Invariant subspaces and explicit Bethe vectors in the integrable open spin 1/2 $XYZ$ chain

Xin Zhang,1 Andreas Klümper,2 and Vladislav Popkov3,2

1Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China
2Department of Physics, University of Wuppertal, Gaussstraße 20, 42119 Wuppertal, Germany
3Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, SI-1000 Ljubljana, Slovenia

We derive a criterion under which splitting of all eigenstates of an open $XYZ$ Hamiltonian with boundary fields into two invariant subspaces, spanned by chiral shock states, occurs. The splitting is governed by an integer number, which has the geometrical meaning of the maximal number of kinks in the basis states. We describe the generic structure of the respective Bethe vectors. We obtain explicit expressions for Bethe vectors, in the absence of Bethe roots, and those generated by one Bethe root, and investigate the single particle subspace. We also describe in detail an elliptic analogue of the spin-helix state, appearing in both the periodic and the open $XYZ$ model, and derive the eigenstate condition. The elliptic analogue of the spin-helix state is characterized by a quasi-periodic modulation of the magnetization profile, governed by Jacobi elliptic functions.

I. INTRODUCTION

Exact solutions are indispensable for our understanding of statistical mechanics of interacting systems [1, 2]. The paradigmatic spin-$1/2$ $XYZ$ chain is one of the most fascinating models in quantum statistical mechanics [1]. Its 2D classical statistical counterpart, the 8-vertex model, has appeared as the first example possessing continuously varying critical exponents. The periodic $XYZ$ spin chain with an even number of sites was solved by Baxter [1]. Takhtajan and Faddeev recovered Baxter’s solution via the generalized algebraic Bethe ansatz method [3]. For open systems, several approaches have been proposed to construct integrable structures [4, 5] and exact solutions [6–8].

Bethe Ansatz equations for the spectrum of the $XYZ$ model with generic integrable boundary conditions (including periodic, anti-periodic and open boundary conditions) were first derived by the off-diagonal Bethe ansatz method [9–11]. Despite many years of studies, little is known about the structure of the $XYZ$ eigenstates (Bethe vectors), especially for an open system.

It is our purpose to show that on special manifolds of parameters, the $XYZ$ eigenstate problem can be significantly advanced, and we are able to explicitly link the solutions of the Bethe ansatz equations (BAE) to the coefficients of the Bethe vectors in a special chiral basis. To this end, we prove a splitting of the whole Hilbert space into two subspaces invariant with respect to the action of the open $XYZ$ Hamiltonian with tuned boundary fields. Along the way, we derive a criterion of such a splitting to occur. For the simplest cases, we calculate explicitly the Bethe vectors for arbitrary system size and unveil their geometrical interpretation.

The analogous Hilbert space splitting in the $XXZ$ open spin chain has been proven with phantom Bethe roots [12, 13]. Thus, our results can be viewed as a generalization of the phantom $XXZ$ Bethe states concept onto the fully anisotropic $XYZ$ spin chain case.

As for the $XXZ$ model, we refer to our finding as the “splitting theorem” which gives us a tool to study the structure of Bethe states in the $XYZ$ model, belonging to each invariant subspace. We name the set of Bethe states belonging to an invariant subspace a multiplet. The number of independent states in the multiplet is equal to the dimension of the respective invariant subspace and is given by $\dim(M) = \binom{N}{0} + \binom{N}{1} + \ldots + \binom{N}{M}$, where $M$ is a nonnegative integer, ranging from 0 to $N - 1$. Choosing $M$ fixes the manifold in the parameter space. There are actually several disconnected submanifolds corresponding to the same $M$, parametrized by another integer $L_0$, see criterion (21).

Each individual state in the multiplet can be parametrized by exactly $M$ Bethe roots. The simplest multiplet ($M = 0$) has just one state in it and this state is an elliptic analogue of the spin-helix state [14–16]. The next simplest case corresponds to the cases $M = 1, 2$ and so forth. Then the multiplet already contains a large, polynomially growing with system size number of states. Investigating this large set of states for large systems can be used for statistical analysis. Here we treat in detail the case $M = 1$, for which the smallest multiplet containing $N + 1$ states. We find the explicit form of Bethe vectors and use them to calculate various observables.

The plan of the manuscript is as follows: After introducing the model we derive a local divergence condition which appears crucial for our study. On the base of it, we describe the simplest possible eigenstate, the elliptic analogue of the spin-helix state. Next, we formulate the criterion (21), under which a splitting of the Hilbert space into two invariant chiral subspaces occurs, and describe the basis states spanning the invariant subspaces. In the final part of
the manuscript we use the gained knowledge to investigate the elliptic analogue of phantom Bethe states belonging to the invariant subspace with dimension \( N + 1 \) where \( N \) is the length of the XXZ spin chain. Details of the proofs are given in the Appendix.

II. FACTORIZED ELLIPTIC SPIN HELIX EIGENSTATES IN XYZ SPIN CHAIN

The Hamiltonian of the XYZ spin chain with generic open boundaries is

\[
H = \sum_{n=1}^{N-1} h_{n,n+1} + \tilde{h}_1 \sigma_1 + \tilde{h}_N \sigma_N,
\]

\[
h_{n,n+1} = J_x \sigma_n^+ \sigma_{n+1}^- + J_y \sigma_n^- \sigma_{n+1}^+ + J_z \sigma_n^z \sigma_{n+1}^z,
\]

where the anisotropy parameter and the boundary magnetic fields are parameterized as in [7, 11] [22]. Hermiticity of the boundary fields we have to demand the following restrictions for the boundary parameters \( \alpha_k \):

\[
\text{Im}[\alpha_1^+ \alpha_1^-] = 0, \quad \text{Im}[\alpha_2^+ \alpha_2^-] = \frac{(2k_1+1)i\pi}{2}, \quad \text{Im}[\alpha_3^+ \alpha_3^-] = \frac{(2k_2+1)i\pi}{2},
\]

\[
\text{Re}[\alpha_1^+ \alpha_1^-] = \frac{2k_1+1}{2}, \quad \text{Re}[\alpha_2^+ \alpha_2^-] = \frac{2k_2+1}{2}, \quad k_1, k_2, k_3, k_4 \in \mathbb{Z}.
\]

Our analysis starts by the following remarkable observation. Define a local state [6]

\[
\psi(u) = \left( \begin{array}{c} \tilde{\theta}_1(u) \\ -\tilde{\theta}_4(u) \end{array} \right),
\]

where \( u \in \mathbb{C} \) is a free parameter. The vector \( \psi(u) \) satisfies the following divergence condition [18]

\[
h \left[ \psi(u) \otimes \psi(u + \eta) \right] = [a(u) \sigma^x \otimes \mathbb{I}_2 - a(u + \eta) \mathbb{I}_2 \otimes \sigma^x + d(u) \mathbb{I}_4] \psi(u) \otimes \psi(u + \eta),
\]

where \( h = \sum_\alpha J_\alpha \sigma^\alpha \otimes \sigma^\alpha \) is a \( 4 \times 4 \) Hamiltonian density operator, and the functions \( a(u), d(u) \) are given by (see Appendix B):

\[
a(u) = \frac{\theta_1(\eta)\theta_2(u)}{\theta_2(0)\theta_1(u)}, \quad d(u) = g(\eta) + g(u) - g(u + \eta), \quad g(u) = \frac{\theta_1(\eta)\theta_1(u)}{\theta_1(0)\theta_1(u)}.
\]
Using Eq. (12), we find a family of spatially inhomogeneous factorizable eigenstates of the XYZ model with boundary fields:

$$\left[ \sum_{n=1}^{N-1} h_{n,n+1} - a(u_1)\sigma_1^z + a(u_N)\sigma_N^z \right] |\Psi_+\rangle = E |\Psi_+\rangle,$$

$$|\Psi_+\rangle = \prod_{n=1}^{N} \psi(u_n), \quad E = \sum_{n=1}^{N-1} d(u_n), \quad u_n = u_1 + (n-1)\eta. \quad (15)$$

Noticing that the Hamiltonian is invariant under $\eta \to -\eta$, we can write another divergence condition, complementary to (12)

$$\hbar \psi(u) \otimes \psi(u - \eta) = [-a(u)\sigma^z \otimes \mathbb{I}_2 + a(u - \eta)\mathbb{I}_2 \otimes \sigma^z + d(-u)\mathbb{I}_4] \psi(u) \otimes \psi(u - \eta), \quad (16)$$

rendering the state $|\Psi_-\rangle = \bigotimes_{n=1}^{N} \psi(u_{2-n})$ an eigenvector for the Hamiltonian $\sum_{n=1}^{N-1} h_{n,n+1} + a(u_1)\sigma_1^z - a(u_{2-N})\sigma_N^z$.

Remarkably, both states $|\Psi_+\rangle$ from (15) and the state $|\Psi_-\rangle$ correspond to periodic modulations of the local magnetization components as exemplified in Fig. 1. Note that the individual qubit states are all pure, and correspondingly, all spins are fully polarized, $\langle \sigma_n^x \rangle^2 + \langle \sigma_n^y \rangle^2 + \langle \sigma_n^z \rangle^2 = 1$ for all $n$.

![FIG. 1: Local magnetization profiles for the factorized eigenstate $|\Psi_+\rangle$ from (15) discussed in detail in section IV. The $x$, $y$, $z$-components of the local magnetization are given by blue, yellow and green points, respectively. The used parameters are: $\eta = 0.43$, $\tau = 0.35i$, $u_1 = 0.9 + 0.23i$, $N = 9$. The curves are exact interpolations by elliptic functions (36)-(38) and are guides for the eye.](image)

Since the magnetization profile of the state (15) is given by elliptic functions, we will call this state an elliptic spin-helix state (elliptic SHS), an elliptic generalization of the spin-helix states of the XXZ model which is governed by trigonometric functions [14–16]. Further physical properties of the elliptic SHS, e.g. the projections of the magnetization vector lying on conic sections are given in section IV.

The elliptic SHS (15) visualized in Fig. 1 is the simplest nontrivial state of an open XYZ Hamiltonian and it is remarkable in many respects. First, due to the local divergence property (16) it is also an eigenstate of the periodic system $H = \sum_{n=1}^{N} h_{n,n+1}$, with $d_{N+1} \equiv d_1$, if periodicity conditions $a(u_1) = a(u_{N+1})$ are fulfilled, which is equivalent to

$$N \eta = 2L_0 \tau + 2K_0, \quad L_0, K_0 \in \mathbb{Z} \quad (17)$$

Note that for the periodic quantum chain, $u_1$ in (15) can be chosen arbitrarily leading to a multiplet of factorized states with the same energy

$$E = \sum_{n=1}^{N} d(u_n) \equiv Ng(\eta).$$

For the Hermitian case, we let $L_0 = 0$ and $\eta = 2K_0/N$. The existence of a remarkably simple elliptic SHS Fig. 1 in a periodic Hermitian XYZ spin chain is related in the case of even length to a special arrangement of Bethe roots $\lambda_j$ in the form of a perfect equidistant string, parallel to the real axis,

$$\lambda_{j+1} = \lambda_j + \frac{1}{M}, \quad j = 1, 2, \ldots, M - 1.$$

Given the boundary fields:

$$\eta^2 = -1,$$

$$\sum_{n=1}^{N} d(u_n) \equiv Ng(\eta).$$

The state $|\Psi_+\rangle$ from (15) is an eigenvector of the periodic magnetization vector:

$$\sum_{n=1}^{N} \sigma_n^z \equiv \mathbb{I}_2 \otimes \mathbb{I}_3 \otimes \mathbb{I}_4 \equiv \mathbb{I}_N \equiv 1.$$
where $M = N/2$ is an integer. The XYZ elliptic SHS string (18) is analogous to the string of phantom Bethe roots appearing in the XXZ model [14]. Other linearly independent states can be obtained by shifting the phases $u_n \rightarrow u_n + \beta$ in (14). We can show that the degeneracy of elliptic SHS in the periodic chain satisfying (17) is $\text{deg} = 2N$. More details will be given elsewhere.

Notably, the elliptic SHS (15) is a quasi-stationary state in any open systems with XYZ bulk dynamics. Indeed, the action of the open Hamiltonian on it

$$
\left( \sum_{n=1}^{N-1} h_{n,n+1} - E \right) |\Psi_+\rangle = [a(u_1)\sigma_1^+ - a(u_N)\sigma_N^-] |\Psi_+\rangle
$$

only affects the state at the boundaries, while the bulk stays intact before the information from the boundaries will spread over all the system, requiring a time of the order $N/v_c$, where $v_c$ is the sound velocity. This quasi-stationarity makes the elliptic SHS long-lived states, thus making them attractive for e.g. cold atom experiments where the anisotropies can be tuned and individual spins can be manipulated, [19, 20].

Third, the elliptic SHS can be generated also dissipatively, in open XYZ spin chains with boundary dissipation projecting the boundary spins onto predefined qubit states. Namely, if the first spin is projected onto the pure qubit state $\psi(u_1)$ and the last spin $N$ onto the state $\psi(u_1 + (N - 1)\eta)$, then the interior spins will relax towards the elliptic SHS (15) with time, provided that the dissipation is sufficiently strong, see [18].

Analogously to (11), we introduce the following bra vector

$$
\phi(u) = \left( \tilde{e}_1(u), -\tilde{e}_4(u) \right) \equiv [\psi(u)]^t.
$$

As $h' = h$, two divergence conditions for $\phi(u) \equiv [\psi(u)]^t$ can be obtained from (12) and (16) by transposition. More properties about $\psi(u)$ and $\phi(u)$ can be found in Appendix C.

III. INVARIANT SUBSPACES FOR XYZ HAMILTONIAN

The properties (12), (16) and (B10)- (B11) are fundamental. They entail the splitting of all eigenstates of the open anisotropic XYZ Heisenberg Hamiltonian on special manifolds into two complementary chiral invariant subspaces. These manifolds are characterized by model parameters satisfying the following criterion, see Appendix:

$$(N - 1 - 2M)\eta = \sum_{\sigma = \pm} \sum_{k=1}^{3} \epsilon_k^\sigma \alpha_k^\sigma - 2L_0\tau + 2K_0, \quad \prod_{\sigma = \pm} \prod_{k=1}^{3} \epsilon_k^\sigma = -1, \quad \epsilon_k^\sigma = \pm 1, \quad L_0, K_0 \in \mathbb{Z}, \quad (21)$$

where $M$ is an integer which takes values $0 \leq M \leq N - 1$. For the generic case $(N - 1 - 2M \neq 0)$, once certain boundary parameters $\{\alpha_i^\pm\}$ are selected, $\eta$ should take certain discrete values in the complex plane. Noticing that

$$
H|_{\eta \rightarrow \eta + 2} = H, \quad H|_{\eta \rightarrow \eta + 2\tau} = e^{-4i\pi(u + \tau)} H,
$$

the integers $L_0$ and $K_0$ in (21) can be restricted to $0 \leq L_0, K_0 < N - 1 - 2M$.

Eq. (21) has an important symmetry, namely the substitution

$$
M \rightarrow N - 1 - M, \quad \epsilon_k^\sigma \rightarrow -\epsilon_k^\sigma, \quad L_0, K_0 \rightarrow -L_0, -K_0
$$

leaves Eq. (21) invariant.

Basis states of these subspaces are given by the factorized products of states of type $\otimes_{n=1}^{N} \psi(u_{\alpha(n)})$ with neighboring sites parameters $\alpha(n), \alpha(n+1)$ satisfying the $\alpha(n + 1) = \alpha(n) \pm 1$ restriction. This fact allows to represent the basis vectors geometrically, plotting the “phase” $\alpha(n)$ versus $n$, and joining the points $\alpha(n)$ by a line. Then, each basis vector corresponds to a trajectory consisting of segments with constant positive or negative slopes as shown in Fig. 2. Each such segment represents a piece of some factorized state of type (15).

Let the boundary parameters in $H$ satisfy the XYZ splitting criterion (21) with $M_+ = M$. Denote

$$
M_- = N - 1 - M_+.
$$

Define two parameters $u_1, v_1$ by

$$
u_1 = \frac{1}{2} - \sum_{k=1}^{3} \epsilon_k^- \alpha_k^-,$$

$$v_1 = -u_1 - \tau.
$$

(25)

(26)
One invariant subspace is spanned by the following ket-vectors
\[
|0,\ldots,0,n_1,\ldots,n_k,N,\ldots,N\rangle = \bigotimes_{r_1=1}^{n_1} \psi(u_{r_1} - 2m_0\eta) \bigotimes_{r_2=n_1+1}^{n_2} \psi(u_{r_2} - 2(m_0 + 1)\eta) \cdots \bigotimes_{r_{k+1}=n_k+1}^{N} \psi(u_{r_{k+1}} - 2(m_0 + k)\eta),
\]
(27)

\[0 < n_1 < n_2 < \cdots < n_k < N, \; m_0, k, m_N \geq 0, \; m_0 + k + m_N = M_+,
\]

and another (complementary) invariant subspace is spanned by bra vectors
\[
\langle 0,\ldots,0,n'_1,\ldots,n'_k,N,\ldots,N|,
\]
(28)

obtained by replacing \(m_0, k, m_N, \psi, u_1, M_+, \{n_1,\ldots,n_k\}\) in (27) by \(m'_0, k', m'_N, \phi, v_1, M_-, \{n'_1,\ldots,n'_{k'}\}\) respectively, with \(M_- = N - M_+ - 1\), and a subsequent transposition.

For convenience, we rewrite the vectors in Eqs. (27)-(28) as
\[
|n_1,\ldots,n_{M_+}\rangle, \; \text{and} \; \langle n'_1,\ldots,n'_{M_-}|.
\]
(29)

Now we formulate our main statement regarding the splitting of the Hilbert space:

**Theorem** The set of linearly independent ket states
\[
|0,\ldots,0,|,|0,\ldots,0,n_1,|,|0,\ldots,0,n_1,n_2,\ldots,|,|n_1,\ldots,n_{M_+},|, \; 1 \leq n_l \leq N, \; n_l < n_{l+1},
\]
(30)

and the set of linearly independent bra states
\[
\langle 0,\ldots,0|,\langle 0,\ldots,0,n'_1,|,\langle 0,\ldots,0,n'_1,n'_2,\ldots,\langle n'_1,\ldots,n'_{M_-}|, \; 1 \leq n'_l \leq N, \; n'_l < n'_{l+1},
\]
(31)

form two bi-orthogonal complementary subspaces \(G_+^M\) and \(G_-^M\) invariant under the action of \(H\) satisfying (21) with \(M_+ := M\) The dimensions are \(\dim G_+^M = \binom{N}{0} + \binom{N}{1} + \cdots + \binom{N}{M_+}\) and \(\dim G_-^M = 2^N - \dim G_+^M\). The parameters \(u_1, v_1\) for the sets (30), (31) are given in (25),(26).

Thus, all the eigenvalues of \(H\) satisfying (21) split into two families: the right eigenvectors for the first family are given by linear combinations of (30) while the left eigenvectors for the (complementary) second family are given by linear combinations of (31).

**Remark.** One notices that the set of independent vectors in the theorem is not symmetric: both coordinates 0 and \(N\) appear several times in (27), but not in (30). So not all vectors in (27) are included in (30). Indeed, the vectors (27) are not all linearly independent; the number of linearly independent vectors is given by dimension \(\dim(G_+^M)\), the number of vectors in (30). We visualize both the symmetric and the minimal (linearly independent) sets in Fig. 2.

The proof of the theorem follows that for the partially anisotropic \(XXZ\) model [12] and is given in Appendix D.

Next we will give the explicit form of the Bethe vectors satisfying the splitting criterion (21), linking the coefficients in the expansion to the solution of the Bethe Ansatz equations.

**IV. ELLIPTIC ANALOGUES OF SPIN-HELIX EIGENSTATES IN THE XYZ MODEL**

If we choose the boundary fields to satisfy our splitting criterion (21) with \(M_+ = 0\), then according to our theorem \(H\) has a 1-dimensional invariant subspace \(G_+^M\) consisting of just one state, a fully factorized state \(|\Psi_+\rangle = \bigotimes_{n=1}^{N} \psi(u_n)\). Indeed, the boundary fields satisfy
\[
\begin{align*}
\hat{h}_1 \sigma_1 \psi(u_1) &= -a(u_1) \sigma_\uparrow \psi(u_1) + b_L(u_1) \psi(u_1), \\
\hat{h}_N \sigma_N \psi(u_N) &= a(u_N) \sigma_\uparrow \psi(u_N) + b_R(u_N) \psi(u_N),
\end{align*}
\]
(32)
(33)

(see Eq. (D7)) making the factorized state \(|\Psi_+\rangle\) from (15) an eigenstate of the Hamiltonian with eigenvalue \(\sum_{n=1}^{N-1} b(u_n) + b_L(u_1) + b_R(u_N)\). The explicit expressions of \(b_L(u), \; b_R(u)\) are given in the Appendix.
FIG. 2: **Upper Panel**: Symmetric set (not all states are linearly independent!) of all states in (27) is represented by all possible trajectories (directed paths), lying within the filled green region, including the boundaries. Each individual path starts in one of $M_{+} + 1$ points (filled black circles) on site $n = 1$ and ends at one of $M_{+} + 1$ points at $n = N$. **Lower Panel** shows the set of linearly independent states (30), which is a subset of (27) in the upper panel. The allowed trajectories end in one of two points at the right boundary site $n = N$, their total number being $(N_{0} + \ldots + (N_{M})_{+}(1,3,5,8)$ and $|0,0,3,8,N⟩$, respectively. The blue trajectory in the upper panel represents a state $|4,N,N,N,N⟩$ which can be expressed via basis states (30). Note that $M_{+}$ gives the maximal number of kinks a trajectory can have.

Since the eigenstate $|Ψ_{+}⟩$ is factorized, it is fully described by its one-point observables, i.e. the components of the magnetization profile, $⟨σ_{α}^{n}⟩$ with $α = x, y, z$. We find

$$\langle σ_{α}^{n} \rangle = -\frac{θ_{1}(β_{n})θ_{5}(iγ)}{|θ_{4}(u_{n})|^2 + |θ_{5}(u_{n})|^2}$$

(34)

and

$$\langle σ_{n}^{z} \rangle = \frac{|θ_{1}(u_{n})|^2 - |θ_{5}(u_{n})|^2}{|θ_{1}(u_{n})|^2 + |θ_{5}(u_{n})|^2}$$

(35)

where $σ_{n}^{+} = (σ_{x}^{n} + iσ_{y}^{n})/2$, and * denotes complex conjugation. Using $θ_{1}(u) = \tilde{θ}_{1}(u^*)$, $θ_{4}(u) = \tilde{θ}_{4}(u^*)$, the identities (A9)-(A11), and the relation between the functions $θ_{α}$ and the Jacobi elliptic functions sn, cn, dn, and assuming $η$ being real, we readily obtain

$$\langle σ_{n}^{x} \rangle = 2\text{Re}[(σ_{n}^{+})] = \frac{θ_{1}(β_{n})θ_{5}(iγ)}{θ_{4}(β_{n})θ_{5}(iγ)} = A_{x} \text{sn}(2K_{k} β_{n}, k)$$

(36)

$$\langle σ_{n}^{y} \rangle = 2\text{Im}[(σ_{n}^{+})] = -\frac{θ_{2}(β_{n})θ_{4}(iγ)}{θ_{4}(β_{n})θ_{3}(iγ)} = A_{y} \text{cn}(2K_{k} β_{n}, k),$$

(37)

$$\langle σ_{n}^{z} \rangle = -\frac{θ_{3}(β_{n})θ_{4}(iγ)}{θ_{4}(β_{n})θ_{3}(iγ)} = A_{z} \text{dn}(2K_{k} β_{n}, k).$$

(38)
where $\beta_n = \text{Re}[u_n] = \text{Re}[u_1] + (n-1)\eta$, $\gamma = \text{Im}[u_n] = \text{Im}[u_1]$, while the elliptic function modulus $k$, quarter period $K_k$ and the coefficients $A_\alpha$ are given by

$$k = \frac{\theta_2'(0)}{\theta_3'(0)}, \quad k' = \sqrt{1 - k^2} = \left(\frac{\theta_2'(0)}{\theta_3'(0)}\right)^2, \quad K_k = \frac{\pi\theta_3'(0)}{2},$$

$$A_x = -\sqrt{k} \frac{\theta_2(i\gamma)}{\theta_3(i\gamma)}, \quad A_y = -i\sqrt{\frac{k}{k'}} \frac{\theta_1(i\gamma)}{\theta_3(i\gamma)}, \quad A_z = -\frac{1}{\sqrt{k'}} \frac{\theta_4(i\gamma)}{\theta_3(i\gamma)}.$$

(39)

(40)

Note that in our physical case (for real $\eta$) $0 \leq k \leq 1$, and $A_\alpha$ are also all real. The periods of the $\text{sn}$, $\text{cn}$ and $\text{dn}$ functions in Eqs. (36)-(38) are given by $2/\eta$, and $1/\eta$, in lattice units.

For the parameterization (5) with generic anisotropy, i.e. generic value of $\tau$ corresponding to $J_x \geq J_y \geq J_z$, we find the following. The projection of the magnetization vector onto the $xy$ plane orbits an ellipse, the projection onto the $yz$ plane lies on a finite sector of an ellipse and the projection onto the $zx$ plane lies on a finite sector of a hyperbola. For the special case of the SHS parameter $\gamma$ taking the value $-i\tau/2$ we have a circular motion in the $xy$ plane with radius 1 and $z$-component 0. For $\gamma = 0$ ($\gamma = -i\tau$) the $y$-component of the magnetization vector is 0, the $x$-component takes values from an interval symmetric around 0 and the $z$-component takes negative (positive) values including $-1$ ($+1$).

In the critical XXZ limit, $\tau \to +i\infty$ with $k = 0$ and $J_x = J_y > J_z$, the projection of the magnetization vector onto the $xy$ plane orbits a circle with radius between 0 and 1, the $z$-component being constant. For the non-critical XXZ limit, $\tau \to 0$ with $k = 1$ and $J_x > J_y = J_z$, the projection of the magnetization vector onto the $yz$ plane lies on straight lines, the projections onto the other planes lie on (sectors of) ellipses. Note however, that for $\eta \neq 0$ most points cluster at $x$-component $\pm 1$ with the $y$- and $z$-components being 0.

We summarize these findings

$$\langle \sigma_{x,n}^2 \rangle^2 + \langle \sigma_{y,n}^2 \rangle^2 = 1, \quad \langle \sigma_{x,n}^2 \rangle^2 + \langle \sigma_{z,n}^2 \rangle^2 = 1, \quad \langle \sigma_{z,n}^2 \rangle^2 - \langle \sigma_{y,n}^2 \rangle^2 = 1 - k^2,$$

(41)

where only $A_z$ takes independent values

$$A_z^2 = 1 - (1 - k^2) A_x^2, \quad A_y^2 = 1 - A_z^2, \quad A_z \in [-1, +1].$$

(42)

These relations are consistent with $\langle \sigma_{x,n}^2 \rangle^2 + \langle \sigma_{y,n}^2 \rangle^2 + \langle \sigma_{z,n}^2 \rangle^2 = 1$.

V. SINGLE-KINK BETHE EIGENSTATES IN THE OPEN XYZ MODEL

Let us specify our general results for the simplest yet nontrivial case $M_+ = 1$ with invariant subspace $G_{M_+}^1$ containing only $N + 1$ basis vectors which we call $|0\rangle, |1\rangle, \ldots, |N\rangle$. The action of the XYZ Hamiltonian on these states straightforwardly gives

$$H |n\rangle = |E_0(1) + X(n) \rangle |n\rangle + 2A_-(n) |n - 1\rangle + 2A_+(n) |n + 1\rangle, \quad n = 1, 2, \ldots, N - 1,$$

(43)

$$H |0\rangle = |E_0(1) + X_L \rangle |0\rangle + 2A_L |1\rangle,$$

(44)

$$H |N\rangle = |E_0(1) + X_R |N\rangle + 2A_R |N - 1\rangle,$$

(45)

where the expressions of some functions in the above formulas are shown in Appendix E.

We search for the Bethe vectors belonging to the invariant subspace in the general form

$$|\Psi(\lambda)\rangle = \sum_{n=0}^{N} F_n(\lambda) |n\rangle, \quad \text{with} \quad H|\Psi(\lambda)\rangle = E(\lambda)|\Psi(\lambda)\rangle,$$

(46)

where $F_n$ are coefficients which depend on the complex parameter $\lambda$ parametrizing the energy $E(\lambda)$ like

$$E(\lambda) = E_0(1) + E_B(\lambda), \quad (47)$$

$$E_B(\lambda) = 2[g(\lambda - \frac{1}{2}) - g(\lambda + \frac{1}{2})].$$

(48)

Substituting Eq. (46) into (43)-(45), we obtain a system of linear equations for $F_n(\lambda)$, namely

$$F_{n+1}(\lambda)A_-(n + 1) + F_{n-1}(\lambda)A_+(n - 1) = Y(\lambda, n)F_n(\lambda),$$

(49)

$$F_0(\lambda)A_L + F_2(\lambda)A_-(2) = Y(\lambda, 1)F_1(\lambda),$$

(50)

$$F_N(\lambda)A_R + F_{N-2}(\lambda)A_+(N - 2) = Y(\lambda, N - 1)F_{N-1}(\lambda),$$

(51)

$$F_1(\lambda)A_-(1) = Y_L(\lambda)F_0(\lambda),$$

(52)

$$F_{N-1}(\lambda)A_+(N - 1) = Y_R(\lambda)F_N(\lambda),$$

(53)
where
\[ 2Y(\lambda, n) = E_B(\lambda) - X(n), \]  
\[ 2Y_L(\lambda) = E_B(\lambda) - X_L, \]  
\[ 2Y_R(\lambda) = E_B(\lambda) - X_R. \]

We propose the following ansatz,
\[ F_n(\lambda) = \kappa_n [B_+ U_n(\lambda) + B_- U_n(-\lambda)], \quad n = 0, \ldots, N, \]  
\[ \kappa_0 = \frac{A_+(0)}{A_L}, \quad \kappa_N = \frac{A_-(N)}{A_R}, \quad \kappa_1 = \kappa_2 = \ldots = \kappa_{N-1} = 1, \]  
\[ U_n(\lambda) = \left[ \frac{\theta_1(\lambda + \frac{n}{2})}{\theta_1(\lambda - \frac{n}{2})} \right]^n \frac{\theta_2(\lambda - u_n + \frac{n}{2})}{\theta_2(u_n-1)\theta_2(u_n)^n}, \]

where \( \{B_{\pm}\} \) are two \( \lambda \)-dependent constants. The functions \( \{U_n(\lambda)\} \) satisfies the identity
\[ U_{n+1}(\pm)A_-(n+1) + U_{n-1}(\pm)A_+(n-1) = Y(\lambda, n)U_n(\pm), \]
for arbitrary \( \lambda, n \). As a consequence, Eqs. (49)-(51) are satisfied automatically. From Eqs. (52),(53) we get
\[ \frac{\kappa_0 Y_L(\lambda)U_0(\lambda) - A_-(1)U_1(\lambda)}{\kappa_0 Y_L(\lambda)U_0(-\lambda) - A_-(1)U_1(-\lambda)} = \frac{\kappa_N Y_R(\lambda)U_N(\lambda) - A_+(N-1)U_{N-1}(\lambda)}{\kappa_N Y_R(\lambda)U_N(-\lambda) - A_+(N-1)U_{N-1}(-\lambda)}. \]  

The consistency condition of the above gives the Bethe ansatz equation (BAE) which determines the Bethe root \( \lambda \)
\[ \frac{\kappa_0 Y_L(\lambda)U_0(\lambda) - A_-(1)U_1(\lambda)}{\kappa_0 Y_L(\lambda)U_0(-\lambda) - A_-(1)U_1(-\lambda)} = \frac{\kappa_N Y_R(\lambda)U_N(\lambda) - A_+(N-1)U_{N-1}(\lambda)}{\kappa_N Y_R(\lambda)U_N(-\lambda) - A_+(N-1)U_{N-1}(-\lambda)}. \]

Recall that
\[ u_1 = \frac{1}{2} - \sum_{k=1}^{3} \epsilon_k^\dagger \alpha_{-k}^- \quad u_{N-2M_{\pm}} = \frac{1}{2} + \sum_{k=1}^{3} \epsilon_k^\dagger \alpha_k^+ - 2L_0 \tau + 2K_0, \quad \prod_{k=1}^{3} \epsilon_k^- = -1, \quad \prod_{k=1}^{3} \epsilon_k^+ = 1. \]

We simplify the expressions of \( \kappa_0 \) and \( \kappa_N \) by substituting Eqs. (25), (E1), (E3), (E4) into (58)
\[ \kappa_0 = \frac{\theta_1(\sum_{k=1}^{3} \epsilon_k^\dagger \alpha_{-k}^- + 2\eta) \prod_{\alpha_1, \alpha_2, \alpha_3} \theta_1(\alpha_1^-)}{\theta_1(\eta) \prod_{\alpha_1, \alpha_2, \alpha_3} \theta_1(\epsilon_j^\dagger \alpha_j^+ + \epsilon_j \alpha_j^- + \epsilon_k \alpha_k^- + \eta)}, \]  
\[ \kappa_N = -\frac{\theta_1(\sum_{k=1}^{3} \epsilon_k^\dagger \alpha_k^+ + 2\eta) \prod_{\alpha_1, \alpha_2, \alpha_3} \theta_1(\alpha_1^+)}{\theta_1(\eta) \prod_{\alpha_1, \alpha_2, \alpha_3} \theta_1(\epsilon_j^\dagger \alpha_j^- + \epsilon_j \alpha_j^+ + \epsilon_k \alpha_k^+ + \eta)}. \]

Especially, when \( \eta = -\epsilon_k \alpha_{-k}^-, k = 1, 2, 3 \), it is straightforward to get \( \kappa_0 = 1 \). Analogously \( \kappa_N = 1 \) when \( \eta = -\epsilon_k^\dagger \alpha_k^-, k = 1, 2, 3 \).

Suppose that our Hamiltonian is hermitian, so its spectrum \( E(\lambda) \) is real. Analyzing the expression for (48) we find that \( E_B(z) \) is an even elliptic function in the complex plane of \( z \) with periods \( 1, \tau \): \( E_B(z) = E_B(-z), E_B(z + 1) = E_B(z + \tau) = E_B(z) \). Consequently, we can restrict the elementary domain of \( z \) to the rectangle in the complex plane with \( 0 \leq \text{Re}[z] \leq \frac{1}{2}, 0 \leq \text{Im}[z] \leq \frac{\pi}{2} \). Moreover, requiring the energies \( E_B(\lambda) \) to be real forbids the \( \lambda \) to lie inside the rectangle. Thus, all physically valid values of \( \lambda \) must lie on the edges of the rectangle \( \text{Re}[\lambda] = 0, \frac{1}{2} \) and \( \text{Im}[\lambda] = 0, \frac{\pi}{2} \).

To check our predictions, we select \( \epsilon_3^\dagger = -1, \epsilon_2^\dagger = 1, k = 1, 2, \epsilon_1^\dagger = 1, l = 1, 2, 3 \) and diagonalize the Hamiltonian inside the invariant subspace \( G_{\dagger}^+ \) for sufficiently large systems, using the system of equations (43)-(45).

The band structure of Eqs (43)-(45) allows to easily solve the problem, namely to obtain the coefficients of the Bethe vector \( F_n \) and the corresponding energies, as well as Bethe roots \( \lambda_k \) for all Bethe vectors belonging to the invariant subspace. Some typical locations of the Bethe roots inside \( G_{\dagger}^+ \) is shown in Fig. 3 for a system of \( N = 100 \) spins, satisfying our criterion (21) for \( M_{\pm} = 1 \). We see that most solutions correspond to either \( \text{Re}[\lambda_k] = 0 \) or \( \text{Re}[\lambda_k] = \frac{1}{2} \), the roots being distributed approximately homogeneously along the imaginary axis. An inspection shows that these roots correspond to the quasi-periodically changing coefficients \( F_n \), which are of order \( O(1) \) for all \( n \). On the other
hand, a few separately located roots at the upper edge $\text{Im}[\lambda_k] = \text{Im}(\tau/2)$ and the lower edge $\text{Im}[\lambda_k] = 0$ (red and green in the Figure) correspond to the “localized” cases, with coefficients $F_n$ or $F_{N-n}$ decreasing exponentially, see Fig. 4. A similar type of solutions was also observed and discussed in the context of XXZ form (see Appendix E for details),

The origin of the “localized” solutions in Fig. 3 becomes clear if we write down the BAE (62) in another, equivalent form (see Appendix E for details),

$$e^{-8i\pi L_0\lambda} \left[ \frac{\theta_1(\lambda + \frac{\eta}{2})}{\theta_1(\lambda - \frac{\eta}{2})} \right]^{2N} \prod_{k=1}^{3} \frac{\theta_1(\lambda - \alpha_k^+ - \frac{\eta}{2})}{\theta_1(\lambda + \alpha_k^+ + \frac{\eta}{2})} \frac{\theta_1(\lambda + \alpha_3^- - \frac{\eta}{2})}{\theta_1(\lambda - \alpha_3^- + \frac{\eta}{2})} \prod_{k=1}^{2} \frac{\theta_1(\lambda - \alpha_l^- - \frac{\eta}{2})}{\theta_1(\lambda + \alpha_l^- + \frac{\eta}{2})} = 1.$$  \hspace{1cm} (65)

It is clear that solutions to (65) with $\frac{\theta_1(\lambda + \frac{\eta}{2})}{\theta_1(\lambda - \frac{\eta}{2})} = d \neq 1$ (meaning $2\text{Re}[\lambda] \neq 0,1$) may lead to divergences for large $N$: if $d > 1$, the term $d^{2N}$ in (65) diverges. Therefore, such a solution can only survive in the limit of $N \to \infty$, if the divergence is compensated by one of factors in the numerator of (65) which becomes zero. Due to $\theta_1(0) = 0$, the above requirement amounts to one of arguments of $\theta_1$ (65) becoming zero, either $\lambda \to \alpha_{1,2,3}^+ + \frac{\eta}{2} \; \text{mod} \; 1$ or $\lambda \to \alpha_{1,2}^+ + \frac{\eta}{2} \; \text{mod} \; 1$, or $\lambda \to -d^+ + \frac{\eta}{2} \; \text{mod} \; 1$. Indeed, in the example shown in Fig. 3, we have four divergent solutions featured in Fig. 4: the corresponding Bethe roots, up to exponentially small corrections are given by $\lambda = \alpha_{1,2}^\pm + \frac{\eta}{2}$.

All the remaining $N - 3$ solutions have the form $\text{Re}(\lambda) = 0$ or $\text{Re}(\lambda) = \frac{\eta}{2}$ corresponding to $\frac{\theta_1(\lambda + \frac{\eta}{2})}{\theta_1(\lambda - \frac{\eta}{2})} = 1$. Their distribution on the segments $[0, \tau/2]$ of the imaginary axis becomes approximately equidistant as $N$ grows. The upper and lower bounds for the respective parts of the “continuous spectrum” in the right panel of Fig. 3 are given by $E_0(1) + E_B(\frac{\tau}{2})$, $E_0(1) + E_B(\frac{\tau}{2})$ for the black (upper) band and $E_0(1) + E_B(\frac{\tau}{2})$, $E_0(1) + E_B(0)$ for the blue (lower) band.

### Discussion

Summarizing, we have proven a splitting of the Hilbert space into invariant manifolds for the XYZ spin chain with boundary fields, and derived the spitting condition (21). Our main result is intrinsically based on a pair of local divergence conditions (12), (16) and is given as the Theorem in section III. Using our theorem, we have demonstrated how one describes in detail the spectrum and the structure of Bethe vectors within the invariant subspaces with $M_+ = 0$ and $M_+ = 1$ (one Bethe root). Generalizations of our results for arbitrary $M_+$ is more technical and will be given elsewhere.

We find that our criterion (21) and our Bethe ansatz equations are the same as the ones given in [7], which proves the consistency of our results. In the limit $\tau \to +i\infty$, the XYZ chain degenerates into the critical XXZ chain and we see the spin-helix structure [14, 18] in the Bethe vectors. The splitting criterion for the XXZ chain has been derived in [12].

It would be interesting to explore the consequences of the existence of the chiral basis for the periodic XYZ chain. We are convinced that our chiral basis will be useful for the periodic system, since some results in [1, 9, 11] show the existence of the homogeneous BAE under certain conditions. As a first step, we derived a condition for a periodic system to have an elliptic SHS in (17).

Another perspective seems to be opening in the cold atom experiments which proved the possibility to create and sustain spin-helix states [19, 20], which are the simplest examples of so-called phantom Bethe states [14] appearing in the XXZ Heisenberg spin chain. It would be very exciting if our novel elliptic SHS can be prepared experimentally.

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FIG. 3: **Upper panel**: Location of the Bethe roots in the multiplet $G^+_1$ with dimension $\text{dim}(G^+_1) = N + 1 = 101$. The respective energies decrease in the counter-clockwise direction, starting with the bottom of the “continuum” in the right. The energies for the multiplet are shown in the **lower panel**, respecting the colour code. Bulk parameters are: $N = 100$, $\eta = 0.43$, $\tau = 0.35i$, and correspond to $J_x \approx 4.51$, $J_y \approx 0.244$, $J_z \approx 0.136$. Boundary parameters are $\{\alpha_1, \alpha_2, \alpha_3\} = \{0.9, 0.86 + \frac{\tau}{2}, 0.53\}$, $\{\alpha_1^+, \alpha_2^+, \alpha_3^+\} = \{0.96, 38.99 + 1.225i, \frac{\tau}{2} + 0.53i\}$, and satisfy (21) with $L_0 = 2$, $K_0 = 0$ and $M_0 = 1$.

FIG. 4: Coefficients $|F_n|$ for the $H$ eigenfunctions corresponding to two red points and two green points in Fig. 3 combined in one plot, on a logarithmic scale. Red, orange, darkgreen, and green symbols corresponding to the energies $E = 81.844$, $75.07$, $70$, $56.43$ respectively.
In this paper, we adopt the notations of elliptic theta functions $\theta_n(u, q)$ following Ref. [17]

\[
\begin{align*}
\vartheta_1(u, q) &= 2 \sum_{n=0}^{\infty} (-1)^n q^{(n+\frac{1}{2})^2} \sin[(2n+1)u], \\
\vartheta_2(u, q) &= 2 \sum_{n=0}^{\infty} q^{(n+\frac{1}{2})^2} \cos[(2n+1)u], \\
\vartheta_3(u, q) &= 1 + 2 \sum_{n=1}^{\infty} q^{n^2} \cos(2nu), \\
\vartheta_4(u, q) &= 1 + 2 \sum_{n=1}^{\infty} (-1)^m q^{n^2} \cos(2nu).
\end{align*}
\]
Recall that $\theta_\alpha(u) \equiv \vartheta_\alpha(\pi u, e^{i\pi \tau})$, $\tilde{\theta}_\alpha(u) \equiv \tilde{\vartheta}_\alpha(\pi u, e^{2i\pi \tau})$. There exist many identities for $\theta_\alpha(u)$ and $\tilde{\theta}_\alpha(u)$. Here we list some useful identities [11, 17, 18, 21]

$$
\begin{align*}
\theta_2(u) &= \theta_1(u + \frac{1}{2}), \\
\theta_3(u) &= e^{i\pi(u + \frac{1}{2})} \theta_1(u + \frac{1}{2}), \\
\theta_4(u) &= -e^{-i\pi(u + \frac{1}{2})} \theta_1(u + \frac{1}{2}), \\
\theta_1(-u) &= -\theta_1(u), \\
\theta_1(u + 1) &= -\theta_1(u), \\
\theta_1(u + \tau) &= -e^{-i\pi(u + \frac{1}{2})} \theta_1(u), \\
\frac{\tilde{\theta}_1(2u)}{\tilde{\theta}_2(2u)} &= \frac{\theta_1(u) \theta_2(u)}{\theta_2(0) \theta_4(0)} = \frac{\theta_3(u) \theta_4(u)}{\theta_2(0) \theta_4(0)}, \\
\theta_1^2(u) \theta_2(0) \theta_3(0) \theta_4(0) &= 2\theta_1(u) \theta_2(u) \theta_3(u) \theta_4(u), \\
\tilde{\theta}_1(u + v) \tilde{\theta}_1(u - v) \tilde{\theta}_2(0) &= \tilde{\theta}_1^2(u) \tilde{\theta}_2^2(v) - \tilde{\theta}_1^2(v) \tilde{\theta}_2^2(u), \\
\tilde{\theta}_4(u + v) \tilde{\theta}_4(u - v) \tilde{\theta}_2(0) &= \tilde{\theta}_4^2(u) \tilde{\theta}_2^2(v) - \tilde{\theta}_4^2(v) \tilde{\theta}_2^2(u), \\
\theta_1(u \pm v) \theta_2(u \mp v) \theta_3(0) \theta_4(0) &= \theta_1(u) \theta_2(v) \theta_3(v) \theta_4(v) \pm \theta_1(v) \theta_2(u) \theta_3(u) \theta_4(u).
\end{align*}
$$

(A2)\hspace{1cm} (A3)\hspace{1cm} (A4)\hspace{1cm} (A5)\hspace{1cm} (A6)\hspace{1cm} (A7)\hspace{1cm} (A8)\hspace{1cm} (A9)\hspace{1cm} (A10)\hspace{1cm} (A11)\hspace{1cm} (A12)\hspace{1cm} (A13)\hspace{1cm} (A14)

where

$$
\begin{align*}
2w' &= -w + x + y + z, \\
2x' &= w - x + y + z, \\
2y' &= w + x - y + z, \\
2z' &= w + x + y - z.
\end{align*}
$$

Define

$$
\zeta(u) = \frac{\theta_1'(u)}{\theta_1(u)}, \quad \tilde{\zeta}(u) = \frac{\tilde{\theta}_1'(u)}{\tilde{\theta}_1(u)}.
$$

(A15)

which possess the following properties

$$
\zeta(u) = -\zeta(-u), \quad \zeta(u + 1) = \zeta(u), \quad \zeta(u + \tau) = \zeta(u) - 2i\pi,
$$

$$
\tilde{\zeta}(u) = -\tilde{\zeta}(-u), \quad \tilde{\zeta}(u + 1) = \tilde{\zeta}(u), \quad \tilde{\zeta}(u + 2\pi) = \tilde{\zeta}(u) - 2i\pi,
$$

$$
2\zeta(2u) = \zeta(u) + \zeta(u + \frac{1}{2}), \quad \zeta(u) = i\pi + \tilde{\zeta}(u) + \tilde{\zeta}(u + \tau),
$$

$$
2\tilde{\zeta}(u) = 2i\pi + \zeta(\frac{u}{2}) + \zeta(\frac{u + 1}{2}) + \zeta(\frac{u + \pi}{2}) + \zeta(\frac{u + \pi + 1}{2}).
$$

(A16)\hspace{1cm} (A17)\hspace{1cm} (A18)\hspace{1cm} (A19)

The functions $\theta_\alpha(u)$, $\tilde{\theta}_\alpha(u)$, $\zeta(u)$, $\tilde{\zeta}(u)$ satisfy identities, e.g.

$$
\begin{align*}
\frac{\theta_2(u)}{\theta_1(u)} &= \frac{\theta_2(0)}{\theta_1'(0)} \left[ \zeta(\frac{u}{2}) + \zeta(\frac{u + 1}{2}) - \zeta(u) \right], \\
\frac{\theta_4(u)}{\theta_1(u)} &= \frac{\theta_4(0)}{\theta_1'(0)} \left[ \zeta(\frac{u}{2}) + \zeta(\frac{u + \pi}{2}) - \zeta(u) + i\pi \right], \\
\frac{\theta_4(u)}{\theta_1(u)} &= \frac{\theta_4(0)}{\theta_1'(0)} \left[ \zeta(\frac{u}{2}) + \zeta(\frac{u + 1 + \pi}{2}) - \zeta(u) + i\pi \right], \\
\frac{\theta_1(x_1 + x_2) \theta_1(x_3)}{\theta_1(x_1) \theta_1(x_2) \theta_1(x_3)} &= \frac{1}{\theta_1'(0)} \left[ \zeta(x_1) + \zeta(x_2) + \zeta(x_3) - \zeta(x_1 + x_2 + x_3) \right], \\
\frac{\tilde{\theta}_1(x_1 + x_2) \tilde{\theta}_1(x_3)}{\tilde{\theta}_1(x_1) \tilde{\theta}_1(x_2) \tilde{\theta}_1(x_3)} &= \frac{\tilde{\theta}_1'(0) \theta_1(x_1)}{\theta_1(x_4) \theta_1(x_4) \theta_1'(0)} \left[ \tilde{\zeta}(x_1) + \tilde{\zeta}(x_2) + \tilde{\zeta}(x_3) - \tilde{\zeta}(x_1 + x_2 + x_3) \right].
\end{align*}
$$

(A20)\hspace{1cm} (A21)\hspace{1cm} (A22)\hspace{1cm} (A23)\hspace{1cm} (A24)
These equations can be proved as follow. The functions on the left and right hand sides are both elliptic functions. According to Liouville’s theorem two meromorphic functions that have same periods, same zeros and poles have constant ratio. If further the two functions coincide at one non-trivial point they are identical everywhere. Thus, the corresponding equation is proved.

**Appendix B: The proof of divergence condition (12)**

Introduce two parameters \( J_{\pm} \) as

\[
J_{\pm} = J_x \pm J_y.
\]

(B1)

First substitute \( a(u + \eta) \) in (12) with \( a'(u) \). The divergence condition (12) thus implies four identities

\[
2[a(u) - a'(u)] = J_- \left[ \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} - \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} \right],
\]

(B2)

\[
2[a(u) + a'(u)] = J_+ \left[ \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} - \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} \right],
\]

(B3)

\[
2d(u) = J_- \left[ \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} + \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} \right],
\]

(B4)

\[
4J_z = J_+ \left[ \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} + \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} \right] + J_- \left[ \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} + \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} \right] = 0.
\]

(B5)

Here we let \( u = u_n \). The above equations can be proved by using elliptic theta function identities. With the help of Eqs. (A9) and (A10), we get

\[
J_- = 2 \frac{\tilde{\theta}_2^2(\eta)}{\theta_2^2(0)}, \quad J_+ = 2 \frac{\tilde{\theta}_4^2(\eta)}{\theta_4^2(0)}.
\]

(B6)

Then, we have

\[
- J_+ \left[ \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} + \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} \right] + J_- \left[ \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} + \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} \right] = \frac{\tilde{\theta}_2^2(\eta)}{\theta_2^2(0)} \left[ \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} + \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} \right] + 2 \frac{\tilde{\theta}_4^2(\eta)}{\theta_4^2(0)} \left[ \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} + \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} \right] + 2 \frac{\tilde{\theta}_2^2(\eta)}{\theta_2^2(0)} \left[ \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} + \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} \right]
\]

(A6)

\[
= -2 \frac{\tilde{\theta}_1(u + \eta)\tilde{\theta}_4(u + \eta)}{\theta_1(u)\theta_4(u)} - 2 \frac{\tilde{\theta}_1(u + \eta)\tilde{\theta}_4(u - \eta)}{\theta_1(u)\theta_4(u)}
\]

(A11)

\[
= -4 \frac{\theta_2(\eta)}{\theta_2(0)} = -4J_z.
\]

(B7)

Thus, the consistency condition (B5) is proved. From Eqs. (B2)-(B5), we get the expression of \( a(u) \)

\[
a(u) = -J_+ \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)} - J_- \frac{\tilde{\theta}_4(u)\tilde{\theta}_4(u + \eta)}{\theta_4(u)\theta_4(u + \eta)}
\]

(A7)

\[
= \frac{\theta_2(\eta)}{\theta_2(0)} + \frac{\tilde{\theta}_2^2(\eta)\tilde{\theta}_4(u + \eta)}{\theta_2(0)\theta_4(u + \eta)} - \frac{\tilde{\theta}_2^2(\eta)\tilde{\theta}_4(u + \eta)}{\theta_2(0)\theta_4(u + \eta)}
\]

(A11)

\[
= \frac{\theta_1(u)\tilde{\theta}_2(u)}{\theta_2(0)\theta_1(u)}
\]

(B8)
Analogously, we can get \( a'(u) \equiv a(u + \eta) \). The expression of \( d(u) \) is obtained as follows

\[
d(u) = -J_z + J_+ + \frac{J_-}{2} \left[ \frac{\hat{\theta}_4(u)}{\hat{\theta}_1(u)} + \frac{\hat{\theta}_4(u)}{\hat{\theta}_4(u)} \right] + \frac{\hat{h}_0}{\hat{\theta}_1(u)} \left[ \frac{\hat{\theta}_4(u)}{\hat{\theta}_1(u)} + \frac{\hat{\theta}_4(u)}{\hat{\theta}_4(u)} \right] + \hat{h}_z^\perp
\]

\[
(\text{A20}) \Rightarrow \frac{\theta_1(\eta)}{\theta_1'(0)} \left[ \zeta(\eta) - 2\zeta'(\eta) \right] + \frac{\theta_4(\eta)\theta_4(\eta + \tau)}{\theta_1(0)\theta_1(\eta + \tau)} \left[ \hat{\theta}_1(u + \tau)\hat{\theta}_1(u + \eta + \tau) + \hat{\theta}_1(u + 2\tau)\hat{\theta}_1(u + \eta + 2\tau) \right]
\]

\[
(\text{A24}) \Rightarrow \frac{\theta_1(\eta)}{\theta_1'(0)} \left[ \zeta(\eta) + \zeta(u + \eta) - \zeta(u + \eta + \tau) - \zeta(u + \eta) \right]
\]

\[
(\text{A18}) \Rightarrow \frac{\theta_1(\eta)}{\theta_1'(0)} \left[ \zeta(\eta) + \zeta(u + \eta) = g(\eta) + g(u) + g(u + \eta). \right]
\]

As noted above, Eq. (12) (or (16)) is proved analytically. For the bra vector \( \phi(u) \), the following equations hold

\[
\phi(u) \otimes \phi(u + \eta) h = \phi(u) \otimes \phi(u + \eta) \left[ a(u) \sigma^z \otimes I_2 - a(u + \eta) \otimes I_2 \right] + d(u) I_4, \quad \text{(B10)}
\]

\[
\phi(u) \otimes \phi(u - \eta) h = \phi(u) \otimes \phi(u - \eta) \left[ -a(u) \sigma^z \otimes I_2 + a(u - \eta) \otimes \sigma^z + d(-u) I_4 \right], \quad \text{(B11)}
\]

where \( a(u) \) and \( d(u) \) are given by (13).

**Appendix C: Properties of \( \psi(u) \) and \( \phi(u) \)**

Apart from the divergence conditions, the two-component vectors \( \psi(u) \) and \( \phi(u) \) also satisfy the following boundary related equations

\[
\hat{h}_1 \sigma_1 \psi(u) = [a_L(u) \sigma_1^z + b_L(u)] \psi(u), \quad \text{(C1)}
\]

\[
\hat{h}_N \sigma_N \psi(u) = [a_R(u) \sigma_N^z + b_R(u)] \psi(u). \quad \text{(C2)}
\]

\[
\phi(u) \hat{h}_1 \sigma_1 = \phi(u) \left[ \hat{a}_L(u) \sigma_1^+ + \hat{b}_L(u) \right], \quad \text{(C3)}
\]

\[
\phi(u) \hat{h}_N \sigma_N = \phi(u) \left[ \hat{a}_L(u) \sigma_N^+ + \hat{b}_R(u) \right], \quad \text{(C4)}
\]

Using Eqs. (A9)-(A11), it is easy to get

\[
\frac{\hat{\theta}_4(u)}{\hat{\theta}_1(u)} + \frac{\hat{\theta}_4(u)}{\hat{\theta}_4(u)} = 2 \frac{\theta_4(u)}{\theta_1(0)}, \quad \text{(C5)}
\]

\[
\frac{\hat{\theta}_4(u)}{\hat{\theta}_1(u)} - \frac{\hat{\theta}_4(u)}{\hat{\theta}_4(u)} = 2 \frac{\theta_4(u)}{\theta_1(0)}. \quad \text{(C6)}
\]

Then the expressions of \( a_L(u) \) and \( b_L(u) \) can be obtained directly from (C1)

\[
a_L(u) = -\frac{\hbar^+}{2} \left[ \frac{\hat{\theta}_4(u)}{\hat{\theta}_1(u)} - \frac{\hat{\theta}_4(u)}{\hat{\theta}_4(u)} \right] + \frac{i\hbar^-}{2} \left[ \frac{\hat{\theta}_4(u)}{\hat{\theta}_1(u)} + \frac{\hat{\theta}_4(u)}{\hat{\theta}_4(u)} \right] + \hat{h}_z^\perp
\]

\[
= -\frac{\theta_1(\eta)\theta_3(u)}{\theta_1(0)} \prod_{l=1}^{3} \theta_3(\alpha_l^-) + \frac{\theta_3(u)}{\theta_1(0)} \prod_{l=1}^{3} \theta_3(\alpha_l^-) - \frac{\theta_1(\eta)}{\theta_1(0)} \prod_{l=1}^{3} \theta_2(\alpha_l^-), \quad \text{(A12)}
\]

\[
= -a(u) + 2 \frac{\theta_1(\eta)}{\theta_2(0)} \prod_{l=1}^{3} \theta_1(\alpha_l^+) = a(u) + 2 \frac{\theta_1(\eta)}{\theta_2(0)} \prod_{l=1}^{3} \theta_1(\alpha_l^-)^{2} \quad \text{or} \quad \frac{\theta_1(\eta)}{\theta_2(0)} \prod_{l=1}^{3} \theta_1(\alpha_l^-)^{2} = a(u), \quad \text{(C7)}
\]

\[
b_L(u) = -\frac{\hbar^-}{2} \left[ \frac{\hat{\theta}_4(u)}{\hat{\theta}_1(u)} + \frac{\hat{\theta}_4(u)}{\hat{\theta}_4(u)} \right] + \frac{i\hbar^+}{2} \left[ \frac{\hat{\theta}_4(u)}{\hat{\theta}_1(u)} - \frac{\hat{\theta}_4(u)}{\hat{\theta}_4(u)} \right]
\]

\[
= -\frac{\theta_1(\eta)\theta_3(u)}{\theta_1(0)} \prod_{l=1}^{3} \theta_3(\alpha_l^-) + \frac{\theta_3(u)}{\theta_1(0)} \prod_{l=1}^{3} \theta_3(\alpha_l^-) \quad \text{or} \quad \frac{\theta_1(\eta)}{\theta_2(0)} \prod_{l=1}^{3} \theta_1(\alpha_l^-) = a(u), \quad \text{(C8)}
\]
With the help of Eqs. (A4)-(A8), we simplify the expression of $L.C.$ denotes linear combination and the following terms will not appear on the RHS of (D9)

$$\chi_0^+ = -\chi_1^+ - \alpha_1^+ - \alpha_2^+ - \alpha_3^+,$$

$$\chi_1^+ = \alpha_1^+ + \alpha_2^+,$$

$$\chi_2^+ = \alpha_1^+ + \alpha_2^+ + \alpha_3^+,$$

$$\chi_3^+ = \alpha_1^+ + \alpha_2^+.$$

(C9)

Analogously, we get the expressions for $a_R(u)$ and $b_R(u)$, and for $\tilde{a}_k(u)$, $\tilde{b}_k(u)$, $k = L, R$

$$\tilde{a}_L(u) = -\frac{h_1^u}{2} \left[ \frac{\theta_1(u) - \theta_1(u)}{\theta_1(u) - \theta_1(u)} \right] - \frac{i h_1^u}{2} \left[ \frac{\theta_2(u) - \theta_3(u)}{\theta_1(u) - \theta_4(u)} \right] + h_2^u,$$

(A13) $\Rightarrow$

$$a_R(u) = -\alpha(u) - 2 \frac{\theta_1(\eta) \prod_{l=0}^{3} \theta_4 \left( \frac{2u - 2\chi_l^+}{4} \right)}{\theta_2(0) \theta_4(0) \prod_{l=1}^{3} \theta_l(\alpha_l)},$$

(C10)

$$\tilde{b}_L(u) = -\frac{h_1^u}{2} \left[ \frac{\theta_1(u) - \theta_1(u)}{\theta_1(u) - \theta_1(u)} \right] - \frac{i h_1^u}{2} \left[ \frac{\theta_2(u) - \theta_3(u)}{\theta_1(u) - \theta_4(u)} \right]$$

$$b_R(u) = -b_L(u) |_{\alpha_k \rightarrow \alpha_k^+},$$

(C12)

$$a_R(u) = -a_L(u) |_{\alpha_k \rightarrow \alpha_k^+},$$

(C13)

Appendix D: Proof of the Theorem in Section III

**Closure** Like for the $XXZ$ chain [12, 13], $\sigma^z \psi(u)$ can be expanded as

$$\sigma^z \psi(u) = p_\pm(u) \psi(u) + q_\pm(u) \psi(u \pm 2\eta),$$

(D1)

$$\phi(u) \sigma^z = p_\pm(u) \phi(u) + q_\pm(u) \phi(u \pm 2\eta).$$

(D2)

From (D1), we have

$$p_\pm(u) = \frac{\theta_3(u + 2\eta) \theta_1(u + 2\eta) \theta_4(u)}{\theta_4(u + 2\eta) \theta_1(u) - \theta_4(u + 2\eta) \theta_4(u)},$$

(D3)

$$q_\pm(u) = -\frac{2 \theta_1(u) \theta_3(u)}{\theta_4(u + 2\eta) \theta_1(u) - \theta_4(u + 2\eta) \theta_4(u)}.$$

(D4)

With the help of Eqs. (A4)-(A8), we simplify the expression of $p_\pm(u)$ and $q_\pm(u)$

$$p_+(u) = -\frac{\theta_2(\eta) \theta_1(u + \eta)}{\theta_1(\eta) \theta_2(u + \eta)},$$

$q_+(u) = \frac{\theta_2(0) \theta_4(u)}{\theta_1(\eta) \theta_2(u + \eta)}.$

(D5)

$$p_-(u) = \frac{\theta_2(\eta) \theta_1(u - \eta)}{\theta_1(\eta) \theta_2(u - \eta)},$$

$q_-(u) = -\frac{\theta_2(0) \theta_4(u)}{\theta_1(\eta) \theta_2(u - \eta)}.$

(D6)

From Eqs. (C7), (C10), (C12) and (C13), we get the closure condition

$$a_L(u_1) = -a(u_1),$$

$$a_R(u_{N-2M_+}) = a(u_{N-2M_+}),$$

$$\tilde{a}(v_1) = -\tilde{a}(v_1),$$

$$\tilde{a}_R(v_{N-2M_+}) = \tilde{a}(v_{N-2M_+}).$$

(D7)

(D8)

Using Eqs. (12)-(16), (C1)-(C2), (D7)-(D8) repeatedly, one can prove

$$H|n_1, \ldots, n_{M_+} \rangle = L.C. \left( |n_1, \ldots, n_{M_+} \rangle, |n_1 - 1, \ldots, n_{M_+} \rangle, |n_1 + 1, \ldots, n_{M_+} \rangle, \ldots, |n_1, \ldots, n_{M_+} - 1 \rangle, |n_1, \ldots, n_{M_+} + 1 \rangle \right),$$

(D9)

where L.C. denotes linear combination and the following terms will not appear on the RHS of (D9)

$$| \ldots, n_l, n_{l+1}, \ldots \rangle, \quad 1 \leq n_l = n_{l+1} \leq N,$$

$$| \ldots, n_k, \ldots \rangle, \quad n_k < 0, \quad \text{or} \quad n_k > N.$$

(D10)
Obviously, the ket vectors in (27) form a closed set. Analogously, the bra vectors form another closed set. The closure condition (D7) determines the values of \(u_1\) and also gives the constraint in (21).

**Orthogonality** We use two sets of parameters \(\{\xi_1, \ldots, \xi_N\}\) and \(\{\xi'_1, \ldots, \xi'_N\}\) to represent the vectors as

\[
\bigotimes_{n=1}^{N} \psi(u_1 + \xi_n \eta), \quad \text{and} \quad \bigotimes_{n=1}^{N} \phi(v_1 + \xi'_n \eta). \tag{D11}
\]

Obviously, we find

\[
\xi_1 + \xi'_1 \leq 0, \quad \xi_N + \xi'_N \geq 0, \quad \xi_{n+1} + \xi'_{n+1} - \xi_n - \xi'_n = 0, \pm 2, \tag{D12}
\]

So equations \(\xi_n + \xi'_n = 0\) (\(\xi_n + \xi'_n\) is an even number) holds at least for one point \(n \ (1 \leq n \leq N)\). Due to the property

\[
\phi(u_1 + x)\psi(v_1 - x) = \phi(u_1 + x)\psi(-u_1 - \tau - x) = 0,
\]

any pair of vectors \(\langle n', \ldots, n'_{M-1}\rangle\) and \(\langle n_1, \ldots, n_{M_+}\rangle\) are mutually orthogonal.

**Independence** Among the ket vectors in (30), there are only \(\sum_{n=0}^{M_+} (\begin{pmatrix} N \cr n \end{pmatrix})\) linearly independent basis vectors

\[
\langle 0, \ldots, 0 \rangle, \quad \langle 0, \ldots, 0, n_1 \rangle, \quad \langle 0, \ldots, 0, n_1, n_2 \rangle, \ldots, \langle n_1, \ldots, n_{M_+} \rangle, \quad 1 \leq n_t \leq N, \quad n_t < n_{t+1}. \tag{D14}
\]

Consider the “unfavoured” case with \(\eta = \frac{1}{2}\). In this case

\[
\phi(u + 2\eta) = -\sigma^z\phi(u), \quad \phi(u + 4\eta) = \phi(u). \tag{D15}
\]

Then, we get

\[
\langle 0, \ldots, 0, n_1 \rangle \propto \prod_{l=1}^{n_1} \sigma_l^z \langle 0, \ldots, 0 \rangle,
\]

\[
\langle 0, \ldots, 0, n_1, n_2 \rangle \propto \prod_{l=n_1+1}^{n_2} \sigma_l^z \langle 0, \ldots, 0 \rangle,
\]

\[
\langle 0, \ldots, 0, n_1, n_2, n_3 \rangle \propto \prod_{l=1}^{n_1} \sigma_l^z \prod_{l_2=n_2+1}^{n_3} \sigma_{l_2}^z \langle 0, \ldots, 0 \rangle, \tag{D16}
\]

We see that even in this special setting all the basis vectors in (30) are linearly independent and form an invariant subspace of the Hamiltonian whose dimension is \(\sum_{n=0}^{M_+} (\begin{pmatrix} N \cr n \end{pmatrix})\). The bra vectors in (28) form another invariant subspace of the Hilbert space whose dimension is \(\sum_{n=0}^{M_-} (\begin{pmatrix} N \cr n \end{pmatrix}) = 2^N - \sum_{n=0}^{M_+} (\begin{pmatrix} N \cr n \end{pmatrix})\). The Hilbert space splits into two invariant subspaces.

**Appendix E: The proof of our ansatz for the \(M_+ = 1\) case**

Using Eqs. (12), (16)-(C2), (D1) repeatedly, we arrive at Eqs. (43)-(45) with

\[
A_+(n) = \frac{\theta_2(u_{n-1})}{\theta_2(u_n)}, \quad A_-(n) = \frac{\theta_2(u_n)}{\theta_2(u_{n-1})}, \tag{E1}
\]

\[
X(n) = 2 \left[ g(u_n + \frac{1}{2}) - g(u_{n-1} + \frac{1}{2}) - 2g(\eta) \right], \tag{E2}
\]

\[
A_L = \frac{1}{2}[a_L(u_{-1}) + a(u_{-1})]q_+(u_{-1}) = \frac{\prod_{l=0}^{3} \theta_1 \left( \frac{2u_l + 2\chi \gamma - 1}{4} \right)}{\theta_2(u_0) \prod_{k=1}^{3} \theta_1 (\alpha_k^+)} \tag{E3}
\]

\[
A_R = \frac{1}{2}[a_R(u_N) - a(u_{-1})]q_-(u_{-1}) = \frac{\prod_{l=0}^{3} \theta_1 \left( \frac{2u_{N-1} + 2\chi \gamma - 1}{4} \right)}{\theta_2(u_{N-1}) \prod_{k=1}^{3} \theta_1 (\alpha_k^+)} \tag{E4}
\]

\[
X_L = b_L(u_{-1}) - b_L(u_1) + g(u_{-1}) - g(u_1) + [a_L(u_{-1}) + a(u_{-1})]q_+(u_{-1}), \tag{E5}
\]

\[
X_R = b_R(u_{-1}) - b_R(u_{N-2}) - g(u_{N-2}) + g(u_{N-2}) + [a_R(u_{-1}) - a(u_{N-1})]q_-(u_{N-1}), \tag{E6}
\]

\[
E_0(M) = b_L(u_1) + b_R(u_{N-2M}) + (N-1)g(\eta) + g(u_1) - g(u_{N-2M}), \tag{E7}
\]
The functional relations in (49)-(53) are fundamental. And Eq. (60) is the key of our ansatz. From Eqs. (54) and (E2), we get the expression for $Y(\lambda, n)$

$$Y(\pm \lambda, n) = g(\lambda - \eta) - g(\lambda + \eta) - g(u_n + \frac{1}{2}) + g(u_{n-1} + \frac{1}{2}) + 2g(\eta)$$

$$= g(\lambda - \eta) + g(u_n + \frac{1}{2}) - g(u_{n-1} + \frac{1}{2}) - g(\lambda + u_n + \frac{1}{2} - \eta) + g(\lambda + u_{n-1} + \frac{1}{2} - \eta)$$

$$= \frac{\theta_1(\lambda + \frac{\eta}{2}) \theta_2(u_n - \frac{\eta}{2}) \theta_1(\lambda - u_n - \frac{3\eta}{2}) + \theta_1(\lambda - \frac{\eta}{2}) \theta_2(u_n) \theta_1(\lambda - u_n - \frac{\eta}{2})}{\theta_1(\lambda - \frac{\eta}{2}) \theta_2(u_n) \theta_1(\lambda + \frac{\eta}{2}) \theta_2(\lambda - u_n - \frac{3\eta}{2})} + \frac{\theta_1(\lambda + \frac{\eta}{2}) \theta_2(u_n - \frac{\eta}{2}) \theta_1(\lambda - u_n - \frac{3\eta}{2}) + \theta_1(\lambda - \frac{\eta}{2}) \theta_2(u_n) \theta_1(\lambda - u_n - \frac{\eta}{2})}{\theta_1(\lambda - \frac{\eta}{2}) \theta_2(u_n) \theta_1(\lambda + \frac{\eta}{2}) \theta_2(\lambda - u_n - \frac{3\eta}{2})}.$$  \hspace{1cm} (E8)

It is straightforward to check that $U_n(\lambda)$ defined in (59) satisfies Eq. (60). Then all our ansatz can be proved analytically.

**Remark.** Numerical evidence suggests the validity of the following expressions:

$$\frac{B_+}{B_-} = \frac{\theta_1(\lambda - \alpha_3 + \frac{\eta}{2}) \theta_1(\lambda + \alpha_3^* + \frac{\eta}{2})}{\theta_1(\lambda + \alpha_3 - \frac{\eta}{2}) \theta_1(\lambda - \alpha_3^* - \frac{\eta}{2})} \prod_{i=1}^{2N} \theta_1(\lambda - \alpha_i + \frac{\eta}{2}) \theta_1(\lambda + \alpha_i^* + \frac{\eta}{2})$$

$$= e^{-8i\pi L_0 \lambda} \left[ \frac{\theta_1(\lambda + \frac{\eta}{2})}{\theta_1(\lambda - \frac{\eta}{2})} \right]^{-2N} \prod_{k=1}^{N} \frac{\theta_1(\lambda - \alpha_k^* + \frac{\eta}{2})}{\theta_1(\lambda + \alpha_k + \frac{\eta}{2})}.$$ \hspace{1cm} (E9)

Based on the above equation, the BAE (E9) should have another equivalent form

$$e^{-8i\pi L_0 \lambda} \left[ \frac{\theta_1(\lambda + \frac{\eta}{2})}{\theta_1(\lambda - \frac{\eta}{2})} \right]^{-2N} \prod_{k=1}^{N} \frac{\theta_1(\lambda - \alpha_k^* + \frac{\eta}{2})}{\theta_1(\lambda + \alpha_k + \frac{\eta}{2})} \frac{\theta_1(\lambda - \alpha_3 + \frac{\eta}{2})}{\theta_1(\lambda + \alpha_3^* + \frac{\eta}{2})} = 1.$$ \hspace{1cm} (E10)

Thus, the BAE (E10) is consistent with the one given by the other approach in Ref. [7].

**Appendix F: Inhomogeneous BAE for the generic case**

The inhomogeneous BAE of the XYZ chain with generic open boundary conditions (pp.192 in [11]) read

$$\sum_{\sigma=\pm} 3 \epsilon_k^\sigma \alpha_k^\sigma + (N + 3 + 2m)\eta + 2 \sum_{j=1}^{N+1+m} \mu_j = 2l_0 \tau + 2k_0, \quad \prod_{\sigma=\pm} 3 \epsilon_k^\sigma = 1,$$ \hspace{1cm} (F1)

$$c e^{-4i\pi l_0 (\mu_j + \eta)} \theta_4^\sigma(\eta) \theta_4^{\mu_j}(\mu_j) \prod_{i=1}^{N+1+m} \theta_1(\mu_j + \eta) \theta_1(2\mu_j + \eta) = \prod_{\sigma=\pm} 3 \epsilon_k^\sigma \theta_4^\sigma \alpha_k^\sigma$$ \hspace{1cm} (F2)

where $c$ is a constant existing in the inhomogeneous term of the $T$-$Q$ relation and $m = 0$ (or $m = 1$) for even (odd) $N$. The energy in terms of Bethe roots is

$$E = -2 \sum_{j=1}^{N+1+m} g(\mu_j + \eta) + (N - 1)g(\eta) - \sum_{\sigma=\pm} 3 \sum_{l=1}^{N+1+m} g(\epsilon_k^\sigma \alpha_k^\sigma) - 4i\pi l_0 \frac{\theta_1(\eta)}{\theta_1(0)}.$$ \hspace{1cm} (F3)

When $c = 0$, it means that the following types of Bethe roots may exist

$$\mu_j = -\mu_l - \eta, \quad \mu_j = -\mu_l - 2\eta, \quad \mu_j = -\epsilon_k^\sigma \alpha_k^\sigma - \eta.$$ \hspace{1cm} (F4)

Suppose that $2m_1$ Bethe roots form pairs as $(\mu_j, -\mu_j + \eta)$, $2m_2$ Bethe roots form pairs as $(\mu_j, -\mu_j + 2\eta)$ and the remaining $m_s = N + 1 + m - 2m_1 - 2m_2$ ($m_s$ is an odd number and $1 \leq m_s \leq 5$) Bethe roots are distributed at discrete points $-\epsilon_k^\sigma \alpha_k^\sigma - \eta$. Then Eq. (F2) becomes

$$(N - 1 - 2m_1)\eta = \sum_{\sigma=\pm} 3 \sum_{k=1}^{N+1+m} \epsilon_k^\sigma \alpha_k^\sigma - 2l_0 \tau - 2k_0, \quad \prod_{\sigma=\pm} 3 \epsilon_k^\sigma = -1.$$ \hspace{1cm} (F5)
To sum up, if the constraint (F5) is satisfied, the $T$-$Q$ relation and the BAE degenerate into the homogeneous ones. Due to that the Bethe roots pair $(\mu, -\mu - 2\eta)$ contributes 0 to the energy. Under condition (F5), the energy becomes

$$E = 2 \sum_{j=1}^{m_1} [g(\mu_j) - g(\mu_j + \eta)] + (N - 1)g(\eta) - \sum_{\sigma = \pm} \sum_{l=1}^{3} g(\tilde{\epsilon}^\sigma l \alpha^\sigma l) - 4i\pi t_0 \frac{\theta_1(\eta)}{\theta'_1(0)}. \quad (F6)$$

The degeneration condition (F5) is consistent with our splitting criterion in Eq. (21), which implies the correspondence between homogeneous $T$-$Q$ relations and invariant subspaces.