Renormalization-group study of high-spin Heisenberg antiferromagnets

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An even-site block renormalization-group method is applied to the spin-1 and spin-$\frac{3}{2}$ anisotropic or alternating Heisenberg antiferromagnets. In the spin-1 case it shows an energy gap $\Delta \cong 0.368\,166$ and ground-state energy $E_0/NJ \cong 1.449\,724$, which are in good agreement with the recent Monte Carlo results. In the spin-$\frac{3}{2}$ case it shows an energy excitation behavior similar to that in the spin-$\frac{1}{2}$ case. Therefore, our study tends to support Haldane's conjecture. In addition, a possible novel property of the spin-1 Heisenberg antiferromagnet has been predicted.

I. INTRODUCTION

Through great effort during the past two decades, the study of one-dimensional, spin-$\frac{1}{2}$ magnets has achieved great success and has borne many interesting results and spectacular theories, such as the exact analytic (Bethe-ansatz) calculations, the Kubo-Anderson spin-wave theory, the Bonner-Fisher finite-chain–extrapolation approach, and the renormalization-group (RG) method, etc. Recently, a quite extensive study of quantum higher-spin chains was stimulated by Haldane's famous conjecture[1] which predicts the existence of a radically different type of ($T=0$) phase behavior for the class of integer-spin one-dimensional (1D) Heisenberg-Ising antiferromagnets (AFM's) when compared with the class of half-odd-integer-spin XXZ chains. For example, an energy gap opens between the ground state and the first excitation state for the case of integer spin; however, for the case of half-odd-integer spin the energy gap is always zero.

Consider the Hamiltonian for the linear antiferromagnet,

$$H = J \sum_{i=1}^{N} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \alpha S_i^z S_{i+1}^z) , \tag{1}$$

where α is the XXZ anisotropy parameter ($\alpha=0$ corresponds to the XY model, $\alpha=1$ to the Heisenberg antiferromagnet, and $\alpha>1$ to uniaxial Ising-like anisotropy). Haldane's conjecture can be schematically represented by the relevant values of the lowest-lying energy levels (Fig. 1),[2] namely, an energy-gap opens up between the ground-state singlet and higher excitations for the class of integer-spin Heisenberg AFM's, whereas the class of half-odd-integer-spin Heisenberg AFM's has a gapless spectrum.

Haldane's conjecture suggests the possibility that there exist some novel quantum effects for higher-spin chains. It naturally attracts, therefore, the great interest of many authors. However, the validity of Haldane's prediction still remains interesting and controversial. It is known rigorously that a gap is absent for the spin-$\frac{1}{2}$ chains. Recently, Botet and Jullien[3] calculated the energy gap of the spin-1 Heisenberg chain by using the finite-chain scaling analysis up to $N_s=12$. They concluded that their results support Haldane's conjecture with the consequence that an energy gap opens up when $N_s \to \infty$.

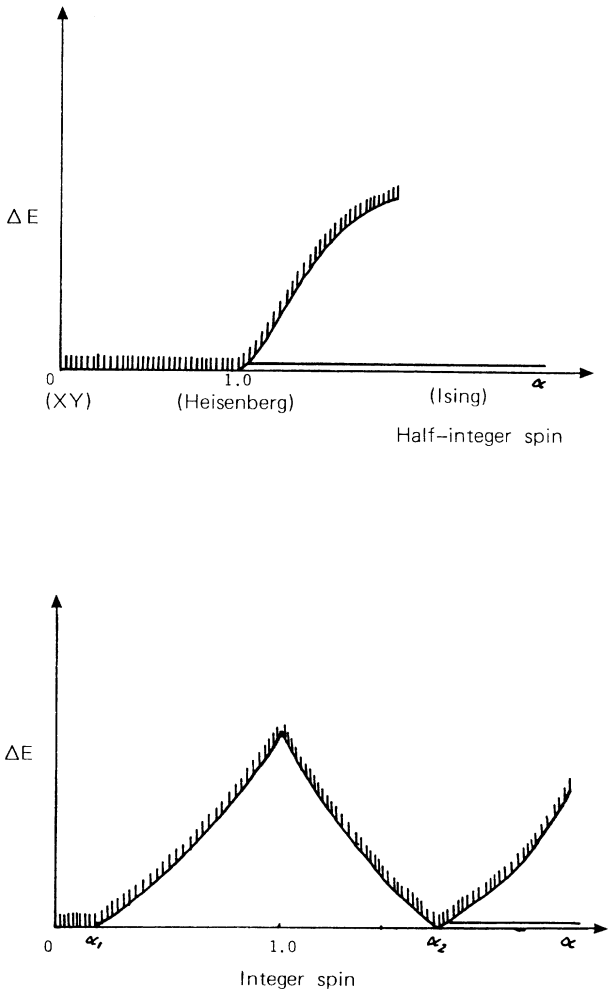

FIG. 1. Low-lying excitations (schematic) as a function of anisotropy α for XXZ Heisenberg spin chains, according to the prediction of Haldane.

However, this conclusion is open to some doubt since Bonner and Muller[4] and independently Sólyom and Ziman[5] seriously questioned it. What raised doubts is that the spin-$\frac{1}{2}$ Heisenberg chain, with size $N_s \leq 12$, when subjected to the same analysis, was found to exhibit behavior strikingly similar to the spin-1 Heisenberg chains, which is in conflict with the known results of the spin-$\frac{1}{2}$ system. Parkinson and Bonner[2] then calculated the energy gap of a finite spin-1 chain up to $N_s = 14$, but they concluded that N_s is still too small to find conclusive evidence for Haldane's conjecture. Moreover, Bonner and Muller predicted that if the lengths of the finite cell become as large as $N_s = 30$, the asymptotic behavior for the spin-1 Heisenberg AFM might be found. Very recently, Nightingale and Blote[6] (NB) successfully obtained the energy gap of the isotropic finite spin-1 Heisenberg chain up to $N_s = 32$ by using a Monte Carlo calculation. Their results support Haldane's conjecture by finding an energy gap in the excitation spectrum when $N_s \to \infty$; the energy gap $\Delta \cong 0.41$ and the ground-state energy $E_0/NJ \cong 1.4015 \pm 0.0005$.

Among very recent research reports we find that Botet and Jullien[3] and Glaus and Schneider[7] claim to support Haldane's conjecture by using the finite-size scaling calculations; however, Sólyom[5,8] and Chui and Ma[9] proposed that the phase diagrams of the spin-1 Heisenberg AFM are in disagreement with Haldane's conjecture. Therefore the validity of Haldane's conjecture still remains an open problem. We also notice that there are many methods adopted to study the linear quantum higher-spin magnets; however, very few use the RG method to treat the problem.

As a matter of fact, Fields, Bonner, and Blöte[10–14] (FBB) have studied the energy spectrum of the linear spin-$\frac{1}{2}$ anisotropic and alternating AFM's by using the block-RG (BRG) approaches, but the results they obtained are not very good. A suitable example of using the BRG method to treat the higher-spin ($S > \frac{1}{2}$) Heisenberg chains does not yet exist.[15] Although the well-known BRG method is not always reliable, we still think it is worth trying to use it to deal with this problem for the following reasons. First, in spite of the fact that the results of the FBB method for the spin-$\frac{1}{2}$ Heisenberg chains are not quantitatively accurate, they are qualitatively correct; second, we find that if we use an even BRG method, it does not keep the uniform chain unchanged, so that the uniform spin-$\frac{1}{2}$ Heisenberg chain shows a small energy gap instead of being gapless ($\Delta = 0.151$ by Fields[10]). We expect for this reason that this even BRG will give a meaningful energy gap, if it exists, for the spin-1 Heisenberg chain due to symmetry breaking of the original uniform chain. The third reason is that this even BRG method can uniformly describe the energy-spectrum behavior of higher-spin chains either for anisotropic or alternating AFM's. It is proved by our calculations that we can get a quite reasonable energy spectrum for higher-spin cases and, therefore, give a global picture of the energy-spectrum behavior of Haldane's conjecture.

In this study we find such an even BRG approach which can obtain the qualitatively good spectrum excitations for the one-dimensional (1D), spin-1 and spin-$\frac{3}{2}$ anisotropic or dimerized Heisenberg chains. For the spin-1 case our results for energy-gap and ground-state energies are in good agreement with the Monte Carlo results of NB.[6] We also find some new anisotropic and alternating spectrum behavior, including a possible novel property of the spin-1 Heisenberg chains. For spin-$\frac{3}{2}$, which is a nontrivial case compared to the spin-$\frac{1}{2}$ case, we find that the spectrum excitation behavior is similar to that in the spin-$\frac{1}{2}$ case, and differs radically from the spin-1 case. Therefore, our result tends to support Haldane's conjecture.

The paper is organized as follows. Section II describes the method in the spin-1 case. Section III gives a brief report on the study in the spin-$\frac{3}{2}$ case. Section IV is devoted to the conclusion and discussion.

II. THE SPIN-1 CASE

The essence of the quantum BRG method is that the original lattice is divided into blocks of spins and the original Hamiltonian of interest is divided into intrablock and interblock parts. The eigenvalues and eigenvectors of the intrablock Hamiltonian can be calculated exactly. A given number of low-lying eigenstates are retained to write the interblock interaction; such iterations are continued until a "fixed point" is reached. We use N_s to indicate the number of spins grouped in one block, and the number of the energy levels retained at each iteration step is indicated by N_l.

The Hamiltonian of the anisotropic and dimerized Heisenberg chain can be described as

$$H = J_1 \sum_{i=1}^{N/2} (S^x_{2i-1} S^x_{2i} + S^y_{2i-1} S^y_{2i} + \alpha S^z_{2i-1} S^z_{2i}) + J_2 \sum_{i=1}^{N/2} (S^x_{2i} S^x_{2i+1} + S^y_{2i} S^y_{2i+1} + \alpha S^z_{2i} S^z_{2i+1}) , \quad (2)$$

where S^x, S^y, and S^z are spin operators, J_1 and J_2 are the interacting constants, and $\alpha = J_{xy}/J_z$ indicates the anisotropic parameter; the alternating parameter is $\gamma = J_2/J_1$ and N is the number of the total sites of the spin chain. The BRG calculations can be naturally divided into two classes; one chooses N_s to be odd- or even-number sites. The odd-BRG method always preserves the invariance with respect to the labeling of J_1 and J_2, while the uniform limit of $J_1 = J_2$ is always found to be an unstable fixed point of the spin systems; hence it makes it impossible to calculate the energy gap. However, the even-BRG method will change the original uniform chain into an alternating one, and this kind of symmetry breaking is observed to be weak for the half-odd-integer-spin chains since the uniform spin-$\frac{1}{2}$ chain is known to be gapless. We find, however, that the above symmetry breaking is stronger for the spin-1 chains since a significant energy gap has been observed.

In the process of symmetry breaking we have to consider the arbitrary possibilities of two kinds of dimerized chains (see Fig. 2); therefore we must symmetrize them

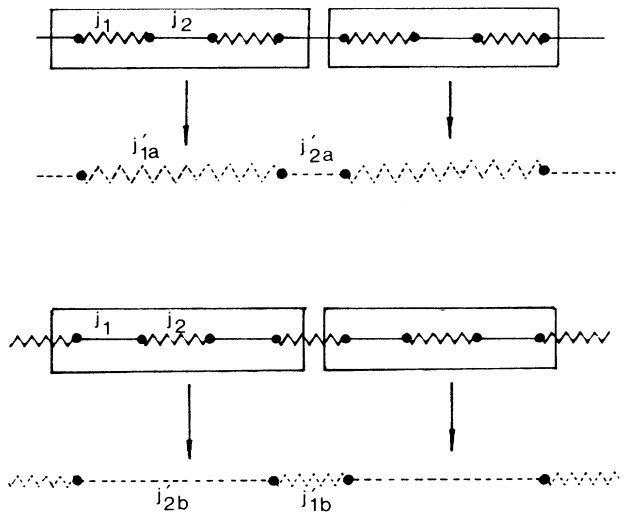

FIG. 2. Two types of mapping in the even BRG procedure, where J_1, J_2, J'_{1a}, J'_{1b}, J'_{2a}, and J'_{2b} are the coupling constants.

in order to preserve the symmetry of the Hamiltonian; namely

$$R(J_1)=\tfrac{1}{2}(J'_{1a}+J'_{1b}),\quad R(J_2)=\tfrac{1}{2}(J'_{2a}+J'_{2b}), \tag{3}$$

where $R(J_1)$ and $R(J_2)$ are symmetrized renormalized coupling constants. This even BRG will keep the dimer as a stable point. We can then calculate the energy gap at the fixed point for different anisotropy parameters.

The ground-state energy can be found by using the well-known formula[10]

$$E_0=\lim_{n\to\infty} C^{(n)}/4^n=\sum_{m=1}^{m\gg 1} E_0^{(m)}/4^m, \tag{4}$$

where $C^{(n)}$ is the nth RG constant term and $E_0^{(m)}$ is the nth ground-state energy.

In practice, the simplest way of performing a BRG calculation is to group four spins into one block and retain the lowest-energy levels in each RG transformation step, i.e., $N_s=4$ and $N_l=2$.

For the two-site block the block Hamiltonian is

$$H'_2=K'_1S_1^{z\prime}S_2^{z\prime}+\tfrac{1}{2}D'_1(S_1^{+\prime}S_2^{-\prime}+S_1^{-\prime}S_2^{+\prime})-h'(S_1^{z\prime}+S_2^{z\prime}), \tag{5a}$$

and the interaction between blocks is

$$V'_{12}=K'_2S_{12}^{z\prime}S_{21}^{z\prime}+\tfrac{1}{2}D'_2(S_{12}^{+\prime}S_{21}^{-\prime}+S_{12}^{-\prime}S_{21}^{+\prime}). \tag{5b}$$

where $S^{\pm}=S^x\pm iS^y$, K, D, and h are interaction constants, and $D/K=\alpha$ is the anisotropy parameter. In the Heisenberg case ($K=D$, $h=0$) the block Hamiltonian (5a) has the eigenstates which include a singlet, a triplet, and a quintet with the lowest-energy levels

$$\begin{aligned}
&|Q+2\rangle=|11\rangle,\quad E_1=K'-2h',\\
&|Q+1\rangle=1/\sqrt{2}(|10\rangle+|01\rangle),\quad E_2=D'-h',\\
&|Q0\rangle=1/\sqrt{1+a}\,[a\,|00\rangle+1/\sqrt{2}(|1-1\rangle+|-11\rangle)],\\
&\qquad E_3=\tfrac{1}{2}[-K'+(K^{2\prime}+8D^{2\prime})^{1/2}],\\
&|Q-1\rangle=1/\sqrt{2}(|-10\rangle+|0-1\rangle),\quad E_4=D'+h',\\
&|Q-2\rangle=|-11\rangle,\quad E_5=K'+2h',\\
&|t+1\rangle=1/\sqrt{2}(|10\rangle-|01\rangle),\quad E_6=-D'-h',\\
&|t_0\rangle=1/\sqrt{2}(|1-1\rangle-|-11\rangle),\quad E_7=-K',\\
&|t-1\rangle=1/\sqrt{2}(|-10\rangle-|0-1\rangle),\quad E_8=-D'+h',\\
&|s\rangle=1/\sqrt{1+a}\,[|00\rangle-a/\sqrt{2}(|1-1\rangle+|-11\rangle)],\\
&\qquad E_9=\tfrac{1}{2}[-K'-(K^{2\prime}+8D^{2\prime})^{1/2}],
\end{aligned} \tag{6}$$

where

$$a=2\sqrt{2}D'/[-K'+(K^{2\prime}+8D^{2\prime})^{1/2}]. \tag{7}$$

The four-site block Hamiltonian is

$$\begin{aligned}
H_4=&K_1(S_1^zS_2^z+S_3^zS_4^z)+\tfrac{1}{2}D_1(S_1^+S_2^-+S_1^-S_2^+\\
&+S_3^+S_4^-+S_3^-S_4^+)\\
&+K_2(S_2^zS_3^z)+\tfrac{1}{2}D_2(S_2^+S_3^-+S_2^-S_3^+)\\
&-h(S_1^z+S_2^z+S_3^z+S_4^z).
\end{aligned} \tag{8}$$

The eigenproblem of the Hamiltonian (8) is easy to solve, which tells us that a singlet $|s\rangle$ and a triplet $|t\pm1\rangle$, $|t_0\rangle$ occupies the lowest energy among the total 81 eigenstates.

In order to carry out the block RG calculation, we have to find out the mapping relation between the original Hamiltonian H_4 (a four-site block Hamiltonian) and the renormalized Hamiltonian H_2. For the zero-order renormalization transformation, from (6) we have

$$\begin{aligned}
&E_{t+1}=A-D'-h',\\
&E_{t_0}=A-K',\\
&E_{t-1}=A-D'+h',\\
&E_s=A-\tfrac{1}{2}[K'+(K^{2\prime}+8D^{2\prime})^{1/2}].
\end{aligned} \tag{9}$$

Solving Eq. (9) we get the following recursion relation:

$$\begin{aligned}
&A=\tfrac{1}{4}[\eta+(\eta^2-8\xi)^{1/2}],\\
&D'=A-\xi,\\
&K'=A-E_{t_0},\\
&h'=\tfrac{1}{2}(E_{t+1}-E_{t-1}),
\end{aligned} \tag{10}$$

where A is the renormalization-group constant and

$$\begin{aligned}
&\xi=\tfrac{1}{2}(E_{t+1}+E_{t-1}),\\
&\eta=4\xi+E_{t_0}-E_s,\\
&\xi=2\xi+E_s(E_{t_0}-E_s).
\end{aligned} \tag{11}$$

In order to obtain the first-order BRG result, we have to check the operator representation of S and S' in the basis of the new truncated lowest eigenstate $|t\pm1\rangle$, $|t_0\rangle$, and $|s\rangle$, whether they only differ from each other by a constant. The result shows that this is true only in an approximate meaning. For example, in case of $K=D$ the representation of $S^{z'}$ in the new basis is

$$S_2^{z'}=\begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{2/3} \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & \sqrt{2/3} & 0 & 0 \end{bmatrix}, \tag{12}$$

and the representation of $S_{L,2}^z$ in the new basis is

$$S_{L,2}^z=\begin{bmatrix} \lambda & 0 & 0 & 0 \\ 0 & \lambda_1 & 0 & \Omega \\ 0 & 0 & -\lambda & 0 \\ 0 & 0 & 0 & \lambda_2 \end{bmatrix},$$

where

$$\begin{aligned} \lambda&=\langle t+1\,|\,S_2^z\,|\,t+1\rangle\ , \\ \lambda_1&=\langle t_0\,|\,S_2^z\,|\,t_0\rangle\ , \\ \lambda_2&=\langle s\,|\,S_2^z\,|\,s\rangle\ , \\ \Omega&=\langle s\,|\,S_2^z\,|\,t_0\rangle\ . \end{aligned} \tag{13}$$

We get $\lambda_1=\lambda_2=0$, $\lambda=0.505\,502$, and $\Omega=0.715\,897$, which approximately correspond to $\frac{1}{2}$ and $\sqrt{2/3}=0.816\,496\,6$, respectively.

III. SPIN-$\frac{3}{2}$ CASE

We use the above even BRG approach to calculate the energy spectrum of the model (2) with spin-$\frac{1}{2}$ and spin-1 either in the anisotropic or the alternating case. We find that the energy-excitation behavior of the model in these two cases is different, which matches Haldane's conjecture; namely, in the spin-$\frac{1}{2}$ case there is no energy gap between the ground state and the first excitation state; however, in the spin-1 case a significant energy gap is observed (see Sec. IV). Now, can we say that our result supports Haldane's conjecture? The answer is not yet. We notice that in the spin-$\frac{1}{2}$ case the model has duality symmetry and it might suppress the energy gap. Therefore, it is better to check the nontrivial spin-$\frac{3}{2}$ case which has no duality symmetry by using the same approach if it behaves like the spin-$\frac{1}{2}$ case. However, the entire calculation is very lengthy. For lack of space we only give a brief summary here.

The forms of the two-site and four-site block Hamiltonians are the same as expressed in (5a) and (5b). Here we use the technique of solving an eigenproblem for a general 2×2 symmetric matrix. Suppose we have a matrix as

$$\begin{bmatrix} A & C \\ C & B \end{bmatrix}.$$

It is well known that its eigenvalues $x_\pm$ and the eigenstates are

$$\begin{aligned} x_\pm&=\tfrac{1}{2}\{A+B\pm[(A-B)^2+4C^2]^{1/2}\}\ , \\ &1/[C^2+(x-A)^2]^{1/2}\begin{bmatrix} C \\ x-A \end{bmatrix}. \end{aligned} \tag{14}$$

By using the above technique we can solve the eigenproblem exactly for the two-site block Hamiltonian in the $S=\frac{3}{2}$ case and get the following four states (one singlet and one triplet) with the lowest energies (for simplicity we omitted the prime for each renormalized coupling constant)

$$\begin{aligned} |t+1\rangle&=\sqrt{2}[\mu-K(\mu)^{1/2}]^{1/2}\begin{bmatrix} \sqrt{3}D(|\frac{3}{2},-\frac{1}{2}\rangle+|-\frac{1}{2},\frac{3}{2}\rangle) \\ \frac{1}{2}(K-\sqrt{\mu})\,|\frac{1}{2},\frac{1}{2}\rangle \end{bmatrix}, \quad E_{t+1}=-\tfrac{1}{4}K-\tfrac{1}{2}\sqrt{\mu}-h\ , \\ |t-1\rangle&=\sqrt{2}/[\mu-K(\mu)^{1/2}]^{1/2}\begin{bmatrix} \sqrt{3}D(|-\frac{3}{2},\frac{1}{2}\rangle+|\frac{1}{2},-\frac{3}{2}\rangle) \\ \frac{1}{2}(K-\sqrt{\mu})\,|-\frac{1}{2},-\frac{1}{2}\rangle \end{bmatrix}, \quad E_{t-1}=-\tfrac{1}{4}K-\tfrac{1}{2}\sqrt{\mu}+h\ , \\ |t_0\rangle&=1/[\nu-2(K+D)(\nu)^{1/2}]^{1/2}\begin{bmatrix} \frac{3}{2}D(|\frac{3}{2},-\frac{3}{2}\rangle+|-\frac{3}{2},\frac{3}{2}\rangle) \\ (K+D-\frac{1}{2}\sqrt{\nu})(|\frac{1}{2},-\frac{1}{2}\rangle+|-\frac{1}{2},\frac{1}{2}\rangle) \end{bmatrix}, \quad E_{t_0}=-\tfrac{5}{4}K+D-\tfrac{1}{2}\sqrt{\nu}\ , \\ |s\rangle&=1/[\lambda-2(K-D)(\lambda)^{1/2}]^{1/2}\begin{bmatrix} \frac{3}{2}D(|\frac{3}{2},-\frac{3}{2}\rangle-|-\frac{3}{2},\frac{3}{2}\rangle) \\ (K-D-\frac{1}{2}\sqrt{\lambda})(|\frac{1}{2},-\frac{1}{2}\rangle-|-\frac{1}{2},\frac{1}{2}\rangle) \end{bmatrix}, \quad E_s=-\tfrac{5}{4}K-D-\tfrac{1}{2}\sqrt{\lambda}\ , \end{aligned} \tag{15}$$

where

$$\begin{aligned} &\mu=K^2+24D^2,\quad \nu=4(K+D)^2+9D^2, \\ &\lambda=4(K-D)^2+9D^2\ . \end{aligned} \tag{16}$$

For the four-site block Hamiltonian we use the numerical method to obtain the energy spectrum and find that the lowest-energy levels are one singlet and one triplet too. Therefore, we truncate all the other energy levels

except for these two lowest-energy levels during the renormalization-group transformation.

The zero-order renormalization-group transformation is

$$\begin{aligned} E_{t+1} &= A - \tfrac{1}{4}K - \tfrac{1}{2}\sqrt{\mu} - h \ , \\ E_{t-1} &= A - \tfrac{1}{4}K - \tfrac{1}{2}\sqrt{\mu} + h \ , \\ E_{t_0} &= A - \tfrac{5}{4}K - \tfrac{1}{2}\sqrt{\nu} + D \ , \\ E_s &= A - \tfrac{5}{4}K - \tfrac{1}{2}\sqrt{\lambda} - D \ . \end{aligned} \tag{17}$$

For the first-order BRG calculation we have to find out the operator presentation of the two-site operator S^+, S^-, S^z and the four-site operator $S^{+\prime}, S^{-\prime}, S^z$ in the new basis of truncated eigenstates $|t\pm1\rangle$, $|t_0\rangle$, and $|s\rangle$, whether they are different from each other by only a constant. The result shows the positive answer. For example, for the operators $S^z_{1,4}$ and $S^{z\prime}_{1,2}$, we have the following representation:

$$S^z_{\substack{1,2\\1,4}} = \begin{pmatrix} \eta & 0 & 0 & 0 \\ 0 & -\eta & 0 & 0 \\ 0 & 0 & 0 & \pm\xi \\ 0 & 0 & \pm\xi & 0 \end{pmatrix} , \tag{18}$$

where $\eta'=0.5$, $\xi'=1.118\,034$ for the two-site operator $S^{z\prime}_{1,2}$; $\eta=0.525\,655$ and $\xi=1.017\,335$ for the four-site operator $S^z_{1,4}$. Therefore, they are almost proportional to each other. We choose the proportional coefficient between these two presentations as

$$\beta_{S^z} = (\eta+\xi)/(\eta'+\xi') \ , \tag{19}$$

where η' and ξ' are the values in (18) for the case of the two-site operator, and η, ξ are the values in (18) for the case of four-site operator. Once we know β, it is easy to obtain the first-order BRG result. For example, we can write the renormalized coupling constants as

$$K' = \beta^2_{S^z} K, \quad D' = \beta^2_{S^+} D \ . \tag{20}$$

Using the above result we have calculated the energy excitation of the anisotropic Heisenberg model in the spin-$\frac{3}{2}$ case, and we get a very similar picture if we compare it with the spin-$\frac{1}{2}$ case.

IV. RESULTS AND DISCUSSION

For the spin-1 chains, Fig. 3 shows the energy gap Δ between the ground-state and excitation spectrum of the spin-1 XXZ Heisenberg AFM, as a function of anisotropy parameter α. At $\alpha=1$, we obtain the ground-state energy $E_0/NJ=1.449\,742$ and the energy gap $\Delta=0.368\,166$, both of which are in good agreement with the Monte Carlo result of NB. We can also see that Fig. 3 agrees with Haldane's picture (see Fig. 1). The $\alpha<\alpha_1=0.4$ region presents the gapless (Kosterlitz-Thouless) phase, and a new phase appears for $\alpha_1<\alpha<\alpha_2=1.135\,31$, which encompasses the Hiesenberg point $\alpha=1$. This novel phase has a nondegenerate ground state and an energy gap to the excited-state continuum. $\alpha>\alpha_2$ presents a double ground-state region. It is interesting to point out that the transition point $\alpha_2=1.135\,31$ is very close to the finite-size scaling result of Botet and Jullien,[3] $\alpha_2=1.18$. One different feature of the energy spectrum shown in Fig. 3 which differs from Fig. 1 is that the locations of the first-excited energy level for the $\alpha>\alpha_2$ region are different from each other. According to our result, it has a shift compared with that shown in Fig. 1. In Fig. 3 for the $1<\alpha<\alpha_2$ region the upper curve indicates the degenerated second-excited energy level; however, the low curve presents the first-excited energy level. In the region for $\alpha>\alpha_2$ the upper curve indicates the degenerated first-excited energy level, and the ground state is double degenerated, as before mentioned. The situation can be seen from Fig. 4 when the anisotropy parameter α varies from an XY-like point to a strong Ising-like point, where the degeneracy of the lowest-energy levels, namely one singlet and one triplet, split accordingly. However, the major behavior of the energy spectrum remains just the same as in Fig. 1.

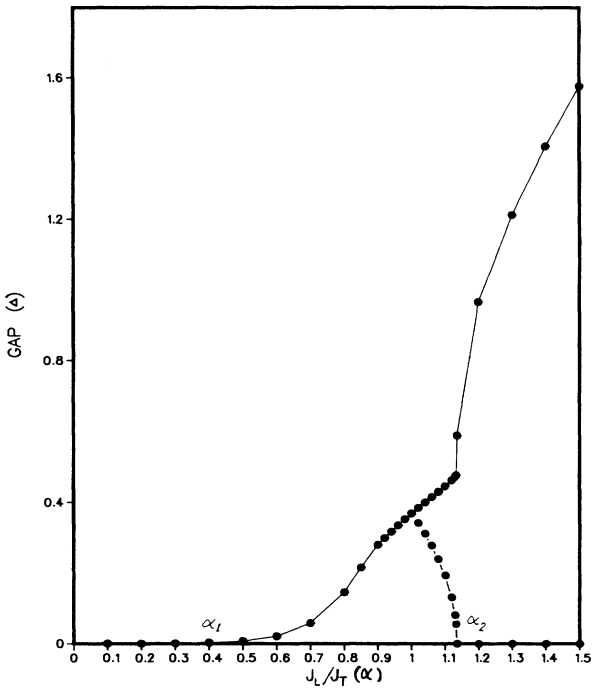

FIG. 3. Energy gap vs anisotropy α for the spin-1 Heisenberg AFM.

As for the alternating spin-1 Heisenberg chain, our result (see Fig. 5) also shows that there is a radical

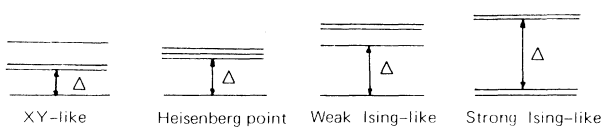

FIG. 4. Lowest-energy levels split when the anisotropy α changes (schematic).

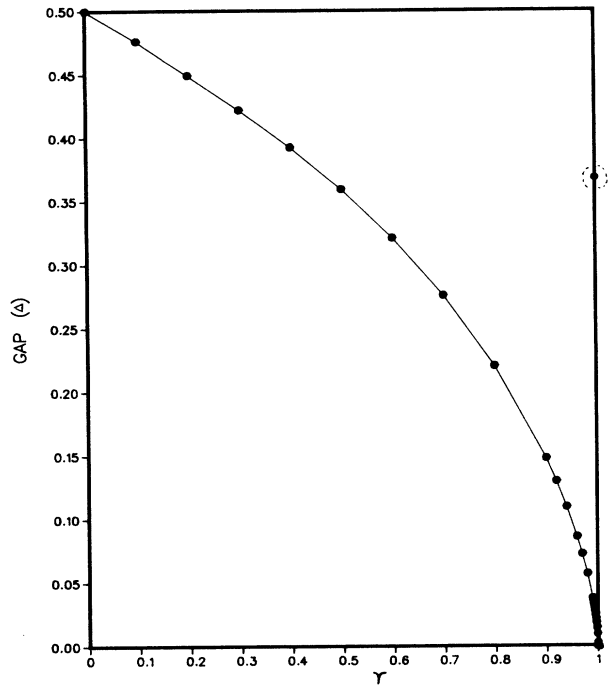

FIG. 5. Energy gap vs alternating parameter γ for the spin-1 Heisenberg AFM.

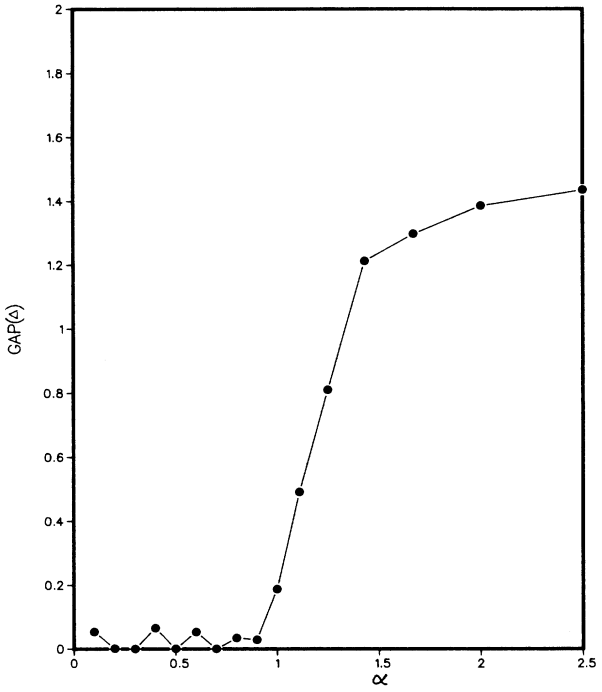

FIG. 6. Energy gap vs anisotropy α for the spin-$\frac{3}{2}$ Heisenberg AFM.

difference between the spin-$\frac{1}{2}$ and spin-1 chains. Instead of a smooth decrease of the energy gap when the alternating parameter γ goes to uniform point 1 in the spin-$\frac{1}{2}$ case, there is an abrupt jump of the finite energy gap, $\Delta=0.368\,166$, when γ changes from $\gamma=1-\epsilon$ to $\gamma=1$ for the spin-1 AFM chain. We also found that the width $\delta=(\gamma+\epsilon)-(\gamma-\epsilon)$ depends on the tolerance that we used to truncate the iteration sequence. This means a measurable energy gap will be observed if the chain shows slight nonuniformity. If this is true, there would be many applications of it. Hence, the other experimental or theoretical checking of this novel property is highly desirable; the study of using the quantum Monte Carlo method to verify this novel property is in progress.

Figure 6 shows the energy spectrum of the spin-$\frac{3}{2}$ anisotropic Heisenberg AFM, which indeed has the similar behavior as in the spin-$\frac{1}{2}$ case. When $\alpha<1$ there are some noises which are indeed caused by the method itself.

Finally, we would like to make a comment about our even-BRG method that has been shown to be able to give a fairly good description for the higher-spin spectrum of the Heisenberg AFM and gives Haldane's famous conjecture positive support. It is obvious that for the purpose of studying higher-spin problems the finite-size scaling method is a powerful and reliable method, but the RG method is also an important and efficient candidate. The reason is that the RG method extracts the physical information of the spin systems from both the energy levels and wave functions of the spin systems; however, the finite-size scaling method looks for the information only from the energy spectrum. Therefore if one can use the RG method more cleverly, one really can obtain more information with less effort.

As a matter of fact, the above method can be extended to treat a series of other spin models in the higher-spin case, such as the Lai-Suthland model, the integrable model,[16] and the pure biquadratic model, etc., which can be formulated in a unified form.[17] The possible novel phase-transition properties of these higher-spin systems are extremely interesting to us, and the relevant research is ongoing.

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[1]F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983).
[2]J. B. Parkinson and J. C. Bonner, Phys. Rev. B **32**, 4703 (1985).
[3]R. Botet and R. Jullien, Phys. Rev. B **27**, 613 (1983); M. Kolb, R. Botet, and R. Jullien, J. Phys. A **16**, L673 (1983); R. Botet, R. Jullien, and N. Kolb, Phys. Rev. B **28**, 3914 (1983).
[4]J. C. Bonner and G. Muller, Phys. Rev. B **29**, 5216 (1984).
[5]J. Sólyom and T. A. L. Ziman, Phys. Rev. B **30**, 3980 (1984).
[6]M. P. Nightingale and H. W. Blöte, Phys. Rev. B **33**, 659 (1986).
[7]U. Glaus and T. Schneider, Phys. Rev. B **30**, 215 (1984).
[8]J. Sólyom, Phys. Rev. B **32**, 7524 (1985).
[9]S. T. Chui and K. B. Ma, Phys. Rev. B **29**, 1287 (1984).
[10]J. N. Fields, Phys. Rev. B **19**, 2637 (1979).
[11]J. N. Fields, H. W. J. Blöte, and J. C. Bonner, J. Appl. Phys. **50**, 1807 (1979).
[12]H. W. J. Blöte, J. C. Bonner, and J. N. Fields, J. Magn. Magn. Mater. **15-18**, 405 (1980).
[13]J. C. Bonner, H. W. J. Blöte, H. Beck, and G. Muller, in *Physics in One Dimension,* Vol. 115 of *Lecture Notes in Physics,* edited by J. Bernasconi and T. Schneider (Springer-Verlag, Berlin, 1981).
[14]J. C. Bonner and H. W. J. Blöte, Phys. Rev. B **25**, 6959 (1982).
[15]J. C. Bonner (private communication).
[16]I. Affleck, Nucl. Phys. **B265**, 409 (1986).
[17]J. C. Bonner and J. P. Parkinson, Bull. Am. Phys. Soc. **32**, 390 (1987).