T19. 1 : Importance of subleading corrections for the Mott critical point

8:00 AM–8:12 AM

A.-M. Tremblay

Patrick Sémon

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UNIVERSITÉ DE SHERBROOKE

VERITATEM IN CHARITATE

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APS-Baltimore, 21 March 2013

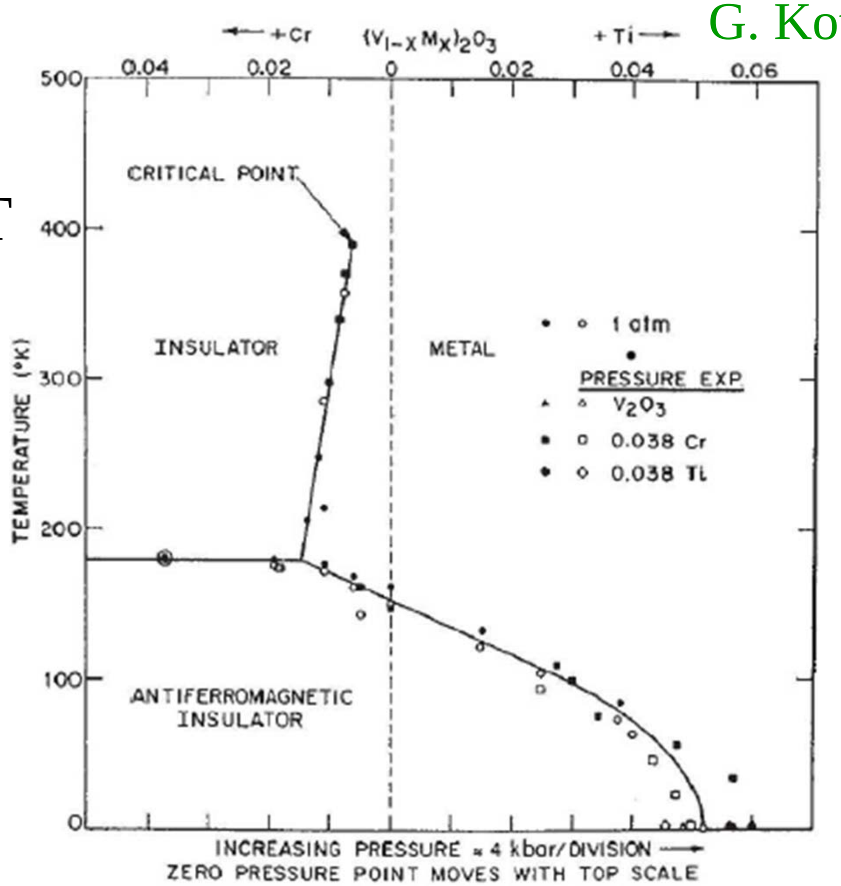
« Conventional » Mott transition

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).

T

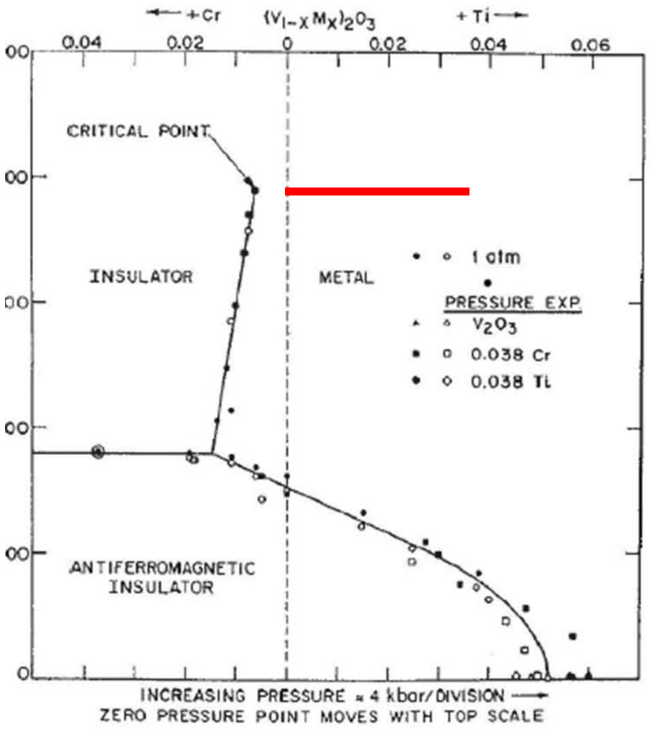


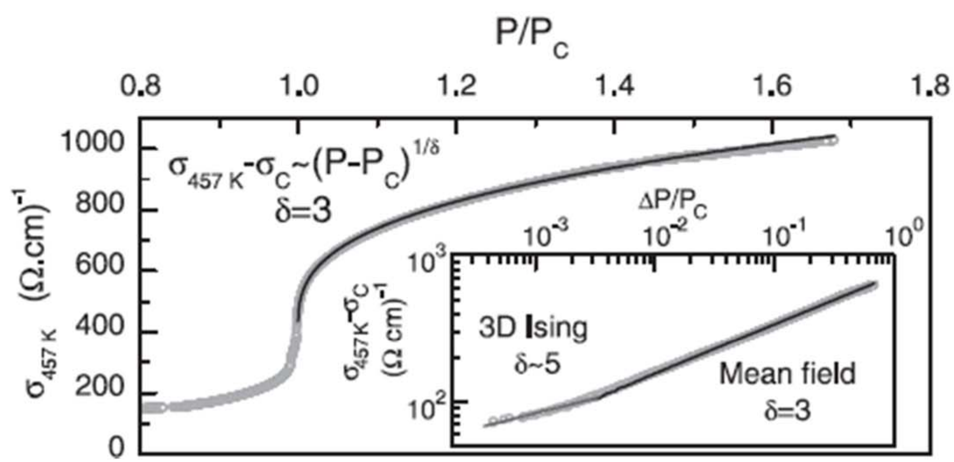
V_2O_3

Figure: McWhan, PRB 1970; Limelette, Science 2003

Critical behavior

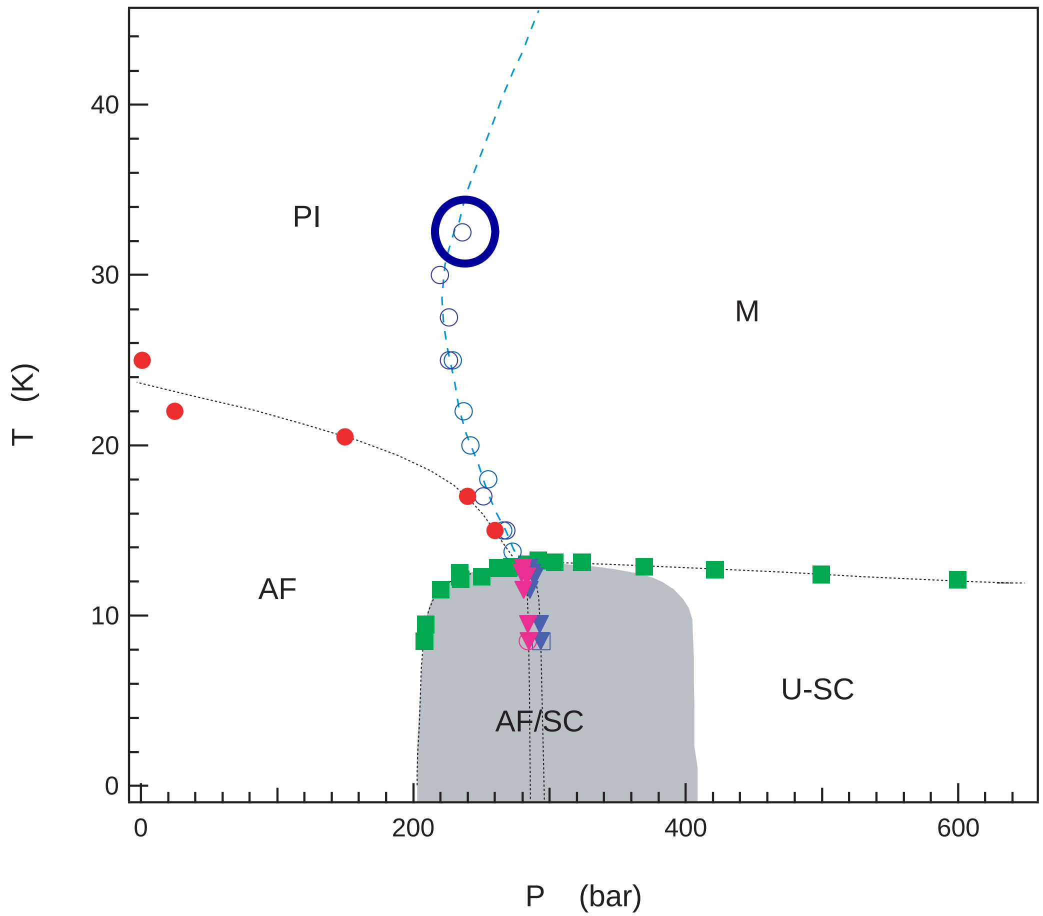
Universality and Critical Behavior at the Mott Transition
P. Limelette, *et al.*
Science **302**, 89 (2003);
DOI: 10.1126/science.1088386





McWhan, PRB 1970; Limelette, Science 2003

Mott critical point in layered organics



THIS TALK

What is the critical behavior?

Phase diagram BEDT-X

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

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

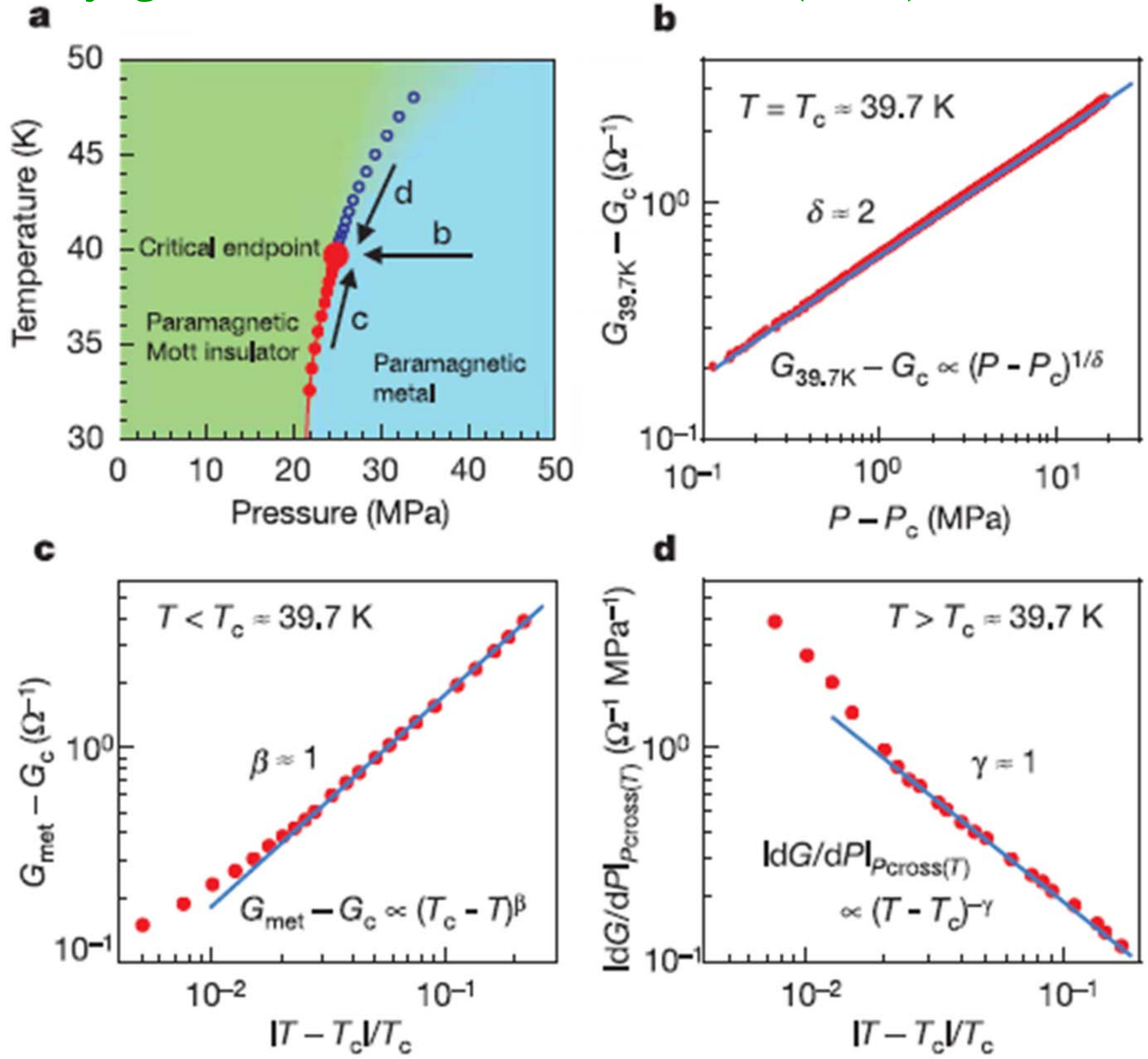
P. Limelette, et al. PRL **91** (2003)

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

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

Surprising critical behavior

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



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

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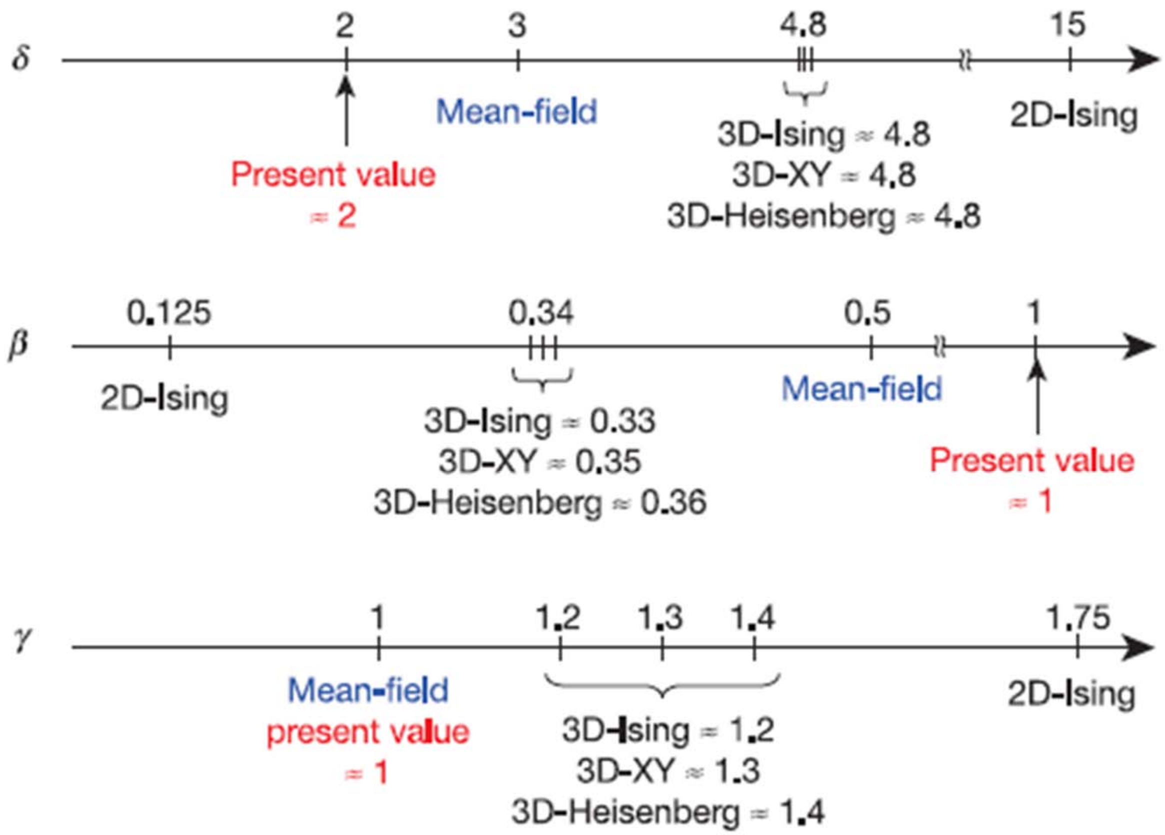
Unconventional behavior

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

Nature
436, 534 (2005)

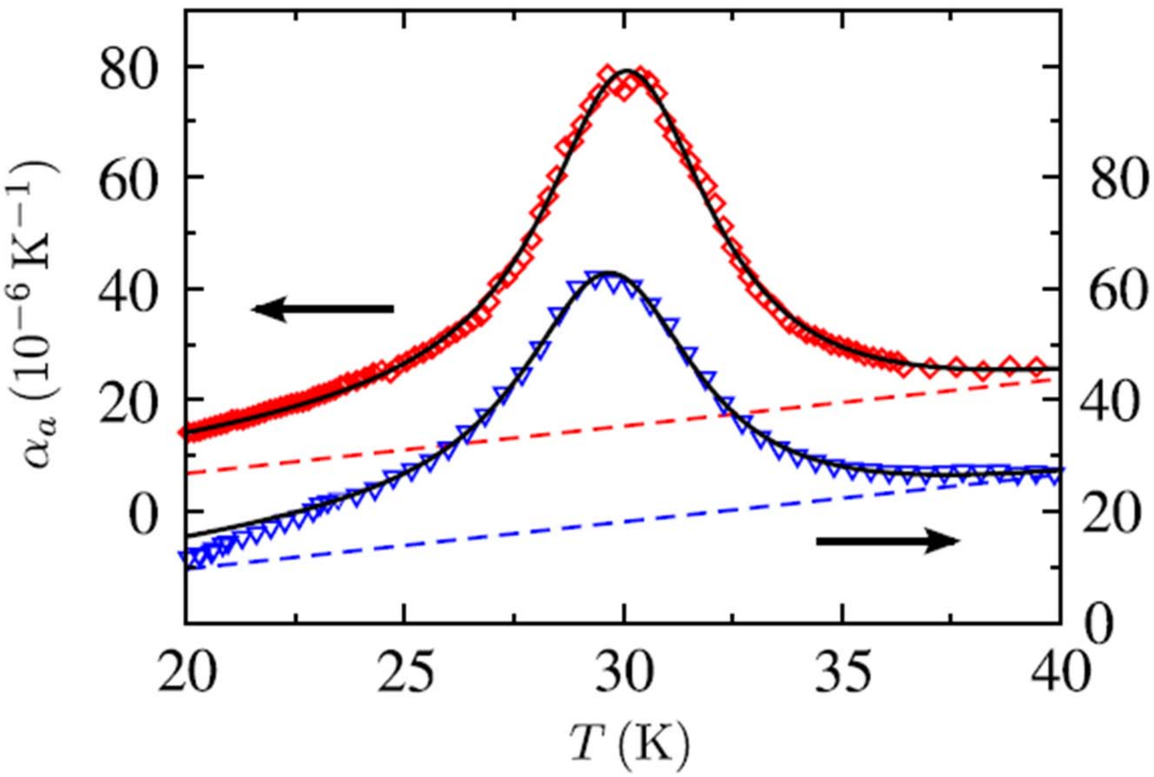
F. Kagawa[1], K. Miyagawa[1,2] & K. Kanoda[1,2]



However, Ising for thermal expansion (Br ion)

M. de Souza et al., Phys. Rev. Lett. **99**, 037003 (2007)
L. Bartosch, M. de Souza, and M. Lang, Phys. Rev. Lett. **104**, 245701 (2010).

Ising



Possible explanations

Control by a $T = 0$ marginal QCP

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

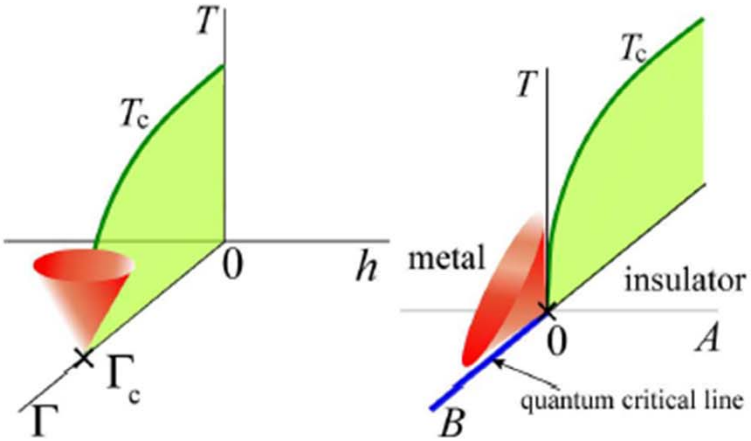


Figure 1. Phase diagram around conventional QCP (a)(left panel), and MQCP (b) (right panel for metal-insulator transition) in the parameter space of temperature T, fields to control transitions h or A and parameters to control quantum fluctuations Γ or B. The cone structures schematically illustrate the quantum critical regions of the QCP (a) and MQCP (b) depicted by the crosses. First-order transitions occur when one crosses shaded (green) walls. Quantum critical line (bold (blue) line) in (b) represents continuous topological transition at $T = 0$.

Coupling to the energy density instead of OP

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

$$\sigma \propto \eta^{\theta}$$

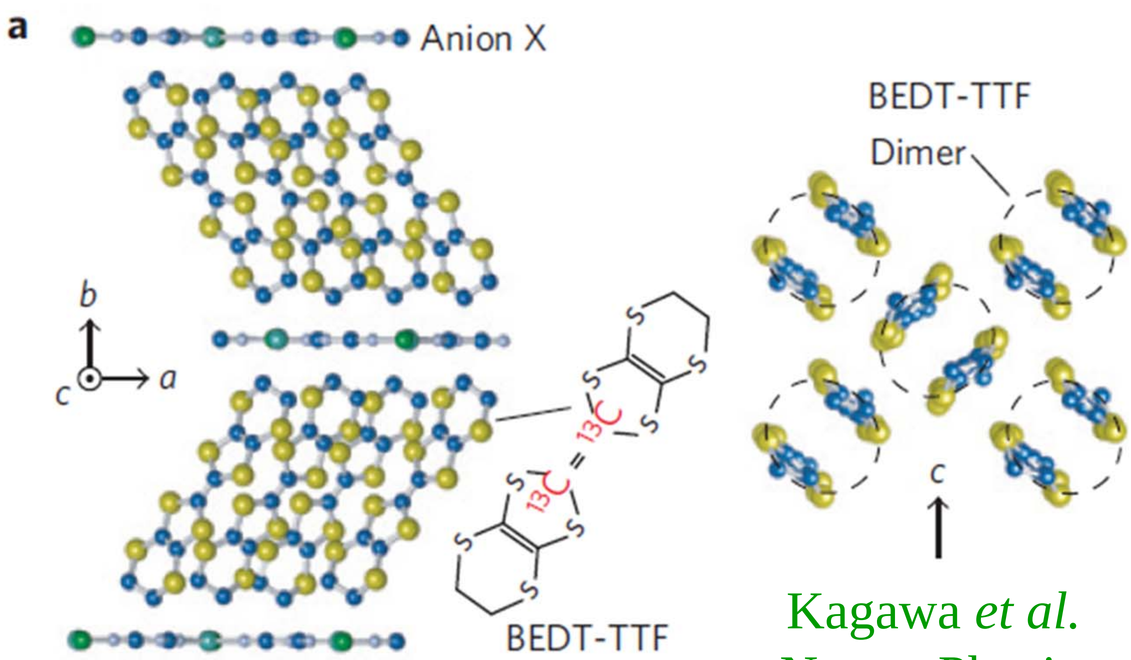
$$\theta = (1 - \alpha)/\beta$$

$$(\beta_\sigma, \gamma_\sigma, \delta_\sigma) = (1, \tfrac{7}{8}, \tfrac{15}{8})$$

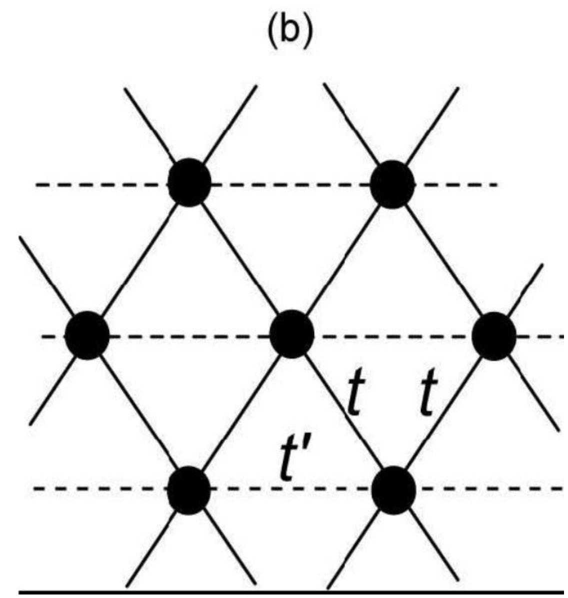
The model

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)



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

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

$t'/t \sim 0.6 - 1.1$

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

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PHYSICAL REVIEW B **85**, 201101(R) (2012)

Importance of subleading corrections for the Mott critical point

Patrick Sémon[1] and A.-M. S. Tremblay[1,2]

The method

Cellular dynamical mean-field theory

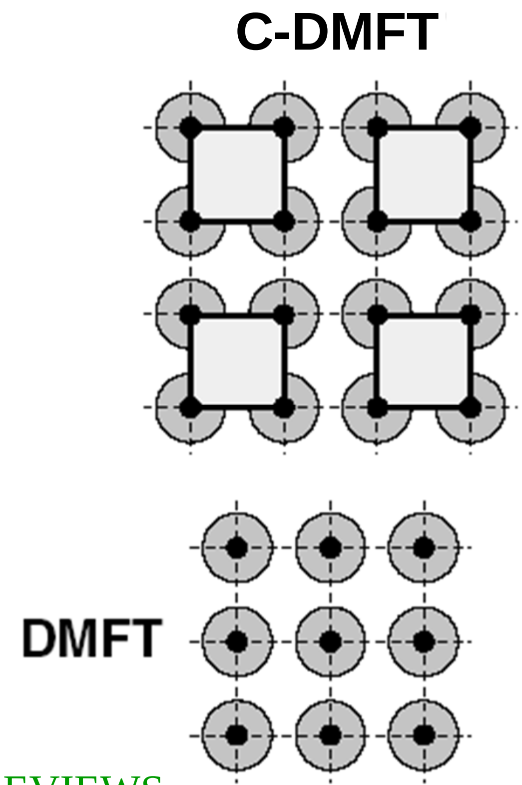
Continuous-time quantum Monte Carlo

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).

2d Hubbard: Quantum cluster method physics

- Observed behavior is a transient from a QCP?
- Quantum fluctuations
- Cluster necessary in *d* = *2* for
- Short-range spatial fluctuations
- 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)

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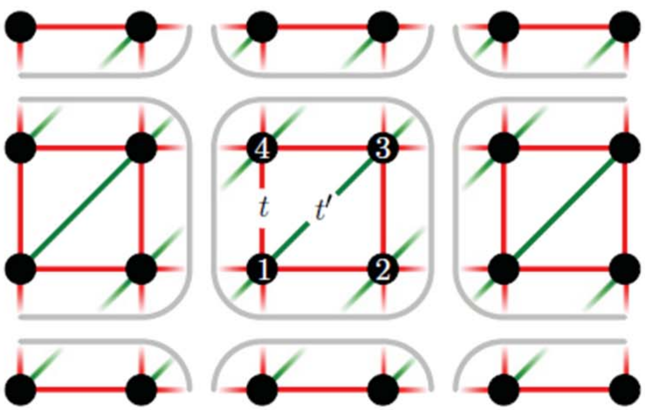
Reducing the sign problem

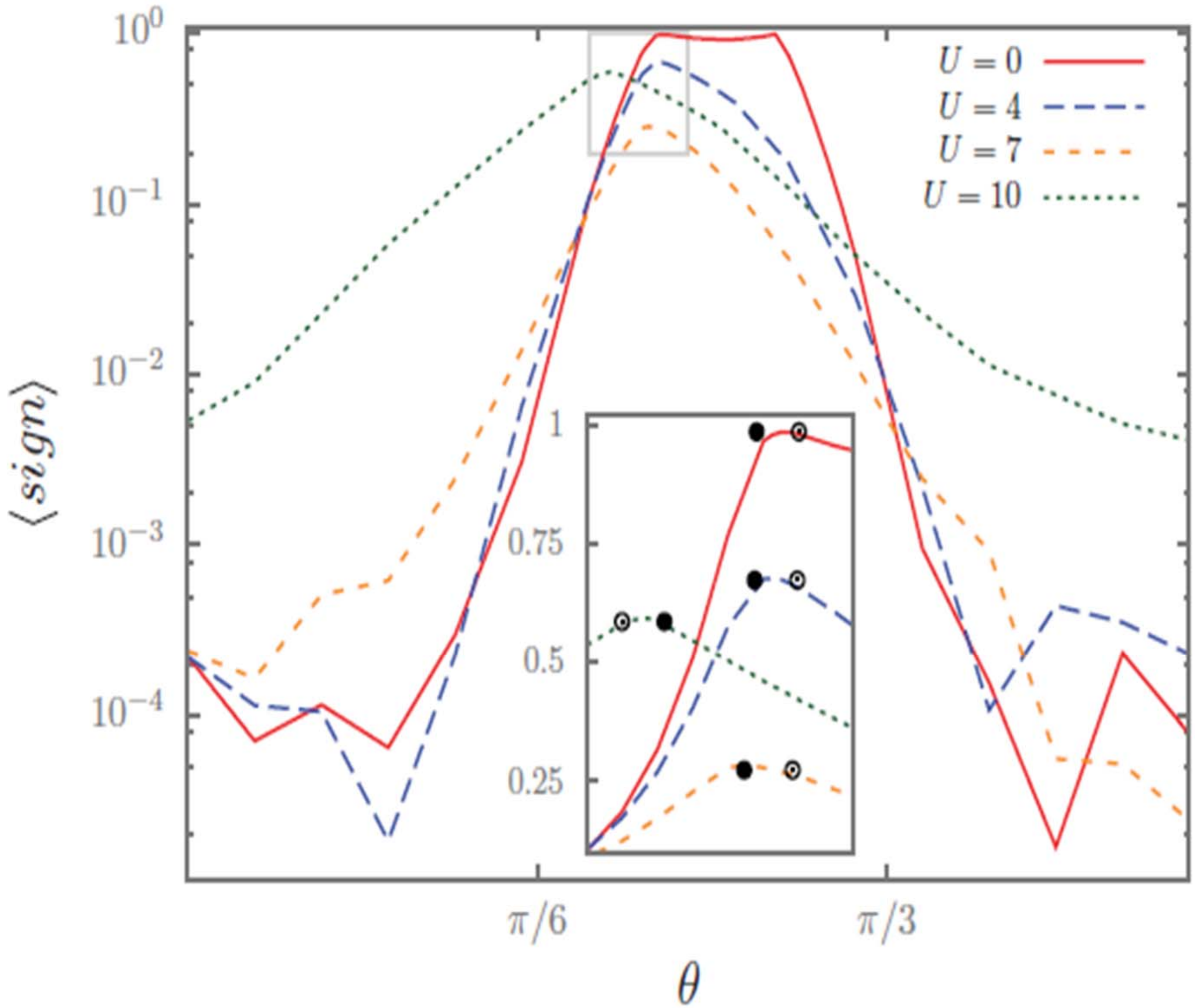
$$\cos\theta c'_{A_1\sigma} - \sin\theta c_{A_1\sigma}, \quad \sin\theta c'_{A_1\sigma} + \cos\theta c_{A_1\sigma}$$



$t'/t = 0.8$

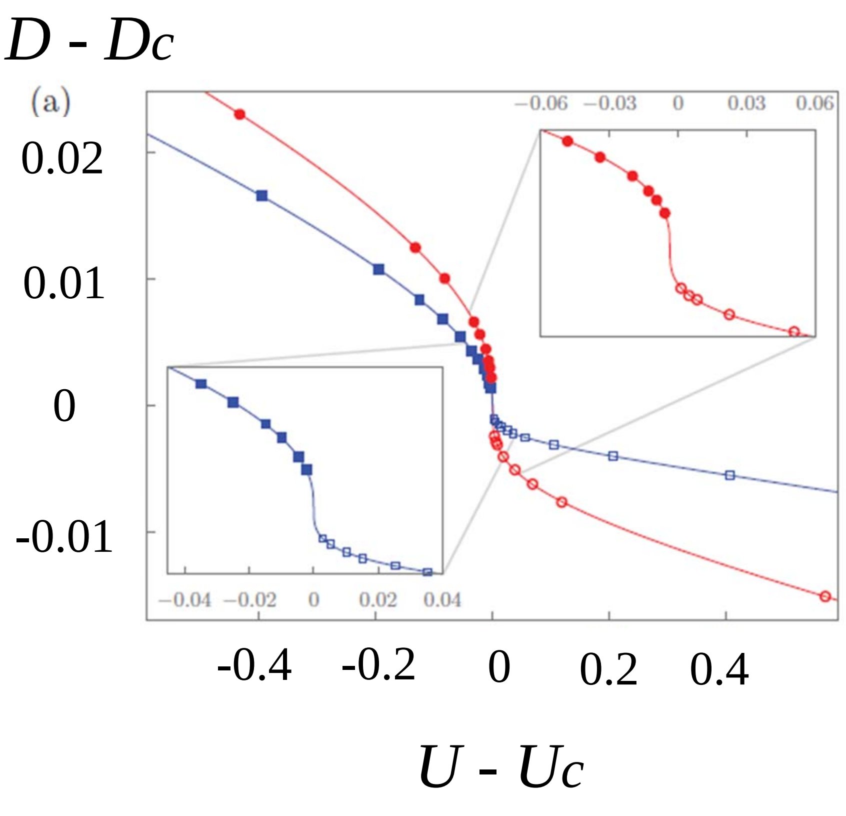
C_{2v}

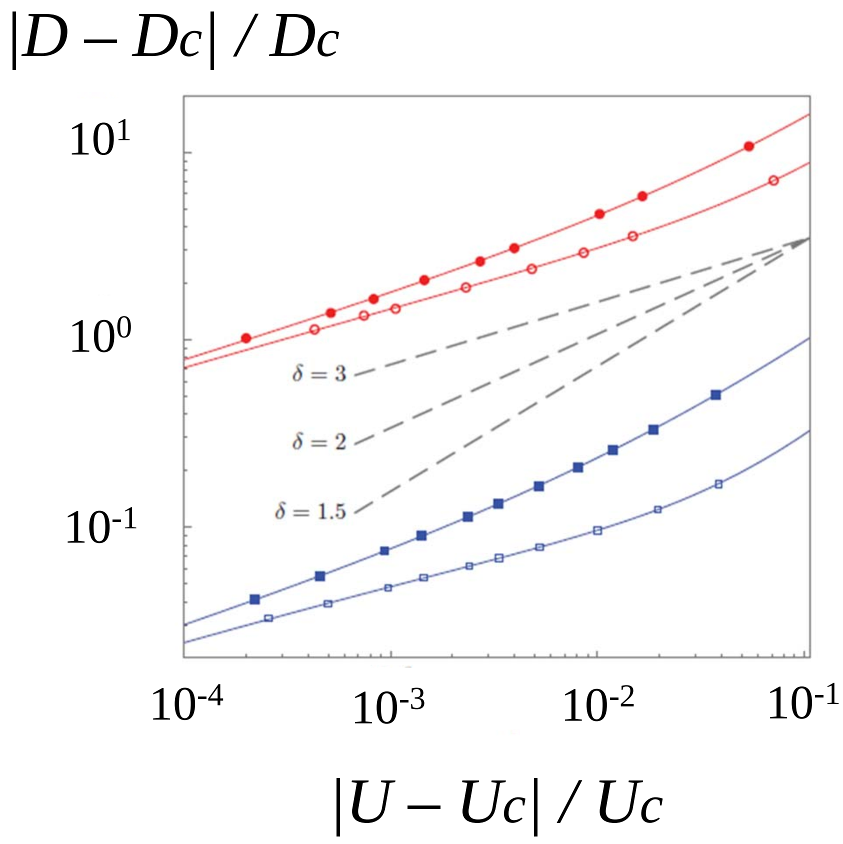
$2A_1, B_1, B_2$



Numerical results

Double occupancy (δ)

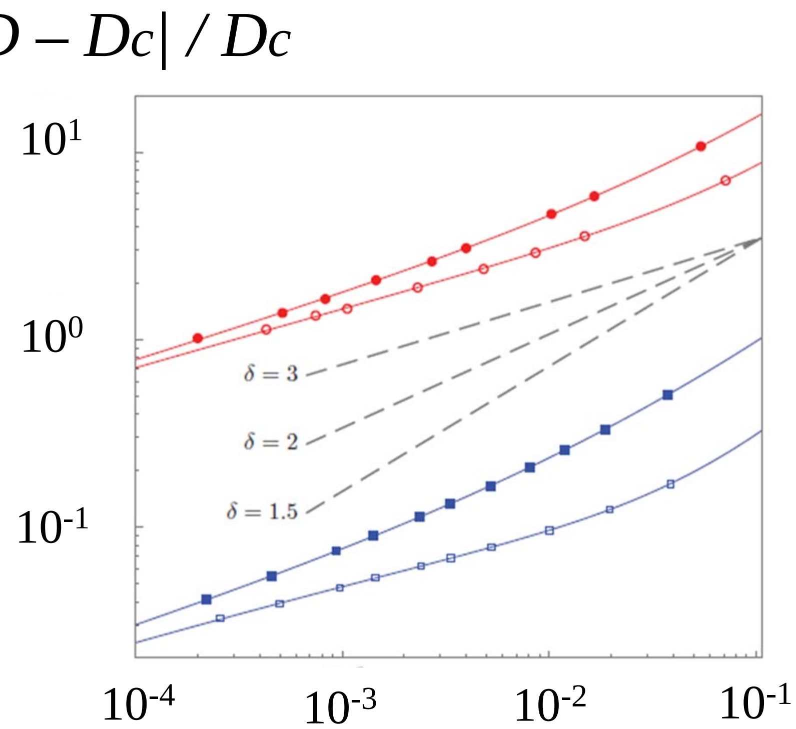




Red circles: CDMFT

Blue squares: single-site DMFT

Double occupancy (δ)



$|U - U_c| / U_c$

M. Sentef, P. Werner, E. Gull, and A. P. Kampf, Phys. Rev. B **84**, 165133 (2011).

Fit with single exponent: δ = 2

Red circles: CDMFT

Blue squares: single-site DMFT : Should give δ = 3

PHYSICAL REVIEW B **85**, 201101(R) (2012)

Importance of subleading corrections for the Mott critical point

Patrick Sémon[1] and A.-M. S. Tremblay[1,2]

Importance of subleading corrections

Subleading corrections to mean-field

VOLUME 84, NUMBER 22 PHYSICAL REVIEW LETTERS 29 MAY 2000

Landau Theory of the Finite Temperature Mott Transition

G. Kotliar,[1] E. Lange,[1] and M. J. Rozenberg[2]

$$p\eta + c\eta^3 = h. \qquad \delta = 3$$

$$p \equiv p_1 (U - U_c) + p_2 (T - T_c)$$

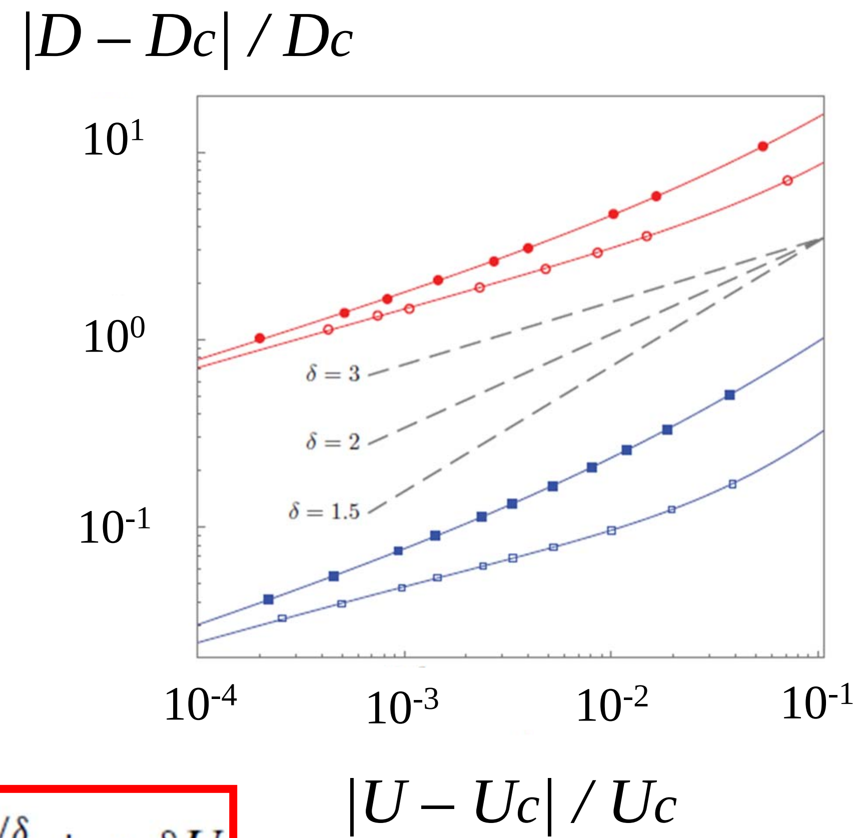
$$p_1 \delta U \eta + c\eta^3 = h_1 \delta U$$

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

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

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

Double occupancy (δ)



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

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

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

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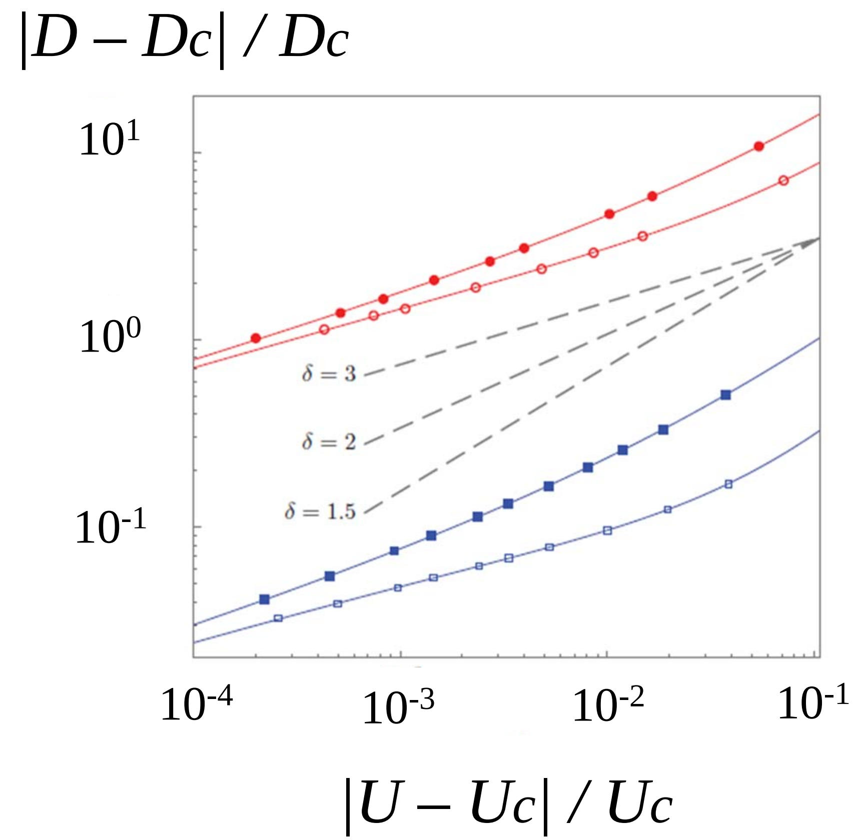
Conclusion

- Drastic reduction of sign problem allows:
- CDMFT and DMFT over almost three decades to give $\delta = 2$
  - If fit over whole range with one exponent.
  - Consistent with experiment.
- Incorrect. Indeed, know that $\delta = 3$ (mean field) in DMFT
  - Must take into account subleading corrections
  - Then, $\delta = 3$ better fits for both DMFT and CDMFT (with same number of parameters as $\delta = 2$)
  - Should reanalyze experiments



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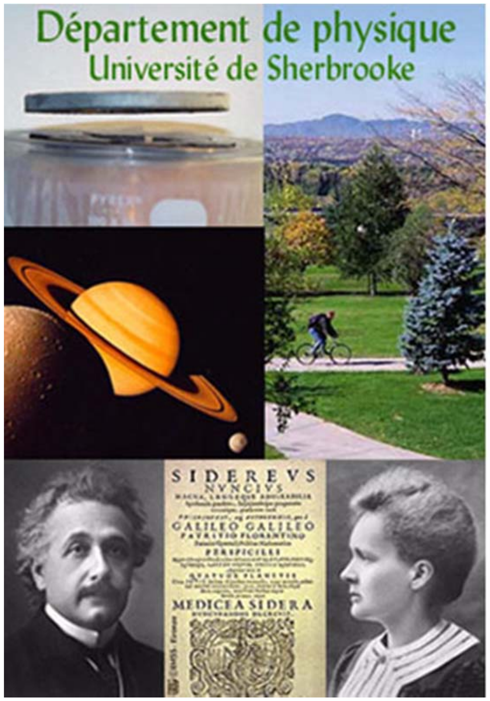

André-Marie Tremblay

CANADA RESEARCH CHAIRS
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Merci

Thank you

Comparisons to experiment

Charles-David Hébert

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FIG. 3. (Color online) Double occupancy as a function of U near the Mott critical point for the Hubbard model on an anisotropic triangular lattice with $t'/t = 0.8$ ($t \equiv 1$) at half filling and fixed critical inverse temperature $\beta = 11.15$ (squares) for DMFT and $\beta = 9.9$ (circles, shiftet by $\times 10^{1.5}$) for CDMFT on a 2×2 plaquette. The solid lines show a fit to $f(U) = c_1 \mathrm{sgn}(\delta U)|\delta U|^{1/\delta} + c_2|\delta U|^{2/\delta} + c_3\delta U + D_c$ ($\delta U \equiv U - U_c$) with the same parameters c_1, c_2, c_3, D_c, U_c, and δ for the metallic (filled symbols) and the insulating region (open symbols). The best fitting values (U_c, D_c, δ) are (10.445,0.0325,2.93) for DMFT and (7.932,0.0679,3.04) for CDMFT. (a) Linear plot centered at (U_c, D_c). The insets zoom on the regions close to the critical point. (b) Logarithmic plot in reduced units relative to the critical point with CDMFT data shifted by a factor of $10^{1.5}$ along the y axis. The dashed lines show the function $\propto|U - U_c|^{1/\delta}$ with δ as indicated. In the critical regime, up to 500 iterations are necessary for convergence in the iterative solution of the (C)DMFT equation. Once convergence is reached, we take the average over hundreds of iterations. Monte Carlo sweeps per iteration: 6×10^9 for DMFT and 10^9 for CDMFT.

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