Entropy Dependence of Correlations in One-Dimensional SU(N) Antiferromagnets

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Motivated by the possibility to load multicolor fermionic atoms in optical lattices, we study the entropy dependence of the properties of the one-dimensional antiferromagnetic SU(N) Heisenberg model, the effective model of the SU(N) Hubbard model with one particle per site (filling $1/N$) in the large U/t limit. Using continuous-time world-line Monte Carlo simulations for $N = 2$–5, we show that characteristic short-range correlations develop at low temperature as a precursor of the ground state algebraic correlations. We also calculate the entropy as a function of temperature, and we show that the first sign of short-range order appears at an entropy per particle that increases with N and already reaches $0.8k_B$ at $N = 4$, in the range of experimentally accessible values.

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Lattice SU(N) models play an ever-increasing role in the investigation of strongly correlated systems. The first systematic use of these models took place in the context of the large-N generalization of the SU(2) Heisenberg model, in which conjugate (or self-conjugate) representations are put on the two sublattices of the square lattice so that a SU(N) singlet can be formed on two sites [1–3]. Over the years, another class of SU(N) models with the same representation at each site has appeared as the relevant description of the low temperature properties in several contexts. In particular, the SU(3) model corresponds to the spin-1 Heisenberg model with equal bilinear and biquadratic interactions [4–6], while the SU(4) model is equivalent to the symmetric version of the Kugel-Khomskii model of Mott insulators with orbital degeneracy [7,8].

These models have attracted renewed attention recently as the appropriate low-energy theory of ultracold fermionic gases loaded in optical lattices [9]. As in Thouless' description of exchange processes in crystalline ^{3}He [10], the dominant process in the Mott insulating phase with one atom per site is the permutation P_{ij} between nearest neighbors i and j. In ^{3}He, the nucleus has a spin $1/2$, and, up to a constant, the resulting model is the standard SU(2) Heisenberg model, since, for spin $1/2$, the permutation can be written $P_{ij} = 2\vec{S}_i\vec{S}_j + 1/2$. For a general nuclear spin I, the number N of different atomic states is equal to $2I + 1$, and the resulting model is the SU(N) Heisenberg model with the N-fold degenerate fundamental representation at each site (see below for details). Alkaline rare earth atoms, in which the nuclear spin can take values from $1/2$ to $9/2$, are the most promising candidates to implement these models with cold atoms in optical lattices.

In that respect, a very important question concerns the possibility to observe correlations typical of the low-energy properties of these models. With cold atoms, since it is the entropy rather than the temperature which is controlled [11], the relevant question is whether the minimum experimentally realizable entropy is larger than that where correlations are likely to become strong. In current state-of-the-art experimental setups, the lower limit for fermions with $N = 2$ is equal to $0.77k_B$ per particle [12]. For the SU(2) case, the first signs of the Mott transition and of nearest-neighbor antiferromagnetic correlations have been predicted to appear below an entropy per atom of about $k_B \ln 2 \simeq 0.693k_B$ [13,14], just below the current experimental limit, and longer-range correlations will be difficult to detect because they develop at lower entropy. For instance, on the cubic lattice, Néel ordering takes place at an entropy per site of $0.338k_B$.

The first hint that increasing the number of colors might help has been obtained in the context of a high temperature investigation of the N-flavor Hubbard model by Hazzard *et al.* [15], who have shown that the effective temperature reached after introducing the optical lattice decreases with N under fairly general conditions. However, to the best of our knowledge, no attempt has been made so far to determine how correlations develop when reducing the entropy and to what extent this depends on N.

In this Letter, we address this issue in the context of the one-dimensional (1D) antiferromagnetic SU(N) Heisenberg model on the basis of extensive quantum Monte Carlo (QMC) simulations. As we shall see, the ground state algebraic correlations lead to characteristic anomalies in the structure factor upon lowering the temperature. These anomalies become visible only at quite low temperature, but, remarkably enough, the corresponding entropy per particle increases with N, leading to observable qualitative effects with current experimental setups for $N \geq 4$.

The SU (N) Heisenberg model.— A good starting point to discuss N-color fermionic atoms loaded in an optical lattice is the SU(N) Hubbard model defined by the Hamiltonian:

$$H = t \sum_{\langle i,j\rangle\alpha} (c^{\dagger}_{\alpha i} c_{\alpha j} + \text{H.c.}) + U \sum_{i,\alpha<\beta} n_{\alpha i} n_{\beta i}, \quad (1)$$

where $c^{\dagger}_{i,\alpha}$ and $c_{i,\alpha}$ are creation and annihilation operators, respectively, of a fermion of color $\alpha = 1 \ldots N$ on site i and the sum is over the first neighbors of a periodic chain of length L. $n_{\alpha i}$ is the number of fermions of color α on site i. At filling $1/N$, i.e., with one fermion per site, the ground state is a Mott insulator for large enough U/t [16–18], and, to second order in t/U, the low-energy effective Hamiltonian is the SU(N) Heisenberg model with the fundamental SU(N) representation at each site and with coupling constant $J = 2t^2/U$. Setting the energy unit by $J = 1$, this Hamiltonian can be written (up to an additive constant)

$$H = \sum_{\langle ij\rangle} P_{ij}, \quad (2)$$

where P_{ij} permutes the colors on sites i and j. If we denote by $S_i^{\alpha\beta}$ the operator that replaces color β by α on site i, this permutation operator can be written as

$$P_{ij} = \sum_{\alpha,\beta} S_i^{\alpha\beta} S_j^{\beta\alpha}. \quad (3)$$

This effective Hamiltonian is an accurate description of the system provided the temperature is much smaller than the Mott gap. In terms of entropy, the criterion is actually quite simple. The high temperature limit of the entropy per site of the SU(N) Hubbard model at $1/N$ filling can be shown to be equal to $k_B[N \ln N - (N-1)\ln(N-1)]$, while that of the SU($N$) Heisenberg model is equal to $k_B \ln N$. So the description in terms of the Heisenberg model can be expected to be accurate when the entropy is below $k_B \ln N$. For $N > 2$, this entropy is much larger than the current experimental limit: For SU(3), it is already equal to $k_B \ln 3 \simeq 1.099 k_B$, and it increases with N. Of course, this is not the whole story, since what really matters is the entropy below which specific correlations develop, but this is encouraging.

A peculiar characteristic of these SU(N) models is that one needs N sites to form a singlet. This is reflected in their ground state properties: plaquette singlet ground state for simplex-based models [19–21] or for the SU(4) model on a ladder [22], 3-sublattice color order for SU(3) on the triangular [4] and square [5] lattices, dimerized ground state with Néel long-range [23] or algebraic [24] order for SU(4) on the square lattice, chiral spin liquids with fractional fluxes for large N [25]. In one dimension, the SU(N) model has been solved with the Bethe ansatz for arbitrary N by Sutherland [26], who showed that there are $N-1$ branches of elementary fractional excitations. They all have the same velocity $v = 2\pi/N$ at small energy [26], and pairs of zero energy elementary fractional excitations have momentum $2\pi n/N$, with n an integer [27]. In the thermodynamic limit, the energy per site is given by

$$E_0(N) = 2 \sum_{k=2}^{\infty} \frac{(-1)^k \zeta(k)}{N^k} - 1, \quad (4)$$

where ζ is Riemann's zeta function [26]. Some values are given in Table I. Affleck has argued that the central charge c should be equal to $N-1$ [29], and Lee [30] has shown that, at low temperature T, the entropy is given by

$$S(T) = \frac{k_B N(N-1)}{6} T + O(T^2), \quad (5)$$

a direct consequence of $c = N-1$ and $v = 2\pi/N$, since the linear coefficient is equal to $\pi c/3v$.

The QMC algorithm.—QMC simulation is the most efficient method to study the finite temperature properties of interacting systems provided one can find a basis where there is no minus sign problem, i.e., a basis in which all off-diagonal matrix elements of the Hamiltonian are nonpositive. For the SU(2) antiferromagnetic Heisenberg model on bipartite lattices, this is easily achieved by a spin rotation by π on one sublattice. For SU(N) with $N > 2$, there is no such general solution, but in 1D one can get rid of the minus sign on a chain with open boundary conditions, as already noticed for the SU(4) model [31]. Let us start from the natural basis consisting of the N^L product states $\otimes_i |\alpha_i\rangle = |\alpha_0, \ldots, \alpha_{L-1}\rangle$, where α_i is the color at site i. In this basis, all off-diagonal elements of the SU(N) model of Eq. (2) are either zero or positive. However, a generalization of the Jordan-Wigner transformation allows us to change all these signs on an open chain. This transformation is defined by

$$|\alpha_0, \ldots, \alpha_{L-1}\rangle \rightarrow (-1)^{r(\alpha_0,\ldots,\alpha_{L-1})} |\alpha_0, \ldots, \alpha_{L-1}\rangle, \quad (6)$$

where $r(\alpha_0, \ldots, \alpha_{L-1})$ is the number of permutations between different color particles on neighboring sites needed to obtain a state such that the α_i are ordered ($\alpha_i \le \alpha_j$ for $i < j$). This basis change is equivalent to a Hamiltonian transformation, the new Hamiltonian being given by

$$H = \sum_{\langle ij\rangle} \sum_{\alpha} \left(S_i^{\alpha\alpha} S_j^{\alpha\alpha} - \sum_{\beta\neq\alpha} S_i^{\alpha\beta} S_j^{\beta\alpha} \right). \quad (7)$$

On a periodic chain, the equivalence with the Hamiltonian of Eq. (2) is not exact, but the difference disappears in the

TABLE I. Ground state energies per site obtained for several N with the Bethe ansatz (BA) in the thermodynamic limit and on a finite size chain [28] and at $T = 0.01$ with the QMC algorithm (see the text) on a $L = 60$ chain with $n = 10^7$ Monte Carlo steps.

N	$BA(L=\infty)$	$BA(L=60)$	$QMC(L=60)$
2	−0.386294		−0.38675(2)
3	−0.703212	−0.7038228	−0.70384(2)
4	−0.8251193		−0.82577(2)
5	−0.884730		−0.88541(2)

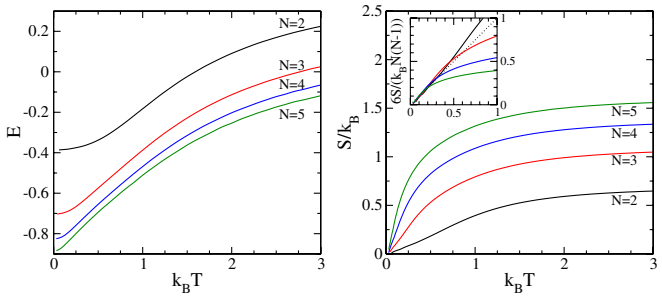


FIG. 1 (color online). Evolution of the energy per site E and of the entropy per site S as a function of the temperature T for different N on a $L = 60$ chain. The inset shows the slope of the entropy at $T = 0$, given in Eq. (5). The curvature being positive at $T = 0$, the curves go higher than the tangent (dashed line).

thermodynamic limit. So in the following we will simulate the Hamiltonian of Eq. (7).

To do so, we have developed a continuous time world-line algorithm with cluster updates [32] adapted to the model of Eq. (7) with N colors [33]. Using this algorithm, we have calculated the energy per site E, which is given by

$$E = \left\langle \frac{H}{L} \right\rangle \simeq \frac{k_B T}{Ln} \sum_{\phi} \left(\sum_{\langle ij \rangle} \int d\tau \delta_{\alpha_i(\tau),\alpha_j(\tau)} - n_c(\phi) \right), \quad (8)$$

where n is the number of Monte Carlo steps and $n_c(\phi)$ the number of world-line crossings in the configuration ϕ, the diagonal correlations defined by

$$C(j) = \left\langle \sum_{\alpha} S_0^{\alpha\alpha} S_j^{\alpha\alpha} \right\rangle - \frac{1}{N} \quad (9)$$

and the associated structure factor defined by

$$\tilde{C}(k) = \frac{1}{2\pi} \frac{N}{N-1} \sum_j C(j) e^{ikj}. \quad (10)$$

This structure factor is normalized in such a way that $\frac{2\pi}{L} \sum_k \tilde{C}(k) = 1$.

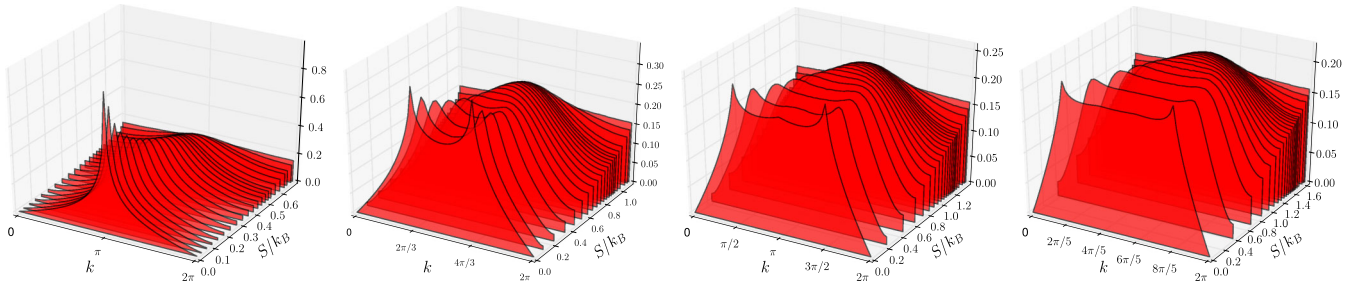
The results.—We have studied chains of length $L = 60$ for T from 0.01 to 20 with a number of colors $N = 2$, 3, 4, and 5. The measurements were based on a number of Monte Carlo steps n at least equal to 10^6. The autocorrelation time measured by the binning method indicates that around N steps are needed to obtain uncorrelated configurations, whatever the temperature, and that the precision on the energy per site E is better than 10^{-4}. This could be confirmed by the comparison of the limit of the energy when $T \to 0$ with the exact finite L value for SU(3) [28]. Moreover, the energy of the ground state differs from that of the thermodynamic limit by less than 8×10^{-4}. So, for our purpose, the finite size effects can be considered to be negligible (see Table I). The entropy per site S has been deduced from the energy E by an integration from high temperature:

$$S(T) = S(\infty) - \int_T^{\infty} d\tau \frac{k_B}{\tau} \frac{dE}{d\tau}, \quad (11)$$

where $S(\infty) = k_B \ln N$. E and S are plotted in Fig. 1 for different N as a function of T. Since the entropy is the result of a numerical integration, it is important to check its accuracy, especially at low temperature, since by construction it has to be correct at high temperature. Now, we know that, at low temperature, the entropy must be linear with a slope equal to $k_B N(N-1)/6$ [see Eq. (5)]. This is confirmed by the inset in Fig. 1(b), in which one clearly sees that the entropies times $6/k_B N(N-1)$ lie on top of each other at low temperature.

Now, the stabilization of the energy at low T occurs at a temperature that decreases when N increases. Thus, one could naively think that it will be more difficult to observe the development of the ground state correlations when N increases. However, this is not true if one considers the entropy. Indeed, the entropy grows much faster at low temperature when increasing N. So, the temperature corresponding to a given entropy decreases very fast when N increases.

We now look at the diagonal correlations $\tilde{C}(k)$. They have been calculated for different temperatures, but, in view of the implications for ultracold fermionic gas, we represent them as a function of the entropy per site S. Since the system is 1D, there is no long-range order and, hence, no Bragg peaks. Nevertheless, short-range correlations develop at low entropy. They translate into finite height peaks in $\tilde{C}(k)$ at finite temperature and singularities at zero



(a) $N = 2$ (b) $N = 3$ (c) $N = 4$ (d) $N = 5$

FIG. 2 (color online). Evolution of the structure factor $\tilde{C}(k)$ as a function of the entropy per site S for different N on a $L = 60$ chain.

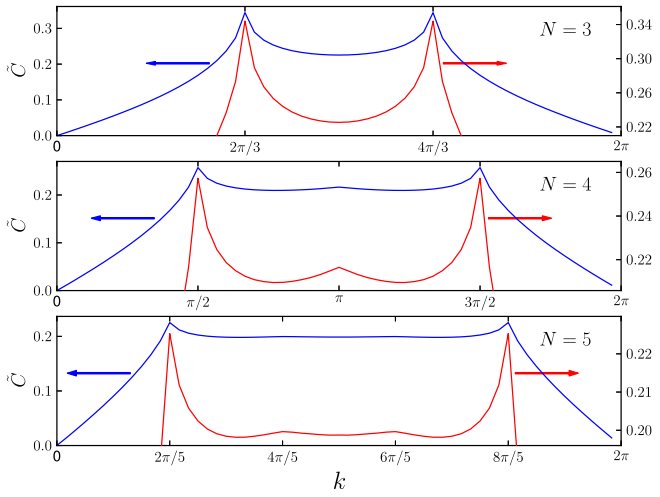


FIG. 3 (color online). Structures factor $\tilde{C}(k)$ at low temperature ($k_BT = 0.01$) for different N on a $L = 60$ chain, with $n = 10^7$ Monte Carlo steps. Small peaks are clearly visible at $k = \pi$ for $N = 4$ and $k = 4\pi/5$ and $6\pi/5$ for $N = 5$. The data for $N = 4$ are in perfect agreement with those of Ref. [31].

temperature. The number and the position of these peaks depend on the number of colors N. From the Bethe ansatz solution, singularities are expected to occur at $k = 2p\pi/N$ with $p = 1, \ldots, N-1$. The results of Fig. 2 agree with this prediction: There is a single peak at π for SU(2), while $N-1$ peaks are indeed present for SU(N) at sufficiently small entropy. Note, however, that all peaks do not have the same amplitude for $N \geq 4$. For $N = 4$ and 5, two types of peaks not related by the symmetry $k \to 2\pi - k$ are present. The peaks at $2\pi/N$ and $2(N-1)\pi/N$ are much more prominent, and they start to be visible at much larger entropy.

At the maximal entropy, the structure factor $\tilde{C}(k)$ is flat (see Fig. 2). At large but finite entropy, it presents a broad maximum at $k = \pi$ for all N. This reflects the simple fact that colors tend to be different on neighboring sites. More specific correlations appear upon lowering the entropy. For SU(2), the peak at $k = \pi$ just gets more pronounced. To observe the development of the singularity typical of the SU(2) ground state, algebraic correlations will, however, require to reach rather low entropy. This should be contrasted with the $N > 2$ cases, where a qualitative change in the structure factor occurs upon reducing the entropy: The broad peak at $k = \pi$ is replaced by peaks at $2\pi/N$ and $2(N-1)\pi/N$. One can in principle read off the corresponding entropy from Fig. 2. To come up with a quantitative estimate, we note that, upon reducing the entropy, the curvature of the structure factor at $k = \pi$ changes sign from positive at high temperature to negative when the peaks at $2\pi/N$ and $2(N-1)\pi/N$ appear. This occurs at $S_c/k_B = 0.58$, 0.87, and 1.08 for $N = 3$, 4, and 5, respectively. This characteristic entropy S_c increases more or less linearly with N as $S_c \simeq 0.2Nk_B$, and for $N = 4$ and 5, it lies in the experimentally accessible range. This is mostly a consequence of the temperature dependence of the entropy, which grows much faster with N at low temperature. The characteristic temperature at which deviations from the broad peak at $k = \pi$ occur depends only weakly on N. Finally, secondary peaks appear at lower temperature (see Fig. 3).

Conclusions.—We have shown that the entropy at which the periodicity characteristic of the zero temperature algebraic order of SU(N) chains is revealed increases significantly with N. For $N = 4$, this entropy is already larger than the entropy per particle recently achieved in the $N = 2$ case in the center of the Mott insulating cloud ($0.77k_B$) [12]. Whether a similar entropy can be achieved for $N > 3$ remains to be seen. As shown by Hazzard *et al.* [15], if the initial temperature is fixed, the initial entropy in a 3D trap increases with N as $N^{1/3}$, implying that one might have to go to values of N larger than 4 to reach a final entropy low enough to observe characteristic correlations. However, evaporative cooling might allow one to reach initial entropies that are less dependent on N. In a recent experiment on ^{173}Yb, the initial entropy reported by Sugawa *et al.* [34] for this $N = 6$ case is not much higher than in $N = 2$ experiments [12]. It is our hope that the present results will encourage the experimental investigation of the $1/N$-filled Mott phase of N-color ultracold fermionic atoms.

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Note added.—After submission of this work, we received a preprint by Bonnes *et al.* [35] in which they consider the same problem in the context of the SU(N) Hubbard model. The approaches are complementary, and the numerical results for $N = 3$ are consistent in the temperature range where they can be compared, yielding a coherent picture from high temperature [35] to very low temperature (present work).

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