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

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(Dated: December 21, 2013)

We determine antiferromagnetic (AF) signatures in the half-filled Hubbard model at strong coupling on 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 $s \equiv S/(Nk_B) = s^* \approx \ln(2)$ per particle and a linear increase of the next-nearest neighbor (NNN) spin correlation function for $s < s^*$. This crossover, driven by a gain in kinetic exchange energy, appears as the essential AF physics relevant for current cold-atom experiments. The onset of long-range AF order (at low $s$ on cubic lattices) is hardly visible in nearest-neighbor spin correlations versus $s$, but could be detected in 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, 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 questions remain open, 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, 10].

Indeed, the Mott metal-insulator transition has recently been demonstrated in two-flavor mixtures of $^{40}$K on cubic optical lattices by experimental observation and quantitative theoretical analysis of signatures in the compressibility [4] and in the double occupancy [6]. This success established that the single-band Hubbard model

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

(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, attempts to realize and detect quantum magnetism in cold lattice fermions have proven extremely challenging. In fact, it is even difficult to verify specific signatures of antiferromagnetic (AF) correlations which are believed to play an important role in high-temperature superconductivity. This type of physics clearly has to be under control before cold fermions on optical lattices can really play a useful role as quantum simulators of materials with strong electronic correlations. The failure to detect AF signals has primarily been attributed to cooling issues [9, 10]. Indeed, the coldest experiments for repulsive fermions on optical lattices have thus far reached central entropies per particle of $s \approx S/(Nk_B) \approx \ln(2) \approx 0.7$ [11, 12] while AF long-range order (LRO) on an isotropic cubic lattice is expected only for entropies $s < s_N \approx 0.4$ [2, 13, 14].

An important feature of cold-atom systems is their inhomogeneity, induced by the trapping potential. On the one hand, this is beneficial for quantum magnetism, since entropy is effectively pushed out of a half-filled core: this aspect is a major theme of current research [11, 14–17]. On the other hand, any AF region will necessarily be of limited spatial extent [18], so that the thermodynamic concept of LRO is not fully applicable. In addition, as we will show, the nearest-neighbor (NN) spin correlation function, which is currently addressed (using modulation spectroscopy [9, 13] or superlattices [20]) in AF related experiments, is hardly sensitive to the onset of LRO even in the thermodynamic limit.

In this situation, one may ask the following: (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”: The essential AF correlation physics emerges already at entropies $s \lesssim \ln(2)$, 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 discuss first an enhancement of the double occupancy $D$ (i.e. also of the interaction energy

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\(E_{\text{int}} \equiv D(U)\) at low temperatures \(T\) which has previously been proposed as an AF signature on the basis of dynamical mean-field theory (DMFT) \[21\]. DMFT results for a half-filled cubic lattice at strong coupling \(U/t = 15\) are compared with direct determinantal quantum Monte Carlo (DQMC) \[22, 23\] simulations. The comparison is extended to the full dimensional range based on DQMC and Bethe ansatz (BA) \[24\] data in dimensions \(d = 2\) and \(d = 1\), respectively. High-precision estimates of the entropy \(s(T)\) allow us to switch to the experimentally relevant entropy representation. An asymptotic collapse of the curves \(D(s)\) is observed with respect to dimensionality, with universal minima at \(s^* \approx \ln(2)\), and no significant features at \(s_N\) in the cubic case. Additional specific signatures of finite-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 \[21\]. As a function of temperature, DMFT predicts nearly flat curves \(D(T)\) in the range \(T \gtrsim T_N^{\text{DMFT}}\), i.e., above its estimate of the Néel temperature, and a sharp increase below, with a kink and absolute minimum at \(T_N^{\text{DMFT}}\). This is clearly seen, for \(U/t = 15\), in Fig.1(a) (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 \[21\].

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 \[25, 26\]. Thus, the sharp kink in \(D(T)\) seen in Fig.1(a) at \(T_N^{\text{DMFT}} \approx 0.4t\) cannot be physical. One might expect a shift of the DMFT results toward 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 does the accuracy of DMFT estimates for \(D\) follow already from series expansions (in \(d = 3\)) \[27\].

**Impact of dimensionality.** — Indeed, DQMC estimates of \(D(T)\) [diamonds in Fig.1(a)] agree with DMFT for \(T/t \gtrsim 1\) within error bars, which are smaller than symbol sizes \[25\]. Surprisingly good agreement is observed also at \(T/t \lesssim 0.3\). As expected \[21\], the DMFT kink is smeared out in the DQMC data toward a broad minimum. At suitably rescaled \[52\] interactions, DQMC data for \(d = 2\) (squares) show remarkably similar behavior. Only the case \(d = 1\) (dotted line) deviates more drastically at intermediate and low \(T\). Note that the position of the minimum in \(D(T)\) shifts upward 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 \[11\], the entropy \(s\) (and not \(T\)) is the experimentally relevant control parameter. Fig.1 shows numerically exact data for \(s(T)\), obtained directly for \(d = 1\) and via the thermodynamic relation \(S(\beta) = \ln(4) + \beta E(\beta) - \int_0^\beta d\beta' E(\beta')\) [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) is close to 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 \[27\], remains far off.

Figure 2 obtained by combining the data of both panels of Fig.1 conveys our first central message: As a function of entropy, the double occupancy is surprisingly universal at strong coupling, with a minimum at \(s^* \approx \ln(2)\) 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 \(s^*\) at constant dimensionality in the strong-coupling limit \(U \to \infty\). Evidently, the minimum in \(D(s)\) separates two regimes with quite different physical properties: (i) the regime \(s > s^*\), which smoothly approaches the Hartree limit (with \(D = \langle n_s \rangle \langle n_{\bar{s}} \rangle = 0.25\)) for \(T \to \infty\), and (ii) a low-temperature regime, with no discernible substructure. It is clear that the latter regime must be characterized by spin coherence, since \(s \ll \ln(2)\) can occur in a two-flavor system at \(n = 1\) only by the development of (possibly short ranged) magnetic correlations.

In fact, any positive deviation of \(D(s)\) from the nonmagnetic background (shaded in Fig.2) should be linked to AF correlations, generalizing Takahashi’s ground state
The experimental quest for AF signatures in cold lattice spin correlations are, so far, playing a central role in this sense, spin correlations at or beyond the NNN distance are much more representative of genuine AF correlations in $s > s^*$ distance are much more representative of genuine AF correlations in $s > s^*$, below which the Heisenberg model (solid lines) becomes applicable. Conclusions concerning 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 $s > s^*$ and take off linearly below in all dimensions. So the mere presence of significant NNN correlations already implies that the Heisenberg regime $s < \ln(2)$ has been reached. Remarkably, the results for $d = 1$ and $d = 2$ are indistinguishable (and close to DMFT) for $s > 0.5$: only those for $d = 3$ are slightly below. The same picture emerges in the Heisenberg model (upper set of curves in the 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 spin correlations decay quickly toward low $d$ (and remain finite in the limit of distance $\delta \to \infty$ at $s > 0$ only for $d \geq 3$) [38], cf. the lower set of curves in the inset of 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 LRO, as illustrated in the Heisenberg limit (chosen due to the higher achievable accuracy) in Fig. 1. While the entropy derivatives of the NN spin correlations in $d = 3$ (squares) are featureless [as those of the spin correlations in $d = 2$ (thin lines)], a distinct
FIG. 4. (Color online) Derivatives of NN (squares) and NNN (circles) spin correlation functions of the Heisenberg model with respect to entropy (main panel) and temperature (inset) in $d = 3$. Thin solid and dashed lines: Heisenberg results in $d = 2$. A 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. As a comparison with corresponding $T$ derivatives (with clear peaks at $T_N$ both in the NN and NNN data – see the inset of Fig. 3) shows, this qualitative difference is associated with the use of the entropy as a control parameter. With experiments being confined to this entropy parametrization, it is clear that a detection of the Néel transition via spin correlations would require measurements at least at NNN distances.

**Conclusion.** We have disentangled generic aspects of antiferromagnetism both from those specific to infinite-range order (which is not attainable, by definition, in finite atomic clouds) and from trivial nearest-neighbor correlations that persist even at high temperatures, where spin models are not adequate. Our results establish that the regime $s \lesssim s^* \approx \ln(2)$ is characterized by “finite-range antiferromagnetism” with remarkably universal properties. It may be detected experimentally, at strong coupling, by a negative slope in $D(s)$ [or $D(T)$] or by the onset of longer-range (beyond NN) spin correlations. Long-range order appears inessential in the cold-atom context and largely decoupled from the basic correlation mechanisms (cf. recent iron layer experiments): The mean-field critical entropy $s^*$ is experimentally more relevant than the critical entropy of an infinite system (in $d = 3$). Thus, reaching $s < s_N \approx 0.4$ in cubic systems would not guarantee additional insight and global equilibration (the time scales for which may exceed experimental life times) is not essential. Tuning the dimensionality (and/or adding frustration) for discriminating AF effects appears much more promising.

We thank M. Inoue for help with the BA code, and P.G.J. van Dongen, U. Schneider, R. P. Singh, and L. Tarruell for valuable discussions. Support under ARO Award W911NF0710576 with funds from the DARPA OLE Program, by CNPq, FAPEJ, and INCT on Quantum Information, and by the DFG through SFB/TRR 49 and FOR 1346 is gratefully acknowledged.

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Our fit for $d = 3$, $\delta = \infty$ is based on the $T = 0$ order parameter $s_N$, and the critical exponents.

Taking derivatives with respect to the average entropy per particle in the inhomogeneous cloud would shift our central-$s$ based results slightly toward the $T$ parametrization.

This is also to be expected for AF signatures in dynamic properties such as optical conductivity.

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