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Sci. Rep. RITU A40 (1995) pp. 239-242
No. 2, January 1995

Haldane to Dimer Phase Transition in the Spin-1 Haldane System with Bond-Alternating Nearest-Neighbor and Uniform Next-Nearest-Neighbor Exchange Interactions

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(Received November 14, 1994)

The Haldane to dimer phase transition is studied in the spin-1 Haldane system with bond-alternating nearest-neighbor and uniform next-nearest-neighbor exchange interactions, where both interactions are antiferromagnetic and thus compete with each other. By using a method of exact diagonalization, the ground-state phase diagram on the ratio of the next-nearest-neighbor interaction constant to the nearest-neighbor one versus the bond-alternation parameter of the nearest-neighbor interactions is determined. It is found that the competition between the interactions stabilizes the dimer phase against the Haldane phase.
KEYWORDS: spin-1 Haldane system, Haldane to dimer phase transition, bond alternation, competing exchange interaction, ground-state phase diagram

1. Introduction

The one-dimensional antiferromagnetic spin-1 Heisenberg system (the spin-1 Haldane system) has been the subject of numerous theoretical and experimental studies. These are motivated mainly by Haldane's prediction [1] that the ground state of the integer-spin case, in contrast to that of the half-integer-spin case, is in a massive phase characterized by a finite gap in the excitation spectrum and by an exponential decay of the two-spin correlation functions. One of the recent topics of this subject is the effect of the bond alternation on the ground-state properties of the system where only the nearest-neighbor exchange interactions are assumed. Several authors [2,3,4,5] have shown that, as the bond-alternation parameter α (for the definition of α, see Eq. (1) below) increases, a transition from the Haldane phase to the dimer phase takes place at a finite critical value $\alpha = \alpha_c$. Another topic is the effect of the antiferromagnetic next-nearest-neighbor exchange interactions on the ground-state properties of the system. Employing a method of exact diagonalization, two of the present authors (T. T. and M. K.) and co-workers [6,7] have demonstrated that the competition between the nearest-neighbor and next-nearest-neighbor interactions enhances the stability of the Haldane phase. Shimaoka and Kuboki [8] have also obtained qualitatively the same result by use of a bosonization method.

In these circumstances we will discuss the ground-state properties of the spin-1 Haldane system with bond-alternating nearest-neighbor and uniform next-nearest-neighbor exchange interactions. We express the Hamiltonian which describes the system as

$$\mathcal{H} = 2\sum_{\ell=1}^{N}\left\{1-(-1)^{\ell}\alpha\right\}\vec{S}_{\ell}\cdot\vec{S}_{\ell+1} + 2j\,(1-\alpha)\sum_{\ell=1}^{N}\vec{S}_{\ell}\cdot\vec{S}_{\ell+2}\,, \qquad (1)$$

where $\vec{S}_{\ell}$ is the spin-1 operator at the ℓth site; α ($0 \le \alpha \le 1$) is the bond-alternation parameter of the nearest-neighbor interactions; j ($j \ge 0$) is the ratio of the next-nearest-neighbor interaction constant to the nearest-neighbor one in the case of $\alpha = 0$; N is the total number of spins in the system and is assumed to be even. We impose periodic boundary conditions ($\vec{S}_{\ell+N} = \vec{S}_{\ell}$). It is noted that the nearest-neighbor and next-nearest-neighbor interactions compete with each other, since both are antiferromagnetic.

As was mentioned before, it has already been known that, in the case of $j = 0$, the Haldane to dimer phase transition occurs at $\alpha = \alpha_c$. According to a pioneering work by Singh and Gelfand [2], who have used a series-expansion method, the value of α_c is given by $\alpha_c = 0.25 \pm 0.03$. Recently, Kato and Tanaka [3] have employed a density-matrix renormalization method [9] to obtain $\alpha_c = 0.25 \pm 0.01$, and Nishiyama *et al.* [4] have analyzed the Binder parameter [10] associated with string order [11], calculated by exact diagonalizations, to obtain $\alpha_c = 0.255 \pm 0.01$. The results of more recent quantum Monte Calro calculation performed by Yamamoto [5] support these results. As can be seen from Fig. 1 in reference [3], the singlet-triplet energy gap $\Delta_{\rm st}(N)$ for finite N ($N = 8,\ 10,\ \cdots$), which will be defined by Eq. (5) below, has a minimum value at $\alpha = \alpha_c(N)$; the minimum value decreases monotonously as N increases and vanishes at $\alpha = \alpha_c$ in the thermodynamic limit ($N \to \infty$) [12]. This is consistent with Affleck and Haldane's argument [13] that the ground state of the system described by the Hamiltonian $\mathcal{H}$ with $j = 0$ and with arbitrary spin magnitude S has $2S$ massless points in the range of $-1 \le \alpha \le 1$.

In the case of $j = 1/2$, on the other hand, Shastry and Sutherland [14] have shown that the following dimer state:

$$\Phi_{\rm dimer} = [1,\ 2]\ [3,\ 4]\ [5,\ 6]\ \cdots\ [N-1,\ N] \qquad (2)$$

is an eigenstate of the Hamiltonian $\mathcal{H}$ and that the en-

ergy eigenvalue $E_{\rm dimer}$ is given by

$$E_{\rm dimer} = -2N(1+\alpha)\,. \qquad (3)$$

(We discuss more general cases in the Appendix.) In Eq. (2) the symbol $[\ell,\ \ell+1]$ denotes the normalized singlet combination of spins $\vec{S}_\ell$ and $\vec{S}_{\ell+1}$, and is explicitly expressed as

$$[\ell,\ \ell+1] = \frac{1}{\sqrt{3}}\left(\alpha_\ell\beta_{\ell+1} - \zeta_\ell\zeta_{\ell+1} + \beta_\ell\alpha_{\ell+1}\right)\,, \qquad (4)$$

where α_ℓ, ζ_ℓ, and β_ℓ represent, respectively, the single-spin states with $S_\ell^z = 1$, 0, and -1. It is apparent that the dimer state $\Phi_{\rm dimer}$ is a singlet state. Furthermore, Shastry and Sutherland [14] have performed a variational calculation and have shown that $\Phi_{\rm dimer}$ is the ground state of the system at least when $\alpha \geq \alpha_{\rm c}^{\rm var} = 1/3$. This suggests that also in the case of $j = 1/2$, the Haldane to dimer phase transition occurs at a critical value $\alpha_{\rm c}$ $\left(0 < \alpha_{\rm c} < \alpha_{\rm c}^{\rm var}\right)$ of α, since the system is in the Haldane phase when $j = 1/2$ and $\alpha = 0$ [15].

In this paper we determine the ground-state phase diagram on the j versus α plane, using a method of exact diagonalization.

2. Numerical Results and Discussion

In order to determine the ground-state phase diagram on the j versus α plane, we diagonalize the Hamiltonian $\mathcal{H}$ for finite-size ($N = 6$, 8, $\cdots$, 18) systems within the subspace determined by the value $M = \sum_{\ell=1}^{N} S_\ell^z$ (= 0, 1, $\cdots$, N) and calculate the lowest energy eigenvalue $E_0(N, M)$ and the second-lowest one $E_1(N, M)$. In these calculations we employ our computer program package KOBEPACK/S coded by using a new coding technique, developed by two of the present authors (M. K. and T. T.) and Nishino [16], of the Lanczös method. The results of our calculation show that the ground state of the finite-size system belongs always to the $M = 0$ subspace and is a singlet state. In other words, the ground-state energy is always given by $E_0(N, 0)$. Thus, the singlet-triplet energy gap $\Delta_{\rm st}(N)$, i.e., the energy difference between the ground state and the lowest state within the $M = 1$ subspace, which belongs to a triplet state, is defined as

$$\Delta_{\rm st}(N) = E_0(N, 1) - E_0(N, 0)\,. \qquad (5)$$

Let us start with the discussion on the case of $j = 1/2$. According to the calculation, as the bond-alternation parameter α decreases from 1, the ground state of the finite-size system changes from the dimer state $\Phi_{\rm dimer}$ to another singlet state at $\alpha = \alpha_{\rm c}(N)$. The values of $\alpha_{\rm c}(N)$ for various N are listed in the seventh column in Table 1. Since they are almost independent of N at least when $N \gtrsim 12$, we can estimate rather accurately the limiting ($N \to \infty$) value $\alpha_{\rm c}$ of $\alpha_{\rm c}(N)$ to be $\alpha_{\rm c} = 0.1583 \pm 0.0001$. As is expected, this value satisfies $0 < \alpha_{\rm c} < \alpha_{\rm c}^{\rm var} (= 1/3)$. It is noted that, as shown in Fig 1, the gap $\Delta_{\rm st}(N)$ takes a minimum value at $\alpha = \alpha_{\rm c}(N)$, the minimum value decreasing monotonously as N increases.

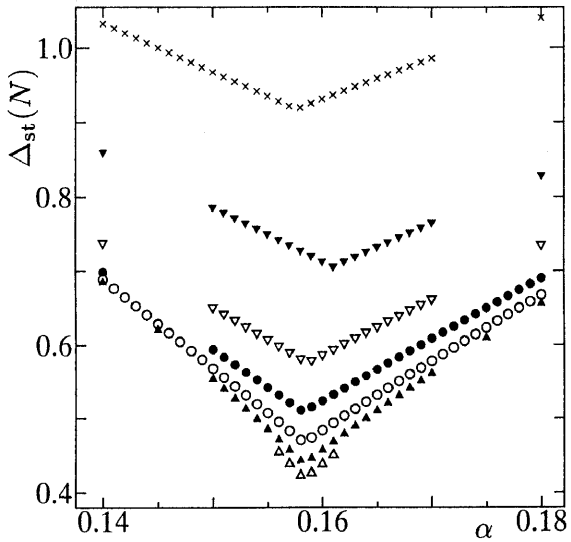

Figure 1: Plot of the singlet-triplet energy gap $\Delta_{\rm st}(N)$ versus α for various values of N, calculated for $j = 0.5$. The symbols, ×, ▼, ▽, ●, ○, ▲, and △, are for $N = 6$, 8, 10, 12, 14, 16, and 18, respectively.

Figure 1 in reference [3] as well as Fig. 1 in this paper suggests that, for arbitrary values of j, the critical value

Table 1: Values of $\alpha_{\rm c}(N)$ for $N = 6$, 8, $\cdots$, 18 and that of $\alpha_{\rm c}$, obtained for representative values of j. Note that, when $N = 6$ and $j = 0.0$, the gap $\Delta_{\rm st}(N)$ is an increasing function of α in the region of $0.0 \leq \alpha \leq 0.5$.

	$j=0.0$	$j=0.1$	$j=0.2$	$j=0.3$	$j=0.4$	$j=0.5$
$\alpha_{\rm c}(6)$	—	0.13270	0.16503	0.17356	0.16602	0.15762
$\alpha_{\rm c}(8)$	0.19129	0.20667	0.20785	0.19858	0.18138	0.16094
$\alpha_{\rm c}(10)$	0.22674	0.22752	0.21995	0.20546	0.18528	0.15862
$\alpha_{\rm c}(12)$	0.24140	0.23607	0.22476	0.20830	0.18703	0.15824
$\alpha_{\rm c}(14)$	0.24872	0.24021	0.22707	0.20972	0.18792	0.15830
$\alpha_{\rm c}(16)$	0.25278	0.24245	0.22831	0.21053	0.18840	0.15832
$\alpha_{\rm c}(18)$	0.25520	0.24374	0.22904	0.21103	0.18869	0.15832
$\alpha_{\rm c}$	0.260± 0.01	0.247± 0.01	0.232± 0.01	0.213± 0.01	0.189± 0.01	0.1583±0.0001

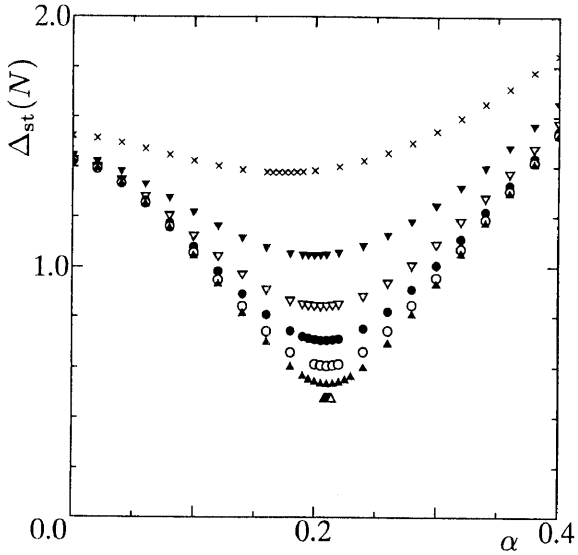

Figure 2: Plot of the singlet-triplet energy gap $\Delta_{st}(N)$ versus α for various values of N, calculated for $j=0.3$. The symbols, ×, ▼, ▽, ●, ○, ▲, and △, are for $N=6$, 8, 10, 12, 14, 16, and 18, respectively.

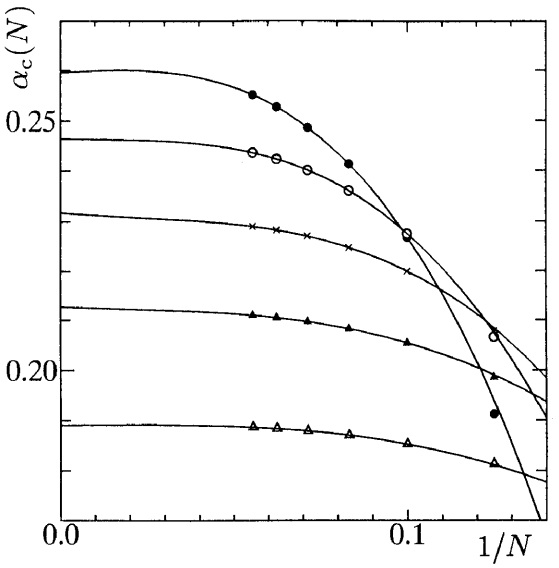

Figure 3: Plot of $\alpha_c(N)$ versus $1/N$ for representative values of j. The symbols, ●, ○, ×, ▲, and △ are for j = 0.0, 0.1, 0.2, 0.3, and 0.4, respectively. The solid lines illustrate the extrapolation of $\alpha_c(12)$, $\alpha_c(14)$, $\alpha_c(16)$, and $\alpha_c(18)$ to $N\to\infty$, the procedure of which is discussed in the text.

α_c of α at which the Haldane to dimer phase transition occurs, can be estimated by extrapolating to the $N\to\infty$ limit the value $\alpha_c(N)$ of α which yields the minimum of $\Delta_{st}(N)$. As an example, we show in Fig. 2 the α-dependence of $\alpha_c(N)$ for N = 6, 8, ···, 18 calculated for $j=0.3$. The values of $\Delta_{st}(N)$ obtained for $j=0.0$, 0.1, 0.2, 0.3, and 0.4 are tabulated, respectively, in the second to sixth columns in Table 1, and are plotted as functions of $1/N$ in Fig. 3. In order to estimate α_c, we make a fit of $\alpha_c(12)$, $\alpha_c(14)$, $\alpha_c(16)$, and $\alpha_c(18)$ to a cubic function of $1/N$, i.e.,

$$\alpha_c(N) = \alpha_c + \frac{c_1}{N} + \frac{c_2}{N^2} + \frac{c_3}{N^3} \qquad (6)$$

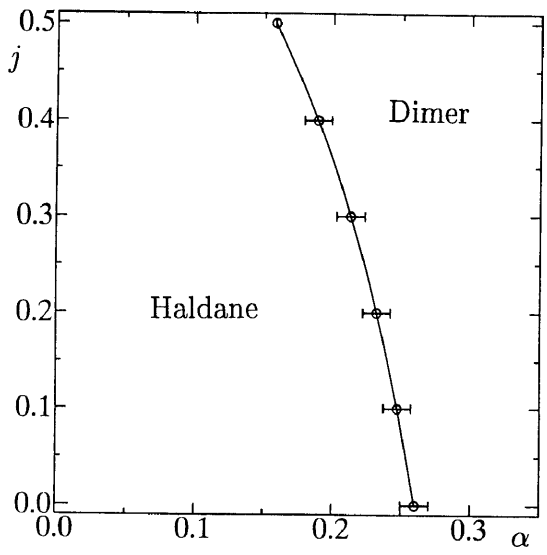

Figure 4: The ground-state phase diagram on the j versus α plane.

with numerical constants c_1, c_2, and c_3. This fitting is illustrated in Fig. 3, and the results for α_c are tabulated in Table 1. It is noted that our result in the case of $j=0$ agrees with the above-mentioned previous results [2,3,4] within the numerical uncertainties.

Figure 4 shows our result for the ground-state phase diagram on the j versus α plane, where the phase boundary line between the Haldane and dimer phases is obtained by connecting smoothly the estimated values of α_c as a function of j. It is clearly seen that the competition between the nearest-nearest-neighbor and next-nearest-neighbor interactions stabilizes the dimer phase against the Haldane phase, as far as the region of $0\le j\le 1/2$ is concerned.

3. Concluding Remarks

We have determined the ground-state phase diagram on the j versus α plane of the system described by the Hamiltonian $\mathcal{H}$, analyzing in the case of $j=1/2$ the finite-size results for the ground-state energy $E_0(N,0)$ and in the case of $0\le j<1/2$ those for the singlet-triplet energy gap $\Delta_{st}(N)$. In order to estimate more accurately the critical value α_c in the latter case, it is necessary to carry out more studies of various physical quantities related to the ground-state eigenfunction. One of the quantities is the Binder parameter associated with string order which has been discussed by Nishiyama *et al.* [4] in the case of $j=0$. Other important quantities are, we believe, the antiferromagnetic equal-time structure factor, which diverges in the $N\to\infty$ limit at least when $j=0$ [2], and also the Binder parameter associated with dimer order. The results of these studies as well as that of the study of how does α_c behave as a function of j in the case of $j>1/2$ will be published in the near future.

The present study suggests that in the spin-1 case, Affleck and Haldane's argument [13] holds even when $j>0$, although it is not clear at present whether the limiting value $\Delta_{st}(\infty)$ of the singlet-triplet energy gap vanishes at $\alpha=\alpha_c$ or not. Both clarifying this and ex-

tending the present study to the larger spin-magnitude cases are left for future investigations.

Acknowledgment

This work has been supported in part by a Grant-in-Aid for Scientific Research on Priority Areas, 'Computational Physics as a New Frontier in Condensed Matter Research', from the Ministry of Education, Science and Culture.

Appendix

Throughout this appendix, we assume that the magnitude of the spin operator $\vec{S}_\ell$ takes an arbitrary value $S\,(=1/2,\ 1,\ 3/2,\ \cdots)$. Let us consider the Hamiltonian,

$$\mathcal{H}_S = 2\sum_{\ell=1}^{N/2}\Big\{\big(J\lambda^2 + J'\lambda'^2\big)\vec{S}_{2\ell-1}\cdot\vec{S}_{2\ell} + \big(J+J'\big)\vec{S}_{2\ell}\cdot\vec{S}_{2\ell+1} + J\vec{S}_{2\ell-1}\cdot\vec{S}_{2\ell+1} + J'\vec{S}_{2\ell}\cdot\vec{S}_{2\ell+2}\Big\}\ , \quad (7)$$

where the first two terms in the braces represent the nearest-neighbor interactions and the third and fourth terms in the braces represent the next-nearest-neighbor ones; the total number N of spins is assumed to be even. We rewrite this Hamiltonian in the following form:

$$\mathcal{H}_S = J\sum_{\ell=1}^{N/2}\Big[\Big\{\lambda\big(\vec{S}_{2\ell-1}+\vec{S}_{2\ell}\big)+\vec{S}_{2\ell+1}/\lambda\Big\}^2 - 2\lambda^2 S(S+1) - S(S+1)/\lambda^2\Big] + J'\sum_{\ell=1}^{N/2}\Big[\Big\{\vec{S}_{2\ell}/\lambda' + \lambda'\big(\vec{S}_{2\ell+1}+\vec{S}_{2\ell+2}\big)\Big\}^2 - 2\lambda'^2 S(S+1) - S(S+1)/\lambda'^2\Big] \quad (8)$$

Then, by using the relation,

$$\big(\vec{S}_{2\ell-1}+\vec{S}_{2\ell}\big)[2\ell-1,\ 2\ell] = 0\ , \quad (9)$$

it is easy to see that $\Phi_{\rm dimer}$ given by Eq. (2) is an eigenstate of $\mathcal{H}_S$ with the energy eigenvalue

$$E_{\rm dimer} = -NS(S+1)\big(J\lambda^2 + J'\lambda'^2\big)\ . \quad (10)$$

The symbol $[2\ell-1,\ 2\ell]$ in Eq. (9) and in the expression of $\Phi_{\rm dimer}$ stands for the normalized singlet combination of two spins $\vec{S}_{2\ell-1}$ and $\vec{S}_{2\ell}$ with magnitude S. In the special case where $J=J'=(1-\alpha)/2$ and $J\lambda^2+J'\lambda'^2 = 1+\alpha$, the Hamiltonian $\mathcal{H}_S$ is reduced to the Hamiltonian $\mathcal{H}$, given by Eq. (1), with $j=1/2$. It is noted that Shastry and Sutherland's variational calculation [14] leads to the result that in the above special case, $\Phi_{\rm dimer}$ becomes the ground state of the system described by $\mathcal{H}_S$ for $S\geq 1$ at least when $\alpha \geq \alpha_{\rm c}^{\rm var} = S/(2+S)$.

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