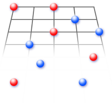
Double occupancy as a universal probe for antiferromagnetic correlations and entropy in cold fermions on optical lattices

Nils Blümer

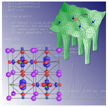
Institut für Physik, Johannes Gutenberg-Universität Mainz

JOHANNES GUTENBERG UNIVERSITÄT MAINZ



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

FOR 1346
LDA+DMFT
Augsburg *et al.*



Outline

Motivation: Ultracold lattice fermions as quantum simulators?

Detection of antiferromagnetic correlations in cold fermions

[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]

Realistic modeling: anisotropic trap ("slab" method $\sim$ GGA)

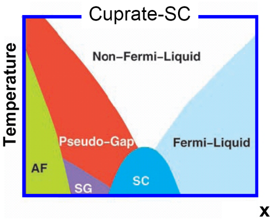
[Gorelik, Blümer, to appear in JLTP]

Characteristic temperature of pseudogap in $2d$ Hubbard model?

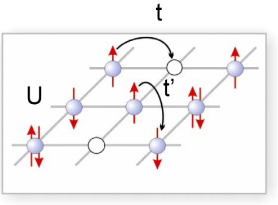
Summary and outlook

Motivation: Ultracold lattice fermions as quantum simulators?

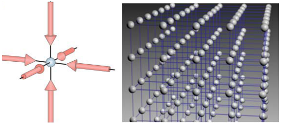
Correlated materials



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)]

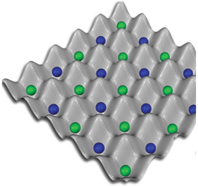
Remaining challenge: antiferromagnetism (staggered order)

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

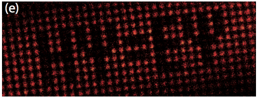


Questions for first part of this talk

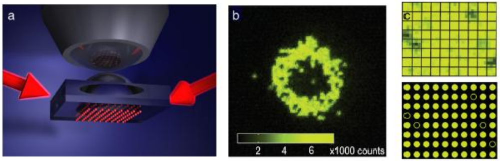
- How to detect AF order/correlations?
- Which entropy range is needed?
- General impact of dimensionality?

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

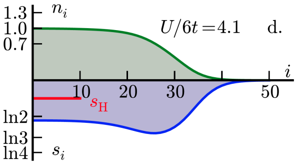
Experimental advantage of 2 dimensions:
single-site resolution (for bosons)



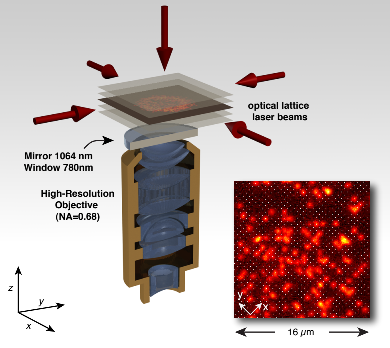
[Würtz et al., PRL **103**, 080404 (2009)]



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

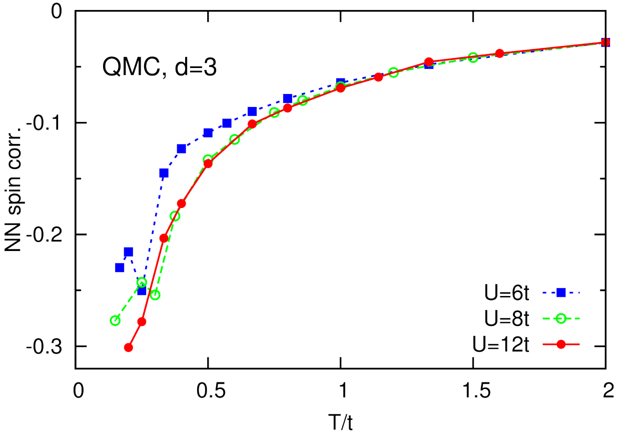


[Jördens et al., PRL **104**, 180401 (2010)]



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

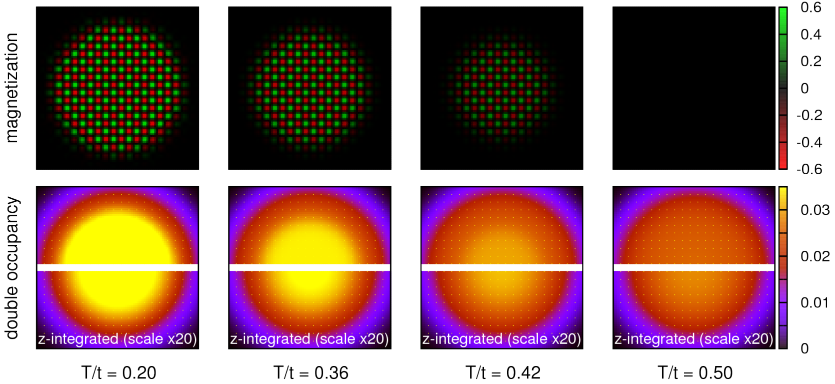
Modulation spectroscopy (Esslinger group), super-lattice (Bloch group)



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

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

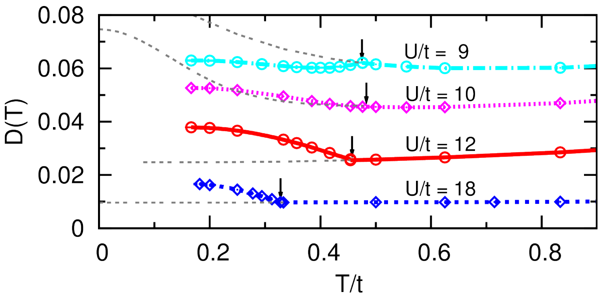
Background: RDMFT-QMC (cubic lattice, $V = 0.05t$, $U = W = 12t$)



Proposal: enhanced double occupancy (i.e. interaction energy) as a signature of antiferromagnetic order at strong coupling

[Gorelik, Titvinidze, Hofstetter, Snoek, Blümer, PRL (2010)]

DMFT-QMC estimates of double occupancy D at half filling



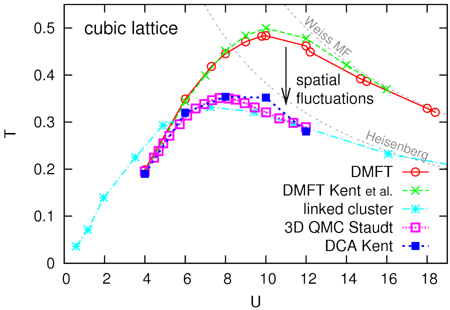
At $U \gtrsim 10t$:

D enhanced below Néel temperature (arrows)

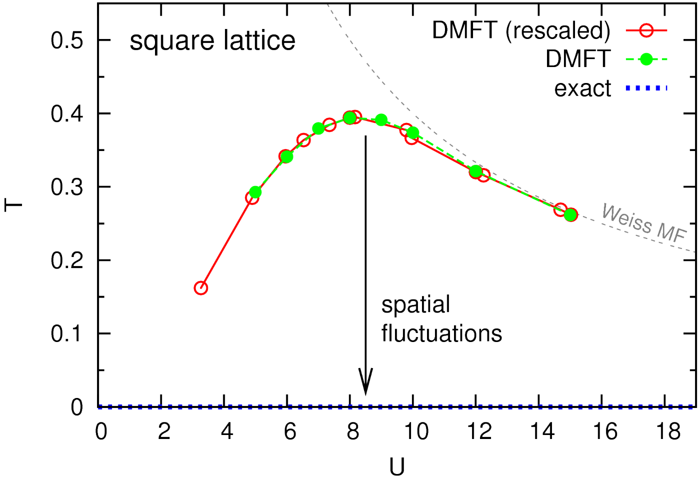
Thin lines: metastable nonmagnetic phase

Problem: DMFT overestimates ordering temperatures

$\rightsquigarrow$ kinks cannot remain at $T = T_{\mathrm{N}}^{\mathrm{DMFT}} > T_{\mathrm{N}}$!



Situation "worse" in 2 dimensions: $T_\mathrm{N} = 0 \ll T_\mathrm{N}^\mathrm{DMFT}$!



Mermin-Wagner theorem excludes AF long-range order at finite temperatures

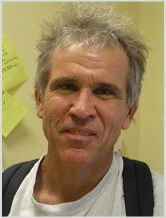
Effects of non-local correlations?
Comparisons with direct QMC + BA

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

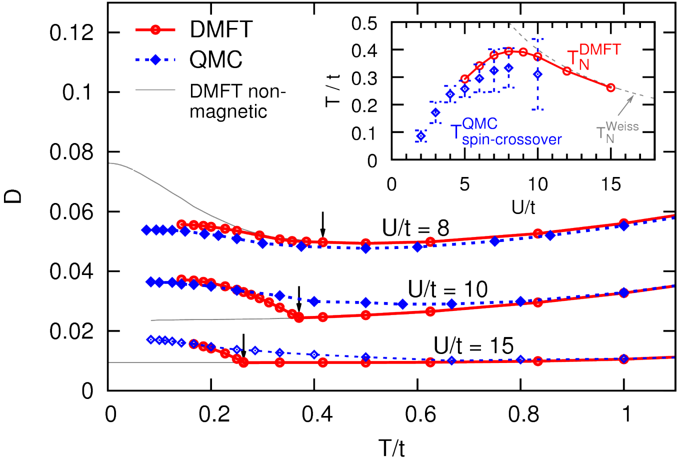
Elena Gorelik
Univ. Mainz

Andreas Klümper
Univ. Wuppertal

Thereza Paiva
Rio de Janeiro



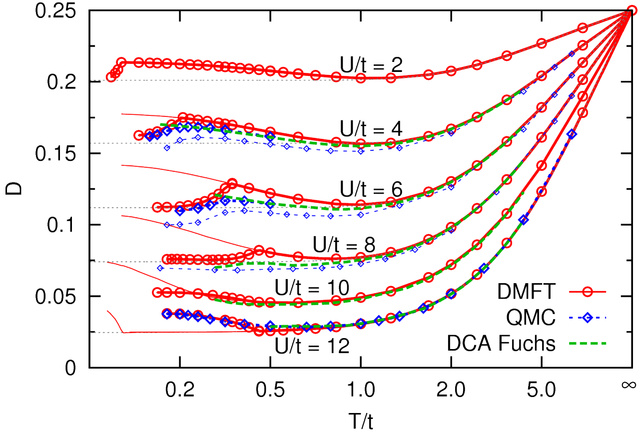
Richard Scalettar
UC Davis



AF DMFT confirmed at high T and at low T, rounding off at $T \approx T_N^{\mathrm{DMFT}}$

Nonmagnetic DMFT completely off at low T!!!

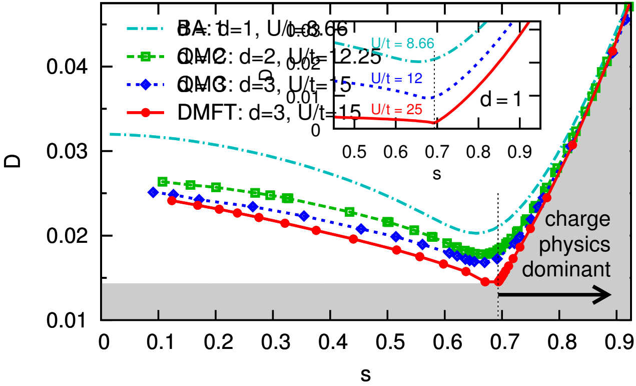
Comparison DMFT – direct QMC for the 3d cubic lattice ($n = 1$)



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!



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

No features seen at $d = 3$ Néel transition

Local probes see only short-range AF $\rightsquigarrow$ needed: $s \lesssim log(2)$, not $s \lesssim log(2)/2$

AF enhancement of D is larger in lower dimensions:

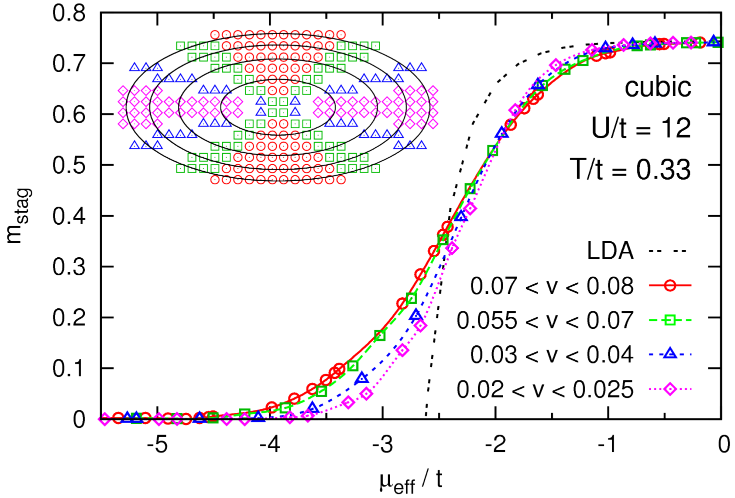
$$D_0 = (1 - \langle \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \rangle)\, Z \frac{t^2}{2U^2} + \mathcal{O}\left(t^4/U^4\right)$$

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

Realistic modeling: anisotropic trap

[Gorelik, Blümer, to appear in JLTP]

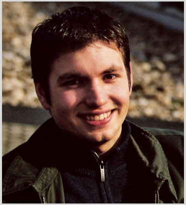
RDMFT for anisotropic trap (aspect ratio 4:1)



Quantification of trap anisotropy: $v = \frac{|\nabla V|^2}{4V} = \frac{V_\parallel^2 (z/a)^2 + V_\perp^2 (\rho/a)^2}{V_\parallel (z/a)^2 + V_\perp (\rho/a)^2}$,

Characteristic temperature of pseudogap in the two-dimensional Hubbard model?

[Preliminary results]



Daniel Rost
Univ. Mainz

Fakher Assaad
Univ. Würzburg

Pseudogap in square lattice Hubbard model from DQMC

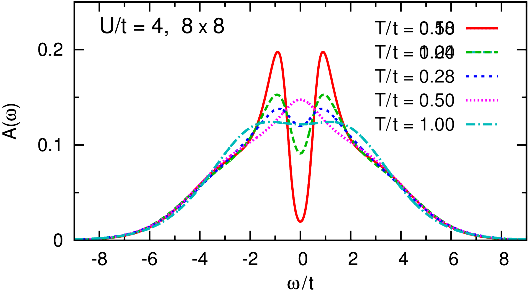
Spectral function (test case for quasi-CT determinantal DQMC and MEM)

At weak coupling ($U = 4t$):

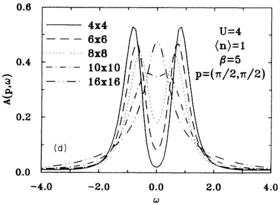
FL peak at intermediate T

Pseudogap for $T \lesssim T_N^{\mathrm{DMFT}}$

– coincidence?

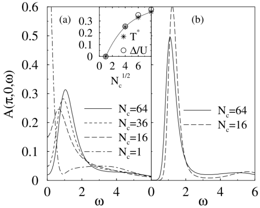


Existence and nature of pseudogap: long controversy!



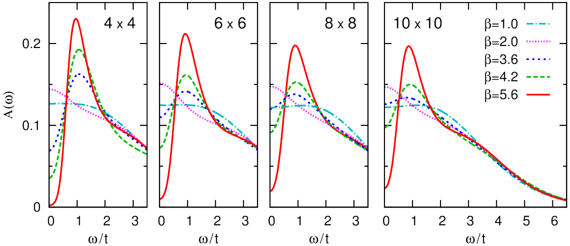
Gap is finite-size effect

[White, PRB (1992)]

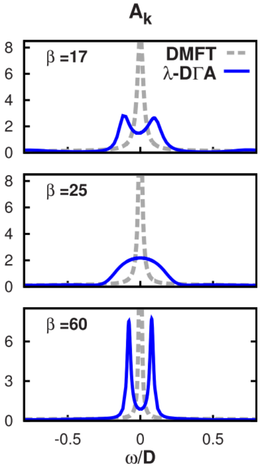


DCA/QMC $\rightsquigarrow$ gap

[Huscroft et al., PRL (2001)]

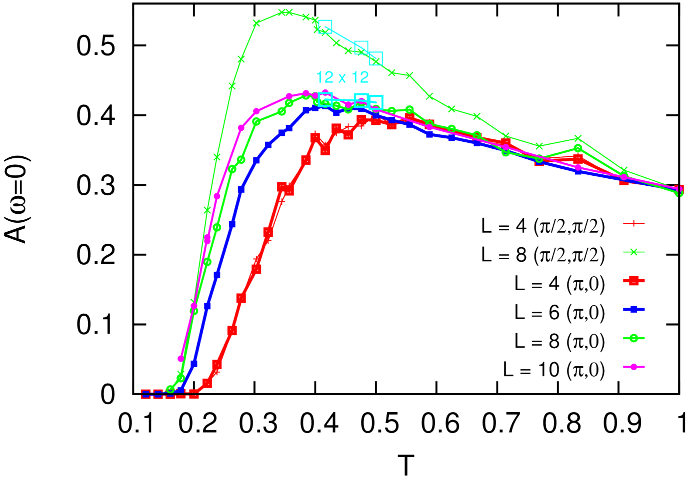


Sweeps + $\Delta\tau$ important; moderate finite-size effects



DΓA: reentrant behavior

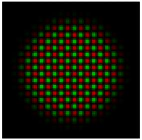
[Katanin et al., PRB (2009)]

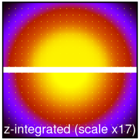


Crossover-temperature seems to converge to $T \gtrsim T_{\mathrm{N}}^{\mathrm{DMFT}} \approx 0.25t$!

Same picture as for double occupancy!

Summary

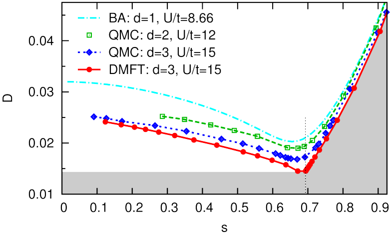


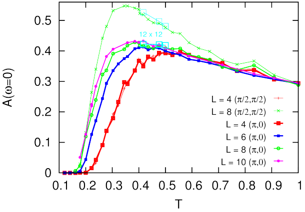


RDMFT: accurate approach for inhomogeneous correlated Fermi systems (cold atoms or materials)

Double occupancy: universal probe of AF correlations and entropy

Relevant **entropy scale** for ultracold experiments (local probes): $s \approx \log(2)$





Characteristic pseudogap temperature in half-filled 2-dimensional Hubbard model

Outlook

New capabilities: entropy, dynamical information, anisotropy, DQMC

Methodological exchange with Hofstetter group (impurity solvers)

Experimental signatures of antiferromagnetic correlations

Impact of dimensionality (DMFT versus DQMC)

Frustration: cold atoms and materials

Inhomogeneities, e.g. impurity atom in harmonic trap

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