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著者	Hatsugai Y., Kohmoto M.
journal or publication title	Physical review B
volume	44
number	21
page range	11789-11794
year	1991-12
権利	(C)1991 The American Physical Society
URL	http://hdl.handle.net/2241/101207

doi: 10.1103/PhysRevB.44.11789

Numerical study of the hidden antiferromagnetic order in the Haldane phase

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(Received 3 July 1991)

We investigate the string correlation functions proposed by den Nijs and Rommelse for $S=1$ Heisenberg antiferromagnets in one dimension. The Hamiltonian with $D\sum_i(S_i^z)^2$ term is diagonalized by the Lanczos method to obtain the ground state. We calculate both the usual spin-spin correlation functions and the string correlation functions not only in the z direction (quantized direction) but also in the x direction to investigate the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry breaking recently proposed by Kennedy and Tasaki. We find that the long-range string correlation, which is argued to exist in the Haldane disordered phase, in fact, exists at the Heisenberg point $D=0$ by a finite-size analysis. We can show explicitly that the string correlation in the x direction signifies the difference between the Haldane phase and the Néel phase, which appears for the $D < 0$, $|D| \gtrsim 1$ case. In the large- D ($D \gtrsim 1$) phase, all spin-spin correlations are short ranged as expected. There is a significant enhancement in the usual and string correlations in the x direction at the boundary between the Haldane phase and the large- D phase.

I. INTRODUCTION

In 1983, Haldane argued that the ground state of the quantum antiferromagnetic Heisenberg chain has an excitation gap when spin S is integral.¹ This proposal is surprising since it was believed that there should be a spin-wave excitation without an energy gap. There are many analytical and numerical studies to confirm this argument and now it is believed that the conjecture is correct.²⁻⁸

An exactly solvable model for the $S=1$ quantum antiferromagnetic chain was discovered by Affleck, Kennedy, Lieb, and Tasaki (AKLT).² The Hamiltonian includes an additional biquadratic term which is not presented in the usual Heisenberg Hamiltonian. The ground state is the valence bond solid (VBS) which is singlet and unique with a finite excitation gap. It is a quantum-disordered state since the usual spin-spin correlation functions decay exponentially. Most of the properties Haldane proposed for the $S=1$ Heisenberg antiferromagnets are realized. Thus the model may prove to be useful in the understanding of the physics of the Haldane phase.

Den Nijs and Rommelse⁹ proposed an order parameter which is long ranged in the VBS of the AKLT model. The order parameter is nonlocal and is called the "string order parameter." Girvin and Arovas¹⁰ calculated the string correlation. It is speculated to remain long ranged at the Heisenberg point. One of the purposes of the present work is to clarify this point by systematic numerical calculations.

The XXZ Hamiltonian with the $D\sum_i(S_i^z)^2$ term [see Eq. (2.5) below] has been investigated in detail using analytical and numerical methods.⁸⁻¹⁴ Several phases are known to exist (see Fig. 1 for a schematic phase diagram). The symmetry breaking which may characterize the Haldane phase was discussed by Kennedy and Tasaki.¹⁵ They discovered a unitary transformation in the $S=1$ antiferromagnetic chain. By the transformation

the original $O(2)$ symmetry is hidden and a $\mathbb{Z}_2 \times \mathbb{Z}_2$ discrete symmetry emerges. They argued that the breakdown of the discrete symmetry brings the Haldane gap. The phases in the antiferromagnetic region have been proposed to be characterized by a full or a partial breaking of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry. We will examine this proposal by numerical calculations.

Up to now, two classes of quantum-disordered states are known. One is the VBS state mentioned above and the other is the Laughlin's quantum liquid state for the fractional quantum Hall effect.^{16,17} Each state is a unique quantum-disordered (liquid) state and there is an excitation gap. There are several similarities between these two types of ground states.^{18,19} The order parameter for the Laughlin state has been discussed by several authors.¹⁷⁻²¹ The important point is that the order parameter is hidden. Girvin and MacDonald¹⁹ argued that the

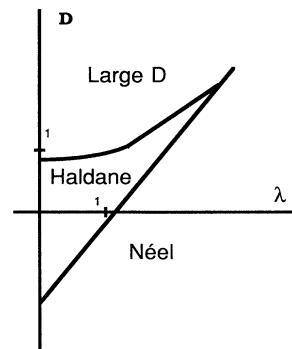


FIG. 1. Schematic phase diagram for the $S=1$ extended Heisenberg Hamiltonian in the $\lambda - D$ plane.

one-body density matrix in the magnetic field is exponentially short ranged but there appears to be a long-range (power law) behavior if one performs a singular gauge transformation. This hidden order may characterize the Laughlin state. The singular gauge transformation used by Girvin and MacDonald can be expressed by a gauge potential of a “string” type.²² The string order parameter found in the VBS state is also hidden in the sense that it is not a local order parameter. It is transformed into a local ferromagnetic order parameter after the nonlocal unitary transformation.¹⁵

In this paper, we investigate the extended Hamiltonians [see Eqs. (2.4) and (2.5) below] by calculating several order parameters in detail and characterize different phases by systematic finite-size studies. In Sec. II we discuss the theoretical background. In Sec. III numerical results are presented. Section IV is a summary.

II. MODEL AND CORRELATION

In this section we discuss the order parameters and the symmetry of the Haldane phase. We consider a spherical symmetric Hamiltonian and a XXZ Hamiltonian with a $D \sum_i (S_i^z)^2$ term for $S=1$ [see Eqs. (2.4) and (2.5)].

A spin chain with an antiferromagnetic coupling is usually characterized by the Néel order parameter defined in the α direction (where $\alpha=x, y, \text{ or } z$) by

$$\begin{aligned} O_{\text{Néel}}^\alpha &= \lim_{|i-j| \rightarrow \infty} O_{\text{Néel}}^\alpha(i, j), \\ O_{\text{Néel}}^\alpha(i, j) &= (-1)^{i-j} \langle S_i^\alpha S_j^\alpha \rangle, \end{aligned} \quad (2.1)$$

where $\langle \rangle$ means the expectation value in the ground state. It is defined by a two-point correlation of the local operator. The symmetry breaking is usually considered for a local order parameter of this type. In the Haldane phase, the ground state is disordered and the usual Néel order parameters vanish. In order to probe the hidden order in the Haldane phase, den Nijs and Rommelse⁹ defined the following nonlocal string order parameter:

$$\begin{aligned} O_{\text{string}}^\alpha &= \lim_{|i-j| \rightarrow \infty} O_{\text{string}}^\alpha(i, j), \\ O_{\text{string}}^\alpha(i, j) &= - \left\langle S_i^\alpha \exp \left[i\pi \sum_{k=i+1}^{j-1} S_k^\alpha \right] S_j^\alpha \right\rangle. \end{aligned} \quad (2.2)$$

It plays a significant role in characterizing the Haldane phase. Kennedy and Tasaki¹⁰ introduced a nonlocal unitary transformation which sheds light on the string order parameter. By the transformation, the Heisenberg Hamiltonian H is transformed to a Hamiltonian \tilde{H} and the string order parameter (2.2) is transformed to a usual ferromagnetic order parameter

$$O_{\text{string}}^\alpha(H) = O_{\text{ferro}}^\alpha(\tilde{H}). \quad (2.3)$$

In the transformed system, the original continuous symmetry [O(2) or O(3)] is hidden and the discrete $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry, which corresponds to the rotation by π around the z and x axes, emerges. This is the only explicit symmetry. The order parameters $O_{\text{ferro}}^\alpha(\tilde{H})$ ($\alpha=x$ and z) determine breakings of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry. If $O_{\text{ferro}}^z(\tilde{H}) \neq 0$, the \mathbb{Z}_2 symmetry corresponding to the rota-

tion of π around the x axis is broken. Similarly, if $O_{\text{ferro}}^x(\tilde{H}) \neq 0$, the \mathbb{Z}_2 symmetry corresponding to the rotation of π around the z axis is broken. Therefore, due to (2.3), the string order parameters in the original Hamiltonian probe the breakings or nonbreakings of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry.

A. Heisenberg Hamiltonian with a biquadratic term

Let us consider the following $S=1$ antiferromagnetic Hamiltonian with a biquadratic term,

$$H = \sum_i [S_i \cdot S_{i+1} - \beta (S_i \cdot S_{i+1})^2]. \quad (2.4)$$

At $\beta=0$, it is the spherically symmetric Heisenberg model. The AKLT Hamiltonian is realized at $\beta=-1/3$. In this case, most of the Haldane’s picture is explicitly realized. There is an excitation gap. The ground state is a unique spin singlet and is disordered in the sense that the usual spin-spin correlation functions decay exponentially.^{2,18} Den Nijs and Rommelse⁹ showed that $O_{\text{string}}^\alpha = 4/9$ ($\alpha=x, y, \text{ or } z$). Thus the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry is fully broken in the AKLT model. One of the main interests is whether such a state is realized in the isotropic Heisenberg model ($\beta=0$). The Hamiltonian (2.4) is also exactly solvable at $\beta=-1$ (Ref. 23) and $\beta=1$ (Ref. 24). There is no excitation gap at these points. Thus, it is a nontrivial problem to determine whether the Heisenberg model ($\beta=0$) is in the same universality class with $\beta=-1/3$. In this paper, we focus on this point, performing systematic numerical calculations of the order parameters.

B. Heisenberg Hamiltonian with a uniaxial anisotropy

Consider the following $S=1$ Heisenberg Hamiltonian with uniaxial anisotropy,

$$H = \sum_i [S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \lambda S_i^z S_{i+1}^z + D (S_i^z)^2]. \quad (2.5)$$

This model was investigated by a number of authors^{8,11-14} and the phase diagram in the D - λ plane was presented.^{9,12,13} Here we assume the model to be antiferromagnetic, i.e., $\lambda > 0$. It is expected to have three phases: a Néel phase, a Haldane phase, and a large- D phase as shown in Fig. 1 schematically. For a negative D and $|D| \gtrsim 1$, $|\uparrow\rangle$ and $|\downarrow\rangle$ states are preferred against the $|0\rangle$ state. Thus there may exist an Ising-like antiferromagnetic correlation and one expects that $O_{\text{Néel}}^z \neq 0$ and $O_{\text{string}}^z \neq 0$ while $O_{\text{Néel}}^x = O_{\text{string}}^x = 0$. Thus only one \mathbb{Z}_2 symmetry, which corresponds to the rotation of π , is broken (the Néel phase). On the other hand, the $|0\rangle$ state is preferred in the large- D phase. thus all the correlation functions are expected to be short ranged ($O_{\text{Néel}}^x = O_{\text{string}}^x = O_{\text{Néel}}^z = O_{\text{string}}^z = 0$).

In the AKLT model [$\beta=-1/3$ in Eq. (2.4)], the usual correlation functions decay exponentially, but one has the hidden order ($O_{\text{string}}^z \neq 0$ and $O_{\text{string}}^x \neq 0$). The $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry is fully broken. the problem is whether this behavior is realized in some of the parameter regions of the Hamiltonian (2.5) which includes the Heisenberg point

TABLE I. Relation between the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry breaking and the three phases: large- D , Haldane, and Néel. (There might be a Kosterlitz-Thouless transition near the $\lambda=0$ boundary.) \circ : The symmetry is not broken in the ground state. \times : The symmetry is broken in the ground state.

Phase	$\mathbb{Z}_2(z)$	O_{string}^z	$\mathbb{Z}_2(x)$	O_{string}^x
Large- D	\circ	zero	\circ	zero
Haldane	\times	finite	\times	finite
Néel	\times	finite	\circ	zero

($\lambda=1, D=0$). The correspondence between the three phases and the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry is summarized in Table I.

III. NUMERICAL RESULTS

We present numerical results to confirm the above scenario. The Lanczos method and the inverse iteration method²⁵ were used to obtain the ground state of (2.4) and (2.5). We restrict ourselves to the sector with $\sum_i S_i^z = 0$ to reduce the maximum required computer memory size for the ground-state calculations. For a spherically symmetric model, there is a degeneracy between sectors with different total S^z . Thus it is sufficient to investigate a sector with $\sum_i S_i^z = 0$ to obtain the ground state. For the cases with $D \neq 0$, this degeneracy is removed. The ground state in these cases, however, lies also in the $\sum_i S_i^z = 0$ sector and is unique when $\lambda=1$ (see the Appendix).

We have calculated several correlation functions including string correlations. In order to calculate string correlations in the x direction, we have to include intermediate states with different total S_z . Thus we take bases of the full Hilbert space for the calculation of the correlation functions in the x direction. In the following, we take the periodic boundary condition.

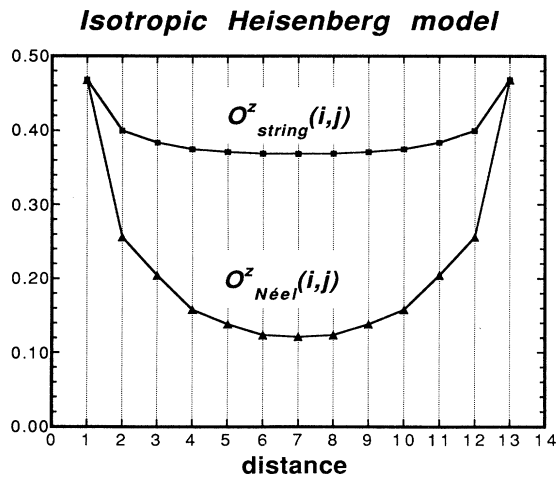


FIG. 2. Correlation functions $O_{N\acute{e}el}^z(i,j)$ and $O_{string}^z(i,j)$ for a 14-site Hamiltonian (2.4) with $\beta=0$.

A. Heisenberg Hamiltonian with a biquadratic term

In Fig. 2 we show the correlation functions $O_{N\acute{e}el}^z(i,j)$ and $O_{string}^z(i,j)$ for a 14-site system with $\beta=0$ for the Hamiltonian (2.4).²⁶ The same result has been obtained by Girvin and Arovas.¹⁰ It suggests that $O_{N\acute{e}el}^z(i,j)$ is short ranged and $O_{string}^z(i,j)$ is long ranged. In Figs. 3(a) and 3(b) we show $O_{N\acute{e}el}^z(i,j)$ and $O_{string}^z(i,j)$ for a 10-site system when we change β from $-1/2$ to 0. The data suggest that there is no phase transition between $\beta=-1/3$ and 0.

B. Heisenberg Hamiltonian with a uniaxial anisotropy

We change D in the Hamiltonian (2.5) to investigate the three phases. For simplicity, λ is fixed to unity.²⁷ We choose $D=4, 0$ and -4 , which will correspond to the large- D , Haldane, and Néel phases, respectively. In Figs. 4(a), 4(b), and 4(c) we show the longest distance behavior, $O_{N\acute{e}el}^\alpha(0, N/2)$ and $O_{string}^\alpha(0, N/2)$ ($\alpha=x$ or z), in finite-size systems as a function of the inverse of the system size $1/N$. It shows that all four order parameters are zero in the large- D phase ($D=4$) in the thermodynamic limit. In the Haldane phase ($D=0$), it suggests that Néel order parameters are zero and string order parameters are nonzero. In the Néel phase ($D=-4$), it shows that only order parameters in the z direction are nonzero. The results confirm the proposed behavior summarized in Table I. In all cases, the string order parameter takes a larger

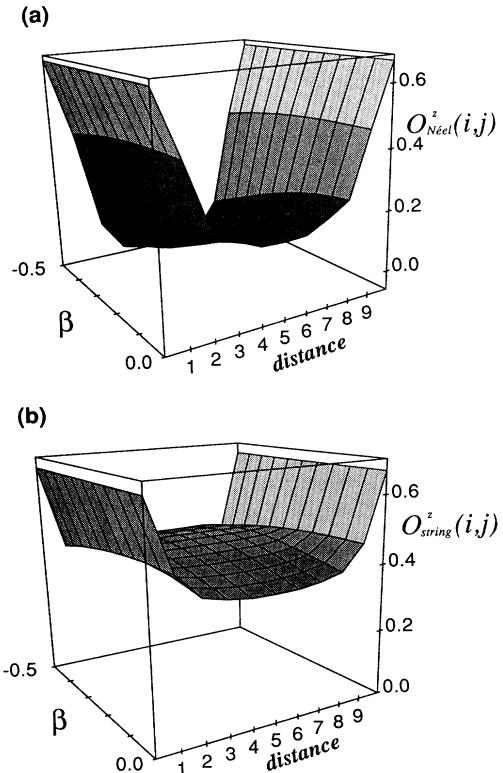


FIG. 3. Correlation functions $O_{N\acute{e}el}^z(i,j)$ and $O_{string}^z(i,j)$ for a 10-site Hamiltonian (2.4) when β is varied from -0.5 to 0. (a) $O_{N\acute{e}el}^z(i,j)$ and (b) $O_{string}^z(i,j)$.

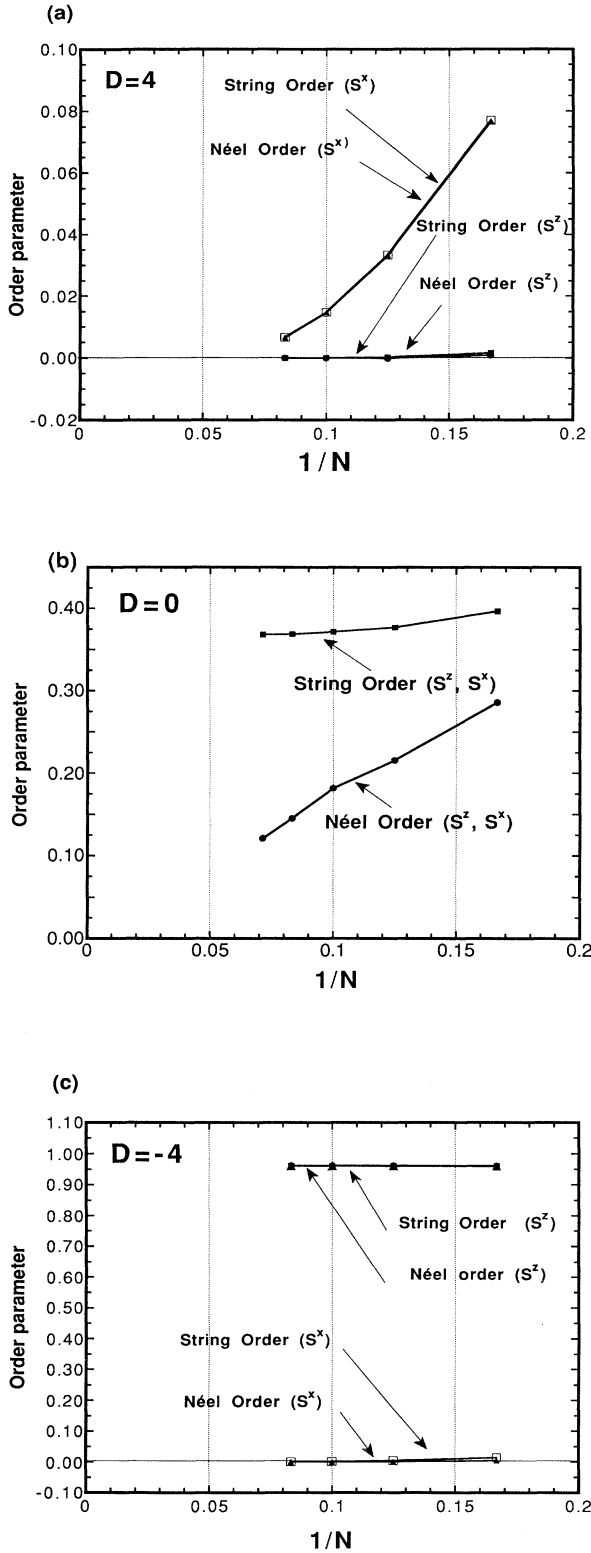


FIG. 4. The longest distance behavior $O_{\text{Néel}}^\alpha(0, N/2)$ and $O_{\text{string}}^\alpha(0, N/2)$ ($\alpha=x$ or z) for the Hamiltonian (2.5) in a finite-size system as a function of the inverse of the system size $1/N$. (a) $D=4$, (b) $D=0$, and (c) $D=-4$.

value than that of the Néel order parameter.¹⁵

In Figs. 5(a)–5(d) we show the correlation functions in the parameter region $D \in [-3, 3]$. The results are consistent with the above discussions. There is an interesting phenomenon not mentioned before when D takes a value near unity where a significant enhancement in the correlation in the x direction [$O_{\text{Néel}}^x(i, j)$ and $O_{\text{string}}^x(i, j)$] is observed.

There is an antiferromagnetic correlation when $D \sim 0$. The antiferromagnetic correlation in the z direction is suppressed if D is increased. It is possible that only the antiferromagnetic correlation in the x direction survives until D takes a large value where the energy gain by spin flip term is overcome by the energy loss of the D term.

In Fig. 6 we show the longest distance behavior, $O_{\text{Néel}}^\alpha(0, N/2)$ and $O_{\text{string}}^\alpha(0, N/2)$ ($\alpha=x$ or z) at $D=1$, as a function of the inverse of the system size. If there is a phase transition between the Haldane phase and the large- D phase, it is natural to imagine that the excitation gap which exists in both phases could collapse at an intermediate value of D . Several authors^{21,22} investigated the phase transition in detail by calculating the excitation gap in finite-size systems. If the system is massless, one expects that the correlation length of some operator diverges. The present numerical data suggest that the correlation function which is responsible for the critical behavior is the Néel correlation in the x direction $O_{\text{Néel}}^x(i, j)$. At this point, we speculate that the correlation length of the Néel correlation in the x direction diverges and it shows a power-law behavior that is exponential in both the large- D and the Haldane phases.

IV. SUMMARY

We focused on the string correlation functions proposed by den Nijs and Rommelse for the $S=1$ Heisenberg antiferromagnets by a numerical diagonalization of finite size systems. We calculated correlation functions for the Hamiltonian with a biquadratic term [Eq. (2.4)] for $\beta \in [-1/3, 0]$. We also treated the Hamiltonian with the $D \sum_i (s_i^z)^2$ term [Eq. (2.5)] and investigated the phases by extensively calculating the string order parameters which show $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry breakings proposed by Kennedy and Tasaki as well as the usual order parameters. These two \mathbb{Z}_2 symmetries are characterized by the string order parameters in the z and x directions. From finite size studies we obtained clear evidence about the correspondence between the three phases: large- D , Haldane, and Néel, and the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry breakings (see Table I). In the Haldane phase, the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry is fully broken, that is, the string order parameters are nonzero in both x and z directions. In the Néel phase, the ground state breaks only one \mathbb{Z}_2 symmetry. Only the string order parameter in the z direction is nonzero. In the large- D phase, the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry is not broken and all string order parameters are zero.

We found that there is a significant enhancement in the spin-spin correlation in the x direction both for string type and usual Néel type when $D \approx 1$. We speculate that the energy gap collapses and the correlation length of the

staggered spin-spin correlations in the x direction diverges at this point.

ACKNOWLEDGMENTS

We thank H. Tasaki for many stimulating discussions, especially for informing us of the importance of the correlation function in the x direction and showing us a proof of the lemma. Y. H. was supported in part by a Grant-in-Aid for Scientific Research on Priority Areas, "Computational Condensed Matter Physics" from the Japanese Ministry of Education, Science and Culture.

APPENDIX

The following lemma guarantees that the ground state of the Heisenberg Hamiltonian with uniaxial anisotropy is within the sector $\sum_i S_i^z = 0$. The proof is due to H. Tasaki.

A "configuration" $\sigma = \{\sigma_i\}$ will mean a choice of $\sigma_i = -1, 0$, or $+1$ at each site i , and Ψ_σ denotes the eigenstate with $S_i^z \Psi_\sigma = \sigma_i \Psi_\sigma$.

We consider the antiferromagnetic Hamiltonian with uniaxial anisotropy

$$H = \sum_i [S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \lambda S_i^z S_{i+1}^z + D(S_i^z)^2].$$

Lemma: For a finite L , the ground state is unique and satisfies $\sum_i S_i^z = 0$ if (i) $\lambda \geq 1$, $D \leq 0$ or (ii) $-1 < \lambda \leq 1$, $D \geq 0$. *Proof:* We simply extend the methods in Ref. 28 and 29. The standard application of the Perron-Frobenius theorem (as in Ref. 28) implies that, for any values of λ and D , the ground state within the sector with $\sum_i S_i^z = M$ is unique, and can be written as a linear combination of all the basis states (within the sector) with nonvanishing coefficients. So, to prove the lemma, we only have to state that the ground state is in the sector with $M = 0$. As for the SO(3) invariant model with $\lambda = 1$ and $D = 0$, this fact has been proved by Lieb and Mattis.²⁸ Following Ref. 29, we will prove that, in the models with (i) and (ii), the ground states are at most two-fold degenerate. In fact, this implies that the ground state is in the sector $M = 0$ for the following reason. Suppose the converse. Then when continuously modifying the Hamiltonian starting from the isotropic one, we must have a level crossing between the $M = 0$ sector and the other sector with $M \neq 0$. Since the sectors with $\sum_i S_i^z = M$ and $\sum_i S_i^z \neq M$ are degenerate, we must have at least

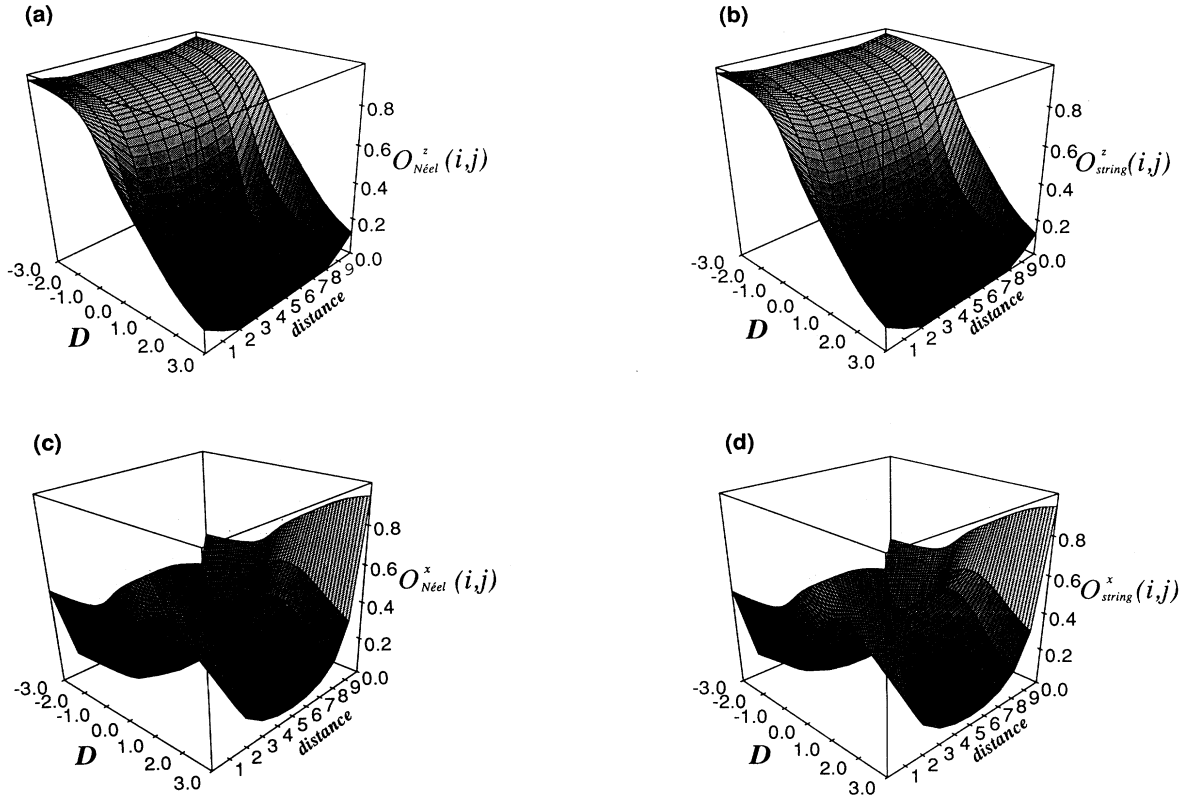


FIG. 5. Correlation functions for a 10-site Hamiltonian (2.5) when we change D from -3 to 3 . (a) $O_{\text{Néel}}^z(i, j)$, (b) $O_{\text{string}}^z(i, j)$, (c) $O_{\text{Néel}}^x(i, j)$, and (d) $O_{\text{string}}^x(i, j)$.

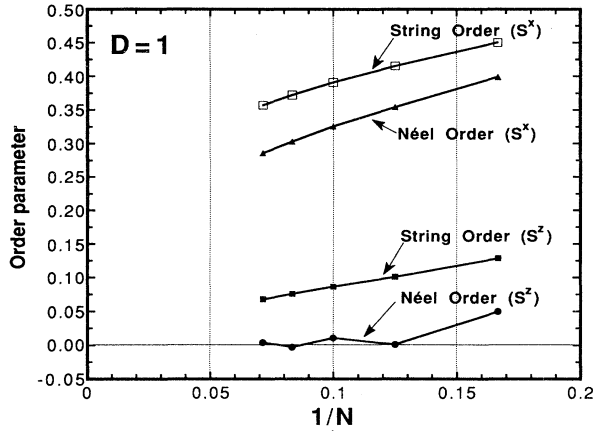


FIG. 6. The longest distance behavior $O_{\text{Néel}}^{\alpha}(0, N/2)$ and $O_{\text{string}}^{\alpha}(0, N/2)$ ($\alpha=x$ or z) for the Hamiltonian (2.5) with $D=1$ in a finite-size system as a function of the inverse system size $1/N$.

threefold degeneracy, which is a contradiction. To prove that there can be at most twofold degeneracy, we interchange the x and z coordinates (as in Ref. 29) to express the Hamiltonian as

$$H' = \sum_i \left\{ \frac{\lambda+1}{4} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) \right. \\ \left. + \frac{\lambda-1}{4} (S_i^+ S_{i+1}^+ + S_i^- S_{i+1}^-) \right. \\ \left. + S_i^z S_{i+1}^z + \frac{D}{4} \{ (S_i^+)^2 + (S_i^-)^2 \right. \\ \left. + (S_i^+ S_i^- + S_i^- S_i^+) \} \right\}.$$

When the parameters in the Hamiltonian satisfy (i) or (ii), we see that the Hamiltonian breaks up the basis states into two blocks with $\sum_i S_i^z = \text{even}$ or odd . (The isotropic point with $\lambda=1$ and $D=0$ is an exception. But this case is already covered in the original work.²⁹) All the basis states in each block are connected with each other by the action of the Hamiltonian. Let $N_{\text{even}} = \sum_j S_{2j}^z$ and $N_{\text{odd}} = \sum_j S_{2j+1}^z$. If we set $\Psi_{\sigma} = (-1)^{N_{\text{even}}} \Psi_{\sigma}$ for case (i) and $\Psi_{\sigma} = (-1)^{N_{\text{even}} - N_{\text{odd}}} \Psi_{\sigma}$ for case (ii), we can show that $\langle \Psi_{\sigma}, H' \Psi_{\sigma'} \rangle \leq 0$ for any σ and σ' . Thus we can apply the Perron-Frobenius theorem to show that the ground state is unique within each sector. Therefore the true ground states are at most twofold degenerate. Q.E.D.

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