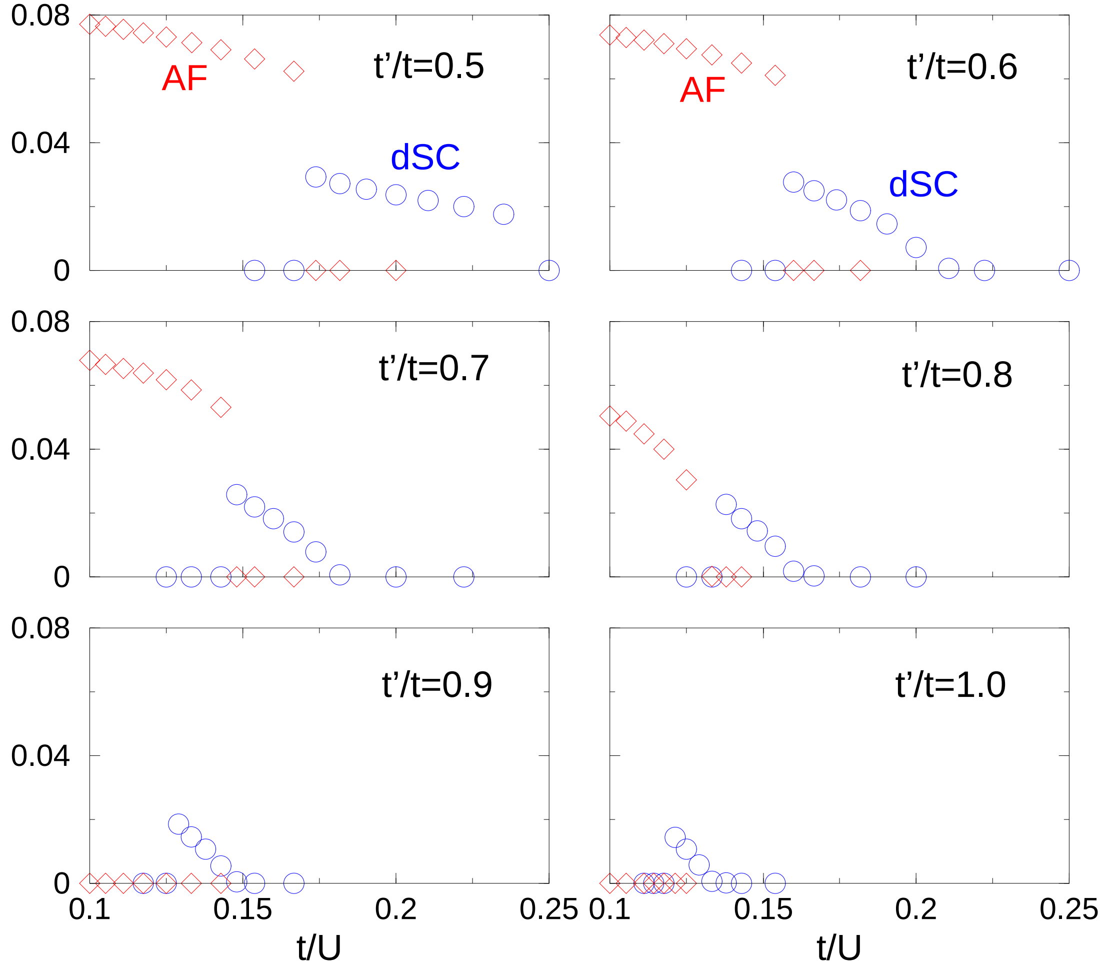
Phys. Rev. Lett. **95**, 177001(2005) Y. Shimizu, et al. Phys. Rev. Lett. **91**, (2003)

AFM and dSC order parameters for various t'/t

- Discontinuous jump
- Maximum order parameter close to insulator.

X	$Cu[N(CN)_2]Br$	$Cu(NCS)_2$	$Cu_2(CN)_3$
t'/t	0.68	0.84	1.06
T_c	11.6	10.4	3.9

AF multiplied by 0.1



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

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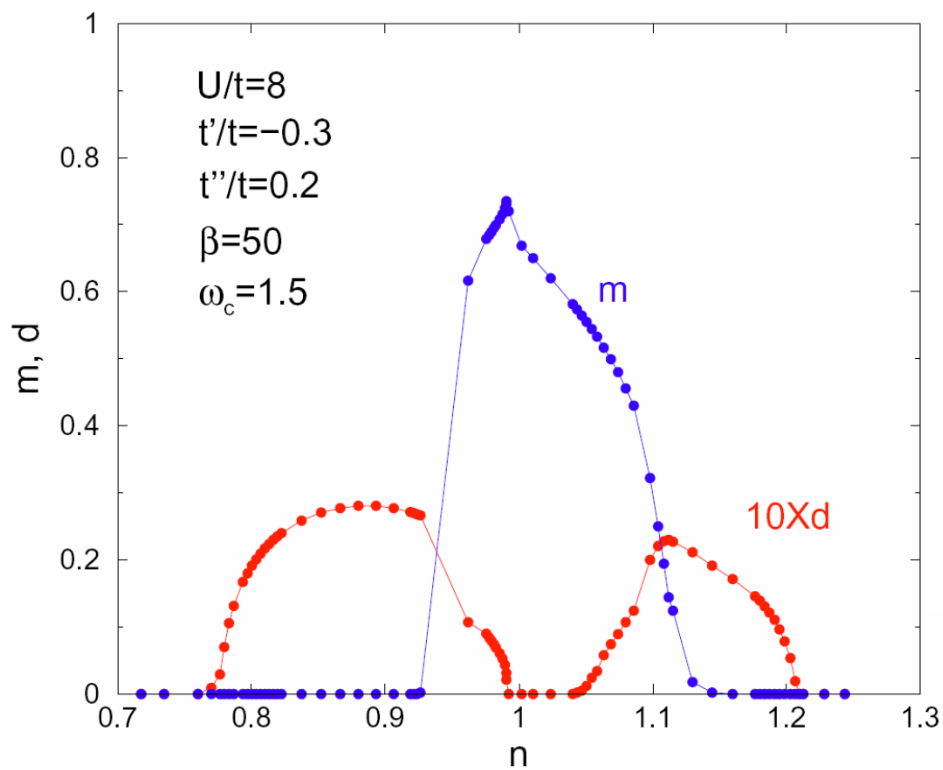
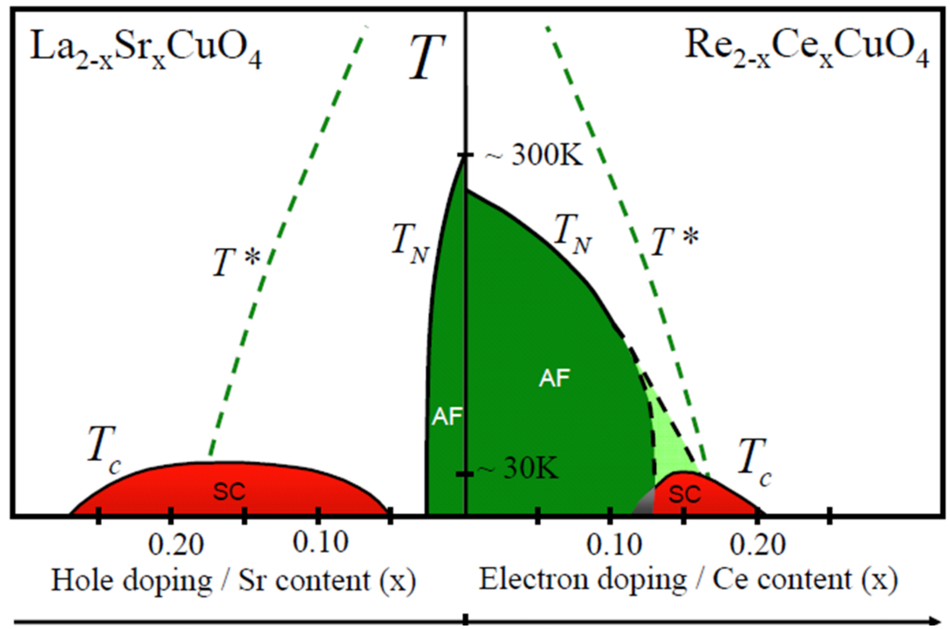
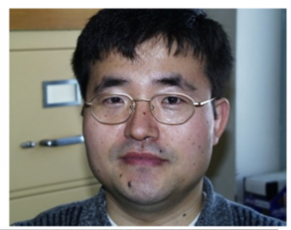
CDMFT cuprate phase diagram

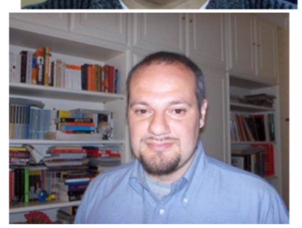


Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008)
AND Capone, Kotliar PRL (2006)



Armitage, Fournier, Greene, RMP (2009)





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Giovanni Sordi

Finite T phase diagram *n = 1* (cuprates)

CTQMC as solver for cluster in a bath (*T=0*).

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Kristjan Haule

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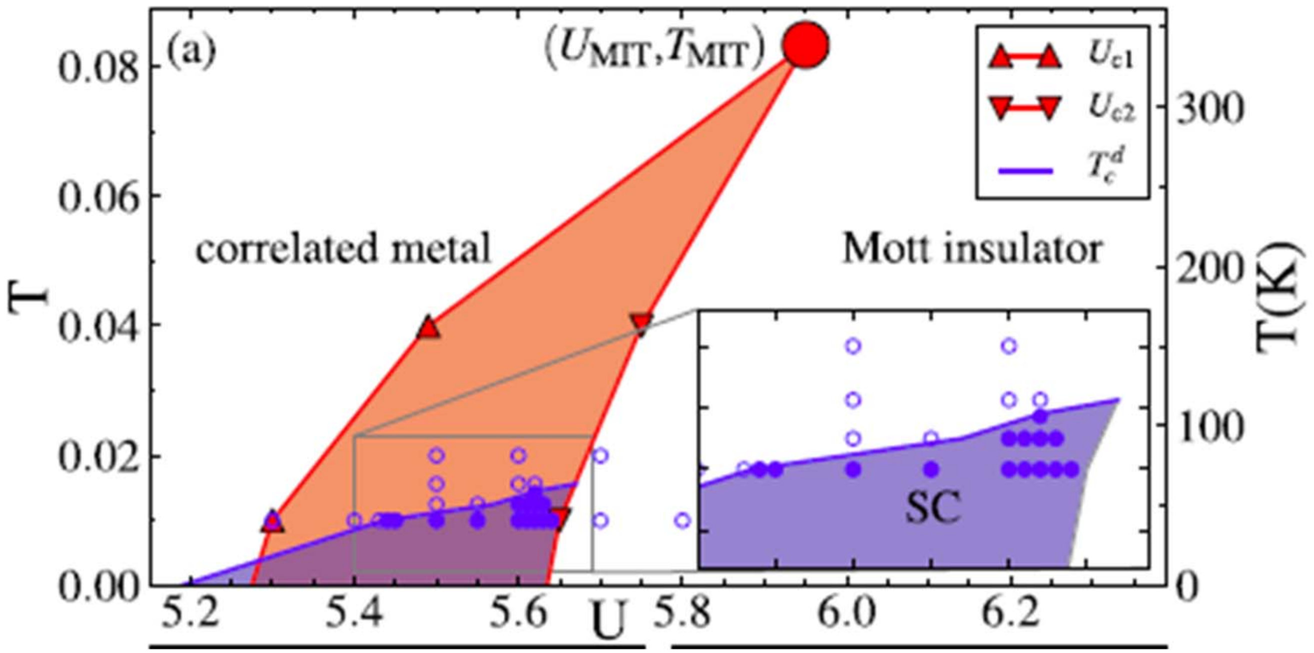
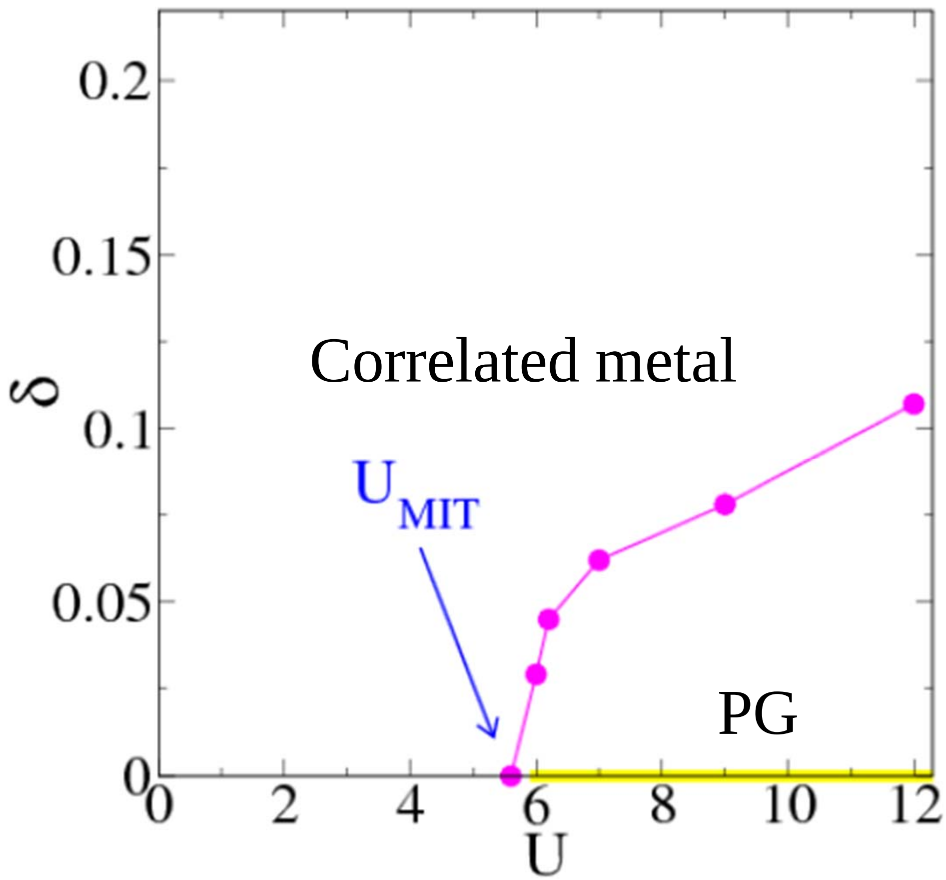
$n = 1$ unfrustrated, $t' = 0$

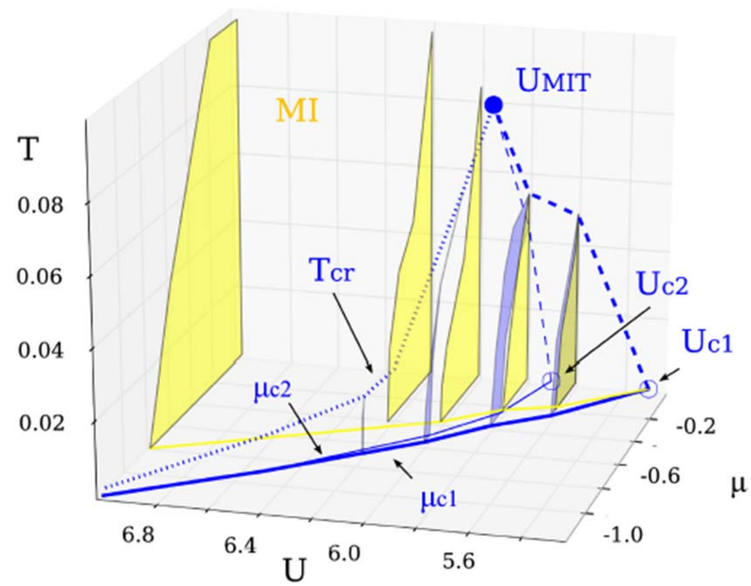


Sordi et al. PRL 108, 216401 (2012)

Link to Mott transition up to optimal doping

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





G. Sordi, P. Sémon, K. Haule, and A.-M.S.T., PRL **104**, 226402 (2010); PRB **84**, 075161 (2011); Sci. Rep. **2**, 547 (2012); PRB **87**, 041101(R) (2013)

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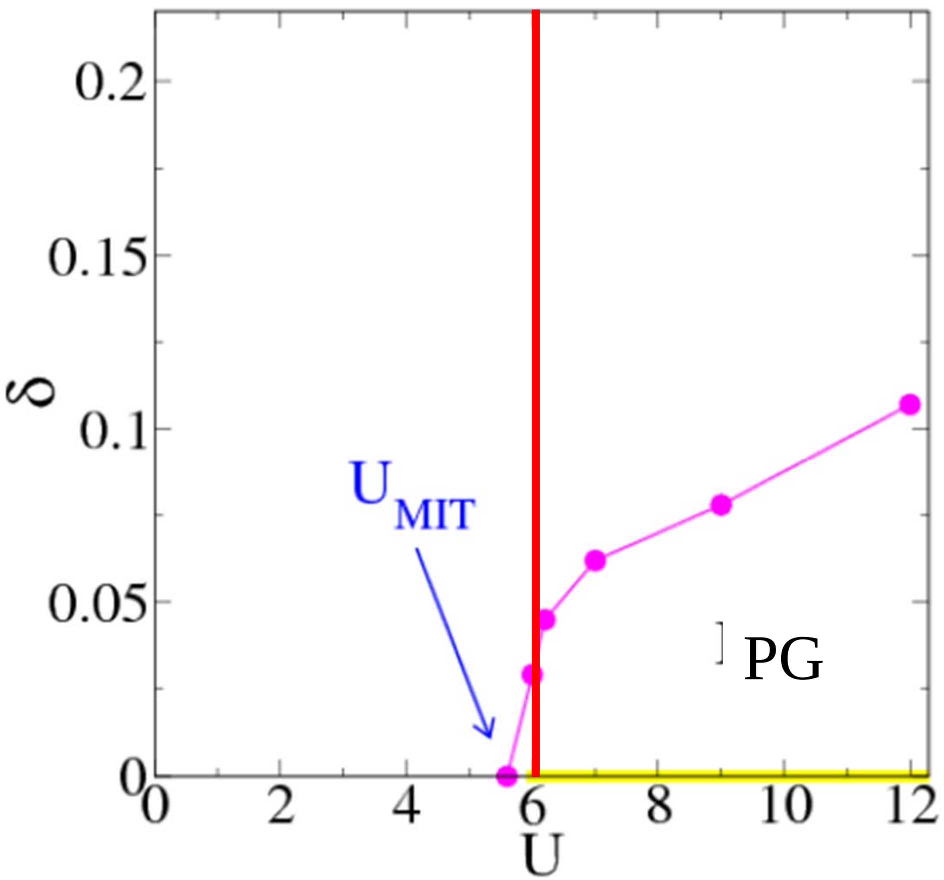
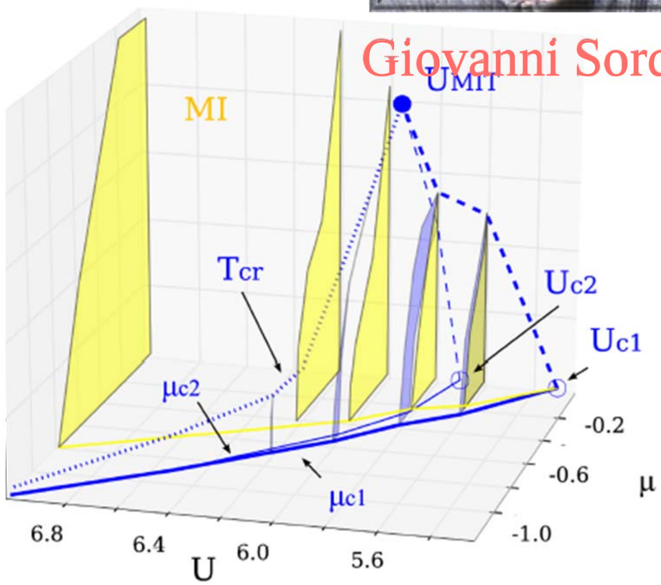
Another phase transition related to Mott

Focus near the Mott transition



Giovanni Sordi



G. Sordi, P. Sémon, K. Haule, and A.-M.S.T., PRL **104**, 226402 (2010); PRB **84**, 075161 (2011); Sci. Rep. **2**, 547 (2012); PRB **87**, 041101(R) (2013)

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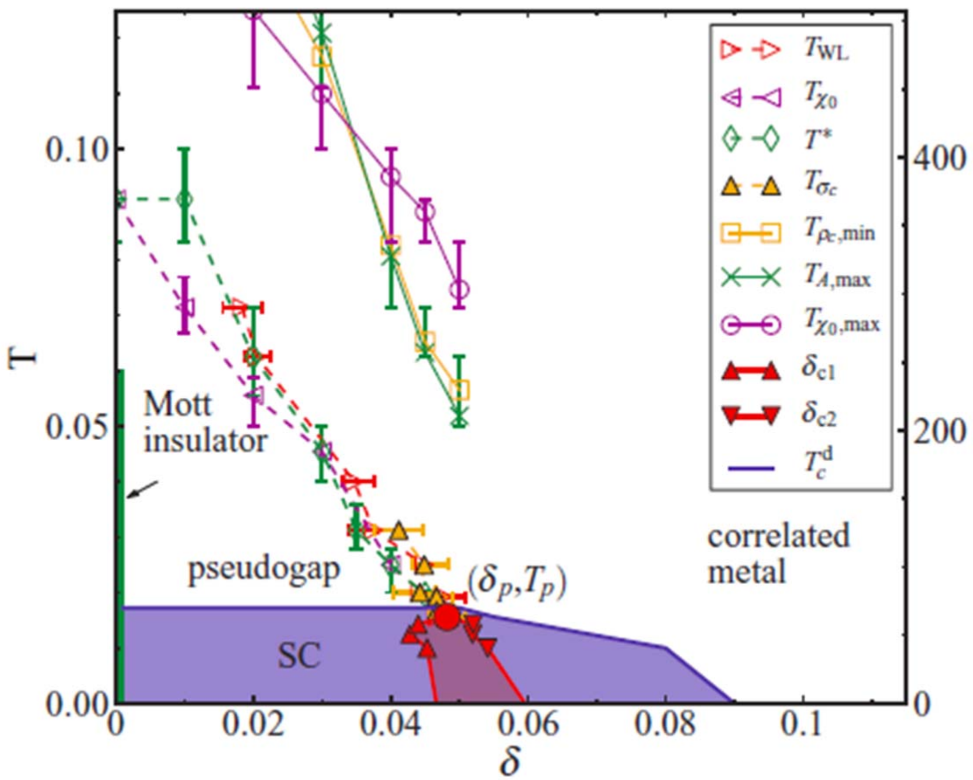
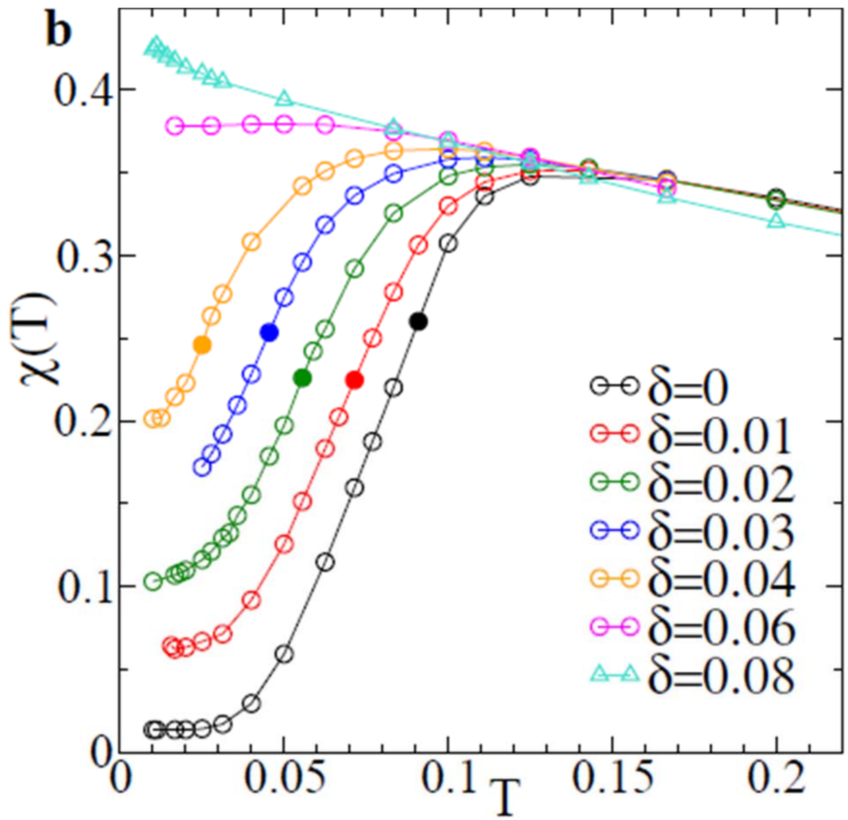
Widom line at end of finite-doping first-order transition

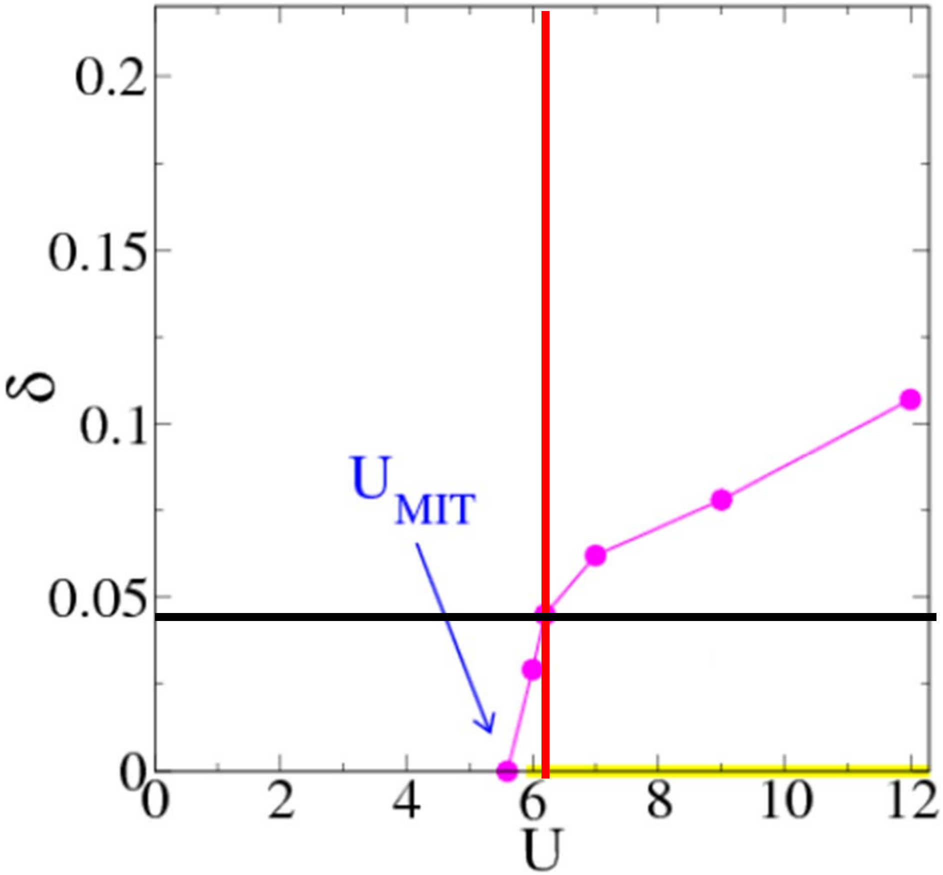


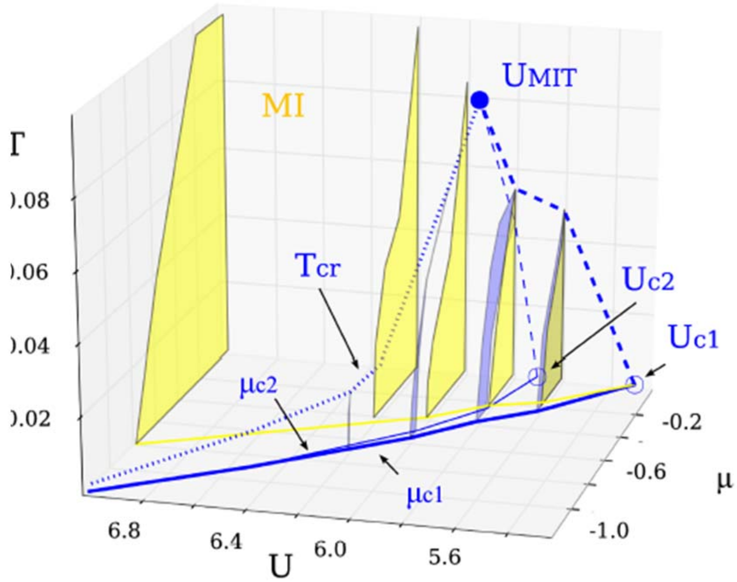


Sordi et al. PRL 108, 216401 (2012)
PRB **87**, 041101(R) (2013)

Link to Mott transition up to optimal doping

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





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G. Sordi, P. Sémon, K. Haule, and A.-M.S.T., PRL **104**, 226402 (2010);
PRB **84**, 075161 (2011); Sci. Rep. **2**, 547 (2012); PRB **87**, 010141 (R) (2013)

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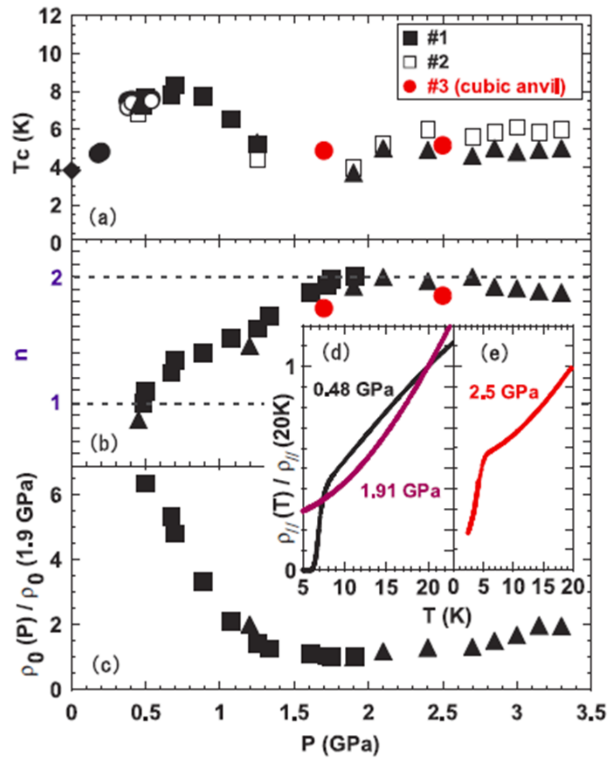
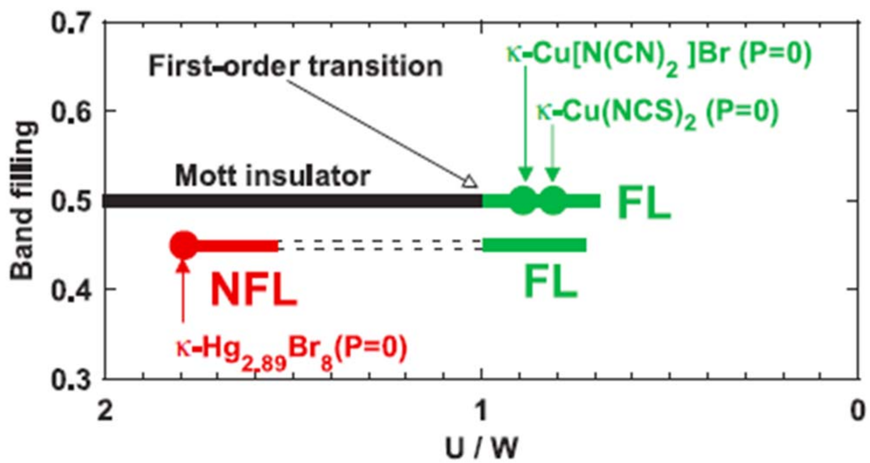
A doped BEDT organic



	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



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

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

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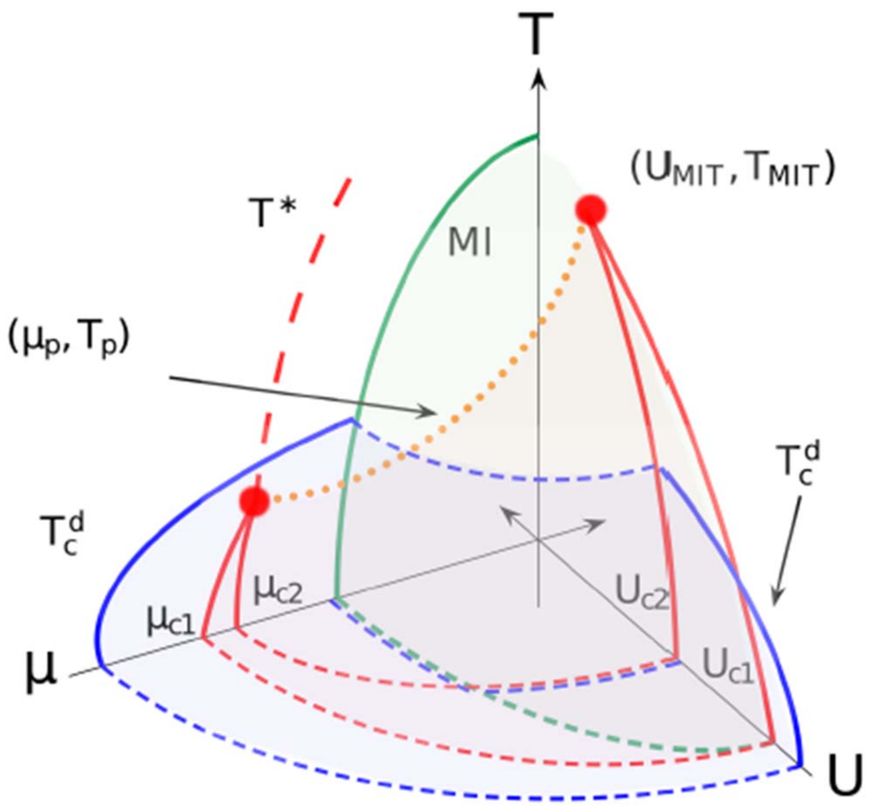
Unified phase diagram



G. Sordi, P. Sémon, K. Haule, and A.-M.S.T., PRL 108, 216401 (2012)

For SCR see: H. Kondo, T. Moriya J. Phys. Soc. Japan, **68**, 3170 (1999)

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Outline

- Model and method
  - $T=0$
  - Finite T
- Phase diagram: Organics and cuprates
  - $T = 0$
  - Finite T
- **The Mott critical point and critical exponents PII-36**

Patrick Sémon

Mott critical point

P. Sémon and A.-M.S. Tremblay,
PRB 85, 201101 (R) (2012)

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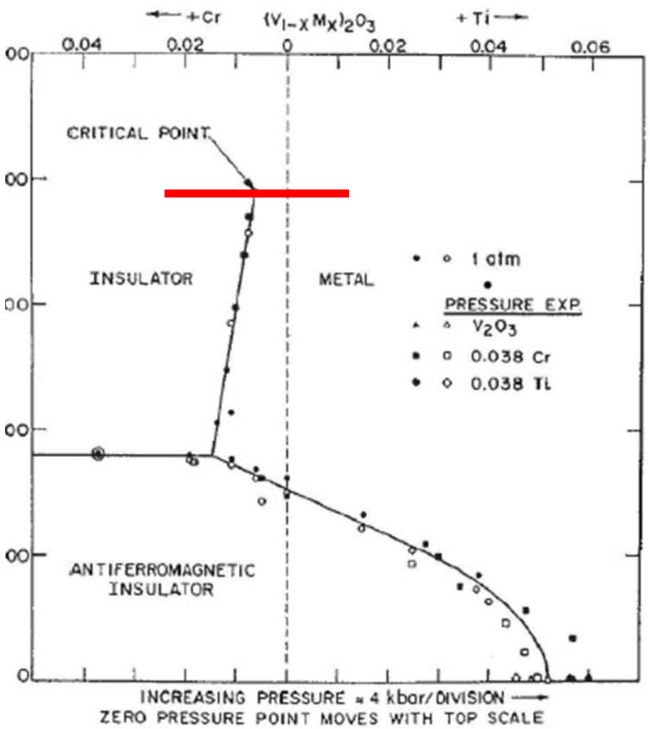
Critical behavior

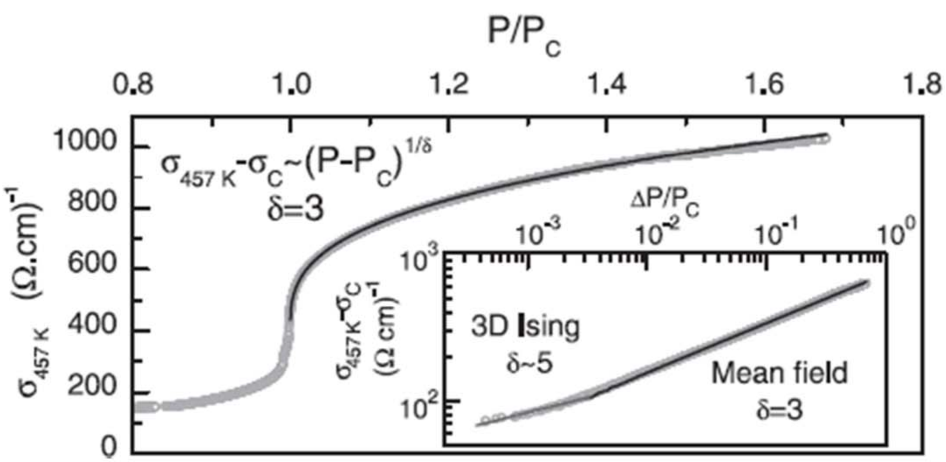
Universality and Critical Behavior at the Mott Transition
P. Limelette, *et al.*
Science **302**, 89 (2003);
DOI: 10.1126/science.1088386



McWhan, PRB 1970; Limelette, Science 2003

Double occupancy: Ising universality class

C. Castellani et al., Phys. Rev. Lett. **43**, 1957 (1979).
G. Kotliar, et al. Phys. Rev. Lett. **84**, 5180 (2000).
Limelette et al. Science (2003)



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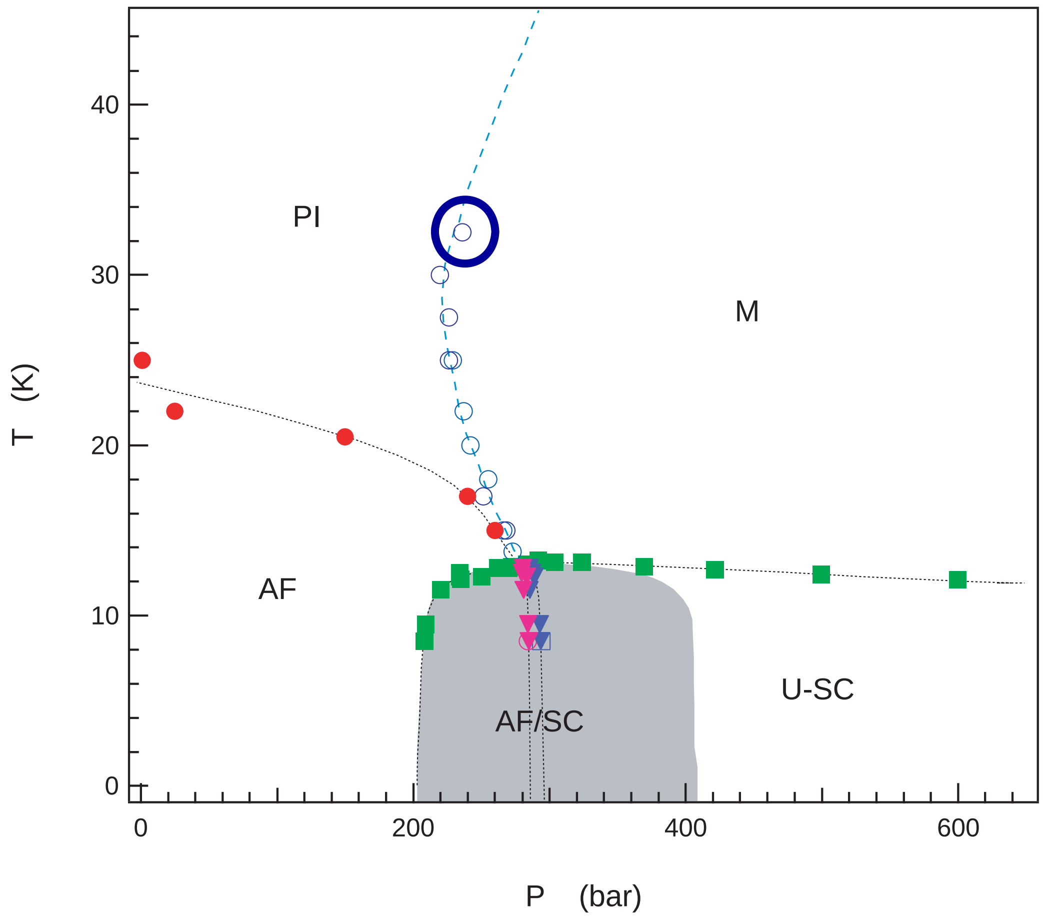
Mott critical point in layered organics



What is the critical behavior?

Phase diagram BEDT-X

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

S. Lefebvre et al. PRL **85**, 5420 (2000),

P. Limelette, et al. PRL **91** (2003)

F. Kagawa, K. Miyagawa, + K. Kanoda

PRB **69** (2004) +Nature **436** (2005)

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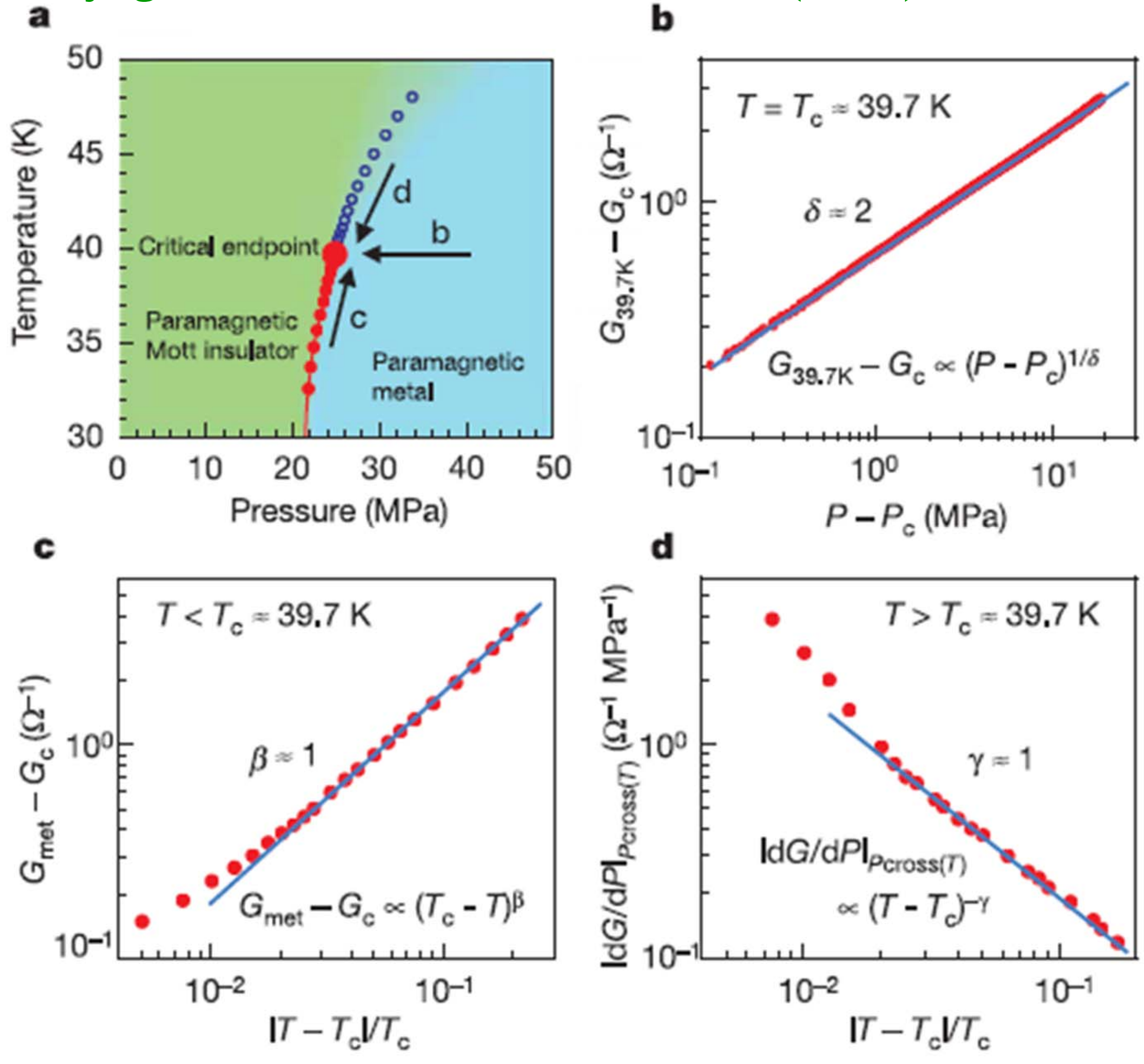
Surprising critical behavior

Kagawa, Miyagawa, Kanoda, Nature **436,** 534 (2005), Nature Physics **5,** 880 (2009)



$$\delta = 1 + (\gamma/\beta)$$

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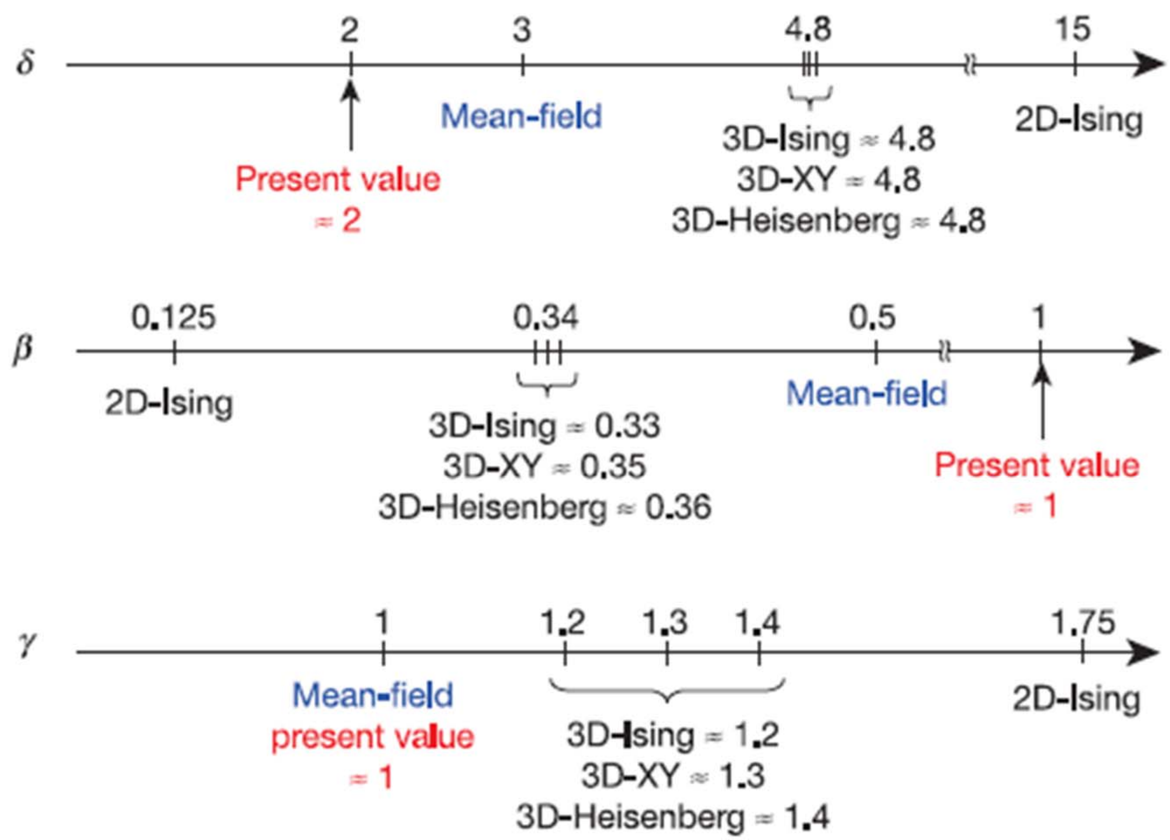
Unconventional behavior

Unconventional critical behaviour in a quasi-two-dimensional organic conductor

Nature
436, 534 (2005)

F. Kagawa[1], K. Miyagawa[1,2] & K. Kanoda[1,2]



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Possible explanations

M. Imada, Phys. Rev. B **72**, 075113 (2005).
M. Imada, et al. J. Phys.: Condens.Matter **22**, 164206 (2010).

S. Papanikolaou, R. M. Fernandes, E. Fradkin, P. W. Phillips, J. Schmalian, and R. Sknepnek, Phys. Rev. Lett. **100**, 026408 (2008).

Numerical results

P. Sémon and A.-M.S.T. PRB **85**, 201101(R)

P. Sémon and A.-M.S.T. PRB **85**, 201101(R)

The method

Cellular dynamical mean-field theory

Continuous-time quantum Monte Carlo

Hybridization expansion

P. Werner, et al., Phys. Rev. Lett. **97**, 076405 (2006).
P. Werner and A. J. Millis, Phys. Rev. B **74**, 155107 (2006).
E. Gull, et al., Rev. Mod. Phys. **83**, 349 (2011).
K. Haule, Phys. Rev. B **75**, 155113 (2007).

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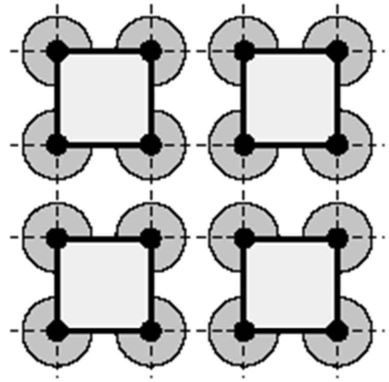
2d Hubbard: Quantum cluster method physics

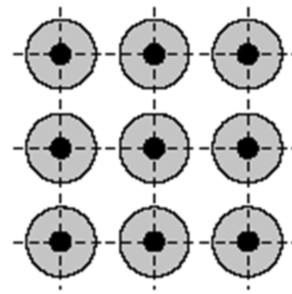
- Observed behavior is a transient from a QCP?

C-DMFT



- Quantum fluctuations
- Cluster necessary in *d* = *2* for
- Short-range spatial fluctuations

DMFT

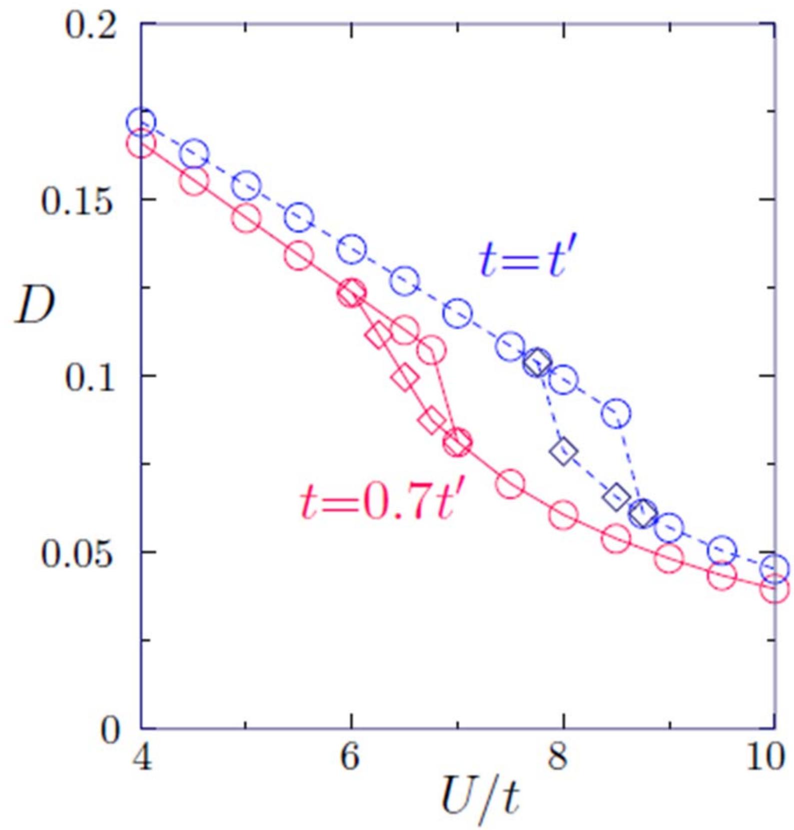


- Disantangle effects of J

- No low q spatial fluctuations

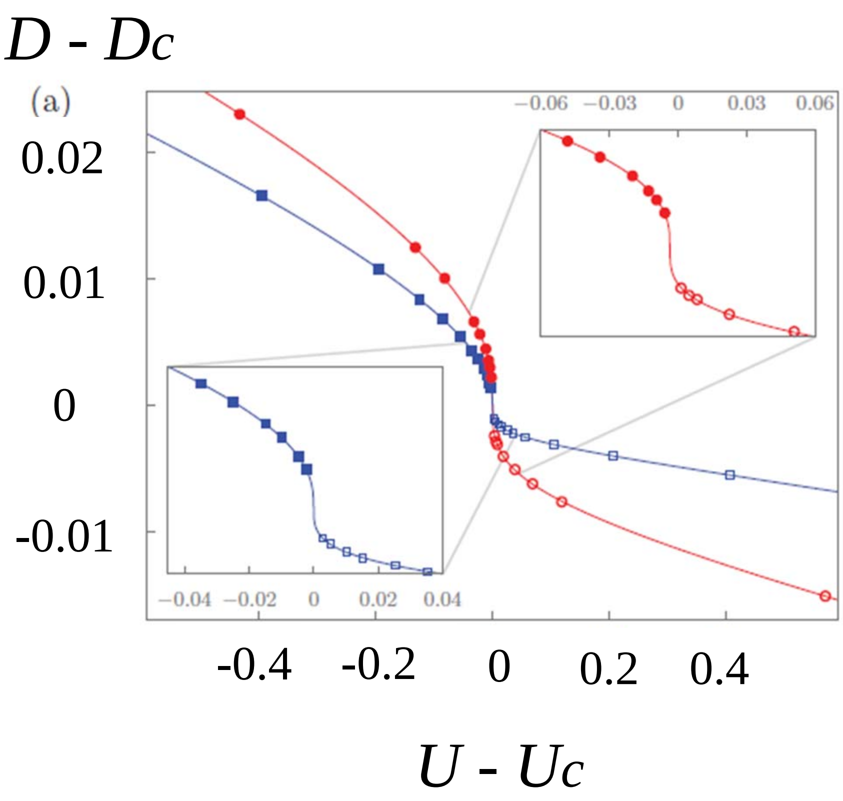
REVIEWS
Maier, Jarrell et al., RMP. (2005)
Kotliar *et al.* RMP (2006)
AMST *et al.* LTP (2006)

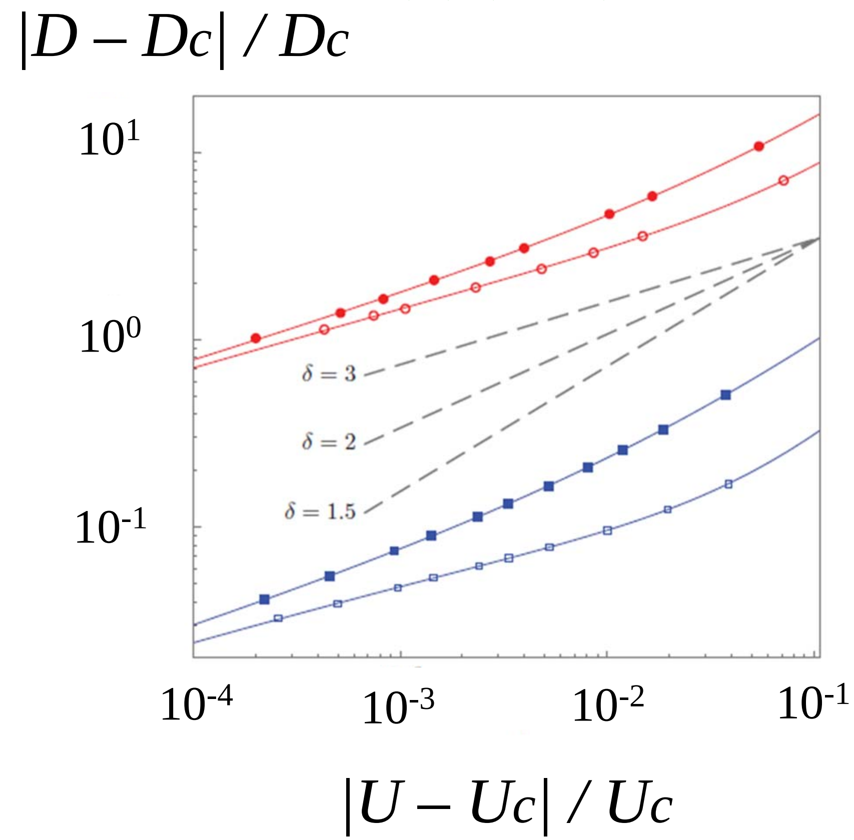
Mott transition, jump in double occupancy



Double occupancy (δ)

- P. Sémon and A.-M.S. Tremblay, PRB 85, 201101 (R) (2012)





Red circles: CDMFT

Blue squares: single-site DMFT

Subleading corrections to mean-field

$\delta = 3$ Kotliar et al. PRL **84**, (2000)

$$\alpha\eta + c\eta^3 = h$$

$$\alpha = \alpha_1(U - U_c) + \alpha_2(T - T_c)$$

$$\alpha_1(U - U_c)\eta + c\eta^3 = h_1(U - U_c)$$

$$\eta = \sum_{i=1}^{\infty} \delta U^{i/3} \eta_i$$

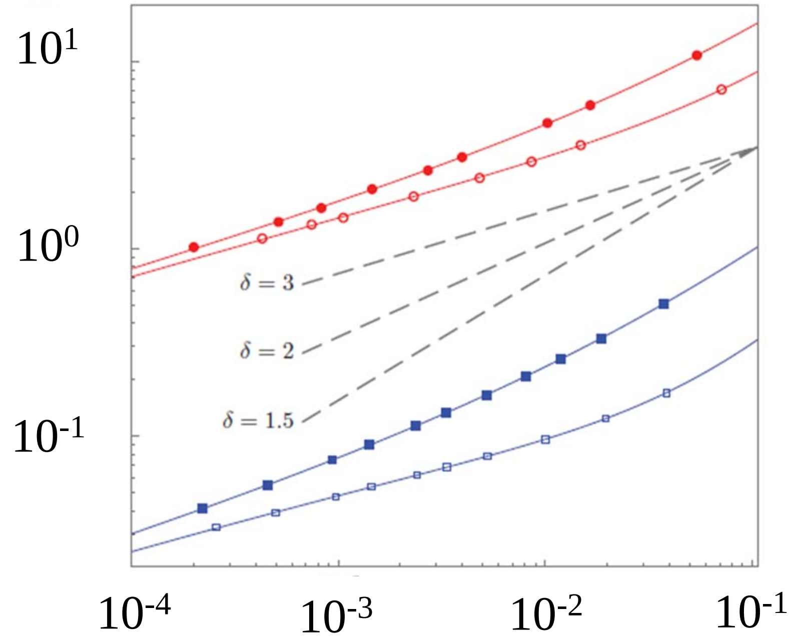
$$D = D_c + a_1\eta + a_2\eta^2$$

$$D - D_c = c_1 \,\mathrm{sgn}(\delta U)|\delta U|^{1/\delta} + c_2|\delta U|^{2/\delta} + c_3\delta U$$

- P. Sémon and A.-M.S. Tremblay, PRB 85, 201101 (R) (2012)

Double occupancy (δ)

$|D - D_c| / D_c$



$|U - U_c| / U_c$

Kotliar et al. PRL **84**, (2000)

$$D - D_c = c_1 \operatorname{sgn}(\delta U)|\delta U|^{1/\delta} + c_2|\delta U|^{2/\delta} + c_3 \delta U$$

Red circles: CDMFT $\delta = 3.04 \pm 0.25$

Blue squares: single-site DMFT $\delta = 2.93 \pm 0.15$

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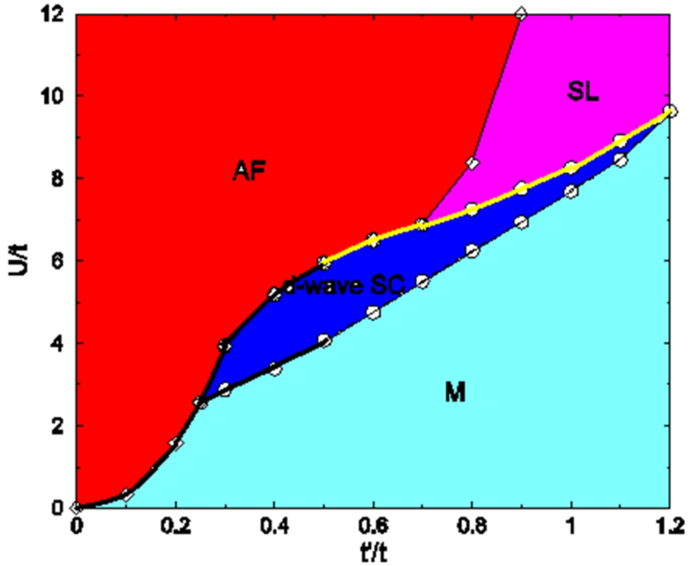
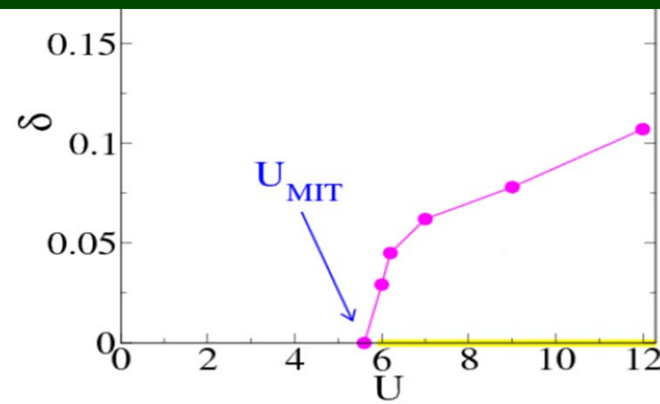
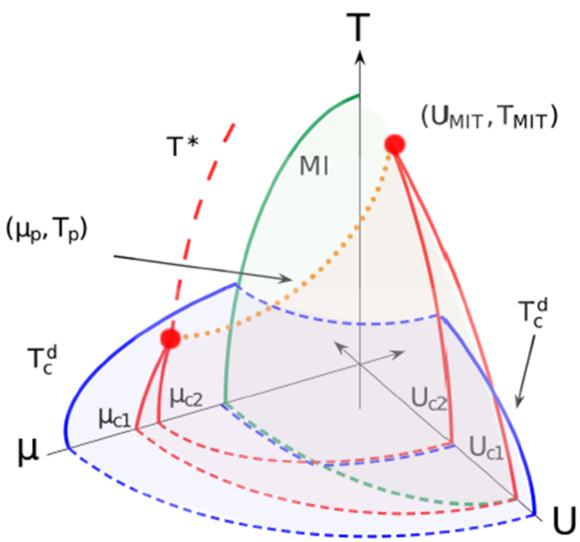
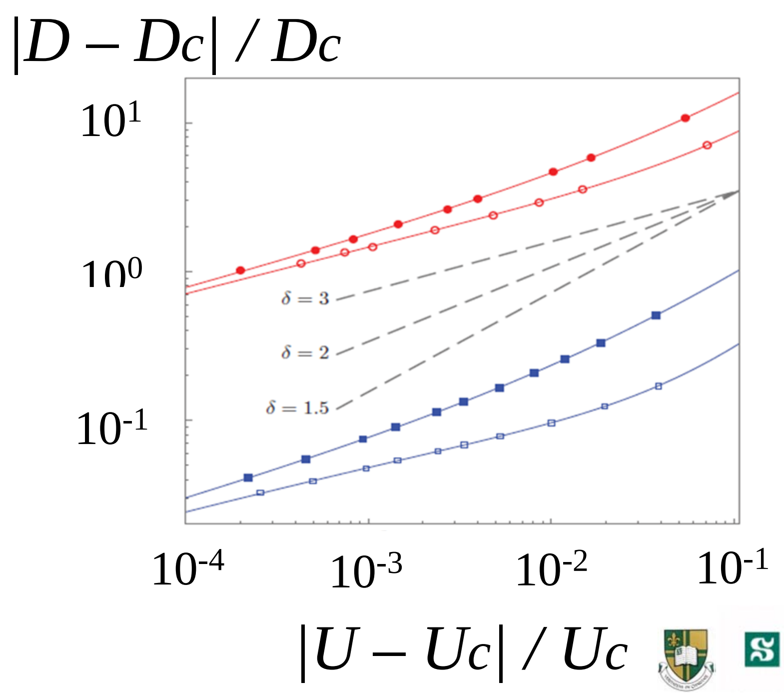
Summary









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Mammouth

Éducation, Loisir et Sport
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Merci

Thank you