

Critical entropy of quantum Heisenberg magnets on simple-cubic lattices

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We analyze the temperature dependence of the entropy of the spin-1/2 Heisenberg model on the three-dimensional simple-cubic lattice, for both the case of antiferromagnetic and ferromagnetic nearest-neighbor exchange interactions. Using optimized extended ensemble quantum Monte Carlo simulations, we extract the entropy at the critical temperature for magnetic order from a finite-size scaling analysis. For the antiferromagnetic case, the critical entropy density equals $0.341(5)k_B$, whereas for the ferromagnet, a larger value of $0.401(5)k_B$ is obtained. We compare our simulation results to estimates put forward recently in studies assessing means of realizing the antiferromagnetic Néel state in ultracold fermion gases in optical lattices.

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I. INTRODUCTION

Ultracold atom gases provide a unique opportunity to study basic models of strongly interacting many-body systems in a highly controlled experimental framework.¹ After the pioneering realization of the superfluid-to-Mott insulator transition of ultracold bosonic atoms,² recently different groups reported the realization of a Mott-insulating state also for ultracold ⁴⁰K fermionic atoms on three-dimensional simple-cubic lattices.^{3,4} A next major step would be the realization and identification of a low-temperature antiferromagnetically ordered Néel state in such systems. In fact, various recent studies explored the prospects of realizing the antiferromagnetic Néel state in an ultracold gas of fermionic atoms confined to an optical lattice.^{5–12} A quantity that is important in assessing the relevant temperature scale is the upper bound on the entropy allowed in order to transfer the atoms into the antiferromagnetically ordered state. For a three-dimensional fermionic Hubbard model on a simple-cubic lattice at half-filling, estimates of the entropy S as a function of temperature, as well as the ratio U/t between the onsite repulsion U and the hopping amplitude t , were obtained within a single-site dynamical mean-field theory (DMFT) approach.⁵ As reported in Ref. 5, DMFT however overestimates the Néel temperature by about 50% in the intermediate coupling regime, as compared to direct quantum Monte Carlo simulations based on systems with up to 10^3 lattice sites.¹³ Obtaining in a similar way the entropy from direct quantum Monte Carlo simulations is challenging and typically involves integration of the specific heat over an extended temperature range.

However, in the limit of large U/t , the spin physics of the Hubbard model is well known to be described by a nearest-neighbor spin-1/2 quantum Heisenberg model, with an antiferromagnetic exchange coupling $J=4t^2/U>0$, obtained within perturbation theory around the strong coupling limit $t=0$. This model is accessible to large scale quantum Monte Carlo simulations and moreover—as shown below—it is possible to provide precise values of the entropy in this large- U limit. In particular, one can obtain the value of the critical entropy density (i.e., the entropy per lattice site) S_C , below which antiferromagnetic order emerges. Nevertheless, thus far no systematic quantum Monte Carlo study concern-

ing the entropy has been reported. On the other hand, different estimates of S_C for the Heisenberg antiferromagnet have been put forward recently. In Ref. 5, a Schwinger boson approach¹⁴ was employed, leading to the estimate that S_C is about 50% of the mean-field value $S_C^{MF}=k_B \ln(2)$. A more recent study⁶ reported a value of S_C obtained from a fluctuation-corrected mean-field approach, leading to a reduction in S_C of only 20% from the mean-field value S_C^{MF} . This rather large discrepancy among current estimates of S_C calls for a clarification based on numerically exact simulations of the Heisenberg model. Here, we present an unbiased estimate of the temperature dependence of the entropy and, in particular, the critical entropy density by combining extended ensemble quantum Monte Carlo simulations with a finite-size scaling analysis based on the known critical properties of the quantum Heisenberg model. For comparison, we consider in the following both the ferromagnetic and the antiferromagnetic spin-1/2 Heisenberg model on the three-dimensional simple-cubic lattice. These models are described by a Hamiltonian

$$H = J \sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1)$$

where \mathbf{S}_i denotes a spin-1/2 degree of freedom on lattice site i , and J is nearest-neighbor exchange interaction, with $J>0$ ($J<0$), for the antiferromagnetic (ferromagnetic) case. From previous studies, the locations of the transition temperatures to the ordered phases have been determined as $k_B T_N/J=0.946(1)$ (Ref. 15) (Néel temperature) for the antiferromagnet, and $k_B T_C/|J|=0.839(1)$ (Ref. 16) (Curie temperature) for the ferromagnet, based on quantum Monte Carlo simulations.

II. METHOD

In order to extract the temperature dependence of the entropy, we use an optimized extended ensemble approach,^{17,18} that is based on a generalization of the Wang-Landau¹⁹ algorithm to the case of quantum Monte Carlo simulations,^{16,20} performed within the stochastic series expansion representation²¹ using multicluster deterministic loop updates.²² Within this approach, one obtains Monte Carlo estimates of the expansion coefficients $g(n)$ of the high-

temperature series expansion of the partition function Z in the inverse temperature $\beta = 1/(k_B T)$

$$Z = \text{Tr} e^{-\beta H} = \sum_{n \geq 0} g(n) \beta^n \quad (2)$$

for a given system of $N = L^3$ lattice sites. Here, L denotes the linear size of the simulated finite cube and we employ periodic boundary conditions in all directions. From the expansion coefficients $g(n)$, the free energy

$$F = -\frac{1}{\beta} \ln Z = -\frac{1}{\beta} \ln \sum_{n \geq 0} g(n) \beta^n \quad (3)$$

the internal energy

$$E = \frac{1}{Z} \sum_{n \geq 0} n g(n) \beta^{n-1} \quad (4)$$

and the entropy

$$S = \frac{E - F}{T} \quad (5)$$

are obtained as continuous functions of the temperature T . In practice, as discussed in Ref. 20, we obtain the expansion coefficients up to a upper cutoff Λ , that is chosen sufficiently large in order to reliably calculate the thermodynamic properties of the finite system based on the coefficients $g(n)$, $n = 0, \dots, \Lambda$ down to a given temperature scale β_Λ . The required Λ scales linear in both β_Λ and the system size N . In our simulations, we consider finite systems up to $L=20$, for which $\Lambda=16\,000$ is required in order to obtain thermodynamic properties down to a temperature of about $k_B T \approx 0.7|J|$. Repeated simulations with independent random streams results in statistical error bars on the thermodynamic quantities.

III. RESULTS

In Fig. 1, we present the results for the entropy from our simulations for both the antiferromagnetic and the ferromagnetic Heisenberg model. For both cases, we show data for systems with $L=8$ and $L=16$. Outside a narrow range around the transition temperature, the entropy curves obtained for the two different system sizes compare well, and thus essentially represent the behavior of the entropy density in the thermodynamic limit. Also shown in Fig. 1 are fits of the numerical data to the low- T scaling $S \propto T^3$ and $S \propto T^{3/2}$ for the antiferromagnet and ferromagnet, respectively. This difference in the low- T scaling behavior relates to the linear (quadratic) dispersion of the magnetic spin-wave excitations in the antiferromagnetic (ferromagnetic) case.¹⁴

However, in order to extract the critical entropy S_C in the thermodynamic limit, we need to perform a finite-size scaling analysis of the finite-size data $S_C(L)$ taken at the transition temperature. For this purpose, we use a finite-size scaling ansatz

$$S_C - S_C(L) \propto L^{1/\nu-d}, \quad (6)$$

where ν is the critical exponent of the correlation length and d the dimensionality of the system. Starting from

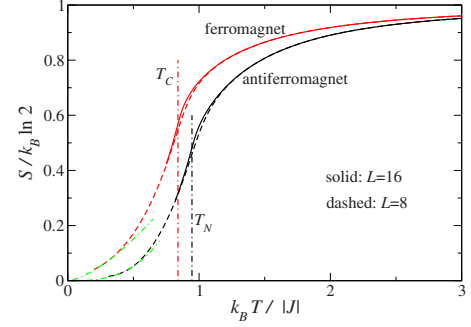


FIG. 1. (Color online) Temperature dependence of the entropy of the spin-1/2 quantum Heisenberg antiferromagnet and ferromagnet on the simple-cubic lattice. For both cases, results from quantum Monte Carlo simulations are shown for finite systems with $L=8$ (dashed lines) and $L=16$ (solid lines). Error bars for the shown data are below the line thickness. Vertical lines show the transition temperatures T_N and T_C for the antiferromagnet and the ferromagnet, respectively. Green dashed-dotted curves denote fits to the algebraic low- T scaling $S \propto T^3$ ($S \propto T^{3/2}$) for the antiferromagnet (ferromagnet).

$S = -\partial F / \partial T$, this relation follows from the scaling behavior of the free energy $F \propto \xi^{-d}$ with the correlation length ξ , that scales as $\xi \propto |t|^{-\nu}$ when the reduced temperature $t \rightarrow 0$, by the usual finite-size scaling ansatz, that at criticality ξ relates to the linear system size L . For the current case of a three-dimensional system ($d=3$) with $O(3)$ symmetry, $\nu = 0.7112(5)$.²³ Figure 2 shows that the finite-size data indeed fits well to the above scaling form in the range of system sizes $L > 6$. From the extrapolated values, we obtain $S_C = 0.341(5)k_B = 0.492(7)S_C^{MF}$ for the antiferromagnetic model, whereas for the ferromagnet, a larger value of $0.401(5)k_B = 0.578(7)S_C^{MF}$ results. We also performed an algebraic fit without biasing the exponent, which returned identical values of S_C within the statistical error bars.

While the ferromagnet has a critical temperature T_C that is about 11% lower than T_N , it orders already below an entropy that is about 17% higher than the critical entropy of the antiferromagnet. The higher critical entropy directly exhibits

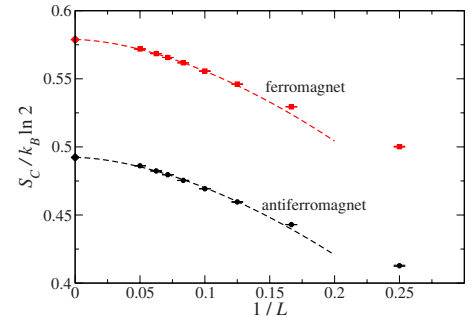


FIG. 2. (Color online) Finite-size scaling of the critical entropy density $S_C(L)$ with the inverse linear system size $1/L$ for the spin-1/2 quantum Heisenberg antiferromagnet and ferromagnet on the simple-cubic lattice. The quantum Monte Carlo data are shown by symbols and the dashed lines represent fits of the finite-size data for $L > 6$ to the finite-size scaling form in Eq. (6). The results for S_C in the thermodynamic limit are indicated by symbols as well.

a reduced efficiency of thermal disorder in destroying long-range magnetic order. The lower transition temperature of the ferromagnetic is due to a significantly enhanced production of entropy upon heating up the system, which follows from both Fig. 1, as well as from the mentioned difference in the low- T behavior of the entropy.

IV. CONCLUSIONS

Based on numerically exact quantum Monte Carlo simulations, we obtained the temperature dependence of the entropy for both the antiferromagnetic and the ferromagnetic spin-1/2 Heisenberg model on the simple-cubic lattice. Focusing on the region close to the magnetic ordering transition, we employed a finite-size scaling analysis to extract the critical entropy density below which long-ranged magnetic order sets in. In case of the antiferromagnetic model, our result for the critical entropy is consistent with a 50% reduc-

tion from the mean-field value that was estimated recently from a Schwinger boson calculation.⁵ This clarifies among the different values of the critical entropy reported previously.^{5,6} In comparison, we found the ferromagnet to be more robust to thermal disorder, which at criticality is about 17% larger for the ferromagnet than for the antiferromagnet in terms of the critical entropy. We consider the current results for the temperature dependence of the magnetic entropy of value also for future calculations of the entropy for the full fermionic Hubbard model beyond the strongly interacting regime.

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