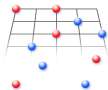


Double occupancy as a universal probe for antiferromagnetic correlations and entropy in cold fermions on optical lattices

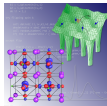
Nils Blümer

Institut für Physik, Johannes Gutenberg-Universität Mainz



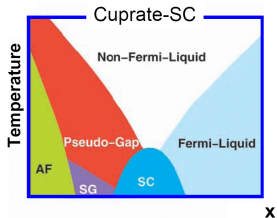
TR 49: *Condensed matter systems
with variable many-body interactions*
Frankfurt / Kaiserslautern / Mainz

FOR 1346
LDA+DMFT
Augsburg *et al.*

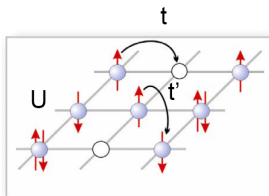


Motivation: Ultracold lattice fermions as quantum simulators?

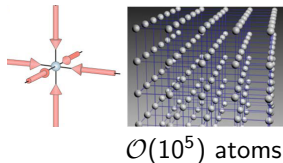
Correlated materials



Fermionic Hubbard model

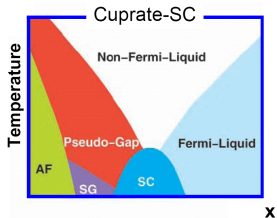


Ultracold fermions on optical lattices

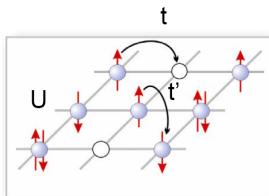


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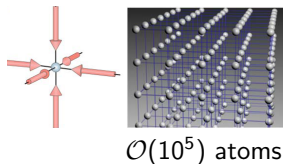
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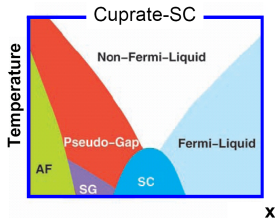


Recent breakthrough: paramagnetic Mott transition in 2-flavor mixtures

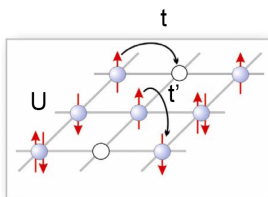
[Schneider et al., Science **322**, 1520 (2008), Jördens et al., Nature **455**, 204 (2008)]

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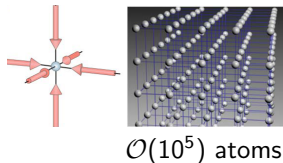
Correlated materials



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Ultracold fermions on optical lattices



$\mathcal{O}(10^5)$ atoms

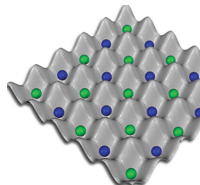
Recent breakthrough: paramagnetic Mott transition in 2-flavor mixtures

[Schneider et al., Science 322, 1520 (2008), Jördens et al., Nature 455, 204 (2008)]

Remaining challenge: antiferromagnetism (staggered order)

Problems:

- (i) difficult to reach sufficiently low temperatures/entropies
- (ii) detection of AF order is not straightforward
- (iii) inhomogeneity, time scale for global (spin) equilibrium

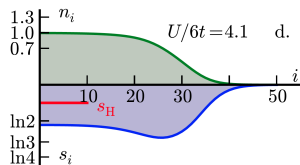


Questions for this talk

- How to detect AF order/correlations?

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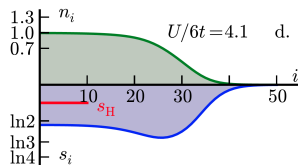


[Jördens et al., PRL **104**, 180401 (2010)]

Questions for this talk

- How to detect AF order/correlations?
- Which entropy range is needed/interesting?
- **General impact of dimensionality?**

Mermin-Wagner: LRO $\leftrightarrow d = 3$



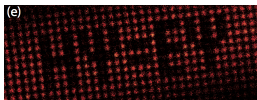
[Jördens et al., PRL **104**, 180401 (2010)]

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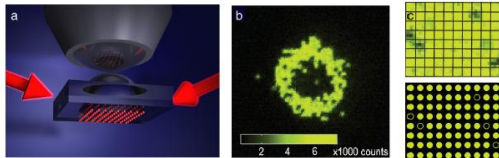
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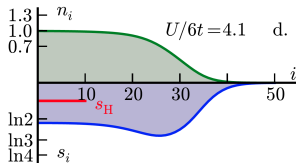
Experimental advantage of 2 dimensions:
single-site resolution (for bosons)



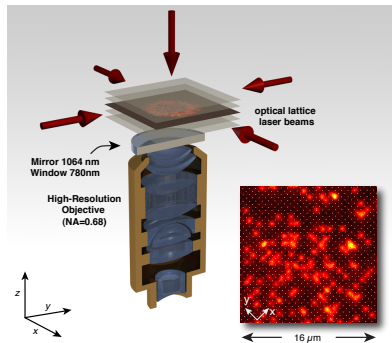
[Würtz et al., PRL 103, 080404 (2009)]



[Bakr et al., Science 329, 547 (2010)]



[Jördens et al., PRL 104, 180401 (2010)]



[Sherson et al., Nature 467, 68 (2010)]

Motivation: Ultracold lattice fermions as quantum simulators?

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Effects of **non-local correlations**? DMFT versus direct QMC + BA

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Other observables: energetics, longer-range correlations; weak coupling

Summary and outlook

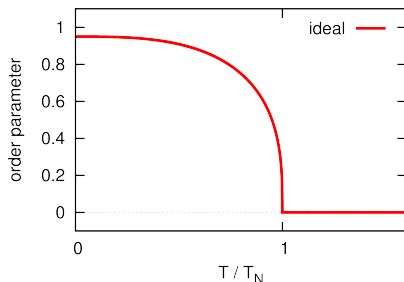
How to detect AF order/correlations?

Obvious choice: order parameter

$$m_{stag}^z = \frac{1}{N} \left[\sum_{i \in A} \langle n_{i\uparrow} - n_{i\downarrow} \rangle - \sum_{i \in B} \langle n_{i\uparrow} - n_{i\downarrow} \rangle \right]$$

(equivalent sublattices A and B)

↪ **specific** and **sharp** signal at/below T_N



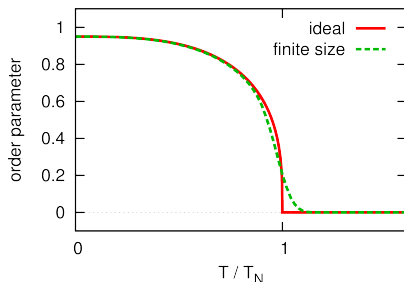
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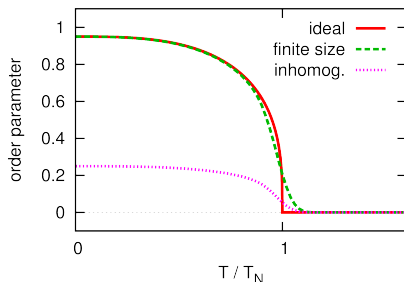
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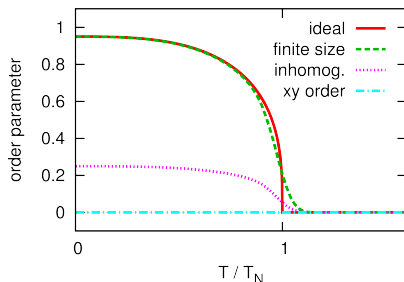
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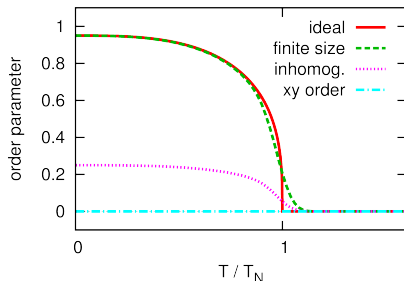
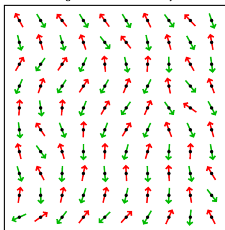


Illustration:

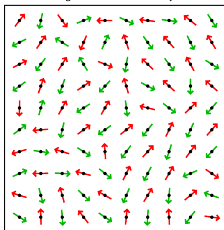
weak order not
apparent in
small snapshot

↪ look at NN
correlations?

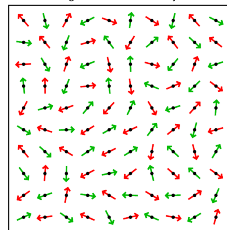
(a) $m_{stag} = 0.9$, $S_i \cdot S_j = -0.85$



(b) $m_{stag} = 0.5$, $S_i \cdot S_j = -0.66$

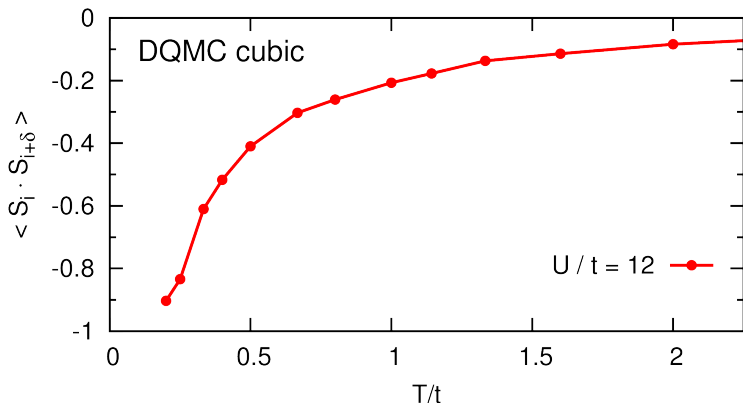


(c) $m_{stag} = 0.0$, $S_i \cdot S_j = -0.55$



Current experimental focus: nearest-neighbor spin correlation function

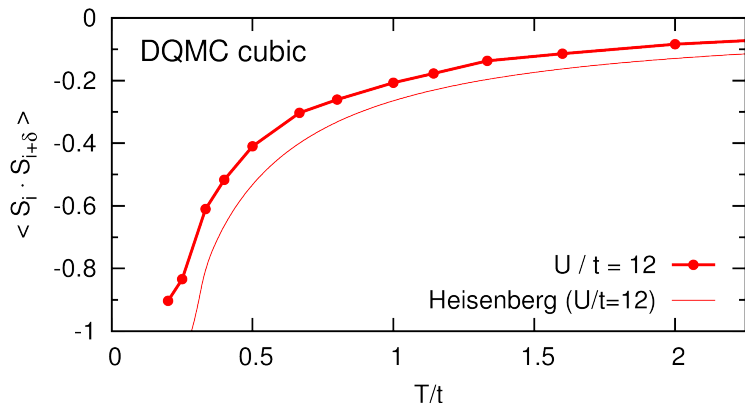
Modulation spectroscopy (Esslinger group), super-lattice (Bloch group)



Note: strong (universal) high-temperature tails, monotonous

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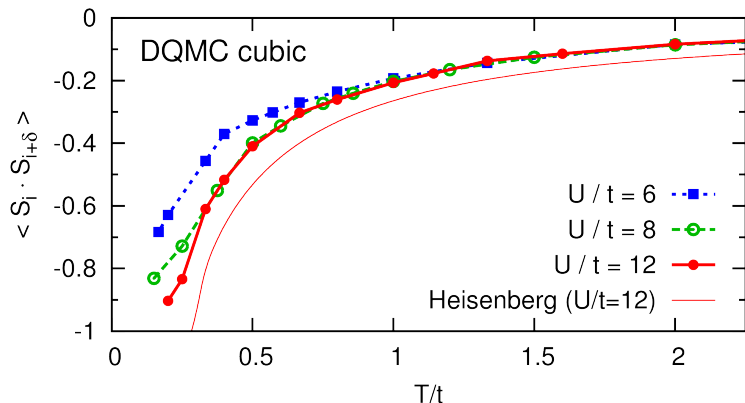
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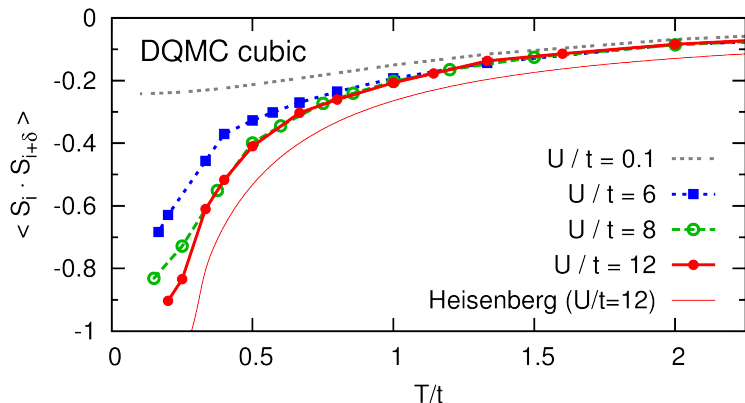
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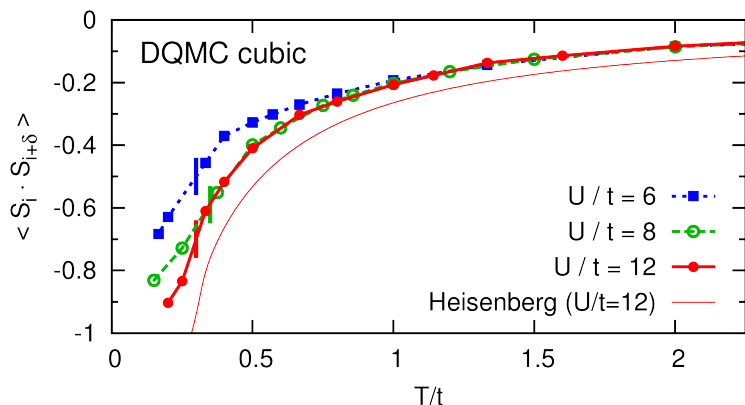
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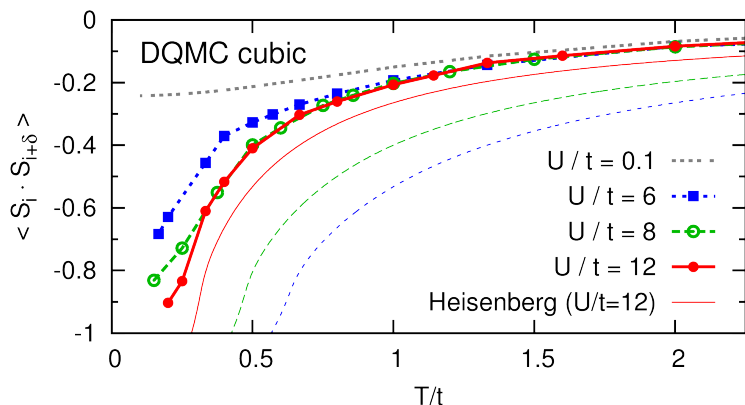
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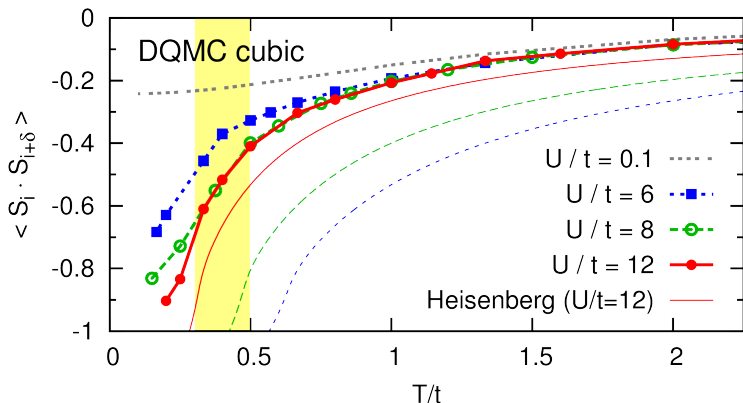
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No distinct features at Néel temperature ($\approx 0.3t$)

Interesting spin physics above T_N , not visible in NN correlations

Néel transition of trapped fermions on cubic optical lattice at (real-space) DMFT level

[Gorelik et al., PRL **105**, 065301 (2010)]



Elena Gorelik
Univ. Mainz



Walter Hofstetter
Univ. Frankfurt

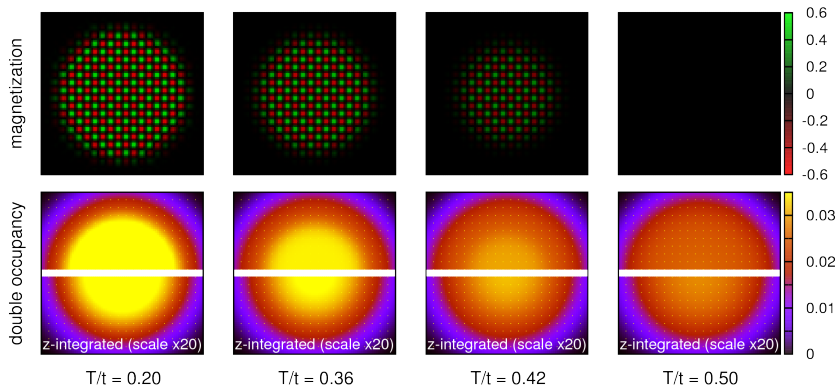


Irakli Titvinidze
Univ. Hamburg



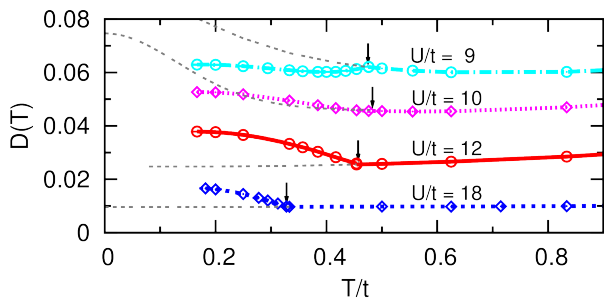
Michiel Snoek
Univ. Amsterdam

RDMFT-QMC results for cubic lattice ($V = 0.05t$, $U = W = 12t$)



Proposal: **enhanced double occupancy** (i.e. interaction energy) as a signature of antiferromagnetic order/correlations **at strong coupling** [Gorelik, Titvinidze, Hofstetter, Snoek, Blümer, PRL (2010)]

DMFT-QMC estimates of double occupancy D at half filling

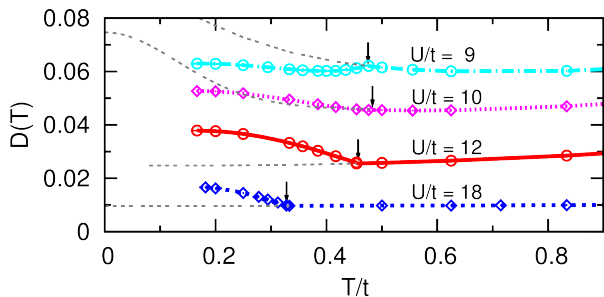


At $U \gtrsim 10t$:

D enhanced below Néel temperature (arrows)

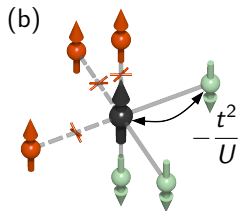
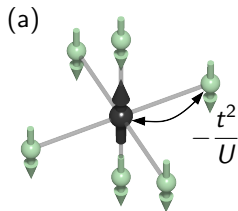
Thin lines: metastable nonmagnetic phase

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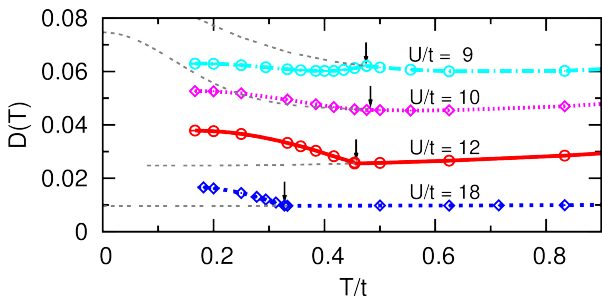


(a) AF state: hopping to all $Z = 6$ neighbors

(b) Para/nonmagnetic state: 1/2 of NN Pauli forbidden

Thus: $D \sim$ NN correlations

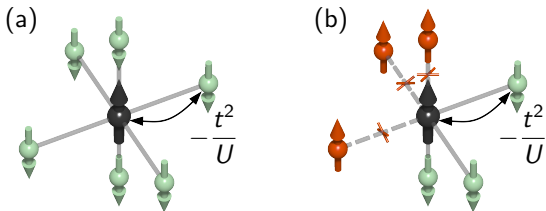
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Exact GS relation (all d) [Takahashi, 1977]: $D_0 = \frac{Zt^2}{2U^2} (1 - \langle \sigma_i \cdot \sigma_j \rangle) + \mathcal{O}\left(\frac{t^4}{U^4}\right)$

Effects of non-local correlations? DMFT versus direct QMC + BA

[Gorelik, Rost, Paiva, Scalettar, Klümper, NB, arXiv:1105.3356]



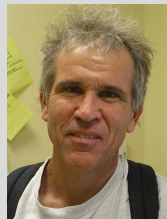
Elena Gorelik
Univ. Mainz



Andreas Klümper
Univ. Wuppertal

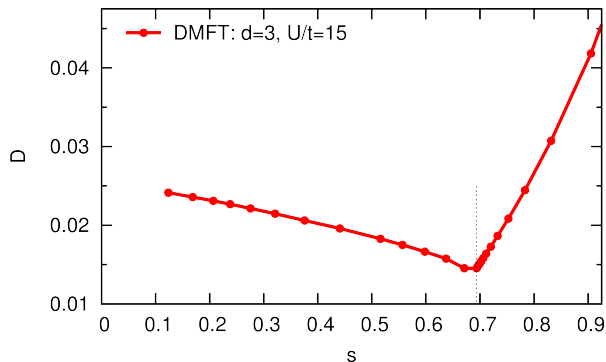


Thereza Paiva
Rio de Janeiro



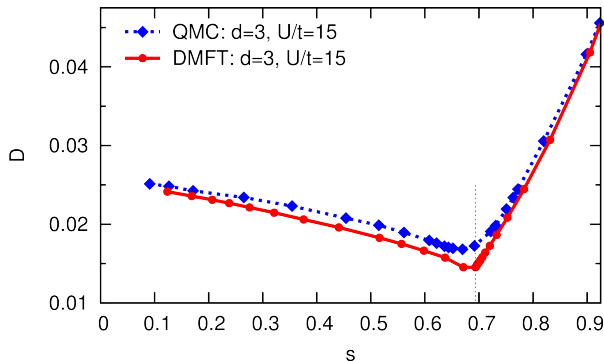
Richard Scalettar
UC Davis

Double occupancy as a universal measure of AF correlations + entropy



DMFT PT at $s \approx \log(2)$

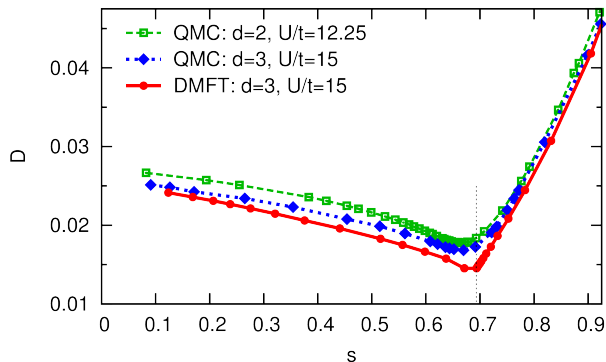
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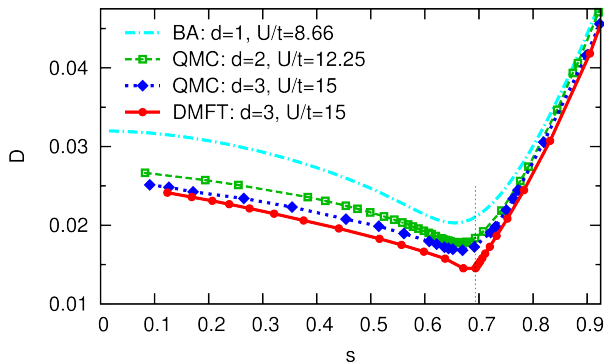
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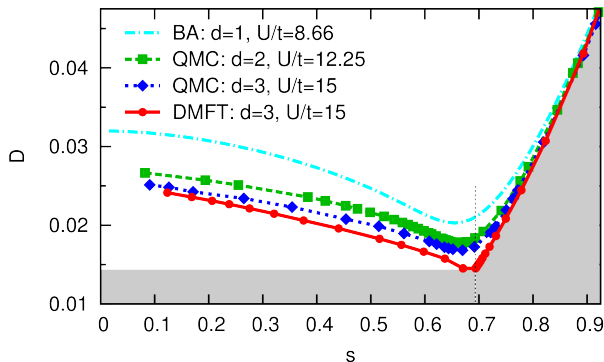
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Minimum of $D(s)$ at
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Interesting physics at
 $\log(2)/2 \lesssim s \lesssim \log(2)$!?

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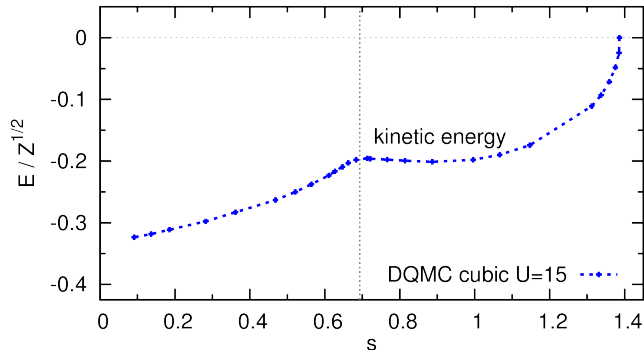
AF enhancement of D is larger

in lower dimensions:

$$D_0 = (1 - \langle \sigma_i \cdot \sigma_j \rangle) Z \frac{t^2}{2U^2} + \mathcal{O}(t^4/U^4)$$

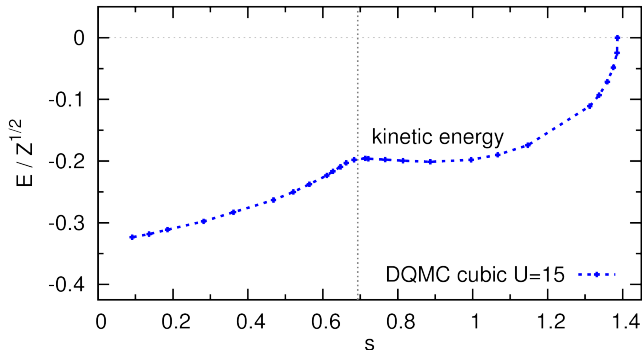
$$\langle \sigma_i \cdot \sigma_j \rangle_0 = \begin{cases} -1.00 & DMFT \\ -1.20 & (d = 3) \\ -1.34 & (d = 2) \\ -1.77 & (d = 1) \end{cases}$$

Related observable: kinetic energy



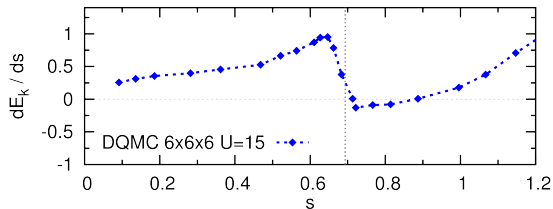
Kink in kinetic energy
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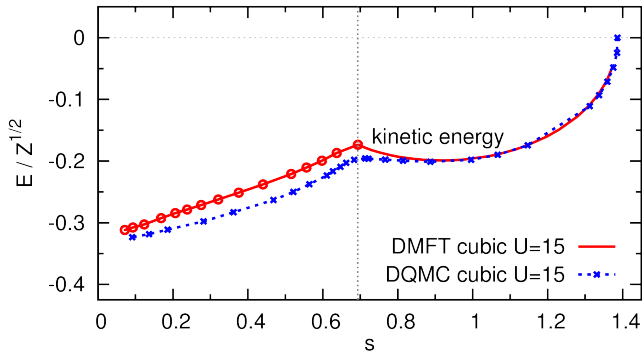


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Negative slope at $s \gtrsim \log(2)$ in $d = 3$?



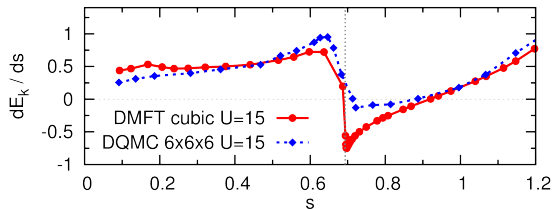
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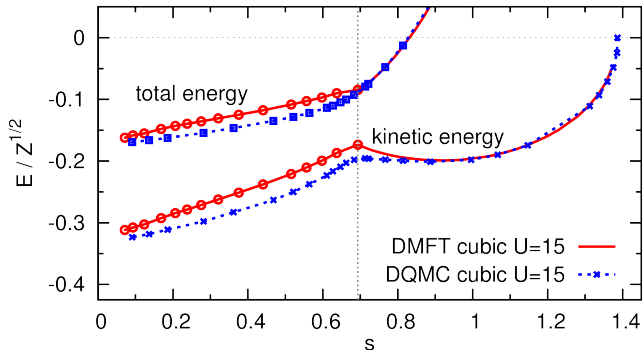
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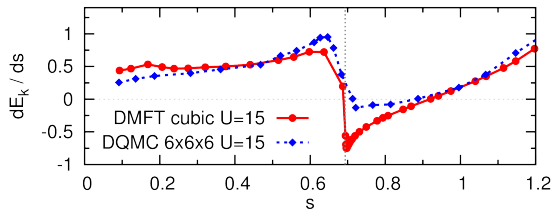


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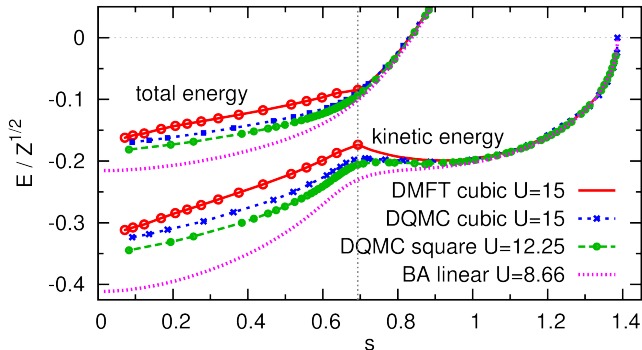
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Check: $dE_{\text{tot}}/ds \geq 0$



Related observable: kinetic energy



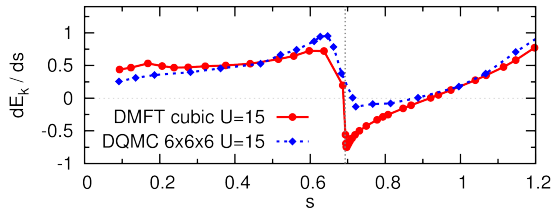
Kink in kinetic energy
(only) at $s \approx \log(2)$

Negative slope at
 $s \gtrsim \log(2)$ in $d = 3$?

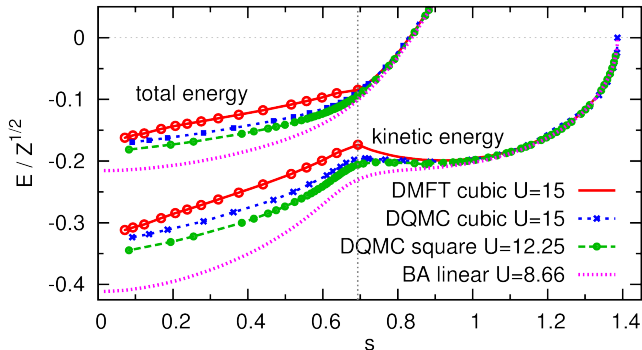
Yes!

Check: $dE_{\text{tot}}/ds \geq 0$

$d = 2$ similar to $d = 3$



Related observable: kinetic energy



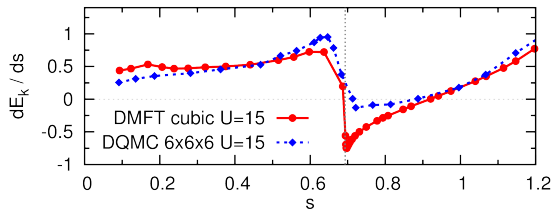
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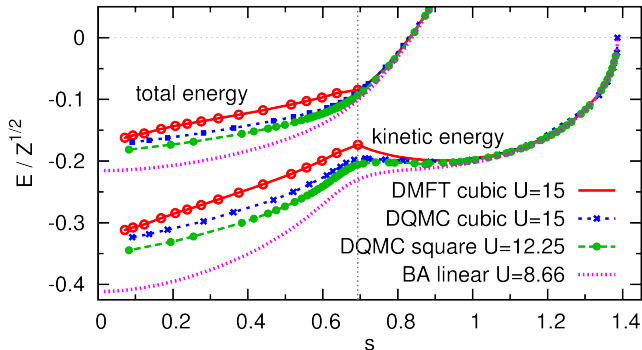
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Why no signature at $d = 3$ phase transition (Ehrenfest)?

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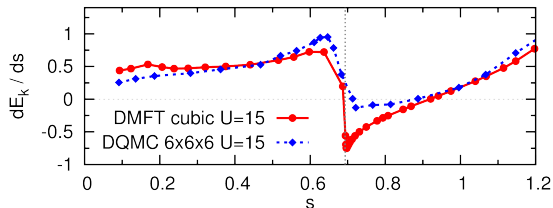
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$d = 2$ similar to $d = 3$



Why no signature at $d = 3$ phase transition (Ehrenfest)?

Finite-size effects, num. noise

Specific heat smoothed vs. s

Illustration: from dE/dT to dE/ds

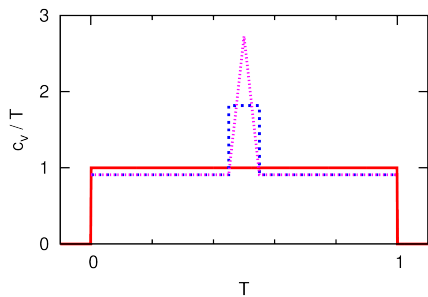


Illustration: from dE/dT to dE/ds

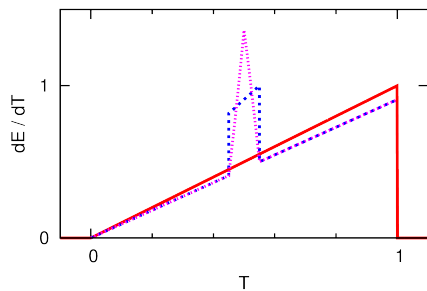
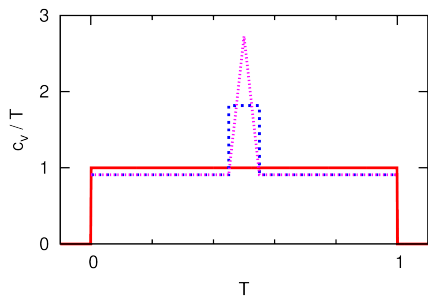


Illustration: from dE/dT to dE/ds

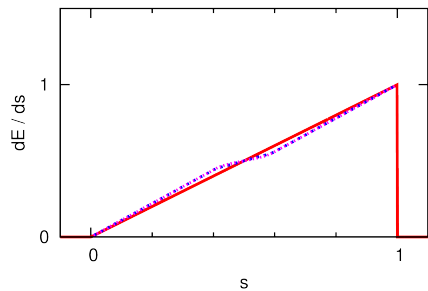
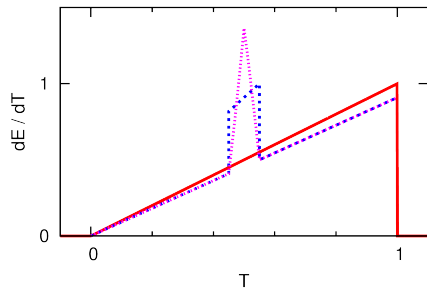
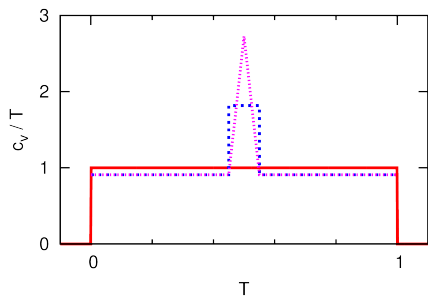
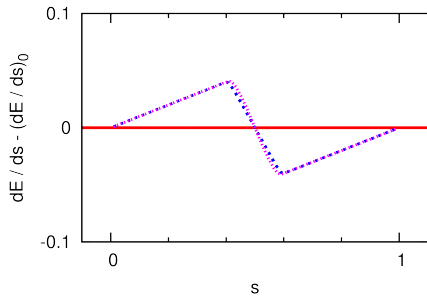
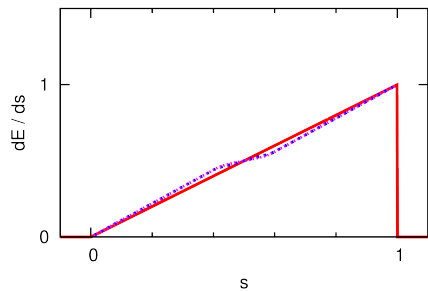
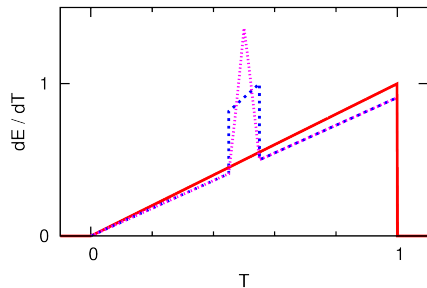
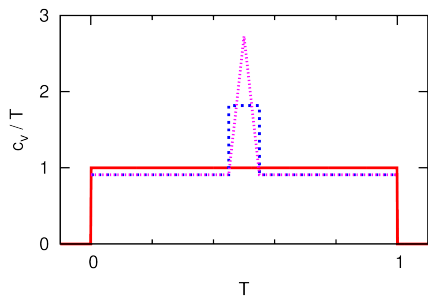
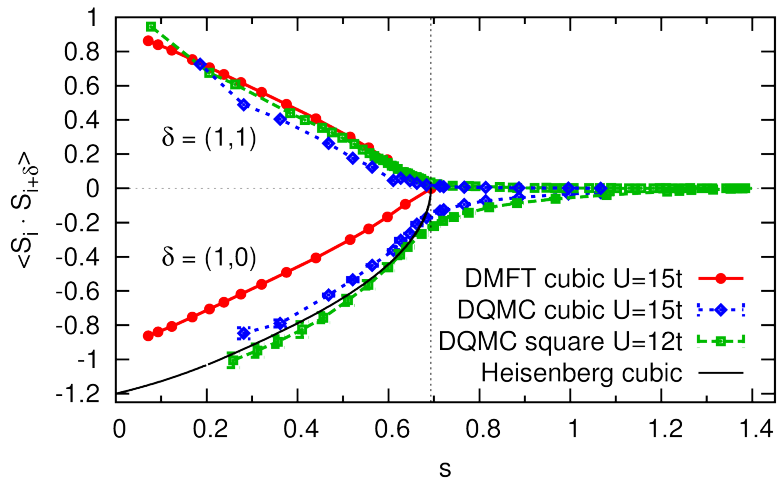


Illustration: from dE/dT to dE/ds

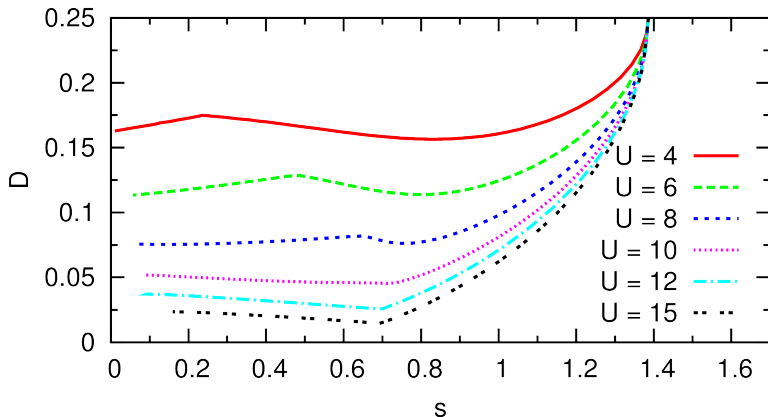


Spin correlation functions: what range is needed?



NNN spin correlation function signals: Heisenberg regime, low entropy

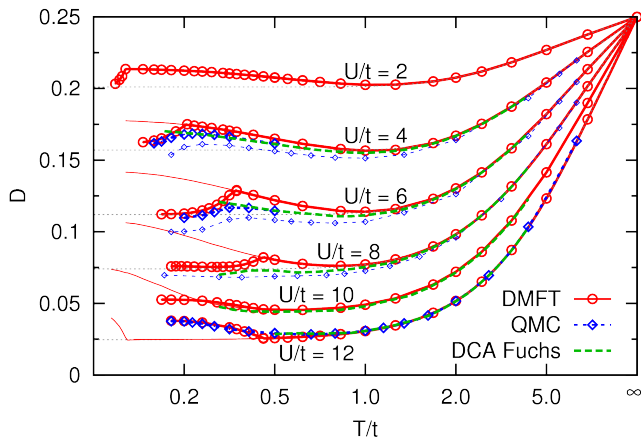
Weak and moderate coupling: qualitatively new physics



AF destroys Fermi liquid low- T enhancement of D at $U \lesssim 10$

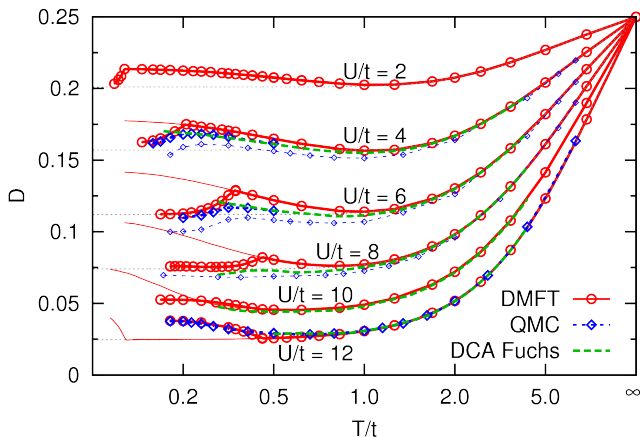
DMFT phase transition at $s = \log(2)$ only in strong coupling limit!

Comparison DMFT – direct QMC for the 3d cubic lattice ($n = 1$)



Excellent general agreement DMFT \leftrightarrow QMC, even at small U

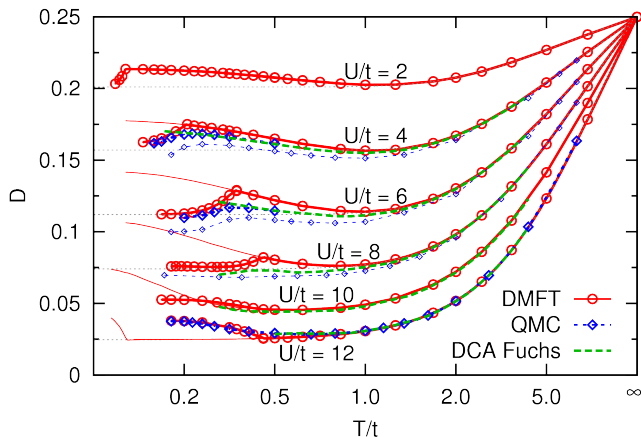
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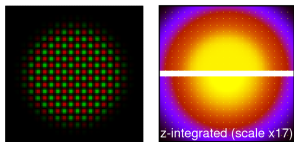


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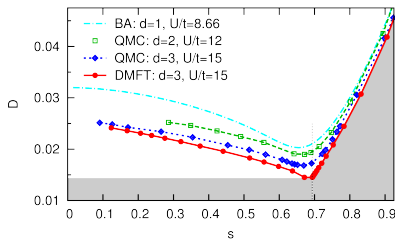
Typical QMC discretization errors (thin lines) larger than DMFT deviations!

Summary and Outlook

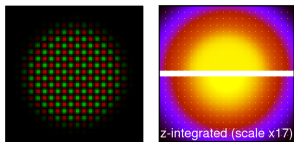


RDMFT: accurate approach for inhomogeneous correlated Fermi systems (cold atoms or materials)

Double occupancy: universal probe of AF correlations and entropy
Relevant **entropy scale** for ultracold experiments (local probes): $s \approx \log(2)$

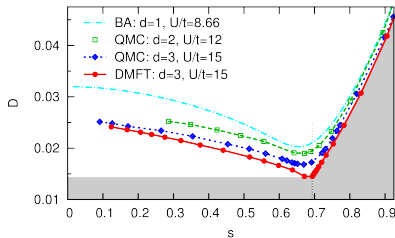


Summary and Outlook



RDMFT: accurate approach for inhomogeneous correlated Fermi systems (cold atoms or materials)

Double occupancy: universal probe of AF correlations and entropy
Relevant **entropy scale** for ultracold experiments (local probes): $s \approx \log(2)$



Frustration: cold atoms [Esslinger group!] and **materials**

Inhomogeneities, e.g. impurity atom in harmonic trap

Inequivalent flavors (\sim orbital-selective Mott transitions), **multi-flavor**