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

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We demonstrate that the signatures of antiferromagnetic (AF) correlations in the double occupancy D persist in all dimensions down to $d = 1$, therefore establishing D as a local probe of AF correlations. As a function of entropy $s = S/(Nk_{\mathrm{B}})$, D is nearly universal with respect to dimension; the minimum in $D(s)$ approaches $s \approx \log(2)$ at strong coupling, also marking the applicability limit of spin models. Long-range order appears hardly relevant for the current search of AF signatures in cold fermions. Thus, experimentalists need not achieve $s < \log(2)/2$ and should consider lower dimensions, for which the AF effects are larger. [D measurable! unique AF signature almost within current s reach, new: weak coupling, cubic T_N nonuniversal (sc vs. bcc)]

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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. 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].

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: both modulation spectroscopy [11, 15] and the superlattice approach [16] address the nearest-neighbor (NN) spin correlation function $\langle\hat{\boldsymbol{\sigma}}_i \cdot \hat{\boldsymbol{\sigma}}_j\rangle$ (for Pauli matrices $\hat{\boldsymbol{\sigma}}$). The same applies for the double occupancy $D \equiv \langle\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\rangle$ at large U/t [see Eq. (2)]. However, as we will show for D, such local observables are nearly insensitive to LRO; given typical noise levels it seems unlikely that their measurement could resolve the Néel transition (when/if low enough s is reached).

Even momentum-space based techniques, e.g. Bragg spectroscopy [17], would have to deal with the fact that (nearly) saturated AF LRO in an infinite system is reached only far below the continuous Néel transition. So a reduction in the entropy by a factor of 3 or 4 would be required for a strong signal, as well as global equilibration within experimental time scales. Moreover, the concept of LRO is not rigorously defined and might be misleading in the finite and inhomogeneous systems realized in fermionic experiments, with a shortest experimental length scale of about 10 lattice spacings [fn]. In contrast, short-range correlations remain well-defined.

Thus, experimentalists should focus (initially) on establishing *local* AF; this is possible, as we will show, via signatures in the double occupancy D: such measurements can not only quantify nearest-neighbor AF correlations, but also define the regime where a spin picture (i.e., the quantum Heisenberg model) is applicable.

Signatures in D have previously been linked to antiferromagnetism within dynamical mean-field theory (DMFT). We will briefly review the DMFT prediction [19] below and discuss arguments [20, 22] against its reliability in dimension $d = 3$. We will show, by comparisons with determinantal quantum Monte Carlo (QMC) simulations [24], that the AF signatures predicted by DMFT survive even on the square lattice ($d = 2$) and are surprisingly precise, up to rounding effects, in the cubic case ($d = 3$). Finally, we will focus on the effects of varying dimensionality and establish the double occupancy as a universal measure of AF correlations and entropy.

AF signatures in the double occupancy – According to DMFT, the low-temperature formation of an AF core in a fermionic cloud on an optical lattice (with central filling $n = 1$) is signaled, at strong coupling, by a distinct enhancement of D in the same region. The absolute increase of D is largest for $U/t \approx 12$; it should be detectable even in experiments integrating over the whole cloud [19].

This DMFT scenario was challenged recently [20] on the basis of the dynamical cluster approximation (DCA) which relaxes the DMFT assumption (valid in the limit of high dimensionality) of a momentum independent self-energy [21]: the DCA estimates of D showed no clear AF related enhancement [20]; however, these calculations excluded AF correlations beyond the cluster size. The reliability of DMFT estimates for D and s (in the nonmagnetic phase) at low temperatures T was also questioned based on comparisons with high-temperature expansions [22]. It was indeed clear from the beginning [19] that not all aspects of the DMFT scenario are realistic: after all, DMFT overestimates the Néel temperature by up to 30% in the simple cubic case, as shown in Fig. 1a. Thus, sharp signatures in $D(T)$ (cf. Fig. 2) cannot remain at $T_{\rm N}^{\rm DMFT}$ (except for the weak-coupling regime $U/t \lesssim 6$). But what is, precisely, the impact of finite dimensionality?

Comparison in $d = 2$ – Let us first turn to the square lattice ($d = 2$), for which the DMFT is *a priori* much less reliable than in $d = 3$. In fact, DMFT predicts AF LRO even in this case, with a maximum in $T_{\rm N}^{\rm DMFT}$ of about $0.4t$ at $U/t \approx 8$ (circles in Fig. 1b), while the Mermin-Wagner theorem excludes LRO for $T > T_N = 0$.

However, in this case it is relatively easy to check the DMFT predictions (circles in Fig. 1c), based on the Hirsch-Fye impurity solver [23], by determinantal QMC simulations [24] of finite clusters (diamonds). In both cases, Trotter errors have been eliminated by extrapolation [26]; for the determinantal results, we have also checked that finite-size effects are negligible (while DMFT is always in the thermodynamic limit). Thus, the latter should be accurate for the Hubbard model (1) within about half symbol size while the former represent exact DMFT solutions within about line width. The previously established accuracy of the DMFT at high temperatures [20, 22] evidently survives in $d = 2$, with no significant deviations from QMC for $T/t \gtrsim 0.8$. Surprisingly good agreement is also found at low temperatures $T/t \lesssim 0.2$, although the stable DMFT solutions (circles) here correspond to the AF phase which at first sight appears unphysical. In contrast, DMFT calculations constrained to the nonmagnetic phase (thin lines) predict low-T features of D which are far off from the exact QMC data. This teaches an important lesson, relevant also for $d = 3$: paramagnetic phases with strong short range order appear much more similar to AF phases (with LRO) than to nonmagnetic solutions (without any AF correlations). Significant deviations from DMFT appear only at $T \approx T_{\rm N}^{\rm DMFT}$, where the kinks are seen to be smoothed out in the QMC data. However, even $T_{\rm N}^{\rm DMFT}$ has physical significance: it (nearly) matches the spin coherence temperature (diamonds in Fig. 1b), defined via the specific heat [30].

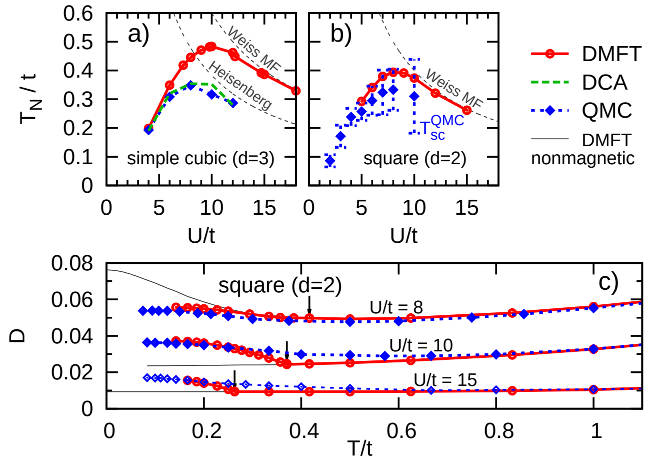

FIG. 1. (Color online) (a) The Néel temperature $T_N(U)$ (determined by QMC [29] and DCA [28]) is up to 30% below the DMFT estimate for $d = 3$. (b) While T_N vanishes in $d = 2$, the spin-crossover temperature [30] agrees with $T_N^{\rm DMFT}(U)$. (c) Double occupancy, estimated from DMFT (circles) and QMC (diamonds) for square lattice. Thin lines: metastable nonmagnetic DMFT results for $T < T_{\rm N}^{\rm DMFT}$ (arrows).

Comparison in $d = 3$ – Approaching the thermodynamic limit using determinantal QMC is much more difficult in the 3 dimensions (as the computational cost scales cubically [check] with the number of cluster sites). Results were obtained for simple-cubic clusters with 6^3 and 8^3 sites and extrapolated to vanishing Trotter discretization $\Delta\tau = 0$ (large diamonds in Fig. 2). Selective studies (with up to 10^3 sites) indicate that finite-size effects in this data are negligible at strong coupling; they might exceed the symbol sizes, however, at weak coupling ($U/t \lesssim 6$) and low temperatures.[supp, fn?] These data show perfect agreement with the DMFT estimates (circles) at $U/t = 12$ both for $T/t \geq 0.7$ and for $T/t \leq 0.4$;

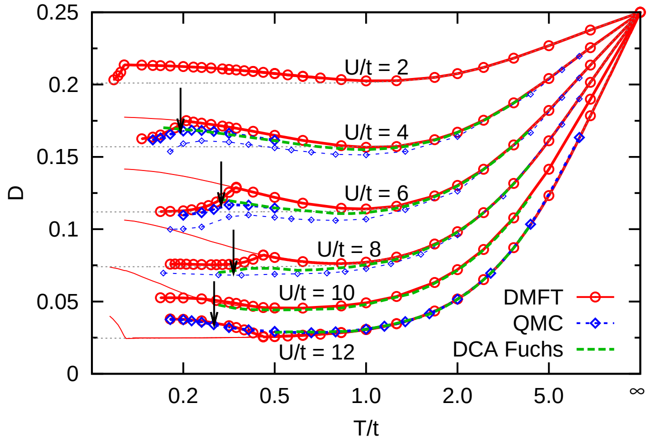

FIG. 2. (Color online) Cubic lattice ($d = 3$): Comparison of DMFT (circles) and direct QMC (diamonds) results for the temperature dependence of the double occupancy $D(T)$ for the cubic lattice. DCA results taken from [20]. Small diamonds: QMC results with finite Trotter discretization bias. Arrows: Néel temperature T_N (QMC estimates [29]). [grey!]

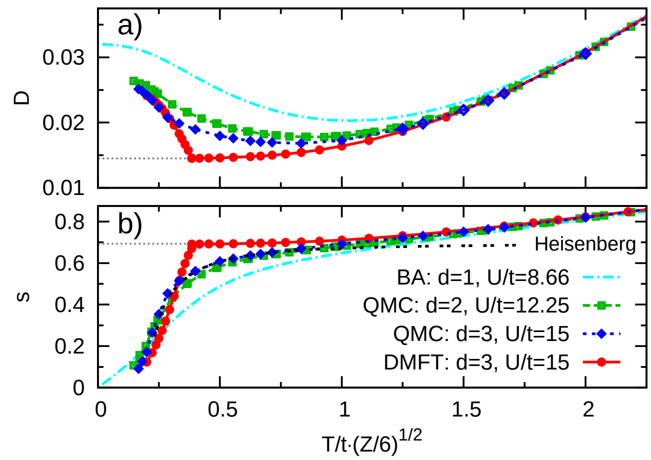

FIG. 3. (Color online) Hypercubic lattice ($1 \leq d \leq 3$) at strong coupling: a) $D(T)$ as estimated from DMFT ($d = 3$, circles), QMC ($d = 2$, 3, diamonds), and BA ($d = 1$, dash-dotted line). b) Corresponding estimates of entropy per particle $s = S/N$. All interactions correspond approximately to the ground state Mott transition at $U/(\sqrt{Z}t) \approx 6$. [grey!]

thus the DMFT prediction of the D enhancement [19] is even quantitatively correct. Only in a narrow range around $T_{\rm N}^{\rm DMFT} \approx 0.45t$ the QMC results deviate visibly.

At relatively weak coupling $U/t \leq 8$, signatures appear in the DMFT data in Fig. 2 which differ fundamentally from the strong-coupling scenario discussed so far: $D(T)$ shows a broad minimum at $T \approx t$; the rise towards lower T breaks down quite abruptly below $T_{\rm N}^{\rm DMFT}$, remarkably approaching exponential fits to the high-T behavior (dotted lines). Apparently the system behaves as a (bad) insulator for $T \gtrsim t$; the Fermi liquid behavior setting in for $T \lesssim t$ enhances D [13], but is destroyed below $T_{\rm N}^{\rm DMFT}$ by AF correlations. Also this weak-coupling DMFT scenario for $D(T)$ is confirmed: QMC predicts (large diamonds) a peak right at $T_{\rm N}^{\rm DMFT} \approx 0.2t$ for $U/t = 4$ and quickly converges towards DMFT for lower T. The deviations in the range $T_{\rm N}^{\rm DMFT} \lesssim T \lesssim t$ can be traced to developing AF correlations which already reduce the Fermi liquid enhancement of D. Note that (at $U/t = 4$) the discrepancies between QMC and DMFT are much smaller than typical QMC discretization errors (data for $\Delta\tau\, t = 1/8$: small diamonds) and that DCA (dashed line) apparently misses the AF physics at $T/t \lesssim 0.2$.

LRO leaves traces in the QMC estimates of $D(T)$ only in the weak-coupling regime $U/t \lesssim 6$ where $T_{\rm N} \approx T_{\rm N}^{\rm DMFT}$ (cf. Fig. 1a). At strong coupling $U/t = 12$, $D(T)$ does not show visible features at $T_{\rm N} \approx 0.3t$, which suggests that local spin correlations (which determine D and current AF observables [11, 16]) are hardly sensitive to LRO and, consequently, dimensionality in this regime.

Impact of dimensionality and entropy – In order to gain more insight into these issues, DMFT and QMC data for the cubic lattice are compared at $U/t = 15$ with QMC results for the square lattice and BA solutions of the infinite chain at equivalent [31] interactions in Fig. 3a. Here, the DMFT data (circles) can also be interpreted as an exact result in infinite dimensions. After rescaling [31], we find rapid convergence with increasing dimensionality at high T and generally similar shapes of $D(T)$ for $1 \leq d \leq \infty$. However, $d \gg 3$ would apparently be needed in order to converge to the DMFT results also at $T_{\rm N}^{\rm DMFT}$. Furthermore, the minimum in $D(T)$ occurs at or above twice $T_{\rm N}^{\rm DMFT}$ in dimensions $1 \leq d \leq 3$. [above too critical?]

[Stress: first reliable entropy data!] It is well-known that nonmagnetic DMFT yields an entropy $s \xrightarrow{T\to 0} \log(2)$ (dotted line in Fig. 3b), which is clearly unphysical [22]. However, the AF DMFT solution (circles for $T < T_{\rm N}^{\rm DMFT}$) recovers the QMC results for the cubic lattice (diamonds) at $T \lesssim T_{\rm N} \approx 0.25t$; remarkably the latter coincide with the Heisenberg limit of $s(T)$ for $T \lesssim 0.8t$. In general, the dimensional dependence of $s(T)$ nearly mirrors that of $D(T)$. Thus, dimensional effects and DMFT errors should be minimal when using s as a (dimensionless) measure of temperature (which is of primary interest to experimentalists anyway).

Indeed, as seen in Fig. 4, $D(s)$ looks strikingly similar in all dimensions; in particular, the minimum in D (at strong coupling) corresponds to $s \approx \log(2) = s_{\rm N}^{\rm DMFT}$ in all cases! While it might appear surprising that this behavior persists down to $d = 1$ it is clear that $s < \log(2)$ 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].

Thus, 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 posi-

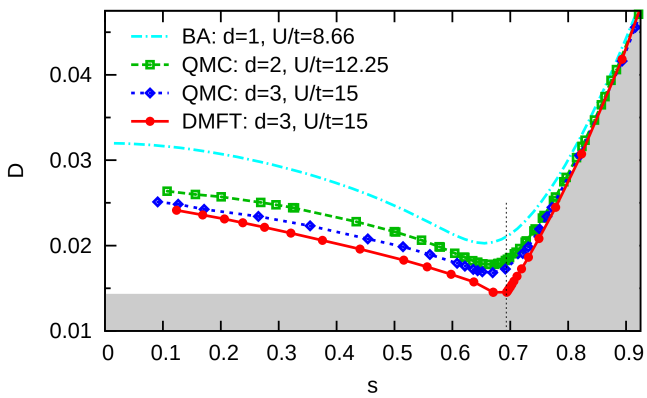

FIG. 4. (Color online) Hypercubic lattice ($1 \leq d \leq 3$) at strong coupling: Double occupancy as a function of entropy per particle. In all cases, the minimum of the double occupancy corresponds to $s \approx \log(2)$ (dotted line). The shaded area indicates the nonmagnetic contribution to D.

tive deviation of $D(s)$ from the nonmagnetic background (shaded in Fig. 4) should be linked to AF correlations, generalizing Takahashi's ground state expression [18]

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

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 ($d = 3$) [32]; -1.34 ($d = 2$) [33, 34]; -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 [35].

Conclusion – As a function of entropy per particle s, the double occupancy is nearly universal with respect to dimensionality; in particular, the minimum in $D(s)$ always occurs at $s \approx \log(2)$ at strong coupling, as predicted by DMFT. Thus, we have established a prominent and specific signal of AF correlations in an entropy range that is in immediate experimental reach, with the prospect of extending the use of $D(s)$ for thermometry [12] to the most interesting range $s \lesssim log(2)$. Our results also validate the RDMFT approach [36–38] for quantitative simulations of inhomogeneous 3-dimensional systems. [boundary within 10 lattice sites, bcc vs. sc, mention spectra?]

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