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Exact solution of an integrable quantum spin chain with competing interactions*

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We construct an integrable quantum spin chain that includes the nearest-neighbor, next-nearest-neighbor, chiral three-spin couplings, Dzyloshinsky–Moriya interactions and unparallel boundary magnetic fields. Although the interactions in bulk materials are isotropic, the spins nearby the boundary fields are polarized, which induce the anisotropic exchanging interactions of the first and last bonds. The $U(1)$ symmetry of the system is broken because of the off-diagonal boundary reflections. Using the off-diagonal Bethe ansatz, we obtain an exact solution to the system. The inhomogeneous T–Q relation and Bethe ansatz equations are given explicitly. We also calculate the ground state energy. The method given in this paper provides a general way to construct new integrable models with certain interesting interactions.

Keywords: quantum spin chain, Bethe ansatz, Yang–Baxter equation

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1. Introduction

Quantum magnetism is an important issue in research of condensed matter physics. Spin–spin interactions can induce many interesting phenomena such as novel magnetic ordered states, fractional spin excitations and quantum phase transitions. The typical spin–spin interactions include the nearest neighbor (NN), next nearest neighbor (NNN), Dzyloshinsky–Moriya (DM) interactions and chirality three-spin couplings.

Focusing on the NN interaction, the most famous model is the Heisenberg model. It is well-known that the elementary excitation of the isotropic Heisenberg model is gapless while that of the anisotropic case has a finite gap in some regions. The Heisenberg model can be solved exactly by the coordinate Bethe ansatz[1] or the quantum inverse scattering method.[2] Nowadays, Bethe ansatz becomes a popular method to calculate exact solutions of one-dimensional quantum many-body systems. The Heisenberg model is also a suitable candidate to check the validity of new numerical simulation technique and new physical pictures such as the spinon and fractional statistics.[3]

When the NNN interaction is involved, the most famous model is the J_1–J_2 model, which cannot be solved exactly. At the Majumdar–Ghosh point, i.e., $J_2/J_1 = 0.5$, the Hamiltonian degenerates into a projector operator and only the ground state can be obtained exactly.[4] The J_1–J_2 model with $J_2/J_1 = 0.241$ possesses a Kosterlitz–Thouless-like quantum phase transition, which is a kind of topological phase transitions and does not have the local order parameter. The corresponding critical point has been studied by many methods such as the density matrix renormalization group[5] and field-theoretical approach.[6–8] Due to the competition between NN and NNN interactions, especially when the NN interaction is ferromagnetic and NNN interaction is antiferromagnetic, some interesting ordered magnetic states are found. The J_1–J_2 model can be explained as the zigzag spin ladder, which is very important in the study of crossover from the one-dimensional to the two-dimensional case. Therefore, much attention has been paid to the quantum spin chain with competing interactions.[9–12]

The DM interaction is a typical antisymmetric spin–spin interaction, which plays an essential role in various fields.[13–15] For example, the DM interaction in the Heisenberg model can induce the spin glasses phase,[16] phase transition[17] and nonlinear excitations.[18] In recent years,

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DM interactions in magnetic systems have been studied extensively.[19,20]

The chiral three-spin couplings are another kind of interesting interactions. The chirality terms are used to characterize the chiral spin liquid state in the system.[21] It is proposed that the expectation value of the spin chirality operator can be used as the order parameter for chiral spin liquids.[22,23] Using the quantum transfer matrix method, researchers have studied the thermodynamic properties of this kind of models.[24,25] Recently, the models with chirality terms have attracted renewed interest in the theory of quantum spin liquids.[26,27]

The magnetic impurity in the strongly correlated systems is the eternal topic in the quantum magnetism theory. Many interesting mechanisms such as the Kondo screen, spiral phase, novel spinon excitation, ghost spin and boundary bound states are induced by the magnetic impurity. The Kondo problems in one dimension are solved by means of Bethe ansatz.[28,29] Using the language of integrable theory, some impurity problems are equivalent to the boundary magnetic fields. Here, we note that if the boundary magnetic fields are parallel, then the $U(1)$ symmetry will be held and the system can be solved by the Bethe ansatz.[30] If the boundary magnetic fields are unparallel, then the $U(1)$ symmetry will be broken and the conventional Bethe ansatz will not work. In this case, the system can be solved by the off-diagonal Bethe ansatz.[31]

In this paper, we put all the above-mentioned interactions (NN, NNN, DM, chiral three-spin couplings and boundary impurities) together and construct a new integrable model. The Hamiltonian is given by Eq. (1). For the most possible applications, we consider the case that the boundary fields are unparallel. Due to the off-diagonal boundary reflection, the total number of quasiparticles with fixed spin-component is not conserved. By means of the off-diagonal Bethe ansatz, we obtain the exact solution of the system. These exact solutions can be used to study some physical quantities such as the ground state, elementary excitations, and boundary energy.

The paper is organized as follows. The model Hamiltonian is explained in Section 2 and the integrability of the system is proved in Section 3. The exact energy spectrum and the Bethe ansatz equations are derived in Section 4. The exact ground state energies in some parameter regions are given in Section 5. Section 6 is attributed to the concluding remarks.

2. Model Hamiltonian

The integrable Hamiltonian considered in this study is

$$\begin{aligned} H = & \sum_{j=1}^{2N-1} \{J_1 \boldsymbol{\sigma}_j \cdot \boldsymbol{\sigma}_{j+1} + J_2 \boldsymbol{\sigma}_j \cdot \boldsymbol{\sigma}_{j+2} \\ & + J_3 (-1)^j \boldsymbol{\sigma}_{j+1} \cdot (\boldsymbol{\sigma}_j \times \boldsymbol{\sigma}_{j+2})\} \\ & + \frac{1-4a^2}{p^2-a^2} \left[p\sigma_1^z - a^2 \sigma_1^z \sigma_2^z - \mathrm{i}ap D_1^z \cdot (\boldsymbol{\sigma}_1 \times \boldsymbol{\sigma}_2) \right] \\ & + \frac{4a^2-1}{a^2\xi^2 + a^2 - q^2} \left[q(\xi \sigma_{2N}^x + \sigma_{2N}^z) \right. \\ & - a^2 (\xi \sigma_{2N-1}^x + \sigma_{2N-1}^z)(\xi \sigma_{2N}^x + \sigma_{2N}^z) \\ & \left. - \mathrm{i}aq(\xi D_{2N}^x + D_{2N}^z) \cdot (\boldsymbol{\sigma}_{2N} \times \boldsymbol{\sigma}_{2N-1}) \right]. \end{aligned} \tag{1}$$

Here σ_j^α $(\alpha = x, y, z)$ represents the Pauli matrix on the j-th site and the total number of sites is $2N$. The first three terms describe the interactions in the bulk which includes the NN, NNN and chiral three-spin interactions with the coupling strengths J_1, J_2 and J_3, respectively. We note that the convention $\boldsymbol{\sigma}_{2N+1} = 0$ has been used. The rest terms are the couplings induced by the unparallel boundary magnetic fields which include the anisotropic and DM interactions of the fist bond and those of the last bond. The boundary field at one side is tuned by the parameter p and the field at the other side is tuned by the parameters q and ξ. The hermitian of Hamiltonian (1) requires that the model parameter a is pure imaginary.

Let us explain Hamiltonian (1) more clearly. The interactions in the bulk are isotropic and the coupling strengths are chosen as

$$\begin{aligned} & J_1 = 1 + c_j(\delta_{j,1} + \delta_{j,2N-1}), \quad J_2 = -2a^2, \quad J_3 = \mathrm{i}a, \\ & c_1 = \frac{a^2(1-2a^2-2p^2)}{p^2-a^2}, \\ & c_{2N-1} = 2a^2 + \frac{a^2(4q^2-\xi^2-1)}{a^2\xi^2+a^2-q^2}. \end{aligned} \tag{2}$$

The integrability requires that the parameters J_1, J_2 and J_3 are not independent. From Eq. (2), we also see that due to the existence of boundary magnetic fields, the couplings of $\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$ and $\boldsymbol{\sigma}_{2N-1} \cdot \boldsymbol{\sigma}_{2N}$ can be enhanced or decreased by the boundary fields. The resulted coupling strengths could be different from that of other bonds in the bulk. The NNN interacting strength J_2 is a constant. Meanwhile, the signs of chiral three-spin interactions change with the changing site number j. Thus the chirality terms are staggered.

Next, we analyze the effects induced by the boundary magnetic field at the first site. Because the interactions in the bulk are isotropic and have the $su(2)$ symmetry, without loss of generality, we can always choose the direction of boundary field at the first site as the z-direction of the whole system. Then the boundary field can be parameterized as $p\sigma_1^z$, where p is the strength of field. The spin state of the first site could be polarized by this boundary field. Due to the NN coupling and the effect of model parameter a, the polarized σ_1^z induces the anisotropic interaction $\sigma_1^z \sigma_2^z$. Thus the coupling of first bond is anisotropic. Meanwhile, the boundary field also induces the DM interaction along the z-direction, which can be read from the term $D_1^z (\boldsymbol{\sigma}_1 \times \boldsymbol{\sigma}_2)^z$, where D_1^z is the unit vector along the z-direction. The strength of DM interaction can be tuned by the strength p of boundary field.

The strength and direction of the boundary magnetic field at the other side are arbitrary. Again, due to the $su(2)$ symmetry of the bulk, we can take the rotation in the xy plane further. After that, the boundary field lies in the xz plane, which is quantified by the term $q(\xi\sigma_{2N}^{x}+\sigma_{2N}^{z})$, where q characterizes the strength and ξ characterizes the direction of the field. The field $q(\xi\sigma_{2N}^{x}+\sigma_{2N}^{z})$ is equivalent to an effective field F_{2N}^{β} along the β-direction, i.e., $q(\xi\sigma_{2N}^{x}+\sigma_{2N}^{z})\equiv F_{2N}^{\beta}$. The equivalent field F_{2N}^{β} will polarize the spin state of the $2N$-th site, thus induce the anisotropic spin-exchanging interaction $F_{2N-1}^{\beta}F_{2N}^{\beta}$ and the DM interaction $F_{2N}^{\beta}(\boldsymbol{\sigma}_{2N}\times\boldsymbol{\sigma}_{2N-1})^{\beta}$ at the boundary.

Every term in Hamiltonian (1) has clear physical meanings. As far as we know, Hamiltonian (1) includes the most typical spin–spin interactions.

3. Integrability

Now, we prove the integrability of Hamiltonian (1). We adopt the standard notations. Throughout this paper, V denotes a two-dimensional linear space. For any matrix $A\in\mathrm{End}(V)$, A_j is an embedded operator in the tensor space $V\otimes V\otimes\cdots$, which acts as A on the j-th space and as identity on the other factor spaces. For $B\in\mathrm{End}(V\otimes V)$, B_{ij} is an embedding operator of B in the tensor space, which acts as identity on the factor spaces except for the i-th and j-th ones.

The integrability of Hamiltonian (1) is related with the R-matrix and the reflection matrices $K^{\pm}(u)$. The R-matrix is

$$\begin{aligned}R_{0,j}(u) &= u+P_{0,j}=u+\frac{1}{2}(1+\boldsymbol{\sigma}_0\cdot\boldsymbol{\sigma}_j)\\ &=\begin{pmatrix}u+1 & 0 & 0 & 0\\ 0 & u & 1 & 0\\ 0 & 1 & u & 0\\ 0 & 0 & 0 & u+1\end{pmatrix},\end{aligned}\tag{3}$$

which satisfies the following relations:

$$\begin{aligned}&\text{Initial condition}\ \ R_{1,2}(0)=P_{1,2},\\ &\text{Unitarity relation}\ \ R_{1,2}(u)R_{2,1}(-u)=(1-u^2)\times\mathrm{i}d,\\ &\text{Crossing relation}\ \ R_{1,2}(u)=-\sigma_1^{y}R_{1,2}^{t_1}(-u-1)\sigma_1^{y},\\ &\text{PT- symmetry}\ \ R_{1,2}(u)=R_{2,1}(u)=R_{1,2}^{t_1t_2}(u),\\ &\text{Fusion condition}\ \ R_{1,2}(-1)=-1+P_{1,2}=-2P_{1,2}^{(-)},\end{aligned}\tag{4}$$

where $P_{1,2}$ is the permutation operator possessing the property $R_{1,2}(u)=P_{0,1}R_{0,2}(u)P_{0,1}$. The R-matrix (3) satisfies the Yang–Baxter equation

$$\begin{aligned}&R_{1,2}(u_1-u_2)R_{1,3}(u_1-u_3)R_{2,3}(u_2-u_3)\\ &=R_{2,3}(u_2-u_3)R_{1,3}(u_1-u_3)R_{1,2}(u_1-u_2).\end{aligned}\tag{5}$$

The reflection matrix $K^{-}(u)$ is

$$K^{-}(u)=\begin{pmatrix}p+u & 0\\ 0 & p-u\end{pmatrix},\tag{6}$$

where p is the boundary parameter which characterizes the strength of boundary field. The matrix $K^{-}(u)$ satisfies the reflection equation

$$\begin{aligned}&R_{1,2}(u-v)K_1^{-}(u)R_{2,1}(u+v)K_2^{-}(v)\\ &=K_2^{-}(v)R_{1,2}(u+v)K_1^{-}(u)R_{2,1}(u-v).\end{aligned}\tag{7}$$

The dual reflection matrix $K^{+}(u)$ is

$$K^{+}(u)=\begin{pmatrix}q+u+1 & \xi(u+1)\\ \xi(u+1) & q-u-1\end{pmatrix},\tag{8}$$

which satisfies the dual reflection equation

$$\begin{aligned}&R_{1,2}(-u+v)K_1^{+}(u)R_{2,1}(-u-v-2)K_2^{+}(v)\\ &=K_2^{+}(v)R_{1,2}(-u-v-2)K_1^{+}(u)R_{2,1}(-u+v),\end{aligned}\tag{9}$$

where q and ξ are the boundary parameters.

The monodromy matrix $T_0(u)$ and the reflecting one $\hat{T}_0(u)$ are

$$\begin{aligned}T_0(u) &= R_{0,2N}(u-\theta_{2N})R_{0,2N-1}(u-\theta_{2N-1})\cdots\\ &\quad\times R_{0,2}(u-\theta_2)R_{0,1}(u-\theta_1),\\ \hat{T}_0(u) &= R_{0,1}(u+\theta_1)R_{0,2}(u+\theta_2)\cdots\\ &\quad\times R_{0,2N-1}(u+\theta_{2N-1})R_{0,2N}(u+\theta_{2N}),\end{aligned}\tag{10}$$

where V_0 is the auxiliary space, $V_1\otimes V_2\otimes\ldots V_{2N}$ is the physical or quantum space, $2N$ is the number of sites, and $\{\theta_j, j=1,\ldots,2N\}$ are the inhomogeneous parameters. The monodromy matrices satisfy the Yang–Baxter relations

$$\begin{aligned}&R_{1,2}(u-v)T_1(u)T_2(v)=T_2(v)T_1(u)R_{1,2}(u-v),\\ &R_{1,2}(u-v)\hat{T}_1(u)\hat{T}_2(v)=\hat{T}_2(v)\hat{T}_1(u)R_{1,2}(u-v).\end{aligned}\tag{11}$$

The double-row monodromy matrix $U_0(u)$ is constructed as

$$U_0(u)=T_0(u)K_0^{-}(u)\hat{T}_0(u),\tag{12}$$

which satisfies the reflection equation

$$\begin{aligned}&R_{1,2}(u-v)U_1(u)R_{1,2}(u+v)U_2(v)\\ &=U_2(v)R_{1,2}(u+v)U_1(u)R_{1,2}(u-v).\end{aligned}\tag{13}$$

Taking the partial trace of double-row monodromy matrix $U_0(u)$ in the auxiliary space V_0, we obtain the transfer matrix of the system as follows:

$$t(u)=\mathrm{tr}_0\{K_0^{+}(u)U_0(u)\}.\tag{14}$$

From the crossing symmetry in Eq. (5), we find the transfer matrix $t(u)$ satisfies the crossing relation

$$t(u)=t(-u-1).\tag{15}$$

From the Yang–Baxter equation (5), reflection equation (7) and its dual one (9), one can prove that the transfer matrices with different spectral parameters commutate with each other,

$$[t(u),t(v)]=0.\tag{16}$$

This implies that the transfer matrix $t(u)$ is the generating function of all the conserved quantities. Hamiltonian (1) is constructed from the transfer matrix $t(u)$ as

$$H = c_2^{-1}\Big\{t(-a)\frac{\partial t(u)}{\partial u}\Big|_{u=a} + t(a)\frac{\partial t(u)}{\partial u}|_{u=-a}\Big\}\Big|_{\{\theta_k\}=\pm a} - c_0, \tag{17}$$

where the subscript $\{\theta_k\} = \pm a$ means $\{\theta_{2k-1} = a, \theta_{2k} = -a | k = 1,\ldots,N\}$ and

$$\begin{aligned} c_0 &= -(2N-1)(2a^2-1) - \frac{2a^4-6a^2+1}{a^2-1}, \\ c_2 &= 8(1-4a^2)^{2N-2}(p^2-a^2)(a^2-1)(a^2\xi^2+a^2-q^2). \end{aligned} \tag{18}$$

Thus the model (1) is integrable.

4. Exact solution

From the construction of Hamiltonian (1), we can see that the dual reflection matrix $K^+(u)$ has the off-diagonal elements. Thus the $U(1)$ symmetry of the system is broken. We use the off-diagonal Bethe ansatz (ODBA) to solve Hamiltonian (1).

The main idea of the ODBA is as follows. From the definition of transfer matrix $t(u)$, we know that $t(u)$ is an operator polynomial of u with the order of $4N+2$. Denote the eigenvalue of the transfer matrix $t(u)$ as $\Lambda(u)$. Then we arrive at the case that the eigenvalue $\Lambda(u)$ must be a polynomial of u with the order of $4N+2$. Our task is to determine the polynomial $\Lambda(u)$, which can be achieved by its values at arbitrary $4N+3$ points (at least) or the $4N+3$ constraints satisfied by $\Lambda(u)$ in principle. From the crossing-unitary relation (15) of the transfer matrix $t(u)$, we also know $\Lambda(u) = \Lambda(-u-1)$. Thus the number of constraints is reduced from $4N+3$ to $2N+2$. If these constraints are obtained, the eigenvalue $\Lambda(u)$ can be completely determined.

Now, we seek these constraints. The matrix $R(u)$ given by Eq. (3) degenerates into the permutation operator at the point of $u = \theta_j$. Using the properties of permutation operator, after tedious calculations, we obtain

$$\begin{aligned} t(\theta_j)t(\theta_j-1) &= \frac{\Delta_q(\theta_j)}{(1-2\theta_j)(1+2\theta_j)} \\ &= a(\theta_j)d(\theta_j-1), \quad j = 1,\ldots,2N, \end{aligned} \tag{19}$$

where $\Delta_q(\theta_j)$ is the value of quantum determinant $\Delta_q(u)$ at the point of $u = \theta_j$, the denominator $(1-2\theta_j)(1+2\theta_j)$ is the structure factor and

$$\begin{aligned} a(u) &= \frac{2u+2}{2u+1}(u+p)[(1+\xi^2)^{\frac{1}{2}}u+q] \\ &\quad\times\prod_{l=1}^{2N}(u+\theta_l+1)(u-\theta_l+1), \\ d(u) &= a(-u-1). \end{aligned} \tag{20}$$

Acting the operators product identities (19) on the eigenstate of transfer matrix $t(u)$, we obtain the $2N$ function relations

$$\Lambda(\theta_j)\Lambda(\theta_j-1) = a(\theta_j)d(\theta_j-1), \quad j = 1,\ldots,2N. \tag{21}$$

Detailed analysis also gives

$$\text{Crossing symmetry}: \Lambda(-u-1) = \Lambda(u), \tag{22}$$

$$\text{Initial condition}: \Lambda(0) = 2pq\prod_{j=1}^{2N}(1-\theta_j)(1+\theta_j) = \Lambda(-1), \tag{23}$$

$$\text{Asymptotic behavior}: \Lambda(u) = 2u^{4N+2} + \cdots, \quad u \to \pm\infty. \tag{24}$$

Then the constraints (21)–(25) give sufficient conditions to determine the eigenvalues $\Lambda(u)$, which can be parameterized as the following inhomogeneous T–Q relation:

$$\begin{aligned} \Lambda(u) &= a(u)\frac{Q(u-1)}{Q(u)} + d(u)\frac{Q(u+1)}{Q(u)} \\ &\quad + 2[1-(1+\xi^2)^{\frac{1}{2}}]u(u+1) \\ &\quad\times\frac{\prod_{l=1}^{2N}(\lambda_j+\theta_l)(\lambda_j-\theta_l)(\lambda_j+\theta_l+1)(\lambda_j-\theta_l+1)}{Q(u)}, \end{aligned} \tag{25}$$

where the function $Q(u)$ is

$$Q(u) = \prod_{j=1}^{2N}(u-\lambda_j)(u+\lambda_j+1), \tag{26}$$

and $\{\lambda_j | j = 1,\ldots,2N\}$ are $2N$ Bethe roots. Because $\Lambda(u)$ is a polynomial, the residues on right-hand side of Eq. (25) should be zero, which gives the constraints of Bethe roots:

$$\begin{aligned} &a(\lambda_j)Q(\lambda_j-1) + d(\lambda_j)Q(\lambda_j+1) \\ &= -2[1-(1+\xi^2)^{\frac{1}{2}}]\lambda_j(\lambda_j+1) \\ &\quad\times\prod_{l=1}^{2N}(\lambda_j+\theta_l)(\lambda_j-\theta_l)(\lambda_j+\theta_l+1)(\lambda_j-\theta_l+1), \\ &\quad j = 1,\ldots,2N. \end{aligned} \tag{27}$$

Solving the Bethe ansatz equations (27), we obtain the values of Bethe roots $\{\lambda_j | j = 1,\ldots,2N\}$. Substituting these values into Eq. (25), we obtain the eigenvalue $\Lambda(u)$ of the transfer matrix $t(u)$.

Now, we are ready to determine the eigenvalue of Hamiltonian (1). Substituting $\{\theta_{2k-1} = a, \theta_{2k} = -a | k = 1,\ldots,N\}$ into Eq. (25), we obtain

$$\begin{aligned} \Lambda(u)|_{\{\theta_k=\pm a\}} &= \bar{a}(u)\frac{Q(u-1)}{Q(u)} + \bar{d}(u)\frac{Q(u+1)}{Q(u)} \\ &\quad + 2[1-(1+\xi^2)^{\frac{1}{2}}]u(u+1) \\ &\quad\times\frac{(u^2-a^2)^{2N}[(u+1)^2-a^2]^{2N}}{Q(u)}, \end{aligned} \tag{28}$$

where

$$\bar{a}(u) = \frac{2u+2}{2u+1}(u+p)[(1+\xi^2)^{\frac{1}{2}}u+q]\,[(u+1)^2-a^2]^{2N},$$

$$\bar{d}(u) = \bar{a}(-u-1). \tag{29}$$

The Bethe ansatz equations (27) degenerate into

$$\begin{aligned}
&\bar{a}(\lambda_j)Q(\lambda_j-1)+\bar{d}(\lambda_j)Q(\lambda_j+1)\\
&= -2[1-(1+\xi^2)^{\frac{1}{2}}]\lambda_j(\lambda_j+1)\\
&\quad\times(\lambda_j^2-a^2)^{2N}[(\lambda_j+1)^2-a^2]^{2N}, \quad j=1,\ldots,2N.
\end{aligned} \tag{30}$$

According to Eqs. (17) and (28), the energy spectrum of Hamiltonian (1) is

$$\begin{aligned}
E &= (1-4a^2)\left\{\frac{p}{p^2-a^2}+\frac{q(1+\xi^2)^{-\frac{1}{2}}}{q^2(1+\xi^2)^{-1}-a^2}\right\}\\
&\quad+\frac{2a^2+1}{a^2-1}+4N(1-2a^2)\\
&\quad-c_0-\sum_{j=1}^{2N}(1-4a^2)\left[\frac{2a+1}{(a-\lambda_j)(a+\lambda_j+1)}\right.\\
&\quad\left.+\frac{2a-1}{(a+\lambda_j)(\lambda_j-a+1)}\right].
\end{aligned} \tag{31}$$

We check the above results numerically for some small site numbers. We first solve the Bethe ansatz equations (30) with randomly chosen model parameters and obtain the values of Bethe roots. Substituting the values of Bethe roots into Eq. (31), we obtain the eigenvalues of Hamiltonian (1). The results are listed in Table 1. Next, we numerically diagonalize Hamiltonian (1) with same model parameters. We find that the eigenvalues obtained by solving the Bethe ansatz equations are exactly the same as those obtained by the exact diagonalization. Meanwhile, the expression (31) gives the complete spectrum of the system.

Table 1. Numerical solutions of the Bethe ansatz equations (30) with $2N=4$, $a=0.7\mathrm{i}$, $p=-0.6$, $q=-0.3$ and $\xi=1.2$. Here n indicates the number of energy levels and E_n is the corresponding energy. The energy E_n obtained from the Bethe ansatz equations is exactly the same as that calculated from the exact diagonalization of Hamiltonian (1).

λ_1	λ_2	λ_3	λ_4	E_n	n
$-0.5000+1.9131\mathrm{i}$	$-0.5000+0.6640\mathrm{i}$	$3.3975-0.6856\mathrm{i}$	$3.3975+0.6856\mathrm{i}$	-10.9019	1
$-0.5000+0.8383\mathrm{i}$	$0.0965-0.0000\mathrm{i}$	$3.4850-1.0458\mathrm{i}$	$3.4850+1.0458\mathrm{i}$	-10.4883	2
$-4.5421-1.2287\mathrm{i}$	$-0.5000+0.5582\mathrm{i}$	$1.1253-0.0000\mathrm{i}$	$3.5421-1.2287\mathrm{i}$	-7.0078	3
$-0.5000-0.9427\mathrm{i}$	$0.8470+0.0000\mathrm{i}$	$3.5183-1.1407\mathrm{i}$	$3.5183+1.1407\mathrm{i}$	-4.9290	4
$-0.9767-1.1079\mathrm{i}$	$-0.9767+1.1079\mathrm{i}$	$3.4335-0.8942\mathrm{i}$	$3.4335+0.8942\mathrm{i}$	-3.0247	5
$-1.1899-0.2527\mathrm{i}$	$-0.5000-1.3600\mathrm{i}$	$0.1899-0.2527\mathrm{i}$	$4.0044-0.0000\mathrm{i}$	-2.3877	6
$-5.0604+0.0000\mathrm{i}$	$-1.1235+1.2725\mathrm{i}$	$-1.0840+0.0000\mathrm{i}$	$0.1235+1.2725\mathrm{i}$	-1.9888	7
$-0.5000-2.1389\mathrm{i}$	$0.1545+0.0000\mathrm{i}$	$3.4323-0.7339\mathrm{i}$	$3.4323+0.7339\mathrm{i}$	0.7990	8
$-2.5042+1.9596\mathrm{i}$	$-0.5000+2.6223\mathrm{i}$	$1.5042+1.9596\mathrm{i}$	$4.2110-0.0000\mathrm{i}$	3.2608	9
$-1.2828+1.6900\mathrm{i}$	$0.2828+1.6900\mathrm{i}$	$0.9279-0.0000\mathrm{i}$	$4.0797+0.0000\mathrm{i}$	3.3143	10
$-2.5996+0.0000\mathrm{i}$	$0.1820+0.0000\mathrm{i}$	$3.5835-1.3725\mathrm{i}$	$3.5835+1.3725\mathrm{i}$	3.5836	11
$-1.3086+0.0772\mathrm{i}$	$0.3086+0.0772\mathrm{i}$	$3.5144-1.1593\mathrm{i}$	$3.5144+1.1593\mathrm{i}$	3.6655	12
$-1.6610+0.0000\mathrm{i}$	$-0.5000-2.3224\mathrm{i}$	$3.4784-0.8026\mathrm{i}$	$3.4784+0.8026\mathrm{i}$	4.2297	13
$-1.4693-0.4209\mathrm{i}$	$0.0845+0.0000\mathrm{i}$	$0.4693-0.4209\mathrm{i}$	$3.8370-0.0000\mathrm{i}$	5.9634	14
$0.6103+0.0000\mathrm{i}$	$1.9297+0.0000\mathrm{i}$	$3.6172-1.4894\mathrm{i}$	$3.6172+1.4894\mathrm{i}$	6.1156	15
$-1.4196-0.7400\mathrm{i}$	$-1.4196+0.7400\mathrm{i}$	$0.0989-0.3472\mathrm{i}$	$0.0989+0.3472\mathrm{i}$	9.7964	16

5. Ground state energy

Now, we study the ground state energy of the system (1). Following the scheme suggested in Refs. [32,33], we find that the contribution of the third term in the inhomogeneous T–Q relation (28) supplies the $o(1/(2N))$ correction which can be neglected in the thermodynamic limit $2N\to\infty$. Thus, we introduce the following homogeneous T–Q relation:

$$\Lambda_h(u) = \bar{a}(u)\frac{Q_h(u-1)}{Q_h(u)}+\bar{d}(u)\frac{Q_h(u+1)}{Q_h(u)}, \tag{32}$$

where the function $Q_h(u)$ is defined as

$$Q_h(u) = \prod_{j=1}^{M}(u-\lambda_j)(u+\lambda_j+1), \quad M=1,\ldots,N, \tag{33}$$

and the corresponding Bethe roots $\{\lambda_j\}$ satisfy the reduced Bethe ansatz equations

$$\frac{\bar{a}(\lambda_j)}{\bar{d}(\lambda_j)} = -\frac{Q_h(\lambda_j+1)}{Q_h(\lambda-1)}, \quad j=1,\ldots,M. \tag{34}$$

We shall note that all the boundary parameters p, q and ξ are included in the homogeneous T–Q relation (32), and Eq. (32) is not the T–Q relation for the system with diagonal boundary reflections. For convenience, we put $u_j=\mathrm{i}(\lambda_j+1/2)$, $\bar{a}=-\mathrm{i}a$, $\bar{p}=p-\frac{1}{2}$ and $\bar{q}=q(1+\xi^2)^{-\frac{1}{2}}-\frac{1}{2}$. The reduced BAEs (34) can be rewritten as

$$\begin{aligned}
&\left[\frac{(u_j+\bar{a}-\mathrm{i}/2)(u_j-\bar{a}-\mathrm{i}/2)}{(u_j+\bar{a}+\mathrm{i}/2)(u_j-\bar{a}+\mathrm{i}/2)}\right]^{2N}\\
&\times\frac{(u_j-\mathrm{i}\bar{p})(u_j-\mathrm{i}\bar{q})}{(u_j+\mathrm{i}\bar{p})(u_j+\mathrm{i}\bar{q})}\\
&=\prod_{l\neq j}^{M}\frac{(u_j-u_l-\mathrm{i})(u_j+u_l-\mathrm{i})}{(u_j-u_l+\mathrm{i})(u_j+u_l+\mathrm{i})},\\
&j=1,\ldots,M.
\end{aligned} \tag{35}$$

Considering the construction (17) of the Hamiltonian and using the homogeneous T–Q relation (32), we obtain

$$E_h = c_2^{-1}\left\{\Lambda_h(-a)\frac{\partial\Lambda_h(u)}{\partial u}\right|_{u=a}$$

$$
\begin{aligned}
&+\Lambda_h(a)\frac{\partial\Lambda_h(u)}{\partial u}\Big|_{u=-a}\Big\}\Big|_{\{\theta_k=\pm a\}}-c_0\\
=\;&(1-4a^2)\Big\{\frac{p}{p^2-a^2}+\frac{q(1+\xi^2)^{-\frac{1}{2}}}{q^2(1+\xi^2)^{-1}-a^2}\Big\}\\
&+\frac{2a^2+1}{a^2-1}+4N(1-2a^2)\\
&-c_0-\sum_{j=1}^{M}(1-4a^2)\\
&\times\Big[\frac{1}{(u_j+a)^2+1/4}+\frac{1}{(u_j-a)^2+1/4}\Big]. \qquad (36)
\end{aligned}
$$

For the finite system size, E_h is the approximation solution of the system. With the increasing system size, the accuracy becomes higher. In the thermodynamic limit, E_h is infinitely tends to the actual value.

Next, we compute the values of E_h. For simplicity, we consider the case that $\bar{p}\geq 0$ and $\bar{q}\geq 0$. In the ground state, all the Bethe roots should take real values. Taking the logarithm of Eq. (35), we arrive at

$$
\begin{aligned}
&\theta_{2\bar{p}}(u_j)+\theta_{2\bar{q}}(u_j)+2N[\theta_1(u_j+\bar{a})+\theta_1(u_j-\bar{a})]\\
=\;&2\pi I_j-\theta_1(u_j)\\
&+\sum_{k=1}^{M}[\theta_2(u_j-u_k)+\theta_2(u_j+u_k)],\quad j=1,\ldots,M, \qquad (37)
\end{aligned}
$$

where the quantum number $\{I_j\}$ are certain integers or half odd integers, and the function $\theta_n(x)$ is defined as

$$
\theta_n(x)=2\arctan\left(\frac{2x}{n}\right). \qquad (38)
$$

In the thermodynamic limit where M also tends to infinity but M/N keeps finite, u_j becomes a continuous variable u. Taking the derivative of Eq. (37) with respect to u and after some calculations, we have

$$
\begin{aligned}
\rho(u)\;=\;&\frac{1}{2}[a_1(u+\bar{a})+a_1(u-\bar{a})]\\
&+\frac{1}{4N}[a_{2\bar{p}}(u)+a_{2\bar{q}}(u)+a_1(u)]\\
&-\frac{1}{4N}[\delta(u)+\delta(u-u^h)+\delta(u+u^h)]\\
&-\int_{-\infty}^{+\infty}a_2(u-v)\rho(v)\,\mathrm{d}v, \qquad (39)
\end{aligned}
$$

where $\rho(u)$ is the density of Bethe roots in the real axis, $a_n(x)$ is given by

$$
a_n(x)=\frac{1}{2\pi}\frac{n}{x^2+n^2/4}, \qquad (40)
$$

and $\delta(u\pm u^h)$ are the boundary holes with the positions $\pm u^h$. In the thermodynamic limit, the positions of holes would tend to infinity, and the holes contribute nothing to the energy. These boundary holes correspond to the Majorana modes at the two boundaries.[34]

We solve Eq. (39) using the Fourier transformation

$$
\begin{aligned}
\tilde{f}(\omega)\;&=\;\int_{-\infty}^{\infty}f(u)\,\mathrm{e}^{\mathrm{i}\omega u}\,\mathrm{d}u, \qquad (41)\\
f(u)\;&=\;\frac{1}{2\pi}\int_{-\infty}^{\infty}\tilde{f}(\omega)\,\mathrm{e}^{-\mathrm{i}\omega u}\,\mathrm{d}\omega. \qquad (42)
\end{aligned}
$$

The Fourier transformation of $a_n(u)$ is

$$
\tilde{a}_n(w)=\mathrm{e}^{\frac{-n|\omega|}{2}}. \qquad (43)
$$

Taking the Fourier transformation of Eq. (39), we have

$$
\begin{aligned}
\tilde{\rho}(\omega)\;=\;&\frac{1}{2}[\mathrm{e}^{\mathrm{i}\omega\bar{a}}+\mathrm{e}^{-\mathrm{i}\omega\bar{a}}]\tilde{a}_1(\omega)-\tilde{a}_2(\omega)\tilde{\rho}(\omega)\\
&+\frac{1}{4N}[\tilde{a}_{2\bar{p}}(\omega)+\tilde{a}_{2\bar{q}}(\omega)+\tilde{a}_1(\omega)\\
&-1-\mathrm{e}^{\mathrm{i}\omega u^h}-\mathrm{e}^{\mathrm{i}\omega u^h}]. \qquad (44)
\end{aligned}
$$

Substituting Eq. (43) into Eq. (44), we obtain the solution of $\tilde{\rho}(\omega)$ as

$$
\begin{aligned}
\tilde{\rho}(\omega)=\;&\frac{\cos(\omega\bar{a})}{2\cosh(\omega/2)}\\
&+\frac{1}{4N}\frac{\mathrm{e}^{-\bar{p}|\omega|}+\mathrm{e}^{-\bar{q}|\omega|}+\mathrm{e}^{-|\omega|/2}-1-2\cos(\omega u^h)}{1+\mathrm{e}^{|\omega|}}. \qquad (45)
\end{aligned}
$$

According to Eqs. (36) and (45), we obtain the ground state energy of the system as follows:

$$
\begin{aligned}
E_g\;=\;&(1-4a^2)\Big\{\frac{p}{p^2-a^2}+\frac{q(1+\xi^2)^{-\frac{1}{2}}}{q^2(1+\xi^2)^{-1}-a^2}\Big\}+\frac{2a^2+1}{a^2-1}+4N(1-2a^2)\\
&-c_0-2N(1-4a^2)\int_{-\infty}^{\infty}\mathrm{e}^{-|\omega|/2}\frac{\cosh^2(\omega a)}{\cosh(\omega/2)}\,\mathrm{d}\omega\\
&-\frac{(1-4a^2)}{2}\int_{-\infty}^{\infty}\cosh(\omega a)\frac{\mathrm{e}^{-p|\omega|}+\mathrm{e}^{-q|\omega|/\sqrt{(1+\xi^2)}}+\mathrm{e}^{-|\omega|}-\mathrm{e}^{-|\omega|/2}}{\mathrm{e}^{-|\omega|/2}\cosh(\omega/2)}\,\mathrm{d}\omega. \qquad (46)
\end{aligned}
$$

In order to show the correctness of Eq. (46), we calculate the ground state energy of the system (1) using the density matrix renomalization group (DMRG) method and compare the results with those obtained from Eq. (46), as shown in Fig. 1. We can see that the energy difference ΔE tends to zero with the increasing system size. The data satisfy the scaling law $\Delta E=\gamma(2N)^m$, where $m<0$. Thus in the thermodynamic limit, the expression (46) gives the actual value of the ground state energy.

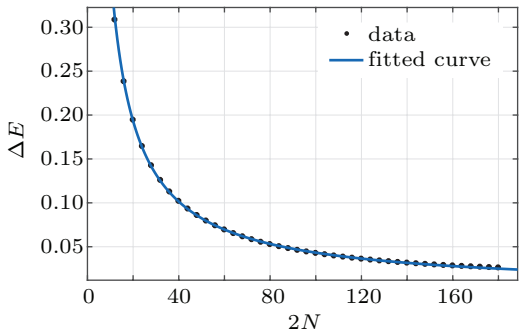


Fig. 1. The energy difference $\Delta E = E_{\rm D} - E_{\rm g}$ with the different system sizes, where $E_{\rm D}$ is the ground state energy calculated by using the DMRG method and $E_{\rm g}$ is the ground state energy calculated by Eq. (46). The model parameters are taken as $a = 0.66{\rm i}$, $p = 1.6$, $q = 1.3$ and $\xi = 1.2$. The ΔE decreases with the increasing system size $2N$ and the data can be fitted as $\Delta E = 3.124(2N)^{-0.9292}$. When the system size tends to infinity, the energy difference ΔE would be zero.

6. Conclusion

In summary, we have proposed a new integrable quantum spin chain which includes the NN, NNN, chiral three-spin couplings, DM interactions and unparallel boundary magnetic fields. By means of the off-diagonal Bethe ansatz, we obtain the exact solution of the system. The inhomogeneous T–Q relation and Bethe ansatz equations are given explicitly. We further calculate the ground state energy in the regime of $\bar{p} \geq 0$ and $\bar{q} \geq 0$.

The method given in this paper can be used to construct other new integrable models with some interesting interactions. For example, if we start from the trigonometric or elliptic R-matrix,[2] we can study the anisotropic version of the integrable Hamiltonian (1). Meanwhile, if we put the alternate inhomogeneous parameters into the R-matrix[35] of the Hubbard model, we can construct an exactly solved strongly correlated electronic model which contains many possible physical processes. For example, besides the electrons hopping and on-site interaction, other terms such as the electron-pairs hopping, extended nearest-neighbor interactions $n_j n_{j+1}$, and spin flipped behavior after reflecting. Due to the competitions among these couplings, some nontrivial phenomena such as the finite critical on-site interaction $U_{\rm c}$ of the metal–insulator transition, new quantum states, novel charge and spin excitations may appear.

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