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Exact solution of an integrable anisotropic $J_1 - J_2$ spin chain model

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Abstract

An integrable anisotropic Heisenberg spin chain with nearest-neighbour couplings, next-nearest-neighbour couplings and scalar chirality terms is constructed. After proving the integrability, we obtain the exact solution of the system. The ground state and the elementary excitations are also studied. It is shown that the spinon excitation of the present model possesses a novel triple arched structure. The elementary excitation is gapless if the anisotropic parameter η is real while the elementary excitation has an enhanced gap by the next-nearest-neighbour and chiral three-spin interactions if the anisotropic parameter η is imaginary. The method of this paper provides a general way to construct integrable models with next-nearest-neighbour interactions.

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

(Some figures may appear in colour only in the online journal)

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1. Introduction

It is well known that the Heisenberg model has played an important role to account for magnetism in condensed matters. An interesting fact is that this model in one-dimension is exactly solvable [1]. Based on Bethe's exact solution, the ground state energy [2], the low-lying excitation spectrum [3] and the magnetization at zero temperature [4] had been studied extensively. This exact solution provided a benchmark to understand a variety of physical phenomena in low-dimensions such as the Luttinger liquid behavior and the fractional excitations. In addition, this model also becomes a typical model in developing new theoretical methods to approach general quantum integrable systems [5–8].

Besides the Heisenberg model with nearest-neighbor (NN) exchanges, its generalization with next-nearest-neighbor (NNN) interactions, known as the $J_1 - J_2$ model, also attracted a lot of attentions [9–15]. The $J_1 - J_2$ model is interesting because there exists a topological phase transition at the point of $J_2/J_1 = 0.241$ [16, 17]. At the Majumdar–Ghosh point, $J_2/J_1 = 0.5$, the model Hamiltonian degenerates into a projector operator and the ground state can be obtained exactly [18]. The ground state is two-fold degenerated and can be expressed by the direct product of spin singlets, supposed the number of site of the system is even.

Another interesting development is that Popkov and Zvyagin proposed an integrable two-chain model, which can be mapped into a spin chain with NNN interaction and spin chirality term [19–22]. Frahm and Rödenbeck constructed an integrable model of two coupled Heisenberg chains by taking the derivative of the logarithm of product of two transfer matrices with different spectral parameters [23]. Using the same idea, Frahm and Seel proposed staggered six-vertex model [24], and Ikhlef, Jacobsen and Saleur constructed the Z_2 staggered vertex model [25, 26]. Arnaudon, Poghossian, Sedrakyan and Sorba constructed a staggered model with staggered R-matrix and studied the integrable boundary terms [27]. The extra scalar chirality terms are introduced in this kind of models for ensuring the integrability. Frahm and Rödenbeck studied the properties of the chiral spin liquid state in the system [28]. Wen, Wilczek and Zee [29] and Baskaran [30] proposed that the expectation value of the spin chirality operator can be used as the order parameter for chiral spin liquids [31]. Tavares and Ribeiro studied the thermodynamic properties of this kind of models by using the quantum transfer matrix method [32, 33]. Recently, the models with chirality terms have attracted renewed interest in the context of quantum spin liquids [34, 35].

In this paper, we propose a systemic method to construct integrable models with the NNN and the scalar chirality terms interactions. We use the anisotropic XXZ quantum spin chain as an example to show the validity of the method. The Hamiltonian of the integrable anisotropic $J_1 - J_2$ spin chain is

$$\begin{aligned} H = \sum_{j=1}^{2N} \Big\{ & \cos(2a)(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y) + \cos\eta\,\sigma_j^z\sigma_{j+1}^z \\ & - \frac{\sin^2(2a)\cos\eta}{2\sin^2\eta}\vec{\sigma}_j\cdot\vec{\sigma}_{j+2} + \frac{(-1)^j i\sin(2a)}{2\sin\eta}\big\{\cos\eta\,\vec{\sigma}_{j+1}\cdot(\vec{\sigma}_j \\ & \times\vec{\sigma}_{j+2}) + [\cos(2a)-\cos\eta]\sigma_{j+1}^z(\sigma_j^x\sigma_{j+2}^y - \sigma_j^y\sigma_{j+2}^x)\big\}\Big\}, \end{aligned} \tag{1.1}$$

where $\vec{\sigma}_j \equiv (\sigma_j^x, \sigma_j^y, \sigma_j^z)$ are the Pauli matrices at site j, a and η are the generic constants describing the coupling strengths, and the periodic boundary condition

$$\vec{\sigma}_{2N+j} = \vec{\sigma}_j, \quad j = 1, \cdots, 2N, \tag{1.2}$$

is imposed. The first two terms describe an anisotropic NN interaction, the third term is an isotropic NNN interaction (i.e. the J_2 term) and the last one corresponds to an anisotropic chiral three-spin interaction. We shall show that the anisotropic $J_1 - J_2$ spin chain with the Hamiltonian (1.1) is integrable and can be exactly solved by the Bethe ansatz.

Some remarks are in order. (i) The hermitian of the Hamiltonian (1.1) requires that a must be real if η is imaginary (gapped regime), and a must be imaginary if η is real (gapless regime). (ii) The NN interactions are anisotropic while the NNN interactions are isotropic. (iii) The anisotropic scalar chirality terms are added to ensure the integrability of the system. (iv) The coupling strengths in the NNN terms and those in the scalar chirality terms are not independent but related by the parameters a and η. (v) The model degenerates into the conventional XXZ spin chain at the points of $a = n\pi$ with integer n. (vi) After parameterizing $a = \bar{a}\,\epsilon$, $\eta = \epsilon$ and then taking the limit of $\epsilon \to 0$, our Hamiltonian (1.1) becomes

$$\begin{aligned} H = \sum_{j=1}^{2N} \{ & \vec{\sigma}_j \cdot \vec{\sigma}_{j+1} - 2\bar{a}^2\, \vec{\sigma}_j \cdot \vec{\sigma}_{j+2} \\ & + (-1)^j i\bar{a}\ \vec{\sigma}_{j+1} \cdot (\vec{\sigma}_j \times \vec{\sigma}_{j+2}) \} . \end{aligned} \tag{1.3}$$

The resulting Hamiltonian describe an integrable isotropic $J_1 - J_2$ spin chain model, which was studied previously by Frahm *et al* [28, 36].

The paper is organized as follows. The model is constructed and the integrability is proved in section 2. The exact energy spectrum and the Bethe Ansatz equations are derived in section 3. The ground state energy and spinon elementary excitation for real η are given in section 4 and the corresponding results with imaginary η are given in section 5. Section 6 is attributed to the concluding remarks. Detailed calculation and the results for the non-hermitian case are given in appendices A and B.

2. Model and integrability

Throughout, V denotes a two-dimensional linear space and let $\{|m\rangle, m = 0, 1\}$ be an orthogonal basis of it. We shall adopt the standard notations: for any matrix $A \in \mathrm{End}(V)$, A_j is an embedding 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.

Let us introduce the R-matrix $R_{0,j}(u) \in \mathrm{End}(V_0 \otimes V_j)$

$$\begin{aligned} R_{0,j}(u) = & \frac{1}{2}\left[\frac{\sin(u+\eta)}{\sin\eta}(1+\sigma_0^z\sigma_j^z) + \frac{\sin u}{\sin\eta}(1-\sigma_0^z\sigma_j^z)\right] \\ & + \frac{1}{2}(\sigma_0^x\sigma_j^x + \sigma_0^y\sigma_j^y) \\ = & \frac{1}{\sin\eta}\begin{pmatrix} \sin(u+\eta) & 0 & 0 & 0 \\ 0 & \sin u & \sin\eta & 0 \\ 0 & \sin\eta & \sin u & 0 \\ 0 & 0 & 0 & \sin(u+\eta) \end{pmatrix}, \end{aligned} \tag{2.1}$$

where u is the spectral parameter. The R-matrix (2.1) satisfies the following relations

$$\begin{aligned}
&\text{Initial condition}: \ R_{0,j}(0) = P_{0,j},\\
&\text{Unitary relation}: \ R_{0,j}(u)R_{j,0}(-u) = \phi(u)\times \mathrm{id},\\
&\text{Crossing relation}: \ R_{0,j}(u) = -\sigma_0^y R_{0,j}^{t_0}(-u-\eta)\sigma_0^y,\\
&\text{PT-symmetry}: \ R_{0,j}(u) = R_{j,0}(u) = R_{0,j}^{t_0\,t_j}(u),
\end{aligned} \tag{2.2}$$

where $\phi(u) = -\sin(u+\eta)\sin(u-\eta)/\sin^2\eta$, t_0 (or t_j) denotes the transposition in the space V_0 (or V_j) and $P_{0,j}$ is the permutation operator possessing the property

$$R_{j,k}(u) = P_{0,j}R_{0,k}(u)P_{0,j}. \tag{2.3}$$

The R-matrix satisfies the Yang–Baxter equation (YBE)

$$\begin{aligned}
&R_{1,2}(u_1-u_2)R_{1,3}(u_1-u_3)R_{2,3}(u_2-u_3)\\
&\quad = R_{2,3}(u_2-u_3)R_{1,3}(u_1-u_3)R_{1,2}(u_1-u_2).
\end{aligned} \tag{2.4}$$

We define the monodromy matrices [8, 37] as

$$\begin{aligned}
T_0(u) &= R_{0,1}(u+a)R_{0,2}(u-a)\cdots R_{0,2N-1}(u+a)\\
&\qquad \times R_{0,2N}(u-a),\\
\hat{T}_0(u) &= R_{0,2N}(u+a)R_{0,2N-1}(u-a)\cdots R_{0,2}(u+a)\\
&\qquad \times R_{0,1}(u-a),
\end{aligned} \tag{2.5}$$

where V_0 is the auxiliary space, $V_1\otimes V_2\otimes\cdots\otimes V_{2N}$ is the physical or quantum space, $2N$ is the number of sites and a is the inhomogeneous parameter. From the YBE (2.4), one can prove that the monodromy matrix $T(u)$ satisfies the Yang–Baxter relation

$$R_{1,2}(u-v)T_1(u)T_2(v) = T_2(v)T_1(u)R_{1,2}(u-v). \tag{2.6}$$

The transfer matrices are the trace of monodromy matrices in the auxiliary space

$$t(u) = tr_0 T_0(u), \quad \hat{t}(u) = tr_0\hat{T}_0(u). \tag{2.7}$$

Using the crossing symmetry in equation (2.2), we obtain the relations between transfer matrices $t(u)$ and $\hat{t}(u)$

$$t(u) = \hat{t}(-u-\eta), \quad \hat{t}(u) = t(-u-\eta). \tag{2.8}$$

From the Yang–Baxter relation (2.6) and equation (2.8), one can prove that the transfer matrices $t(u)$ [or $\hat{t}(u)$] with different spectral parameters commute with each other. Meanwhile, the transfer matrices $t(u)$ and $\hat{t}(u)$ also commute with each other

$$[t(u), t(v)] = [\hat{t}(u), \hat{t}(v)] = [t(u), \hat{t}(u)] = 0. \tag{2.9}$$

Therefore, both $t(u)$ and $\hat{t}(u)$ serve as the generating functions of all the conserved quantities of the system. We note that the transfer matrices $t(u)$ and $\hat{t}(u)$ can be diagonalized simultaneously.

The model Hamiltonian (1.1) can be constructed as (for details, see appendix A)

$$\begin{aligned}
H = &-\frac{N\cos\eta[\cos^2(2a)-\cos(2\eta)]}{\sin^2\eta} + \phi^{1-N}(2a)\sin\eta\\
&\times\left\{\hat{t}(-a)\frac{\partial\, t(u)}{\partial u}\Big|_{u=a} + \hat{t}(a)\frac{\partial\, t(u)}{\partial u}\Big|_{u=-a}\right\}.
\end{aligned} \tag{2.10}$$

From the construction (2.10) and the commutation relation (2.9) of generating functions $t(u)$ and $\hat{t}(u)$, we conclude that the quantum spin chain (1.1) with the periodic boundary condition is integrable.

We note that if $2a = \eta$, the transfer matrix $t(a)$ is not a full rank matrix and does not have the inverse matrix. Thus we use two commutative transfer matrices $t(u)$ and $\hat{t}(u)$ to construct the Hamiltonian.

3. Exact solution

Based on the integrability discussed in the previous section, the Hamiltonian (1.1) can be solved exactly via the algebraic Bethe Ansatz [6]. The matrix form of monodromy matrix $T_0(u)$ in the auxiliary space is

$$T_0(u) = \begin{pmatrix} A(u) & B(u) \\ C(u) & D(u) \end{pmatrix} \tag{3.1}$$

where $A(u)$, $B(u)$, $C(u)$ and $D(u)$ are the operators acting in the quantum space. We denote the all spins aligning up state as the vacuum state $|0\rangle$

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_1 \otimes \cdots \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}_{2N}. \tag{3.2}$$

The matrix elements of the monodromy matrix $T_0(u)$ acting on the vacuum state gives

$$\begin{aligned} &A(u)|0\rangle = a(u)|0\rangle, \quad B(u)|0\rangle \neq 0, \\ &C(u)|0\rangle = 0, \quad D(u)|0\rangle = d(u)|0\rangle, \end{aligned} \tag{3.3}$$

where

$$\begin{aligned} a(u) &= \frac{\sin^N(u+a+\eta)\sin^N(u-a+\eta)}{\sin^{2N}\eta}, \\ d(u) &= \frac{\sin^N(u+a)\sin^N(u-a)}{\sin^{2N}\eta}. \end{aligned}$$

From equation (3.3), we know that the operator $B(u)$ can be regarded as the creation operator of all the eigenstates of the system. Assume the eigenstates take the form

$$|\lambda_1, \cdots, \lambda_M\rangle = \prod_{j=1}^{M} B(\lambda_j)|0\rangle, \tag{3.4}$$

where M is the number of flipped spins and $\{\lambda_j\}$ are the Bethe roots. From the Yang–Baxter relation (2.6), we obtain the commutative relations among the elements of monodromy matrix as

$$\begin{aligned} &[A(u), A(v)] = [B(u), B(v)] = [C(u), C(v)] = [D(u), D(v)] = 0, \\ &A(u)B(v) = \frac{\sin(u-v-\eta)}{\sin(u-v)}B(v)A(u) + \frac{\sin\eta}{\sin(u-v)}B(u)A(v), \\ &D(u)B(v) = \frac{\sin(u-v+\eta)}{\sin(u-v)}B(v)D(u) - \frac{\sin\eta}{\sin(u-v)}B(u)D(v), \\ &[B(u), C(v)] = \frac{\sin\eta}{\sin(u-v)}[D(v)A(u) - D(u)A(v)]. \end{aligned} \tag{3.5}$$

From the definition (2.7), the transfer matrix $t(u)$ is

$$t(u) = A(u) + D(u). \tag{3.6}$$

Acting the transfer matrix $t(u)$ on the Bethe state (3.4) and with the help of the commutation relations (3.5), we have

$$\begin{aligned} t(u)|\lambda_1, \cdots, \lambda_M\rangle = \Lambda(u)|\lambda_1, \cdots, \lambda_M\rangle \\ + \sum_{j=1}^{M} \Lambda_j(u) B(\lambda_1) \cdots, B(\lambda_{j-1}) B(u) B(\lambda_{j+1}) \cdots \\ \times B(\lambda_M)|0\rangle, \end{aligned} \tag{3.7}$$

where

$$\Lambda(u) = a(u) \prod_{j=1}^{M} \frac{\sin(u - \lambda_j - \eta)}{\sin(u - \lambda_j)} + d(u) \prod_{j=1}^{M} \frac{\sin(u - \lambda_j + \eta)}{\sin(u - \lambda_j)}, \tag{3.8}$$

$$\begin{aligned} \Lambda_j(u) = \frac{\sin\eta}{\sin(u - \lambda_j)} \left\{ a(\lambda_j) \prod_{l \neq j}^{M} \frac{\sin(\lambda_j - \lambda_l - \eta)}{\sin(\lambda_j - \lambda_l)} - d(\lambda_j) \right. \\ \left. \times \prod_{l \neq j}^{M} \frac{\sin(\lambda_j - \lambda_l + \eta)}{\sin(\lambda_j - \lambda_l)} \right\}. \end{aligned}$$

The first term in equation (3.7) corresponds to the eigenvalue term, while the last terms in equation (3.7) are the unwanted ones. The state (3.4) becomes an eigenstate (or the Bethe state) of the transfer matrix provided that the parameters $\{\lambda_j | j = 1, \cdots, M\}$ satisfy the Bethe Ansatz equations (BAEs)

$$\begin{aligned} \left[\frac{\sin(\lambda_j + a + \eta) \sin(\lambda_j - a + \eta)}{\sin(\lambda_j + a) \sin(\lambda_j - a)} \right]^N = \prod_{l \neq j}^{M} \frac{\sin(\lambda_j - \lambda_l + \eta)}{\sin(\lambda_j - \lambda_l - \eta)}, \\ j = 1, \cdots, M. \end{aligned} \tag{3.9}$$

For convenience, we put $\lambda_j = iu_j/2 - \eta/2$ and $a = ib$ for real η and $\lambda_j = u_j/2 - \eta/2$ for imaginary $\eta = i\gamma$. The BAEs become

$$\begin{aligned} \left[\frac{\sinh \frac{1}{2}(u_j - 2b - i\eta) \sinh \frac{1}{2}(u_j + 2b - i\eta)}{\sinh \frac{1}{2}(u_j - 2b + i\eta) \sinh \frac{1}{2}(u_j + 2b + i\eta)} \right]^N \\ = \prod_{l \neq j}^{M} \frac{\sinh \frac{1}{2}(u_j - u_l - 2\eta i)}{\sinh \frac{1}{2}(u_j - u_l + 2\eta i)}, \quad j = 1, \cdots, M \end{aligned} \tag{3.10}$$

for real η. The period of Bethe roots is $2\pi i$, thus the real part of Bethe roots locate in the interval $(-\infty, \infty)$, and

$$\begin{aligned} \left[\frac{\sin \frac{1}{2}(u_j - 2a - i\gamma) \sin \frac{1}{2}(u_j + 2a - i\gamma)}{\sin \frac{1}{2}(u_j - 2a + i\gamma) \sin \frac{1}{2}(u_j + 2a + i\gamma)} \right]^N \\ = \prod_{l \neq j}^{M} \frac{\sin \frac{1}{2}(u_j - u_l - 2\gamma i)}{\sin \frac{1}{2}(u_j - u_l + 2\gamma i)}, \quad j = 1, \cdots, M \end{aligned} \tag{3.11}$$

for imaginary $\eta = i\gamma$. The period of Bethe roots is 2π, thus we fix the real part of Bethe roots in the interval $[-\pi, \pi)$. From equations (2.8), (2.10) and (3.8) we obtain the eigenvalue of the Hamiltonian (1.1) in terms of the Bethe roots as

$$\begin{aligned} E = & \frac{N\cos\eta[\cosh^2(2b) - \cos(2\eta)]}{\sin^2\eta} - [\cosh(4b) - \cos(2\eta)] \\ & \times \sum_{j=1}^{M} \left\{ \frac{1}{\cosh(u_j + 2b) - \cos\eta} + \frac{1}{\cosh(u_j - 2b) - \cos\eta} \right\}, \end{aligned} \tag{3.12}$$

where η is real and $\{u_j\}$ should satisfy the BAEs (3.10), or

$$\begin{aligned} E = & \frac{N\cosh\gamma[\cosh(2\gamma) - \cos^2(2a)]}{\sinh^2\gamma} - [\cosh(2\gamma) - \cos(4a)] \\ & \times \sum_{j=1}^{M} \left\{ \frac{1}{\cosh\gamma - \cos(u_j + 2a)} + \frac{1}{\cosh\gamma - \cos(u_j - 2a)} \right\}, \end{aligned} \tag{3.13}$$

where $\eta = i\gamma$ is imaginary and $\{u_j\}$ should satisfy the BAEs (3.11).

Next, we check above results numerically. Numerical solutions of the BAEs and exact diagonalization of the Hamiltonian (1.1) are performed for the case of $2N = 4$ and randomly choosing of model parameters. The results are listed in table 1 for real η and table 2 for imaginary η. The missing lines mean there is no Bethe roots. The number of Bethe roots is equal to the number of flipped spins M. We note that the eigenvalues obtained by solving the BAEs are exactly the same as those obtained by the exact diagonalization of the Hamiltonian (1.1). The energies of the system are degenerated and there are only eight separated energy level. Therefore, the expression (3.12) or (3.13) gives the complete spectrum of the system.

4. Ground state and elementary excitations for real η

In this section we study the ground state and elementary excitations of the system. First, we consider the real η case. Taking the logarithm of BAEs (3.10), we have

$$\begin{aligned} & N[\theta_1(u_j+2b)+\theta_1(u_j-2b)] = 2\pi I_j + \sum_{k=1}^{M} \theta_2(u_j-u_k), \\ & j = 1, \ldots, M, \end{aligned} \tag{4.1}$$

where

$$\theta_n(x) = 2\arctan\frac{\tanh(x/2)}{\tan(n\eta/2)}. \tag{4.2}$$

Here the quantum number $\{I_j\}$ are certain integers (or half odd integers) if M is odd (or even). For convenience, we define the counting function

$$Z(u) = \frac{1}{4\pi}\left[\theta_1(u+2b)+\theta_1(u-2b) - \frac{1}{N}\sum_{k=1}^{M}\theta_2(u-u_k)\right]. \tag{4.3}$$

Obviously, $Z(u_j) = I_j/2N$ corresponds to the equation (4.1). In the thermodynamic limit, $N \to \infty$, $M \to \infty$ and N/M finite, taking the derivative of equation (4.3) with respect to u, we obtain

Table 1. Numerical solutions of the BAEs (3.10) for real η case, where $\eta = 1$, $b = 1$, $2N = 4$, n indicates the number of the energy levels and E_n is the corresponding energy. The energy E_n calculated from the Bethe roots is exactly the same as that from the exact diagonalization of the Hamiltonian (1.1).

u_1	u_2	E_n	n
$-2.0080 + 0.0000i$	$2.0080 + 0.0000i$	-100.4304	1
$2.6286 + 0.0000i$	$---$	-20.0748	2
$-2.0253 - 3.1416i$	$2.0253 + 0.0000i$	-20.0748	2
$0.0000 + 0.0000i$	$---$	5.0260	3
$0.0000 - 3.1416i$	$0.0000 + 0.0000i$	17.9135	4
$0.0000 - 1.3032i$	$0.0000 + 1.3032i$	18.1853	5
$---$	$---$	22.2360	6
$0.0000 - 3.1416i$	$---$	35.1235	7
$-2.0777 - 3.1416i$	$2.0777 - 3.1416i$	60.0091	8

Table 2. Numerical solutions of the BAEs (3.11) for imaginary η case, where $\gamma = 1$, $a = 1$ and $2N = 4$.

u_1	u_2	E_n	n
$-1.9566 + 0.0000i$	$1.9566 + 0.0000i$	-12.1765	1
$-3.1416 + 0.0000i$	$0.0000 + 0.0000i$	-4.3247	2
$-1.8439 + 0.0000i$	$---$	-1.8476	3
$-1.5708 - 0.9497i$	$-1.5708 + 0.9497i$	-1.8476	3
$-3.1416 + 0.0000i$	$---$	0.1830	4
$-3.1416 - 1.1002i$	$-3.1416 + 1.1002i$	1.1932	5
$0.0000 - 1.3426i$	$0.0000 + 1.3426i$	2.9633	6
$0.0000 + 0.0000i$	$---$	3.5122	7
$---$	$---$	8.0199	8

$$\begin{aligned}\frac{\mathrm{d}Z(u)}{\mathrm{d}u} &= \frac{1}{2}\left[a_1(u+2b)+a_1(u-2b)\right] - \int_{-\infty}^{\infty} a_2(u-\lambda) \\ &\quad \times \rho(\lambda)\mathrm{d}\lambda \\ &\equiv \rho(u) + \rho^h(u),\end{aligned} \tag{4.4}$$

where

$$a_n(x) = \frac{1}{2\pi}\frac{\sin(n\eta)}{\cosh u - \cos(n\eta)}, \tag{4.5}$$

$\rho(x)$ and $\rho^h(x)$ are the densities of particles and holes, respectively.

4.1. Ground state

From the analysis of equation (4.1), we know that at the ground state, $M = N$ which is half of the number of sites. Meanwhile, all the Bethe roots constrained by equation (4.1) are real and the corresponding quantum numbers are

$$I_j = -\frac{N-1}{2}, -\frac{N-3}{2}, \cdots, \frac{N-1}{2}. \tag{4.6}$$

From equation (3.12), we learn that each real Bethe root u_j contributes a negative energy. At the ground state, the Bethe roots should fill the whole real axis and leave no hole, i.e. $\rho^h(u) = 0$. This means that the density of particles $\rho_g(u)$ at the ground state satisfies

$$\rho_g(u) = \frac{1}{2}\left[a_1(u+2b) + a_1(u-2b)\right] - \int_{-\infty}^{\infty} a_2(u-\lambda) \times \rho_g(\lambda)\mathrm{d}\lambda. \tag{4.7}$$

Let us define the following Fourier transformation

$$\tilde{f}(\omega) = \int_{-\infty}^{\infty} f(u)\mathrm{e}^{\mathrm{i}\omega u}\mathrm{d}u,$$
$$f(u) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \tilde{f}(\omega)\mathrm{e}^{-\mathrm{i}\omega u}\mathrm{d}\omega. \tag{4.8}$$

Without losing generality, we consider the case $\eta \in (0, \pi)$. Taking the Fourier transformation of equation (4.7), we obtain

$$\tilde{a}_n(\omega) = \frac{\sinh(\pi\omega - 2\delta_n\pi\omega)}{\sinh \pi\omega}.$$
$$\tilde{\rho}_g(\omega) = \frac{\cos(2b\,\omega)}{2\cosh(\eta\,\omega)}, \tag{4.9}$$

with $\delta_n \equiv \frac{n\eta}{2\pi} - \lfloor\frac{n\eta}{2\pi}\rfloor$ denoting the fractional part of $\frac{n\eta}{2\pi}$. Thus the solution of equation (4.7) is

$$\rho_g(u) = \frac{1}{8\eta}\left[\frac{1}{\cosh(\frac{\pi(u+2b)}{2\eta})} + \frac{1}{\cosh(\frac{\pi(u-2b)}{2\eta})}\right]. \tag{4.10}$$

The Bethe root distribution at the ground state is shown in figure 1. The magnetization at the ground state is

$$\frac{1}{2} - \int_{-\infty}^{\infty} \rho_g(u)\mathrm{d}u = 0, \tag{4.11}$$

indicating a singlet ground state. The energy density at the ground state reads

$$\begin{aligned} e_g &= \frac{\cos\eta[\cosh^2(2b) - \cos(2\eta)]}{2\sin^2\eta} - \frac{\cosh(4b) - \cos(2\eta)}{\sin\eta} \\ &\quad \times 2\pi\int_{-\infty}^{\infty} [a_1(u+2b) + a_1(u-2b)]\rho_g(u)\mathrm{d}u \\ &= \frac{\cos\eta[\cosh^2(2b) - \cos(2\eta)]}{2\sin^2\eta} - \frac{\cosh(4b) - \cos(2\eta)}{\sin\eta} \\ &\quad \times \int_{-\infty}^{\infty} \frac{\sinh(\pi\omega - \eta\omega)\cos^2(2b\omega)}{\sinh(\pi\omega)\cosh(\eta\omega)}\mathrm{d}\omega. \end{aligned} \tag{4.12}$$

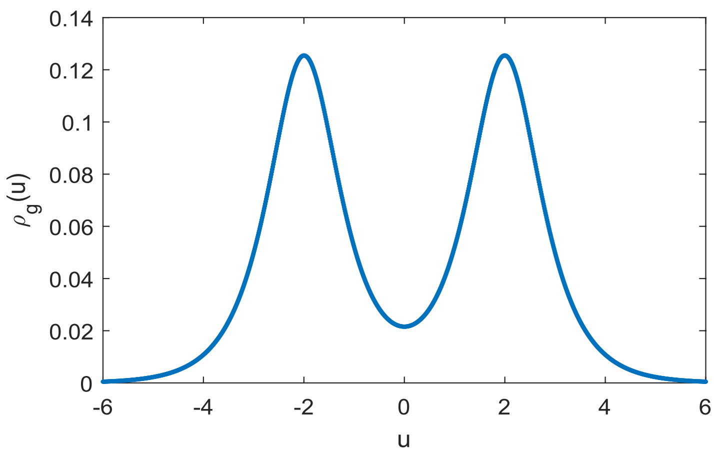

Figure 1. The density of Bethe roots at the ground state with $\eta = 1$ and $b = ia = 1$.

4.2. Spinon excitations

Now we consider the elementary excitations. The simplest excitation is the case of one less spin flipped, i.e. $M = N - 1$. Such a configuration is described by putting two holes in the Fermi sea. Meanwhile, all the Bethe roots constrained by equation (4.1) are real and the corresponding quantum numbers are

$$\begin{aligned} I_j = &-\frac{N}{2}, -\frac{N}{2}+1, \cdots, -\frac{N}{2}+r-1, -\frac{N}{2}+r+1, \cdots, \\ &-\frac{N}{2}+s-1, -\frac{N}{2}+s+1, \cdots, \frac{N}{2}-1, \frac{N}{2}, \end{aligned} \tag{4.13}$$

where $0 < r < s < N$. The positions of holes are denoted as u_r^h and u_s^h. In this case all $N - 1$ quasi-momentum are real numbers and the total momentum is $\Delta K = \pi(r+s)/N$. In the thermodynamic limit, the momentum of this excitation is calculated as

$$\begin{aligned} K &= 2\pi \int_{u_r^h}^{\infty} \rho_g(u)\mathrm{d}u + 2\pi \int_{u_s^h}^{\infty} \rho_g(u)\mathrm{d}u \\ &= \arctan\left[\mathrm{e}^{-\frac{\pi(u_r^h-2b)}{2\eta}}\right] + \arctan\left[\mathrm{e}^{-\frac{\pi(u_r^h+2b)}{2\eta}}\right] \\ &\quad + \arctan\left[\mathrm{e}^{-\frac{\pi(u_s^h-2b)}{2\eta}}\right] + \arctan\left[\mathrm{e}^{-\frac{\pi(u_s^h+2b)}{2\eta}}\right]. \end{aligned} \tag{4.14}$$

The density of holes is

$$\rho^h(u) = \frac{1}{2N}\left[\delta_1(u - u_r^h) + \delta_1(u - u_s^h)\right]. \tag{4.15}$$

The corresponding Bethe root density becomes $\rho_e(u) = \rho_g(u) + \delta\rho(u)$ [7]. The density $\rho_e(u)$ will deviate from $\rho_g(u)$ by $\delta\rho(u)$ because of the presence of the two holes. From equations (4.4) and (4.15), we obtain

$$\begin{aligned} \rho_e(u) + \rho^h(u) = &\frac{1}{2}\left[a_1(u+2b) + a_1(u-2b)\right] \\ &- \int_{-\infty}^{\infty} a_2(u-\lambda)\rho_e(\lambda)\mathrm{d}\lambda. \end{aligned} \tag{4.16}$$

After some calculations, we have

$$\delta\tilde{\rho}(\omega) = -\frac{1}{2N}\frac{e^{i\omega u_r^h}+e^{i\omega u_s^h}}{1+\tilde{a}_2(\omega)}. \tag{4.17}$$

The excitation energy is

$$\begin{aligned}\Delta E = &-\frac{4\pi N[\cosh(4b)-\cos(2\eta)]}{\sin\eta}\int_{-\infty}^{\infty}[a_1(u+2b) \\ &+a_1(u-2b)]\delta\rho(u)\mathrm{d}u \\ &= \frac{4\pi[\cosh(4b)-\cos(2\eta)]}{\sin\eta}[\rho_g(u_r^h)+\rho_g(u_s^h)] \\ &= \varepsilon(u_r^h)+\varepsilon(u_s^h),\end{aligned} \tag{4.18}$$

where

$$\varepsilon(u) = \frac{4\pi[\cosh(4b)-\cos(2\eta)]}{\sin\eta}\rho_g(u). \tag{4.19}$$

We see that the energy of such an excitation is the summation of the energies of two holes. Here the two holes together carry spin-1, and each of them carries spin-$\frac{1}{2}$. These excitations are usually called spinons [38], a typical fractional excitation in the one-dimensional quantum systems. Spinon excitations are spin-triplet elementary excitations. Relative to the Neel state, the net spin carried by the flipped domain is one. Each domain boundary (kink or anti-kink) carries a spin of $\frac{1}{2}$.

The dispersion relation of the spinon excitations can be derived from equations (4.14) and (4.18). The numerical results are shown in figure 2. From it, we see that the spinon excitation is gapless which can be reached by putting the holes at the points 0 or $\pm\pi$. Meanwhile, if b is very small, the excitation spectrum is quite similar to that of the conventional XXZ model [7]. With the increasing of b, the excitation spectrum turns to the triple arched structure, which means the structure of the spinon excitation spectrum consists of overlapping continua with a triple arched upper boundary. Unlike the conventional $J_1 - J_2$ model, there is no dimerization in the present model for any real b. If b takes some imaginary values, dimerization indeed occurs as hinted from the solution of the BAE's. However, in such a case the Hamiltonian is non-hermitian.

5. Ground state and elementary excitations for imaginary η

In this section we study the ground state and elementary excitations of the system for imaginary $\eta = i\gamma$. Without losing generality, we assume $\gamma > 0$. Similarly, let us introduce

$$a_n(x) = \frac{1}{2\pi}\frac{\sinh(n\gamma)}{\cosh(n\gamma)-\cos x}. \tag{5.1}$$

The Fourier transformation of $a_n(x)$ is

$$\tilde{a}_n(\omega) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i\omega x}\frac{\sinh(n\gamma)}{\cosh(n\gamma)-\cos x}\mathrm{d}x = e^{-n\gamma|\omega|}. \tag{5.2}$$

Note that ω takes values of integers. From the energy expression (3.13), we know that at the ground state the Bethe roots still take real values and fill the region $(-\pi, \pi]$. Using the similar procedure mentioned above, we find the density of Bethe roots at the ground state satisfies

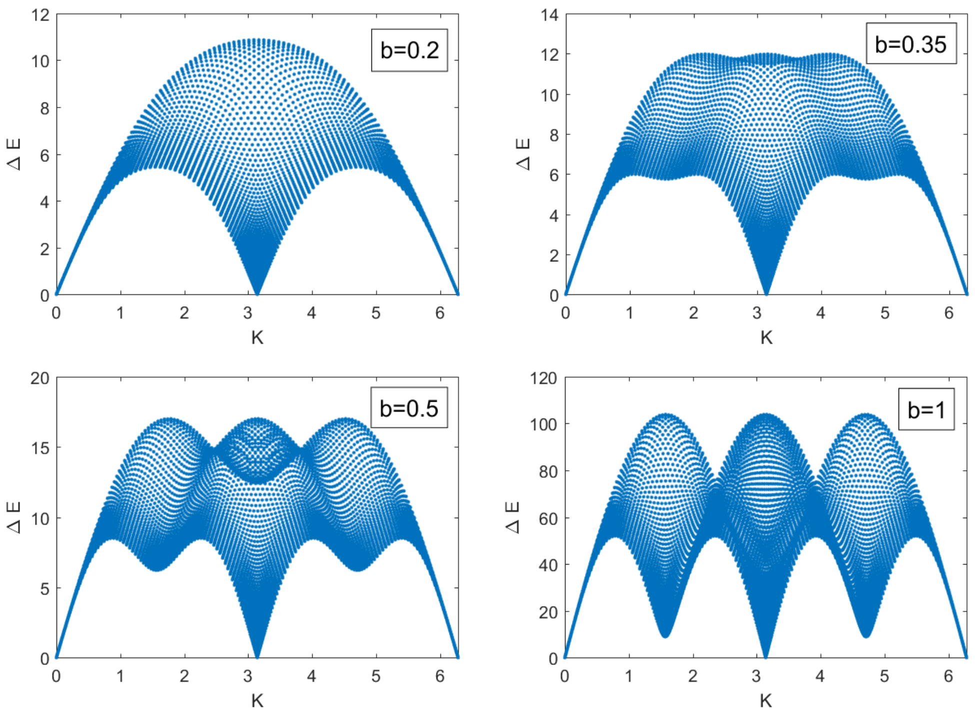

Figure 2. The dispersion relations between energy ΔE and momentum K of spinon excitations with $\eta = 1, b = ia$.

$$\rho_g(u) = \frac{1}{2}\left[a_1(u+2a) + a_1(u-2a)\right] - \int_{-\pi}^{\pi} a_2(u-\lambda) \times \rho_g(\lambda)\mathrm{d}\lambda. \tag{5.3}$$

Using Fourier transformation we have

$$\begin{aligned} \tilde{\rho}_g(\omega) &= \frac{\cos(2a\,\omega)}{2\cosh(\gamma\,\omega)}, \\ \rho_g(u) &= \frac{1}{2\pi}\sum_{\omega=-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}u\omega}\,\frac{\cos(2a\,\omega)}{2\cosh(\gamma\omega)}. \end{aligned} \tag{5.4}$$

The Bethe root distribution at the ground state is shown in figure 3. Interestingly, we find $\rho_g(\pm\pi) = \rho_g(0)$ if $a = \pi/4 + k\pi/2$, and k is an arbitrary integer. Please see the left one in figure 3. The total magnetization at the ground state is still zero. The energy density at the ground state reads

$$e_g = \frac{\cosh\gamma[\cosh(2\gamma) - \cos^2(2a)]}{2\sinh^2\gamma} + \frac{\cos(4a) - \cosh(2\gamma)}{\sinh\gamma} \times \sum_{\omega=-\infty}^{\infty} \frac{\cos^2(2a\omega)\mathrm{e}^{-\gamma|\omega|}}{\cosh(\gamma\omega)}. \tag{5.5}$$

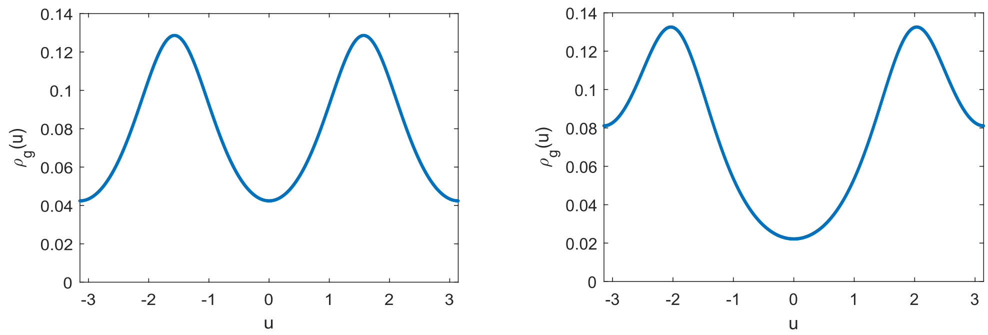

Figure 3. The densities of Bethe roots at the ground state with $\gamma = 1$, $a = \pi/4$ (left); and $\gamma = 1$, $a = 1$ (right).

In the thermodynamic limit, the momentum of spinion excitation is calculated as

$$\begin{aligned} K &= 2\pi \int_{u_r^h}^{\pi} \rho_g(u)\mathrm{d}u + 2\pi \int_{u_s^h}^{\pi} \rho_g(u)\mathrm{d}u \\ &= \sum_{\substack{\omega=-\infty,\\ \omega\neq 0}}^{\infty} \frac{\cos(2a\omega)}{2i\omega\cosh(\gamma\omega)} [2(-1)^{\omega} - \mathrm{e}^{\mathrm{i}\omega u_r^h} - \mathrm{e}^{\mathrm{i}\omega u_s^h}] \\ &\quad + \pi - \frac{u_r^h + u_s^h}{2}. \end{aligned} \tag{5.6}$$

After some calculations similar with above real η case, we obtain the excitation energy

$$\Delta E = \varepsilon(u_r^h) + \varepsilon(u_s^h), \tag{5.7}$$

where

$$\varepsilon(u) = \frac{4\pi[\cosh(2\gamma) - \cos(4a)]}{\sinh\gamma} \rho_g(u). \tag{5.8}$$

The dispersion relation of the spinon excitations can be derived from equations (5.6) and (5.7). The numerical results are shown in figure 4. From it, we see that if a is very small, the excitation spectrum is quite similar to that of the conventional XXZ model [7]. With the increasing of a, the excitation spectrum turns to the triple arched structure. Similar with real η case, there is also no dimerization in the present model for any imaginary η and real a.

From the excitation spectrum in figure 4, we also find that the elementary excitations possess a finite gap. Now we determine the values of the gap. Without losing generality, we assume $a \in [0, \pi]$. We should consider the positions of holes first. From figure 3, we know that there are two minimal points located at $u = 0$ and $u = \pi$. As we mentioned before, $\rho_g(\pi) = \rho_g(0)$ if $a = \pi/4$ or $a = 3\pi/4$. By detailed analysis, we conclude that $\rho_g(\pi) < \rho_g(0)$ if $0 < a < \pi/4$ or $3\pi/4 < a < \pi$ and $\rho_g(\pi) > \rho_g(0)$ if $\pi/4 < a < 3\pi/4$. Thus we put the holes at the point of π if $a \in [0, \pi/4] \cup [3\pi/4, \pi]$, and put the holes at the point of 0 if $a \in (\pi/4, 3\pi/4)$. We note that only in the thermodynamic limit, two holes can be put at the same position. After some calculations, we obtain the energy gap of the model (1.1) in these intervals as

$$\Delta = \frac{4[\cosh(2\gamma) - \cos(4a)]}{\sinh\gamma} \sum_{\omega=-\infty}^{\infty} \frac{(-1)^{\omega}\cos(2a\omega)}{2\cosh(\gamma\omega)}, \tag{5.9}$$

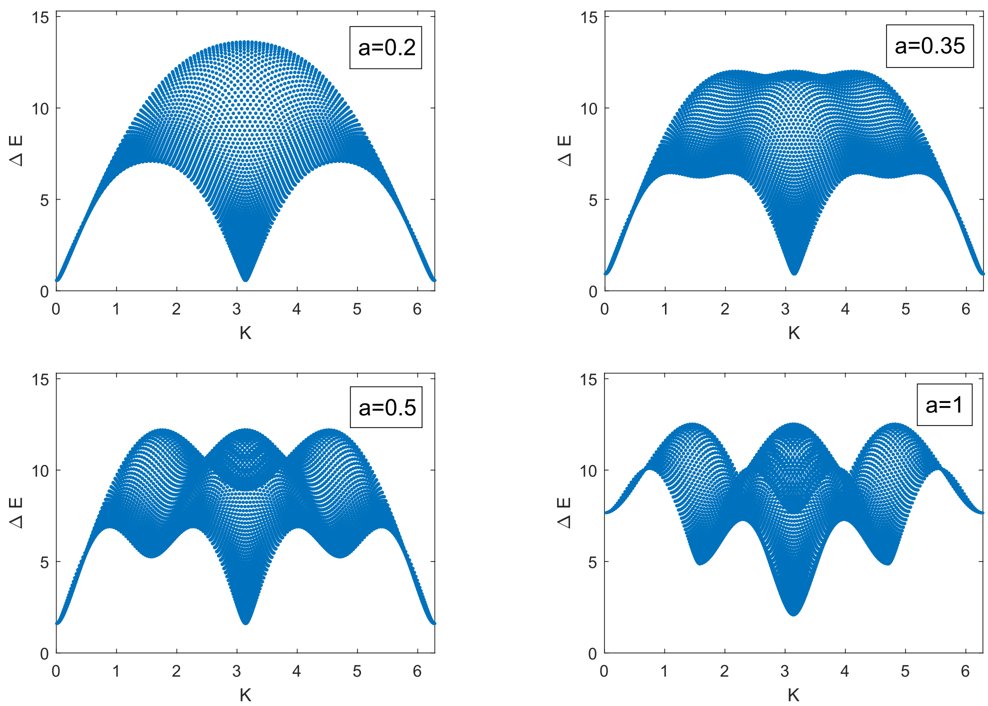

Figure 4. The dispersion relations between energy ΔE and momentum K of spinon excitations with $\gamma = 1$.

if $a \in [0, \pi/4] \cup [3\pi/4, \pi]$, and

$$\Delta = \frac{4[\cosh(2\gamma) - \cos(4a)]}{\sinh\gamma} \sum_{\omega=-\infty}^{\infty} \frac{\cos(2a\omega)}{2\cosh(\gamma\omega)}, \tag{5.10}$$

if $a \in (\pi/4, 3\pi/4)$.

The gap is shown in figure 5. From it, we see that the gap is enhanced by the NNN and chiral three-spin interactions. At the points of $a = 0$ and $a = \pi$, the gap takes its minimum, which is the same as that of the conventional XXZ spin chain, because that the model (1.1) degenerates into the conventional XXZ spin chain at these points. At the point of $a = \frac{\pi}{2}$, the gap also takes its minimum. In this case the model (1.1) degenerates into the XXZ spin chain only with NN interaction where the couplings along the x and y directions are negative. At the points of $a = \frac{\pi}{4}$ and $a = \frac{3\pi}{4}$, the gap arrives at its maximal value. This is because at the these points, the coupling strengths of NNN and chiral three-spin interactions reach their maximum and the NN couplings along the x and y directions are zero. Besides, the gap also has the property

$$\Delta(a) = \Delta(\frac{\pi}{2} - a) = \Delta(\frac{\pi}{2} + a) = \Delta(\pi - a),$$

which means that the gap is symmetric with respect to the points of $\frac{\pi}{4}$, $\frac{\pi}{2}$ and $\frac{3\pi}{4}$. This symmetry is different from that of the Hamiltonian, where the Hamiltonian is symmetric only with respect to π, i.e.

$$H(a) = H(\pi + a).$$

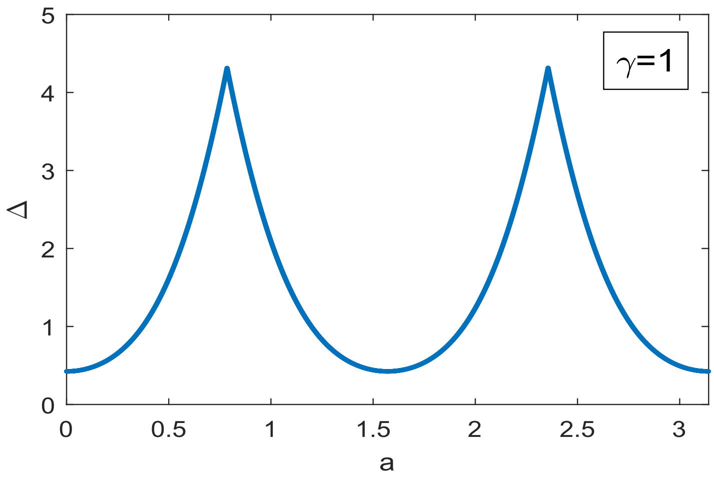

Figure 5. The gap with $\gamma = 1$.

6. Conclusion

In this paper, we study an integrable anisotropic $J_1 - J_2$ spin chain model with extra scalar chirality terms. By means of the Bethe Ansatz method, we obtain the exact solution of the system. The ground state and the novel structure of the elementary excitation spectrum are obtained. We find that the elementary excitation is gapless if the anisotropic parameter is real while the elementary excitation has a gap if the anisotropic parameter is imaginary. Moreover, it is shown that the spinon excitation spectrum of the model possesses a novel triple arched structure, which could be observed in experiments (e.g. inelastic neutron scattering of some quasi-one-dimensional magnetic materials). The method of this paper can be used to construct other integrable models with next-nearest-neighbour couplings.

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Appendix A. Derivation of the Hamiltonian

Using the initial condition (2.2) of the R-matrix $R(u)$ given by (2.1), we can evaluate the values of the transfer matrix $\hat{t}(u)$ at some points: $u = \pm a$:

$$\hat{t}(-a) = R_{2N,2N-1}(-2a)\cdots R_{2N,2}(0)R_{2N,1}(-2a),$$
$$\hat{t}(a) = R_{1,2N}(2a)R_{1,2N-1}(0)\cdots R_{1,2}(2a). \tag{A.1}$$

Taking the derivative of the transfer matrix $t(u)$ with respect to u at the point of $u = a$, we have

$$\begin{aligned}\frac{\partial\, t(u)}{\partial u}\Big|_{u=a} = &\sum_{j=1}^{N-1} R_{2N,1}(2a)R_{2N,2}(0)\cdots[R'_{2N,2j-1}(2a)R_{2N,2j}(0) + R_{2N,2j-1}(2a)R'_{2N,2j}(0)]\\ &\cdots R_{2N,2N-1}(2a) + R_{2N,1}(2a)R_{2N,2}(0)\cdots R'_{2N,2N-1}(2a)\\ &+ R_{2,3}(2a)R_{2,4}(0)\cdots R_{2,2N-1}(2a)R'_{2,2N}(0)R_{2,1}(2a),\end{aligned} \tag{A.2}$$

where $R'_{i,j}(u) = \frac{\partial}{\partial u}R_{i,j}(u)$. Similarly we can calculate the derivative of $t(u)$ at the point of $u = -a$

$$\begin{aligned}\frac{\partial\, t(u)}{\partial u}\Big|_{u=-a} = &\sum_{j=1}^{N} R_{1,2}(-2a)\cdots[R'_{1,2j-1}(0)R_{1,2j}(-2a) + R_{1,2j-1}(0)R'_{1,2j}(-2a)]\\ &\cdots R_{1,2N-1}(0)R_{1,2N}(-2a) + R_{1,2}(-2a)R_{1,3}(0)\cdots R_{1,2N}(-2a)\\ &+ R_{3,4}(-2a)R_{3,5}(0)\cdots R_{3,2N}(-2a)R'_{3,1}(0)R_{3,2}(-2a).\end{aligned} \tag{A.3}$$

Substituting the above relations (A.1)–(A.3) into the expression (2.10), we obtain

$$\begin{aligned}H = &\sum_{j=1}^{N}\{R_{2j,2j-1}(-2a)R'_{2j,2j-1}(2a) + \phi_1 R_{2j+1,2j}(2a)R'_{2j+1,2j}(-2a)\\ &+ R_{2j+2,2j+1}(-2a)P_{2j+2,2j}R'_{2j+2,2j}(0)R_{2j+2,2j+1}(2a)\\ &+ R_{2j+1,2j}(2a)P_{2j+1,2j-1}R'_{2j+1,2j-1}(0)R_{2j+1,2j}(-2a)\}\\ &- \frac{N\cos\eta[\cos^2(2a) - \cos(2\eta)]}{\sin^2\eta}.\end{aligned} \tag{A.4}$$

The derivative of the R-matrix (2.1) reads

$$R'_{0,j}(u) = \frac{1}{2}\left[\frac{\cos(u+\eta)}{\sin\eta}(1 + \sigma_0^z\sigma_j^z) + \frac{\cos u}{\sin\eta}(1 - \sigma_0^z\sigma_j^z)\right]. \tag{A.5}$$

The commutative relation between the permutation operators is

$$\begin{aligned}[P_{2,1}, P_{2,0}] &= \frac{1}{4}[(1 + \vec{\sigma}_2\cdot\vec{\sigma}_1), (1 + \vec{\sigma}_2\cdot\vec{\sigma}_0)]\\ &= \frac{\mathrm{i}}{2}(\sigma_2^z\sigma_1^x\sigma_0^y - \sigma_2^y\sigma_1^x\sigma_0^z - \sigma_2^z\sigma_1^y\sigma_0^x\\ &\quad \sigma_2^x\sigma_1^y\sigma_0^z + \sigma_2^y\sigma_1^z\sigma_0^x - \sigma_2^x\sigma_1^z\sigma_0^y)\\ &= \frac{\mathrm{i}}{2}\vec{\sigma}_2\cdot(\vec{\sigma}_1\times\vec{\sigma}_0).\end{aligned} \tag{A.6}$$

Substituting equations (2.1), (A.5) and (A.6) into (A.4) and after some tedious calculations, we arrive at the form of the Hamiltonian (1.1).

Appendix B. Non-hermitian case

In this section, we consider the case that both a and η are real, which implies that the Hamiltonian (1.1) is non-hermitian. By the analysis of possible couplings in the Hamiltonian (1.1), we restrict the values of a in the interval $[0,\pi]$. It is easy to check that following identity holds

$$H(a,\pi+\eta)=H(\pi-a,\pi-\eta). \tag{B.1}$$

This means that the values of η can also be restricted in the interval $(0,\pi)$. Then the parameters $a\in[0,\pi]$ and $\eta\in(0,\pi)$ can describe all the coupling strengths.

The Hamiltonian (1.1) possesses the PT-symmetry. However, the corresponding eigenvalues are real only if all the eigenfunctions are chosen as simultaneous eigenfunctions of the PT-operator [39]. Now, we study the condition of real energy spectrum.

Using the direct diagonalization method, up to $2N=12$, we find that all the eigenvalues of the Hamiltonian (1.1) are real if a takes the values in some intervals. After detailed calculation, the intervals are determined as $a\in[0,\eta/2]\cup[(\pi-\eta)/2,(\pi+\eta)/2]\cup[\pi-\eta/2,\pi]$. We note that if $\eta>\pi/2$, these intervals are connected with each other and the parameter a fills the whole interval $[0,\pi]$, which means that with an arbitrary a, all the eigenvalues of the model (1.1) are real.

The BAEs (3.9) are true for real a and real η. Put $\lambda_j=iu_j/2-\eta/2$ and the BAEs become

$$\begin{aligned}&\left[\frac{\sinh\frac{1}{2}(u_j-i(2a+\eta))\sinh\frac{1}{2}(u_j+i(2a-\eta))}{\sinh\frac{1}{2}(u_j+i(2a+\eta))\sinh\frac{1}{2}(u_j-i(2a-\eta))}\right]^N\\&\quad=\prod_{l\neq j}^{M}\frac{\sinh\frac{1}{2}(u_j-u_l-2\eta i)}{\sinh\frac{1}{2}(u_j-u_l+2\eta i)},\quad j=1,\cdots,M.\end{aligned} \tag{B.2}$$

From equations (2.10) and (3.8) we obtain the eigenvalue of the Hamiltonian (1.1) in terms of the Bethe roots as

$$\begin{aligned}E=&\frac{N\cos\eta[\cos^2(2a)-\cos(2\eta)]}{\sin^2\eta}-[\cos(4a)-\cos(2\eta)]\\&\times\sum_{j=1}^{M}\left\{\frac{1}{\cosh(u_j+2ai)-\cos\eta}+\frac{1}{\cosh(u_j-2ai)-\cos\eta}\right\}.\end{aligned} \tag{B.3}$$

Solving the BAEs (B.2) with $2N=6$ and substituting the values of Bethe roots into (B.3), we find that the eigenvalues calculated from the Bethe roots are exactly the same as those obtained from the exact diagonalization of the Hamiltonian (1.1). The energy spectrum is complete. Meanwhile, the intervals that all the eigenvalues are real keep unchanged.

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