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

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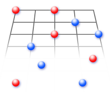
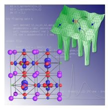


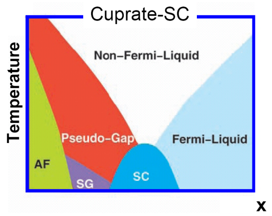
TR 49: *Condensed matter systems with variable many-body interactions*
Frankfurt / Kaiserslautern / Mainz

FOR 1346
LDA+DMFT
Augsburg *et al.*

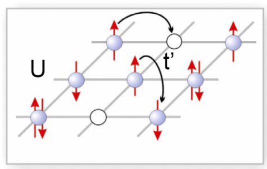


Motivation: Ultracold lattice fermions as quantum simulators?

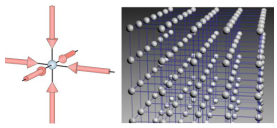
Correlated materials



Fermionic Hubbard model



Ultracold fermions on optical lattices



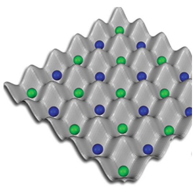
$\mathcal{O}(10^5)$ atoms

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:

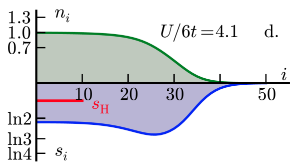
(i) difficult to reach sufficiently low temperatures/entropies
(ii) detection of AF order is not straightforward
(iii) inhomogeneity, time scale for global (spin) equilibrium



Questions for this talk

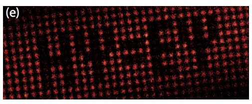
- How to detect AF order/correlations?
- Which entropy range is needed/interesting?
- General impact of dimensionality?

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

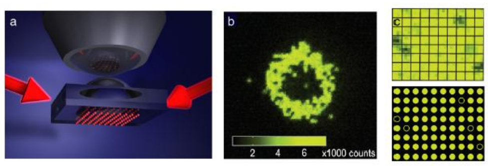


[Jördens et al., PRL **104**, 180401 (2010)]

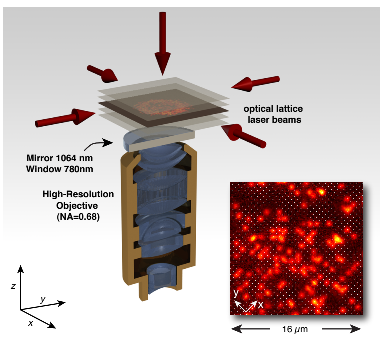
Experimental advantage of 2 dimensions: single-site resolution (for bosons)



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



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



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

Outline

Motivation: Ultracold lattice fermions as quantum simulators?

How to detect AF order/correlations? Is NN spin correlation useful?

Néel transition of lattice fermions in a harmonic trap
[Gorelik, Titvinidze, Hofstetter, Snoek, Blümer, PRL (2010)]

Effects of non-local correlations? DMFT versus direct QMC + BA
[Gorelik, Paiva, Scalettar, Klümper, Blümer, arXiv:1105.3356]

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

Summary and outlook

How to detect AF order/correlations?

Obvious choice: order parameter

$$m^z_{stag} = \frac{1}{N}\Big[\sum_{i\in A}\langle n_{i\uparrow}-n_{i\downarrow}\rangle - \sum_{i\in B}\langle n_{i\uparrow}-n_{i\downarrow}\rangle\Big]$$

(equivalent sublattices A and B)

$\rightsquigarrow$ specific and sharp signal at/below T_N

but: need right orientation, $T \lesssim T_N$

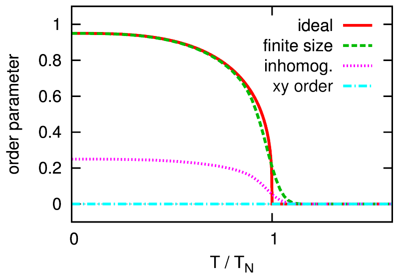
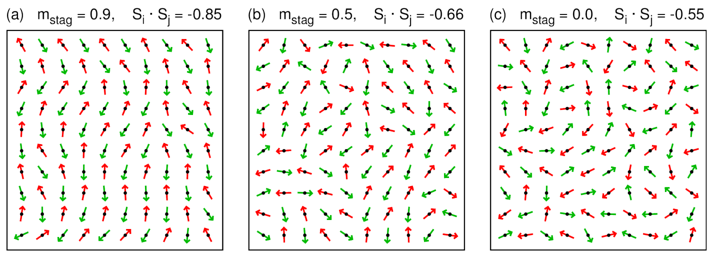


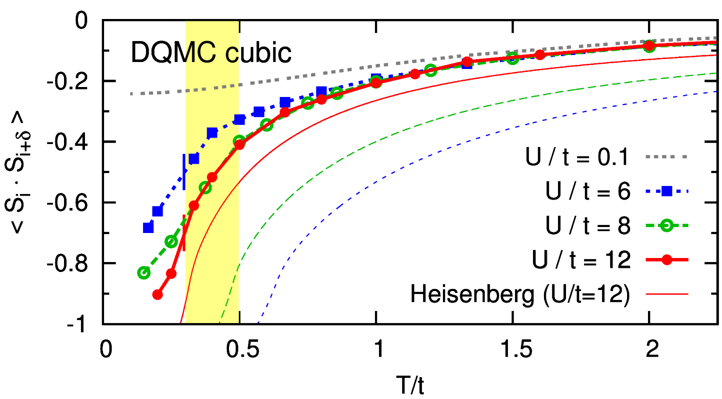
Illustration: weak order not apparent in small snapshot

$\rightsquigarrow$ look at NN correlations?



Current experimental focus: nearest-neighbor spin correlation function

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



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

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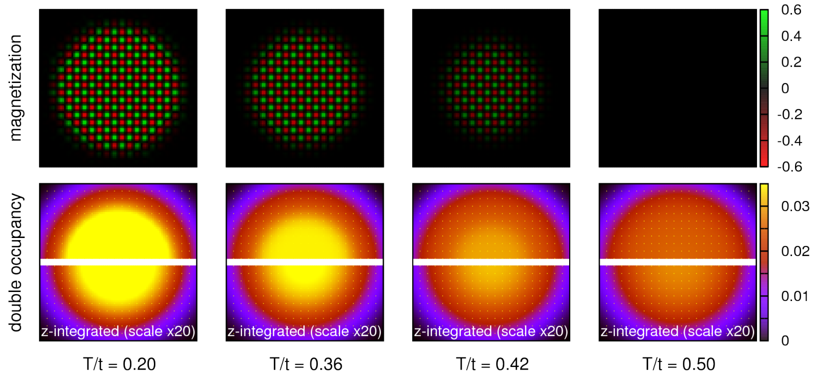
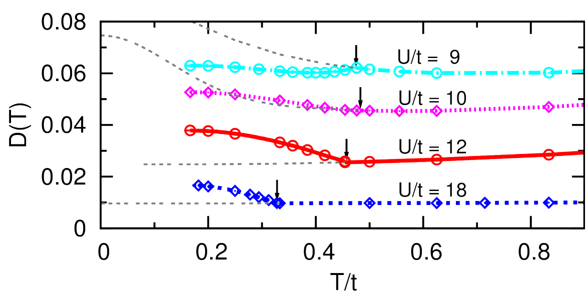
RDMFT-QMC results for cubic lattice ($V = 0.05t$, $U = W = 12t$)



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)]

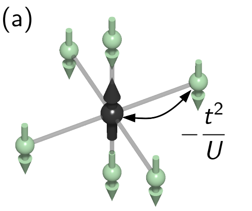
DMFT-QMC estimates of double occupancy D at half filling



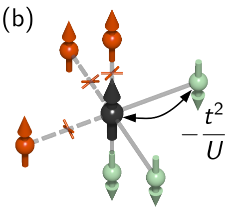
At $U \gtrsim 10t$: D enhanced below Néel temperature (arrows)

Thin lines: metastable nonmagnetic phase

(a)



(b)



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

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

Thus: $D \sim$ NN correlations

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

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

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

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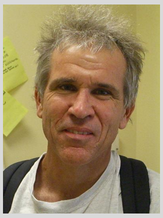
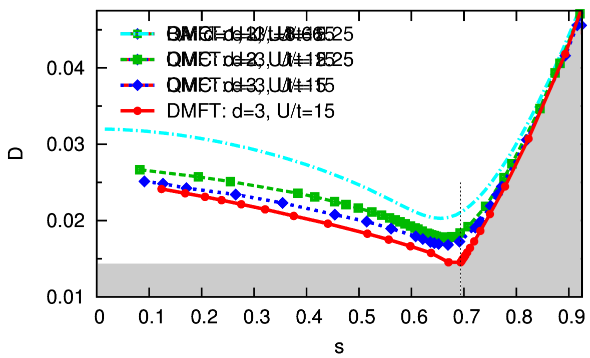


Richard Scalettar
UC Davis

Double occupancy as a universal measure of AF correlations + entropy



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

No features seen at $d = 3$ Néel transition

Minimum of $D(s)$ at $s \approx \log 2$ for all d!

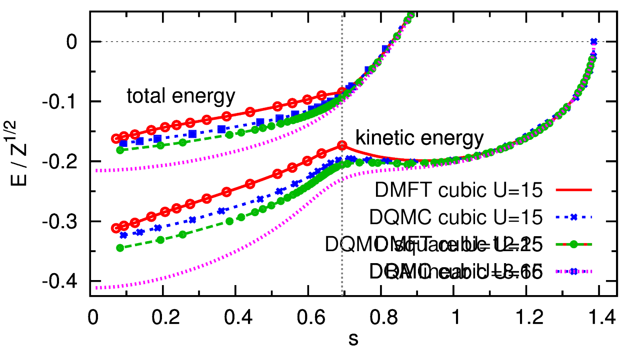
Interesting physics at $\log(2)/2 \lesssim s \lesssim \log(2)$!?

AF enhancement of D is larger in lower dimensions:

$$D_0 = (1 - \langle \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \rangle)\, Z \frac{t^2}{2U^2} + \mathcal{O}\left(t^4/U^4\right)$$

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

Related observable: kinetic energy

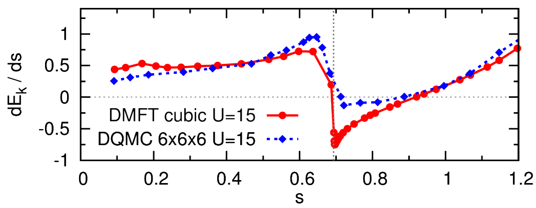


Kink in kinetic energy (only) at $s \approx \log(2)$

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

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

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

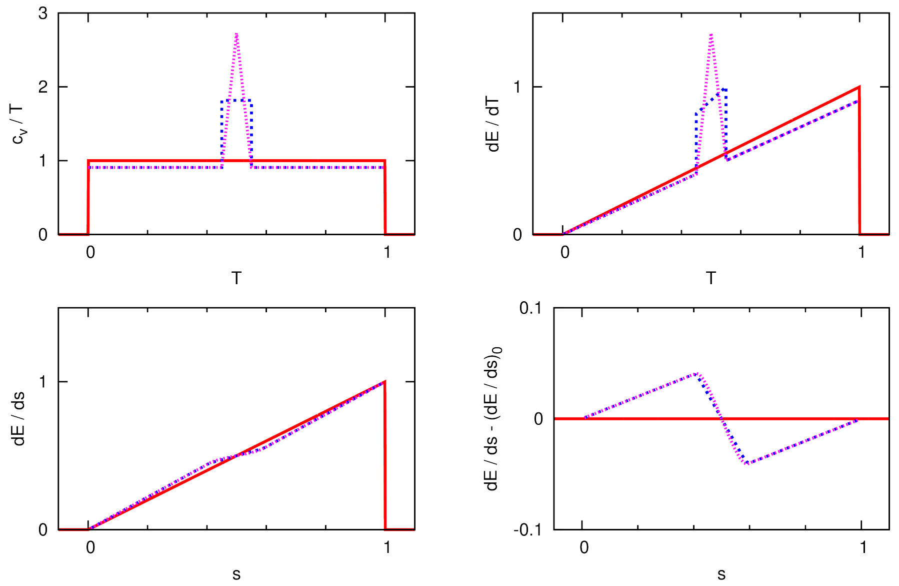


Why no signature at $d = 3$ phase transition (Ehrenfest)?

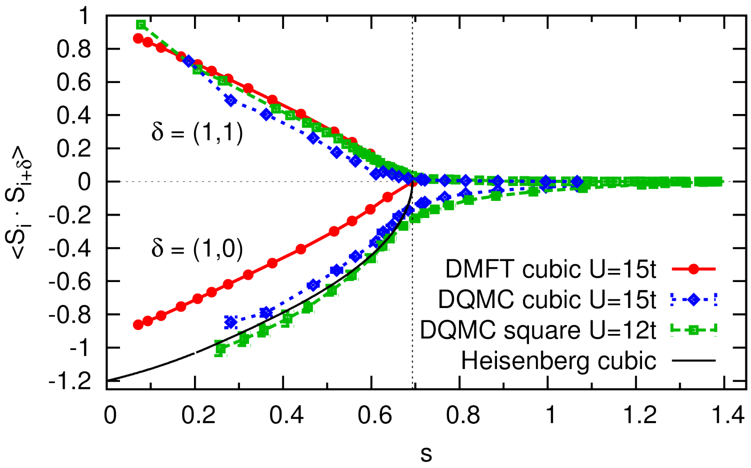
Finite-size effects, num. noise

Specific heat smoothed vs. s

Illustration: from dE/dT to dE/ds

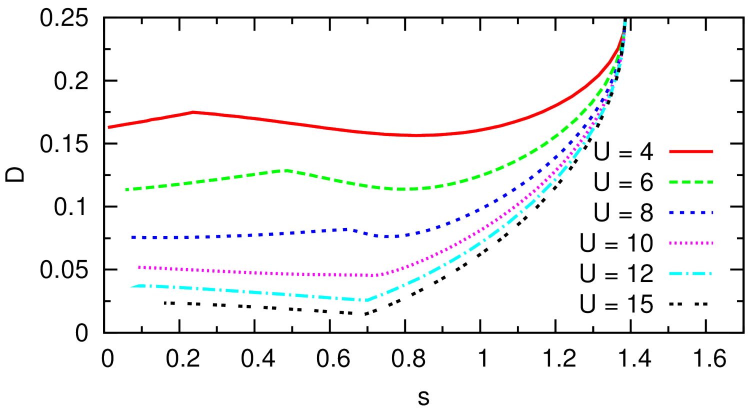


Spin correlation functions: what range is needed?



NNN spin correlation function signals: Heisenberg regime, low entropy

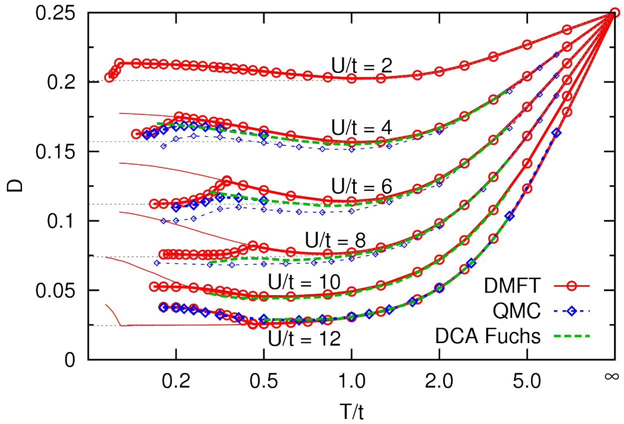
Weak and moderate coupling: qualitatively new physics



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 ($n = 1$)

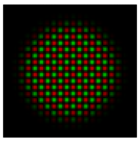
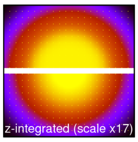


Excellent general agreement DMFT ↔ QMC, even at small U

DCA study [Fuchs et al., PRL (2011)] misses AF signatures

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

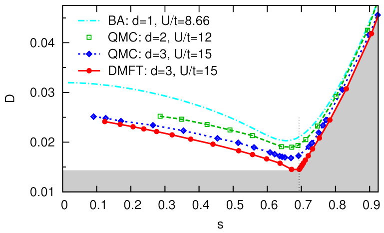
Summary and Outlook

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): $s \approx \log(2)$



Frustration: cold atoms [Esslinger group!] and materials

Inhomogeneities, e.g. impurity atom in harmonic trap

Inequivalent flavors (∼ orbital-selective Mott transitions), multi-flavor