Ground-state wave function of antiferromagnetic $S = \frac{1}{2}$ Heisenberg chains

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We have proposed an approach to solve the eigenvalue problem of the isotropic $S = \frac{1}{2}$ Heisenberg chain. Many interesting properties of the antiferromagnetic ground state have been reanalyzed by our technique. These results show our method is an appropriate technique.

I. INTRODUCTION

It is well known that the famous Bethe ansatz is in common use to solve the eigenvalue problem of the one-dimensional $S = \frac{1}{2}$ Heisenberg chains,¹ but the procedure is very complicated. Recently, we have developed another method for the same objective, which is completely based on permutation group theory and completely different from the Bethe ansatz.² Our method can deal with not only the $S = \frac{1}{2}$ chain, but also q -deformed chains, and the general spin chain in principle, especially the $S = 1$ chain. Furthermore, the above-mentioned method can be used conveniently to write the exact wave function of the Heisenberg chain, which is rather difficult in the Bethe Ansatz technique. To inspect the validity of our method, in this paper we will focus our attention on discussions of the ground-state properties of the $S = \frac{1}{2}$ isotropic antiferromagnetic Heisenberg chain. From the analysis, we can rederive many important conclusions. This means that our method is a suitable technique.

II. THE WAVE FUNCTION OF ANTIFERROMAGNETIC CHAINS AND ITS PROPERTIES

The $S = \frac{1}{2}$ Heisenberg chain with nearest-neighbor interaction and without external magnetic field is specified by the Hamiltonian

$$H = J \sum_{j=1}^{N-1} \mathbf{S}_j \cdot \mathbf{S}_{j+1}. \quad (1)$$

We define total spin operators S^z and $S^\pm$ by

$$S^z = \sum_{j=1}^N S_j^z, \quad S^\pm = \sum_{j=1}^N S_j^\pm. \quad (2)$$

They generate SU(2) algebra and satisfy

$$[H, S^z] = 0, \quad [H, S^\pm] = 0. \quad (3)$$

When $S = \frac{1}{2}$ it is well known that Eq. (1) can be written as

$$H = \frac{J}{4} \sum_{j=1}^{N-1} (2P_{j,j+1} - 1), \quad (4)$$

where $P_{j,j+1}$ ($j = 1, 2, \dots, N-1$) is the generator of the permutation group S_N , which is related to $\mathbf{S}_j \cdot \mathbf{S}_{j+1}$ by

$$P_{j,j+1} = \frac{1}{2}(4\mathbf{S}_j \cdot \mathbf{S}_{j+1} + 1). \quad (5)$$

Therefore we can solve Eq. (1) with the help of the S_N technique. The key point of our method is to reduce the dimension of the configuration space of Hamiltonian (1) from 2^N to the direct sum of $d_{[N-n,n]} h_{[N-n,n]}$,

$$2^N = \sum_n \otimes d_{[N-n,n]} h_{[N-n,n]}, \quad (6)$$

where $d_{[N-n,n]}$ is the dimension of the representation $[N-n,n]$ of the permutation group,

$$d_{[N-n,n]} = \frac{N!(N-2n+1)}{n!(N-n+1)!}, \quad (6')$$

$h_{[N-n,n]}$ is the dimension of the representation of the SU(2) group, $h_{[N-n,n]} = 2S + 1$, S is the total spin of the spin chain, and $S = N/2 - n$. From Eq. (3) we know that Hamiltonian (1) commutes with S^z and $S^\pm$, so states with different S^z but the same S are degenerate. We can diagonalize Hamiltonian (1) in the space whose dimension is $d_{[N-n,n]}$. The basis vector of the space is

$$|Y_r^{[N-n,n]}, S, S^z\rangle, \quad r = 1, 2, \dots, d_{[N-n,n]}, \quad (7)$$

$$S = N/2 - n, \quad S^z = S,$$

FIG. 1. Weights of SR-RVB state and Néel state in the ground state. $\square$ SR-RVB, $\blacksquare$ Néel state.

where $Y_r^{[N-n,n]}$ represents a Young tableau. More detailed discussions about basis vectors of the representation of the permutation group can be found in Ref. 2.

According to our calculation, we find that the ground state of the antiferromagnetic Heisenberg chain belongs to the representation with $n = [N/2]$,

$$|g.s.\rangle = \sum_r C_r |Y_r^{[N/2,N/2]}, S=0, S^z=0\rangle, \quad \text{if } N \text{ is even}, \quad (8a)$$

$$|g.s.\rangle = \sum_r C_r |Y_r^{[(N+1)/2,(N-1)/2]}, S=\frac{1}{2}, S^z=\frac{1}{2}\rangle, \quad \text{if } N \text{ is odd}. \quad (8b)$$

Hence, the ground state is a singlet when N is even and a

$$|g.s.\rangle = 0.9221 |Y_1^{[3,3]}, S=0, S^z=0\rangle - 0.2593 |Y_3^{[3,3]}, S=0, S^z=0\rangle - 0.2593 |Y_3^{[3,3]}, S=0, S^z=4\rangle \\ + 0.1222 |Y_4^{[3,3]}, S=0, S^z=0\rangle - 0.0187 |Y_5^{[3,3]}, S=0, S^z=0\rangle. \quad (9c)$$

(4) For $N=8$,

$$|g.s.\rangle = 0.8746 |Y_1^{[4,4]}, S=0, S^z=0\rangle \\ - 0.2609 |Y_2^{[4,4]}, S=0, S^z=0\rangle \\ + \dots \quad (14 \text{ terms}). \quad (9d)$$

(5) For $N=10$,

$$|g.s.\rangle = 0.8262 |Y_1^{[5,5]}, S=0, S^z=0\rangle \\ - 0.2496 |Y_3^{[5,5]}, S=0, S^z=0\rangle \\ + \dots \quad (42 \text{ terms}). \quad (9e)$$

We can see from these examples that the first basis vector is most significant in the ground state, which is the short-range resonating valence bond states (SR-RVB) of Anderson.³ Figure 1 shows its weight in the ground state. In the same figure, the Néel state is also shown. From Fig. 1 we see clearly that the weight of the Néel

doublet when N is odd. It is well known that the ground state of the antiferromagnetic chain is unclear up to date. People consider the Néel state as an approximation to the ground state of the antiferromagnetic system, but it is not a good approximation³ and not even an eigenstate of Hamiltonian (1).

The following are some concrete examples of Eq. (8a).

(1) For $N=2$,

$$|g.s.\rangle = |Y_1^{[1,1]}, S=0, S^z=0\rangle. \quad (9a)$$

(2) For $N=4$,

$$|g.s.\rangle = 0.9659 |Y_1^{[2,2]}, S=0, S^z=0\rangle \\ + 0.2588 |Y_2^{[2,2]}, S=0, S^z=0\rangle. \quad (9b)$$

(3) For $N=6$,

state decreases exponentially with increasing N , so it is not appropriate to consider it as an approximate ground state of the antiferromagnetic chain. Although the SR-RVB state is a better approximation than the Néel state, it is also not an exact ground state. The SR-RVB state has an interesting feature. It is asymmetric when the spins at site k and $k+1$ are exchanged, where k is odd.

To uncover the relations between the ground state and the Néel state, we write the ground state (9) as a combination of the products of single-body wave functions. Due to the limitation of space, here we only give the ground state of the chains with $N=2, 4$, and 6.

(i) For $N=2$, the ground state is the Néel state exactly.

(ii) For $N=4$, the ground state is

$$|g.s.\rangle = 0.1494 (\uparrow\uparrow\downarrow\downarrow + \downarrow\downarrow\uparrow\uparrow) + 0.4082 (\uparrow\downarrow\uparrow\downarrow + \downarrow\uparrow\downarrow\uparrow) \\ - 0.5577 (\uparrow\downarrow\downarrow\uparrow + \uparrow\downarrow\uparrow\downarrow). \quad (10a)$$

(iii) For $N=6$, the ground state is

$$|g.s.\rangle = -0.0094 (\uparrow\uparrow\uparrow\downarrow\downarrow - \downarrow\downarrow\uparrow\uparrow\uparrow) + 0.0607 (\uparrow\uparrow\downarrow\uparrow\downarrow - \downarrow\downarrow\uparrow\uparrow\uparrow) \\ - 0.1315 (\uparrow\uparrow\downarrow\uparrow\downarrow - \downarrow\downarrow\uparrow\uparrow\uparrow - \uparrow\downarrow\uparrow\downarrow\uparrow + \uparrow\uparrow\downarrow\uparrow\downarrow) + 0.802 (\uparrow\uparrow\downarrow\uparrow\downarrow - \uparrow\downarrow\downarrow\uparrow\uparrow - \downarrow\downarrow\uparrow\uparrow\downarrow + \downarrow\uparrow\uparrow\downarrow\downarrow) \\ - 0.3085 (\uparrow\downarrow\uparrow\downarrow\uparrow - \uparrow\downarrow\uparrow\downarrow\uparrow - \uparrow\downarrow\uparrow\uparrow\downarrow + \downarrow\uparrow\uparrow\downarrow\downarrow) \\ - 0.2376 (\uparrow\downarrow\uparrow\uparrow\downarrow - \downarrow\uparrow\uparrow\downarrow\uparrow) + 0.4494 (\uparrow\downarrow\uparrow\uparrow\downarrow - \downarrow\uparrow\uparrow\downarrow\uparrow). \quad (10b)$$

TABLE I. Ground-state energy of antiferromagnetic chains.

N		N	
2	-0.3750	3	-0.3333
4	-0.4040	5	-0.3856
6	-0.4156	7	-0.4052
8	-0.4219	9	-0.4151
10	-0.4258	11	-0.4211
12	-0.4285		

TABLE II. Energy gap between ground state and lowest-lying excited states.

N		N	
2	0.5000	3	0.3333
4	0.3295	5	0.1441
6	0.1639	7	0.0796
8	0.0982	9	0.0503
10	0.0655	11	0.0347

FIG. 2. Ground-state energy of antiferromagnetic chains. $\square$ N odd, $\blacksquare$ N even.

FIG. 3. Energy gap between ground state and lowest-lying excited states. $\square$ N odd, $\blacksquare$ N even.

The last two terms of (10a) and (10b) are the Néel state.

From (10) we find that the antiferromagnetic ground state is very complicated and it is impossible to treat any one of the products of single-particle wave functions as its approximation.

Table I and Fig. 2 show the ground-state energies for even N . From Fig. 2 we can conclude that the ground-state energy per spin, E/NJ , approaches -0.44 when N is infinite, which is in better agreement with other authors.⁴

Table II and Fig. 3 show the energy gap between the ground state and the lowest-lying excited singlet states. It is clear that this gap tends to zero when N is infinite. Since the energy of the lowest-lying excited singlet state is always higher than that of the lowest excited states, there is no energy gap between the ground state and the lowest excited states for the infinite chain. This conclusion is in agreement with the famous Haldane conjecture.⁵

In addition, from our calculation we draw the conclusion that the lowest excited state is still a doublet when N is odd but triplet when N is even. In other words, the ground state and lowest excited state do not belong to the same representation of the permutation group for even N . This is a very interesting feature of the antiferromagnetic system because it means that the two states do not share the same permutational symmetry.

III. SUMMARY

In summary, we have presented many results for the isotropic $S = \frac{1}{2}$ Heisenberg finite chain with the help of our technique. Although some of the results are not new in terms of physics, they show that our technique is a reliable approach. Since our wave function is exact, the following two conclusions are also reliable. (1) The SR-RVB state is a better approximate ground state than the Néel state for the one-dimensional $S = \frac{1}{2}$ isotropic antiferromagnetic chain, but it also is not an exact ground state. (2) Our calculation shows that the Haldane conjecture applies for $S = \frac{1}{2}$ chains.

Our calculation is only limited to $N = 12$. Owing to the dimensions of the diagonalized matrix rapidly increasing with N ($d = 144$ for $N = 12$, $d = 16796$ for $N = 20$), it is necessary to have a big computer for large N . Once that is available, we think we would be able to attack many relevant problems which are both interesting and important in low-dimensional condensed-matter physics.

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