Pedestrian's way to Baxter's Bethe ansatz for the periodic XYZ chain

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A chiral coordinate Bethe ansatz method is developed to study the periodic XYZ chain. We construct a set of chiral vectors with fixed number of kinks. All vectors are factorized and have simple structures. Under roots of unity conditions, the Hilbert space has an invariant subspace, and our vectors form a basis of this subspace. We propose a Bethe ansatz solely based on the action of the Hamiltonian on the chiral vectors, avoiding the use of transfer matrix techniques. This allows us to parametrize the expansion coefficients and derive the homogeneous Bethe ansatz equations, whose solutions give the exact energies and eigenstates. Our analytic results agree with earlier approaches, notably by Baxter, and are supported by numerical calculations.

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I. INTRODUCTION

The XYZ model, an integrable system in quantum statistical mechanics, has been a constant source of fascination for researchers since Baxter's discovery of its integrability and his groundbreaking work on the solution [1–8]. The exact solution for the eigenvalues of the eight vertex model's transfer matrix and of the Hamiltonian of the related XYZ quantum chain with even number of sites and periodic boundary conditions was first obtained in [3,8], then a coordinate Bethe ansatz for the eigenstates was presented in [5–7], which was argued in [9] to be complete.

Takhtadzhan and Faddeev successfully tackled the model using the algebraic Bethe ansatz method [10]. Related equations for the eigenvectors of the eight-vertex model were addressed by researchers in Refs. [11,12]. The role of additional algebraic structures appearing at special anisotropy parameters (roots of unity), especially in view of the completeness of the spectrum of the transfer matrix, were studied in [13–17].

The absence of a suitable vacuum state has long hindered the application of conventional Bethe ansatz methods to the XYZ model. Exact solutions are only attainable in specific scenarios, such as the periodic XYZ chain with an even number of lattice sites (N) [8,10], or in root of unity cases or open XYZ chains [9,10,18,19].

The introduction of the off-diagonal Bethe ansatz method (ODBA) led to the derivation of Bethe ansatz equations (BAE) for the spectrum of the XYZ chain with various integrable boundary conditions [20–22], although this approach yielded limited information about the eigenstates.

Over the past two years we conducted a series of studies on open XXZ and XYZ chains with boundary fields [23–26]. We demonstrated the existence of two invariant subspaces in anisotropic Heisenberg chains under certain criteria [23,26]. A set of chiral vectors with kinks was constructed to expand the invariant subspace. Subsequently, we proposed a Bethe ansatz method to derive the coefficients of Bethe vectors in the chiral basis and the corresponding eigenvalues [23–26]. A recent study [27] shows that quantum states with helicity are protected from certain types of noise over intermediate timescales even better than the ground state, making chiral states attractive for experimental applications [28,29]. Finally, chiral states, both in XXZ and XYZ open chains, can be targeted by boundary-localized strong dissipation [25].

Following our investigation of the open XYZ chain [26], we realized that similar invariant subspaces and chiral bases exist in the periodic XYZ chain. This is the motive for the present work.

In this communication we verify that the Hilbert space of the periodic XYZ chain has invariant subspace(s) at roots of unity, expandable by a generating set of chiral vectors. Unlike the open chain, the vectors in this case include a free parameter, and the closure of our basis is ensured by the periodicity of elliptic functions at roots of unity. We employ a chiral coordinate Bethe ansatz to diagonalize the Hamiltonian within this subspace. The solutions of the resulting BAE determine the coefficients for the respective eigenstates in our chiral basis. During our calculations, we observe two distinct scenarios. When $M \neq \frac{N}{2}$, the subspace's dimension correlates with binomial coefficients, resulting in degenerate energy levels. Conversely, when $M = \frac{N}{2}$, we successfully construct most of the eigenstates of the Hamiltonian. The dimension of the invariant subspace is numerically proven to be equal to the number of regular solutions of the BAE. We also conjecture that the missing eigenstates in our chiral basis correspond to special bound pair BAE solutions [9]. All our analytic results are validated through numerical checks.

Upon completing our calculations, we recognized an overlap between our results and the earlier work of Baxter [6,7,9]. Our chiral basis is a subset of Baxter's, which is a truly complete basis of states containing two independent free parameters. All states have the structure of the elliptic spin-helix state with insertions of kinks. The number of kinks is conserved under the action of the transfer matrix as shown in [6] by the property "pair propagation through a vertex," see also Ref. [8]. Based on this property, Baxter set up the Bethe ansatz [7] for the transfer matrix. This program was successful in the presence of two free parameters. In contrast, our chiral basis and the Bethe ansatz method are based solely on the local divergence condition (7, 18) for the local Hamiltonian and the local vectors [25,26], which are allowed to depend only on one free parameter instead of two. Notably, our approach is independent of the transfer matrix, representing a distinct methodology. While Baxter exclusively investigated the periodic XYZ chain, our work extends to both periodic and open chains. Furthermore, this paper serves as a complement to Baxter's previous research. For instance, we explicitly identify the bound pair solutions of the BAE and correlate them with the missing eigenstates in our chiral subspace. The existence of the invariant subspace of lower dimension may facilitate the study of certain physical phenomena, such as quantum quenching.

The structure of this paper is as follows: We begin by revisiting the parametrization of the XYZ model and postulating the conditions necessary for the existence of a chiral invariant subspace. In Sec. III we define the chiral basis vectors, which serve as the foundation of the invariant subspace. Subsequently, we introduce a Bethe ansatz method to parameterize the eigenvalues and eigenstates of the Hamiltonian. We explore specific cases, including $M = 0$ and $M = 1, 2$, in Secs. IV and V, respectively, and then proceed to generalize our findings to arbitrary values of M in Sec. VI. In Sec. VII we delve into the XXZ and XX limits of the model. Lastly, we provide useful identities and technical proofs in the Appendices.

II. XYZ MODEL AND CHIRAL SUBSPACE CONDITIONS

The quantum spin-$\frac{1}{2}$ XYZ chain with periodic boundary condition, defined by the following Hamiltonian,

$$H = \sum_{n=1}^{N} \mathbf{h}_{n,n+1} = \sum_{n=1}^{N} J_x\, \sigma_n^x \sigma_{n+1}^x + J_y\, \sigma_n^y \sigma_{n+1}^y + J_z\, \sigma_n^z \sigma_{n+1}^z, \tag{1}$$

is one of the most famous integrable models without $U(1)$ symmetry [8,10]. Here N is the length of the system, and $\sigma^x, \sigma^y, \sigma^z$ are the Pauli matrices and the periodic boundary condition implies $\vec{\sigma}_{N+1} \equiv \vec{\sigma}_1$. The exchange coefficients $\{J_x, J_y, J_z\}$ are parameterized by the crossing parameter η as [19–21]

$$J_x = \frac{\theta_4(\eta)}{\theta_4(0)}, \quad J_y = \frac{\theta_3(\eta)}{\theta_3(0)}, \quad J_z = \frac{\theta_2(\eta)}{\theta_2(0)}, \tag{2}$$

where $\theta_\alpha(u) \equiv \vartheta_\alpha(\pi u, e^{i\pi\tau})$, $\alpha = 1, 2, 3, 4$ are elliptic θ functions [30] defined in Appendix A, and τ is a quasiperiod of $\theta_\alpha(u)$ with $\text{Im}[\tau] > 0$.

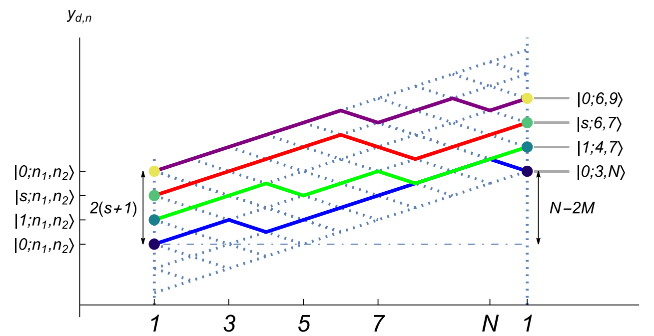

FIG. 1. Visualization of the vectors $\{|d; n_1, n_2\rangle\}$ for $M = 2$, $s = 2$. Any state in (16) corresponds to a directed path. Here we denote $\otimes_{n=1}^{N} \psi(\eta y_{d,n}) \equiv |d; n_1, n_2, \ldots, n_M\rangle$.

In this paper we study periodic XYZ chains, with η taking the following discrete values:

$$(N - 2M)\eta = 2L\tau + 2K, \quad 0 \leqslant M \leqslant N, \quad L, K \in \mathbb{Z}, \tag{3}$$

$$2(s+1)\eta = 2L_0\tau + 2K_0, \quad s \in \mathbb{N}, \quad L_0, K_0 \in \mathbb{Z}, \tag{4}$$

where s is the *smallest nonnegative integer* satisfying Eq. (4).

Equation (4) demands that η, τ and 1 are commensurate. Furthermore, a canonical set of integers with smallest value for the factor of η defines the non-negative integer s as well as L_0 and K_0.

As (4) is satisfied, Eq. (3) may have more than the solution $M = N/2$ (for even N). For any integer M that satisfies (3), we are going to set up a set of chiral states for which a Bethe ansatz can be derived. These states contain a fixed number M of what we call kinks. There are $s + 1$ many linearly independent kink states with the same locations of the kinks.

In the following we show that the conditions (3), (4) guarantee the existence of an invariant subspace of the XYZ Hamiltonian, spanned by the factorized helix states with kinks, of type shown in Fig. 1. The number of basis states (the number of trajectories in Fig. 1 with kinks at arbitrary positions) $(s+1)\binom{N}{M}$ typically coincides with the dimension of the invariant subspace $d_{M,s}$ (the exception $N = 2M$ will be discussed separately). Our aim is to find the eigenvectors of the Hamiltonian and the corresponding spectrum within the invariant subspace.

For odd N, $s + 1 < \frac{|N-2M|}{2}$ or $s + 1 = |N - 2M|$. For even N, $s + 1 \leqslant \frac{|N-2M|}{2}$. It can be verified that the dimension of the invariant subspace is strictly smaller than the Hilbert space dimension, $d_{M,s} = (s+1)\binom{N}{M} < 2^N$. For the exceptional case $N = 2M$, Eq. (3) is satisfied for any η with the choice $K = L = 0$; then, s from (4) can become arbitrarily large, leading to possible $(s+1)\binom{N}{N/2} > 2^N$, and consequently, a linear dependence of states in the generating system.

Hermiticity condition. Only when τ is purely imaginary and η is real or purely imaginary, the Hamiltonian is Hermitian, specifically as follows:

(i) when $\text{Im}[\eta] = \text{Re}[\tau] = 0$, $|J_x| \geqslant |J_y| \geqslant |J_z|$,

(ii) when $\text{Re}[\eta] = \text{Re}[\tau] = 0$, $|J_x| \leqslant |J_y| \leqslant |J_z|$.

One of particular examples of a system satisfying (3), (4) is an XYZ spin chain on special manifold of couplings $J_xJ_y + J_yJ_z + J_zJ_x = 0$, corresponding to $\eta = 2/3$ or to

$\eta = 2\tau/3$ in our parametrization (2) and discussed in detail in [31].

III. CHIRAL BASIS VECTORS

Introduce the following local ket vector [7,8]:

$$\psi(u) = \begin{pmatrix} \tilde\theta_1(u) \\ -\tilde\theta_4(u) \end{pmatrix}, \tag{5}$$

where $u \in \mathbb{C}$ is a free parameter and $\tilde\theta_\alpha(u) \equiv \vartheta_\alpha(\pi u, e^{2i\pi\tau})$, $\alpha = 1, 2, 3, 4$ are elliptic theta functions defined in Appendix A. The state $\psi(u)$ possesses the quasiperiodicity property:

$$\psi(u + 2k + 2l\tau) = \exp[-i\pi l(2u + 2l\tau + 1)]\psi(u), k, l \in \mathbb{Z}. \tag{6}$$

The following identities hold [25,26]:

$$\mathbf{h}_{n,n+1}\psi_n(u)\psi_{n+1}(u \pm \eta) = \big[\pm f(u)\sigma_n^z \mp f(u \pm \eta)\sigma_{n+1}^z + w(\pm u)\big]\psi_n(u)\psi_{n+1}(u \pm \eta), \tag{7}$$

where $\mathbf{h}_{n,n+1}$ is the local density of the XYZ Hamiltonian (1), and the functions $f(u)$, $w(u)$ are

$$g(u) = \frac{\theta_1(\eta)\theta_1'(u)}{\theta_1'(0)\theta_1(u)}, \quad f(u) = \frac{\theta_1(\eta)\theta_2(u)}{\theta_2(0)\theta_1(u)}, \tag{8}$$

$$w(u) = g(\eta) + g(u) - g(u + \eta). \tag{9}$$

The state $\psi(u)$ satisfies another equation [26],

$$f(u)\sigma^z\psi(u) = a_\pm(u)\psi(u) + b_\pm(u)\psi(u \pm 2\eta), \tag{10}$$

with

$$a_\pm(u) = \mp\frac{\theta_2(\eta)\theta_2(u)\theta_1(u \pm \eta)}{\theta_2(0)\theta_1(u)\theta_2(u \pm \eta)}, \quad b_\pm(u) = \pm\frac{\theta_2(u)}{\theta_2(u \pm \eta)}. \tag{11}$$

Denote

$$u_m = u_0 + m\eta, \quad u_0 \in \mathbb{C} \tag{12}$$

and then define the global states [7]

$$|d; n_1, n_2, \dots, n_M\rangle = \bigotimes_{k_1=1}^{n_1} \psi(u_{2d+k_1}) \bigotimes_{k_2=n_1+1}^{n_2} \psi(u_{2d+k_2-2}) \cdots \bigotimes_{k_M=n_{M-1}+1}^{n_M} \psi(u_{2d+k_M-2M+2}) \bigotimes_{k_{M+1}=n_M+1}^{N} \psi(u_{2d+k_{M+1}-2M}), \quad 1 \leqslant n_1 < n_2 < \cdots < n_M \leqslant N. \tag{13}$$

Using Eqs. (3), (4), (7), and (10), one can prove that $H|d; n_1, \dots, n_M\rangle$ is a linear combination of

$$|d; n_1, \dots, n_M\rangle \text{ and } |d; \dots, n_{k-1}, n_k \pm 1, n_{k+1}, \dots\rangle, \quad k = 1, \dots, M, \tag{14}$$

where $|d; \dots, n_j, n_{j+1} = n_j, \dots\rangle \equiv 0$. The periodicity of the θ functions implies

$$\begin{aligned} &|d; n_1, \dots, n_{M-1}, N+1\rangle \propto |d+1; 1, n_1, \dots, n_{M-1}\rangle, \\ &|d; 0, n_2, \dots, n_M\rangle \propto |d-1; n_2, \dots, n_M, N\rangle, \\ &|d; n_1, \dots, n_M\rangle \propto |d+s+1; n_1, \dots, n_M\rangle, \end{aligned} \tag{15}$$

where the last identity follows from Eq. (4) (note that above we have extended the definition of vectors (13) for $n_1 = 0$ or $n_M = N + 1$). Therefore the vectors

$$|d; n_1, n_2, \dots, n_M\rangle, \quad d = 0, 1, \dots, s, \quad 1 \leqslant n_1 < n_2 < \cdots < n_M \leqslant N, \tag{16}$$

form an invariant subspace of H.

The qubit phase u of the state (13) increases linearly by the amount η at each site along the chain, except at the kink positions $n_1, \dots, n_M$, where it decreases by the same amount. The chiral vectors (16) can be represented in a form of trajectories, see Fig. 1, each trajectory having exactly M kinks. The total number of kinks M thus serves as a conserved charge. In the following sections we diagonalize the Hamiltonian within the invariant subspace spanned by the vectors (16). The total number of eigenstates thus constructed is equal to the dimension of the invariant subspace, and provided $M \neq N/2$, it is given by

$$d_{M,s} = (s+1)\binom{N}{M}. \tag{17}$$

Remark A. Changing the sign of the chirality $\eta \to -\eta$, we get another set of linearly independent basis vectors, of the same dimension as in (17), provided $N \neq 2M$. The vectors with positive and negative chirality are all linearly independent, so that we have two invariant subspaces, with opposite chiralities, of the dimension $d_{M,s}$ each. Any state obtained from the set (16) by a shift of the initial phase is not independent and can be expanded as a linear combination of the $2d_{M,s}$ vectors. This is our numerical observation, and for the moment we do not have an analytical proof.

Remark B. Baxter proposed a similar basis in [7], which contains two free parameters. In comparison, there is only one free parameter u_0 in our chiral basis (16). The generating system of our chiral states (16) has a simpler structure and is an invariant subset of Baxter's states in [7,9]. More details are given in Appendix G.

If the Hermiticity conditions at the end of Sec. II are not satisfied, the Hamiltonian (1) is non-Hermitian, and the bra-vectors need to be constructed separately. The bra-vector analog of the basis (16) can be built using identities for the bra-vector $\phi(u) = (\tilde\theta_1(u), -\tilde\theta_4(u))$ analogous to (7):

$$\phi_n(u)\phi_{n+1}(u \pm \eta)\mathbf{h}_{n,n+1} = \phi_n(u)\phi_{n+1}(u \pm \eta) \times \big[\pm f(u)\sigma_n^z \mp f(u \pm \eta)\sigma_{n+1}^z + w(\pm u)\big], \tag{18}$$

$$f(u)\phi(u)\sigma^z = a_\pm(u)\phi(u) + b_\pm(u)\phi(u \pm 2\eta). \tag{19}$$

The bra-vectors of type (16) constituting the basis of the chiral invariant subspace for bra-vectors can then be constructed by replacement of all $\psi_n(u) \to \phi_n(u)$ in (13).

IV. $M = 0$ CASE: PERFECT HELIX WITHOUT KINKS

Let us introduce the following states:

$$|\Psi_0^{\pm}(u)\rangle = \bigotimes_{n=1}^{N} \psi(u \pm n\eta). \tag{20}$$

The state $|\Psi_0^{\pm}(u)\rangle$ is chiral (the sign $\pm$ in (20) indicates the sign of chirality) and can be viewed as an elliptic analog of the spin-helix eigenstate of the periodic XXZ model at root of unity anisotropies [32].

Both elliptic spin-helix states (20) are eigenstates of the XYZ Hamiltonian. Indeed, Eq. (3) with $M = 0$ gives

$$\psi(u \pm N\eta) \propto \psi(u), \quad f(u \pm N\eta) = f(u), \tag{21}$$

for arbitrary u. Acting by the Hamiltonian on $|\Psi_0^{\pm}(u)\rangle$ and using Eq. (7), we obtain

$$H\,|\Psi_0^{\pm}(u)\rangle = E_0\,|\Psi_0^{\pm}(u)\rangle\,, \quad E_0 = Ng(\eta) + 4\mathrm{i}\pi L\,\frac{\theta_1(\eta)}{\theta_1'(0)}. \tag{22}$$

Due to $\tilde{\theta}_\alpha(1-u) = \tilde{\theta}_\alpha(u)$, $\alpha = 1, 4$, it is easy to prove $|\Psi_0^{-}(u)\rangle = |\Psi_0^{+}(1-u)\rangle$. The eigenvalue E_0 is consistent with those given by other approaches [10,20]. Since E_0 is u-independent, the eigenvalue is degenerate. Linearly independent eigenstates are obtained by choosing different u in (20). One can prove that the energy level E_0 is at least $2N$-fold degenerate, see Appendix F. Rather remarkably, the elliptic spin-helix state (20) can be targeted in an open XYZ chain with strong local dissipation applied to edge spins in the quantum Zeno regime [26], the inverse strength of dissipation playing the role of an effective temperature, and the state (20) playing the role of an effective ground state.

V. ONE-KINK AND TWO-KINKS CASES $M = 1, 2$

One-kink case $M = 1$.
Using Eqs. (3), (4) with $M = 1$ we get

$$f(u + N\eta - 2\eta) = f[u + 2(s+1)\eta] = f(u),$$
$$|d+s+1;n\rangle \propto |d;n\rangle\,,$$

for arbitrary u, d, n. Acting Hamiltonian H on $\{|d;n\rangle\}$ and using Eqs. (7) and (10) repeatedly, we arrive at

$$\begin{aligned}
H|d;n\rangle &= A(u_{2d+n})|d;n\rangle + 2A_-(u_{2d+n})|d;n-1\rangle + 2A_+(u_{2d+n})|d;n+1\rangle, \quad n = 1,\dots,N-1,\\
H|d;N\rangle &= A(u_{2d+N})|d;N\rangle + 2A_-(u_{2d+N})|d;N-1\rangle + 2A_+(u_{2d+2})|d+1;1\rangle,\\
H|d;1\rangle &= A(u_{2d+1})|d;1\rangle + 2A_+(u_{2d+1})|d;2\rangle + 2A_-(u_{2d+N-1})\mathrm{e}^{4\mathrm{i}\pi L\eta}|d-1;N\rangle,\\
H\,|s;N\rangle &= A(u_{2s+N})|s;N\rangle + 2A_-(u_{2s+N})|s;N-1\rangle + 2A_+(u_0)\mathrm{e}^{4\mathrm{i}\pi L_0\eta}W|0;1\rangle,\\
H|0;1\rangle &= A(u_1)|0;1\rangle + 2A_+(u_1)|0;2\rangle + 2A_-(u_{2s+N+1})W^{-1}\mathrm{e}^{4\mathrm{i}\pi L\eta}|s;N\rangle,
\end{aligned} \tag{23}$$

where $A_\pm(u)$, $A(u)$, and W are given by

$$A_-(u) = \frac{\theta_2(u)}{\theta_2(u-\eta)}, \quad A_+(u) = \frac{\theta_2(u-\eta)}{\theta_2(u)}, \quad A_\pm(u + 2l\tau + 2k) = \mathrm{e}^{\pm 4\mathrm{i}\pi l\eta}A_\pm(u),$$

$$A(u) = E_0 + 2\left[g\left(u + \frac{1}{2}\right) - g\left(u - \eta + \frac{1}{2}\right) - 2g(\eta)\right],$$

$$\begin{aligned}
W &= (-1)^{NL_0}\exp\left[-2\mathrm{i}\pi L_0\left(2\eta + \sum_{n=1}^{N} u_{n-2} + NL_0\tau\right)\right]\\
&= \exp\left[-2\mathrm{i}\pi(sL + L + L_0)(2u_{s+1} + L\tau - \eta) - 4\mathrm{i}\pi L_0\eta\right].
\end{aligned}$$

Equations (23) explicitly show that the states $|d;n\rangle$ with $n = 1,\dots,N$ and $d = 0, 1,\dots,s$ form an invariant subspace of H. The respective chiral eigenstates are constructed as a linear combination of $\{|d;n\rangle\}$

$$|\Psi(\lambda)\rangle = \sum_{d=0}^{s}\sum_{n=1}^{N} F_{d,n}(\lambda)\,|d;n\rangle\,, \quad \text{with} \quad H|\Psi(\lambda)\rangle = E(\lambda)|\Psi(\lambda)\rangle. \tag{24}$$

Here we assume both the eigenstate and the energy to depend on the Bethe root λ. $E(\lambda)$ is parametrized as

$$E(\lambda) = E_0 + E_b(\lambda), \tag{25}$$

$$E_b(\lambda) = 2\left[g\left(\lambda - \frac{\eta}{2}\right) - g\left(\lambda + \frac{\eta}{2}\right)\right], \tag{26}$$

where E_0 is a "vacuum" energy (22). Substituting (24) into the eigenequation of H and using (23) we obtain the following functional recursive relations:

$$\begin{aligned}&A_-(u_{2d+n+1})F_{d,n+1}(\lambda)+A_+(u_{2d+n-1})F_{d,n-1}(\lambda)=B(\lambda,u_{2d+n})F_{d,n}(\lambda),\\&\mathrm{e}^{4\mathrm{i}\pi L\eta}A_-(u_{2d+N+1})F_{d+1,1}(\lambda)+A_+(u_{2d+N-1})F_{d,N-1}(\lambda)=B(\lambda,u_{2d+N})F_{d,N}(\lambda),\\&A_+(u_{2d})F_{d-1,N}(\lambda)+A_-(u_{2d+2})F_{d,2}(\lambda)=B(\lambda,u_{2d+1})F_{d,1}(\lambda),\\&\mathrm{e}^{4\mathrm{i}\pi L_0\eta}WA_+(u_0)F_{s,N}(\lambda)+F_{0,2}(\lambda)A_-(u_2)=B(\lambda,u_1)F_{0,1}(\lambda),\\&W^{-1}\mathrm{e}^{4\mathrm{i}\pi L\eta}A_-(u_{2s+N+1})F_{0,1}+A_+(u_{2s+N-1})F_{s,N-1}(\lambda)=B(\lambda,u_{2s+N})F_{s,N}(\lambda),\end{aligned}\tag{27}$$

where

$$B(\lambda,u)=\frac{\theta_1\left(\lambda+\frac{\eta}{2}\right)}{\theta_1\left(\lambda-\frac{\eta}{2}\right)}\frac{\theta_2(u-\eta)\theta_2\left(\lambda-u-\frac{\eta}{2}\right)}{\theta_2(u)\theta_2\left(\lambda-u+\frac{\eta}{2}\right)}+\frac{\theta_1\left(\lambda-\frac{\eta}{2}\right)}{\theta_1\left(\lambda+\frac{\eta}{2}\right)}\frac{\theta_2(u)\theta_2\left(\lambda-u+\frac{3\eta}{2}\right)}{\theta_2(u-\eta)\theta_2\left(\lambda-u+\frac{\eta}{2}\right)}.$$

We propose the following ansatz for the coefficients $F_{d,n}(\lambda)$:

$$F_{d,n}(\lambda)=\alpha_d\,U^{(n)}_{2d+n}(\lambda),\tag{28}$$

$$\alpha_d=\exp\left[2\mathrm{i}\pi Ld(2u_d+2L\tau+\eta)-d\xi\right],\tag{29}$$

$$U^{(n)}_m(\lambda)=\left[\frac{\theta_1\left(\lambda+\frac{\eta}{2}\right)}{\theta_1\left(\lambda-\frac{\eta}{2}\right)}\right]^n\frac{\theta_2\left(\lambda-u_m+\frac{\eta}{2}\right)}{\theta_2(u_{m-1})\theta_2(u_m)},\tag{30}$$

where ξ is an unknown parameter. The function $U^{(n)}_m(\lambda)$ satisfies the following identity:

$$\begin{aligned}&A_-(u_{m+1})U^{(n+1)}_{m+1}(\lambda)+A_+(u_{m-1})U^{(n-1)}_{m-1}(\lambda)\\&=B(\lambda,u_m)U^{(n)}_m(\lambda),\end{aligned}\tag{31}$$

for arbitrary λ, m, n. Due to (31), the first of Eqs. (27) is satisfied automatically. Inserting our ansatz (28) into the remaining Eqs. (27), we get the following BAE for λ and ξ:

$$\left[\frac{\theta_1\left(\lambda+\frac{\eta}{2}\right)}{\theta_1\left(\lambda-\frac{\eta}{2}\right)}\right]^N\exp(4\mathrm{i}\pi L\lambda+\xi)=1,\tag{32}$$

$$\exp[4\mathrm{i}\pi L_0\lambda-(s+1)\xi]=1.\tag{33}$$

When N is even, $L_0\leqslant|L|$. For odd N, $L_0<|L|$ or $L_0=|2L|$. Our BAE (32), (33) are consistent with those given by the off-diagonal Bethe ansatz method [20].

For the Hermitian case when τ is purely imaginary and η is real, entailing $L=L_0=0$, our BAE (32), (33) simplify as

$$\mathrm{e}^{\xi}\left[\frac{\theta_1\left(\lambda+\frac{\eta}{2}\right)}{\theta_1\left(\lambda-\frac{\eta}{2}\right)}\right]^N=1,\tag{34}$$

$$\mathrm{e}^{(s+1)\xi}=1,\tag{35}$$

while the coefficient $F_{d,n}(\lambda)$ becomes

$$F_{d,n}(\lambda)=\mathrm{e}^{-d\xi}\left[\frac{\theta_1\left(\lambda+\frac{\eta}{2}\right)}{\theta_1\left(\lambda-\frac{\eta}{2}\right)}\right]^n\frac{\theta_2\left(\lambda-u_{2d+n}+\frac{\eta}{2}\right)}{\theta_2(u_{2d+n-1})\theta_2(u_{2d+n})}.$$

An example of BAE solutions is given in Table I. It is noteworthy to point out that some Bethe roots in Table I have an obvious tight connection with τ, e.g., $\mathrm{Im}[\lambda]=\frac{\tau}{2\mathrm{i}}$. In the limit $\tau\to+\mathrm{i}\infty$, the XYZ model with parameters listed in the left panel of Table I degenerates into the XXZ model with $\Delta=\cos(\pi\eta)=-\frac{1}{2}$, see Eq. (54). Some Bethe roots will tend to $\pm\mathrm{i}\infty$, becoming so-called phantom Bethe roots, i.e., special roots contributing zero energy [32] and thus leading to extra degeneracies in the spectrum of the XXZ Hamiltonian. For more examples of the sort, see Tables VI and VII.

Remark A1. If $\{\lambda,\xi\}$ is a solution of BAE (32), (33), then $\{\lambda+1,\xi\}$ and $\{\lambda+\tau,\xi'\}$ are also BAE solutions. Since

$$F_{d,n}(\lambda+1)=-F_{d,n}(\lambda),\quad \mathrm{e}^{\xi}=\mathrm{e}^{\xi'-4\mathrm{i}\pi\eta},$$
$$F_{d,n}(\lambda+\tau)|_{\xi=\xi'}=\mathrm{e}^{-2\mathrm{i}\pi\left(\lambda-u_0+\frac{\eta}{2}+\frac{\tau}{2}\right)}F_{d,n}(\lambda),\tag{36}$$

these solutions are equivalent. So we restrict the Bethe root λ to the rectangle $0\leqslant\mathrm{Re}[\lambda]<1$, $0\leqslant\mathrm{Im}[\lambda]<\mathrm{Im}[\tau]$.

Remark B1. Due to the identity $E_b(m+m'\tau-u)=E_b(u)$, $m,m'=0,1$, the solutions $\{\lambda,\xi\}$ and $\{m+m'\tau-\lambda,\xi''\}$, $m,m'=0,1$ correspond to the same energy; see Table I for an example.

Next we consider the case of two-kink states.

Two-kink case $M=2$.

We proceed analogously in the case $M=2$. The vectors $\{|d;n_1,n_2\rangle\}$ with $1\leqslant n_1<n_2\leqslant N$, $d=0,\dots,s$ form an invariant subspace (see Appendix C for details). The corresponding eigenstates can be expanded as

$$|\Psi(\lambda_1,\lambda_2)\rangle=\sum_{d=0}^{s}\sum_{1\leqslant n_1<n_2\leqslant N}F_{d,n_1,n_2}(\lambda_1,\lambda_2)\,|d;n_1,n_2\rangle\,,\tag{37}$$

$$\begin{aligned}&H|\Psi(\lambda_1,\lambda_2)\rangle=E(\lambda_1,\lambda_2)|\Psi(\lambda_1,\lambda_2)\rangle,\\&E(\lambda_1,\lambda_2)=E_0+E_b(\lambda_1)+E_b(\lambda_2),\end{aligned}\tag{38}$$

where E_0 and $E_b(\lambda)$ are defined in (22) and (26), respectively. Substituting Eq. (37) in the eigenvalue equation (38), we obtain functional recursive equations for F_{d,n_1,n_2}, see Appendix C. The recursive equations are solved by the following ansatz:

$$\begin{aligned}F_{d,n_1,n_2}(\lambda_1,\lambda_2)=\alpha_d\big[&C_{1,2}\,U^{(n_1)}_{2d+n_1}(\lambda_1)\,U^{(n_2)}_{2d+n_2-2}(\lambda_2)\\&+C_{2,1}\,U^{(n_1)}_{2d+n_1}(\lambda_2)\,U^{(n_2)}_{2d+n_2-2}(\lambda_1)\big],\end{aligned}\tag{39}$$

where $U^{(n)}_m(\lambda)$ is defined in (30). After some tedious calculations, we obtain the two-body scattering matrix, see Appendix D:

$$S_{1,2}=\frac{C_{2,1}}{C_{1,2}}=\frac{\theta_1(\lambda_1-\lambda_2-\eta)}{\theta_1(\lambda_1-\lambda_2+\eta)},\tag{40}$$

TABLE I. Left: Numerical solutions of BAE (34)–(35) with $N = 5$, $M = 1$, $\tau = 1.47\mathrm{i}$, $\eta = \frac{2}{3}$, and $s = 2$. The exchange coefficients are $\{J_x, J_y, J_z\} = \{1.0302, 0.9710, -0.4999\}$. Right: Numerical solutions of BAE (32)–(33) with $N = 5$, $M = 1$, $\tau = 1.47\mathrm{i}$, $\eta = \frac{2\tau}{3}$, and $s = 2$. The exchange coefficients are $\{J_x, J_y, J_z\} = \{-3.7333, 5.5542, 11.3876\}$. Here $\boxed{\cdots}$ represents the ground-state energy which is degenerate and belongs to the chiral invariant manifold. We see that the Bethe roots λ are distributed on the segment $\mathrm{Re}[\lambda] = 0, \frac{1}{2}$ or $\mathrm{Im}[\lambda] = 0, \frac{\tau}{2\mathrm{i}}$. Since the Hamiltonian is an even function of η, there exists another set of Bethe ansatz solutions with $\eta \to -\eta$, $\lambda \to \lambda$, $\xi \to -\xi$, which corresponds to the same set of energies but different eigenvectors. Thus all the energies in any of the tables are degenerate. The total number of solutions is $2(s+1)N = 30$.

λ	ξ	E
1.4114i	0	$\boxed{-4.4167}$
0.0586i	$4\mathrm{i}\pi\eta$	$\boxed{-4.4167}$
0.2025i	0	−3.7422
1.2675i	$4\mathrm{i}\pi\eta$	−3.7422
$\frac{\tau}{2}$	$2\mathrm{i}\pi\eta$	−2.6195
$\frac{1}{2}+\frac{\tau}{2}$	$2\mathrm{i}\pi\eta$	−2.3825
$\frac{1}{2}$+1.2283i	0	−0.9141
$\frac{1}{2}$+0.2417i	$4\mathrm{i}\pi\eta$	−0.9141
$\frac{1}{2}$+0.1422i	0	0.7378
$\frac{1}{2}$+1.3278i	$4\mathrm{i}\pi\eta$	0.7378
$\frac{1}{2}$+0.0837i	$2\mathrm{i}\pi\eta$	2.1776
$\frac{1}{2}$+1.3863i	$2\mathrm{i}\pi\eta$	2.1776
$\frac{1}{2}$+1.4307i	0	3.1550
$\frac{1}{2}$+0.0393i	$4\mathrm{i}\pi\eta$	3.1550
$\frac{1}{2}$	0	3.5007

λ	ξ	E
0.9209	1.4315i	$\boxed{-39.0981}$
0.0791	−1.4315i	$\boxed{-39.0981}$
0.7417	−2.1637i	−35.4475
0.2583	2.1637i	−35.4475
$\frac{1}{2}$	0	−32.3420
$\frac{1}{2}+\frac{\tau}{2}$	$2\mathrm{i}\pi\eta$	−9.0082
0.6857+$\frac{\tau}{2}$	$2\mathrm{i}\pi\eta$ − 0.5384i	−3.2905
0.3143+$\frac{\tau}{2}$	$2\mathrm{i}\pi\eta$+0.5384i	−3.2905
0.1977+$\frac{\tau}{2}$	$2\mathrm{i}\pi\eta$+1.6559i	7.6856
0.8023+$\frac{\tau}{2}$	$2\mathrm{i}\pi\eta$ − 1.6559i	7.6856
0.8815+$\frac{\tau}{2}$	$2\mathrm{i}\pi\eta$ − 3.0874i	18.2039
0.1185+$\frac{\tau}{2}$	$2\mathrm{i}\pi\eta$+3.0874i	18.2039
0.9440+$\frac{\tau}{2}$	$2\mathrm{i}\pi\eta$+1.6253i	25.5295
0.0560+$\frac{\tau}{2}$	$2\mathrm{i}\pi\eta$ − 1.6253i	25.5295
$\frac{\tau}{2}$	$2\mathrm{i}\pi\eta$	28.1417

and the chiral BAE for the Bethe roots λ_1, λ_2:

$$\exp\left(4\mathrm{i}\pi L\lambda_j + \xi\right)\left[\frac{\theta_1(\lambda_j + \frac{\eta}{2})}{\theta_1(\lambda_j - \frac{\eta}{2})}\right]^N \prod_{k\neq j}^{M} \frac{\theta_1(\lambda_j - \lambda_k - \eta)}{\theta_1(\lambda_j - \lambda_k + \eta)} = 1,$$

$$j = 1, 2, \dots, M, \tag{41}$$

$$\exp[4\mathrm{i}\pi L_0(\lambda_1 + \lambda_2) - (s+1)\xi] = 1. \tag{42}$$

The coefficient α_d in (39) is parameterized in terms of ξ and d as

$$\alpha_d = \exp\left[2\mathrm{i}\pi Ld(2u_d + 2L\tau + \eta) - d\xi\right]. \tag{43}$$

The complete set of solutions of BAE (41), (42) for a special case is given in Table II.

In the next section, Sec. VI, we show that a multibody scattering process between multiple kinks can be factorized as a product of two-body scatterings governed by the chiral S matrix (40), which is typical for integrable systems. Formally, a generalization to the arbitrary M case can be done analogously to the conventional coordinate Bethe ansatz method.

VI. GENERALIZATION OF THE CHIRAL BETHE ANSATZ TO ARBITRARY M CASE

For arbitrary M, the eigenstates are expanded as

$$|\Psi(\lambda_1, \dots, \lambda_M)\rangle = \sum_{d=0}^{s} \sum_{\substack{1\leqslant n_1 < n_2 < \cdots \\ \cdots < n_M \leqslant N}} F_{d,n_1,n_2,\dots,n_M}(\lambda_1, \dots, \lambda_M) \times |d; n_1, \dots, n_M\rangle,$$

where the corresponding energy is

$$E(\lambda_1, \dots, \lambda_M) = E_0 + \sum_{k=1}^{M} E_b(\lambda_k).$$

We propose the following ansatz:

$$F_{d,n_1,n_2,\dots,n_M}(\lambda_1, \dots, \lambda_M) = \alpha_d \sum_{x_1,\dots,x_M} C_{x_1,\dots,x_M} \prod_{k=1}^{M} U^{(n_k)}_{2d-2k+n_k+2}(\lambda_{x_k}), \tag{44}$$

where $U_m^{(n)}(\lambda)$ is defined in (30) and $\{x_1, \dots, x_M\}$ is a permutation of $\{1, \dots, M\}$. The coefficients $\{C_{x_1,\dots,x_M}\}$ in terms of Bethe roots $\{\lambda_1, \dots, \lambda_M\}$ satisfy

$$\frac{C_{\dots,x_{n+1},x_n,\dots}}{C_{\dots,x_n,x_{n+1},\dots}} = \frac{\theta_1\left(\lambda_{x_n} - \lambda_{x_{n+1}} - \eta\right)}{\theta_1\left(\lambda_{x_n} - \lambda_{x_{n+1}} + \eta\right)}. \tag{45}$$

The Bethe roots and the parameter ξ satisfy the following BAE:

$$\exp(4\mathrm{i}\pi L\lambda_j + \xi)\left[\frac{\theta_1\left(\lambda_j + \frac{\eta}{2}\right)}{\theta_1\left(\lambda_j - \frac{\eta}{2}\right)}\right]^N \prod_{k\neq j}^{M} \frac{\theta_1(\lambda_j - \lambda_k - \eta)}{\theta_1(\lambda_j - \lambda_k + \eta)} = 1,$$

$$j = 1, 2, \dots, M, \tag{46}$$

$$\exp\left(4\mathrm{i}\pi L_0 \sum_{k=1}^{M} \lambda_k - (s+1)\xi\right) = 1. \tag{47}$$

The coefficient α_d in (44) can be parameterized in terms of ξ as

$$\alpha_d = \exp\left[2\mathrm{i}\pi Ld(2u_d + 2L\tau + \eta) - d\xi\right].$$

Remark A2. One can verify that $\{\lambda_1, \lambda_2, \dots, \lambda_M, \xi\}$, $\{\lambda_1 + 1, \lambda_2, \dots, \lambda_M, \xi\}$, and $\{\lambda_1 + \tau, \lambda_2, \dots, \lambda_M, \xi + 4\mathrm{i}\pi\eta\}$

TABLE II. Numerical solutions of BAE (41), (42) with $N = 7, M = 2, \tau = 0.38\mathrm{i}, \eta = \frac{2\tau}{3}$, and $s = 2$. The exchange coefficients are $\{J_x, J_y, J_z\} = \{-0.8500, 1.6986, 1.7012\}$. The total number of solutions in the tables is $(s+1)\binom{N}{2} = 63$. Another 63 solutions/eigenvectors corresponding to the same set of energies are obtained by a symmetry operation, i.e., replacement $\xi \to -\xi$ in the tables, and the replacements $\eta \to -\eta$, $\xi \to -\xi$ and $\lambda_{1,2} \to \lambda_{1,2}$ in the chiral basis (16) and the expansion coefficients (39). The total number of chiral solutions is $2(s+1)\binom{N}{2} = 126$. The entries of the table inside boxes $\boxed{\cdots}$ represent the ground-state energy. For all entries, the real part of ξ is given by $2i\pi\eta m$, where $m = 0, 1, 2$.

λ_1	λ_2	ξ	E
0.9417	0.0220	1.7902i	$\boxed{-11.7526}$
0.0583	0.9780	−1.7902i	$\boxed{-11.7526}$
0.1106	0.0112	1.0206i	−10.6912
0.8894	0.9888	−1.0206i	−10.6912
0.1021	0.8979	0	−9.0419
0.0506	0.5068	0.4805i	−8.6817
0.9494	0.4932	−0.4805i	−8.6817
$0.5068+\frac{\tau}{2}$	0.0506	$2i\pi\eta+0.4808\mathrm{i}$	−8.6706
$0.4932+\frac{\tau}{2}$	0.9494	$2i\pi\eta-0.4808\mathrm{i}$	−8.6706
0.0125	$0.8831+\frac{\tau}{2}$	$2i\pi\eta+1.2194\mathrm{i}$	−7.6183
0.9875	$0.1169+\frac{\tau}{2}$	$2i\pi\eta-1.2194\mathrm{i}$	−7.6183
$0.9158+\frac{\tau}{2}$	0.9715	$2i\pi\eta-0.9443\mathrm{i}$	−5.9926
$0.0842+\frac{\tau}{2}$	0.0285	$2i\pi\eta+0.9443\mathrm{i}$	−5.9926
$\frac{1}{2}+\frac{\tau}{2}$	$\frac{1}{2}$	$2i\pi\eta$	−5.9497
$\frac{1}{2}+0.0951\mathrm{i}$	$\frac{1}{2}+0.2849\mathrm{i}$	$4i\pi\eta$	−5.9497
$0.1106+\frac{\tau}{2}$	0.4336	$2i\pi\eta+0.3696\mathrm{i}$	−4.0638
0.5664	$0.8894+\frac{\tau}{2}$	$2i\pi\eta-0.3696\mathrm{i}$	−4.0638
$0.5669+\frac{\tau}{2}$	$0.8890+\frac{\tau}{2}$	$4i\pi\eta-0.3696\mathrm{i}$	−4.0621
$0.4331+\frac{\tau}{2}$	$0.1110+\frac{\tau}{2}$	$4i\pi\eta+0.3696\mathrm{i}$	−4.0621
$0.9263+\frac{\tau}{2}$	0.0969	$2i\pi\eta+0.1940\mathrm{i}$	−3.7988
$0.0737+\frac{\tau}{2}$	0.9031	$2i\pi\eta-0.1940\mathrm{i}$	−3.7988
0.0437	$0.9463+\frac{\tau}{2}$	$2i\pi\eta-2.1785\mathrm{i}$	−3.2901
0.9563	$0.0537+\frac{\tau}{2}$	$2i\pi\eta+2.1785\mathrm{i}$	−3.2901
0.9502+0.1265i	0.9502+0.2535i	$4i\pi\eta-0.8350\mathrm{i}$	−3.2592
0.0498+0.1265i	0.0498+0.2535i	$4i\pi\eta+0.8350\mathrm{i}$	−3.2592
0.0158+0.1267i	0.0158+0.2533i	$4i\pi\eta-1.8298\mathrm{i}$	−2.6256
0.9842+0.1267i	0.9842+0.2533i	$4i\pi\eta+1.8298\mathrm{i}$	−2.6256
$0.9581+\frac{\tau}{2}$	0	$2i\pi\eta+1.7432\mathrm{i}$	−2.5499
$0.0419+\frac{\tau}{2}$	0	$2i\pi\eta-1.7432\mathrm{i}$	−2.5499
$0.0392+\frac{\tau}{2}$	0.0638	$2i\pi\eta+0.8629\mathrm{i}$	−1.2544
$0.9608+\frac{\tau}{2}$	0.9362	$2i\pi\eta-0.8629\mathrm{i}$	−1.2544
0.9653	$0.0153+\frac{\tau}{2}$	$2i\pi\eta+1.9316\mathrm{i}$	0.5804
0.0347	$0.9847+\frac{\tau}{2}$	$2i\pi\eta-1.9316\mathrm{i}$	0.5804
0.0190	$0.0116+\frac{\tau}{2}$	$2i\pi\eta-1.8375\mathrm{i}$	0.5941
0.9810	$0.9884+\frac{\tau}{2}$	$2i\pi\eta+1.8375\mathrm{i}$	0.5941
$0.9767+\frac{\tau}{2}$	0.0918	$2i\pi\eta+0.5736\mathrm{i}$	1.1487
$0.0233+\frac{\tau}{2}$	0.9082	$2i\pi\eta-0.5736\mathrm{i}$	1.1487
0.5063	$0.9655+\frac{\tau}{2}$	$2i\pi\eta-0.2368\mathrm{i}$	1.6849
0.4937	$0.0345+\frac{\tau}{2}$	$2i\pi\eta+0.2368\mathrm{i}$	1.6849
$0.5063+\frac{\tau}{2}$	$0.9655+\frac{\tau}{2}$	$4i\pi\eta-0.2369\mathrm{i}$	1.6944
$0.4937+\frac{\tau}{2}$	$0.0345+\frac{\tau}{2}$	$4i\pi\eta+0.2369\mathrm{i}$	1.6944
$0.0493+\frac{\tau}{2}$	$0.8925+\frac{\tau}{2}$	$4i\pi\eta+1.6063\mathrm{i}$	2.0519
$0.9507+\frac{\tau}{2}$	$0.1075+\frac{\tau}{2}$	$4i\pi\eta-1.6063\mathrm{i}$	2.0519
0.9158	$0.9923+\frac{\tau}{2}$	$2i\pi\eta-0.7697\mathrm{i}$	2.1506
0.0842	$0.0077+\frac{\tau}{2}$	$2i\pi\eta+0.7697\mathrm{i}$	2.1506
$0.0703+\frac{\tau}{2}$	$0.9297+\frac{\tau}{2}$	$4i\pi\eta$	2.1783
$\frac{1}{2}$	$\frac{\tau}{2}$	$2i\pi\eta$	4.2446

TABLE II. (*Continued.*)

λ_1	λ_2	ξ	E
$\frac{1}{2}+\frac{\tau}{2}$	$\frac{\tau}{2}$	$4i\pi\eta$	4.2550
$0.0242+\frac{\tau}{2}$	$0.1004+\frac{\tau}{2}$	$4i\pi\eta-1.0503\mathrm{i}$	5.1168
$0.9758+\frac{\tau}{2}$	$0.8996+\frac{\tau}{2}$	$4i\pi\eta+1.0503\mathrm{i}$	5.1168
$0.1046+\frac{\tau}{2}$	$0.9907+\frac{\tau}{2}$	$4i\pi\eta-1.2961\mathrm{i}$	6.1318
$0.8954+\frac{\tau}{2}$	$0.0093+\frac{\tau}{2}$	$4i\pi\eta+1.2961\mathrm{i}$	6.1318
$0.0198+\frac{\tau}{2}$	$0.9321+\frac{\tau}{2}$	$4i\pi\eta-0.4029\mathrm{i}$	7.5138
$0.9802+\frac{\tau}{2}$	$0.0679+\frac{\tau}{2}$	$4i\pi\eta+0.4029\mathrm{i}$	7.5138
$0.9864+\frac{\tau}{2}$	$0.9348+\frac{\tau}{2}$	$4i\pi\eta-0.6600\mathrm{i}$	8.2335
$0.0136+\frac{\tau}{2}$	$0.0652+\frac{\tau}{2}$	$4i\pi\eta+0.6600\mathrm{i}$	8.2335
$0.0469+\frac{\tau}{2}$	$0.9681+\frac{\tau}{2}$	$4i\pi\eta+2.2203\mathrm{i}$	8.2419
$0.9531+\frac{\tau}{2}$	$0.0319+\frac{\tau}{2}$	$4i\pi\eta-2.2203\mathrm{i}$	8.2419
$0.9552+\frac{\tau}{2}$	$0.9967+\frac{\tau}{2}$	$4i\pi\eta-2.4978\mathrm{i}$	10.6968
$0.0448+\frac{\tau}{2}$	$0.0033+\frac{\tau}{2}$	$4i\pi\eta+2.4978\mathrm{i}$	10.6968
$0.0069+\frac{\tau}{2}$	$0.9700+\frac{\tau}{2}$	$4i\pi\eta+1.9014\mathrm{i}$	12.2719
$0.9931+\frac{\tau}{2}$	$0.0300+\frac{\tau}{2}$	$4i\pi\eta-1.9014\mathrm{i}$	12.2719
$0.0178+\frac{\tau}{2}$	$0.9822+\frac{\tau}{2}$	$4i\pi\eta$	12.8134

are equivalent solutions. If not stated otherwise, all the Bethe roots are distinct and lie within the rectangle $0 \leqslant \mathrm{Re}[\lambda_j] < 1$, $0 \leqslant \mathrm{Im}[\lambda_j] < \mathrm{Im}[\tau]$.

Remark B2. Our results are independent of whether the XYZ Hamiltonian is Hermitian or not. The only constraints are Eqs. (3) and (4). We have explicitly constructed the ket eigenstates. With the help of Eqs. (18) and (19), we can similarly construct the corresponding bra eigenstates.

Remark C2. The Hamiltonian is invariant under the substitution $\eta \to -\eta$. Once M, η satisfy Eq. (3), another set of solutions exists with $M \to M$, $\eta \to -\eta$. More generally, there may exist a set of integers $\{M_1, \ldots, M_r\}$ satisfying Eq. (3). In this case the r chiral invariant subspaces exist, and for each of them our procedure to construct eigenstates remains valid.

Remark D2. Only part of the eigenstates (equal to the dimension of the chiral invariant subspace) can be constructed with our method. Note, however, that the energy does not depend on the free parameter u_0 which parametrizes the chiral eigenstates via (12), rendering some energy levels degenerate. The degeneracies may be related to the $\mathfrak{sl}_2$ loop algebra [12,33,34].

Remark E2. When N is even and $M = \frac{N}{2}$, Eq. (3) always holds and s in Eq. (4) can be arbitrary large. For the Bethe ansatz with $M = \frac{N}{2}$, an additional selection rule for $\{\lambda_1, \ldots, \lambda_M\}$ is necessary to ensure the eigenstate to be nontrivial. Based on numerics, see e.g., Tables III and IV, we conjecture the following selection rule for the valid Bethe roots:

$$2\sum_{j=1}^{M} \lambda_j = k + l\tau, \quad k, l \in \mathbb{Z}, \tag{48}$$

while the solutions violating the selection rule correspond to invalid eigenstates. The sum rule (48) does not hold for $M \neq \frac{N}{2}$, which can be seen from Tables I and II. The sum rule (48) is consistent with Baxter's observation in [9].

Let us analyze the special case $N = 2M$ presented in Table IV in some more detail. The number of generating states $(s+1)\binom{N}{M} = 30$ is larger than the dimension of the

TABLE III. Left: Numerical solutions of BAE (46)–(47) with $N=2, M=1, \tau=0.38\mathrm{i}, \eta=\frac{2}{5}$, and $s=4$. The exchange coefficients are $\{J_x,J_y,J_z\}=\{3.6415, 0.3172, 0.2155\}$. Right: Numerical solutions of BAE (46)–(47) with $N=2, M=1, \tau=0.38\mathrm{i}, \eta=\frac{2\tau}{5}$, and $s=4$. The exchange coefficients are $\{J_x,J_y,J_z\}=\{0.3741, 1.2093, 1.2116\}$.

λ_1	$2\lambda_1$	ξ	E
0	0	0	−8.3486
$\frac{\tau}{2}$	τ	$2i\pi\eta$	−6.2176
$\frac{1}{2}+\frac{\tau}{2}$	$1+\tau$	$2i\pi\eta$	7.0797
$\frac{1}{2}$	1	0	7.4865

λ_1	$2\lambda_1$	ξ	E
0	0	0	−5.5890
$\frac{1}{2}$	1	0	0.7436
$\frac{1}{2}+\frac{\tau}{2}$	$1+\tau$	$2i\pi\eta$	0.7526
$\frac{\tau}{2}$	τ	$2i\pi\eta$	4.0938

Hilbert space $2^N=16$, so one may think that all eigenstates can be obtained. Nevertheless, we find that among 30 generating states $\{|d;n,m\rangle\}$, only 15 are linearly independent, regardless of the choice of the overall phase u_0 or chirality. Any of the states $|1,2\rangle, |1,4\rangle, |2,3\rangle, |3,4\rangle$ where $|k,l\rangle = \sigma_k^-\sigma_l^-|\uparrow\uparrow\ldots\uparrow\rangle$, cannot be expanded by the states $\{|d;n,m\rangle\}$ alone. It can be proved that

$$\begin{aligned}H|3,4\rangle &= H|2,3\rangle = H|1,4\rangle = H|1,2\rangle\\ &= (J_x-J_y)(|\uparrow\uparrow\uparrow\uparrow\rangle + |\downarrow\downarrow\downarrow\downarrow\rangle)\\ &\quad + (J_x+J_y)(|2,4\rangle + |1,3\rangle).\end{aligned}$$

Therefore, $\kappa_1|3,4\rangle+\kappa_2|2,3\rangle+\kappa_3|1,4\rangle-(\kappa_1+\kappa_2+\kappa_3)|1,2\rangle$ for any $\kappa_1,\kappa_2,\kappa_3$ is an eigenstate of H with eigenvalue 0. We verify that $|1,2\rangle-|3,4\rangle$ and $|2,3\rangle-|1,4\rangle$ are linear combinations of $\{|d;n,m\rangle\}$ so that the missing eigenstate can be constructed by letting $\kappa_2\neq-\kappa_3$. With this degree of freedom in mind, the missing eigenstate is given by

$$|\Omega\rangle = |1,2\rangle - |2,3\rangle, \quad H|\Omega\rangle = 0. \tag{49}$$

For a larger system size $N=2M=6$, $s>3$, again $(s+1)\binom{N}{M}>2^N$, but the set of chiral states in (16) contains 60 linearly independent states, while the Hilbert space dimension is $2^6=64$. Denoting $(\sum a_{n_1n_2\ldots n_j}|n_1,n_2,\ldots,n_j\rangle)' = \sum a_{n_1n_2\ldots n_j}|n_1,n_2,\ldots,n_j\rangle'$, where

$$|n_1,\ldots,n_j\rangle = \prod_{k=1}^{j}\sigma_{n_k}^-|\uparrow\uparrow\ldots\uparrow\rangle,$$

$$|n_1,\ldots,n_j\rangle' = \prod_{k=1}^{j}\sigma_{n_k}^+|\downarrow\downarrow\ldots\downarrow\rangle,$$

we find that the remaining four eigenstates of H have a remarkably simple form:

$$\begin{aligned}&|\Omega_1\rangle = |\Phi\rangle + |\Phi\rangle', \quad |\Omega_2\rangle = |\Phi\rangle - |\Phi\rangle',\\ &|\Omega_3\rangle = |\Psi\rangle + |\Psi\rangle', \quad |\Omega_4\rangle = |\Psi\rangle - |\Psi\rangle',\\ &|\Phi\rangle = |1,2\rangle - |2,3\rangle + |3,4\rangle - |4,5\rangle + |5,6\rangle - |1,6\rangle,\\ &|\Psi\rangle = |1,2,4\rangle - |1,4,6\rangle - |2,3,6\rangle - |2,4,5\rangle\\ &\qquad + |2,5,6\rangle + |3,4,6\rangle,\\ &H|\Omega_1\rangle = 2(J_x-J_y+J_z)|\Omega_1\rangle,\\ &H|\Omega_2\rangle = -2(J_x-J_y-J_z)|\Omega_2\rangle,\\ &H|\Omega_3\rangle = 2(J_x+J_y-J_z)|\Omega_3\rangle,\\ &H|\Omega_4\rangle = -2(J_x+J_y+J_z)|\Omega_4\rangle.\end{aligned} \tag{50}$$

At this point it is instructive to compare our approach with Baxter's classical work [9]. When $\mathrm{Im}[\eta]=0$, our BAE coincides with those obtained in [9], where evidence for the

TABLE IV. Left: Numerical solutions of BAE (46)–(47) with $N=4, M=2, \tau=0.38\mathrm{i}, \eta=\frac{2}{5}$, and $s=4$. The exchange coefficients are $\{J_x,J_y,J_z\}=\{3.6415, 0.3172, 0.2155\}$. Right: Numerical solutions of BAE (46)–(47) with $N=4, M=2, \tau=0.38\mathrm{i}, \eta=\frac{2\tau}{5}$, and $s=4$. The exchange coefficients are $\{J_x,J_y,J_z\}=\{0.3741, 1.2093, 1.2116\}$. The missing eigenstate "—" is given by $(\sigma_1^-\sigma_2^- - \sigma_2^-\sigma_3^-)|\uparrow\uparrow\uparrow\uparrow\rangle$. Note that the Bethe roots in both tables satisfy (48).

λ_1	λ_2	$2(\lambda_1+\lambda_2)$	ξ	E
0.0862i	0.2938i	2τ	$4i\pi\eta$	−14.7204
0	$\frac{\tau}{2}$	τ	$2i\pi\eta$	−14.5662
0	$\frac{1}{2}+\frac{\tau}{2}$	$1+\tau$	$2i\pi\eta$	−1.2689
0	$\frac{1}{2}$	1	0	−0.8621
$0.8002+\frac{3\tau}{4}$	$0.1998+\frac{3\tau}{4}$	$2+3\tau$	$6i\pi\eta$	0.0000
$0.8002+\frac{\tau}{4}$	$0.1998+\frac{\tau}{4}$	$2+\tau$	$2i\pi\eta$	0.0000
0.2903i	$\frac{1}{2}$+0.0897i	$1+2\tau$	$4i\pi\eta$	0.0000
0.0897i	$\frac{1}{2}$+0.2903i	$1+2\tau$	$4i\pi\eta$	0.0000
0.0914i	$\frac{1}{2}$+0.0986i	$1+\tau$	$2i\pi\eta$	0.0000
0.2886i	$\frac{1}{2}$+0.2814i	$1+3\tau$	$6i\pi\eta$	0.0000
–	–	–	–	0.0000
$0.7994+\frac{\tau}{2}$	$0.2006+\frac{\tau}{2}$	$2+2\tau$	$4i\pi\eta$	0.1486
$\frac{\tau}{2}$	$\frac{1}{2}+\frac{\tau}{2}$	$1+2\tau$	$4i\pi\eta$	0.8621
$\frac{1}{2}$	$\frac{\tau}{2}$	$1+\tau$	$2i\pi\eta$	1.2689
$\frac{1}{2}$	$\frac{1}{2}+\frac{\tau}{2}$	$2+\tau$	$2i\pi\eta$	14.5662
$\frac{1}{2}$+0.0933i	$\frac{1}{2}$+0.2867i	$2+2\tau$	$4i\pi\eta$	14.5719

λ_1	λ_2	$2(\lambda_1+\lambda_2)$	ξ	E
0.0434	0.9566	2	0	−7.6363
0	$\frac{1}{2}$	1	0	−4.8464
0	$\frac{1}{2}+\frac{\tau}{2}$	$1+\tau$	$2i\pi\eta$	−4.8374
0	$\frac{\tau}{2}$	τ	$2i\pi\eta$	−1.4962
0.8891	$0.6109+\frac{\tau}{2}$	$3+\tau$	$2i\pi\eta$	0.0000
0.1109	$0.3891+\frac{\tau}{2}$	$1+\tau$	$2i\pi\eta$	0.0000
0.8880	0.6120	3	0	0.0000
0.1120	0.3880	1	0	0.0000
0.9488	$0.0512+\frac{\tau}{2}$	$2+\tau$	$2i\pi\eta$	0.0000
0.0512	$0.9488+\frac{\tau}{2}$	$2+\tau$	$2i\pi\eta$	0.0000
–	–	–	–	0.0000
$\frac{1}{2}$	$\frac{1}{2}+\frac{\tau}{2}$	$2+\tau$	$2i\pi\eta$	1.4962
$\frac{1}{2}$+0.2850i	$\frac{1}{2}$+0.0950i	$2+2\tau$	$4i\pi\eta$	1.4962
$\frac{1}{2}$	$\frac{\tau}{2}$	$1+\tau$	$2i\pi\eta$	4.8374
$\frac{\tau}{2}$	$\frac{1}{2}+\frac{\tau}{2}$	$1+2\tau$	$4i\pi\eta$	4.8464
$0.0622+\frac{\tau}{2}$	$0.9378+\frac{\tau}{2}$	$2+2\tau$	$4i\pi\eta$	6.1401

TABLE V. Bound pair solutions of BAE (46)–(47) with $N = 8, M = 4, \tau = 0.38\mathrm{i}, \eta = \frac{2}{5}$, and $s = 4$. The exchange coefficients are $\{J_x, J_y, J_z\} = \{3.6415, 0.3172, 0.2155\}$.

λ_1	λ_2	λ_3	λ_4	$2\sum_k \lambda_k$	ξ	E
$\frac{\eta}{2}$	$-\frac{\eta}{2}$	0.0424i	0.3376i	2τ	$4\mathrm{i}\pi\eta$	−16.1265
$\frac{\eta}{2}$	$-\frac{\eta}{2}$	$\frac{\tau}{2}$	0	τ	$2\mathrm{i}\pi\eta$	−14.5662
$\frac{\eta}{2}$	$-\frac{\eta}{2}$	0.1366i	0.2434i	2τ	$4\mathrm{i}\pi\eta$	−13.1249
$\frac{\eta}{2}$	$-\frac{\eta}{2}$	$\frac{1}{2}+\frac{\tau}{2}$	0	$1+\tau$	$2\mathrm{i}\pi\eta$	−1.2689
$\frac{\eta}{2}$	$-\frac{\eta}{2}$	$\frac{1}{2}$	0	1	0	−0.8621
$\frac{\eta}{2}$	$-\frac{\eta}{2}$	$0.8000+\frac{\tau}{2}$	$0.2000+\frac{\tau}{2}$	$2+2\tau$	$4\mathrm{i}\pi\eta$	0.0759
$\frac{\eta}{2}$	$-\frac{\eta}{2}$	$\frac{\tau}{2}$	$\frac{1}{2}+\frac{\tau}{2}$	$1+2\tau$	$4\mathrm{i}\pi\eta$	0.8621
$\frac{\eta}{2}$	$-\frac{\eta}{2}$	$\frac{1}{2}$	$\frac{\tau}{2}$	$1+\tau$	$2\mathrm{i}\pi\eta$	1.2689
$\frac{\eta}{2}$	$-\frac{\eta}{2}$	$\frac{1}{2}$+0.2425i	$\frac{1}{2}$+0.1375i	$2+2\tau$	$4\mathrm{i}\pi\eta$	14.2999
$\frac{\eta}{2}$	$-\frac{\eta}{2}$	$\frac{1}{2}+\frac{\tau}{2}$	$\frac{1}{2}$	$2+\tau$	$2\mathrm{i}\pi\eta$	14.5662
$\frac{\eta}{2}$	$-\frac{\eta}{2}$	$\frac{1}{2}$+0.0422i	$\frac{1}{2}$+0.3378i	$2+2\tau$	$4\mathrm{i}\pi\eta$	14.8756

completeness of the Bethe ansatz for the periodic XYZ model with even N was presented. If the BAE solutions are complete, where do the eigenstates and the respective eigenvalues missing in our chiral subspace come from? We propose that in the case $N = 2M \geqslant 4$ the missing eigenstates are generated by bound pair solutions of BAE when two Bethe roots form a pair as

$$\lambda_1 = \frac{\eta}{2}, \quad \lambda_2 = -\frac{\eta}{2}, \quad \frac{\theta_1\left(\lambda_1 + \frac{\eta}{2}\right)}{\theta_1\left(\lambda_1 - \frac{\eta}{2}\right)} \to \infty,$$
$$\frac{\theta_1\left(\lambda_2 + \frac{\eta}{2}\right)}{\theta_1\left(\lambda_2 - \frac{\eta}{2}\right)} \to 0, \quad \frac{\theta_1\left(\lambda_1 + \frac{\eta}{2}\right)}{\theta_1\left(\lambda_1 - \frac{\eta}{2}\right)}\frac{\theta_1\left(\lambda_2 + \frac{\eta}{2}\right)}{\theta_1\left(\lambda_2 - \frac{\eta}{2}\right)} = -1,$$

and the remaining Bethe roots $\{\lambda_3, \ldots, \lambda_{N/2}\}$ satisfy

$$\mathrm{e}^{\xi}\left[\frac{\theta_1\left(\lambda_j + \frac{\eta}{2}\right)}{\theta_1\left(\lambda_j - \frac{\eta}{2}\right)}\right]^{N-1}\frac{\theta_1\left(\lambda_j - \frac{3\eta}{2}\right)}{\theta_1\left(\lambda_j + \frac{3\eta}{2}\right)}\prod_{\substack{k=3\\k\neq j}}^{N/2}\frac{\theta_1(\lambda_j - \lambda_k - \eta)}{\theta_1(\lambda_j - \lambda_k + \eta)} = 1,$$
$$j = 3, \ldots, \tfrac{N}{2}, \tag{51}$$

$$\exp\left(4\mathrm{i}\pi L_0\sum_{k=3}^{N/2}\lambda_k - (s+1)\xi\right) = 1. \tag{52}$$

A bound pair $\lambda_1 = -\lambda_2 = \frac{\eta}{2}$ contributes $-4g(\eta)$ to the energy and leads to

$$E\left(\frac{\eta}{2}, -\frac{\eta}{2}, \lambda_3, \ldots, \lambda_{N/2}\right) = E_0 - 4g(\eta) + \sum_{k=3}^{N/2}E_b(\lambda_k)$$
$$= (N-4)g(\eta) + \sum_{k=3}^{N/2}E_b(\lambda_k). \tag{53}$$

A possibility of such bound pair solutions was envisaged in [9] and there studied explicitly for the XXZ chain. Here we explicitly point them out: for $N = 4$, the only bound pair solution (corresponding to one "missing" eigenstate) is

$$\lambda_1 = \frac{\eta}{2}, \quad \lambda_2 = -\frac{\eta}{2}, \quad \xi = 0, \quad E = 0.$$

For $N = 6$ there are four bound pair BAE solutions (corresponding to four "missing" eigenstates):

$$(1): \lambda_1 = \frac{\eta}{2}, \quad \lambda_2 = -\frac{\eta}{2}, \quad \lambda_3 = 0, \quad \xi = 0, \quad E = -2(J_x + J_y + J_z),$$
$$(2): \lambda_1 = \frac{\eta}{2}, \quad \lambda_2 = -\frac{\eta}{2}, \quad \lambda_3 = \frac{1}{2}, \quad \xi = 0, \quad E = 2(J_x + J_y - J_z),$$
$$(3): \lambda_1 = \frac{\eta}{2}, \quad \lambda_2 = -\frac{\eta}{2}, \quad \lambda_3 = \frac{\tau}{2}, \quad \xi = 2\mathrm{i}\pi\eta, \quad E = -2(J_x - J_y - J_z),$$
$$(4): \lambda_1 = \frac{\eta}{2}, \quad \lambda_2 = -\frac{\eta}{2}, \quad \lambda_3 = \frac{1+\tau}{2}, \quad \xi = 2\mathrm{i}\pi\eta, \quad E = 2(J_x - J_y + J_z).$$

When $N = 8$, we find 11 BAE solutions with bound pairs corresponding to 11 "missing" eigenvalues, listed in Table V. Remarkably, the missing eigenstates always correspond to the bound pair BAE solutions. We conjecture that this correspondence holds for larger systems with $N = 2M \geqslant 10$ as well. For $N = 2M = 4, 6, 8, 10, 12$, the total number of missing eigenstates (i.e., not expandable by our set of chiral states) is 1,4,11,37,66, respectively, according to a numerical analysis, provided that $d_{M,s}$ (17) is larger than 2^N. The relative fraction of missing eigenstates $\frac{1}{16}, \frac{4}{2^6}, \frac{11}{2^8}, \frac{37}{2^{10}}, \frac{66}{2^{12}}$ for $N = 4, 6, 8, 10, 12$ is getting smaller with the system size.

Summarizing, we propose that the standard BAE for periodic XYZ and even N contain two types of solutions: the regular ones (constituting the vast majority), and those with a bound pair $\lambda_1 = -\lambda_2 = \frac{\eta}{2}$. Remarkably, all eigenstates corresponding to regular BAE solutions can be understood in terms of our simple chiral basis with kinks (16); see also Fig. 1. Unlike regular eigenstates, the bound pair eigenstates seem to lack such an appealing representation, although we can readily construct them using the generalized basis from [7], see Appendix G. Explicit expressions for the bound pair eigenstates (49), (50) suggest that actually these eigenstates might have a simpler representation in the usual computational basis. Further technical details concerning bound pair eigenstates, are given in Appendix G.

Our findings readily reduce to the partially anisotropic Heisenberg Hamiltonian, see Sec. VII.

VII. XXZ AND XX LIMITS OF THE XYZ MODEL

By letting $\tau \to +\mathrm{i}\infty$, the XYZ chain degenerates into the partially anisotropic XXZ chain as

$$J_x \to 1, \quad J_y \to 1, \quad J_z \to \cos(\pi\eta). \tag{54}$$

In the limit $u \to \tilde{u} + \frac{\tau}{2}$, $\tau \to +\mathrm{i}\infty$ ($\tilde{u}$ being finite), we get

$$\lim_{\substack{\tau\to+\mathrm{i}\infty \\ u\to\tilde{u}+\frac{\tau}{2}}} \frac{\theta_2(u)}{\theta_1(u)} = -\mathrm{i}, \qquad \lim_{\substack{\tau\to+\mathrm{i}\infty \\ u\to\tilde{u}+\frac{\tau}{2}}} \frac{\tilde{\theta}_4(u)}{\tilde{\theta}_1(u)} = -\mathrm{e}^{\mathrm{i}\pi(\tilde{u}+\frac{1}{2})},$$

$$\lim_{\substack{\tau\to+\mathrm{i}\infty \\ u\to\tilde{u}+\frac{\tau}{2}}} f(u) = -\mathrm{i}\sin(\pi\eta), \qquad \lim_{\substack{\tau\to+\mathrm{i}\infty \\ u\to\tilde{u}+\frac{\tau}{2}}} w(u) = \cos(\pi\eta).$$

The divergence condition (7) degenerates into the XXZ divergence condition [23,24,32,35]

$$\mathbf{h}^{\mathrm{XXZ}}_{n,n+1}\tilde{\psi}_n(\tilde{u})\tilde{\psi}_{n+1}(\tilde{u}\pm\eta) = \left[\mp\mathrm{i}\sin(\pi\eta)\,\sigma^z_n \pm \mathrm{i}\sin(\pi\eta)\,\sigma^z_{n+1} + \cos(\pi\eta)\right]\tilde{\psi}_n(\tilde{u})\tilde{\psi}_{n+1}(\tilde{u}\pm\eta), \tag{55}$$

where $\mathbf{h}^{\mathrm{XXZ}}_{n,n+1} = \sigma^x_n\sigma^x_{n+1} + \sigma^y_n\sigma^y_{n+1} + \cos(\pi\eta)\,\sigma^z_n\sigma^z_{n+1}$ and $\tilde{\psi}(u) = (1,\ \mathrm{e}^{\mathrm{i}\pi(u+\frac{1}{2})})^T$.

The parameter η now can only take some discrete real values according to Eqs. (3) and (4):

$$(N-2M)\eta = 2K, \quad 0 \leqslant M \leqslant N, \quad K \in \mathbb{Z},$$
$$2(s+1)\eta = 2K_0, \quad s \in \mathbb{N}, \quad K_0 \in \mathbb{Z}. \tag{56}$$

Equations (56) are constraints under which a chiral invariant subspace exists for a periodic XXZ spin-$\frac{1}{2}$ chain. Thus we can follow the same procedure to study the periodic XXZ chain at roots of unity [33,34,36]. The corresponding BAE obtained from our chiral coordinate Bethe ansatz are deformed ones [32,36]:

$$\mathrm{e}^{\bar{\xi}}\left[\frac{\sinh\left(\bar{\lambda}_j + \frac{\bar{\eta}}{2}\right)}{\sinh\left(\bar{\lambda}_j - \frac{\bar{\eta}}{2}\right)}\right]^N \prod_{k\neq j}^{M} \frac{\sinh(\bar{\lambda}_j - \bar{\lambda}_k - \bar{\eta})}{\sinh(\bar{\lambda}_j - \bar{\lambda}_k + \bar{\eta})} = 1,$$
$$\mathrm{e}^{(s+1)\bar{\xi}} = 1, \quad \bar{\eta} = \mathrm{i}\pi\eta, \quad j = 1,\ldots,M. \tag{57}$$

From Eq. (56) we find the parameter $\bar{\xi}$ in (57) can take values $\pm 2\bar{m}\bar{\eta}$, $\bar{m} \in \mathbb{Z}$. It implies that the conventional BAE for the periodic XXZ chain at root of unity (56) may have solutions with $\bar{m}_0$ phantom Bethe roots and M regular Bethe roots [32], and $\pm$ represents different chirality. In the six-vertex model limit $\tau \to +\mathrm{i}\infty$, the Bethe roots in Eqs. (46), (47) will degenerate into the ones for the XXZ model in (57) as

$$\lim_{\tau\to+\mathrm{i}\infty} \mathrm{i}\pi\lambda_j = \bar{\lambda}_j, \qquad \lim_{\tau\to+\mathrm{i}\infty} \xi = \bar{\xi}. \tag{58}$$

If $\mathrm{i}\,\mathrm{Im}[\lambda_j]/\tau$ tends toward a finite but nonzero number in the limit $\tau \to +\mathrm{i}\infty$, the corresponding Bethe root $\bar{\lambda}_j$ will be a phantom one with $\mathrm{Re}[\bar{\lambda}_j] \to \pm\infty$ [32]. To demonstrate this phenomenon, we do some simple numerical calculations for the $M = 1, 2$ cases with details shown in Tables VI and VII.

TABLE VI. Left: Numerical solutions of BAE (46)–(47) with $N = 5$, $M = 1$, $\tau = 1.8\mathrm{i}$, $\eta = \frac{2}{3}$, and $s = 2$. The exchange coefficients are $\{J_x, J_y, J_z\} = \{1.0106, 0.9896, -0.5000\}$. Right: Numerical solutions of BAE (57) with $N = 5$, $M = 1$, $\eta = \frac{2}{3}$, and $s = 2$. The exchange coefficients are $\{J_x, J_y, J_z\} = \{1, 1, -\frac{1}{2}\}$. Here we let the Bethe root λ lie within a proper range in order to compare the solutions of BAE for the XYZ and XXZ model in a better way. Although the parameter τ we chose is not too large, one can still see the correspondence in (58) approximately. We can verify that BAE in (57) has two phantom solutions.

λ	$\xi/(2\mathrm{i}\pi\eta)$	E	$\bar{\lambda}$	$\bar{\xi}/(2\bar{\eta})$	E
$-0.0586\mathrm{i}$	1	-4.4131	0.1841	1	-4.4126
$0.0586\mathrm{i}$	-1	-4.4131	-0.1841	-1	-4.4126
$0.2027\mathrm{i}$	0	-3.7368	0.6369	0	-3.7361
$-0.2027\mathrm{i}$	0	-3.7368	-0.6369	0	-3.7361
$\frac{\tau}{2}$	1	-2.5421	$-\infty$	1	-2.5000
$\frac{1}{2}-\frac{\tau}{2}$	-1	-2.4581	$\infty+\frac{\mathrm{i}\pi}{2}$	-1	-2.5000
$\frac{1}{2}-0.2420\mathrm{i}$	1	-0.9176	$0.7602+\frac{\mathrm{i}\pi}{2}$	1	-0.9181
$\frac{1}{2}+0.2420\mathrm{i}$	-1	-0.9176	$-0.7602+\frac{\mathrm{i}\pi}{2}$	-1	-0.9181
$\frac{1}{2}+0.1423\mathrm{i}$	0	0.7363	$-0.4470+\frac{\mathrm{i}\pi}{2}$	0	0.7361
$\frac{1}{2}-0.1423\mathrm{i}$	0	0.7363	$0.4470+\frac{\mathrm{i}\pi}{2}$	0	0.7361
$\frac{1}{2}+0.0837\mathrm{i}$	1	2.1767	$-0.2630+\frac{\mathrm{i}\pi}{2}$	1	2.1765
$\frac{1}{2}-0.0837\mathrm{i}$	-1	2.1767	$0.26295+\frac{\mathrm{i}\pi}{2}$	-1	2.1765
$\frac{1}{2}-0.0393\mathrm{i}$	1	3.1543	$0.1233+\frac{\mathrm{i}\pi}{2}$	1	3.1542
$\frac{1}{2}+0.0393\mathrm{i}$	-1	3.1543	$-0.1233+\frac{\mathrm{i}\pi}{2}$	-1	3.1542
$\frac{1}{2}$	0	3.5001	$\frac{\mathrm{i}\pi}{2}$	0	3.5000

The eigenstates constructed by using the chiral basis with fixed number of kinks are not eigenstates of the magnetization operator. However, in the XXZ limit one may project such an eigenstate onto any of the subspaces with fixed magnetization. The result is either 0 or an eigenstate of the Hamiltonian with well-defined magnetization. In this way several eigenstates with same energy, but different magnetizations, respectively different numbers of Bethe rapidities in the conventional Bethe ansatz, are obtained. The degeneracy of the energy eigenvalue in the chiral Bethe ansatz is seen by the different choices of the parameter u_0 that enters the eigenstate, but not the eigenvalue expression.

For $\eta = 0$, the XYZ model degenerates into the isotropic XXX model. In the isotropic case, the spin helical structure disappears and our basis vectors become indistinguishable. The corresponding eigenstates can now be constructed by the conventional Bethe ansatz with the number of Bethe

TABLE VII. Left: Numerical solutions of BAE (46)–(47) with $N = 4$, $M = 2$, $\tau = 1.8\mathrm{i}$, $\eta = \frac{2}{5}$, and $s = 4$. The exchange coefficients are $\{J_x, J_y, J_z\} = \{1.0128, 0.9874, 0.3090\}$. Here the Bethe roots satisfy the sum rule in (48). Right: Numerical solutions of BAE (57) with $N = 4$, $M = 2$, $\eta = \frac{2}{5}$, and $s = 4$. The exchange coefficients are $\{J_x, J_y, J_z\} = \{1, 1, 0.3090\}$. Here "—" represents the bound pair solution. One can see a lot of phantom solutions in the XXZ case. In some solutions, both $\bar{\lambda}_1$ and $\bar{\lambda}_2$ are phantom and they form a string. Such phantom strings will appear in the $M \geqslant 2$ cases. Here $\boxed{\cdots}$ represents the missing bound pair solution.

λ_1	λ_2	$\xi/(2\mathrm{i}\pi\eta)$	E
$0.1141\mathrm{i}$	$-0.1141\mathrm{i}$	0	−6.3093
0	$\frac{\tau}{2}$	1	−4.0510
0	$\frac{1}{2}-\frac{\tau}{2}$	−1	−3.9497
0	$\frac{1}{2}$	0	−1.2360
$-0.1347\mathrm{i}$	$\frac{1}{2}+0.1347\mathrm{i}$	0	0.0000
$0.1347\mathrm{i}$	$\frac{1}{2}-0.1347\mathrm{i}$	0	0.0000
$-0.2764\mathrm{i}$	$\frac{1}{2}+\frac{\tau}{2}+0.2764\mathrm{i}$	1	0.0000
$0.2764\mathrm{i}$	$\frac{1}{2}-\frac{\tau}{2}-0.2764\mathrm{i}$	−1	0.0000
$0.3193\mathrm{i}$	$\frac{\tau}{2}-0.3193\mathrm{i}$	1	0.0000
$-0.3193\mathrm{i}$	$-\frac{\tau}{2}+0.3193\mathrm{i}$	−1	0.0000
$\frac{\eta}{2}$	$-\frac{\eta}{2}$	0	$\boxed{0.0000}$
$0.2486+\frac{\tau}{2}$	$0.7514+\frac{\tau}{2}$	2	1.2356
$\frac{1}{2}-\frac{\tau}{2}$	$-\frac{\tau}{2}$	−2	1.2360
$\frac{\tau}{2}$	$\frac{1}{2}$	1	3.9497
$\frac{1}{2}-\frac{\tau}{2}$	$\frac{1}{2}$	−1	4.0510
$\frac{1}{2}-0.1637\mathrm{i}$	$\frac{1}{2}+0.1637\mathrm{i}$	0	5.0737

$\bar{\lambda}_1$	$\bar{\lambda}_2$	$\bar{\xi}/(2\bar{\eta})$	E
−0.3584	0.3584	0	−6.3085
0	$-\infty$	1	−4.0000
0	$\infty+\frac{\mathrm{i}\pi}{2}$	−1	−4.0000
0	$\frac{\mathrm{i}\pi}{2}$	0	−1.2361
0.4232	$-0.4232+\frac{\mathrm{i}\pi}{2}$	0	0.0000
−0.4232	$0.4232+\frac{\mathrm{i}\pi}{2}$	0	0.0000
0.9214	$-\infty+\frac{\mathrm{i}\pi}{2}$	1	0.0000
−0.9214	$\infty+\frac{\mathrm{i}\pi}{2}$	−1	0.0000
−0.9214	$-\infty$	1	0.0000
0.9214	∞	−1	0.0000
$\frac{\bar{\eta}}{2}$	$-\frac{\bar{\eta}}{2}$	0	$\boxed{0.0000}$
$-\infty+\frac{\mathrm{i}\pi}{4}$	$-\infty+\frac{3\mathrm{i}\pi}{4}$	2	1.2361
∞	$\infty+\frac{\mathrm{i}\pi}{2}$	−2	1.2361
$-\infty$	$\frac{\mathrm{i}\pi}{2}$	1	4.0000
$\infty+\frac{\mathrm{i}\pi}{2}$	$\frac{\mathrm{i}\pi}{2}$	−1	4.0000
$0.5142+\frac{\mathrm{i}\pi}{2}$	$-0.5142+\frac{\mathrm{i}\pi}{2}$	0	5.0725

roots M ranging from 0 to $N/2$ and by use of $SU(2)$ operators.

Another interesting case is the XX model ($\eta = \frac{1}{2}$), which can be transformed to a free fermion model via the Jordan-Wigner transformation. From Eqs. (3) and (4), our chiral generating states work for the XX model with an even N, specifically as follows [37]:

$$N = 4m, \quad s = 1, \quad M = 0, 2, \ldots, N, \quad m \in \mathbb{N}^+,$$
$$N = 4m + 2, \quad s = 1, \quad M = 1, 3, \ldots, N - 1, \quad m \in \mathbb{N}.$$

Under the condition $\eta = \frac{1}{2}$, the following identity holds: $\psi(u + 2\eta) = -\sigma^z\psi(u)$, rendering the basis vectors with the argument shift $2\eta = 1$ linearly independent and orthogonal to the nonshifted ones. Remarkably, the joined set of "shifted" and original chiral basis vectors for even N turns out to be orthonormal and complete [37], the latter feature resulting from

$$2\sum_{k=0}^{2m}\binom{N}{2k} = 2^N, \quad \text{if } N = 4m, \quad m \in \mathbb{N}^+,$$
$$2\sum_{k=0}^{2m}\binom{N}{2k+1} = 2^N, \quad \text{if } N = 4m+2, \quad m \in \mathbb{N}.$$

VIII. CONCLUSION

In this paper we studied the periodic XYZ chain under the conditions (3) and (4), which is the elliptic analog of the root of unity conditions for anisotropy of the partially anisotropic XXZ case. Under these conditions, a chiral subspace invariant under the action of the Hamiltonian exists, consisting of chiral vectors with a fixed number of kinks. We propose a coordinate Bethe ansatz to find all eigenstates corresponding to the chiral invariant manifold. The solution of the homogeneous BAE in Eqs. (46) and (47) for the Bethe roots gives the eigenvalues and generates the coefficients of the respective eigenstates in the chiral basis. This renders the chiral basis more natural for the diagonalization problem of the XYZ chain than the standard computational basis.

We studied two parametrizations of the XYZ chain with real and also with imaginary values of η. Remarkably, the obtained BAE for the case of real valued η coincide with those obtained by earlier alternative methods [9,10,20]. In case of imaginary values of η, we obtain BAE with non–root of unity twist factors. By use of the conjugate modulus transformation this can be reconciled completely with the results obtained in Baxter's parametrization using real values for η.

The solutions of these BAE for our invariant chiral subspace (and $M = N/2$) are regular solutions: the states outside the invariant subspace are given by Bethe root distributions containing a bound pair which appear in Baxter's treatment.

The integer M in Eq. (3) denotes the number of kinks in a chiral invariant subspace and serves as a quantum number, which should correspond to a certain symmetry. It is challenging to understand the origin of this symmetry and the resulting degeneracies of the energy levels. More work in this direction needs to be done.

Notably, in some of our examples (Tables VI and VII) we treat both the XYZ chain and its XXZ counterpart (arising as the XYZ limit for $\tau \to +\mathrm{i}\infty$), demonstrating the "XYZ" origin of phantom Bethe roots in the periodic XXZ chain [32]. The XXZ limit is of additional interest since its open chain version with appropriately chosen boundary fields describes a paradigmatic classical stochastic system (ASEP) where the usage of chiral states was also found to be beneficial; see [38] and the references therein.

Another interesting open question is how to construct the eigenstates of the XYZ model with generic integrable boundary conditions. Based on the known inhomogeneous T-Q relation, a reasonable approach would be to retrieve the Bethe-type eigenstate via Sklyanin's separation of variables (SoV) method [39,40].

Finally, we'd like to note that recent experiments in cold atoms [28,29] showed a feasible way to create spin-helix states, the partially anisotropic counterparts of the states forming our chiral invariant subspace basis.

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APPENDIX A: ELLIPTIC θ FUNCTIONS

We adopt the notations of elliptic θ functions $\vartheta_\alpha(u,q)$ from Ref. [30]:

$$\vartheta_1(u,q)=2\sum_{n=0}^{\infty}(-1)^n q^{(n+\frac{1}{2})^2}\sin[(2n+1)u],\quad \vartheta_2(u,q)=2\sum_{n=0}^{\infty}q^{(n+\frac{1}{2})^2}\cos[(2n+1)u],$$
$$\vartheta_3(u,q)=1+2\sum_{n=1}^{\infty}q^{n^2}\cos(2nu),\quad \vartheta_4(u,q)=1+2\sum_{n=1}^{\infty}(-1)^n q^{n^2}\cos(2nu). \tag{A1}$$

For convenience, we use the following shorthand notations θ_α, $\tilde{\theta}_\alpha$:

$$\theta_\alpha(u)\equiv\vartheta_\alpha(\pi u,e^{i\pi\tau}),\quad \tilde{\theta}_\alpha(u)\equiv\vartheta_\alpha(\pi u,e^{2i\pi\tau}),\quad \mathrm{Im}[\tau]>0,\quad \alpha=1,2,3,4. \tag{A2}$$

The elliptic functions $\theta_\alpha(u)$ possess important properties [20,30]:

$$\theta_2(u)=\theta_1\left(u+\frac{1}{2}\right),\quad \theta_3(u)=e^{i\pi(u+\frac{\tau}{4})}\theta_1\left(u+\frac{1+\tau}{2}\right),\quad \theta_4(u)=-e^{i\pi(u+\frac{\tau}{4}+\frac{1}{2})}\theta_1\left(u+\frac{\tau}{2}\right), \tag{A3}$$
$$\theta_1(-u)=-\theta_1(u),\quad \theta_\alpha(-u)=\theta_\alpha(u),\quad \alpha=2,3,4, \tag{A4}$$
$$\theta_\alpha(u+1)=-\theta_\alpha(u),\quad \theta_{\alpha'}(u+1)=\theta_{\alpha'}(u),\quad \alpha=1,2,\quad \alpha'=3,4, \tag{A5}$$
$$\theta_\alpha(u+\tau)=-e^{-i\pi(2u+\tau)}\theta_\alpha(u),\quad \theta_{\alpha'}(u+\tau)=e^{-i\pi(2u+\tau)}\theta_{\alpha'}(u),\quad \alpha=1,4,\quad \alpha'=2,3. \tag{A6}$$

Define the useful function

$$\zeta(u)=\frac{\theta_1'(u)}{\theta_1(u)}, \tag{A7}$$

which satisfies the following equations [25,26]:

$$\zeta(u)=-\zeta(-u),\quad \zeta(u+1)=\zeta(u),\quad \zeta(u+\tau)=\zeta(u)-2i\pi, \tag{A8}$$
$$\frac{\theta_1(v_1+v_2)\theta_1(v_1+v_3)\theta_1(v_2+v_3)}{\theta_1(v_1)\theta_1(v_2)\theta_1(v_3)\theta_1(v_1+v_2+v_3)}=\frac{1}{\theta_1'(0)}[\zeta(v_1)+\zeta(v_2)+\zeta(v_3)-\zeta(v_1+v_2+v_3)]. \tag{A9}$$

From Eq. (A9) we get useful identities frequently used in this paper:

$$\frac{\theta_1(v_1+v_2)\theta_1(v_1+\eta)\theta_1(v_2+\eta)}{\theta_1(v_1)\theta_1(v_2)\theta_1(v_1+v_2+\eta)}=g(v_1)+g(v_2)+g(\eta)-g(v_1+v_2+\eta), \tag{A10}$$
$$\frac{\theta_2(\eta)\theta_2(u)\theta_1(u\pm\eta)}{\theta_2(0)\theta_1(u)\theta_2(u\pm\eta)}=\pm\left[g(u)\mp g(\eta)-g\left(u\pm\eta+\frac{1}{2}\right)\right]. \tag{A11}$$

APPENDIX B: EXPRESSIONS OF SOME FUNCTIONS

Using the equations shown in Appendix A, we derive the expression of some functions as follows:

$$a_+(u)=-\left[g(u)+g(\eta)-g\left(u+\eta+\frac{1}{2}\right)\right], \tag{B1}$$
$$a_-(u)=-\left[g(u)-g(\eta)-g\left(u-\eta+\frac{1}{2}\right)\right], \tag{B2}$$

$$
\begin{aligned}
A(u_{2d+n}) &= \sum_{k=1}^{n-1} w(u_{2d+k}) + \sum_{k=n+1}^{N} w(u_{2d-2+k}) + w(-u_{2d+n}) - 2a_-(u_{2d+n}) + 2a_+(u_{2d+n-1}) \\
&= E_0 - 2g(u_{2d+n}) + 2g(u_{2d+n-1}) - 2a_-(u_{2d+n}) + 2a_+(u_{2d+n-1}) \\
&\overset{(A11)}{=} E_0 + 2\left[g\left(u_{2d+n} + \frac{1}{2}\right) - g\left(u_{2d+n-1} + \frac{1}{2}\right) - 2g(\eta)\right],
\end{aligned}
\tag{B3}
$$

$$
\begin{aligned}
B(\lambda, u) &= \frac{E(\lambda) - A(u)}{2} \\
&= g\left(\lambda - \frac{\eta}{2}\right) + g\left(-\lambda - \frac{\eta}{2}\right) + g\left(-u - \frac{1}{2}\right) + g\left(u - \eta + \frac{1}{2}\right) + 2g(\eta) \\
&\overset{(A10)}{=} \frac{\theta_1\left(\lambda + \frac{\eta}{2}\right)}{\theta_1\left(\lambda - \frac{\eta}{2}\right)} \frac{\theta_2(u-\eta)\theta_2\left(\lambda - u - \frac{\eta}{2}\right)}{\theta_2(u)\theta_2\left(\lambda - u + \frac{\eta}{2}\right)} + \frac{\theta_1\left(\lambda - \frac{\eta}{2}\right)}{\theta_1\left(\lambda + \frac{\eta}{2}\right)} \frac{\theta_2(u)\theta_2\left(\lambda - u + \frac{3\eta}{2}\right)}{\theta_2(u-\eta)\theta_2\left(\lambda - u + \frac{\eta}{2}\right)},
\end{aligned}
\tag{B4}
$$

$$
B(\lambda_1, \lambda_2, u, v) = \frac{E(\lambda_1, \lambda_2) - A(u, v)}{2} = B(\lambda_1, u) + B(\lambda_2, v) = B(\lambda_1, v) + B(\lambda_2, u),
\tag{B5}
$$

$$
\begin{aligned}
\overline{B}(\lambda_1, \lambda_2) &= \frac{E(\lambda_1, \lambda_2) - E_0 + 4g(\eta)}{2} \\
&= g\left(\lambda_1 - \frac{\eta}{2}\right) - g\left(\lambda_1 + \frac{\eta}{2}\right) + g\left(\lambda_2 - \frac{\eta}{2}\right) - g\left(\lambda_2 + \frac{\eta}{2}\right) + 2g(\eta) \\
&\overset{(A10)}{=} \frac{\theta_1\left(\lambda_1 + \frac{\eta}{2}\right)}{\theta_1\left(\lambda_1 - \frac{\eta}{2}\right)} \frac{\theta_1\left(\lambda_2 + \frac{\eta}{2}\right)}{\theta_1\left(\lambda_2 - \frac{\eta}{2}\right)} \frac{\theta_1(\lambda_1 + \lambda_2 - \eta)}{\theta_1(\lambda_1 + \lambda_2)} + \frac{\theta_1\left(\lambda_1 - \frac{\eta}{2}\right)}{\theta_1\left(\lambda_1 + \frac{\eta}{2}\right)} \frac{\theta_1\left(\lambda_2 - \frac{\eta}{2}\right)}{\theta_1\left(\lambda_2 + \frac{\eta}{2}\right)} \frac{\theta_1(\lambda_1 + \lambda_2 + \eta)}{\theta_1(\lambda_1 + \lambda_2)}.
\end{aligned}
\tag{B6}
$$

APPENDIX C: DERIVATION OF THE XYZ EIGENSTATES AND BAE FOR THE $M = 2$ CASE

With the acting Hamiltonian on the vectors $\{|d; n_1, n_2\rangle\}$ we arrive at

$$
\begin{aligned}
H\,|d; n_1, n_2\rangle =& A(u_{2d+n_1}, u_{2d+n_2-2})|d; n_1, n_2\rangle + 2A_-(u_{2d+n_1})|d; n_1 - 1, n_2\rangle + 2A_+(u_{2d+n_1})|d; n_1 + 1, n_2\rangle \\
&+ 2A_-(u_{2d+n_2-2})|d; n_1, n_2 - 1\rangle + 2A_+(u_{2d+n_2-2})|d; n_1, n_2 + 1\rangle, \quad 1 < n_1 < n_2 < N, \quad n_2 > n_1 + 1,
\end{aligned}
\tag{C1}
$$

$$
H\,|d; n, n+1\rangle = [E_0 - 4g(\eta)]|d; n, n+1\rangle + 2A_-(u_{2d+n})|d; n-1, n+1\rangle + 2A_+(u_{2d+n-1})|d; n, n+2\rangle, \quad 1 < n < N - 1,
\tag{C2}
$$

$$
\begin{aligned}
H\,|d; n, N\rangle =& A(u_{2d+n}, u_{2d+N-2})|d; n, N\rangle + 2A_-(u_{2d+n})|d; n - 1, N\rangle + 2A_+(u_{2d+n})|d; n + 1, N\rangle \\
&+ 2A_-(u_{2d+N-2})|d; n, N - 1\rangle + 2A_+(u_{2d+2})|d + 1; 1, n\rangle, \quad 1 < n < N - 1,
\end{aligned}
\tag{C3}
$$

$$
H\,|d; N - 1, N\rangle = [E_0 - 4g(\eta)]|d; N - 1, N\rangle + 2A_-(u_{2d+N-1})|d; N - 2, N\rangle + 2A_+(u_{2d+2})|d + 1; 1, N - 1\rangle,
\tag{C4}
$$

$$
\begin{aligned}
H\,|d; 1, n\rangle =& A(u_{2d+1}, u_{2d+n-2})|d; 1, n\rangle + 2A_-(u_{2d+n-2})|d; 1, n - 1\rangle + 2A_+(u_{2d+n-2})|d; 1, n + 1\rangle \\
&+ 2A_+(u_{2d+1})|d; 2, n\rangle + 2A_-(u_{2d+N-3})e^{4i\pi L\eta}|d - 1; n, N\rangle, \quad 1 < n < N - 1,
\end{aligned}
\tag{C5}
$$

$$
H\,|d; 1, 2\rangle = [E_0 - 4g(\eta)]|d; 1, 2\rangle + 2A_+(u_{2d})|d; 1, 3\rangle + 2A_-(u_{2d+N-3})e^{4i\pi L\eta}|d - 1; 2, N\rangle,
\tag{C6}
$$

$$
H\,|d; 1, N\rangle = A(u_{2d+1}, u_{2d+N-2})|d; 1, N\rangle + 2A_-(u_{2d+N-2})|d; 1, N - 1\rangle + 2A_+(u_{2d+1})|d; 2, N\rangle,
\tag{C7}
$$

$$
\begin{aligned}
H\,|s; n, N\rangle =& A(u_{2s+n}, u_{2s+N-2})|s; n, N\rangle + 2A_-(u_{2s+n})|s; n - 1, N\rangle + 2A_+(u_{2s+n})|s; n + 1, N\rangle \\
&+ 2A_-(u_{2s+N-2})|s; n, N - 1\rangle + 2A_+(u_0)e^{4i\pi L_0\eta}\widetilde{W}_n|0; 1, n\rangle, \quad 1 < n < N - 1,
\end{aligned}
\tag{C8}
$$

$$
H\,|s; N - 1, N\rangle = [E_0 - 4g(\eta)]|s; N - 1, N\rangle + 2A_-(u_{2s+N-1})|s; N - 2, N\rangle + 2A_+(u_0)e^{4i\pi L_0\eta}\widetilde{W}_{N-1}|0; 1, N - 1\rangle,
\tag{C9}
$$

$$
\begin{aligned}
H\,|0; 1, n\rangle =& A(u_1, u_{n-2})|0; 1, n\rangle + 2A_-(u_{n-2})|0; 1, n - 1\rangle + 2A_+(u_{n-2})|0; 1, n + 1\rangle \\
&+ 2A_+(u_1)|0; 2, n\rangle + 2A_-(u_{2s+N-1})\widetilde{W}_n^{-1}e^{4i\pi L\eta}|s; n, N\rangle, \quad 1 < n < N - 1,
\end{aligned}
\tag{C10}
$$

$$
H\,|0; 1, 2\rangle = [E_0 - 4g(\eta)]|0; 1, 2\rangle + 2A_+(u_0)|d; 1, 3\rangle + 2A_-(u_{2s+N-1})\widetilde{W}_2^{-1}e^{4i\pi L\eta}|s; 2, N\rangle,
\tag{C11}
$$

where

$$A(u_1,u_2)=E_0+2\sum_{k=1}^{2}\left[g\left(u_k+\frac{1}{2}\right)-g\left(u_k-\eta+\frac{1}{2}\right)-2g(\eta)\right], \tag{C12}$$

and

$$\widetilde{W}_n=\exp\{-\mathrm{i}\pi L_0[2Nu_{s+1}+(N^2-7N+4n+4)\eta]\}. \tag{C13}$$

The vectors in (16) form a basis of the Hilbert space and the corresponding eigenstates can be expanded as

$$|\Psi(\lambda_1,\lambda_2)\rangle=\sum_{d=0}^{s}\sum_{1\leqslant n_1<n_2\leqslant N}F_{d,n_1,n_2}(\lambda_1,\lambda_2)\,|d;n_1,n_2\rangle\,,\quad \text{with}\quad H|\Psi(\lambda_1,\lambda_2)\rangle=E(\lambda_1,\lambda_2)|\Psi(\lambda_1,\lambda_2)\rangle. \tag{C14}$$

Here we assume

$$E(\lambda_1,\lambda_2)=E_0+E_b(\lambda_1)+E_b(\lambda_2), \tag{C15}$$

where E_0 and $E_b(\lambda)$ are defined in (22) and (26), respectively.

For convenience, we assume that $F_{d,n,n}\equiv F_{d,n,n+N}\equiv 0$. The eigenequation of H gives the following identities:

$$\begin{aligned}&F_{d,n_1+1,n_2}(\lambda_1,\lambda_2)A_-(u_{2d+n_1+1})+F_{d,n_1-1,n_2}(\lambda_1,\lambda_2)A_+(u_{2d+n_1-1})+F_{d,n_1,n_2-1}(\lambda_1,\lambda_2)A_+(u_{2d+n_2-3})\\&\quad+F_{d,n_1,n_2+1}(\lambda_1,\lambda_2)A_-(u_{2d+n_2-1})=B(\lambda_1,\lambda_2,u_{2d+n_1},u_{2d+n_2-2})F_{d,n_1,n_2}(\lambda_1,\lambda_2),\quad 1<n_1<n_2<N,\quad n_2>n_1+1,\end{aligned} \tag{C16}$$

$$F_{d,n-1,n+1}(\lambda_1,\lambda_2)A_+(u_{2d+n-1})+F_{d,n,n+2}(\lambda_1,\lambda_2)A_-(u_{2d+n})=\overline{B}(\lambda_1,\lambda_2)F_{d,n,n+1}(\lambda_1,\lambda_2),\quad 1<n<N-1, \tag{C17}$$

$$\begin{aligned}&F_{d,n+1,N}(\lambda_1,\lambda_2)A_-(u_{2d+n+1})+F_{d,n-1,N}(\lambda_1,\lambda_2)A_+(u_{2d+n-1})+F_{d,n,N-1}(\lambda_1,\lambda_2)A_+(u_{2d+N-3})\\&\quad+F_{d+1,1,n}(\lambda_1,\lambda_2)\mathrm{e}^{4\mathrm{i}\pi L\eta}A_-(u_{2d+N-1})=P(\lambda_1,\lambda_2,u_{2d+n},u_{2d+N-2})F_{d,n,N}(\lambda_1,\lambda_2),\quad 1\leqslant n<N,\end{aligned} \tag{C18}$$

$$\begin{aligned}&F_{d,2,n}(\lambda_1,\lambda_2)A_-(u_{2d+2})+F_{d-1,n,N}(\lambda_1,\lambda_2)A_+(u_{2d})+F_{d,1,n-1}(\lambda_1,\lambda_2)A_+(u_{2d+n-3})\\&\quad+F_{d,1,n+1}(\lambda_1,\lambda_2)A_-(u_{2d+n-1})=P(\lambda_1,\lambda_2,u_{2d+1},u_{2d+n-2})F_{d,1,n}(\lambda_1,\lambda_2),\quad 1<n\leqslant N,\end{aligned} \tag{C19}$$

$$\begin{aligned}&F_{s,n+1,N}(\lambda_1,\lambda_2)A_-(u_{2s+n+1})+F_{s,n-1,N}(\lambda_1,\lambda_2)A_+(u_{2s+n-1})+F_{s,n,N-1}(\lambda_1,\lambda_2)A_+(u_{2s+N-3})\\&\quad+F_{0,1,n}(\lambda_1,\lambda_2)\widetilde{W}_n^{-1}\mathrm{e}^{4\mathrm{i}\pi L\eta}A_-(u_{2s+N-1})=P(\lambda_1,\lambda_2,u_{2s+n},u_{2s+N-2})F_{s,n,N}(\lambda_1,\lambda_2),\quad 1\leqslant n<N,\end{aligned} \tag{C20}$$

$$\begin{aligned}&F_{0,2,n}(\lambda_1,\lambda_2)A_-(u_2)+F_{s,n,N}(\lambda_1,\lambda_2)A_+(u_0)\widetilde{W}_n\mathrm{e}^{4\mathrm{i}\pi L_0\eta}+F_{0,1,n-1}(\lambda_1,\lambda_2)A_+(u_{n-3})\\&\quad+F_{0,1,n+1}(\lambda_1,\lambda_2)A_-(u_{n-1})=P(\lambda_1,\lambda_2,u_1,u_{n-2})F_{0,1,n}(\lambda_1,\lambda_2),\quad 1<n\leqslant N,\end{aligned} \tag{C21}$$

where

$$B(\lambda_1,\lambda_2,u,v)=B(\lambda_1,u)+B(\lambda_2,v)=B(\lambda_1,v)+B(\lambda_2,u), \tag{C22}$$

$$\overline{B}(\lambda_1,\lambda_2)=\frac{\theta_1\left(\lambda_1+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_1-\frac{\eta}{2}\right)}\frac{\theta_1\left(\lambda_2+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_2-\frac{\eta}{2}\right)}\frac{\theta_1(\lambda_1+\lambda_2-\eta)}{\theta_1(\lambda_1+\lambda_2)}+\frac{\theta_1\left(\lambda_1-\frac{\eta}{2}\right)}{\theta_1\left(\lambda_1+\frac{\eta}{2}\right)}\frac{\theta_1\left(\lambda_2-\frac{\eta}{2}\right)}{\theta_1\left(\lambda_2+\frac{\eta}{2}\right)}\frac{\theta_1(\lambda_1+\lambda_2+\eta)}{\theta_1(\lambda_1+\lambda_2)}, \tag{C23}$$

$$P(\lambda_1,\lambda_2,v+\eta,v)=\overline{B}(\lambda_1,\lambda_2),\quad P(\lambda_1,\lambda_2,u,v)=B(\lambda_1,\lambda_2,u,v),\quad u\neq v+\eta. \tag{C24}$$

We propose the following ansatz:

$$F_{d,n_1,n_2}(\lambda_1,\lambda_2)=\alpha_d\big[C_{1,2}\,U^{(n_1)}_{2d+n_1}(\lambda_1)\,U^{(n_2)}_{2d+n_2-2}(\lambda_2)+C_{2,1}\,U^{(n_1)}_{2d+n_1}(\lambda_2)\,U^{(n_2)}_{2d+n_2-2}(\lambda_1)\big], \tag{C25}$$

where $U^{(m)}_d(\lambda)$ is defined in (30). Using the property of $U^{(n)}_m(\lambda)$ in Eq. (31), one can prove that our ansatz (C25) satisfies Eq. (C16) automatically. From Eq. (C17), we get

$$\begin{aligned}&\big[C_{1,2}U^{(n+1)}_{k'+1}(\lambda_1)U^{(n+1)}_{k'-1}(\lambda_2)+C_{2,1}U^{(n+1)}_{k'+1}(\lambda_2)U^{(n+1)}_{k'-1}(\lambda_1)\big]A_-(u_{k'+1})+\big[C_{1,2}U^{(n)}_{k'}(\lambda_1)U^{(n)}_{k'-2}(\lambda_2)+C_{2,1}U^{(n)}_{k'}(\lambda_2)U^{(n)}_{k'-2}(\lambda_1)\big]A_+(u_{k'-2})\\&\quad=[B(\lambda_1,\lambda_2,u_{k'},u_{k'-1})-\overline{B}(\lambda_1,\lambda_2)]\big[C_{1,2}U^{(n)}_{k'}(\lambda_1)U^{(n+1)}_{k'-1}(\lambda_2)+C_{2,1}U^{(n)}_{k'}(\lambda_2)U^{(n+1)}_{k'-1}(\lambda_1)\big],\end{aligned} \tag{C26}$$

where

$$\begin{aligned}\big[B(\lambda_1,\lambda_2,u_k,u_{k-1})-\overline{B}(\lambda_1,\lambda_2)\big]&=2g(\eta)-g\left(u_k+\frac{1}{2}\right)+g\left(u_{k-2}+\frac{1}{2}\right)\\&=\frac{\theta_2(\eta)\theta_2(u_{k-1})\theta_1(u_k)}{\theta_2(0)\theta_2(u_k)\theta_1(u_{k-1})}+\frac{\theta_2(\eta)\theta_2(u_{k-1})\theta_1(u_{k-2})}{\theta_2(0)\theta_2(u_{k-2})\theta_1(u_{k-1})}.\end{aligned} \tag{C27}$$

After tedious calculations, the "two-body scattering matrix" S is obtained, see Appendix D:

$$S_{1,2}=\frac{C_{2,1}}{C_{1,2}}=\frac{\theta_1(\lambda_1-\lambda_2-\eta)}{\theta_1(\lambda_1-\lambda_2+\eta)}. \tag{C28}$$

To satisfy Eqs. (C18)–(C21), the following BAE for $\lambda_1,\ \lambda_2$, and ξ should be satisfied:

$$\left[\frac{\theta_1\left(\lambda_j+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_j-\frac{\eta}{2}\right)}\right]^N\prod_{k\neq j}\frac{\theta_1(\lambda_j-\lambda_k-\eta)}{\theta_1(\lambda_j-\lambda_k+\eta)}\exp(4i\pi L\lambda_j+\xi)=1,\quad j=1,2, \tag{C29}$$

$$\exp[4i\pi L_0(\lambda_1+\lambda_2)-(s+1)\xi]=1. \tag{C30}$$

The coefficient α_d in (C25) is parameterized in terms of ξ and d as

$$\alpha_d=\exp\left[2i\pi Ld(2u_d+2L\tau+\eta)-d\xi\right]. \tag{C31}$$

APPENDIX D: DERIVATION OF THE *S* MATRIX IN (40)

Introduce the useful identity [20]

$$\theta_1(u+x)\theta_1(u-x)\theta_1(v+y)\theta_1(v-y)-\theta_1(u+y)\theta_1(u-y)\theta_1(v+x)\theta_1(v-x)=\theta_1(u+v)\theta_1(u-v)\theta_1(x+y)\theta_1(x-y). \tag{D1}$$

Equation (C26) can then be rewritten as

$$J(\lambda_1,\lambda_2)C_{1,2}+J(\lambda_2,\lambda_1)C_{2,1}=0. \tag{D2}$$

The expression of $J(\lambda_1,\lambda_2)$ can be derived as follows:

$$\begin{aligned}
J(\lambda_1,\lambda_2)&=A_-(u_{k'+1})U_{k'+1}^{(n+1)}(\lambda_1)U_{k'-1}^{(n+1)}(\lambda_2)+A_+(u_{k'-2})U_{k'}^{(n)}(\lambda_1)U_{k'-2}^{(n)}(\lambda_2)\\
&\quad-[B(\lambda_1,\lambda_2,u_{k'},u_{k'-1})-\overline{B}(\lambda_1,\lambda_2)]U_{k'}^{(n)}(\lambda_1)U_{k'-1}^{(n+1)}(\lambda_2)\\
&=\left[\frac{\theta_1\left(\lambda_1+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_1-\frac{\eta}{2}\right)}\frac{\theta_1\left(\lambda_2+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_2-\frac{\eta}{2}\right)}\right]^{n+1}\frac{\theta_2\left(\lambda_1-u_{k'+1}+\frac{\eta}{2}\right)\theta_2\left(\lambda_2-u_{k'-1}+\frac{\eta}{2}\right)}{\theta_2^2(u_{k'})\theta_2(u_{k'-2})\theta_2(u_{k'-1})}\\
&\quad+\left[\frac{\theta_1\left(\lambda_1+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_1-\frac{\eta}{2}\right)}\frac{\theta_1\left(\lambda_2+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_2-\frac{\eta}{2}\right)}\right]^{n}\frac{\theta_2\left(\lambda_1-u_{k'}+\frac{\eta}{2}\right)\theta_2\left(\lambda_2-u_{k'-2}+\frac{\eta}{2}\right)}{\theta_2(u_{k'})\theta_2(u_{k'-1})\theta_2^2(u_{k'-2})}\\
&\quad-\left[\frac{\theta_1\left(\lambda_1+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_1-\frac{\eta}{2}\right)}\right]^{n}\left[\frac{\theta_1\left(\lambda_2+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_2-\frac{\eta}{2}\right)}\right]^{n+1}\frac{\theta_2\left(\lambda_1-u_{k'}+\frac{\eta}{2}\right)\theta_2\left(\lambda_2-u_{k'-1}+\frac{\eta}{2}\right)}{\theta_2^2(u_{k'})\theta_2(u_{k'-1})\theta_2(u_{k'-2})}\frac{\theta_2(\eta)\theta_1(u_{k'})}{\theta_2(0)\theta_1(u_{k'-1})}\\
&\quad-\left[\frac{\theta_1\left(\lambda_1+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_1-\frac{\eta}{2}\right)}\right]^{n}\left[\frac{\theta_1\left(\lambda_2+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_2-\frac{\eta}{2}\right)}\right]^{n+1}\frac{\theta_2\left(\lambda_1-u_{k'}+\frac{\eta}{2}\right)\theta_2\left(\lambda_2-u_{k'-1}+\frac{\eta}{2}\right)}{\theta_2(u_{k'})\theta_2(u_{k'-1})\theta_2^2(u_{k'-2})}\frac{\theta_2(\eta)\theta_1(u_{k'-2})}{\theta_2(0)\theta_1(u_{k'-1})}\\
&=\chi\,\frac{\theta_1\left(\lambda_2-u_{k'-1}+\frac{1+\eta}{2}\right)}{\theta_1\left(u_{k'}+\frac{1}{2}\right)}\frac{\theta_1\left(\lambda_2+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_2-\frac{\eta}{2}\right)}\left\{\frac{\theta_1\left(\lambda_1+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_1-\frac{\eta}{2}\right)}\theta_1\left(\lambda_1-u_{k'+1}+\frac{1+\eta}{2}\right)\right.\\
&\quad\left.-\frac{\theta_1\left(\eta+\frac{1}{2}\right)\theta_1(u_{k'})}{\theta_1\left(\frac{1}{2}\right)\theta_1(u_{k'-1})}\theta_1\left(\lambda_1-u_{k'}+\frac{1+\eta}{2}\right)\right\}+\chi\,\frac{\theta_1\left(\lambda_1-u_{k'}+\frac{1+\eta}{2}\right)}{\theta_1\left(u_{k'-2}+\frac{1}{2}\right)}\\
&\quad\times\left[\theta_1\left(\lambda_2-u_{k'-2}+\frac{1+\eta}{2}\right)-\frac{\theta_1\left(\lambda_2+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_2-\frac{\eta}{2}\right)}\frac{\theta_1\left(\eta+\frac{1}{2}\right)\theta_1(u_{k'-2})}{\theta_1\left(\frac{1}{2}\right)\theta_1(u_{k'-1})}\theta_1\left(\lambda_2-u_{k'-1}+\frac{1+\eta}{2}\right)\right]\\
&\overset{(D1)}{=}-\chi\,\frac{\theta_1(\eta)\theta_1\left(\lambda_2+\frac{\eta}{2}\right)\theta_1\left(\lambda_2-u_{k'-1}+\frac{1+\eta}{2}\right)\theta_1\left(\lambda_1-u_{k'}+\frac{\eta}{2}\right)\theta_1\left(\lambda_1-\frac{\eta}{2}+\frac{1}{2}\right)}{\theta_1\left(\lambda_2-\frac{\eta}{2}\right)\theta_1\left(\lambda_1-\frac{\eta}{2}\right)\theta_1\left(\frac{1}{2}\right)\theta_1(u_{k'-1})}\\
&\quad+\chi\,\frac{\theta_1(\eta)\theta_1\left(\lambda_1-u_{k'}+\frac{1+\eta}{2}\right)\theta_1\left(\lambda_2+\frac{\eta}{2}+\frac{1}{2}\right)\theta_1\left(\lambda_2-u_{k'}+\frac{3\eta}{2}\right)}{\theta_1\left(\lambda_2-\frac{\eta}{2}\right)\theta_1\left(\frac{1}{2}\right)\theta_1(u_{k'-1})}\\
&\overset{(D1)}{=}\chi\,\frac{\theta_1(\eta)\theta_1(\lambda_2-\lambda_1+\eta)\theta_2(\lambda_1+\lambda_2-u_{k'-1})}{\theta_1\left(\lambda_2-\frac{\eta}{2}\right)\theta_1\left(\lambda_1-\frac{\eta}{2}\right)},
\end{aligned} \tag{D3}$$

where

$$\chi = \left[\frac{\theta_1\left(\lambda_1+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_1-\frac{\eta}{2}\right)}\frac{\theta_1\left(\lambda_2+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_2-\frac{\eta}{2}\right)}\right]^n \theta_2^{-1}(u_{k'})\theta_2^{-1}(u_{k'-1})\theta_2^{-1}(u_{k'-2}). \tag{D4}$$

Thus, we get the two-body scattering matrix:

$$S_{1,2} = \frac{C_{2,1}}{C_{1,2}} = -\frac{J(\lambda_1,\lambda_2)}{J(\lambda_2,\lambda_1)} = \frac{\theta_1(\lambda_1-\lambda_2-\eta)}{\theta_1(\lambda_1-\lambda_2+\eta)}. \tag{D5}$$

APPENDIX E: DERIVATION OF BAE

The quasiperiodicity of $\theta_\alpha(u)$ gives rise to

$$\frac{\theta_\alpha(u+2l\tau+2k)}{\theta_\alpha(u)} = \exp\left[-4\mathrm{i}\pi l(u+l\tau)\right], \quad \alpha = 1,2. \tag{E1}$$

When

$$(N-2M)\eta = 2L\tau+2K, \quad 2(s+1)\eta = 2L_0\tau+2K_0, \tag{E2}$$

it is straightforward to get

$$\frac{U^{(n)}_{m+2s+2}(\lambda)}{U^{(n)}_m(\lambda)} = \exp\left[2\mathrm{i}\pi L_0(2\lambda+2u_{m+s+1}-\eta)\right], \tag{E3}$$

$$\frac{U^{(n+N)}_{m+N-2M}(\lambda)}{U^{(n)}_m(\lambda)} = \left[\frac{\theta_1\left(\lambda+\frac{\eta}{2}\right)}{\theta_1\left(\lambda-\frac{\eta}{2}\right)}\right]^N \exp\left[2\mathrm{i}\pi L(2\lambda+2u_m+2L\tau-\eta)\right]. \tag{E4}$$

1. $M = 1$ case

Property (31) of $U^{(n)}_m(\lambda)$ ensures that the first of Eq. (27) is satisfied for arbitrary m, n. The remaining (27) give the following identities:

$$\mathrm{e}^{-4\mathrm{i}\pi L\eta}\frac{F_{d,N+1}(\lambda)}{F_{d+1,1}(\lambda)} = \frac{F_{d,N}(\lambda)}{F_{d+1,0}(\lambda)} = 1, \tag{E5}$$

$$\mathrm{e}^{-4\mathrm{i}\pi L_0\eta}\frac{F_{0,0}(\lambda)}{F_{s+1,0}(\lambda)} = \frac{F_{0,1}(\lambda)}{F_{s+1,1}(\lambda)} = W. \tag{E6}$$

The BAE (32), (33) are derived from the above equations directly.

2. $M = 2$ case

With the help of Eqs. (31) and (C28), the functional relations (C16) and (C17) hold for arbitrary d, n_1, n_2. Thus, to satisfy Eqs. (C18)–(C21), one has

$$\frac{F_{d,n,N}(\lambda_1,\lambda_2)}{F_{d+1,0,n}(\lambda_1,\lambda_2)} = \mathrm{e}^{-4\mathrm{i}\pi L\eta}\frac{F_{d,n,N+1}(\lambda_1,\lambda_2)}{F_{d+1,1,n}(\lambda_1,\lambda_2)} = 1, \tag{E7}$$

$$\frac{F_{s+1,0,n}(\lambda_1,\lambda_2)}{F_{0,0,n}(\lambda_1,\lambda_2)} = \mathrm{e}^{-4\mathrm{i}\pi L_0\eta}\frac{F_{s+1,1,n}(\lambda_1,\lambda_2)}{F_{0,1,n}(\lambda_1,\lambda_2)} = \widetilde{W}_n^{-1}\exp(-4\mathrm{i}\pi L_0\eta). \tag{E8}$$

The above equations are equivalent to

$$\frac{\alpha_d\, C_{1,2}\, U^{(N)}_{2d+N-2}(\lambda_2)}{\alpha_{d+1}\, C_{2,1}\, U^{(0)}_{2d+2}(\lambda_2)} = \frac{\alpha_d\, C_{2,1}\, U^{(N)}_{2d+N-2}(\lambda_1)}{\alpha_{d+1}\, C_{1,2}\, U^{(0)}_{2d+2}(\lambda_1)} = 1, \tag{E9}$$

$$\frac{\alpha_{s+1}\, U^{(n)}_{2s+n}(\lambda_1)\, U^{(0)}_{2s+2}(\lambda_2)}{\alpha_0\, U^{(n)}_{n-2}(\lambda_1)\, U^{(0)}_0(\lambda_2)} = \frac{\alpha_{s+1}\, U^{(n)}_{2s+n}(\lambda_2)\, U^{(0)}_{2s+2}(\lambda_1)}{\alpha_0\, U^{(n)}_{n-2}(\lambda_2)\, U^{(0)}_0(\lambda_1)} = \widetilde{W}_n^{-1}\exp(-4\mathrm{i}\pi L_0\eta). \tag{E10}$$

Using Eqs. (E3) and (E4), we finally arrive at the BAE (C29), (C30) after straightforward calculations.

APPENDIX F: DEGENERATION OF THE INHOMOGENEOUS BAE

For the periodic XYZ chain, the eigenvalue of the transfer matrix $\Lambda(u)$ can be given by the following inhomogeneous T-Q relation [20,21]:

$$\Lambda(u) = e^{2i\pi l_0 u+\kappa}\,\theta_1^N(u+\eta)\frac{\mathcal{Q}_1(u-\eta)}{\mathcal{Q}_2(u)} + e^{-2i\pi l_0(u+\eta)-\kappa}\,\theta_1^N(u)\frac{\mathcal{Q}_2(u+\eta)}{\mathcal{Q}_1(u)} + c\,\theta_1^m\left(u+\frac{\eta}{2}\right)\frac{\theta_1^N(u+\eta)\theta_1^N(u)}{\mathcal{Q}_1(u)\mathcal{Q}_2(u)}, \tag{F1}$$

where l_0 is an integer, and M_0 and m are two non-negative integers which satisfy the relation $N+m=2M_0$. The $\mathcal{Q}$ functions $\mathcal{Q}_{1,2}(u)$ are defined by

$$\mathcal{Q}_1(u) = \prod_{j=1}^{M_0}\theta_1(u-\mu_j), \quad \mathcal{Q}_2(u) = \prod_{j=1}^{M_0}\theta_1(u-\nu_j). \tag{F2}$$

The BAE for the generic periodic XYZ chain read [20,21]

$$\exp\left\{i\pi\left[(N-2M_0)\eta - 2\sum_{j=1}^{M_0}(\mu_j-\nu_j)\right]\right\} = \exp(2i\pi l_0\tau), \tag{F3}$$

$$c\,\exp\left\{2i\pi\left[M_0\eta + \sum_{j=1}^{M_0}(\mu_j+\nu_j)\right]\right\} = c, \tag{F4}$$

$$\frac{c\,\theta_1^m\left(\mu_j+\frac{\eta}{2}\right)\theta_1^N(\mu_j+\eta)}{\exp[-2i\pi l_0(\mu_j+\eta)-\kappa]} = -\prod_{l=1}^{M_0}\theta_1(\mu_j-\nu_l+\eta)\theta_1(\mu_j-\nu_l), \tag{F5}$$

$$\frac{c\,\theta_1^m\left(\nu_j+\frac{\eta}{2}\right)\theta_1^N(\nu_j)}{\exp(2i\pi l_0\nu_j+\kappa)} = -\prod_{l=1}^{M_0}\theta_1(\nu_j-\mu_l-\eta)\theta_1(\nu_j-\mu_l), \tag{F6}$$

$$e^{\kappa}\prod_{j=1}^{M_0}\frac{\theta_1(\mu_j+\eta)}{\theta_1(\nu_j)} = e^{\frac{2i\pi k}{N}}, \quad k\in\mathbb{Z}. \tag{F7}$$

Under the condition

$$(N-2M)\eta = 2L\tau + 2K, \quad L, K\in\mathbb{Z}, \tag{F8}$$

the Bethe roots have to satisfy the following relations:

$$\mu_j = \nu_j \equiv \lambda_j - \frac{\eta}{2}, \quad j=1,\ldots,M, \tag{F9}$$

$$\mu_{j+M} = \nu_{j+M} - \eta, \quad j=1,\ldots,M_0-M. \tag{F10}$$

The inhomogeneous term vanishes with $l_0 = L$, and the resulting homogeneous BAE are

$$\exp(4i\pi L\lambda_j + 2\kappa)\left[\frac{\theta_1\left(\lambda_j+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_j-\frac{\eta}{2}\right)}\right]^N \prod_{k\neq j}^{M}\frac{\theta_1(\lambda_j-\lambda_k-\eta)}{\theta_1(\lambda_j-\lambda_k+\eta)} = 1, \quad j=1,2,\ldots,M, \tag{F11}$$

$$e^{\kappa}\prod_{j=1}^{M}\frac{\theta_1\left(\lambda_j+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_j-\frac{\eta}{2}\right)} = e^{\frac{2i\pi k}{N}}, \quad k\in\mathbb{Z}. \tag{F12}$$

From Eqs. (F11)–(F12) we get

$$\prod_{j=1}^{M}\left[\frac{\theta_1\left(\lambda_j+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_j-\frac{\eta}{2}\right)}\right]^N \exp\left(4i\pi L\sum_{j=1}^{M}\lambda_j + 2M\kappa\right) = 1, \quad e^{N\kappa}\prod_{j=1}^{M}\left[\frac{\theta_1\left(\lambda_j+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_j-\frac{\eta}{2}\right)}\right]^N = 1, \tag{F13}$$

leading to

$$\exp\left[4i\pi L\sum_{j=1}^{M}\lambda_j - (N-2M)\kappa\right] = 1. \tag{F14}$$

The case we consider in this paper belongs to the degenerate case (F8) and an additional identity (4) is needed. By letting $e^{\kappa} = \pm e^{\frac{\xi}{2}}$, we see that our BAE in (46)–(47) are consistent with Eqs. (F11) and (F14).

Under the condition (F8), the T-Q relation (F1) reduces to a conventional homogeneous one:

$$\Lambda(u) = \mathrm{e}^{2\mathrm{i}\pi Lu+\kappa}\,\theta_1^N(u+\eta)\prod_{j=1}^{M}\frac{\theta_1\big(u-\lambda_j-\frac{\eta}{2}\big)}{\theta_1\big(u-\lambda_j+\frac{\eta}{2}\big)} + \mathrm{e}^{-2\mathrm{i}\pi L(u+\eta)-\kappa}\,\theta_1^N(u)\prod_{j=1}^{M}\frac{\theta_1\big(u-\lambda_j+\frac{3\eta}{2}\big)}{\theta_1\big(u-\lambda_j+\frac{\eta}{2}\big)}, \tag{F15}$$

where $\{\lambda_j\}$ and κ are given by Eqs. (F11) and (F14).

Remark: When $M=0$ and $N\eta = 2L\tau + 2K,\ \ L, K \in \mathbb{Z}$, $\Lambda(u)$ in (F15) reads

$$\Lambda(u) = \mathrm{e}^{2\mathrm{i}\pi Lu+\kappa}\,\theta_1^N(u+\eta) + \mathrm{e}^{-2\mathrm{i}\pi L(u+\eta)-\kappa}\,\theta_1^N(u), \quad \kappa = \frac{2\mathrm{i}\pi k}{N}, \quad k\in\mathbb{Z}. \tag{F16}$$

The selection of κ in (F16) shows that the transfer matrix has N factorized eigenstates which are exactly our elliptic spin-helix states in (20) [8,10], and they all correspond to the same energy E_0 in (22). Replacing η, L, K with $-\eta, -L, -K$ leaves the Hamiltonian invariant. Therefore, we can construct another set of N independent elliptic spin-helix states with different chirality. Consequently, the minimal degeneracy of E_0 is $2N$.

APPENDIX G: BAXTER'S GENERALIZED BETHE ANSATZ

Baxter proposed a basis and a Bethe ansatz solution for the periodic XYZ chain in [7,9]. In this section we will recall his results and then explain the relation between our Bethe ansatz and Baxter's.

First, recall Baxter's result in [7]. Define a local state

$$\psi'(u) = \begin{pmatrix}\tilde{\theta}_1(u)\\ \tilde{\theta}_4(u)\end{pmatrix}. \tag{G1}$$

Let us introduce the following notations:

$$r_m = r - v - \frac{1}{2}\eta + m\eta, \quad t_m = t + v - \frac{3}{2}\eta + m\eta, \quad \omega_m = \frac{r+t}{2} + m\eta, \tag{G2}$$

where r, t, and v are arbitrary. Then the following global state is constructed:

$$|d; n_1,\ldots,n_M\rangle_I = \bigotimes_{k_1=1}^{n_1-1}\psi'\big(r_{d+k_1}\big)\bigotimes\psi'\big(t_{d+n_1}\big)\bigotimes_{k_2=n_1+1}^{n_2-1}\psi'\big(r_{d+k_2-2}\big)\bigotimes\psi'\big(t_{d+n_2-2}\big)\cdots$$
$$\bigotimes\psi'\big(t_{d+n_M-2M+2}\big)\bigotimes_{k_{M+1}=n_M+1}^{N}\psi'\big(r_{d+k_{M+1}-2M}\big). \tag{G3}$$

Under the condition

$$Q\eta = 2m_1 + 2m_2\tau, \quad (N-2M')\eta = 2m_1' + 2m_2'\tau, \quad Q\in\mathbb{N}^+, \quad m_1, m_2, m_1', m_2' \in \mathbb{Z}, \tag{G4}$$

Baxter has proved that the following states

$$|d; n_1, n_2, \ldots, n_{M'}\rangle_I, \quad d = 1, 2, \ldots, Q, \quad 1 \leqslant n_1 < n_2 < \cdots < n_{M'} \leqslant N, \tag{G5}$$

form a closed subspace for the transfer matrix of the eight-vertex model, corresponding to the XYZ Hamiltonian [7].

When $M' = \frac{N}{2}$, the eigenstate of the Hamiltonian can be expanded as [7,9]

$$|\Psi\rangle_I = \sum_{d=1}^{Q}\sum_{\substack{1\leqslant n_1<n_2<\cdots\\ \cdots<n_{M'}\leqslant N}}\sum_{P}\varpi^d\,Y(P)\,G_{p_1}(d,n_1)G_{p_2}(d-2,n_2)\cdots$$
$$\times\, G_{p_{M'}}(d-2M'+2, n_{M'})\,|d; n_1, n_2, \ldots, n_{M'}\rangle_I, \tag{G6}$$

$$G_j(d,x) = \left[\frac{\theta_1\big(\mu_j+\frac{\eta}{2}\big)}{\theta_1\big(\mu_j-\frac{\eta}{2}\big)}\right]^x \frac{\theta_2\big(\mu_j - \omega_{l+x-1}+\frac{\eta}{2}\big)}{\theta_2(\omega_{l+x-1})\theta_2(\omega_{l+x-2})}, \tag{G7}$$

$$Y(P) = \epsilon_P\prod_{1\leqslant j\leqslant m\leqslant M'}\theta_1(\mu_{p_j}-\mu_{p_m}+\eta), \tag{G8}$$

where $P=\{p_1,\ldots,p_{M'}\}$ is the permutation of integers $\{1,\ldots,M'\}$, ϵ_P is the signature of the permutation P, and ω_m is defined in (G2). The Bethe roots $\{\mu_1,\ldots,\mu_{M'}\}$ satisfy the BAE:

$$\varpi^{-2}\left[\frac{\theta_1\big(\mu_j+\frac{\eta}{2}\big)}{\theta_1\big(\mu_j-\frac{\eta}{2}\big)}\right]^N\prod_{k\neq j}^{N/2}\frac{\theta_1(\mu_j-\mu_k-\eta)}{\theta_1(\mu_j-\mu_k+\eta)} = 1, \quad \varpi^Q = 1, \quad j = 1,\ldots,N/2. \tag{G9}$$

Our Bethe ansatz equations for the $M=\frac{N}{2}$ case are

$$\mathrm{e}^{\xi}\left[\frac{\theta_1\left(\lambda_j+\frac{\eta}{2}\right)}{\theta_1\left(\lambda_j-\frac{\eta}{2}\right)}\right]^N\prod_{k\neq j}^{N/2}\frac{\theta_1(\lambda_j-\lambda_k-\eta)}{\theta_1(\lambda_j-\lambda_k+\eta)}=1,\quad j=1,2,\dots,N/2, \tag{G10}$$

$$\exp\left(4\mathrm{i}\pi L_0\sum_{k=1}^{N/2}\lambda_k-(s+1)\xi\right)=1. \tag{G11}$$

Remark: When $\eta=\frac{m}{m'}(L_0=0)$, $m,m'\in\mathbb{Z}$, we find that the solutions of the BAE (G9) and (G10), (G11) have the following correspondence:

$$\{\mu_1,\dots,\mu_{N/2}\}=\{\lambda_1,\dots,\lambda_{N/2}\},\quad Q=2(s+1),\quad \varpi=\pm\mathrm{e}^{-\frac{\xi}{2}}. \tag{G12}$$

For a nonzero L_0 in Eq. (G11), i.e., $\mathrm{Im}[\eta]\neq 0$, our BAE appear to be *not* equivalent to Baxter's. The parameter ϖ in Baxter's BAE (G9) is always a root of unity, while the parameter $\mathrm{e}^{-\frac{\xi}{2}}$ in our BAE (G10), (G11) is not for a nonzero L_0. Obvious examples are the right panels of Tables III and IV. This inconsistency seems to contradict Eq. (G12): for the $M=\frac{N}{2}=2$ and $L_0\neq 0$ case, we prove numerically that the solution of our BAE (G10), (G11) and the correspondence Eq. (G12) still give the correct expansion coefficients in (G6). The apparent disagreement can be understood.

By applying the conjugate modulus transformation, we find that the same XYZ chain with parameters η,τ can be parameterized with η/τ, $-1/\tau$ plus a unitary transformation interchanging the J_x and J_z coefficients as follows:

$$\bar{\theta}_\alpha(u)=\vartheta_\alpha(\pi u,\mathrm{e}^{-\frac{\mathrm{i}\pi}{\tau}}),\quad \alpha=1,2,3,4,$$

$$\theta_1(u)=\mathrm{i}\sqrt{\frac{\mathrm{i}}{\tau}}\,\mathrm{e}^{-\frac{\mathrm{i}\pi u^2}{\tau}}\bar{\theta}_1\left(\frac{u}{\tau}\right),\quad \theta_\alpha(u)=\sqrt{\frac{\mathrm{i}}{\tau}}\,\mathrm{e}^{-\frac{\mathrm{i}\pi u^2}{\tau}}\bar{\theta}_{6-\alpha}\left(\frac{u}{\tau}\right),\quad \alpha=2,3,4, \tag{G13}$$

$$J_x|_{\eta,\tau}=\mathrm{e}^{-\frac{\mathrm{i}\pi\eta^2}{\tau}}J_z|_{\eta/\tau,-1/\tau},\quad J_y|_{\eta,\tau}=\mathrm{e}^{-\frac{\mathrm{i}\pi\eta^2}{\tau}}J_y|_{\eta/\tau,-1/\tau},\quad J_z|_{\eta,\tau}=\mathrm{e}^{-\frac{\mathrm{i}\pi\eta^2}{\tau}}J_x|_{\eta/\tau,-1/\tau}. \tag{G14}$$

Interestingly, τ and $-1/\tau$ are from $\mathrm{i}\mathbb{R}^+$, and for the real (imaginary) value of η the parameter η/τ is imaginary (real). This means that the case of imaginary η is transformed into the case of Baxter's treatment, where he uses real values for this parameter. Now the question comes up as to how the Bethe ansatz equations transform? When η is purely imaginary, we do the conjugate modulus transformation for the BAE (G10):

$$\exp\left(\xi-\frac{4\mathrm{i}\pi\eta}{\tau}\sum_{k=1}^{N/2}\lambda_k\right)\left[\frac{\bar{\theta}_1\left[\frac{1}{\tau}\left(\lambda_j+\frac{\eta}{2}\right)\right]}{\bar{\theta}_1\left[\frac{1}{\tau}\left(\lambda_j-\frac{\eta}{2}\right)\right]}\right]^N\prod_{k\neq j}^{N/2}\frac{\bar{\theta}_1\left[\frac{1}{\tau}(\lambda_j-\lambda_k-\eta)\right]}{\bar{\theta}_1\left[\frac{1}{\tau}(\lambda_j-\lambda_k+\eta)\right]}$$

$$\overset{(\mathrm{G11})}{=}\exp\left(\frac{2\mathrm{i}\pi n}{s+1}\right)\left[\frac{\bar{\theta}_1\left[\frac{1}{\tau}\left(\lambda_j+\frac{\eta}{2}\right)\right]}{\bar{\theta}_1\left[\frac{1}{\tau}\left(\lambda_j-\frac{\eta}{2}\right)\right]}\right]^N\prod_{k\neq j}^{N/2}\frac{\bar{\theta}_1\left[\frac{1}{\tau}(\lambda_j-\lambda_k-\eta)\right]}{\bar{\theta}_1\left[\frac{1}{\tau}(\lambda_j-\lambda_k+\eta)\right]}=1,\quad j=1,2,\dots,N/2,\quad n\in\mathbb{Z}. \tag{G15}$$

The real part of the parameter ξ in (G11) now disappears and a root of unity factor results.

By letting Q in (G4) be $2(s+1)$, we can divide the states in (G5) into two subsets:

$$\{|d;n_1,n_2,\dots,n_{M'}\rangle_I\}=\{|d';n_1,n_2,\dots,n_{M'}\rangle_{II}\}\cup\{|d';n_1,n_2,\dots,n_{M'}\rangle_{III}\},\quad d=1,\dots,Q,\quad d'=1,\dots,(s+1),$$

$$|d';n_1,n_2,\dots,n_{M'}\rangle_{II}=|2d'-1;n_1,n_2,\dots,n_{M'}\rangle_I,\quad |d';n_1,n_2,\dots,n_{M'}\rangle_{III}=|2d';n_1,n_2,\dots,n_{M'}\rangle_I. \tag{G16}$$

One sees that the state $|d;n_1,n_2,\dots,n_{M'}\rangle_{III}$ can be obtained from $|d;n_1,n_2,\dots,n_{M'}\rangle_{II}$ by shifting an overall phase for all local states as $\psi'(u)\to\psi'(u+\eta)$. Since $\psi'(u)$ is a linear combination of $\psi'(v)$ and $\psi'(v+2\eta)$ with $u,v\in\mathbb{C}$ as

$$\psi'(u)=\beta_1(u,v)\psi'(v+2\eta)+\beta_2(u,v)\psi'(v), \tag{G17}$$

$$\beta_1(u,v)=\frac{\theta_1\left(\frac{u-v}{2}\right)\theta_2\left(\frac{u+v}{2}\right)}{\theta_1(\eta)\theta_2(v+\eta)},\quad \beta_2(u,v)=-\frac{\theta_1\left(\frac{u-v}{2}-\eta\right)\theta_2\left(\frac{u+v}{2}+\eta\right)}{\theta_1(\eta)\theta_2(v+\eta)}, \tag{G18}$$

one can verify that the set $\{|d;n_1,n_2,\dots,n_{M'}\rangle_{II}\}$ in (G16) is exactly our chiral basis in (16) when $M=0,1$ by letting $r_1=u_0\pm 1$.

The difference between our set of generating states (16) (see also Fig. 1) and the set $\{|d;n_1,n_2,\dots,n_{M'}\rangle_{II}\}$ appears when

$M > 1$. For $M = 2$, we have

$$
\begin{aligned}
|d;n_1,n_2\rangle_{II} &= \bigotimes_{k_1=1}^{n_1-1}\psi'(r_{2d+k_1-1})\bigotimes\psi'(t_{2d+n_1-1})\bigotimes_{k_2=n_1+1}^{n_2-1}\psi'(r_{2d+k_2-3})\bigotimes\psi'(t_{2d+n_2-3})\bigotimes_{k_3=n_2+1}^{N}\psi'(r_{2d+k_3-5})\\
&= (-1)^N\beta_1(\rho_1,\varrho_1)\beta_2(\rho_2,\varrho_2)\underline{\bigotimes_{k_1=1}^{n_1}\psi'(r_{2d+k_1-1})\bigotimes_{k_2=n_1+1}^{n_2-1}\psi'(r_{2d+k_2-3})\bigotimes_{k_3=n_2}^{N}\psi'(r_{2d+k_3-5})}\\
&\quad+(-1)^N\beta_1(\rho_1,\varrho_1)\beta_1(\rho_2,\varrho_2)\,|d-1;n_1,n_2\rangle+(-1)^N\beta_2(\rho_1,\varrho_1)\beta_1(\rho_2,\varrho_2)\,|d-1;n_1-1,n_2\rangle\\
&\quad+(-1)^N\beta_2(\rho_1,\varrho_1)\beta_2(\rho_2,\varrho_2)\,|d-1;n_1-1,n_2-1\rangle\,,
\end{aligned}
\tag{G19}
$$

$$
\rho_1=t_{2d+n_1-1},\quad \varrho_1=r_{2d+n_1-3},\quad \rho_2=t_{2d+n_2-3},\quad \varrho_2=r_{2d+n_2-5},
$$

where we let $r_1 = u_0 \pm 1$. The underlined part in (G19) is beyond our set of generating states in (16) when $n_2 = n_1 + 1$. In this case, indeed, the underlined part becomes

$$
\underline{\bigotimes_{k_1=1}^{n_1}\psi'(r_{2d+k_1-1})\bigotimes_{k_2=n_1+1}^{N}\psi'(r_{2d+k_2-5})},
\tag{G20}
$$

which corresponds to a *double* drop of phase over a single link $n_1, n_1 + 1$ (i.e., two kinks on one link, in our notation), which is not allowed in our basis, see Fig. 1 and (16). For larger $M > 2$ the set $\{|d;n_1,n_2,\ldots,n_{M'}\rangle_{II}\}$, expanded as in (G19), will produce states of type "some double kinks plus some ordinary kinks," while triple, quadruple, etc. kinks on one link will never occur. In addition, double kinks (double drop of phase) cannot occur on consecutive links.

Consequently, the set $\{|d;n_1,n_2,\ldots,n_{M'}\rangle_{II}\}$ contains extra vectors when $M \geqslant 2$ so that Baxter's basis (G5) is a more general one. The sets $\{|d;n_1,n_2,\ldots,n_{M'}\rangle_{II}\}$ and $\{|d;n_1,n_2,\ldots,n_{M'}\rangle_{III}\}$ in basis (G5) reduce respectively to our chiral basis in (16) as follows:

$$
\begin{aligned}
&\{|d;n_1,\ldots,n_{M'}\rangle\}_{II}\to\{|d;n_1,n_2,\ldots,n_M\rangle\}: \quad v=\frac{\eta+r-t}{2}+1,\quad u_0=\frac{r+t}{2},\quad M=M',\\
&\{|d;n_1,\ldots,n_{M'}\rangle\}_{III}\to\{|d;n_1,n_2,\ldots,n_M\rangle\}: \quad v=\frac{\eta+r-t}{2}+1,\quad u_0=\frac{r+t}{2}+\eta,\quad M=M'.
\end{aligned}
\tag{G21}
$$

When $N = 2M$, the basis (G5) with generic r, t, and v is argued to be complete [9]. As a consequence, we can use it to expand the remaining eigenstates beyond our chiral basis. From our analysis in Appendix F, we conjecture that the remaining eigenstates ($M \geqslant 2$) correspond to the bound pair solutions of (G9) [9] with

$$
\mu_1=\frac{\eta}{2},\quad \mu_2=-\frac{\eta}{2},\quad \frac{\theta_1\left(\mu_1+\frac{\eta}{2}\right)}{\theta_1\left(\mu_1-\frac{\eta}{2}\right)}\to\infty,\quad \frac{\theta_1\left(\mu_2+\frac{\eta}{2}\right)}{\theta_1\left(\mu_2-\frac{\eta}{2}\right)}\to 0,\quad \frac{\theta_1\left(\mu_1+\frac{\eta}{2}\right)}{\theta_1\left(\mu_1-\frac{\eta}{2}\right)}\frac{\theta_1\left(\mu_2+\frac{\eta}{2}\right)}{\theta_1\left(\mu_2-\frac{\eta}{2}\right)}=-1,
\tag{G22}
$$

$$
\theta_1(\mu_2-\mu_1+\eta)=-\theta_1(2\eta)\varpi^2\left[\frac{\theta_1\left(\mu_1+\frac{\eta}{2}\right)}{\theta_1\left(\mu_1-\frac{\eta}{2}\right)}\right]^{-N}\prod_{k\neq 1,2}^{N/2}\frac{\theta_1\left(\mu_k-\frac{3\eta}{2}\right)}{\theta_1\left(\mu_k+\frac{\eta}{2}\right)}.
\tag{G23}
$$

Now the expansion coefficients of the basis in (G6) all vanish, so that we need to extract the terms with slowest decay. By substituting the bound pair solution (G22), (G23) into Eqs. (G6)–(G8) and eliminating an overall factor, the analytic expression of the remaining eigenstates can be derived.

For instance, when $N = 2M = 4$, the remaining eigenstate in Table IV can be written as

$$
\begin{aligned}
|\Psi\rangle_R &= \sum_{d=1}^{Q}\left[\frac{|d;1,2\rangle_I}{\theta_2(\omega_d)\theta_2(\omega_{d-2})}-\frac{|d;2,3\rangle_I}{\theta_2(\omega_{d+1})\theta_2(\omega_{d-1})}+\frac{|d;3,4\rangle_I}{\theta_2(\omega_{d+2})\theta_2(\omega_d)}-\frac{|d;1,4\rangle_I}{\theta_2(\omega_{d-1})\theta_2(\omega_{d+1})}\right]\\
&\propto |1,2\rangle-|2,3\rangle+|3,4\rangle-|1,4\rangle\,.
\end{aligned}
\tag{G24}
$$

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