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

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We compute short-range properties of the half-filled Hubbard model at strong coupling using determinantal quantum Monte Carlo (DQMC) and within dynamical mean-field theory (DMFT) for the cubic lattice as well as for the square lattice and Hubbard chain using DQMC and Bethe ansatz. When parametrized by entropy, as is appropriate in the cold-atom context, these observables are surprisingly insensitive to dimensionality and long-range order. In particular, the entrance into the regime of local antiferromagnetism (AF) is signaled by a universal minimum of the double occupancy at entropy $s \approx \log(2)$ and the onset of next-nearest neighbor spin correlations below. Thus, unique AF signatures are (almost) within reach of cold-atom experiments with current cooling techniques. Comparisons with the Heisenberg model and the weak-coupling case are included.

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A thorough understanding of materials with strong electronic correlations is not only desirable on intellectual grounds, but also due to their increasing technological importance, e.g., in magnetoresistive and superconducting devices [1, 2]. Theoretical investigations of corresponding Hubbard type models have already shed light on many strong-coupling phenomena including metal-insulator transitions, heavy-fermion and non-Fermi-liquid behavior, and various types of magnetic and orbital order [3]. However, there are still important open questions, most notably regarding high-temperature superconductivity, for which so far no mechanism could conclusively 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, within a few years after the first achievement of quantum degeneracy in (single flavor) fermionic atoms on optical lattices [7], the Mott metal-insulator transition (MIT) was observed in two-flavor mixtures, based on signatures in the compressibility [8] and a suppression of the integrated double occupancy [9]. As a result, it is now 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, onsite 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.

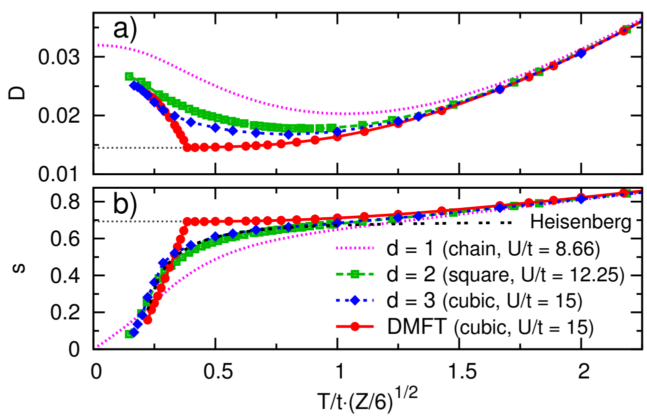

FIG. 1. (Color online) Hypercubic lattice ($1 \leq d \leq 3$) at strong coupling $U/(\sqrt{Z}t) \approx 6$: a) Double occupancy $D(T)$ as estimated from DMFT ($d = 3$, circles), DQMC ($d = 3$: diamonds, $d = 3$: squares), and BA ($d = 1$, dotted line). b) Corresponding estimates of entropy per particle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

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 [10, 11]. Indeed, the coldest systems achieved so far have central entropies per particle of $s \equiv S/(Nk_B) \approx \log(2) \approx 0.69$ [12] while AF long-range order (LRO) on a cubic lattice is expected only for entropies $s < s_{\mathrm{N}} \approx 0.34$ [11, 13, 14].

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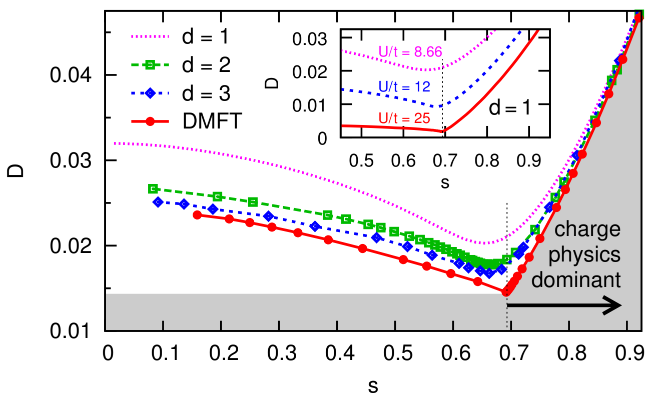

FIG. 2. (Color online) Hypercubic lattice at strong coupling: Double occupancy versus entropy. In all cases, the minimum of the double occupancy corresponds to $s \approx \log(2)$ (dotted line). The shaded area indicates the nonmagnetic contribution to D. Inset: $D(s)$ in $d = 1$ for various interactions.

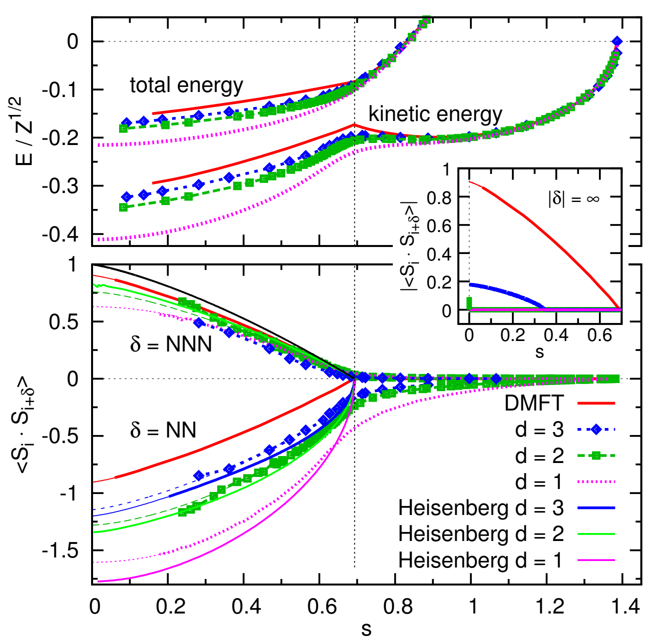

FIG. 3. (Color online) Hypercubic lattice at strong coupling: a) Rescaled total and kinetic energy versus entropy. b) Spin correlations $\langle S_i \cdot S_{i+\delta}\rangle$ between nearest neighbours [$\delta_{d=1} = 1$, $\delta_{d=2} = (1,0)$, $\delta_{d=3} = (1,0,0)$)] and between next-nearest neighbours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

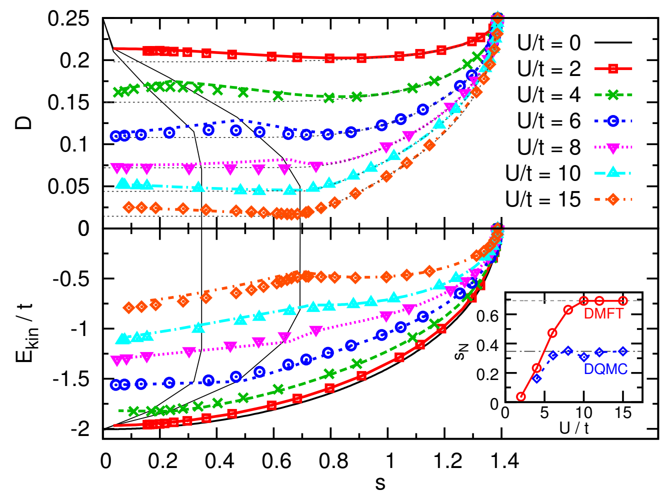

FIG. 4. (Color online) Cubic lattice ($d = 3$): DMFT (lines) and DQMC (symbols) results for a) double occupancy $D(s)$ [thin dotted lines: extrapolations of high-s asymptotics], and b) kinetic energy $E_{kin}(s)$. Inset: Néel entropy per particle $s_N(U)$, [fn: Staudt T_N + our $s(T)$], also indicated by thin solid lines in the main panels.

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