Universal probes for antiferromagnetic correlations and entropy in cold fermions on optical lattices

E. V. Gorelik,[1] D. Rost,[1] T. Paiva,[2] R. Scalettar,[3] A. Klümper,[4] and N. Blümer[1]

[1] *Institute of Physics, Johannes Gutenberg University, Mainz, Germany*
[2] *Instituto de Fisica, Universidade Federal do Rio de Janeiro, Brazil*
[3] *Department of Physics, UC Davis, USA*
[4] *University of Wuppertal, Wuppertal, Germany*

(Dated: December 29, 2011)

We determine antiferromagnetic (AF) signatures in the half-filled Hubbard model at strong coupling for a cubic lattice and in lower dimensions. Upon cooling, the transition from the charge-excitation regime to the AF Heisenberg regime is signaled by a universal minimum of the double occupancy at entropy $S/(Nk_\mathrm{B}) \approx \log(2)$ per particle and a linear increase of the next-nearest neighbor (NNN) spin correlation function below. This crossover, driven by a gain in kinetic exchange energy, appears as the essential AF physics relevant for current cold-atom experiments. The detection of long-range AF order requires measurements of spin correlations at or beyond NNN distances.

PACS numbers: 67.85.-d, 03.75.Ss, 71.10.Fd, 75.10.-b

Materials with strong electronic correlations are, due to their increasing technological importance, e.g., in magnetoresistive and superconducting devices, a prime subject of current research [1, 2]. Theoretical investigations of corresponding Hubbard type models have shed light on many strong-coupling phenomena including metal-insulator transitions, non-Fermi-liquid behavior, and various types of magnetic and orbital order [3]. However, important open questions remain, most notably regarding high-temperature superconductivity, for which so far no mechanism could be established. Recently, a novel class of correlated Fermi systems, namely ultracold fermionic atoms (such as ^{40}K and ^{6}Li) on optical lattices, has opened a new promising direction of research: cold atoms are predicted to serve as *quantum simulators* for the Hubbard type solid-state Hamiltonians of interest [4–6].

Indeed, the Mott metal-insulator transition was recently demonstrated in two-flavor mixtures of ^{40}K on cubic optical lattices by experimental observation and quantitative theoretical analysis of signatures in the compressibility [7] and in the double occupancy [8]. This success established that the single-band Hubbard model

$$\hat{H} = -t \sum_{\langle ij\rangle,\sigma} \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \qquad (1)$$

(with hopping amplitude t, on-site interaction U, and $\hat{n}_{i\sigma} = \hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma}$) can be realized to a reasonable accuracy using ultracold fermions in the interesting interaction range, which certainly supports the hopes of accessing also less understood Hubbard physics in similar ways.

However, all attempts of realizing and detecting *quantum magnetism* in cold lattice fermions have failed so far. In fact, it has not even been possible yet to verify specific signatures of antiferromagnetic (AF) correlations which are ubiquitous in correlated electrons and believed to play an important role in high-temperature superconductivity. This type of physics clearly has to be under control before cold fermions can really play a useful role as *quantum simulators*. Up to now the failures to detect AF signals have primarily been attributed to cooling issues [9, 10]. Indeed, the coldest systems achieved so far have central entropies per particle of $s \equiv S/(Nk_B) \approx \log(2) \approx 0.69$ [11] while AF long-range order (LRO) on a cubic lattice is expected only for entropies $s < s_\mathrm{N} \approx 0.34$ [9, 12, 13].

We will argue in the following that this discrepancy, by a factor of 2, is *not* the primary issue for current AF related cold-atom experiments, which try to extract information about the nearest-neighbor (NN) spin correlation function $\langle\hat{\boldsymbol{\sigma}}_i \cdot \hat{\boldsymbol{\sigma}}_j\rangle$ (for Pauli matrices $\hat{\boldsymbol{\sigma}}$) from modulation spectroscopy measurements [9, 14] or a superlattice approach [15]. While this observable should, in principle, reveal the Néel transition at least in the Heisenberg limit (where it corresponds to the energy), already the role of the entropy as the relevant thermodynamic variable in the cold-atom context makes this route impractical, with overly subtle features in $\langle\hat{\boldsymbol{\sigma}}_i \cdot \hat{\boldsymbol{\sigma}}_j\rangle(s)$ at s_N even in the thermodynamic limit (cf. Fig. 4). For the inhomogeneous systems realized in fermionic experiments, with a shortest experimental length scale of about 10 lattice spacings [16], the concept of LRO appears of limited value anyway.

Accepting that true LRO, defined by the infinite-distance limit of spin correlations, is not directly relevant for cold atoms, one may ask: (i) is there a threshold distance beyond which spin correlations have "long-range characteristics" and (ii) can we define "finite-range antiferromagnetism" as a unique scenario with universal properties, appearing only in a certain entropy range? The answer to both questions is "yes": quite interesting AF correlation physics emerges at entropies $s \lesssim \log(2)$, i.e. in reach of current cooling techniques. Since, in addition, the threshold distance turns out to be rather small (but larger than one lattice spacing), our quantitative predictions should enable experimentalists to verify specific AF signatures with current system sizes, i.e., to get the long-sought grip on *quantum magnetism*.

In the following, we will first discuss an enhancement of the double occupancy D (i.e. also of the interaction energy $D\,U$) at low temperatures T which has previously been proposed as an AF signature on the basis of dynamical mean-field theory (DMFT) [17]. DMFT results for a half-filled cubic lattice at strong coupling $U/t = 15$ are, then, compared with numerically exact determinantal quantum Monte Carlo (DQMC) [18] data. The comparison is extended to the full dimensional range based on DQMC and Bethe ansatz (BA) [19] results in dimensions $d = 2$ and $d = 1$. In addition to $D(T)$, we obtain high-precision estimates of the entropy $s(T)$ in all cases, enabling us to switch to the experimentally relevant entropy representation. An asymptotic collapse of the curves $D(s)$ is observed as a function of dimensionality, with universal minima at $s \approx \log(2)$ and no significant features at $s_{\rm N}$ in the cubic case. Additional specific signatures of short-range AF order are found in the kinetic energy and in spin correlation functions, with different degrees of universality. Finally, the perspectives for detecting LRO are discussed using stochastic series expansion (SSE) results for the Heisenberg model.

AF signatures in the double occupancy – According to DMFT, the low-T formation of an AF core in a fermionic cloud on an optical lattice (with central half filling, $n = 1$) is signaled, at strong coupling, by a distinct enhancement of D in the same region [17]. Such relation between double occupancy and AF correlations follows for a half-filled system in the ground state from second-order perturbation theory [cf. Eq. (2)]. As a function of temperature, DMFT predicts nearly flat curves $D(T)$ in the range $T \gtrsim T_{\rm N}^{\rm DMFT}$, i.e. above its estimate of the Néel temperature, and a sharp increase below, with a kink and absolute minimum at $T_{\rm N}^{\rm DMFT}$. This is clearly seen, for $U/t = 15$, in Fig. 1a (circles). The absolute low-T increase of D is largest for $U/t \approx 12$; it should be detectable, according to real-space DMFT, even in experiments integrating over the inhomogeneous cloud [17].

Not all aspects of this DMFT scenario are, however, realistic: after all, DMFT is exact only in the limit of infinite coordination number $Z \to \infty$ (with $Z = 2d$ for hypercubic lattices) and overestimates the Néel temperature by up to 30% in the simple cubic case [20, 21]. Thus, the sharp kink in $D(T)$ seen in Fig. 1a at $T_{\rm N}^{\rm DMFT} \approx 0.4t$ cannot be physical. One might expect a shift of the DMFT results towards *lower* temperatures, as well as some broadening in the cubic case and more radical changes (at least) for $d \leq 2$; only at high temperatures the accuracy of DMFT estimates for D follows already from series expansions (in $d = 3$) [22].

Impact of dimensionality – Indeed, DQMC estimates of $D(T)$ (diamonds in Fig. 1a) agree with DMFT for $T/t \gtrsim 1$ within error bars, which are smaller than symbol sizes (after elimination of Trotter errors both from the DQMC results and from the Hirsch-Fye QMC [23, 24]

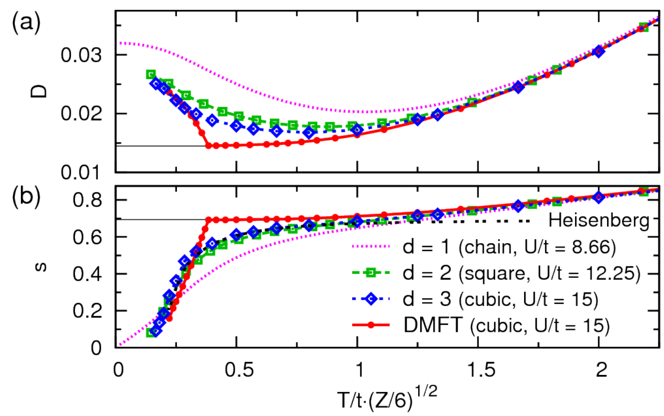

FIG. 1. (Color online) Hypercubic lattice ($1 \leq d \leq 3$) at strong coupling $U/(\sqrt{Z}t) \approx 6$: a) Double occupancy $D(T)$ as estimated from DMFT ($d = 3$, circles), DQMC ($d = 3$: diamonds, $d = 3$: squares), and BA ($d = 1$, dotted line). b) Corresponding estimates of entropy per particle $s = S/(Nk_{\rm B})$.

DMFT data) [25]. Surprisingly good agreement is observed also at $T/t \lesssim 0.3$; only the DMFT kink is smeared out in the DQMC data towards a broad minimum. This trend continues when going to $d = 2$ (squares) at suitably rescaled [26] interactions; however, the quantitative differences between $d = 3$ and $d = 2$ are minimal. The case $d = 1$ (dotted line) deviates more drastically (at intermediate and low T), with still similar general shape. Note that the position of the minimum in $D(T)$ shifts *upwards* with decreasing d, i.e. opposite to the naive expectation.

As optical lattice and interactions are switched on for the ultracold atoms in a nearly adiabatic process, the entropy s (and not T) is the experimentally relevant control parameter. Fig. 1b shows numerically exact data for $s(T)$, obtained directly for $d = 1$ and via the thermodynamic relation $S(\beta) = \log(4) + \beta E(\beta) - \int_0^\beta d\beta' E(\beta')$ [valid for $n = 1$, with $\beta = 1/(k_B T)$ and energy E] for $d = 2, 3$ and DMFT. Again, the agreement between $d = 2$ and $d = 3$ is striking; the latter results converge to the Heisenberg limit for $T \lesssim 0.8t$. Remarkably, the proper DMFT solution (circles) approaches the DQMC result for the cubic lattice (diamonds) at $T \lesssim 0.3t$; only the (metastable) nonmagnetic DMFT solution (thin solid lines), considered in previous studies [22], remains far off.

Fig. 2, obtained by combining the data of both panels of Fig. 1 illustrates our first central message: as a function of entropy, the double occupancy is surprisingly universal at strong coupling, with a minimum at $s \approx \log(2)$ in all dimensions (and generally similar shapes). At constant rescaled interaction U, the curvature around the minimum increases with increasing dimensionality until it becomes sharp in the DMFT limit, where it corresponds to the Néel transition. As seen in the inset (for $d = 1$), the minimum becomes also sharp and approaches $\log(2)$ at constant dimensionality in the strong-coupling limit $U \to \infty$. Evidently, the minimum in

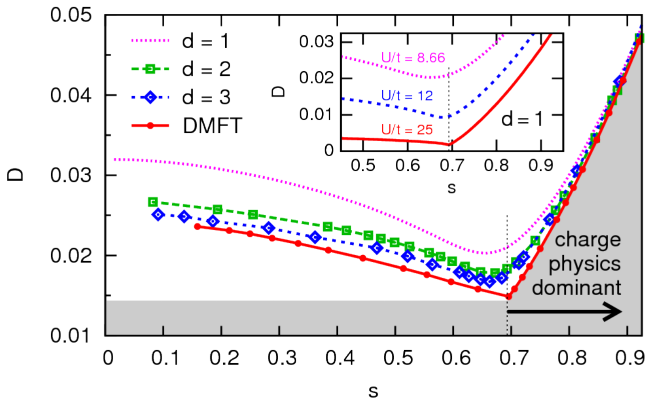

FIG. 2. (Color online) Hypercubic lattice at strong coupling: Double occupancy versus entropy. In all cases, the minimum of the double occupancy corresponds to $s \approx \log(2)$ (dotted line). The shaded area indicates the nonmagnetic contribution to D. Inset: $D(s)$ in $d = 1$ for various interactions.

$D(s)$ separates two regimes with quite different physical properties: (i) the regime $s > \log(2)$ which is adiabatically connected with the uncorrelated Hartree regime with $D = \langle n_\uparrow \rangle \langle n \downarrow \rangle = 0.25$ in the high-temperature limit and (ii) a low-temperature regime, with no discernible sub-structure. It is clear that the latter regime must be characterized by spin coherence, since $s < \log(2)$ is possible for a two-flavor system at $n = 1$ only by the development of (possibly short ranged) AF correlations.

In fact, any positive deviation of $D(s)$ from the non-magnetic background (shaded in Fig. 2) should be linked to AF correlations, generalizing Takahashi's ground state expression [28]

$$D_0 = \frac{Zt^2}{2U^2}\left(1 - \langle \hat{\boldsymbol{\sigma}}_i \cdot \hat{\boldsymbol{\sigma}}_j \rangle_0\right) + \mathcal{O}\left(\frac{t^4}{U^4}\right). \qquad (2)$$

Here, $\langle \hat{\boldsymbol{\sigma}}_i \cdot \hat{\boldsymbol{\sigma}}_j \rangle_0$ is the nearest-neighbor correlation in the quantum Heisenberg model (at $T = 0$): $\langle \hat{\boldsymbol{\sigma}}_i \cdot \hat{\boldsymbol{\sigma}}_j \rangle_0 = -1.00$ ($d = \infty$, Weiss MF); -1.20 ($d = 3$) [29]; -1.34 ($d = 2$) [30, 31]; -1.77 ($d = 1$) [28], which is stronger in lower d, consistent with our finite-T results. Thus, irrespective of the measurement technique, signatures of AF correlations may be easier to detect experimentally (at fixed s) for lower (effective) dimensionality. Conversely, a tuning of the hopping amplitude in z direction could help to discriminate magnetic effects from those of charge excitations; similar ideas including frustration will be explored in a separate publication [32].

Energetics and spin correlations – Up to a numerical prefactor (of $15/\sqrt{6}$), the curves in Fig. 2 represent the rescaled interaction energy $E_{\text{int}}/(\sqrt{Z}t)$. Corresponding AF signatures appear also in the kinetic energy, shown in Fig. 3a. In particular, $E_{\text{kin}}(s)$ exhibits a maximum at $s \approx \log(2)$ for $d \geq 3$ [while the total energy $E(s) = E_{\text{int}}(s) + E_{\text{kin}}(s)$ is always monotonous, as required by thermodynamic consistency]. The associated redistribution of quasi momentum at $s \lesssim \log(2)$ might be a worthwhile experimental target.

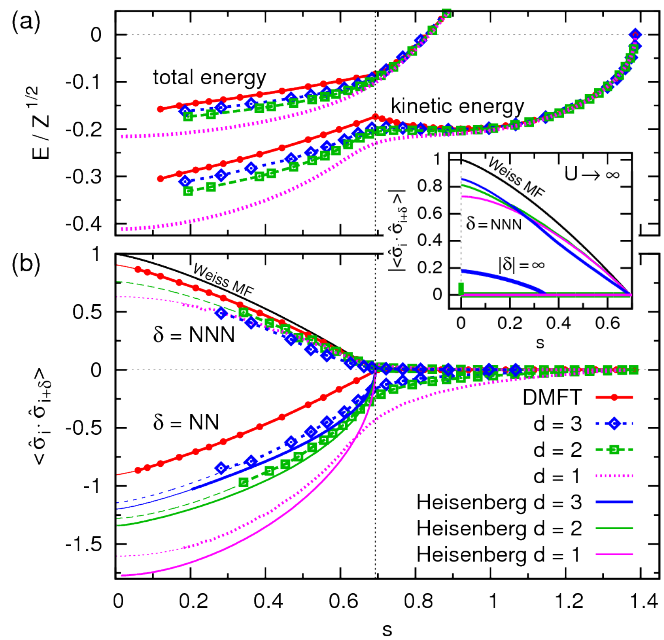

FIG. 3. (Color online) Hypercubic lattice at strong coupling: a) Rescaled total and kinetic energy versus entropy. b) Spin correlations $\langle \hat{\boldsymbol{\sigma}}_i \cdot \hat{\boldsymbol{\sigma}}_{i+\delta} \rangle$ between nearest [$\delta_{d=1} = 1$, $\delta_{d=2} = (1, 0)$, $\delta_{d=3} = (1, 0, 0)$)] and next-nearest [$\delta_{d=1} = 2$, $\delta_{d=2} = (1, 1)$, $\delta_{d=3} = (1, 1, 0)$] neighbours. Inset: NNN and infinite-range spin correlations for Heisenberg model.

As discussed in the introduction, nearest-neighbor (NN) spin correlations are, so far, central in the experimental quest for AF signatures in cold lattice fermions. However, as seen in (the lower part of) Fig. 3b, the NN spin correlation function (symbols and dashed/dotted lines) has strong high-entropy tails in all physical dimensions $d \leq 3$, with only trivial features at $s \approx \log(2)$, below which the Heisenberg model (solid lines) becomes applicable. Conclusions about the presence or proximity of AF order could be drawn from corresponding experimental data only via theoretical look-up tables.

In contrast, the next-nearest-neighbor (NNN) spin correlation functions are essentially zero for $s > \log(2)$ and take off linearly below. So the mere presence of significant NNN correlations already implies that the Heisenberg regime $s < \log(2)$ has been reached. Very remarkably, the results for $d = 1, 2$, and DMFT are indistinguishable for $s \gtrsim 0.5$; only $d = 3$ is slightly below. The same picture emerges in the Heisenberg model (upper set of curves in inset of Fig. 3), with slightly larger absolute values. This near-universality with respect to d establishes that the crossing point between short-range physics, where spin correlations increase with lowering d, and long-range physics, where correlations quickly decay towards low d (and remain finite in the limit $\delta \to \infty$ at $s > 0$ only for $d \geq 3$, cf. lower set of curves in inset of

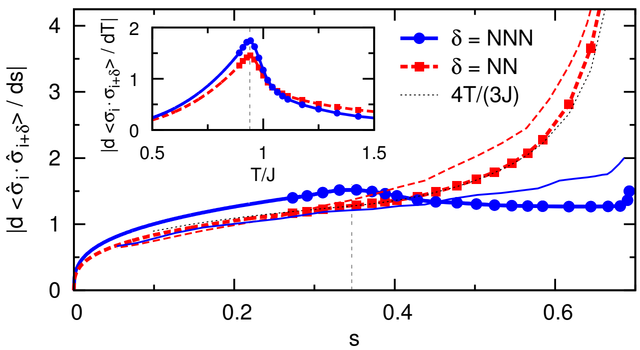

FIG. 4. (Color online) Derivatives of NN (squares) and NNN (circles) spin correlation functions of the Heisenberg model w.r.t. entropy (main panel) and temperature (inset) in $d = 3$. Thin solid and dashed lines: Heisenberg results in $d = 2$.

Fig. 3) is essentially at the NNN distance.

In this sense, spin correlations at or beyond the NNN distance are much more representative of genuine AF physics than the unspecific NN correlations. This is true even regarding the infinite-range limit, as shown in Fig. 4 for the Heisenberg model: While the entropy derivatives of the NN spin correlations in $d = 3$ are featureless [and quite similar to the spin correlations in $d = 2$ (thin lines)], a distinct peak at the critical entropy s_{N} for AF LRO in $d = 3$ is visible in the NNN data (circles), with a nearly flat plateau above. This qualitative difference is specific to the (experimentally motivated) use of the entropy as a control paramater: in temperature derivatives, both NN and NNN spin correlations reveal the specific-heat peak at T_{N} (see inset of Fig. 4). These conclusions are certainly also valid for the Hubbard model at $U/t = 15$; however, unavoidable noise in the DQMC data of Fig. 3b makes their illustration more difficult. Extrapolating to experiments, with still much larger errors and being confined to the entropy parametrization [33], a detection of the Néel transition via spin correlations would require measurements at least at NNN distances.

Summary and Conclusion – In this Letter, we have studied the half-filled Hubbard model and the Heisenberg model in the full dimensional range, combining the most reliable theoretical methods available today. Thereby we could, for the first time, disentangle generic aspects of antiferromagnetism both from those specific to long-range order (which is not attainable, by definition, in finite atomic clouds) and from trivial correlations between nearest neighbors that persist even in the high-temperature regime where spin models are not adequate. Our results establish that "finite-range antiferromagnetism" is, indeed a useful picture in the regime $s \lesssim \log(2)$ which may be detected experimentally, at strong coupling, by a negative slope in $D(s)$ [or $D(T)$] or by the onset of spin correlations between next-nearest neighbors. This small distance, of roughly two lattice spacings, appears as the threshold beyond which spin correlations are representative of ordering phenomena and increase with increasing dimensionality.

Thus, essential aspects of antiferromagnetism are clearly in experimental reach with current system sizes [16]; tuning dimensionality to $d < 3$ would not suppress, but even enhance AF signatures. Long-range order appears inessential in this scenario; similar conclusions have recently been reached for the magnetism in thin iron layers [38].

Results for weak to intermediate coupling will be presented elsewhere, together with elaborate studies of finite-size effects . . .

[1] Y. Tokura, Phys. Today **56**, 50 (2003).
[2] E. Dagotto, Science **309**, 257 (2005).
[3] V. Anisimov and Y. Izyumov, *Electronic Structure of Strongly Correlated Materials*, Springer Series in Solid-State Sciences, Vol. 163 (Springer, Berlin, 2010).
[4] W. Hofstetter, J. I. Cirac, P. Zoller, E. Demler, and M. D. Lukin Phys. Rev. Lett. **89**, 220407 (2002).
[5] D. Jaksch and P. Zoller, Ann. Phys. (NY) **315**, 52 (2005).
[6] T. Esslinger, Ann. Rev. Cond. Matt. Phys. **1**, 129 (2010).
[7] U. Schneider *et al.*, Science **322**, 1520 (2008).
[8] R. Jördens, N. Strohmaier, K. Günter, H. Moritz, and T. Esslinger, Nature **455**, 204 (2008).
[9] D. Greif, L. Tarruell, T. Uehlinger, R. Jördens, and T. Esslinger, Phys. Rev. Lett. **106**, 145302 (2011).
[10] D. C. McKay and B. DeMarco, Rep. Prog. Phys. **74**, 054401 (2011).
[11] R. Jördens *et al.*, Phys. Rev. Lett. **104**, 180401 (2010).
[12] F. Werner, O. Parcollet, A. Georges, and S. R. Hassan, Phys. Rev. Lett. **95**, 056401 (2005).
[13] S. Wessel, Phys. Rev. B **81**, 052405 (2010).
[14] C. Kollath, A. Iucci, I. P. McCulloch, and T. Giamarchi, Phys. Rev. A **74**, 041604(R) (2006).
[15] S. Trotzky, Yu-Ao Chen, U. Schnorrberger, P. Cheinet, and I. Bloch, Phys. Rev. Lett. **105**, 265303 (2010).
[16] Current experimental trap geometries ($\sim 10^5$ fermions) imply AF cores smaller than $40 \times 40 \times 20$ lattice sites, i.e. each AF site will "feel" a boundary within 10 sites.
[17] E. V. Gorelik, I. Titvinidze, W. Hofstetter, M. Snoek, and N. Blümer, Phys. Rev. Lett. **105**, 065301 (2010).
[18] R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D **24**, 2278 (1981).
[19] G. Jüttner, A. Klümper, and J. Suzuki, Nucl. Phys. B **522**, 471 (1998).
[20] P. R. C. Kent, M. Jarrell, T. A. Maier, and Th. Pruschke, Phys. Rev. B **72**, 060411(R) (2005).
[21] R. Staudt, M. Dzierzawa, and A. Muramatsu, Eur. Phys. J. B **17**, 411 (2000).
[22] L. De Leo, J. Bernier, C. Kollath, A. Georges, and V. W. Scarola, Phys. Rev. A **83**, 023606 (2011).
[23] J. Hirsch and R. Fye, Phys. Rev. Lett. **56**, 2521 (1986).
[24] N. Blümer, Phys. Rev. B **76**, 205120 (2007).
[25] See Supplemental Material at . . . for an analysis of finite-size and Trotter errors.
[26] All scales are set by the root mean square energy $\langle \epsilon^2 \rangle^{1/2}_{U=0} = \sqrt{Z}t$ (for coordination number Z) [27].
[27] E. V. Gorelik and N. Blümer, J. Low Temp. Phys. **165**,

195 (2011).
[28] M. Takahashi, J. Phys. C **10**, 1289-7301 (1977).
[29] J. Oitmaa, C. J. Hamer, and Z. Weihong, Phys. Rev. B **50**, 3877 (1994).
[30] Z. Weihong, J. Oitmaa, and C. J. Hamer, Phys. Rev. B **43**, 8321 (1991).
[31] A. W. Sandvik, Phys. Rev. B **56**, 11678 (1997).
[32] E. V. Gorelik and N. Blümer, in preparation.
[33] Exact correspondence with experiments would require derivatives w.r.t. the *average* (not *central*) entropy per particle in the inhomogeneous cloud, shifting our picture slightly towards T derivatives.
[34] M. Pickel, A. B. Schmidt, M. Weinelt, and M. Donath, Phys. Rev. Lett. **104**, 237204 (2010).
[35] T. Corcovilos, S. Baur, J. Hitchcock, E. Mueller, and R. Hulet, Phys. Rev. A **81**, 013415 (2010).
[36] Th. Paiva, R. Scalettar, M. Randeria, and N. Trivedi, Phys. Rev. Lett. **104**, 066406 (2010).
[37] N. Blümer and E. V. Gorelik, Comp. Phys. Comm. **118**, 115 (2011).
[38] K. G. L. Pedersen, B. M. Andersen, G. M. Bruun, O. F. Syljuåsen, and A. S. Sørensen, Phys. Rev. A **84**, 041603(R) (2011).
[39] S. Fuchs *et al.*, Phys. Rev. Lett. **106**, 030401 (2011).