

# Highest weight state description of the isotropic spin-1 chain

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We introduce an overcomplete highest weight state basis as a calculational tool for the description of the isotropic spin-1 chain with bilinear exchange coupling  $J_1$  and biquadratic coupling  $J_2$ . The ground state can be expressed exactly at the three special points in the phase diagram where the Hamiltonian corresponds to a sum of nearest neighbor total spin projection operators ( $J_1=0 > J_2$ ,  $J_1=-J_2 < 0$ , and  $J_1=-J_2/3 > 0$ ). In particular, at the phase transition point  $J_1=-J_2 < 0$ , it is possible to exactly compute the ground states, excited states, expectation values, and correlation functions by using the new total spin basis.

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## I. INTRODUCTION

There has been a large interest in the isotropic one-dimensional spin-1 chain ever since Haldane's prediction<sup>1,2</sup> that the excitation spectrum in integer spin Heisenberg chains should show a gap in strong contrast to the model with half-integer spins. The general  $SU(2)$  invariant spin-1 chain model with nearest neighbor coupling is given by

$$H = \sum_{i=1}^N [J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} - J_2 (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2] \\ = J \sum_{i=1}^N [\cos \Theta \mathbf{S}_i \cdot \mathbf{S}_{i+1} - \sin \Theta (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2], \quad (1)$$

where  $\mathbf{S}_i$  are the spin-1 operators at site  $i$  in a one-dimensional periodic lattice with  $N$  sites. Exact analytical solutions at special points were obtained by Affleck, Kennedy, Lieb and Tasaki (AKLT),<sup>3,4</sup> Sutherland,<sup>5</sup> Klümper,<sup>6-8</sup> and Barber and Batchelor,<sup>9</sup> which supported Haldane's hypothesis and established an interesting phase diagram<sup>10,11</sup> as shown in Fig. 1. Experimental results on quasi-one-dimensional spin-1 compounds such as "NENP,"  $\text{CsNiCl}_3$ , or  $\text{AgVP}_2\text{S}_6$  also confirmed the gap and the existence of effective  $s=\frac{1}{2}$  spins near boundaries.<sup>12,13</sup> The spin-1 chain was also one of the driving forces in the development of the density matrix renormalization group algorithm, which in turn provided very accurate estimates of the excitation spectrum and the correlation lengths at the Heisenberg point.<sup>14,15</sup>

By changing the ratio of the Heisenberg coupling  $J_1$  and biquadratic exchange term  $J_2$ , the system can be tuned through at least three antiferromagnetic regions<sup>11</sup> and one ferromagnetic phase, as shown in Fig. 1. The three established antiferromagnetic regions are called Trimer, Haldane, and Dimer, of which the last two are gapped. Because in most substances the biquadratic exchange term is much smaller compared to the bilinear term, the experimental realization in regions with dominant biquadratic exchange term was not possible for a long time. First experimental success was achieved with  $\text{LiVGe}_2\text{O}_2$ , which appears to be well described by a large positive value of  $J_2$ .<sup>16</sup>

The similarity of the phase diagrams of the spin-1 chain compared to the spin- $\frac{1}{2}$  chain with next nearest neighbor cou-

pling is striking. The spin- $\frac{1}{2}$  model of a periodic chain with sites  $N$  is given by

$$H = \sum_{i=1}^N (J_1 \mathbf{s}_i \cdot \mathbf{s}_{i+1} + J_2 \mathbf{s}_i \cdot \mathbf{s}_{i+2}) \\ = J \sum_{i=1}^N (\cos \vartheta \mathbf{s}_i \cdot \mathbf{s}_{i+1} + \sin \vartheta \mathbf{s}_i \cdot \mathbf{s}_{i+2}), \quad (2)$$

where  $\mathbf{s}_i$  are the spin- $\frac{1}{2}$  operators at site  $i$ . The spin- $\frac{1}{2}$  chain also shows three antiferromagnetic regions, two of which are believed to be gapped, and one ferromagnetic phase as shown in Fig. 1. It is known that the AKLT point in the spin-1 chain is in the same phase as the Majumdar-Ghosh point<sup>17</sup> in the spin- $\frac{1}{2}$  chain, i.e., the two points  $B$  and  $b$  in Fig. 1 can be connected in a more general parameter space.<sup>18</sup> We also see that the two gapped phases in both the spin-1 and the spin- $\frac{1}{2}$  chain are separated by an integrable point with  $SU(2)_2$  symmetry (points  $G$  and  $g$ ). Moreover, in both cases,

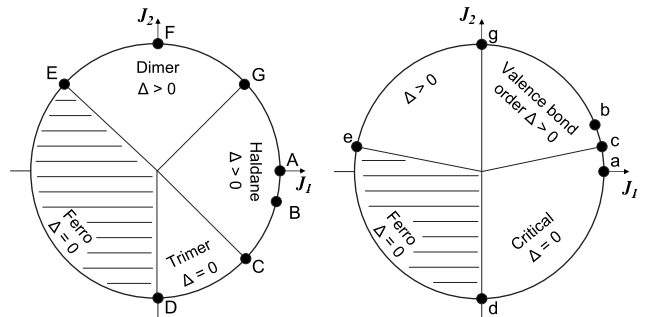


FIG. 1. (Left) Phase diagram of the spin-1 chain as function of  $\Theta$ :  $A(0)$ , pure Heisenberg chain;  $B(-\arctan 1/3)$ , AKLT point (Refs. 3 and 4);  $C(-\pi/4)$ , Sutherland model (Ref. 5);  $D(-\pi/2)$ , phase transition (Ref. 19);  $E(3\pi/4)$ , phase transition (Refs. 20–22);  $F(\pi/2)$ , exactly solvable (Refs. 6–8); and  $G(\pi/4)$ ,  $SU(2)_2$  integrable point (Refs. 23–25). (Right) Phase diagram of the spin- $\frac{1}{2}$  chain as function of  $\vartheta$ :  $a(0)$ , Heisenberg chain (Ref. 26);  $b(\arctan 1/2)$ , Majumdar-Ghosh point (Ref. 17);  $c(\sim 0.24)$ , critical point (Ref. 27);  $d(-\pi/2)$ , phase transition;  $g(\pi/2)$ , two independent chains,  $SU(2)_1 \times SU(2)_1$  integrable; and  $e(\pi - \arctan 1/4)$ , phase transition (Ref. 28). The gaps are generically denoted by  $\Delta$ . The points  $B$ ,  $D$ , and  $E$  are projection points treated in this paper.

the phase transition to the ferromagnetic behavior occurs at points where the Hamiltonian (1) can be written in terms of total spin projection operators of neighboring spins (points  $D$ ,  $d$ ,  $E$ , and  $e$ ). Therefore, the main difference between the two phase diagrams is that in the spin-1 chain the isotropic point  $A$  happens to be in a gapped phase, while the isotropic point  $a$  falls in a gapless phase in the spin- $\frac{1}{2}$  chain.

In this paper, we develop a highest weight state basis which can be used to calculate a number of exact properties, especially at the “projection points”  $B$ ,  $D$ , and  $E$ , where the Hamiltonian can be written as a sum over quintet, triplet, or singlet projection operators of two neighboring spins, respectively. In Sec. II, we introduce the general total spin basis, which is in spirit similar to the valence bond basis for spin- $\frac{1}{2}$  systems where the total spin of pairs of spins in the system is specified. In Sec. III, we demonstrate how to calculate the ferromagnetic excitations with total spin  $s=N-1$  in the new basis as a simple illustration. At the singlet projection point  $D$ , the ferromagnetic excitations become dispersionless and it is possible to construct excitations with spin  $s=N-2$  in agreement with earlier results<sup>19</sup> as shown in Sec. IV. In Sec. V, we consider the triplet projection point  $E$  at  $J_1=-J_2<0$  ( $\Theta=\frac{3\pi}{4}$ ) in a system with an even number of sites  $N$ . At this phase transition, the antiferromagnetic  $s=0$  and ferromagnetic  $s=N$  ground states are degenerate, but also ground states with any even total spin  $s$  exist, leading to a large degeneracy. We are able to calculate the correlation functions exactly, which remarkably do not decay along the chain, even for the antiferromagnetic ground state. Using the highest weight state basis, excited states can also be constructed exactly at this point. For completeness, we also show how to express the AKLT state at the quintet projection point  $B$  ( $\Theta=-\arctan 1/3$ ) in the new basis in Sec. VI. We conclude in Sec. VII. The appendixes explain how operators are applied and scalar products are computed in the highest weight state basis.

**II. TOTAL SPIN BASIS FOR SPIN-1 SYSTEMS**

In this section, a basis set of highest weight states with given total spin  $s$  is introduced. Similar to the valence bond basis for spin- $\frac{1}{2}$  systems, it is possible to specify pairs of spins (so-called valence bonds) which have definite total spin. In spin-1 systems, pairs of spins can now be quintets ( $s=2$ ), triplets ( $s=1$ ), or singlets ( $s=0$ ). The most important difference to an ordinary  $S^z$  basis is that in this construction, “bonds” are specified instead of local quantum numbers.

We use a notation similar to the conventional one for the spin- $\frac{1}{2}$  chain by Majumdar and Ghosh<sup>17</sup>  $\{|i_1, i_2\rangle_{m=0} \equiv |s=0, m=0\rangle$ ,  $[i_1, i_2]_m \equiv |s=1, m\rangle$ , and  $(i_1, i_2)_m \equiv |s=2, m\rangle$ , where  $s$  is the total spin of the pair of spins at sites  $i_1$  and  $i_2$ , and  $m$  is the  $S^z$  eigenvalue. An important simplification for  $SU(2)$  invariant systems is that only highest weight states (hws) with  $m=s$  have to be considered as representatives of degenerate multiplets, since it is possible to construct an entire degenerate multiplet by applying the total spin lowering operator  $S^- = \sum_i S_i^-$ , which commutes with  $H$ .

Accordingly, it is useful to define bonds as pairs of two spins, which are in a highest weight state of total spin 2, 1, or 0,

$$(i_1, i_2)_2 = |++\rangle,$$

$$[i_1, i_2]_1 = (|+0\rangle - |0+\rangle)/\sqrt{2},$$

$$\{i_1, i_2\}_0 = (|+-\rangle + |-+\rangle - |00\rangle)/\sqrt{3}. \tag{3}$$

Singlet and quintet bonds have even parity under exchange of indices, while the triplet bonds are odd. Using this notation, it is now possible to construct a highest weight state of the total system by specifying all bonds as follows:

$$|\psi_s(i_1, \dots, i_N)\rangle = \overbrace{(i_1, i_2)_2 \dots (i_{2Q-1}, i_{2Q})_2}^Q \overbrace{[i_{2Q+1}, i_{2Q+2}]_1}^T \overbrace{\{i_{2Q+3}, i_{2Q+4}\}_0 \dots \{i_{N-1}, i_N\}_0}^S, \tag{4}$$

assuming an even number of lattice sites  $N$ . The number of quintet, triplet, and singlet bonds,  $Q$ ,  $T$ , and  $S$ , defines the total spin  $s=2Q+T$ . The wave function is a function of the pairwise different ordered indices  $i_1, i_2, \dots, i_N$ , which are used to specify the bonds. The order of the quintet indices does not matter since all spins in quintet bonds are in the state  $|+\rangle$ , so Eq. (4) can be simplified by only specifying which spins belong to the quintets  $(i_1, \dots, i_{2Q})_{2Q}$ . Also, the order within each singlet and triplet bracket is irrelevant up to a possible minus sign. To simplify the calculations, it is sometimes useful to specify the bonds graphically as follows:

$$\{i_1, i_2\}_0 = \text{---} \overset{\frown}{\text{---}} \text{---} \quad [i_1, i_2]_1 = \text{---} \overline{\text{---}} \text{---} \quad (i_1, i_2)_2 = \bullet \bullet, \tag{5}$$

$i_1 \quad i_2 \qquad i_1 \quad i_2 \qquad i_1 \quad i_2$

where no bond connections are assigned to quintets.

Clearly, states of the form Eq. (4) are indeed highest weight states of the entire system, since

$$S_{\text{tot}}^z |\psi_s\rangle = m |\psi_s\rangle,$$

$$S_{\text{tot}}^2 |\psi_s\rangle = s(s+1) |\psi_s\rangle, \tag{6}$$

where  $s=m=2Q+T$ . Here, the first line is obvious from Eq. (3), and the second line follows since the total spin  $s$  has to be at least  $m$ , but can be at most the sum of the individual bond spins  $s=2Q+T$ .

States of the form Eq. (4) can now be used as basis states in order to express any hws of the system. For this purpose, it is sufficient to only consider basis states with no triplets  $T=0$  (for  $s=2Q$  even) or one triplet pair  $T=1$  (for  $s=2Q+1$  odd), since states with  $T>1$  can be expressed by the following linear combination:

$$\begin{aligned}
 [1,2]_1[3,4]_1 &\propto (2,3)_2\{1,4\}_0 + (1,4)_2\{2,3\}_0 - (1,3)_2\{2,4\}_0 \\
 &\quad - (2,4)_2\{1,3\}_0 \\
 \square\square &\propto \text{---} + \text{---} - \text{---} - \text{---} \dots
 \end{aligned} \tag{7}$$

In the hws basis defined in this way, it is possible to determine the action of any  $SU(2)$  invariant operator involving two spins, i.e., linear combinations of  $\mathbf{S}_i \cdot \mathbf{S}_{i+1}$  and  $(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2$ . For example, for states with two singlet bonds, we find the following relations:

$$\mathbf{S}_i \cdot \mathbf{S}_{i+1} \{j, i\}_0 \{i+1, k\}_0 = \{j, i+1\}_0 \{i, k\}_0 - \{j, k\}_0 \{i, i+1\}_0,$$

$$(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \{j, i\}_0 \{i+1, k\}_0 = \{j, i\}_0 \{i+1, k\}_0 + \{j, k\}_0 \{i, i+1\}_0, \tag{8}$$

or, equivalently,

$$\begin{aligned}
 \mathbf{S}_i \cdot \mathbf{S}_{i+1} \begin{array}{c} \text{---} \\ j \quad i \quad i+1 \quad k \end{array} &= \begin{array}{c} \text{---} \\ j \quad i \quad i+1 \quad k \end{array} - \begin{array}{c} \text{---} \\ j \quad i \quad i+1 \quad k \end{array} \\
 (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \begin{array}{c} \text{---} \\ j \quad i \quad i+1 \quad k \end{array} &= \begin{array}{c} \text{---} \\ j \quad i \quad i+1 \quad k \end{array} + \begin{array}{c} \text{---} \\ j \quad i \quad i+1 \quad k \end{array}
 \end{aligned} \tag{9}$$

Since the terms in the Hamiltonian (1) operate only on two spins at a time, it is always sufficient to consider clusters of two bonds irrespective of the length of the chain. A complete list how  $\mathbf{S}_i \cdot \mathbf{S}_{i+1}$  and  $(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2$  operate on the states can be found in Appendix A.

From those relations (A) it is clear that the representation of linear combinations in the hws basis in Eq. (4) is closed under the operation of any local  $SU(2)$  operator, including permutations. Therefore, starting with any hws, all other states in the corresponding sector of the Hilbert space can be represented as a linear combination in the hws basis (4). However, the linear combinations are not necessarily unique since the hws basis is overcomplete and not orthogonal. In particular, for the  $s=0$  sector, the hws basis is linearly independent up to  $N=6$  spin, while for  $N=8$ , the basis becomes overcomplete. This means that no relation between singlet states with three singlet bonds exists, while there are 14 (relatively complicated) relations involving four singlet bonds, which will not be discussed here. In general, there are  $N!/[2^{(N-s)/2}(\frac{N-s}{2})!s!]$  basis states of the form Eq. (4) for a given even spin  $s=2Q$ . For comparison, if only the quantum number in the  $z$  direction  $S^z=0$  in the ordinary  $S^z$  basis is specified, the number of basis states is given by  $1 + \sum_{N_+=1}^{N/2} \frac{N!}{(N-2N_+)!N_+!N_+!}$ , which is a larger basis than the  $s=0$  hws basis up to  $N=18$ . The situation for  $N=4$  spins is discussed in detail in Appendix B as an example.

It is also possible to determine scalar products in the hws basis using a straightforward algorithm as presented in Appendix C. In particular, the scalar product between two total spin  $s=0$  states can be obtained by the minimum number  $\gamma$  of index exchanges  $V_{i_k, i_l}$  needed to transform the indices  $i_1, \dots, i_N$  into an equivalent bond configuration corresponding to indices  $i'_1, \dots, i'_N$ ,

$$\begin{aligned}
 \langle \psi_{s=0}(i_1, \dots, i_N) | \psi_{s=0}(i'_1, \dots, i'_N) \rangle \\
 = \langle \psi_{s=0}(i_1, \dots, i_N) | \overbrace{V \dots V}^{\gamma} | \psi_{s=0}(i_1, \dots, i_N) \rangle = \frac{1}{3^\gamma}.
 \end{aligned} \tag{10}$$

Interestingly, this means that any basis state in the  $s=0$  sector is never orthogonal to any other  $s=0$  basis state.

### III. FERROMAGNETIC EXCITATIONS

In order to demonstrate how to apply the new basis, we consider as an example excitations on the ferromagnetic state  $|F\rangle = (1, 2, \dots, N)_N$ , which is always an eigenstate with energy  $E_0 = N(J_1 - J_2) = JN(\cos \Theta - \sin \Theta)$ . In order to construct a spin-wave excitation  $|k\rangle$  with total spin  $s=N-1$ , we can write

$$|k\rangle = \sum_{i_1 \neq i_2} e^{tki_1} [i_1, i_2]_1 (i_3, \dots, i_N)_{N-1}. \tag{11}$$

Here, we require  $k \neq 0$  since the  $k=0$  ‘‘excitation’’ of the ordinary spin-wave construction actually corresponds to an  $s=N$  multiplet state. We will now show explicitly that the state in Eq. (11) is an eigenstate of the Hamiltonian (1) for any  $J_1$  and  $J_2$ . In order to apply the operators  $\mathbf{S}_i \cdot \mathbf{S}_{i+1}$  and  $(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2$ , we write states involving triplet bonds with the sites  $i$  or  $i+1$  separately,

$$\begin{aligned}
 |k\rangle &= e^{tki} [i, i+1]_1 (\dots)_{N-1} + e^{tk(i+1)} [i+1, i]_1 (\dots)_{N-1} \\
 &+ \sum_{i_3 \neq i+1} e^{tki} [i, i_3]_1 (\dots, i+1, \dots)_{N-1} \\
 &+ \sum_{i_3 \neq i} e^{tk(i+1)} [i+1, i_3]_1 (\dots, i, \dots)_{N-1} \\
 &+ \sum_{i_3 \neq i+1} e^{tki_3} [i_3, i]_1 (\dots, i+1, \dots)_{N-1} \\
 &+ \sum_{i_3 \neq i} e^{tki_3} [i_3, i+1]_1 (\dots, i, \dots)_{N-1} \\
 &+ \sum_{i_4, i_3 \neq i, i+1} e^{tki_3} [i_3, i_4]_1 (\dots, i, i+1, \dots)_{N-1}.
 \end{aligned} \tag{12}$$

Now we use the relation from Appendix A

$$\mathbf{S}_i \cdot \mathbf{S}_{i+1} (j, i)_2 [i+1, k]_1 = (j, i+1)_2 [i, k]_1,$$

$$(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 (j, i)_2 [i+1, k]_1 = (j, i)_2 [i+1, k]_1. \tag{13}$$

By summing over all  $i$ , we obtain

$$\sum_{i=1}^N \mathbf{S}_i \cdot \mathbf{S}_{i+1} |k\rangle = N|k\rangle + 2[\cos(k) - 1]|k\rangle,$$

$$\sum_{i=1}^N (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 |k\rangle = N|k\rangle. \tag{14}$$

This means that for a general Hamiltonian (1),

$$H|F\rangle = E_0|F\rangle, \quad H|k\rangle = E_0|k\rangle + 2J_1[\cos(k) - 1]|k\rangle, \tag{15}$$

which is the well-known ferromagnetic dispersion.

#### IV. MODEL AT $J_1=0 > J_2$ ( $\Theta=-\frac{\pi}{2}$ )

One immediate consequence of the dispersion relation (15) is that the excitations become dispersionless at the phase transition point  $D$  for  $J_1=0$ ,

$$H = -J_2 \sum_{i=1}^N (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2, \quad (16)$$

where we assume  $J_2 < 0$ . At this point, it is also possible to express the Hamiltonian in terms of a total spin  $s=0$  projection operator of two neighboring spins  $P_0(\mathbf{S}_i, \mathbf{S}_{i+1}) = -\frac{1}{3} + \frac{1}{3}(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2$ ,

$$H = E_0 - 3J_2 \sum_{i=1}^N P_0(\mathbf{S}_i, \mathbf{S}_{i+1}), \quad (17)$$

where  $E_0 = -NJ_2$ . For this model, we are able to compare with known results,<sup>19</sup> which serves as an illustration of how to use the hws basis. We know from Eq. (13) that *any* state with total spin  $s=N-1$  is an eigenstate and degenerate with the ground state. Excitations of the form  $|k\rangle = \sum_{i_1} \exp(ik i_1) \times \{i_1, i_1+1\}_0(i_3, i_4, \dots, i_N)_{N-2}$ , with total spin  $s=N-2$ , also become eigenstates at this point. This can be shown again by decomposing  $|k\rangle$  in the following form:

$$\begin{aligned} |k\rangle &= \sum_{i_1=1}^N e^{ik i_1} \{i_1, i_1+1\}_0(\dots, \dots, \dots)_{N-2} \\ &= e^{ik i_1} \{i_1, i_1+1\}_0(\dots, \dots, \dots)_{N-2} \\ &\quad + e^{ik(i-1)} \{i-1, i\}_0(\dots, \dots, \dots)_{N-2} \\ &\quad + e^{ik(i+1)} \{i+1, i+2\}_0(\dots, \dots, \dots)_{N-2} \\ &\quad + \sum_{i_3 \neq i-1, i, i+1} e^{ik i_3} \{i_3, i_3+1\}_0(\dots, i, i+1, \dots)_{N-2}. \end{aligned} \quad (18)$$

Using Eq. (A2) from Appendix A, we find

$$\begin{aligned} (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 |k\rangle &= 3e^{ik i_1} \{i_1, i_1+1\}_0(\dots, \dots, \dots)_{N-2} \\ &\quad + (e^{ik} + e^{-ik}) e^{ik i_1} \{i_1, i_1+1\}_0(\dots, \dots, \dots)_{N-2} + |k\rangle. \end{aligned} \quad (19)$$

Finally, we sum over all  $i$ , and obtain the dispersion relation  $E_2(k) = -J_2[3 + 2 \cos(k)] + E_0$ , which is gapped in agreement with earlier results from Ref. 19.

#### V. MODEL AT $J_1=-J_2 < 0$ ( $\Theta=\frac{3\pi}{4}$ )

We now turn to the other ferro-antiferromagnetic phase transition point  $E$  at  $J_1=-J_2 < 0$ , which has been studied in different contexts.<sup>5,11,20-22</sup> Using the basis of hws in Eq. (4), we are now not only able to describe all degenerate ferro- and antiferromagnetic ground states explicitly, but also calculate correlation functions and excited states exactly at that point. The model is given by the Hamiltonian

$$H = J_1 \sum_{i=1}^N [\mathbf{S}_i \cdot \mathbf{S}_{i+1} + (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2] \quad (20)$$

for a periodic chain with even number of sites  $N$ . It is possible to express the Hamiltonian (20) in terms of triplet projection operator of two neighboring spins  $P_1(\mathbf{S}_i, \mathbf{S}_{i+1}) = 1 - \frac{1}{2}(\mathbf{S}_i \cdot \mathbf{S}_{i+1}) - \frac{1}{2}(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2$ ,

$$H = E_0 - 2J_1 \sum_{i=1}^N P_1(\mathbf{S}_i, \mathbf{S}_{i+1}), \quad (21)$$

where  $E_0 = 2NJ_1$ . Since the operator  $P_1$  can only have positive eigenvalues and  $J_1 < 0$ , the system has so-called optimum ground states,<sup>29</sup> which must be in a configuration where no two neighboring spins are in a triplet configuration, so that  $P_1|0\rangle = 0$  for all nearest neighbors.

Another useful representation can be obtained by using the operator  $V_{i,i+1}$ , which exchanges the quantum numbers of two neighboring sites. Since both singlets and quintets are even under exchange, we have  $P_1(\mathbf{S}_i, \mathbf{S}_{i+1}) = (1 - V_{i,i+1})/2$  and, therefore, the Hamiltonian becomes

$$H = J_1 N + J_1 \sum_{i=1}^N V_{i,i+1}, \quad (22)$$

which is, in fact,  $SU(3)$  invariant.<sup>5,11</sup> Hence, ground states of the Hamiltonian (22) can be constructed by requiring  $V_{i,i+1}|0\rangle = |0\rangle$  for all  $i$ , i.e., the ground states are invariant under the application of all permutation operators  $V_{i,i+1}$ .<sup>11,21</sup> In order to construct such a ground state, we use the hws notation (4) to describe the antiferromagnetic and ferromagnetic ground states as follows:

$$\begin{aligned} |F\rangle &= (1, 2, \dots, N-1, N)_N, \\ |AF\rangle &\propto \sum_P \{i_1, i_2\}_0 \{i_3, i_4\}_0 \{i_5, i_6\}_0 \dots, \end{aligned} \quad (23)$$

where  $\sum_P$  is the sum over all possible permutations of  $i_1, \dots, i_N$ . It is clear that the states defined in this way are eigenstates of all permutations  $V_{i,i+1}$  and, therefore, immediately ground states of the Hamiltonian (20) with definite total spin  $s=N$  and  $s=0$ , respectively. Therefore, the energies of the ferro- and antiferromagnetic states cross at the phase transition point as expected, but, in addition, we find that it is possible to construct a ground state for each sector with an even spin  $s$  by simply combining permutations of quintet and singlet bonds

$$|0\rangle_s \propto \sum_P (i_1, i_2, \dots, i_{s-1}, i_s)_s \{i_{s+1}, i_{s+2}\}_0 \dots \{i_{N-1}, i_N\}_0, \quad (24)$$

which is in accordance with  $SU(3)$  invariance.<sup>11</sup> There are no other ground states.

It is interesting to note that in the spin- $\frac{1}{2}$  chain at the phase transition point  $e$  in Fig. 1, the ground state can also be written as a permutation over all possible valence bonds.<sup>28</sup>

For each ground state, all pairs of spins are equally entangled with each other. Consequentially, also the correlation

function is the same between any two spins in the chain, *independent of distance*,

$${}_s\langle 0 | \mathbf{S}_i \cdot \mathbf{S}_j | 0 \rangle_s = \frac{s(s+1) - 2N}{N(N-1)}, \quad (25)$$

which follows from expanding  $\langle \mathbf{S}_{\text{tot}}^2 \rangle = \langle \sum_{i \neq j} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_i \mathbf{S}_i^2 \rangle$  and can also be verified by direct calculation with the help of the scalar product in Appendix C. The correlation function varies from  $\langle AF | \mathbf{S}_i \cdot \mathbf{S}_j | AF \rangle = -\frac{2}{N-1}$  up to  $\langle F | \mathbf{S}_i \cdot \mathbf{S}_j | F \rangle = 1$ . Higher order correlation functions can then also be determined iteratively by the use of  $P_1(\mathbf{S}_i, \mathbf{S}_j) | 0 \rangle_s = [1 - \mathbf{S}_i \cdot \mathbf{S}_j / 2 - (\mathbf{S}_i \cdot \mathbf{S}_j)^2 / 2] | 0 \rangle_s = 0$  for any pair of spins, so that, e.g.,  $\langle (\mathbf{S}_i \cdot \mathbf{S}_j)^2 \rangle = 2 - \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ .

A magnon excitation can now be constructed in a similar spirit as in Eq. (11) on any of the ground states. For example, a spin-1 excitation on the antiferromagnetic state is given by

$$|k\rangle_{AF} = \sum_{i_1 \neq i_2} e^{ik i_1} [i_1, i_2]_1 \sum_{P'} \{i_3, i_4\}_0 \dots, \quad (26)$$

with  $k \neq 0$ . In order to show that this state is an eigenstate of the Hamiltonian (22), a decomposition as in Eq. (12) can be used. Applying  $V_{i, i+1}$  and then summing again over all  $i$ , we obtain

$$H|k\rangle_s = E_1(k)|k\rangle_s, \quad E_1(k) = 2J_1[\cos(k) - 1] + E_0, \quad (27)$$

where  $|k\rangle_s$  is now the corresponding excitation on the ground state  $|0\rangle_s$  with any even spin  $s$  in Eq. (24).

Interestingly, the permutational ground states in Eq. (24) are, in fact, independent of the individual coupling strengths along the chain and are even ground states of higher dimensional models as long as  $J_1 = -J_2$  for all couplings. However, the excited states in Eq. (26) require translational invariance.

## VI. MODEL AT $J_1 = -J_2/3 > 0$ ( $\Theta = -\arctan \frac{1}{3}$ )

Finally, we consider the famous AKLT model<sup>3,4</sup> at point  $B$  in the phase diagram,

$$H = J_1 \sum_{i=1}^N \left( \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{3} (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \right) = E_0 + 2J_1 \sum_{i=1}^N P_2(\mathbf{S}_i, \mathbf{S}_{i+1}), \quad (28)$$

where  $J_1 > 0$ ,  $E_0 = -\frac{2}{3}NJ_1$ , and  $P_2(\mathbf{S}_i, \mathbf{S}_{i+1}) = \frac{1}{3} + \frac{1}{2}(\mathbf{S}_i \cdot \mathbf{S}_{i+1}) + \frac{1}{6}(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2$  is the projection operator onto the quintet state of two neighboring spins. It is of course well known how to express the ground state  $|0\rangle$  at this point,<sup>3,4</sup> but it is instructive to gain an alternative description in terms of the hws basis.

Analogously to the other projection points, the Hamiltonian (28) has an optimum ground state  $|0\rangle$ , which must obey  $P_2(\mathbf{S}_i, \mathbf{S}_{i+1})|0\rangle = 0$  for all adjacent spins. Using the relations in Appendix A, we know

$$\begin{aligned} P_2(\mathbf{S}_i, \mathbf{S}_{i+1}) \{i, i+1\}_0 &= 0, \\ P_2(\mathbf{S}_i, \mathbf{S}_{i+1}) (\{j, i\}_0 \{i+1, k\}_0 - \{j, i+1\}_0 \{i, k\}_0) &= 0, \\ \text{i.e. :} \\ P_2(\mathbf{S}_i, \mathbf{S}_{i+1}) (\text{---} \text{---} \text{---} - \text{---} \text{---} \text{---}) &= 0. \end{aligned} \quad (29)$$

Accordingly, we can construct the ground state by ensuring that for neighboring spins which are not coupled by a singlet bond, the corresponding crossed state is subtracted. The following state is therefore a ground state:

$$|0\rangle \propto \sum_P (-1)^{\text{No. of crossings}(P)} \{1, 2\}_0 \{3, 4\}_0 \dots \{N-1, N\}_0, \quad (30)$$

where the number of crossings is defined as the crossing of singlet bonds in the graphical representation in Eq. (5). For example, in the  $N=4$  chain, the ground state is given by

$$\begin{aligned} |0\rangle &\propto (\{1, 2\}_0 \{3, 4\}_0 + \{1, 4\}_0 \{2, 3\}_0 - \{2, 4\}_0 \{1, 3\}_0) \\ &\propto \text{---} \text{---} \text{---} + \text{---} \text{---} \text{---} - \text{---} \text{---} \text{---}. \end{aligned}$$

For a finite chain with open boundary conditions, the Hamiltonian (28) has four degenerate ground states, one singlet, and one triplet. The singlet is given by Eq. (30) with  $s=0$ . By using the relation from Appendix A, we find for triplet states

$$P_2(\mathbf{S}_i, \mathbf{S}_{i+1}) [i, i+1]_1 = 0$$

$$P_2(\mathbf{S}_i, \mathbf{S}_{i+1}) ([j, i]_1 \{i+1, k\}_0 - [j, i+1]_1 \{i, k\}_0) = 0$$

$$\text{i.e. : } P_2(\mathbf{S}_i, \mathbf{S}_{i+1}) (\text{---} \text{---} \text{---} - \text{---} \text{---} \text{---}) = 0.$$

(31)

Hence, the triplet ground state is analogously given by

$$|0\rangle = \sum_{P'} (-1)^{\text{No. of crossings}(P')} [1, 2]_1 \{3, 4\}_0 \dots \{N-1, N\}_0, \quad (32)$$

where the permutations  $P'$  are restricted so that the indices in the triplet bond always remain in ascending order. This ground state is a triplet of total spin  $s=1$ , in accordance with previous results.<sup>3,4</sup>

## VII. CONCLUSIONS

We have introduced a highest weight state basis as a total spin representation for the Hilbert space of spin-1 systems. In this basis, it is possible to compute scalar products and the action of  $SU(2)$  invariant operators for analytical and numerical calculations. However, the new basis states are not orthogonal and overcomplete.

In the ferromagnetic phase and at the phase transition point  $D$  ( $\Theta = -\pi/2$ ), it is possible to construct spin-wave excitations explicitly in the new basis. Also, the AKLT ground states at point  $B$  ( $\tan \Theta = -1/3$ ) can be explicitly expressed using the highest weight states.

At the phase transition point  $E$  ( $\Theta = 3\pi/4$ ), we find all degenerate ground states which are multiplets of even total spin  $s=0, 2, \dots, N$ . Using the hws basis, it is now possible to express all ground states exactly as permutations over hws bonds. The spin correlation functions  $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$  have been determined, which remarkably do not decay along the chain even for the antiferromagnetic state. The hws basis also allows the explicit construction of excited states with odd spin

and the corresponding dispersion relation, which is gapless. There is some hope that these results at point  $E$  can be used in future works as an ansatz for wave functions in the anti-ferromagnetic region in order to investigate the phase between points  $E$  and  $F$ , which is still not fully understood.<sup>20-22</sup>

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### APPENDIX A: ACTION OF $SU(2)$ INVARIANT OPERATORS

The action of  $h_{i,i+1} = \mathbf{S}_i \cdot \mathbf{S}_{i+1}$  on bonds where both indices are in the same singlet, triplet, or quintet coupling is immediately given by the respective eigenvalues

$$\begin{aligned} h_{i,i+1}\{|i, i+1\rangle_0\} &= -2\{|i, i+1\rangle_0\}, \\ h_{i,i+1}\{|i, i+1\rangle_1\} &= -\{|i, i+1\rangle_1\}, \\ h_{i,i+1}\{|i, i+1\rangle_2\} &= \{|i, i+1\rangle_2\}. \end{aligned} \quad (\text{A1})$$

Using the definition in Eq. (3), it is straightforward to determine the action of  $h_{i,i+1} = \mathbf{S}_i \cdot \mathbf{S}_{i+1}$  on all possible hws states as follows:

$$\begin{aligned} h_{i,i+1}\{|j, i\rangle_0\{|i+1, k\rangle_0\} &= \{|j, i+1\rangle_0\{|i, k\rangle_0\} - \{|j, k\rangle_0\{|i, i+1\rangle_0\}, \\ h_{i,i+1}\{|j, i\rangle_1\{|i+1, k\rangle_0\} &= \{|j, i+1\rangle_1\{|i, k\rangle_0\} - \{|j, k\rangle_1\{|i, i+1\rangle_0\}, \\ h_{i,i+1}\{|j, i\rangle_2\{|i+1, k\rangle_0\} &= \{|j, i+1\rangle_2\{|i, k\rangle_0\} - \{|j, k\rangle_2\{|i, i+1\rangle_0\}, \\ h_{i,i+1}\{|j, i\rangle_2\{|i+1, k\rangle_1\} &= \{|j, i+1\rangle_2\{|i, k\rangle_1\}. \end{aligned} \quad (\text{A2})$$

The application of  $h_{i,i+1}^2 = (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2$  is then given by applying  $\mathbf{S}_i \cdot \mathbf{S}_{i+1}$  twice

$$\begin{aligned} h_{i,i+1}^2\{|j, i\rangle_0\{|i+1, k\rangle_0\} &= \{|j, i\rangle_0\{|i+1, k\rangle_0\} + \{|j, k\rangle_0\{|i, i+1\rangle_0\}, \\ h_{i,i+1}^2\{|j, i\rangle_1\{|i+1, k\rangle_0\} &= \{|j, i\rangle_1\{|i+1, k\rangle_0\} + \{|j, k\rangle_1\{|i, i+1\rangle_0\}, \\ h_{i,i+1}^2\{|j, i\rangle_2\{|i+1, k\rangle_0\} &= \{|j, i\rangle_2\{|i+1, k\rangle_0\} + \{|j, k\rangle_2\{|i, i+1\rangle_0\}, \\ h_{i,i+1}^2\{|j, i\rangle_2\{|i+1, k\rangle_1\} &= \{|j, i\rangle_2\{|i+1, k\rangle_1\}. \end{aligned} \quad (\text{A3})$$

In this way, the action of any  $SU(2)$  invariant operator involving two spins can be calculated as a linear combination of  $\mathbf{S}_i \cdot \mathbf{S}_{i+1}$  and  $(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2$  using the above relations.

### APPENDIX B: HIGHEST WEIGHT STATES BASIS FOR $N=4$ SPINS

We consider a spin-1 system consisting of four sites and find all hws states of the form Eq. (4), using at most one triplet bond. In the spin  $s=0$  sector, we find

$$\{|1, 2\rangle_0\{|3, 4\rangle_0\}, \{|1, 3\rangle_0\{|2, 4\rangle_0\}, \{|1, 4\rangle_0\{|2, 3\rangle_0\}; \quad (\text{B1})$$

in the spin  $s=1$  sector, we find

$$\begin{aligned} \{|1, 2\rangle_1\{|3, 4\rangle_0\}, \{|1, 3\rangle_1\{|2, 4\rangle_0\}, \{|1, 4\rangle_1\{|2, 3\rangle_0\}, \\ \{|3, 4\rangle_1\{|1, 2\rangle_0\}, \{|2, 4\rangle_1\{|1, 3\rangle_0\}, \{|2, 3\rangle_1\{|1, 4\rangle_0\}; \end{aligned} \quad (\text{B2})$$

in the spin  $s=2$  sector, we find

$$\begin{aligned} \{|1, 2\rangle_2\{|3, 4\rangle_0\}, \{|1, 3\rangle_2\{|2, 4\rangle_0\}, \{|1, 4\rangle_2\{|2, 3\rangle_0\}, \\ \{|3, 4\rangle_2\{|1, 2\rangle_0\}, \{|2, 4\rangle_2\{|1, 3\rangle_0\}, \{|2, 3\rangle_2\{|1, 4\rangle_0\}; \end{aligned} \quad (\text{B3})$$

in the spin  $s=3$  sector, we find

$$\begin{aligned} \{|1, 2\rangle_3\{|3, 4\rangle_1\}, \{|1, 3\rangle_3\{|2, 4\rangle_1\}, \{|1, 4\rangle_3\{|2, 3\rangle_1\}, \\ \{|3, 4\rangle_3\{|1, 2\rangle_1\}, \{|2, 4\rangle_3\{|1, 3\rangle_1\}, \{|2, 3\rangle_3\{|1, 4\rangle_1\}; \end{aligned} \quad (\text{B4})$$

and the ferromagnetic state is

$$\{|1, 2, 3, 4\rangle_4\}. \quad (\text{B5})$$

Using the addition rules for angular momenta  $\mathbf{1} \otimes \mathbf{1} \otimes \mathbf{1} \otimes \mathbf{1} = 3 \cdot \mathbf{0} \oplus 6 \cdot \mathbf{1} \oplus 6 \cdot \mathbf{2} \oplus 3 \cdot \mathbf{3} \oplus 1 \cdot \mathbf{4}$ , we see that the states of spin  $s=0$ ,  $s=1$ ,  $s=2$ , and  $s=4$  are linearly independent, as can also be checked directly using Eq. (3). For the  $s=3$  sector, we obtain the following linear relations:

$$\begin{aligned} \begin{array}{c} \boxed{\bullet} \\ \bullet \end{array} \bullet &= \bullet \begin{array}{c} \boxed{\bullet} \\ \bullet \end{array} \bullet + \begin{array}{c} \boxed{\bullet} \\ \bullet \end{array} \bullet \bullet, \\ \bullet \begin{array}{c} \boxed{\bullet} \\ \bullet \end{array} &= \bullet \begin{array}{c} \boxed{\bullet} \\ \bullet \end{array} \bullet + \bullet \bullet \begin{array}{c} \boxed{\bullet} \\ \bullet \end{array}, \\ \begin{array}{c} \boxed{\bullet} \\ \bullet \bullet \end{array} &= \bullet \begin{array}{c} \boxed{\bullet} \\ \bullet \end{array} \bullet + \bullet \bullet \begin{array}{c} \boxed{\bullet} \\ \bullet \end{array} + \begin{array}{c} \boxed{\bullet} \\ \bullet \bullet \end{array} \bullet \bullet. \end{aligned} \quad (\text{B6})$$

### APPENDIX C: SCALAR PRODUCT

First, we note that only states with equal total spin, i.e., states with equal number of singlet  $S$ , triplet  $T$ , and quintet  $Q$  bonds, have a nonvanishing scalar product. Using Eq. (3), we write the hws (4) in the expanded form

$$\begin{aligned} |\psi_s\rangle &= \frac{1}{\sqrt{2^T 3^S}} \sum_{(t_1, t_2) \in \tau, (s_1, s_2) \in \Sigma} |+\langle i_1 \rangle \dots + \langle i_{2Q} \rangle\rangle |t_1^{i(2Q+1)} t_2^{i(2Q+2)}\rangle \\ &\quad \times |s_1^{i(2Q+3)} s_2^{i(2Q+4)}\rangle \dots |s_1^{i(N-1)} s_2^{i(N)}\rangle, \end{aligned} \quad (\text{C1})$$

where  $\tau \equiv \{(+, 0), -(0, +)\}$  and  $\Sigma \equiv \{(+, -), (-, +), -(0, 0)\}$ . The algorithm on how to compute the scalar product is based on determining the number of different combinations of  $S^z$  product states in the decomposition (C1) that are the same in the two states in the scalar product. This number multiplied by the corresponding normalization factors gives the scalar product.

For illustration, let us consider two states in a chain of length  $N=10$  as an example,

$$|1\rangle = (1, 2, 3, 4)_4 |5, 6\rangle_1 |7, 8\rangle_0 |9, 10\rangle_0,$$

$$|2\rangle = (1, 2, 5, 7)_4 |3, 6\rangle_1 |4, 8\rangle_0 |9, 10\rangle_0.$$

In order to calculate the scalar product  $\langle 1|2\rangle$ , we simply count the number of states that agree on both sides after the

decomposition (C1) and then multiply by the normalization. The quintet spins  $(1,2,3,4)_4$  on the left hand side and  $(1,2,5,7)_4$  on the right hand side must all be in the state  $|+\rangle$ . Therefore, according to Eq. (3), only states can agree on both sides of the scalar product where the  $S^z$  eigenvalues of the spins at site 6 is  $|0\rangle$  and at site 8 it must be  $|-\rangle$ . We have exactly one possibility of different combinations of product states to agree, which must be multiplied by the respective normalizations in Eq. (3). The spins with the label 9 and 10 are already in the same state and do not change the scalar product (or, alternatively speaking, this bond contributes a factor of 3 both in the numerator and denominator). Therefore, we obtain, after multiplying by the normalization factors,  $\langle 1|2\rangle = 3/(2 \cdot 3^2) = 1/(2 \cdot 3)$ . Obviously, scalar products factorize according to “connected clusters” and the analysis can be done for each connected cluster separately. From this, it also follows that in order for the scalar product to be non-zero, at least one spin of each singlet bond must again be in a singlet bond on the other side of the scalar product.

The application of this algorithm on connected clusters with  $s=0$  gives a scalar product which is determined by the minimum number of index exchanges  $\gamma$  between bonds in order to bring the two states into the same hws state,

$$\begin{aligned} & \langle \psi_{s=0}(i_1, \dots, i_N) | \psi_{s=0}(i'_1, \dots, i'_N) \rangle \\ &= \langle \psi_{s=0}(i_1, \dots, i_N) | \overbrace{V \dots V}^{\gamma} | \psi_{s=0}(i_1, \dots, i_N) \rangle = \frac{1}{3^\gamma}, \end{aligned} \quad (\text{C2})$$

where  $V_{i,j}\{.,i\}_0\{j,.\}_0 = \{.,j\}_0\{i,.\}_0$  exchanges the indices be-

tween two singlet bonds. This rule can most easily be understood by first considering two equal states with  $\langle \psi | \psi \rangle = 1$ . Then by successively changing indices with  $V_{i,j}$  in order to create

$$|\psi'\rangle = \overbrace{V \dots V}^{\gamma} |\psi\rangle$$

it is clear that the product state with  $|00\rangle$  remains the same, while product states involving  $|+-\rangle$  no longer agree. Each application of  $V$ , therefore, reduces the scalar product by a factor of 3. In an  $s=0$  connected cluster of  $N$  sites, there are  $N/2$  singlet bonds. The exchange operator  $V$  can at most be applied  $N/2 - 1$  times between bonds in order to bring the states into an equivalent form. Therefore, the scalar product must be at least  $1/3^{N/2-1}$  or larger between such states.

As an example, let us consider the states

$$|3\rangle = \{1,2\}_0\{3,4\}_0\{5,6\}_0\{7,8\}_0\{9,10\}_0,$$

$$|4\rangle = \{1,10\}_0\{2,5\}_0\{4,6\}_0\{7,8\}_0\{3,9\}_0.$$

The scalar product  $\langle 3|4\rangle$  can be obtained from the number of exchange operators which we need to transform the state  $|4\rangle$  into the state  $|3\rangle$ ,

$$\langle 3|4\rangle = \langle 3|V_{3,6}V_{5,9}V_{2,10}|3\rangle = \frac{1}{3^3}. \quad (\text{C3})$$

There are other possible choices of exchange operators  $V_{i,j}$ , but the minimum number of exchanges is always  $\gamma=3$  in this case.

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