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

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We determine short-range antiferromagnetic (AF) signatures in the half-filled Hubbard model at strong coupling using dynamical mean-field theory and numerically exact methods for a cubic lattice and at lower dimensionality. 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 rapid 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. In larger systems, the detection of long-range AF order requires measurements of spin correlations at NNN (or longer) distances.

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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 $s < s_{\mathrm{N}} \approx 0.34$ [10, 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 [10, 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). [It is even less promising] in the finite and inhomogeneous systems realized in fermionic experiments, with a shortest experimental length scale of about 10 lattice spacings [17], for which the concept of LRO appears of limited value.

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" (in a sense to be specified) and (ii) can we define "short-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 and, thereby, 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) [19]. New 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) data. The analysis of the discrepancies is extended to the full dimensional range based on DQMC and Bethe ansatz (BA) 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 picture. 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 [19]. 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 thin solid line, visible for $T < T_{\rm N}^{\rm DMFT} \approx 0.4t$, corresponds to a nonmagnetic DMFT calculation in which all AF correlations are suppressed]. The absolute low-T increase of D is largest for $U/t \approx 12$; it should remain detectable, according to real-space DMFT, even in experiments integrating over the whole inhomogeneous cloud [19].

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 [28, 29]. Thus, the sharp kink in $D(T)$ seen in Fig. 1a at $T_{\rm N}^{\rm DMFT}$ 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 $d \le 2$; only at high temperatures the accuracy

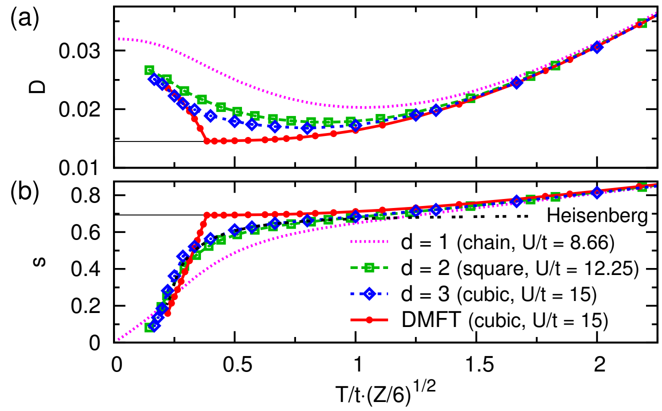

FIG. 1. (Color online) Hypercubic lattice ($1 \le d \le 3$) at strong coupling $U/(\sqrt{Z}t) \approx 6$: a) Double occupancy $D(T)$ as estimated from DMFT ($d = 3$, circles), DQMC ($d = 3$: diamonds, $d = 3$: squares), and BA ($d = 1$, dotted line). b) Corresponding estimates of entropy per particle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

of DMFT estimates for D already follows from series expansions (in $d = 3$) [22].

Impact of dimensionality – Indeed, DQMC estimates for $D(T)$ (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 DMFT data) [31]. Surprisingly good agreement is observed also at $T \lesssim 0.3$; 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 [32] 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 from about $2\,T_{\rm N}^{\rm DMFT}$ in $d = 3$ to $3\,T_{\rm N}^{\rm DMFT}$ in $d = 1$.

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, valid for $n = 1$, $S(\beta) = \log(4) + \beta E(\beta) - \int_0^\beta d\beta' E(\beta')$ [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 AF DMFT solution (circles for $T < T_{\rm N}^{\rm DMFT}$) approaches the DQMC result for the cubic lattice (diamonds) at $T \lesssim 0.3t$; only the nonmagnetic solution (thin solid line), considered in previous studies [22], is far off.

In Fig. 2 we present the experimentally relevant curves $D(s)$, obtained by combining the data of both panels of Fig. 1. While the overall general agreement between the data sets and the regular dimensional convergence at both high and low s already appear striking, our study

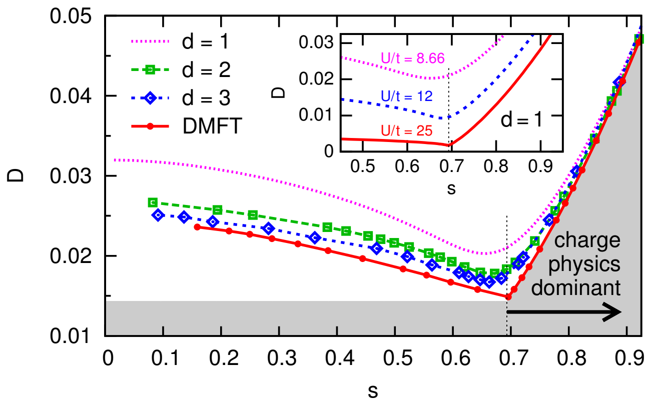

FIG. 2. (Color online) Hypercubic lattice at strong coupling: Double occupancy versus entropy. In all cases, the minimum of the double occupancy corresponds to $s \approx \log(2)$ (dotted line). The shaded area indicates the nonmagnetic contribution to D. Inset: $D(s)$ in $d = 1$ for various interactions.

reveals an important physical fact not realized so far: the minimum in D (at strong coupling) corresponds to $s \approx \log(2) = s_{\mathrm{N}}^{\mathrm{DMFT}}$ in all dimensions, down to $d = 1$. *A posteriori,* this behavior is easy to understand: $s < \log(2)$ is only possible for a two-flavor system at $n = 1$ by spin coherence, i.e. the development of (possibly short ranged) AF correlations; these, in turn, enhance D [19]. A practical consequence of our finding is that, contrary to earlier expectation, cooling to $s < \log(2)$ will give experimental access to AF physics in any dimension at strong coupling; $s < \log(2)/2$ is not needed.

More generally, the evolution of D is a near-perfect thermometer for ultracold atoms measuring AF correlations and (in $d = 3$) the proximity to AF LRO. 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 expression [18]

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

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 ($d = 3$) [33]; -1.34 ($d = 2$) [34, 35]; -1.77 ($d = 1$) [18], 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 [36].

Although going beyond the strong coupling regime may, from the first sight, seem favourable due to the higher values of D, it does not bring any real advan-

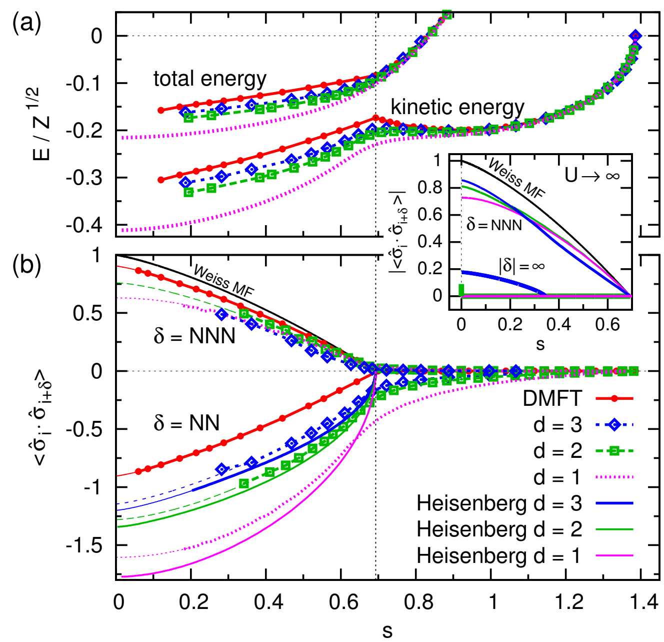

FIG. 3. (Color online) Hypercubic lattice at strong coupling: a) Rescaled total and kinetic energy versus entropy. b) Spin correlations $\langle \hat{\boldsymbol{\sigma}}_i \cdot \hat{\boldsymbol{\sigma}}_{i+\delta} \rangle$ between nearest [$\delta_{d=1} = 1$, $\delta_{d=2} = (1,0)$, $\delta_{d=3} =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

tages. The AF features are less pronounced in double occupancy, as well as in other local observables (i.e. in totel or kinetic energy, spin correlations). Moreover, decreasing the onsite interaction beyond $U/(\sqrt{Z}t) \lesssim 4$ reduce the critical entropy.

AF signatures in other observables – As we just demonstrated above, in the strong coupling regime the onset of local antiferromagnetism is signaled by the minimum in double occupancy at $s \approx s_{\mathrm{N}}^{\mathrm{DMFT}} = \log(2)$. Corresponding signatures appear also in other local observables. So, the kinetic energy E_{kin} in $d = 1$ exhibit shoulder at $s \approx s_{\mathrm{N}}^{\mathrm{DMFT}}$, which transforms into the maximum with increasing the dimensionality, see Fig. 3a. The total energy $E = E_{kin} + UD$ being a monotonous function of entropy shows a kink in this entropy interval. Neither the total energy, nor its kinetic and potential components reveal any visible signature at the Néel phase transition $s_{\mathrm{N}} = \log(2)/2$ in $d = 3$. Although this could be attributed to the finite-size effects or numerical noise in DQMC calculations, the main begetter here is the entropy representation. Indeed, it is easy to show that peaks in specific heat, as appear due to the phase transitions, are heavily suppressed and smoothed when energy is considered as a function of entropy. Our "local probes for local order" conclusion is also supported by the recent experimental observation, that even as a function of temperature local properties are unaffected by magnetic phase transition [41].

Spin correlation functions, and especially the one between the nearest neighbors (NN), are probably the most discussed observables in the context of experimental detection of AF in lattice fermions [10, 14, 15, 40]. The NN spin correlation function appears also as a natural choice from the perspective of the Heisenberg model, describing the relevant spin physics in the strong coupling limit. However, if the onsite interaction is strong-but-finite, NN spin correlation function possess strong high-entropy tails for all finite dimensions d, see Fig. 3b. It does not provide any specific signal, neither by the onset of local spin order at $s_{\mathrm{N}}^{\mathrm{DMFT}} = \log(2)$ nor at the Néel critical entropy in three dimensions $s_{\mathrm{N}} = \log(2)/2$. Therefore it is rather of minor usefullness as an experimental observable to monitor the onset of AF.

It is clear, that the only explicit indication of AF LRO may come from the infinite-range spin correlations, as shown on the inset of Fig. 3 (for the Heisenberg model). However, the experimental relevance of this signal and of the LRO itself is not obvious on the length scale of the experimentally realized systems. And even in the best case, the decrease of the central entropy per particle by factor of 3 to 4 respective to the current state-of-art will be recuired for a detectable signal in $d = 3$, lower dimensions will give no signal at all.

The opposite dimensional tendencies in these two limiting cases (NN vs. LRO) forced us to look in detail into the "intermediate" range. And indeed, already the spin correlations between the next-nearest neighbors (NNN) provide the perfect signal of the local AF: with the dimesion-independent onset at $s \approx s_{\mathrm{N}}^{\mathrm{DMFT}}$ and the absence of high-entropy tails. The entropy dependence of NNN spin correlations is shown in Fig. 3b for the Hubbard model at strong coupling $U/(\sqrt{Z}t) \approx 6$, and on the inset of Fig. 3 for Heisenberg model. Going to larger spin-spin distances will (i) further suppress the amplitude of signal, and (ii) shift down the entropy of the signal onset, with both changes being more pronounced for lower dimensions.

The detailed analysis of spin correlations for the Heisenberg model in $d = 3$ illustrates this special role of the NNN spin correlations. The first temperature derivatives of both NN and NNN spin correlations show typical peak behaviour in the vicinity of the Néel phase transition, see the inset of Fig. 4. In the entropy representation the NN correlation function does not show any discernible feature at the Néel transition, even if one looks at the corresponding derivative (squares in the main panel of Fig. 4). In contrast, the derivative of the NNN correlation function shows a nice peak on a nearly flat background (circles in the main panel of Fig. 4).

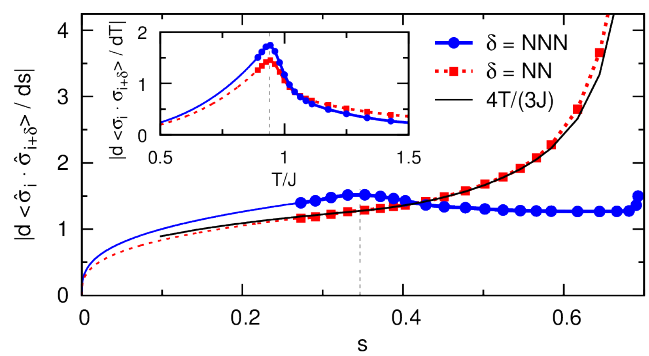

FIG. 4. (Color online) Derivatives of NN (squares) and NNN (circles) spin correlation functions of the Heisenberg model w.r.t. entropy (main panel) and temperature (inset) in $d = 3$.

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