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LETTER TO THE EDITOR

Applications of permutation group theory to Heisenberg spin-1/2 chain

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Abstract. Making use of permutation group technique, the eigenvalue problem of Heisenberg spin- $\frac{1}{2}$ chains can be solved. Especially the ground state of the antiferromagnetic chains can be easily written.

A large body of literature on the Heisenberg spin- $\frac{1}{2}$ chain has now appeared, and has presented many techniques to solve its eigenvalue problems [1]. In the present letter we develop another method which is completely based on the permutation group theory. This method possesses three main characteristics:

(1) It is easy to write the ground state of the antiferromagnetic chain. We know that it is difficult in the Bethe Ansatz method.

(2) It is easily translated into programs, and computer facilities can be well utilized.

(3) It can be conveniently extended to the spin-1 chain and q -deformed chain, and so on.

The Hamiltonian of this model is given by

$$H = J \sum_{k=1}^{N-1} s_k \cdot s_{k+1} \quad (1)$$

Defining total spin operators S_0 and S_{\pm}

$$S_0 = \sum_{k=1}^N s_k^z \quad S_{\pm} = \sum_{k=1}^N s_k^{\pm} \quad (2)$$

They generate $SU(2)$ algebra and satisfy

$$[H, S_0] = 0 \quad [H, S_{\pm}] = 0 \quad (3)$$

It is well known that (1) can be rewritten as

$$H = \frac{1}{4} J \sum_{k=1}^{N-1} (2p_k - 1) \quad (4)$$

where $p_k(k=1, 2, \dots, N-1)$ are the generators of the permutation group S_N , which is related to $s_k \cdot s_{k+1}$ by

$$p_k = \frac{1}{2} (1 + 4s_k \cdot s_{k+1}). \tag{5}$$

To our knowledge, there is no further development for solving (4) with the help of the S_N technique.

According to the $U(g)$ and S_N group theory, the basis vectors can be expressed as [2, 3]

$$|Y_r^{[f]}; W_m^{[f]}\rangle. \tag{6}$$

Here $[f] = [f_1, f_2, \dots, f_g]$, the f_1, f_2, \dots, f_g are g integers and a partition of N obeying $f_1 \geq f_2 \geq \dots \geq f_g$ and $f_1 + f_2 + \dots + f_g = N$. We can introduce a graphical representation (Young diagram) of the partitions: a Young diagram consists of N boxes arranged with f_1 boxes in the first row, f_2 boxes in the second row and so on. Such diagram labels an irreducible representation of the groups S_N and $U(g)$. $Y_r^{[f]}$ represents a standard Young tableau (SYT). A SYT is an arrangement of the numbers $1, 2, \dots, N$ in a Young diagram in which the numbers increase as we read from left to right in each row and as we read down in each column. And the $r(r=1, 2, \dots, \dim([f]))$ is an index of SYT which represents a possible filling of the numbers $1, 2, \dots, N$ in a $[f]$ according to the above rules. For example,

$$Y_1^{[31]} = \begin{array}{|c|c|c|} \hline 1 & 3 & 4 \\ \hline 2 & & \\ \hline \end{array} \quad Y_2^{[31]} = \begin{array}{|c|c|c|} \hline 1 & 2 & 4 \\ \hline 3 & & \\ \hline \end{array} \quad Y_3^{[31]} = \begin{array}{|c|c|c|} \hline 1 & 2 & 3 \\ \hline 4 & & \\ \hline \end{array}$$

$W_m^{[f]}$ represents a standard Weyl tableau (swt) which can be constructed by writing the g numbers m_1, m_2, \dots, m_g in the Young diagram corresponding to the above $[f]$. The filling rules are as follows:

- (1) The same m value may not appear in any single column, which means that the Young diagram can be characterized only by a partition with at most g rows. For example, in the case of $SU(2)$, $g=2$, then $[f] = [N-n, n]$ or $[N]$.
- (2) The m values must in increasing order (based on a presumed order: first all the m_1 s, then m_2 s, and so on) as we read from left to right in any row and from top to bottom in any column. For $SU(2)$, $m = \uparrow$ and \downarrow (or $\frac{1}{2}$ and $-\frac{1}{2}$), thus the Weyl tableau are

$$\begin{array}{|c|c|c|c|c|} \hline \uparrow & \dots & \uparrow & \uparrow & \dots & \uparrow \\ \hline \downarrow & \dots & \downarrow & & & \\ \hline \end{array}, \quad \begin{array}{|c|c|c|c|c|} \hline \uparrow & \dots & \uparrow & \uparrow & \dots & \downarrow \\ \hline \downarrow & \dots & \downarrow & & & \\ \hline \end{array}, \dots, \quad \begin{array}{|c|c|c|c|c|} \hline \uparrow & \dots & \uparrow & \downarrow & \dots & \downarrow \\ \hline \downarrow & \dots & \downarrow & & & \\ \hline \end{array}$$

From (3) we know that we can diagonalize the H in the set of basis vector (6) with a fixed Weyl tableau, i.e. the states with the same total spin $S = (N-2n)/2$ (same Young diagram) and different S_0 values (different Weyl tableau) are degeneracy.

Accordingly we can take a particular Weyl tableau in which all boxes of the first row are filled by \uparrow , those in the second row by \downarrow , i.e. the so-called highest weight state of $SU(2)$,

$$\begin{array}{|c|c|c|c|c|c|} \hline \uparrow & \uparrow & \uparrow & \dots & \uparrow & \dots & \uparrow \\ \hline \downarrow & \downarrow & \downarrow & \dots & \downarrow & & \\ \hline \end{array} = |S = (N - 2n)/2, S = S\rangle \tag{7}$$

According to the standard theory of S_N , the non-vanishing matrix elements of the transposition p_k acting in the syr's are as follows:

(1) the diagonal matrix elements are

$$\langle Y_r^{[f]} | p_k | Y_r^{[f]} \rangle = 1/d_{k, k+1}(r) \tag{8a}$$

(2) the non-diagonal matrix elements of p_k between two states $|Y_r^{[f]}\rangle$ and $|Y_s^{[f]}\rangle$ have a non-vanishing value only if the positions of k and $k+1$ are interchanged in going from the tableau r to the tableau s , in which case

$$\langle Y_s^{[f]} | p_k | Y_r^{[f]} \rangle = (1 - 1/(d_{k, k+1}(r))^2)^{1/2}. \tag{8b}$$

The integer $d_{k, k+1}(r)$ is the 'axial distance' of k and $k+1$ in the tableau r , and is defined as

$$d_{k, k+1}(r) = \text{col}(k+1) - \text{col}(k) - \text{row}(k+1) + \text{row}(k) \tag{9}$$

where $\text{col}(k)$ and $\text{row}(k)$ are the column and row numbers of the k th number in tableau r , respectively.

Due to the limitation of the space, here we only discuss the cases $n = 1$ and $n = 0$. The aim is to show the main points of our method. The general discussion will appear elsewhere.

For $n = 1$ there are $N - 1$ different Young tableaux corresponding to a fixed Young diagram. So the basis vectors (6) become

$$\begin{aligned}
 |Y_1^{[N-1, 1]}; S, S\rangle &= \left| \begin{array}{|c|c|c|c|} \hline 1 & 3 & \dots & N \\ \hline 2 & & & \\ \hline \end{array} \right\rangle ; S, S \\
 |Y_2^{[N-1, 1]}; S, S\rangle &= \left| \begin{array}{|c|c|c|c|} \hline 1 & 2 & \dots & N \\ \hline 3 & & & \\ \hline \end{array} \right\rangle ; S, S \\
 \dots & \dots \dots \dots \\
 |Y_{N-2}^{[N-1, 1]}; S, S\rangle &= \left| \begin{array}{|c|c|c|c|} \hline 1 & 2 & \dots & N \\ \hline N' & & & \\ \hline \end{array} \right\rangle ; S, S \quad N' = N - 1 \\
 |Y_{N-1}^{[N-1, 1]}; S, S\rangle &= \left| \begin{array}{|c|c|c|c|} \hline 1 & 2 & \dots & N' \\ \hline N & & & \\ \hline \end{array} \right\rangle ; S, S \quad N' = N - 1
 \end{aligned} \tag{10}$$

Notice that now the index r is equal to $x - 1$, the x is a number filling the box of the second row in (10).

Using the standard technique of S_N , every state in (10) can be rewritten as $a_1 | \uparrow \uparrow \dots \uparrow \uparrow \downarrow \rangle + a_2 | \uparrow \uparrow \dots \uparrow \downarrow \uparrow \rangle + \dots + a_N | \downarrow \uparrow \dots \uparrow \uparrow \uparrow \rangle$

where the $| \uparrow \downarrow \dots \uparrow \uparrow \uparrow \rangle, \dots,$ is a possible arrangement of the up and down spin in the same chain. The coefficients a_1, a_2, \dots, a_N can be easily obtained by means of the standard technique of S_N .

Making use of (8) and (9) the matrix

$$M \left(\sum_{k=1}^{N-1} p_k \right) \text{ of } \sum_{k=1}^{N-1} p_k$$

in the basis vectors (10) can be written as

$$M \left(\sum_{k=1}^{N-1} p_k \right) = N - 3 + M(N) \tag{11a}$$

$$M(N) = \begin{pmatrix} -1/2 & \sqrt{3}/2 & & & & & & \\ \sqrt{3}/2 & -1/2 \cdot 3 & \sqrt{8}/3 & & & & & \\ & \sqrt{8}/3 & -1/3 \cdot 4 & & & & & \\ & & & \ddots & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & -1/N'' \cdot N' & (N'^2 - 1)^{1/2} N' \\ & & & & & & (N'^2 - 1)^{1/2} / N' & N'' / N' \end{pmatrix} \tag{11b}$$

where $N' = N - 1, N'' = N - 2$. It can be shown that

- (a) Trace $(M(N)) = 0,$
- (b) Making use of

$$\det(M(N)) = (N - 2)A_{N-2} / (N - 1) - (N^2 - 2N)A_{N-3} / (N - 1)^2 \quad N \geq 3$$

and

$$A_k = -A_{k-1} / k(k + 1) - (k^2 - 1)A_{k-2} / k^2 \quad k = 2, 3, \dots, (N - 2)$$

$$A_0 = 1 \quad A_1 = -1/2$$

we obtain

$$\det(M(N)) = \begin{cases} 0 & \text{if } N \geq 2; \text{ even integer numbers} \\ (-1)^{N-1/2} & \text{if } N \geq 3; \text{ odd integer numbers.} \end{cases} \tag{12}$$

Let $\lambda(k, N) (k = 1, 2, \dots, N - 1)$ represent the eigenvalues of $M(N)$, then

$$\sum_{k=1}^{N-1} \lambda(k, N) = 0 \quad \prod_{k=1}^{N-1} \lambda(k, N) = \det(M(N)). \tag{13}$$

Since $2 \cos(k\pi/N) (k = 1, 2, \dots, N - 1)$ also satisfy the same relation as (13), we can write

$$\lambda(k, N) = 2 \cos(k\pi/N) \quad k = 1, 2, \dots, N - 1. \tag{14}$$

This means that the eigenvalues are

$${}^1E(k, N) = \frac{1}{4} J \{ (N - 5) + 4 \cos(k\pi/N) \} \quad k = 1, 2, \dots, N - 1. \tag{15}$$

This result is in agreement with [4, 5] if $\Delta = 1$ and $p, p' = 0$ in [4], which means that our method is reasonable. Notice that the physical implication of quantum number k here is very different from that in [4, 5]. Our k is only the index of syts. Another strong point of our method is that the states of the system may be written conveniently. For $J < 0$ and arbitrary N , the lowest state |L.s.) is

$$|L.s.) = \sum_r C_r |Y_r^{[N-1, 1]}; S, S\rangle \tag{16a}$$

where

$$C_r = \frac{r}{2(r^2 - 1)^{1/2}} \left\{ \left[\frac{2}{r(r-1)} + 4E(k=1, N)/J - N + 5 \right] C_{r-1} - \frac{2(r^2 - 2r)^{1/2}}{r-1} C_{r-2} \right\}$$

$$r = 2, 3, \dots, N-1. \tag{16b}$$

The parameter C_1 can be determined by a normalized procedure. For example

(1) $N = 4; S_0 = S = 1; {}^1E(1, 4) = 0.4571J$

$$|L.s.) = 0.2706 |Y_1^{[31]}; 1, 1\rangle + 0.5981 |Y_2^{[31]}; 1, 1\rangle + 0.7543 |Y_3^{[31]}; 1, 1\rangle$$

(2) $N = 5; S_0 = S = 3/2; {}^1E(1, 5) = 0.8090J$

$$|L.s.) = 0.1625 |Y_1^{[41]}; 3/2, 3/2\rangle + 0.3973 |Y_2^{[41]}; 3/2, 3/2\rangle$$

$$+ 0.6029 |Y_3^{[41]}; 3/2, 3/2\rangle + 0.6725 |Y_4^{[41]}; 3/2, 3/2\rangle$$

(3) $N = 10; S_0 = S = 4; E(1, 10) = 2.2011J$

$$|L.s.) = 0.0306 |Y_1^{[91]}; 4, 4\rangle + 0.0848 |Y_2^{[91]}; 4, 4\rangle$$

$$+ 0.1580 |Y_3^{[91]}; 4, 4\rangle + 0.2414 |Y_4^{[91]}; 4, 4\rangle$$

$$+ 0.3248 |Y_5^{[91]}; 4, 4\rangle + 0.3977 |Y_6^{[91]}; 4, 4\rangle$$

$$+ 0.4503 |Y_7^{[91]}; 4, 4\rangle + 0.4747 |Y_8^{[91]}; 4, 4\rangle$$

$$+ 0.4656 |Y_9^{[91]}; 4, 4\rangle$$

For $n = 0, S = N/2$ and the Young tableau is unique, $\boxed{1 \mid 2 \mid \dots \mid N-1 \mid N}$. The eigenenergy and the lowest state, are, respectively

$${}^0E(N) = J(N-1)/4 \tag{17}$$

$$|L.s.) = \left| \boxed{1 \mid 2 \mid 3 \mid \dots \mid N} ; N/2, N/2 \right\rangle \tag{18}$$

The general case ($n \neq 0, 1$) eigenenergies and eigenstates can also be given. Further discussions will be reported in later papers, especially the relations between the ground state |g.s.) and the Neel state in antiferromagnetic spin chains.

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