Magnetism in low/finite dimensions
–
can DMFT be relevant?

Nils Blümer and Elena Gorelik, Univ. Mainz

Outline

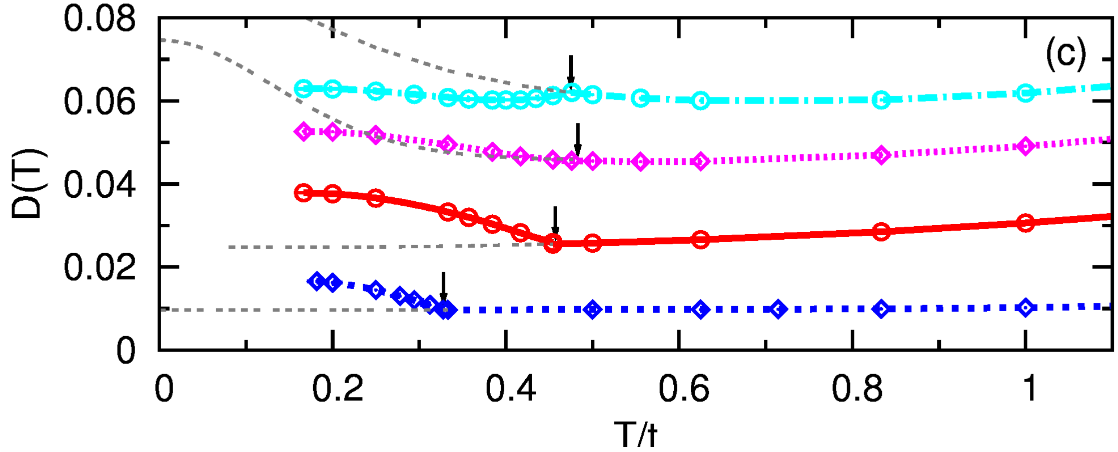
Modification of DMFT predictions by spatial fluctuations: how?

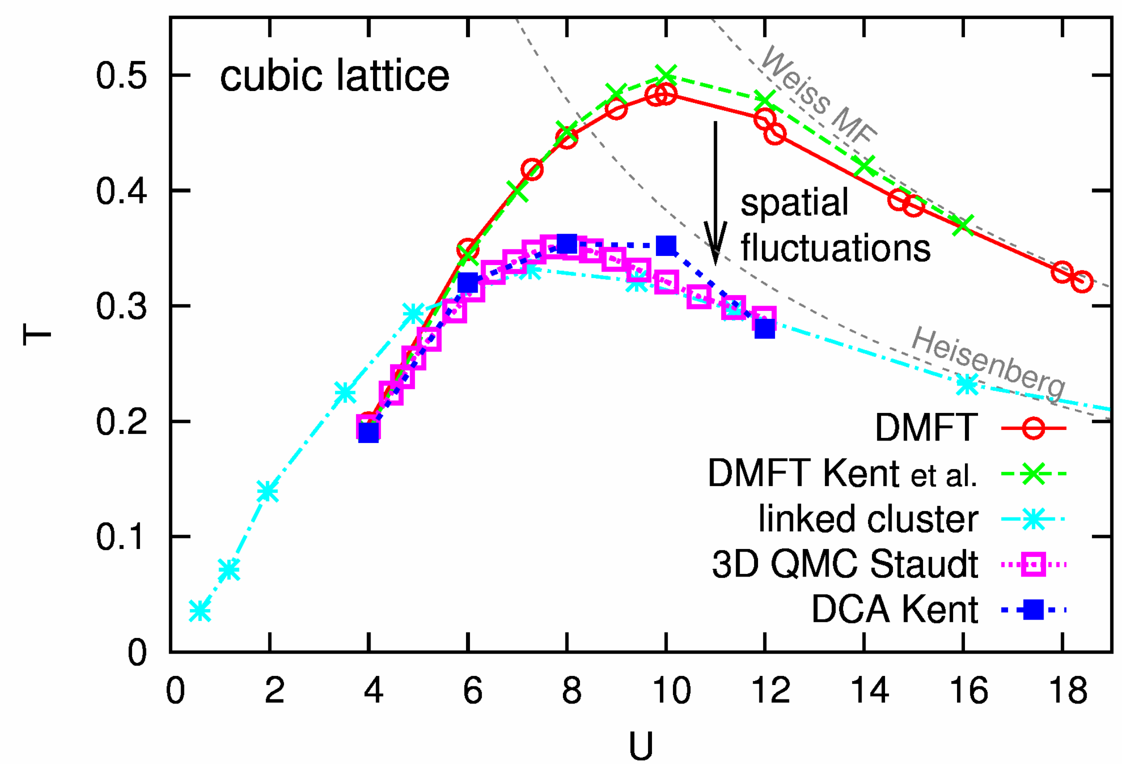
Antiferromagnetism in 2 dimensions at finite T?

How relevant is the Néel temperature?

Summary and outlook

Modification of DMFT predictions by spatial fluctuations in 3d: how?





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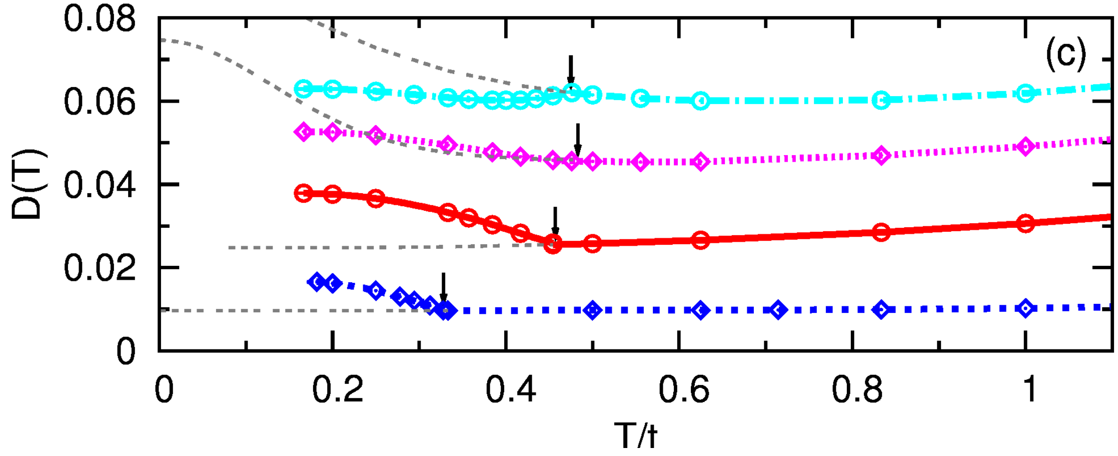

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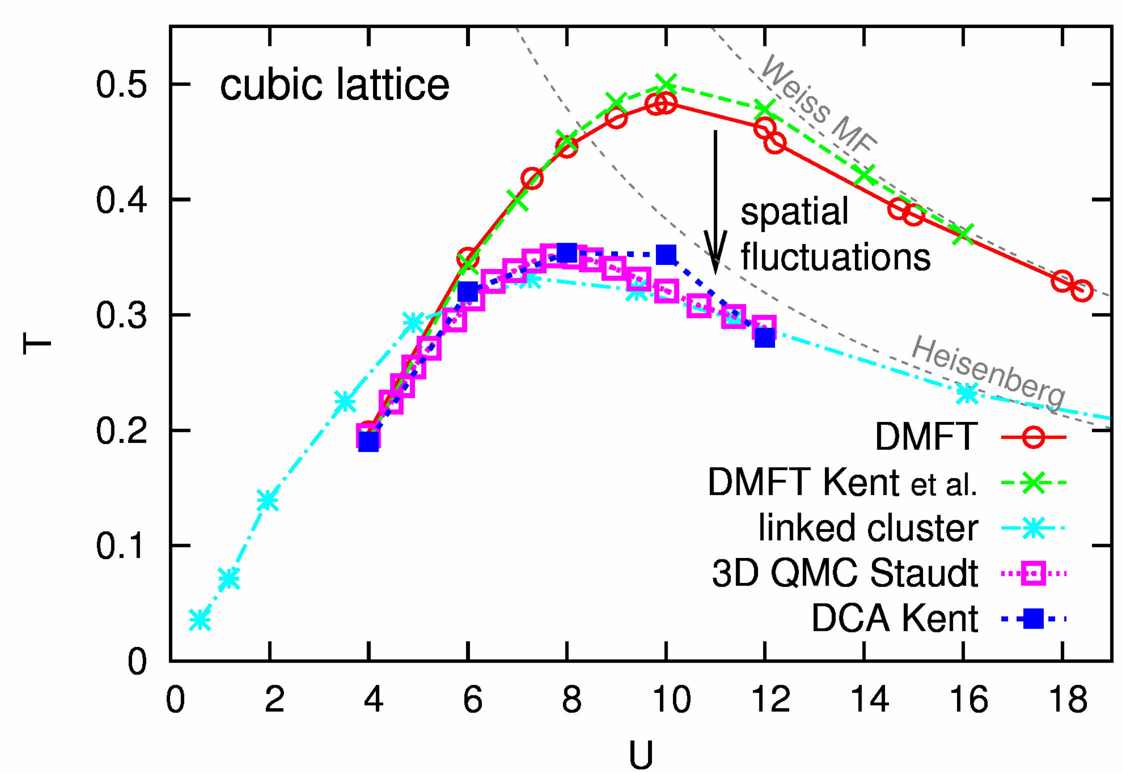

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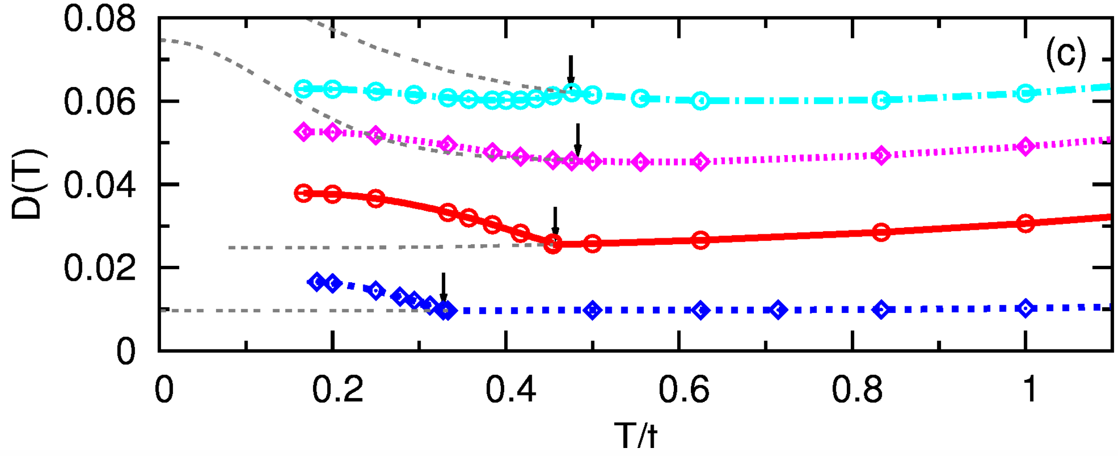

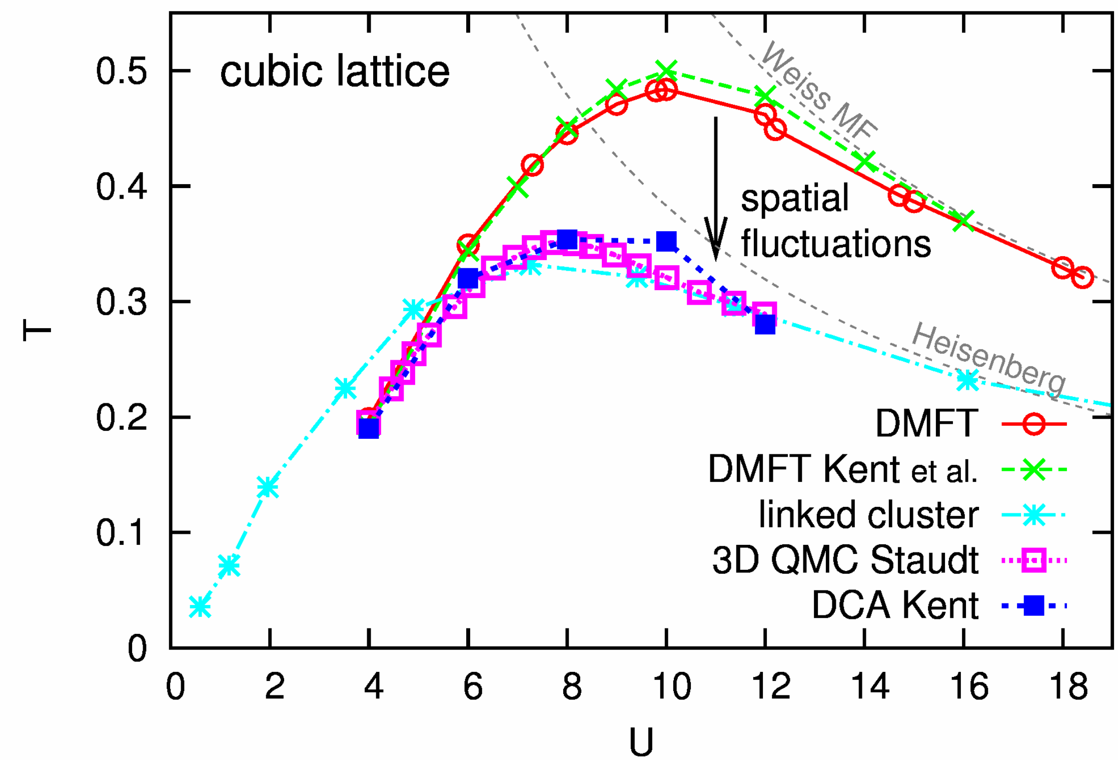

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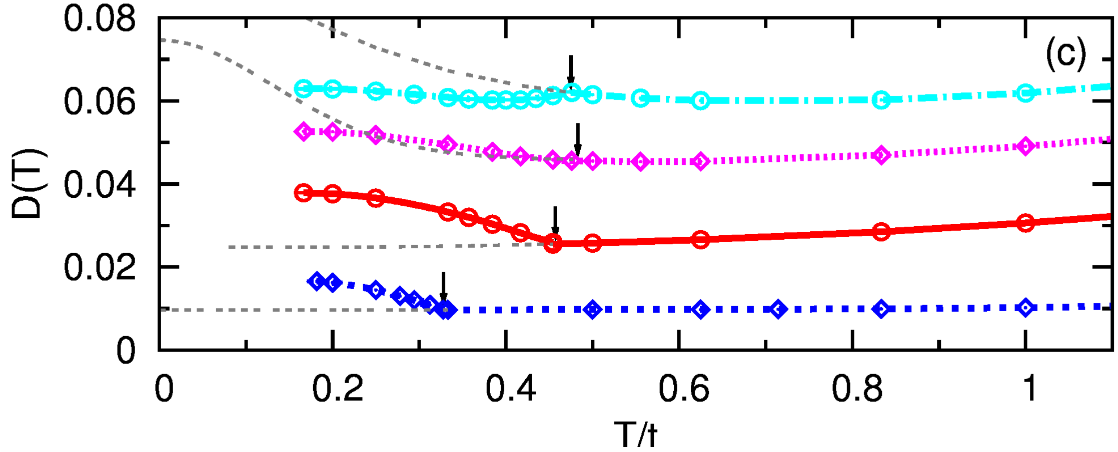

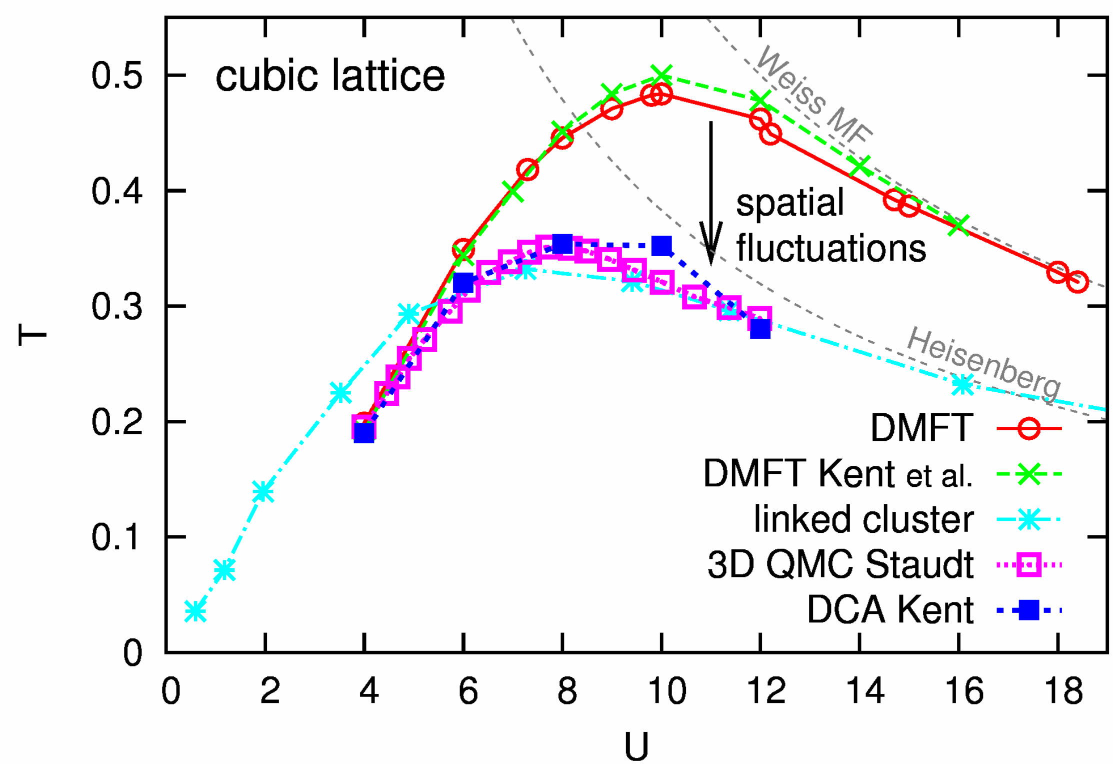

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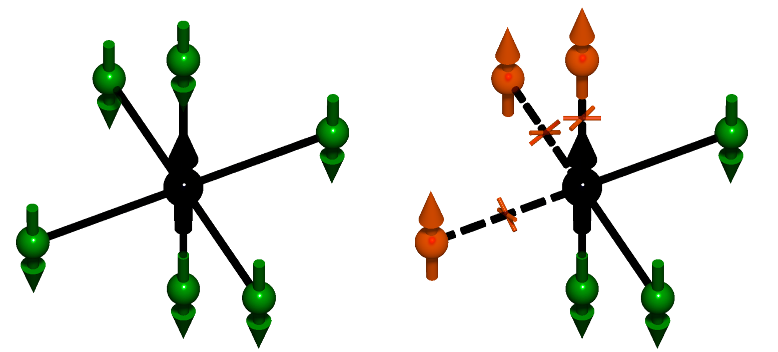

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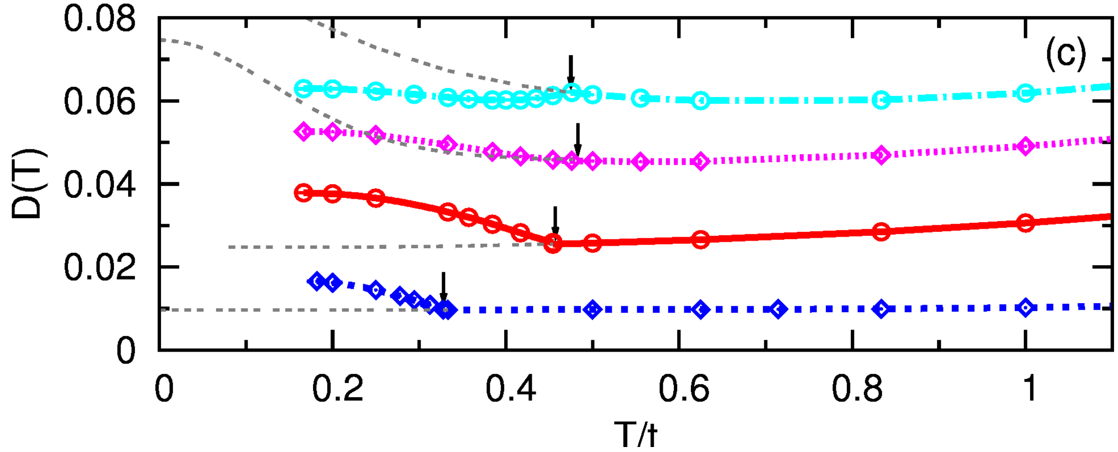

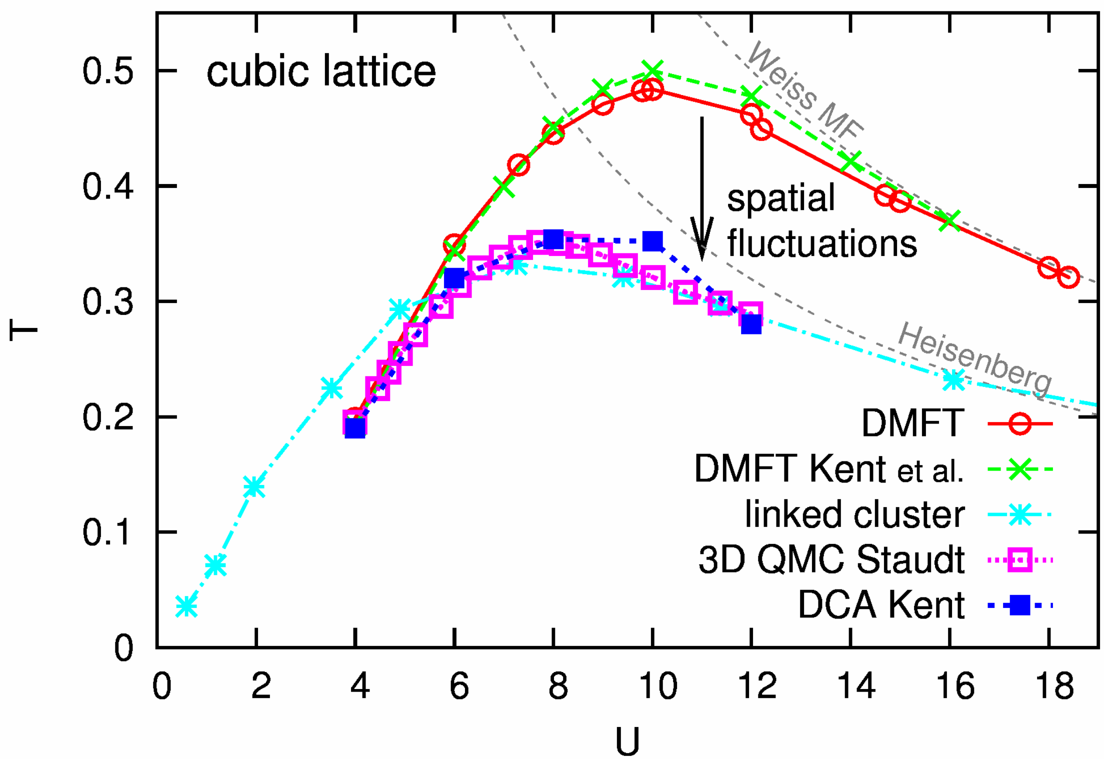

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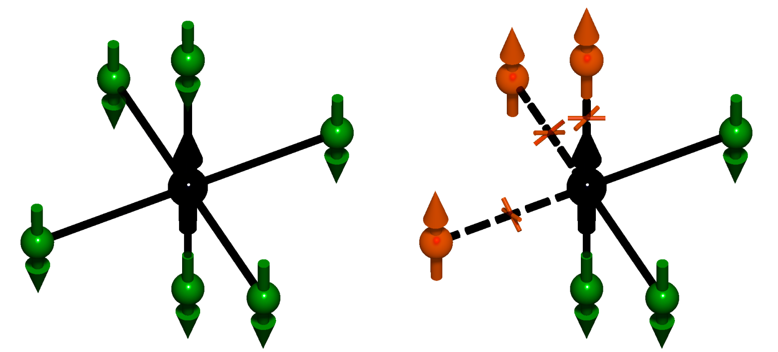
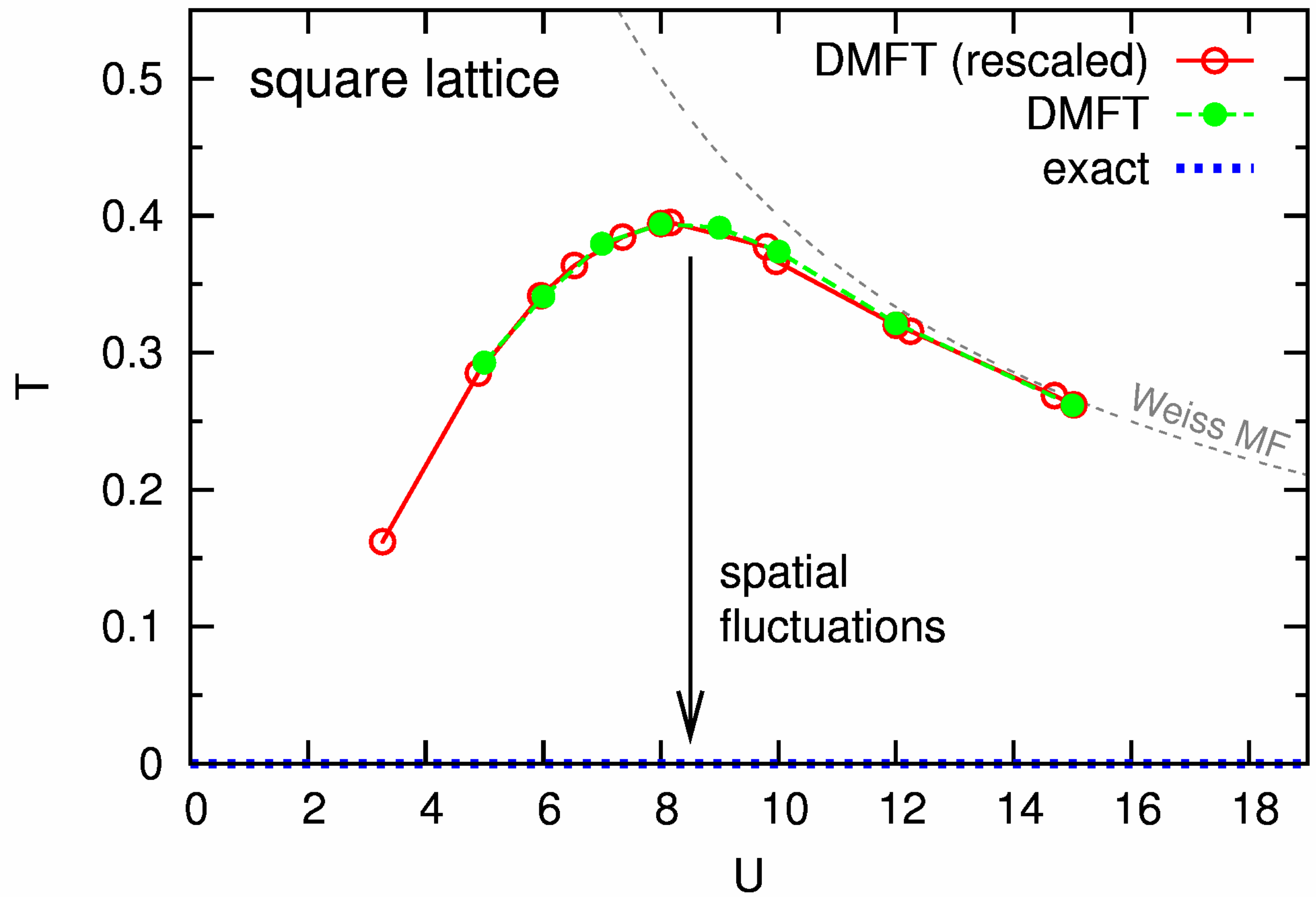


and independ. of long-range order

Situation "worse" in 2d: no antiferromagnetism at finite T!



Will any enhancement of D at low T remain? At which temperature scale?

How large are the DMFT errors in $D(T)$ for $T \gtrsim T_N^{\mathrm{DMFT}}$?

PRL 104, 066406 (2010) PHYSICAL REVIEW LETTERS week ending 12 FEBRUARY 2010

Fermions in 2D Optical Lattices: Temperature and Entropy Scales for Observing Antiferromagnetism and Superfluidity

Thereza Paiva,[1] Richard Scalettar,[2] Mohit Randeria,[3] and Nandini Trivedi[3]

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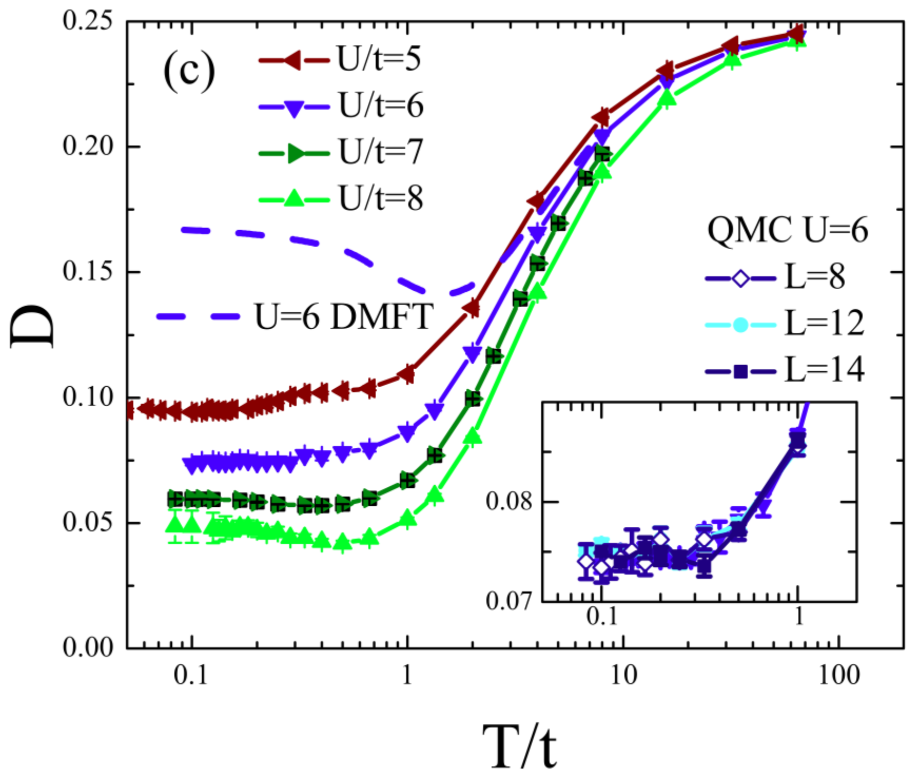

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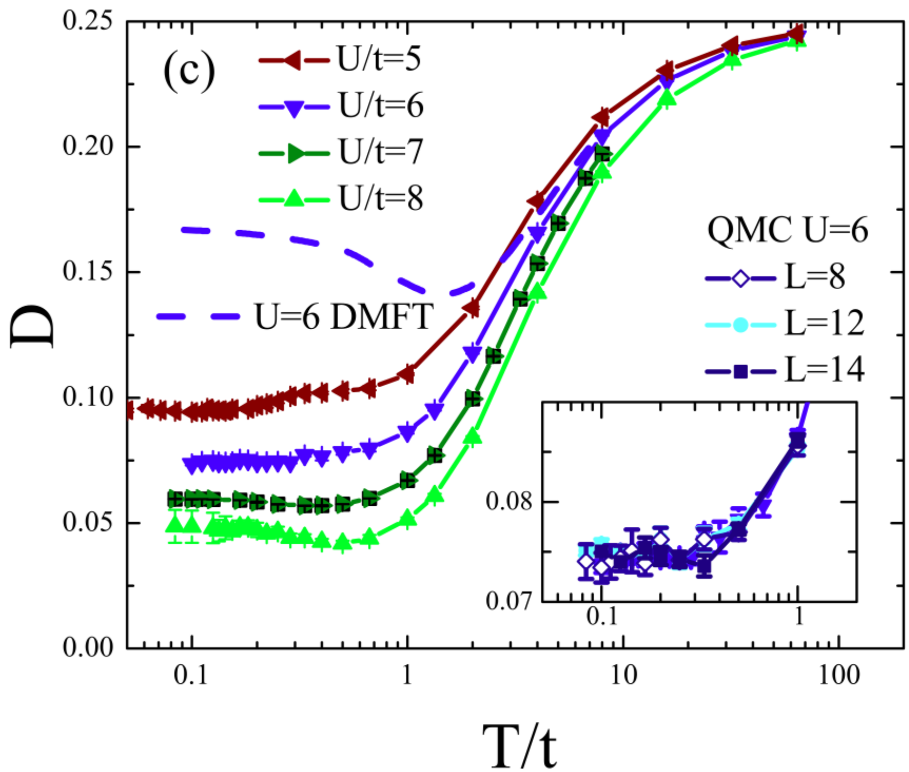

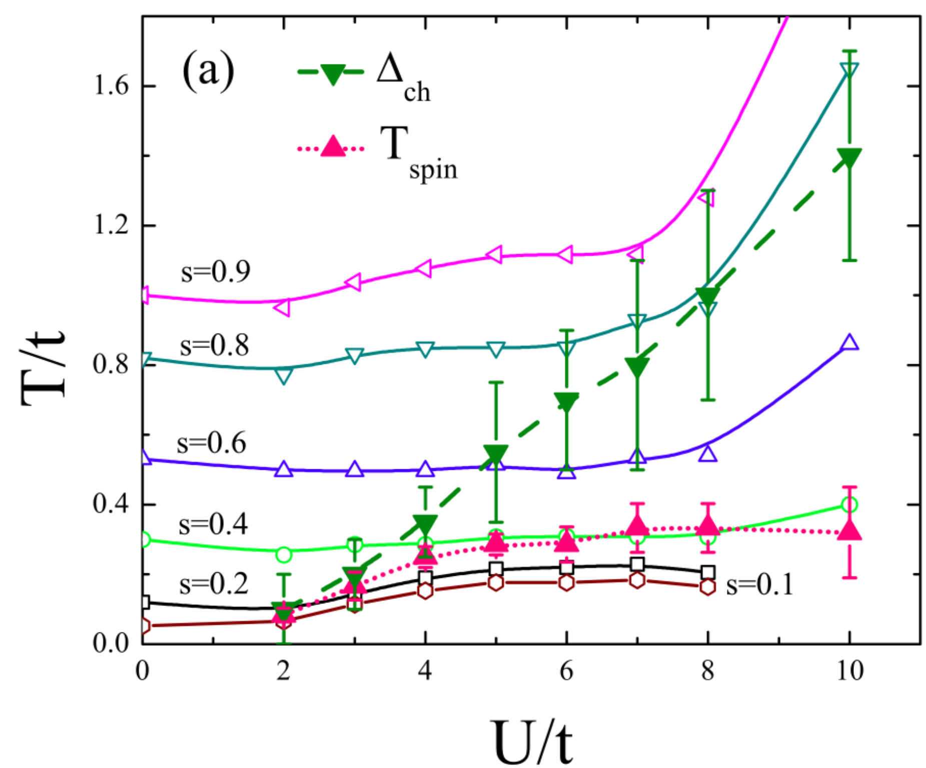

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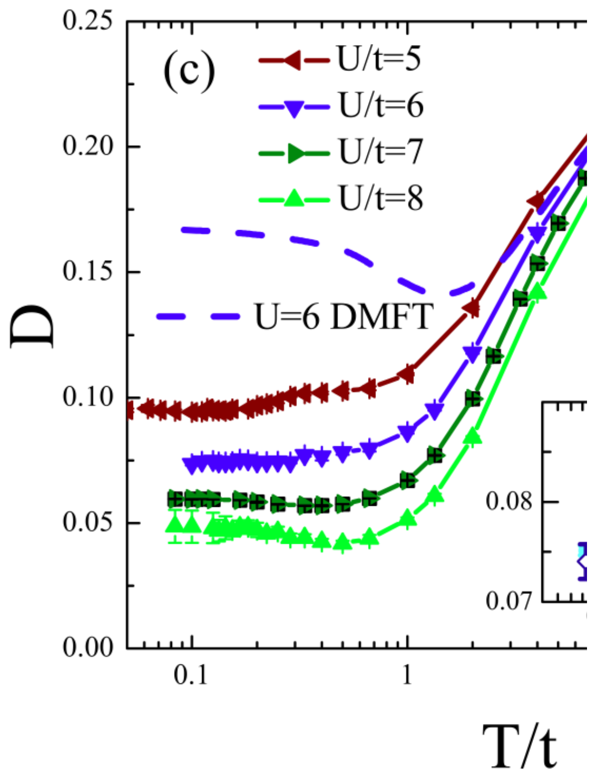
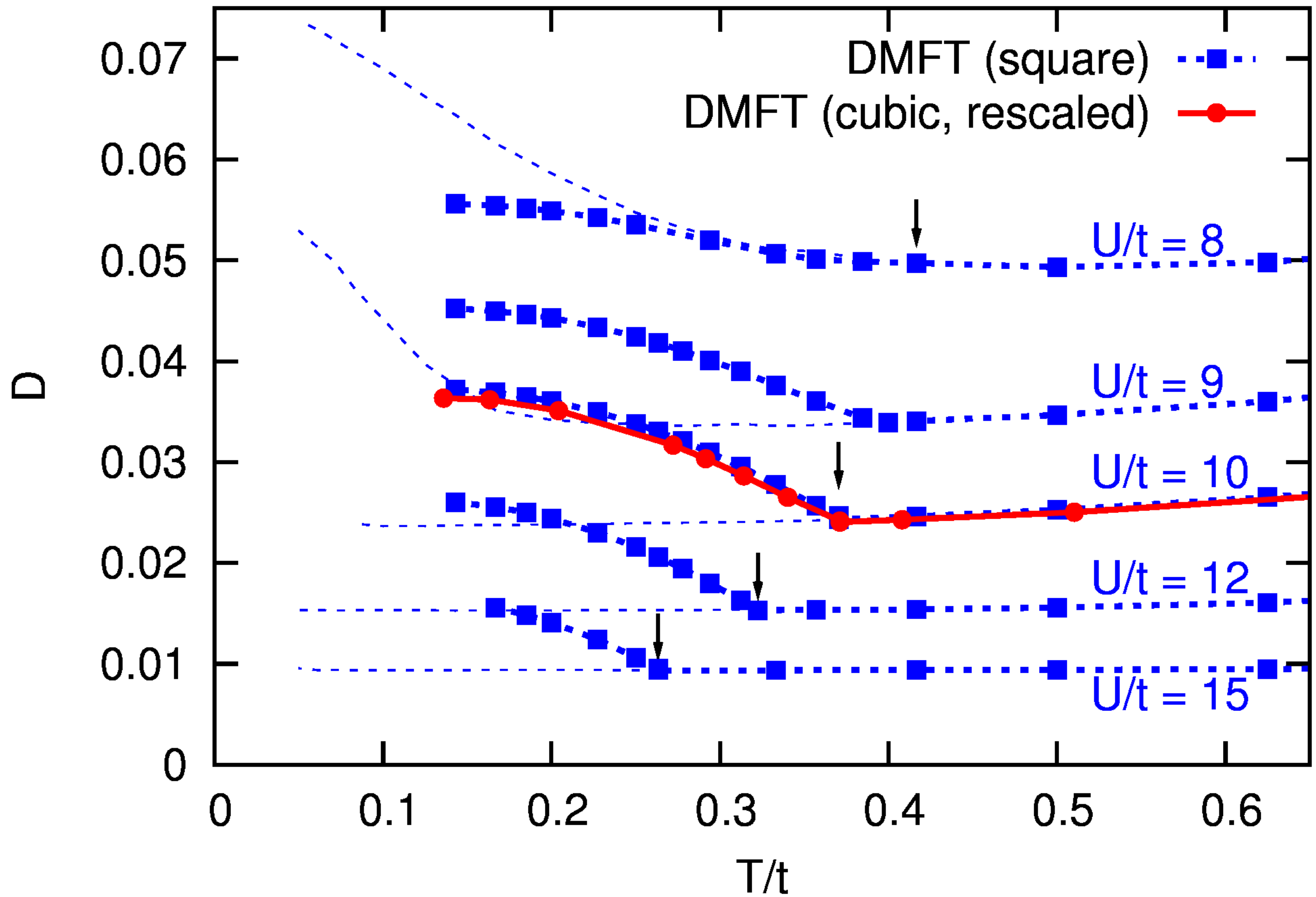
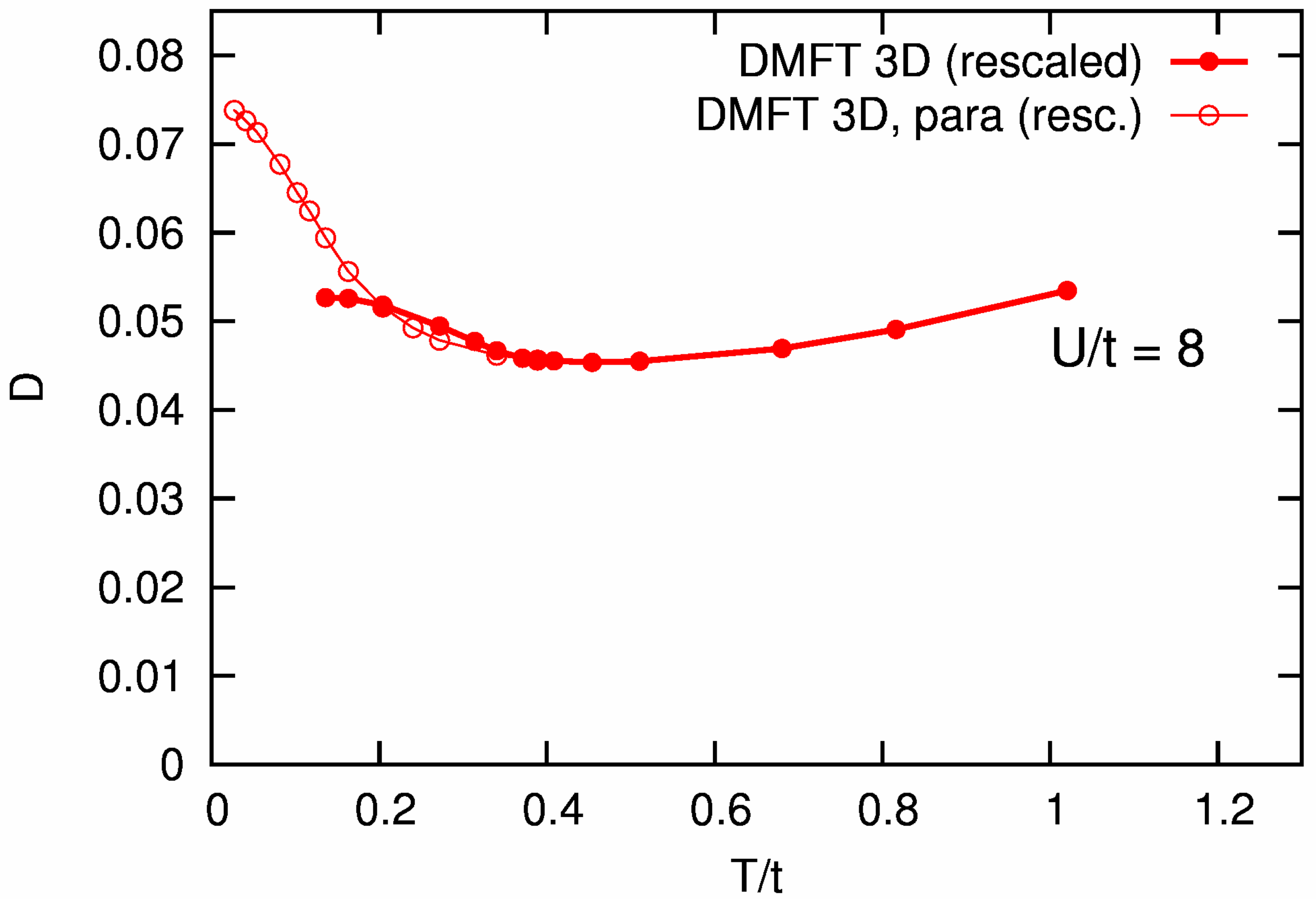




Comparison DMFT – direct QMC for the 2d square lattice



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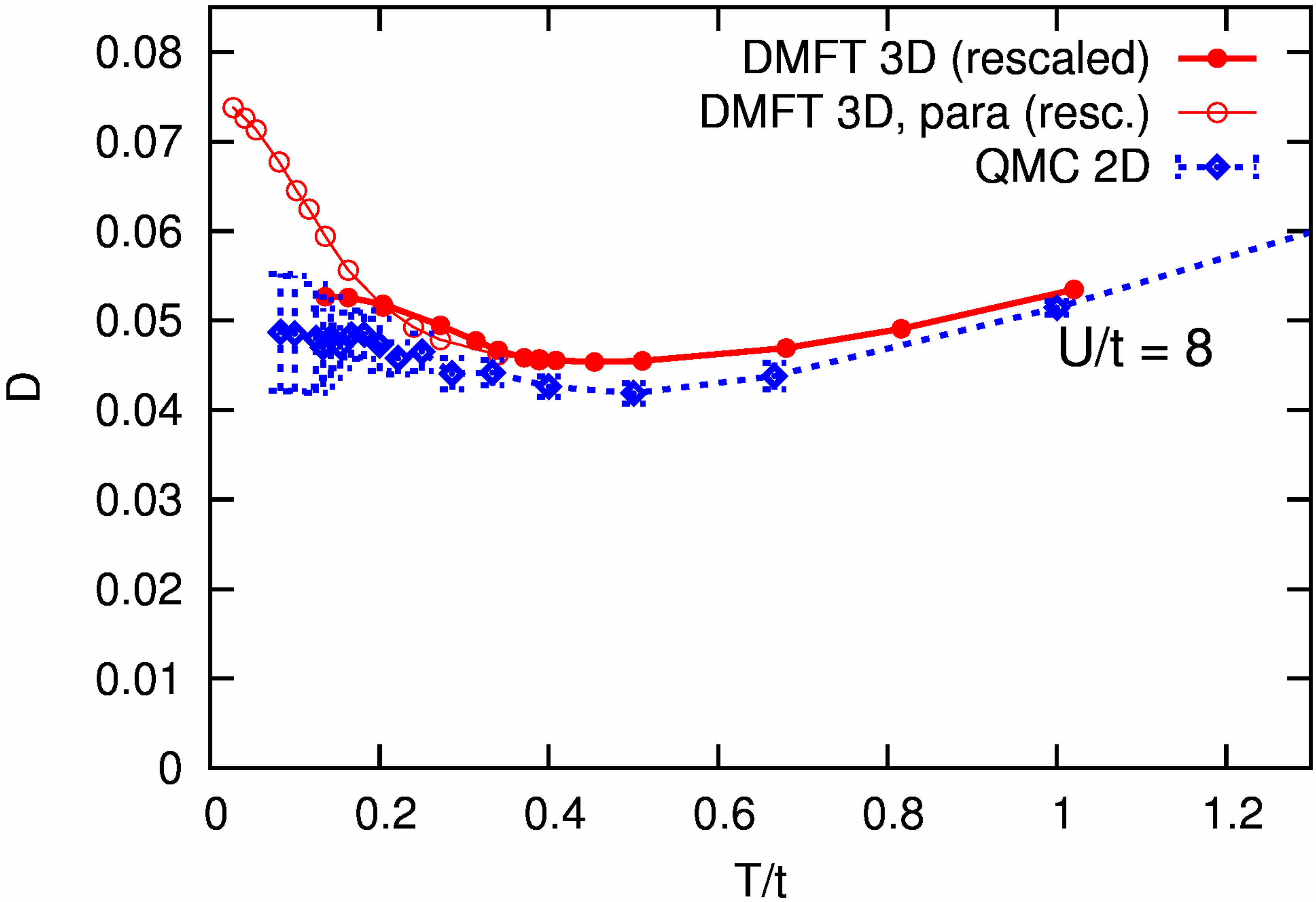

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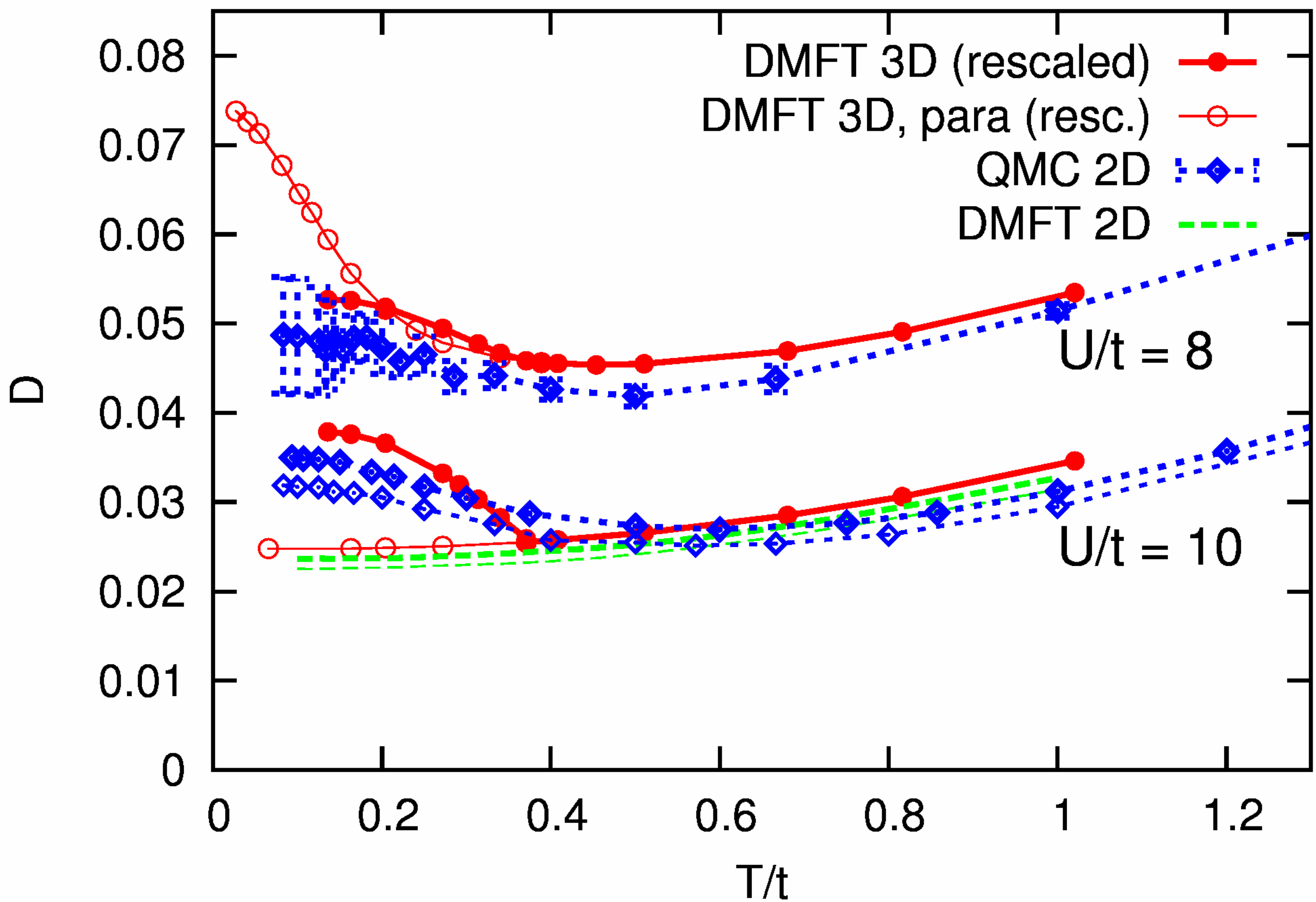
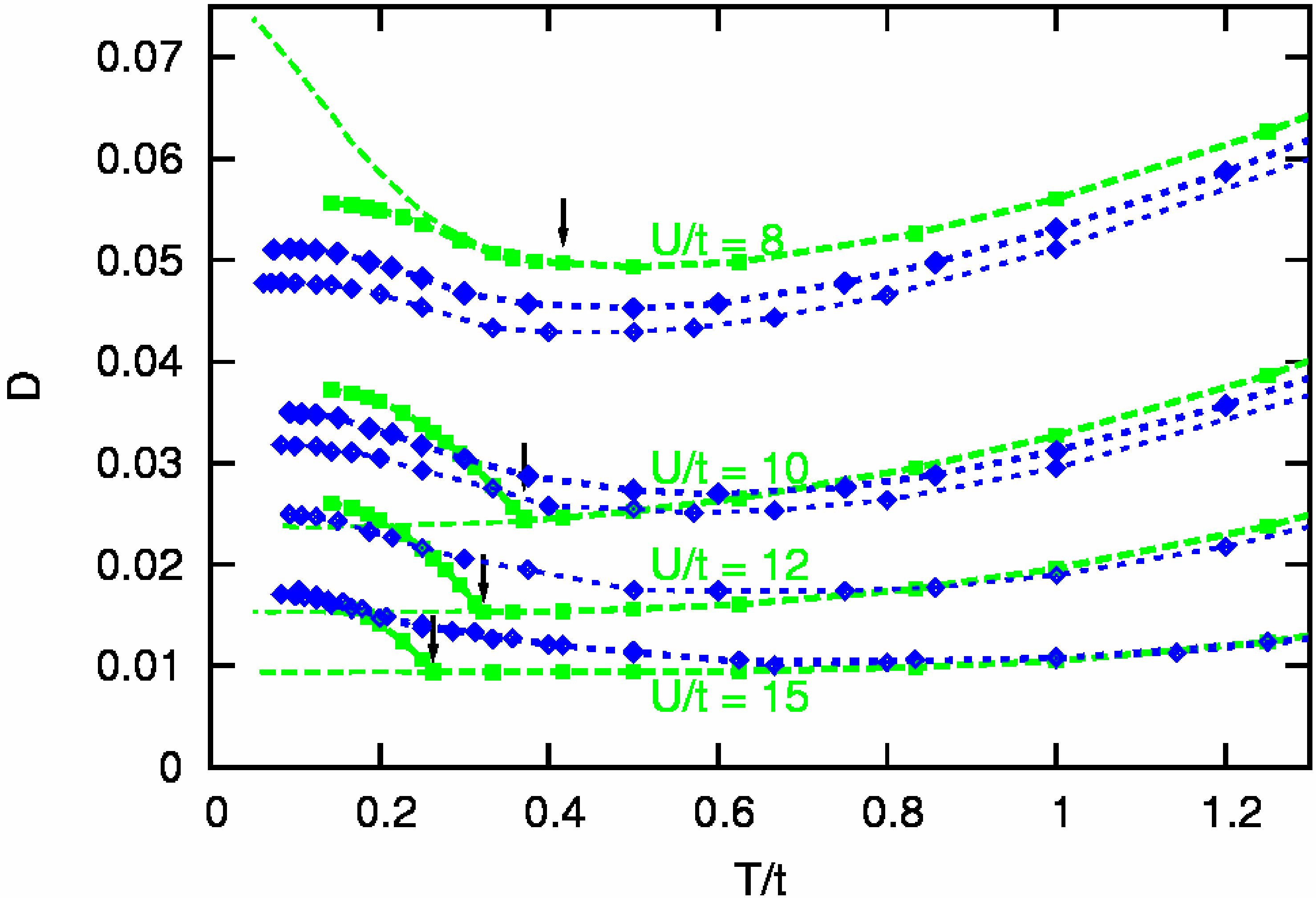
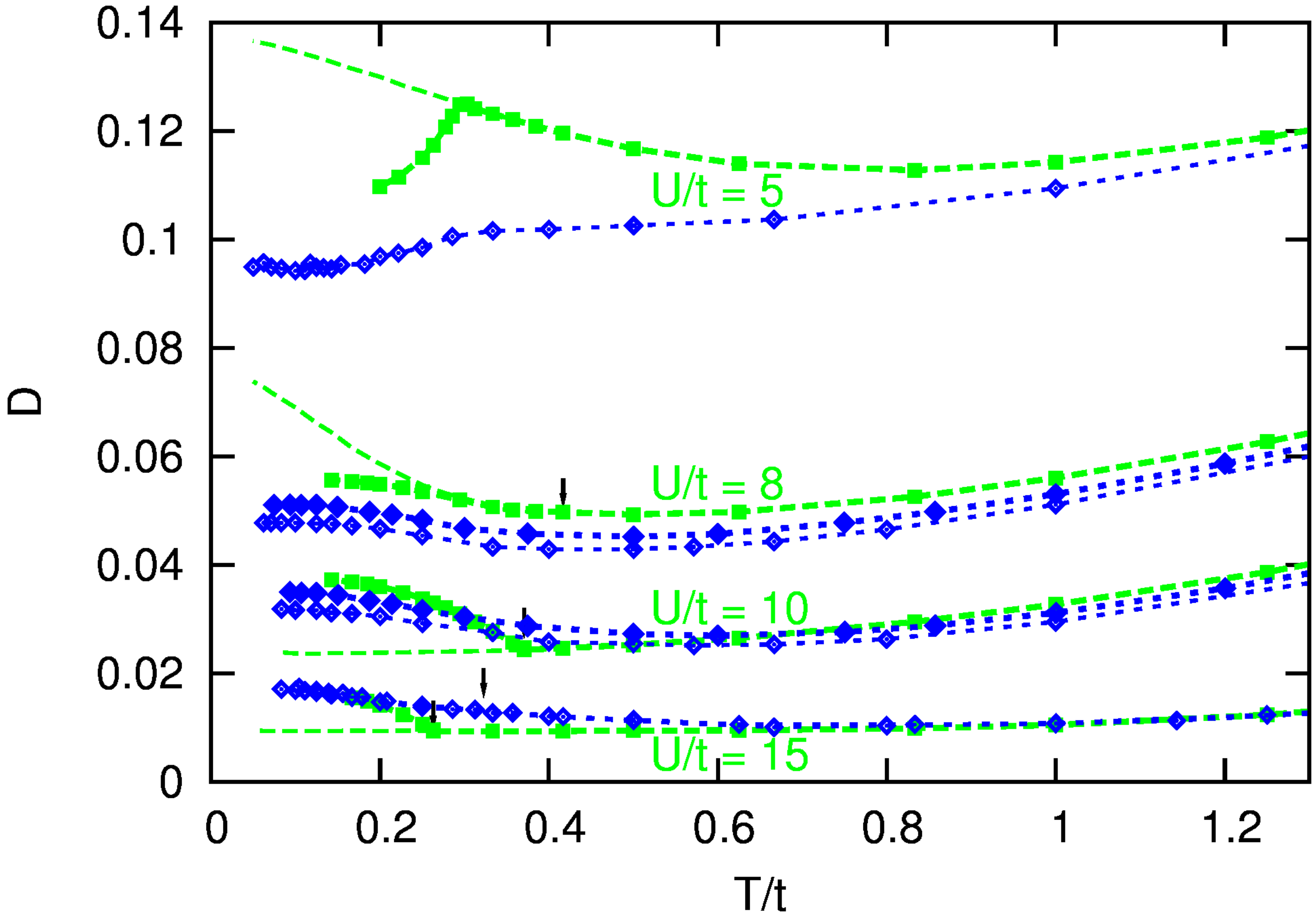




green: DMFT, blue: BSS-QMC (thicker lines: smaller $\Delta\tau$)

excellent agreement at $U = 8$; rounding off at $T \gtrsim T_N^{\text{DMFT}}$ for larger U

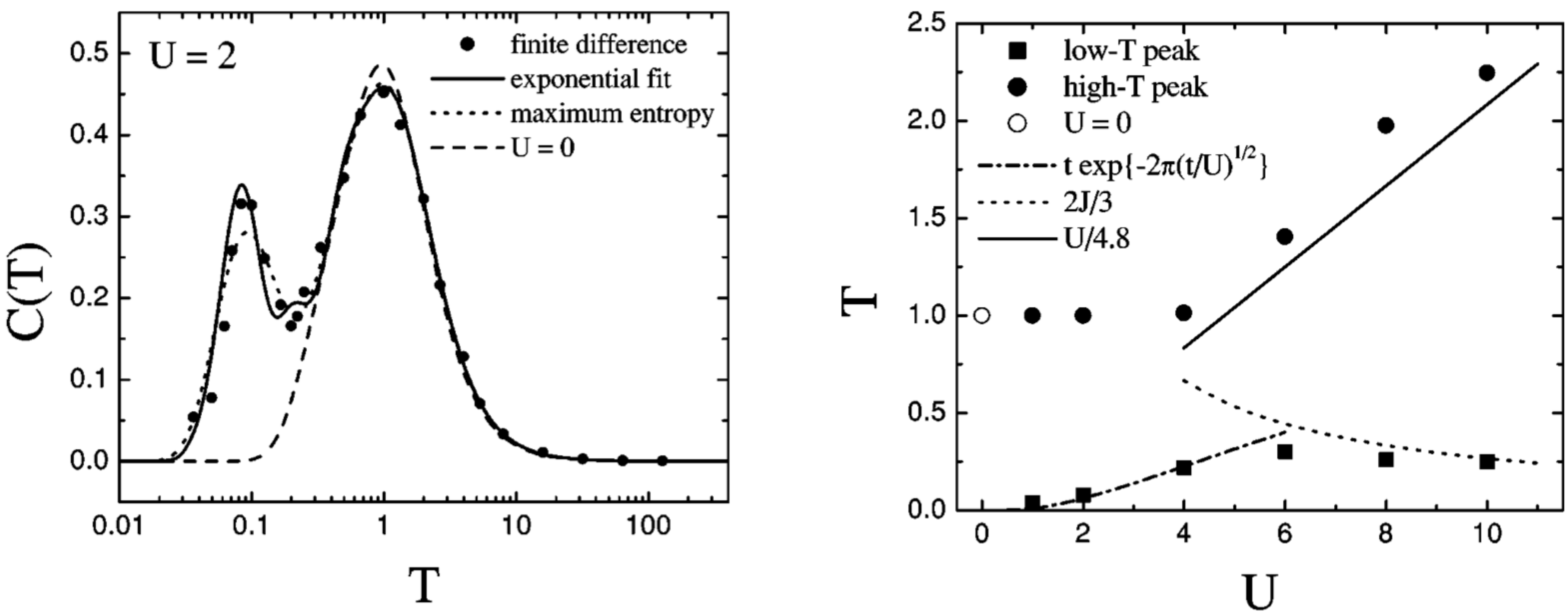
Even the low-T suppression of D at small U corresponds with direct QMC:



How is this possible? How much better is the agreement in 3 dimensions?

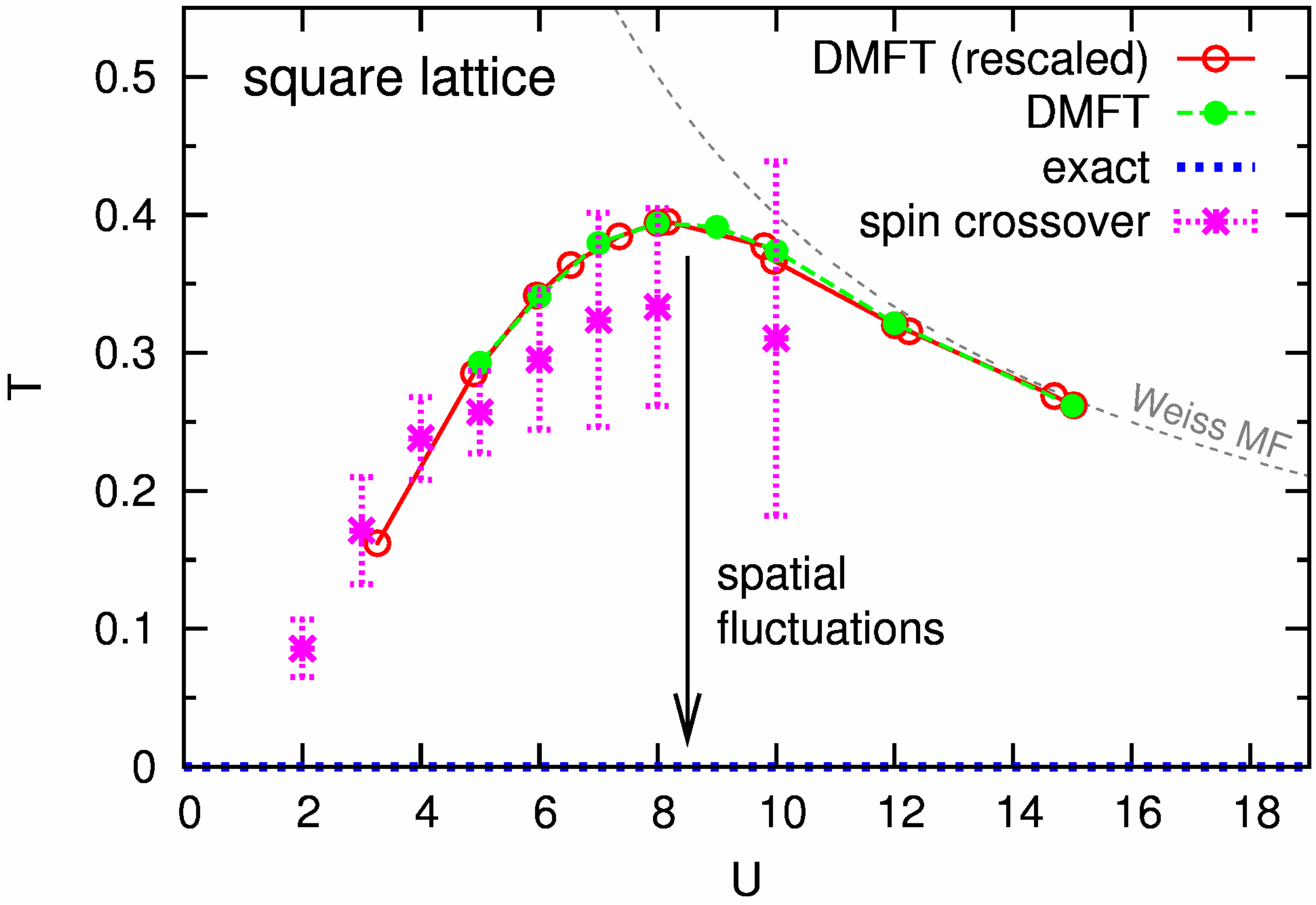
Spin crossover scale in 2 dimensions – definition?

PAIVA, SCALETTAR, HUSCROFT, AND MCMAHAN PHYSICAL REVIEW B **63** 125116



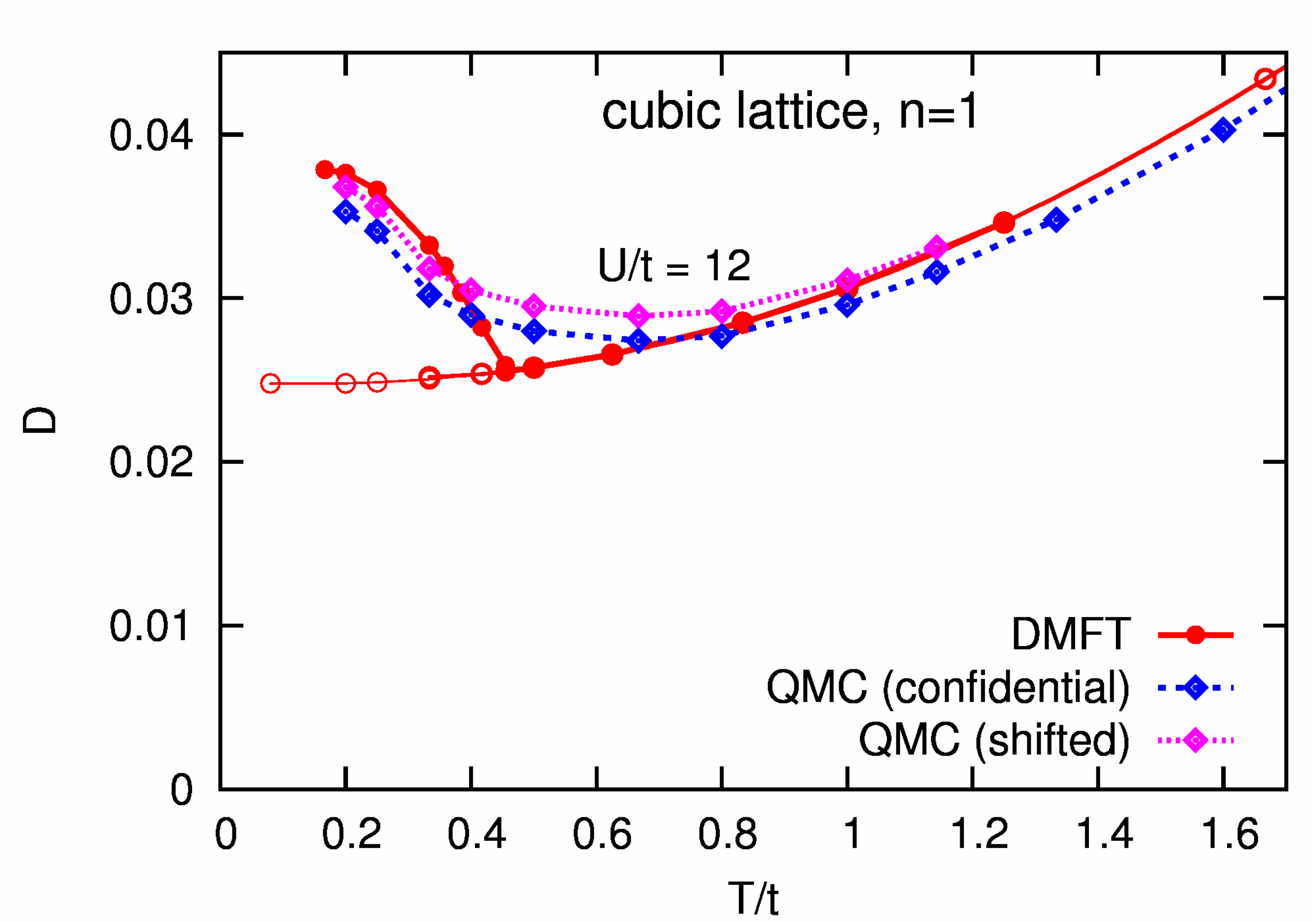
[Paiva, Scalettar, Huscroft, McMahan, PRB (2001)]

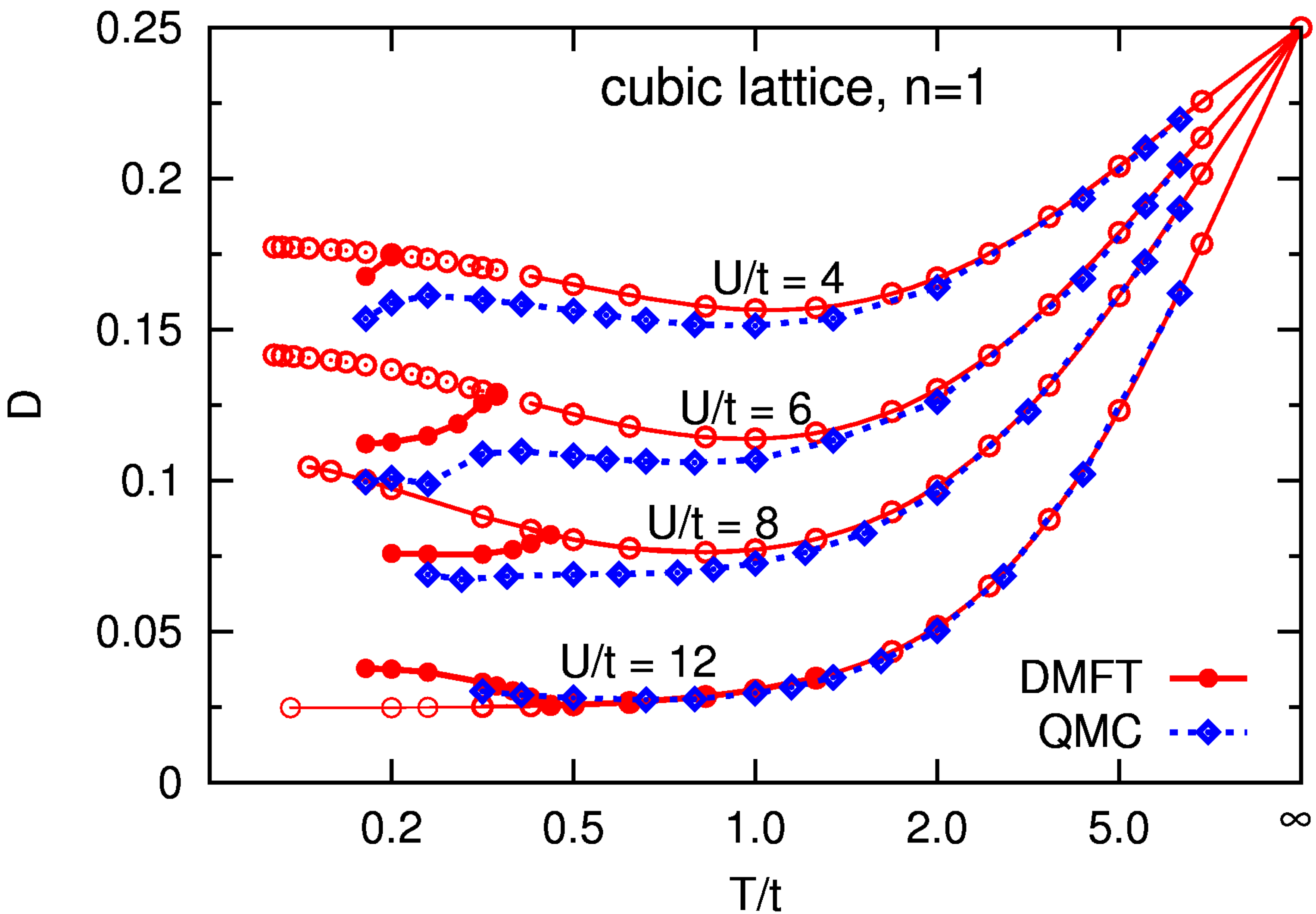
Comparison for square lattice: spin crossover temperature vs. T_N^{DMFT}



Nearly perfect agreement!!!

Comparison in 3 dimensions





Discretization corrections unknown – larger at intermediate U!

Note: nonuniform discretization $\Delta\tau$ at large T

Summary

DMFT predicts $D(T)$ more accurately in $d=3$, $d=2$ than expected

AF induced enhancement/suppression of D survives; U scale correct

Near-perfect precision at $T \gg T_N^{\text{DMFT}}$ and $T \to 0$ (at least for $U \gtrsim W$)

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Extend study to triangular and other frustrated lattices

Analyze/verify BSS-QMC results for $\langle S_i \cdot S_j \rangle$

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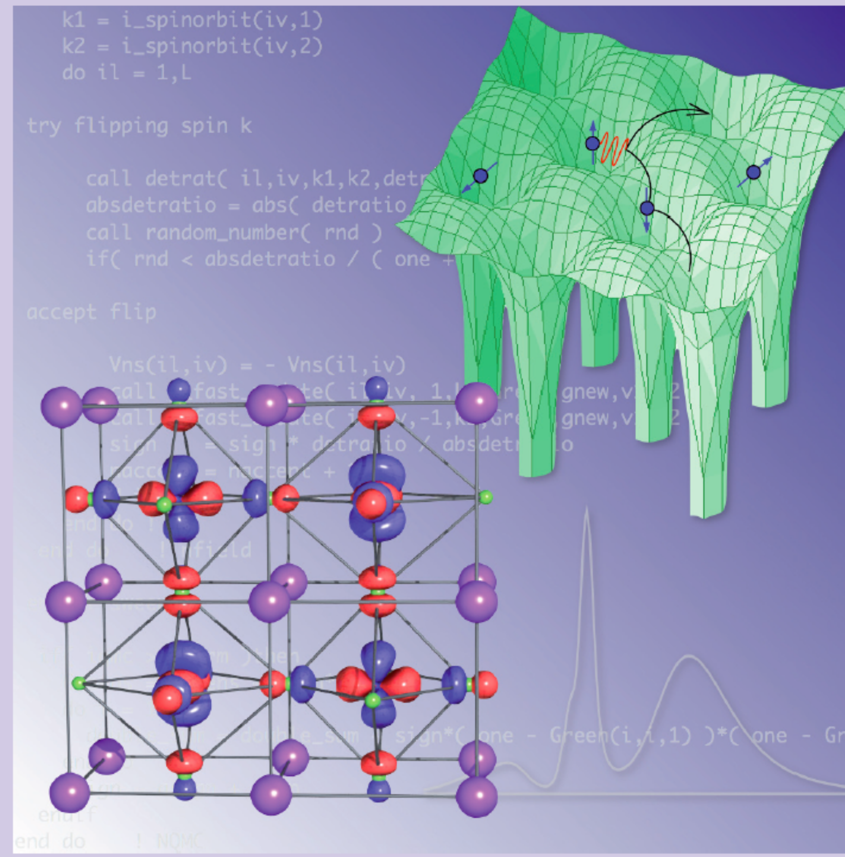
Thanks to: T. Paiva and R. Scalettar and DFG (TR49)

General method development: new initiative DFG-FG 1346

Positive evaluation on 2010/04/15+16, senate decision on 2010/07/06.

FOR 1346:
Dynamical Mean-Field Approach with Predictive Power for Strongly Correlated Materials



Dieter Vollhardt, University of Augsburg (Spokesperson)
Alexander Lichtenstein, University of Hamburg (Co-Spokesperson)

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P8: QMC impurity solvers
(F. Assaad, N. Blümer, P. Werner)

- most efficient QMC impurity solver for important problem classes?
- study impact of neglected interactions
- generalize CT-QMC solvers for frequency-dependent interactions
- eliminate systematic errors in BSS solver (linear in $1/T$) using multigrid approach

P7: GW+DMFT (Held,Toschi,Kresse)

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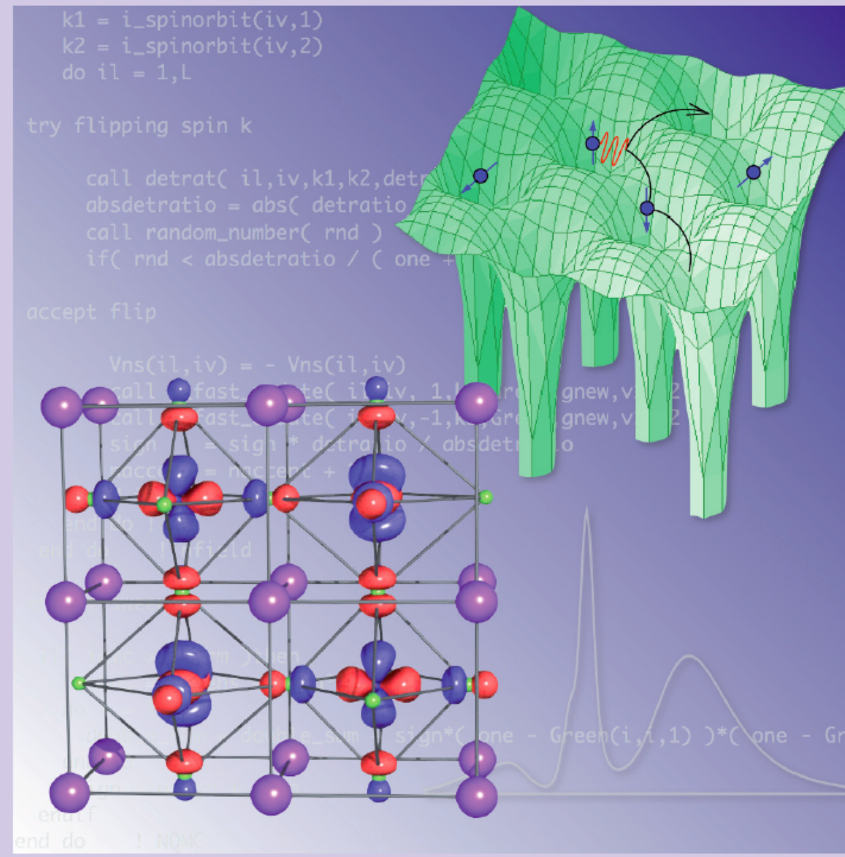

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