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String correlation functions in the anisotropic spin-1 Heisenberg chain

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We study the string correlation functions proposed by den Nijs and Rommelse for the $S=1$ XXZ Hamiltonian by an exact diagonalization method. Using a finite size analysis, we estimate values of the string order parameters in the thermodynamic limit. Using the extrapolated values of the string order parameter we investigate the phase boundary between the two expected phases of the model, namely, the massive Haldane phase and the x-y–like massless phase. In the massless phase the exponent of the string correlation functions on the periodic system seems to be given by dimensions, which normally occur in the operator content of the chain when antiperiodic boundary condition is imposed.

I. INTRODUCTION

An extensive study of one-dimensional quantum spin chains describing the dynamics of spin S larger than 1/2 has been done in recent years. Let us focus our attention on the Heisenberg model in one dimension. In 1983, Haldane conjectured that the ground-state wave function of the isotropic Heisenberg model, or XXX chain, exhibits different behavior depending on whether the spin is integer or half integer.[1] In the case of half-integer spins, the ground state is disordered but has correlation functions that decay as power laws due to the existence of gapless excitations and the model is in a critical (massless) phase. On the other hand, in the case of integer spins, although the model is still disordered, the quantum fluctuations are sufficiently strong to destroy the massless excitations (spin waves) appearing in the former case, producing a finite energy gap and rendering the system off critical.

After the conjecture was enunciated, many studies were performed both analytically and numerically[2–9] to test these ideas. Although the above conjecture was derived based on the large spin-S arguments, it has been confirmed for the $S=1$ case experimentally and numerically (see Ref. 10 for a review). An important step in the direction of understanding the physics of these models was achieved by the introduction of an exactly solvable model by Affleck, Kennedy, Lieb, and Tasaki (AKLT model[2]). This is a rotational invariant spin-1 model but in order to ensure an exact integrability, other terms are included in the Hamiltonian beyond that of the standard Heisenberg chains. This model has the virtue that many of Haldane's conjectures can be proved exactly. Consequently, many of the Haldane conjectures would be proved if both models are in the same universality class. The exact ground-state wave function of the AKLT model, although disordered like the Heisenberg model, has a hidden order characterized by alternating signs in the successive nonzero spins (take for example, the S^z basis). den Nijs and Rommelse[11] proposed an order parameter that takes a nonzero value in the phase with the above mentioned hidden symmetry. This operator is of nonlocal nature and is called the string order parameter.

Several studies of the string order operator and some extensions of this order parameter for higher spin can be found in recent literature.[12–16] In Ref. 9, Kennedy and Tasaki found that the long-range order of this string order is related to the break down of a discrete $Z_2\times Z_2$ symmetry.[9] Hatsugai and Kohmoto[12] numerically investigated this string order parameter in an extended parameter space, which include the uniaxial anisotropy $+D\sum_j(S_j^z)^2$. This order parameter was shown to be quite useful in distinguishing the three phases of the model, namely, the large-D phase, the Haldane phase, and the Néel phase.

In this paper, we are going to study the spin-1 anisotropic Heisenberg model or XXZ chain, with anisotropy constant λ. We expect the massive Haldane phase to extend into a region of xy anisotropy $\lambda>\lambda_c$ and for $-1<\lambda<\lambda_c$ a disordered massless phase with no hidden symmetry will occur. Recently Alcaraz and Moreo,[17] by exploring the conformal invariance of the model in the gapless regime, conjectured that λ_c is exactly 0 and the entire gapless phase could be described by a $c=1$ conformal field theory of the Gaussian type.[18,19] In this paper, we report an independent calculation of the phase diagram obtained by evaluating directly the string order parameter. Our results ($\lambda_c\approx 0$) are in favor of the above conjecture. We also show that in the massless regime, the string order parameter has a power-law decay with exponents given by the Coulomb gas picture, obtained in Ref. 17, but with half-integer spin-wave index.

II. MODEL AND STRING CORRELATION FUNCTION

In this paper, we study the anisotropic Heisenberg spin-1 model, or XXZ chain, defined by the Hamiltonian

$$H=J\sum_j(S_j^xS_{j+1}^x+S_j^yS_{j+1}^y+\lambda S_j^zS_{j+1}^z)\ , \tag{2.1}$$

where S_j^x, S_j^y, and S_j^z ($j=0,1,2,\dots$) are spin-1 operators at site j, and λ is the anisotropy constant. At $\lambda=1$ (isotropic), this model is expected to be in the massive Haldane phase where the usual spin-spin correlation functions of Néel type[3–5,12]

$$\mathcal{O}^{\alpha}_{\text{Néel}}(j)=(-1)^{j-1}\langle S_1^{\alpha}S_j^{\alpha}\rangle\ ,\quad (\alpha=x,y,z) \tag{2.2}$$

decay exponentially as a function of the distance $(j-1)$.[3–5,9,12] In contrast, in the other limit where $-1<\lambda$ and $\lambda\approx-1$, we do expect massless behavior, since, as $\lambda\to-1$ the sector of Hilbert space characterized by different z components of the total spin $S^z=\sum_j S_j^z$ become degenerate producing gapless excitations around this point. Consequently, we should expect the existence of a critical value $\lambda=\lambda_c$ separating the Haldane phase and the massless phase.

As shown by previous works,[9,12] the Haldane phase for the $S=1$ model, although does not have long-range order of the Néel type $[\mathcal{O}_{\text{Néel}}(j)=0, j\to\infty]$ it still has a hidden antiferromagnetic order. This can be characterized by the string correlation functions

$$\mathcal{O}^{\alpha}_{\pi}(j)=\left\langle S_1^{\alpha}\exp\left[i\pi\sum_{k=1}^{j-1}S_k^{\alpha}\right]S_j^{\alpha}\right\rangle_H\ ,\quad \alpha=x,y,z\ , \tag{2.3}$$

where $\langle A\rangle_H$ means an expectation of A in the ground state of H. The above string correlation functions were first introduced by den Nijs and Rommelse.[11] Subsequent works[9,12] showed that the Haldane phase can be characterized by a long-range order in these string correlation functions,

$$\lim_{j\to\infty}\mathcal{O}^{\alpha}_{\pi}(j)\neq 0\ ,\quad (\alpha=x,y,z) \tag{2.4}$$

Recently Kennedy and Tasaki[9] made an important observation about the long-range order of the string type given in (2.4). They showed that the long-range order of the string order parameters is related to a breakdown of a discrete $Z_2\times Z_2$ symmetry of the model. In order to see this, they introduced a nonlocal unitary transformation U, which transforms the Hamiltonian (2.1) into a local ferromagnetic Hamiltonian $\tilde{H}$ given by

$$\tilde{H}=UHU^{-1}=-J\sum_j[S_j^xS_{j+1}^x+S_j^ye^{i\pi C_{j,j+1}}S_{j+1}^y+\lambda S_j^zS_{j+1}^z]\ , \tag{2.5}$$

where

$$C_{j,j+1}=S_j^z+S_{j+1}^x-1\ . \tag{2.6}$$

This Hamiltonian, although different from the usual ferromagnetic Hamiltonian by the factor $C_{j,j+1}$ given by (2.6), still has the virtue of inducing a ferromagnetic order. It is also interesting to observe that the explicit symmetry of this transformed Hamiltonian $\tilde{H}$ is not a usual continuous $U(1)$ but the discrete $Z_2\times Z_2$, which corresponds to global rotations around the z and x axis. This symmetry arises due to the independent commutation of $\tilde{H}$ with the nonlocal Z_2 operators $Q_z=\exp i\pi\sum_k S_k^z$ and $Q_x=\exp i\pi\sum_k S_k^x$. The important properties of this transformation is that the string order parameters (2.3) along x and z directions are transformed into the usual spin-spin correlation functions in the transformed Hamiltonian $\tilde{H}$,

$$\mathcal{O}^{\alpha}_{\pi}(j)=\langle S_1^{\alpha}S_j^{\alpha}\rangle_{\tilde{H}}\ ,\quad \alpha=x,z\ . \tag{2.7}$$

Consequently, the long-range order of the strong correlation function implies a ferromagnetic order in $\tilde{H}$, and we should expect a breakdown of the above described Z_2 symmetry. In the Haldane phase, we do expect long-range order in the string order parameters along x,y,z directions. This implies full breakdown of the $Z_2\times Z_2$ symmetry in the Haldane phase.

In this paper, we are interested in the phase boundary between the Haldane phase and the massless phase. Since the massless phase should have full $Z_2\times Z_2$ symmetry, it is enough, for our purposes, to investigate the correlation function

$$\mathcal{O}^{z}_{\pi}=\left\langle S_1^{z}\exp\left[i\pi\sum_{k=1}^{j-1}S_k^{z}\right]S_j^{z}\right\rangle\ . \tag{2.7'}$$

Before closing this section, let us consider the particular case of (2.1) where $\lambda=0$. By making the canonical transformation

$$S_j^x\to S_j^x\ ,\quad S_j^y\to S_j^z\ ,\quad S_j^z\to -S_j^y\ ,$$

we obtain

$$H=-\sum_j(S_j^xS_{j+1}^x+S_j^zS_{j+1}^z)\ . \tag{2.8}$$

If we now make the same nonlocal unitary transformation U described above [see (2.5)], we obtain the transformed Hamiltonian $\tilde{H}=-H$. Using (2.7), we obtain

$$\mathcal{O}^{x}_{\pi}(j)=\langle S_1^xS_j^x\rangle_{-H}=(-1)^{j-1}\langle S_1^xS_j^x\rangle_H \tag{2.9a}$$

and

$$\mathcal{O}^{z}_{p}(j)=\langle S_1^zS_j^z\rangle_{-H}=(-1)^{j-1}\langle S_1^zS_j^z\rangle_H\ , \tag{2.9b}$$

where in the last equations we have made the canonical transformation

$$S_j^x\to(-1)^jS_j^x\ ,\quad S_j^z\to(-1)^jS_j^z\ ,\quad S_j^y\to S_j^y\ .$$

The above relations state that the string correlation functions $\mathcal{O}^{x}_{\pi}(j)$ and $\mathcal{O}^{z}_{\pi}(j)$ will have long-range order only if the models also have an antiferromagnetic order of the Néel type. Since we expect no antiferromagnetic order of Néel type in the Haldane phase, (2.9a and b) imply that the particular point $\lambda=0$ (XY model) should be in the massless disordered regime with no hidden antiferromagnetic order.

III. NUMERICAL RESULTS

We calculate numerically the ground-state wave function of (2.1) with periodic boundary conditions using the Lanczos method, supplemented by hashing techniques,[20] for the lattice sizes up to $N=14$.

In Fig. 1, we plot for two values of λ ($\lambda=-0.5$ and $\lambda=1.0$) the spin-spin correlation function for the lattice size $N=14$. As we clearly see, this correlation function shows different behavior at $\lambda=1$ and $\lambda=-0.5$. At $\lambda=1$, it alternates in sign, while at $\lambda=-0.5$ the sign is fixed. Using the conformal invariance[21] of (2.1) in the massless regime, we can show that the above nonalternating behavior at $\lambda=-0.5$ is consistent with the Gaussian pic-

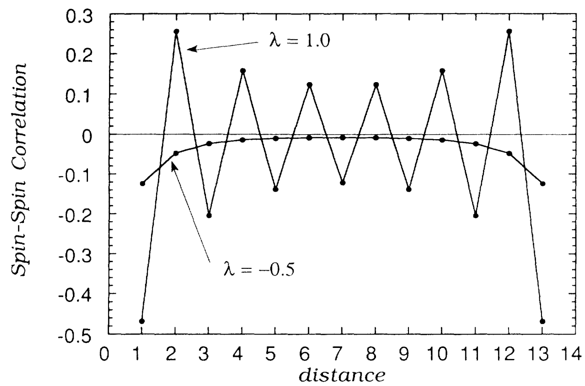

FIG. 1. Spin-spin correlation function $\langle S_1^z S_j^z \rangle$ as a function of j for the chain with 14 sites and anisotropies $\lambda=1.0$ and $\lambda=-0.5$.

ture proposed in Ref. 17. The conformal invariance in this gapless regime[22] and the Gaussian picture imply that the spin-spin correlation function should behave as $j \rightarrow \infty$ as,

$$\langle S_1^z S_j^z \rangle \sim \frac{A}{|j-1|^4} + \frac{B \cos\pi(j+1)}{|j-1|^{2x_{0,1}}} , \tag{3.1}$$

where $x_{0,1}=\pi/(\pi-\cos^{-1}\lambda)$ is the anomalous dimension of the operator with spin-wave number 1 in the Gaussian picture.[18] According to (3.1), the lack of oscillatory behavior should occur for all the negative values of λ. Our numerical results for other values of λ are also consistent with (3.1).

In Fig. 2, we also plot the string correlation function $\mathcal{O}_\pi^z(j)$ given in (2.7) for $\lambda=1$ and $\lambda=-0.5$ and the system size $N=14$. In contrast to Fig. 1, we clearly see that this correlation function does not alternate in sign, showing the same type of behavior for both values of λ. This suggests that the string correlation function changes continuously as we move from the Haldane phase to the massless phase, giving us a good order parameter to distinguish the two phases. Exploiting this idea, we calculate the string correlation function (2.7) for the farthest points compatible with the periodic boundary condition, namely $\mathcal{O}_\pi(j=N/2+1)$, for $N=6,8,\cdots,14$. In Fig. 3, we show the results as a function of $1/N$. We see from this figure that the string correlation grows quickly as we move from the negative to the positive values of λ. In order to better see this change of behavior, we show in Fig. 4 the extrapolated ($N \rightarrow \infty$) values of Fig. 3. These results are obtained assuming the following functional form:

$$\mathcal{O}(N/2+1)=C_0+C_1\frac{1}{N^\alpha} , \tag{3.2}$$

and evaluating C_1, C_2, and α by the least-squares method. The results of Fig. 4 clearly show that the string order parameter $\mathcal{O}_\pi^z(\infty)$ is zero for $\lambda<\lambda_c\approx 0$.

We can also calculate numerically the exponent α appearing in (3.2), in the massless phase.

In Fig. 5, we show these results. According to the Gaussian picture of Ref. 17, the possible correlation functions of local operators, when (2.1) is in a periodic chain, should have a power-law decay with exponents given in terms of the dimensions

$$x_{m,n}=n^2 x_p+\frac{m^2}{4x_p} , \quad x_p=\frac{\pi-\cos^{-1}(\lambda)}{4\pi} , \tag{3.3}$$

and $n,m=0,\pm 1,\pm 2,\cdots$. We checked that the above dimensions do not explain the results of Fig. 5. This is not

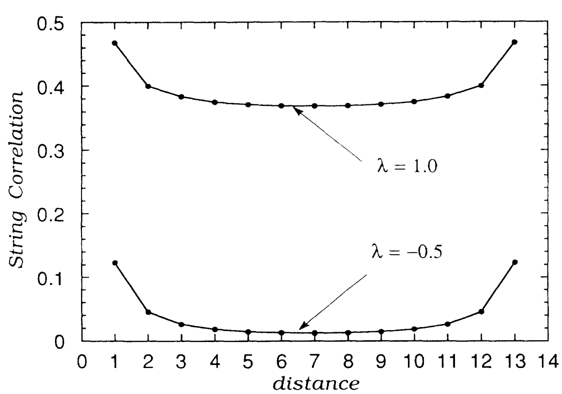

FIG. 2. String correlation function

$$\left\langle S_1^z \exp\left[i\pi \sum_{k=1}^{j-1} S_k^z \right] S_j^z \right\rangle ,$$

as a function of j for the 14 sites chain with $\lambda=1.0$ and $\lambda=-0.5$.

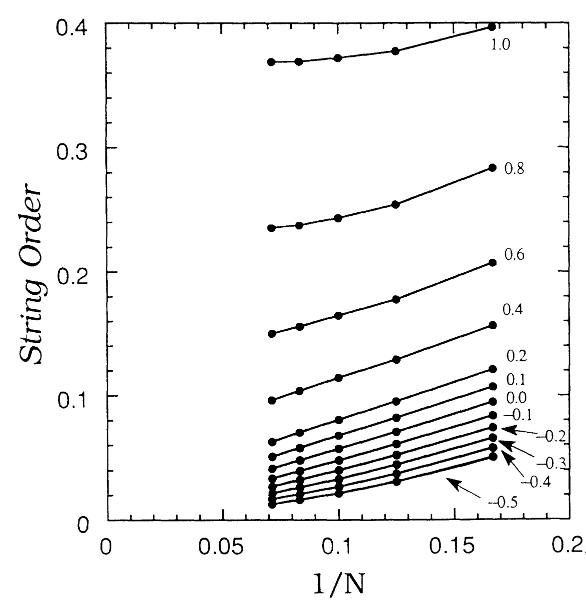

FIG. 3. String order parameter in the finite-size system

$$\mathcal{O}_\pi^z(j)=\left\langle S_1^z \exp\left[i\pi \sum_{k=1}^{j-1} S_k^z \right] S_j^z \right\rangle , \quad j=N/2+1$$

as a function of the inverse of the system size for various values of λ. The numbers in the figure are values of λ.

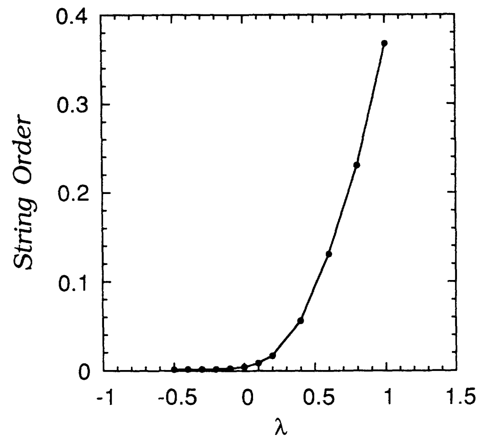

FIG. 4. The extrapolated ($N \to \infty$) values of the string order parameter as a function of the anisotropy λ.

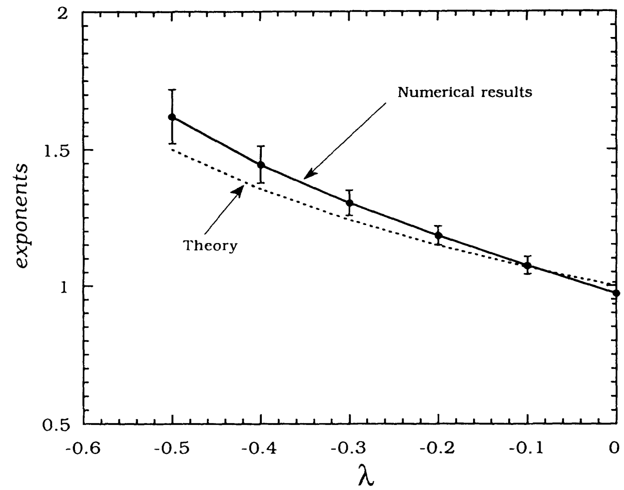

FIG. 5. Exponents of the string order parameter as a function of the anisotropy λ. The theoretical predictions is given by $x_{0,1/2}$ in Eq. (3.3).

a surprise, since the string correlation function is in fact two point correlation function of the nonlocal operators,

$$\mathcal{S}_j = \exp\left[i\pi \sum_{k=1}^{j-1} S_k^z \right] S_j^z \,. \tag{3.4}$$

Since this operator is nonlocal, in order to estimate its dimensions, or the exponent α in (3.2) by conformal invariance, we should consider (2.1) not only with periodic boundary condition, but also with other toroidal boundary conditions. Nonlocal operators, in general, may connect sectors of the Hilbert space corresponding to different boundary conditions.[23] Using the Gaussian picture of Ref. 17 a similar calculation as that of Ref. 23 show us that the exponent α in (3.2) should be related with the lowest dimension appearing in (2.1) when antiperiodic boundary condition are imposed. The dimensions of (2.1) in the antiperiodic case are given by (3.3) where now $n = 0, \pm 1, \pm 2, \cdots$ but $m = \pm 1/2, \pm 3/2, \cdots$ and, consequently

$$\alpha = 2x_{0,1/2} = \pi / 2(\pi - \cos^{-1}\lambda) \,.$$

In Fig. 5 we also show these results. Although the agreement is not complete, it is consistent with the analytical results taking into account the finite-size effects neglected when fitting the correlation function by (3.2).

IV. SUMMARY AND CONCLUSION

In this paper we have investigated the phase diagram of the spin-1 anisotropic Heisenberg model or *XXZ* chain, given in (2.1). Our study was done by calculating numerically the string correlation functions introduced by den Nijs and Rommelse. We show that the asymptotic behavior of these correlation functions are good order parameters to distinguish the massless phase and the massive Haldane phase.

In Sec. II, we presented the string correlation and also gave some arguments, which imply that the Haldane phase should start in a non-negative value of the anisotropy $\lambda = \lambda_c$. In Sec. III, our numerical calculations (see Fig. 4) indicate that $\lambda_c \approx 0$, which is consistent with the conjectured value of $\lambda_c = 0$.

Our results for the string correlation functions in the massless phase are in agreement with the Gaussian picture proposed for this model in the Ref. 17. We also calculate the exponent governing the power-law behavior of the string function (2.7) in the massless phase. These results indicate that these exponents are given by the anomalous dimensions of the Gaussian operator with spin-wave index equal to 1/2, normally obtained by studying (2.1) with antiperiodic boundary condition.

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