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ON EXACT SOLUTIONS OF HEISENBERG SPIN MODEL WITH NEXT-to-NEAREST NEIGHBOUR INTERACTIONS

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On Exact Solutions of Heisenberg Spin Model with Next-to-Nearest Neighbour Interactions[1]

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Abstract

The symmetries of the isotropic Heisenberg spin-$\frac{1}{2}$ model in one dimension with next nearest interactions are investigated. It is shown that the model can be exactly solved. Some detailed calculations and results are presented.

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It is well known that the XXZ 1-D Heisenberg spin-$\frac{1}{2}$ chain with nearest interactions can be exactly solved in terms of Bethe ansatz [1], which gives rise to the general forms of the energy and eigenstates but the explicit solutions are difficult to obtain. In [2] Levy presented a systematic method in dealing with this model exactly and analytically by using its Temperley-Lieb-Jones (TLJ) [3] algebraic structures. This method is related to the $SU_q(2)$ group symmetries [4] of this model in [5] [6] and some detailed calculations are given in [7].

In this paper, we investigate the isotropic 1-D Heisenberg spin chain with next nearest interactions. It is not known how to cope with this case by Bethe ansatz. But we find that the Levy's discussions can be easily applied.

We consider a chain with $N+1$ spins. The spin operators $S^{\pm}$ and S^3 of every spin constitute the $SU(2)$ algebra

$$[S^+, S^-] = 2S^3 , \qquad [S^3, S^{\pm}] = \pm S^{\pm} , \tag{1}$$

with the Casimir operator $C = S^+S^- - S^3(S^3-1)$ and co-multiplication map Δ

$$\begin{aligned} \Delta(S^3) &= S^3 \otimes 1 + 1 \otimes S^3 , \\ \Delta(S^{\pm}) &= S^{\pm} \otimes 1 + 1 \otimes S^{\pm} , \\ \Delta 1 &= 1 \otimes 1, \end{aligned} \tag{2}$$

which is the algebra homomorphism.

For spin-$\frac{1}{2}$,

$$S^{\pm} = \sigma^{\pm} , \quad S^3 = \frac{1}{2}\sigma^3 , \tag{3}$$

where $\sigma^{\pm,3}$ are Pauli matrices. It is easy to find that

$$\Delta(2-C) = \frac{1}{2}1 \otimes 1 - \left[\sigma^+ \otimes \sigma^- + \sigma^- \otimes \sigma^+ + \frac{1}{2}\sigma^3 \otimes \sigma^3\right]. \tag{4}$$

which is just the terms describing two nearest spin interactions up to a constant term. From (4) one has the trivial representation of TLJ algebra,

$$e_i = 1^{(1)} \otimes 1^{(2)} \otimes \cdots \otimes 1^{(i-1)} \otimes \Delta(2-C)^{(i,i+1)} \otimes 1^{(i+2)} \otimes \cdots \otimes 1^{(N+1)} , \tag{5}$$

which represents the interactions of spin at site i and $i+1$ and satisfies TLJ algebraic relations

$$e_i^2 = 2e_i\ , \qquad e_i e_{i\pm1} e_i = e_i\ ,$$
$$e_i e_j = e_j e_i\ , \quad \text{if} \quad |i-j| \geq 2\ . \tag{6}$$

From eqs. (4) and (5) it is obvious that e_i commutes with the total spin operators

$$S^\alpha_{tot} = \sum_{i=1}^{N+1} 1_1 \otimes 1_2 \otimes \cdots \otimes 1_{i-1} \otimes S^\alpha_i \otimes 1_{i+1} \otimes \cdots \otimes 1_{N+1}\ , \tag{7}$$

where $\alpha = \pm, 3$. Therefore the Hamiltonian constituted of e_i will have $SU(2)$ symmetry. Its eigenvalues and eigenstates can be studied in terms of the TLJ algebraic properties and classified according to the highest weight representations of $SU(2)$ algebra.

The Hamiltonian for spin chain with nearest interactions is simply

$$H_n = \frac{J}{2}\sum_{i=1}^{N} e_i = -\frac{J}{2}\sum_{i=1}^{N}\left[\sigma_i^+\sigma_{i+1}^- + \sigma_i^-\sigma_{i+1}^+ + \frac{1}{2}\sigma_i^3\sigma_{i+1}^3\right] + N1 \tag{8}$$

It is the usual ferromagnetic(antiferromagnetic) Heisenberg spin chain, up to a constant term, when J is positive(negative).

Let $e_{i,i+2}$ denote the next nearest interactions between spins at site i and $i+2$. We find that $e_{i,i+2}$ can be expressed in terms of the interactions between spins at $\{i, i+1\}$ and $\{i+1, i+2\}$, i.e., e_i and e_{i+1},

$$e_{i,i+2} = e_i + e_{i+1} - \{e_i, e_{i+1}\}\ , \quad i = 1, 2, \cdots, N-1\ , \tag{9}$$

where $\{\cdot,\cdot\}$ denotes the anticommutator. Therefore the isotropic Heisenberg spin Hamiltonian with next nearest interactions are

$$\begin{aligned} H_{nn} &= \frac{J}{2}\left[\sum_{i=1}^{N} e_i + g\sum_{i=1}^{N-1} e_{i,i+2}\right] \\ &= \frac{J}{2}\sum_{i=1}^{N-1}\left[(1+g)e_i + g(e_i + e_{i+1} - e_i e_{i+1} - e_{i+1}e_i)\right] + \frac{J}{2}e_N\ , \end{aligned} \tag{10}$$

where g is a coupling constant of interactions between next nearest spins. For the convenience of writing, we will omit the factor $\frac{J}{2}$ in the following.

The Hamiltonian system of (10) can be studied according to the independent bases of the left ideal of TLJ algebra [2] [7]. Let $|x_1\ x_2\ \cdots\ x_n\rangle$, $1 \leq x_1 < x_2 < \cdots < x_n \leq N+1$, denote the state with n down spins and x_is denote the locations of the down spins of the chain. The bases for n down spin states with the highest weight j are

$${}^nC_{(m)}Z_n^N|1\ 3\ 5\ \cdots\ (2n-1)\rangle, \quad n \leq \frac{(N+1)}{2}, \tag{11}$$

where

$$\begin{aligned} &{}^nC_{(m)} = C_1^{m_1}C_3^{m_2}\cdots C_{2n-1}^{m_n}, \quad 1 \leq m_1 < m_2 < \cdots < m_n \leq N, \quad m_i \geq (2n-1) \\ &C_i^m = e_m e_{m-1}\cdots e_i, \quad j = \tfrac{1}{2}(N-2n-1). \end{aligned} \tag{12}$$

Z_n^N is a polynomial of e_i's with property $e_k Z_n^N = 0$ if $k \geq 2n$. The action of Z_n^N on $|1\ 3\ 5\ \cdots\ (2n-1)\rangle$ gives rise to a constant factor. Therefore the bases of eigenstates for n spins down case are simply

$${}^n\Phi_{(m)} = {}^nC_{(m)}|1\ 3\ 5\ \cdots\ (2n-1)\rangle. \tag{13}$$

The eigenstates of the Hamiltonian are the combinations of ${}^n\Phi_{(m)}$ with the same n,

$${}^n\Psi = \sum_{(m)} a_{(m)}\Phi_{(m)}. \tag{14}$$

For every $n \leq (N+1)/2$, there are $\begin{pmatrix} N \\ n \end{pmatrix} - \begin{pmatrix} N \\ n-2 \end{pmatrix}$ eigenvalues of energy ${}^nE$ from Hamiltonian equation

$$H\ {}^n\Psi = {}^nE\ {}^n\Psi. \tag{15}$$

The degenerate states with respect to every eigenvalue can be obtained by acting the total spin operator S^-_{tot} on the corresponding eigenstate of the highest weight.

All the eigenvalues and eigenstates can be exactly obtained in terms of recipe above for given spins of the chain. Here we only give detailed calculations for some special cases.

First we consider n=1, the case of $N+1$ spins chain with 1 spin down. The eigenstates are simply of the form

$$^{1}\Psi = \sum_{m=1}^{N} a_m C_1^m |1\rangle \tag{16}$$

Accounting to the relations (6) and (15) we have

$$-ga_{m+2} + a_{m+1} + [2(1+g) - E]a_m + a_{m-1} - ga_{m-2} = 0, \quad m = 1, 2, \cdots, N. \tag{17}$$

Where comparing to the Hamiltonian equations about $m = 1, 2, N-1$ and N, we have

$$a_0 = 0,\ a_{-1} = a_1 + a_2,\ a_{N+1} = 0,\ a_{N+2} = a_{N-1} + a_N. \tag{18}$$

The reduction equation (17) can be easily manipulated by simply setting $a_m = \eta^m$, which gives rise to an equation of η with four solutions,

$$\begin{aligned} \eta_{1,2} &= \frac{\pm 2\sqrt{-A - 2gE + 4g + 1} - A\sqrt{2} + \sqrt{2}}{4\sqrt{2}g} \\ \eta_{3,4} &= \frac{A\sqrt{2} \pm 2\sqrt{A - 2gE + 4g + 1} + \sqrt{2}}{4\sqrt{2}g} \end{aligned} \tag{19}$$

where $A = \sqrt{16g^2 - 4gE + 8g + 1}$. Therefore $a_m = b_1\eta_1^m + b_2\eta_2^m + b_3\eta_3^m + b_4\eta_4^m$. The coefficients b_1, b_2, b_3, b_4 and energy E are determined by conditions (18).

Or explicitly

$$a_{m+2} = \left[(\beta_m + \gamma_m) - (\alpha_m + \gamma_m)\frac{\beta_{N-1} + \gamma_{N-1}}{\alpha_{N-1} + \gamma_{N-1}}\right] \quad m = 1, \cdots, N, \tag{20}$$

where α_m, β_m, γ_m are determinants of $(m+3) \times (m+3)$ matrices,

$$\alpha_m = \frac{1}{(-g)^m} det \begin{pmatrix} 1 & c & 1 & -g & & & & & & & \\ -g & 1 & c & 1 & -g & & & & & & \\ & -g & 1 & c & 1 & -g & & & & & \\ & & & \cdot & \cdot & \cdot & \cdot & & & & \\ & & & & & & -g & 1 & c & 1 & -g \\ & & & & & & & 0 & 1 & 0 & 0 \\ & & & & & & & 0 & 0 & 1 & 0 \\ & & & & & & & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$\beta_m = \frac{1}{(-g)^m} det \begin{pmatrix} 1 & c & 1 & -g & & & & & & & \\ -g & 1 & c & 1 & -g & & & & & & \\ & -g & 1 & c & 1 & -g & & & & & \\ & & & \cdot & \cdot & \cdot & \cdot & & & & \\ & & & & & & -g & 1 & c & 1 & -g \\ & & & & & & & 1 & 0 & 0 & 0 \\ & & & & & & & 0 & 0 & 1 & 0 \\ & & & & & & & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$\gamma_m = \frac{1}{(-g)^m} det \begin{pmatrix} 1 & c & 1 & -g & & & & & & & \\ -g & 1 & c & 1 & -g & & & & & & \\ & -g & 1 & c & 1 & -g & & & & & \\ & & & \cdot & \cdot & \cdot & \cdot & & & & \\ & & & & & & -g & 1 & c & 1 & -g \\ & & & & & & & 0 & 1 & 0 & 0 \\ & & & & & & & 0 & 1 & 0 & 0 \\ & & & & & & & 0 & 0 & 0 & 1 \end{pmatrix},$$

and $c = 2(1+g) - E$.

The condition

$$\begin{aligned}
&\left[(\beta_N+\gamma_N)-(\alpha_N+\gamma_N)\frac{\beta_{N-1}+\gamma_{N-1}}{\alpha_{N-1}+\gamma_{N-1}}\right] \\
&=\left[(\beta_{N-2}+\gamma_{N-2})-(\alpha_{N-2}+\gamma_{N-2})\frac{\beta_{N-1}+\gamma_{N-1}}{\alpha_{N-1}+\gamma_{N-1}}\right] \\
&+\left[(\beta_{N-3}+\gamma_{N-3})-(\alpha_{N-3}+\gamma_{N-3})\frac{\beta_{N-1}+\gamma_{N-1}}{\alpha_{N-1}+\gamma_{N-1}}\right]
\end{aligned} \tag{21}$$

determines the energy E.

If $g=0$, the Hamiltonian (10) becomes (8) with only nearest interactions and

$$\begin{aligned}
a_m &= (-)^{m-1}\frac{\sin\left(\frac{mk\pi}{N+1}\right)}{\sin\left(\frac{k\pi}{N+1}\right)}, \\
E &= 2\left(1-\cos\frac{k\pi}{N+1}\right), \quad k=0,1,2,\cdots,N .
\end{aligned} \tag{22}$$

For each k, there is an energy E and a set of coefficients a_m that gives rise to an eigenstate (16) of the highest weight state. The degenerate states with lower weights are obtained by the actions of the lowering operator of the symmetry algebra $SU(2)$, S^-_{tot}, on the highest weight state.

The solutions of the case with one spin down in the chain, $n=1$, corresponds to the eigenstates and energies of the ground and lower exciting states of the ferromagnetic chain when J is positive. And when J is negative it corresponds to the solutions of some excited states of antiferromagnetic chains.

For $n\geq 2$ and general N the equation (15) becomes a set of reduction equations. It will be a bit more difficult to solve. However, for a given finite N the problem becomes the solving of a set of linear and homogeneous equations. The energies can be immediately obtained from the condition that the coefficient determinant of the equation set equals to zero.

Let us consider, for example, the case of four spins ($N=3$). The Hamiltonian

(10) is simply

$$H_{nn}=(g+1)(e_1+e_3)+(2g+1)e_2-g(e_1e_2+e_2e_1+e_2e_3+e_3e_2). \tag{23}$$

For $n=0$, there is only one state ${}^0\Psi=|0\rangle$ with all spins up. It is the eigenstate of both Hamiltonian and angular momentum with eigenvalues $E_0=0$ and $j=2$ respectively.

For n=1, there are four independent states. One of them is of energy $E_0=0$, and eigenstate

$${}^1\Psi_0=S^-_{tot}\,{}^0\Psi=\sum_{i=1}^{4}|i\rangle\ , \tag{24}$$

where $|i\rangle$ represents that the spin at location i is down and others are up.

From (16) the rest three eigenstates are

$${}^1\Psi_0=(a_1e_1+a_2e_2e_1+a_3e_3e_2e_1)|1\rangle\ . \tag{25}$$

By use of (6) and (15) it is easy to get

$$\begin{aligned}
(g+2-E)a_1 &+ (1+g)a_2 - ga_3=0 \\
a_1 &+ (2-E+2g)a_2 + a_3=0 \\
-ga_1 &+ (1-g)a_2 + (2+g-E)a_3=0
\end{aligned} \tag{26}$$

Therefore we have solutions

$$\begin{aligned}
&E_1=2+g-\sqrt{g^2-2g+2},\quad a_2=2a_1(\sqrt{g^2-2g+2}+g)^{-1},\quad a_3=a_1\ ; \\
&E_3=2(g+1),\quad a_2=0\ (or\ \ arbitrary\ \ if\ \ g=1),\quad a_3=-a_1; \\
&E_4=2+g+\sqrt{g^2-2g+2},\quad a_2=2a_1(\sqrt{g^2-2g+2}-g)^{-1},\quad a_3=a_1\ .
\end{aligned} \tag{27}$$

Explicitly the corresponding eigenstates are

$$\begin{aligned}
{}^1\Psi_1 &= |1\rangle-\left(1+2(\sqrt{g^2-2g+2}+g)^{-1}\right)|2\rangle \\
&\quad+\left(1+2(\sqrt{g^2-2g+2}+g)^{-1}\right)|3\rangle-|4\rangle \\
{}^1\Psi_3 &= |1\rangle-|2\rangle-|3\rangle+|4\rangle \\
{}^1\Psi_4 &= |1\rangle-\left(1+2(\sqrt{g^2-2g+2}-g)^{-1}\right)|2\rangle \\
&\quad+\left(1+2(\sqrt{g^2-2g+2}-g)^{-1}\right)|3\rangle-|4\rangle
\end{aligned} \tag{28}$$

For n=2, there are six independent states. Four of them are obtained by the actions of the lowering operator S^-_{tot} on above four states of $n = 1$,

$$
\begin{aligned}
{}^2\Psi_0 = S^-_{tot}\,{}^1\Psi_0 &= 2(|12\rangle + |13\rangle + |14\rangle + |23\rangle + |24\rangle + |34\rangle) \\
{}^2\Psi_1 = S^-_{tot}\,{}^1\Psi_1 &= (1 - \left(1 + 2(\sqrt{g^2 - 2g + 2} + g)^{-1}\right))(|12\rangle - |34\rangle) \\
&\quad +(1 + \left(1 + 2(\sqrt{g^2 - 2g + 2} + g)^{-1}\right))(|13\rangle - |24\rangle) \\
{}^2\Psi_3 = S^-_{tot}\,{}^1\Psi_3 &= 2(|14\rangle - |23\rangle) \\
{}^2\Psi_4 = S^-_{tot}\,{}^1\Psi_4 &= (1 - \left(1 + 2(\sqrt{g^2 - 2g + 2} - g)^{-1}\right))(|12\rangle - |34\rangle) \\
&\quad +(1 + \left(1 + 2(\sqrt{g^2 - 2g + 2} - g)^{-1}\right))(|13\rangle - |24\rangle)
\end{aligned}
\tag{29}
$$

with energies E_0, E_1, E_3, and E_4 respectively.

From (14) the rest two states are of the form

$$
{}^2\Psi = (a_{13}C_1^1C_3^3 + a_{23}C_1^2C_3^3)|13\rangle = (a_{13}e_3e_1 + a_{23}e_2e_3e_1)|13\rangle \tag{30}
$$

Using (15) we get energies

$$
\begin{aligned}
E_2 &= 2g + 3 - \sqrt{4g^2 - 6g + 3} \\
E_5 &= 2g + 3 + \sqrt{4g^2 - 6g + 3}
\end{aligned}
\tag{31}
$$

with respect to eigenstates

$$
\begin{aligned}
{}^2\Psi_2 &= (1 - \frac{1 + \sqrt{4g^2 - 6g + 3}}{2g - 2})|13\rangle + (\frac{1 + \sqrt{4g^2 - 6g + 3}}{2g - 2} - 1)|14\rangle \\
&\quad +(1 + \frac{1 + \sqrt{4g^2 - 6g + 3}}{2g - 2})|24\rangle - |23\rangle - \frac{1 + \sqrt{4g^2 - 6g + 3}}{2g - 2}|34\rangle \\
{}^2\Psi_5 &= (1 - \frac{1 - \sqrt{4g^2 - 6g + 3}}{2g - 2})|13\rangle + (\frac{1 - \sqrt{4g^2 - 6g + 3}}{2g - 2} - 1)|14\rangle \\
&\quad +(1 + \frac{1 - \sqrt{4g^2 - 6g + 3}}{2g - 2})|24\rangle - |23\rangle - \frac{1 - \sqrt{4g^2 - 6g + 3}}{2g - 2}|34\rangle
\end{aligned}
\tag{32}
$$

In this way we get all the eigenstates and energy levels of the 1-D Heisenberg spin system (N=3) with next nearest interactions. It is worthwhile to note that when g=0,

$$
\begin{aligned}
E_0 = 0, \quad E_1 = 2 - \sqrt{2}, \quad E_2 = 3 - \sqrt{3} \\
E_3 = 2, \quad E_4 = 2 + \sqrt{2}, \quad E_5 = 3 + \sqrt{3}
\end{aligned}
\tag{33}
$$

Hence if J is positive we have,

$$
E_0 < E_1 < E_2 < E_3 < E_4 < E_5 \,. \tag{34}
$$

However, when $g = \frac{1}{2}$, $E_2 = E_3 = 3$. The energy level 2 and 3 become degenerate. This also takes place when $g = 1$ (at this moment the eigenstate ${}^1\Psi_4$ in eq. (28) is no longer correct. By solving the eq. (26) again one gets $a_3 = -a_1$ and a_2 is arbitrary. Similar recalculations for ${}^2\Psi_2$ and ${}^2\Psi_5$ are also needed). In fact we have

$$
\begin{aligned}
E_2 = E_3 \quad if \quad g = \frac{1}{2} \;\; or \;\; g = 1 \\
E_2 < E_3 \quad if \quad 0 < g < \frac{1}{2} \\
E_2 > E_3 \quad if \quad \frac{1}{2} < g < 1
\end{aligned}
\tag{35}
$$

Therefore it is manifest that the interactions between the next nearest spins may change the order of energy levels and result in phase transitions.

It is also interesting to have a look at the case of $g < 0$. When $g = \frac{1}{3}$, $E_0 = E_1$, the original ground state and first exited state become degenerate. And when $1 < g < \frac{1}{3}$, one has $E_0 > E_1 > E_2$. The energy levels 1, 2 and 3 are reversed.

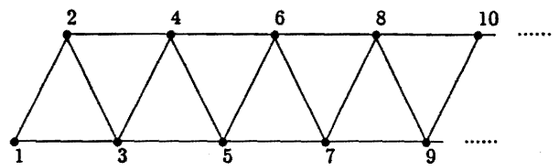
Here the boundary conditions of Hamiltonian (10) are open. The cyclic boundary conditions may be also considered by adding a boundary term $e_{1,4}$ of interactions between spin 1 and 4, which is easily deduced from relation (9)

$$
\begin{aligned}
e_{1,4} &= e_{1,3} + e_3 - \{e_{1,3}, e_3\} \\
&= e_1 + e_2 + e_3 - \{e_1, e_2\} - \{e_2, e_3\} - \{e_1, e_3\} \\
&\quad +\{e_1, \{e_2, e_3\}\}
\end{aligned}
\tag{36}
$$

It is directly to get all the eigenfunctions and energy levels for this Hamiltonian system of cyclic boundary condition from similar calculations above.

It should be noted that the lower dimensional Heisenberg spin model with higher order non-nearest interactions corresponds to higher dimensional ones with

lower order non-nearest interactions. Here the 1-D chain with next nearest interactions is the same as the 2-D strip with triangular nearest interactions, i.e.,



Different selections of non-nearest interactions of 1-D chain will correspond to different kinds of 2-D or higher dimension lattice interactions. Similarly higher dimensional Heisenberg spin models may be exactly solved by reducing them to be 1-D problems. In any way the Hamiltonians are always the polynomials of the elements of Temperley-Lied algebra and hence their eigenstates are of the form (14). The 2-D isotropic Heisenberg model, which is related to the Hubbard model [8] in high T_c superconductivity theory [9], can be also be exactly solved in this way [10].

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