Chiral coordinate Bethe ansatz for phantom eigenstates in the open XXZ spin-$\frac{1}{2}$ chain

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We construct the coordinate Bethe ansatz for all eigenstates of the open spin-$\frac{1}{2}$ XXZ chain that fulfill the phantom roots criterion (PRC). Under the PRC, the Hilbert space splits into two invariant subspaces and there are two sets of homogeneous Bethe ansatz equations (BAE) to characterize the subspaces in each case. We propose two sets of vectors with chiral shocks to span the invariant subspaces and expand the corresponding eigenstates. All the vectors are factorized and have symmetrical and simple structures. Using several simple cases as examples, we present the core elements of our generalized coordinate Bethe ansatz method. The eigenstates are expanded in our generating set and show clear chirality and certain symmetry properties. The bulk scattering matrices, the reflection matrices on the two boundaries and the BAE are obtained, which demonstrates the agreement with other approaches. Some hypotheses are formulated for the generalization of our approach.

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I. INTRODUCTION

Quantum integrable systems [1–3] play important roles in various fields, such as low-dimensional condensed-matter physics, quantum field theory, statistical physics, and Yang-Mills theory. Many methods have been developed for the analysis of integrable systems. Among them, the two most classic ones are the coordinate Bethe ansatz and the algebraic Bethe ansatz (ABA). The usage of the conventional coordinate Bethe ansatz and ABA has so far been restricted to one-dimensional integrable systems with $U(1)$ symmetry that guarantees the existence of some obvious reference states. For integrable systems without $U(1)$ symmetry, there are no obvious reference states and the conventional BA fails. Several methods including Baxter's T-Q relation [1] and Sklyanin's separation of variables (SoV) method [4] have been developed to approach this remarkable problem.

In this paper we focus on the XXZ spin-$\frac{1}{2}$ chain with open boundaries. The nondiagonal boundary fields break the $U(1)$ symmetry which makes the problem of constructing Bethe vectors rather unusual. It was proved in Refs. [5–7] for the boundary parameters obeying a certain constraint, that the modified algebraic Bethe ansatz (MABA) can be applied, and homogeneous conventional T-Q relations exist. The eigenvalue problem of the open XXZ spin chain with generic integrable boundary conditions was first solved via the off-diagonal Bethe ansatz (ODBA) method [8,9]. The Bethe-type eigenstates were then retrieved in Ref. [10] based on the ODBA solution and a convenient SoV basis [11–13]. Although the analytical form of the Bethe state with generic or constrained boundaries has been given, little is known about their inner structure.

In our recent papers [14,15], we studied the eigenstates of the open XXZ chain under the phantom roots criterion (PRC). The PRC is equivalent to the constrained boundary condition proposed in Refs. [5,6]. The PRC restricts the system parameters to a set of manifolds parametrized by an integer number M but does not introduce any obvious symmetry, such as $U(1)$ symmetry. Under the PRC, the Hilbert space splits into two invariant subspaces whose dimensions are determined by the integer M. Two sets of factorized chiral states are selected here to span the subspaces, respectively. In Refs. [14,15] we constructed the phantom Bethe states in some simple cases and analyzed their properties, such as the chirality and the corresponding spin current.

In this paper, the coordinate Bethe ansatz method is generalized in full detail. Here we report on a formulation of "generalized" chiral coordinate Bethe ansatz (CCBA) in an open XXZ spin chain with nondiagonal boundary fields. We do this on the example of the system satisfying the PRC.

Our approach inherits the core ideas of the conventional coordinate Bethe ansatz method. Its main two features are (i) We find that it is appropriate to use the basis vectors with chiral shocks, instead of the usual conventional computational basis; for this reason we also call it a chiral Bethe ansatz, (ii) it turns out to be appropriate to enlarge the basis into a symmetric one by including linearly dependent "auxiliary" vectors.

The paper is organized as follows. First, we introduce the open XXZ spin-$\frac{1}{2}$ chain under the phantom roots conditions. Two symmetrically enlarged sets of vectors are then constructed based on which we can expand the phantom eigenstates of the Hamiltonian. Next, we demonstrate how the chiral coordinate Bethe ansatz works in terms of these vectors for the $M = 0$–2 cases and generalize our method to the arbitrary M case. In the last part of the main text, we specifically study the spin helix eigenstates. Some necessary proofs are given in the appendices.

II. THE OPEN XXZ MODEL UNDER PHANTOM ROOTS CONDITIONS

We study the spin-$\frac{1}{2}$ XXZ chain with open boundary conditions,

$$H=\sum_{n=1}^{N-1} h_{n,n+1}+h_1+h_N, \tag{1}$$

where

$$h_{n,n+1}=\sigma_n^x\sigma_{n+1}^x+\sigma_n^y\sigma_{n+1}^y+\cosh\eta\;\sigma_n^z\sigma_{n+1}^z-\cosh\eta, \tag{2}$$

$$h_1=\frac{\sinh\eta}{\sinh(\alpha_-)\cosh(\beta_-)}[\cosh(\theta_-)\sigma_1^x+i\sinh(\theta_-)\sigma_1^y+\cosh(\alpha_-)\sinh(\beta_-)\sigma_1^z], \tag{3}$$

$$h_N=\frac{\sinh\eta}{\sinh(\alpha_+)\cosh(\beta_+)}[\cosh(\theta_+)\sigma_N^x+i\sinh(\theta_+)\sigma_N^y-\cosh(\alpha_+)\sinh(\beta_+)\sigma_N^z], \tag{4}$$

and $\alpha_\pm$, $\beta_\pm$, $\theta_\pm$ are boundary parameters. We parametrize the anisotropy parameter of the exchange interaction as $\Delta\equiv\cosh\eta\equiv\cos\gamma$ with $\eta=i\gamma$.

This model is one of the most famous integrable systems [1,2,16,17] without $U(1)$ symmetry. The exact solutions of this model have been given by the ODBA method [8,9]. A set of inhomogeneous Bethe ansatz equations (BAE) with, at least, N Bethe roots were constructed [8–10] to solve the eigenvalue problem, and the Bethe-type eigenstates were then retrieved [9,10] based on the ODBA solution.

An interesting observation is that some Bethe roots in the original inhomogeneous BAE can be chosen "phantom", i.e., with an infinite value of the root and, hence, not contributing to the energy, under some specific conditions, such as

$$(N-2M-1)\eta=\alpha_-+\beta_-+\alpha_++\beta_++\theta_--\theta_+\mod 2\pi i, \tag{5}$$

where M is an integer ranging from 0 to $N-1$. Under the PRC (5), the inhomogeneous BAE can reduce to homogeneous ones with M or $\widetilde{M}=N-1-M$ preserved finite Bethe roots [5–7,9] and the Hilbert space splits into two invariant subspaces G_M^+ and G_M^-, whose dimensions are determined by the integer M [14,15]. The PRC also serve as the compatibility condition of the MABA method [5,18].

Under the constraint (5), the Hermiticity of Hamiltonian (1) requires in the case $|\Delta|<1$ (the easy-plane regime),

$$\mathrm{Re}[\alpha_\pm]=\mathrm{Re}[\theta_\pm]=\mathrm{Re}[\eta]=0,$$
$$\mathrm{Im}[\beta_\pm]=0\quad\text{and}\quad\beta_+=-\beta_-, \tag{6}$$

and in the case $\Delta>1$ (the easy axis regime),

$$\mathrm{Im}[\alpha_\pm]=\mathrm{Im}[\beta_\pm]=\mathrm{Im}[\eta]=0,$$
$$\mathrm{Re}[\theta_\pm]=0\quad\text{and}\quad\theta_+=\theta_-\mod 2i\pi. \tag{7}$$

In the following we show that the two sets of homogeneous BAE correspond to two invariant subspaces G_M^+ and G_M^-, respectively, and we argue that their solutions constitute the complete set of eigenstates and eigenvalues under the criterion (5). In addition, we construct explicit phantom Bethe vectors via a chiral coordinate Bethe ansatz, see below.

III. ADDITION OF EXTRA AUXILIARY VECTORS TO THE BASES OF $G_M^\pm$.

Here we explain a perhaps most important and subtle feature of the chiral coordinate Bethe ansatz for open systems with nondiagonal boundary fields, satisfying the phantom roots criterion. Namely, we have two invariant subspaces G_M^+ and G_M^-, and the eigenvectors of H for each subspace will be given by separate CCBA. Furthermore, the Bethe eigenvectors will be given not as a linear combination of independent original basis vectors but as a linear combination of the original basis vectors plus other extra auxiliary vectors, which are linearly dependent and are added for convenience. Adding the extra vectors allows to symmetrize the basis and to make the CCBA coefficients elegant and simple. Below we recall the definition of the basis vectors and show how the extra auxiliary vectors are constructed.

Define the following local left vectors on each site n:

$$\phi_n(x)=(1,-e^{\theta_-+\alpha_-+\beta_-+(2x-n+1)\eta})\equiv(1,e^{z_{n,x}}), \tag{8}$$

$$z_{n,x}=\theta_-+\alpha_-+\beta_-+(2x-n+1)\eta+i\pi. \tag{9}$$

Here the second component of these states depends on the position index n, and $z_{n,x}$ serves as a phase factor of state $\phi_n(x)$. Let us introduce a set of factorized states,

$$\langle\underbrace{0,\ldots,0}_{m_0},\underbrace{n_1,\ldots,n_k}_{k},\underbrace{N,\ldots,N}_{m_N}|=\exp\left[\eta\left(Nm_N+\sum_{j=1}^k n_j\right)\right]\bigotimes_{l_1=1}^{n_1}\phi_{l_1}(m_0)\bigotimes_{l_2=n_1+1}^{n_2}\phi_{l_2}(m_0+1)\cdots\bigotimes_{l_{k+1}=n_k+1}^{N}\phi_{l_{k+1}}(m_0+k),$$
$$0<n_1<n_2<\cdots<n_k<N,\qquad k\geqslant 0. \tag{10}$$

The structure of the states (10) is particular and is very different from the usual computational basis of up and down spins, used, for instance, to describe the Bethe eigenstates of a periodic XXZ spin chain. The number m_0 defines the initial phase of the first qubit, and the phases of the subsequent qubits increment by an amount η from site to site except at the points $n_1,\ldots,n_k$, where kinks occur. The states (10) are conveniently graphically represented in a form of trajectories, see Fig. 1. The nature of any state even in the presence of kinks is chiral. The full set of Bethe vectors (all eigenstates of the Hamiltonian) will be expressed by a chiral set (10) as explained below.

It was proved in Ref. [14] that the bra vectors (10) with

$$m_0+k+m_N=M,$$
$$m_0=0,1,\ldots,M,\qquad m_N=0,1, \tag{11}$$

are all independent and form a basis of the invariant subspace G_M^+ with the dimension $\dim G_M^+=d_+(M)=\sum_{n=0}^M\binom{N}{n}$. The Hamiltonian H has $d_+(M)$ left eigenvectors which are linear combinations of the G_M^+ basis states. The G_M^+ basis (11) consists of factorized states with 0 kink, 1 kink, etc. $\cdots$ up to M kinks, see Fig. 1, upper panel.

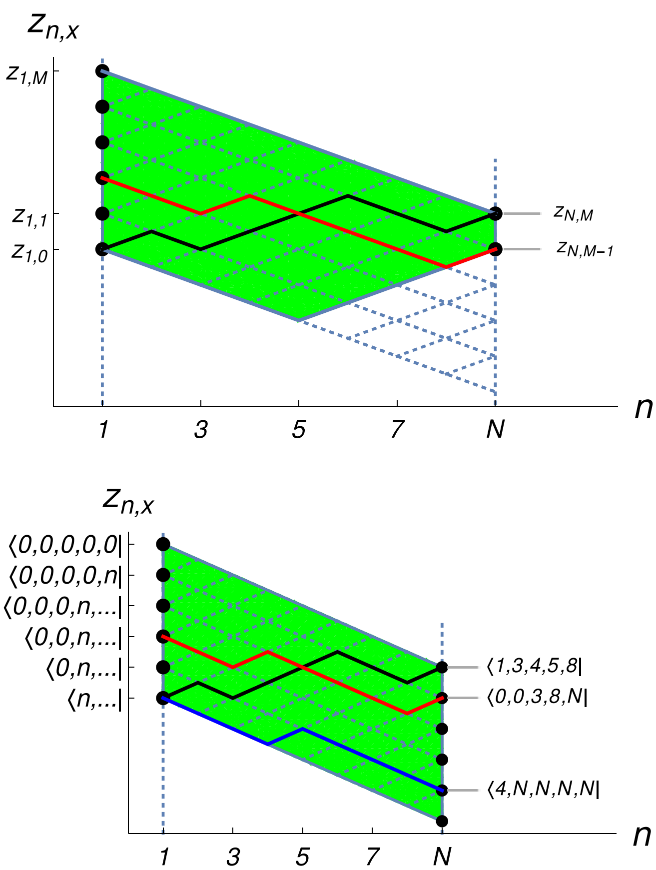

FIG. 1. Visualization of the invariant subspace G_M^+ (upper panel) and of the symmetrically enlarged G_M^+ with auxiliary states added (lower panel) for $N = 9$, $M = 5$ and showing the phase factor $z_{n,x}$ from (8) versus site number n. Any state (10) corresponds to some directed path (backward moves are forbidden). Upper panel: Illustration of the linearly independent states (11) that realize a basis of G_M^+. Directed paths start at one of $M + 1$ points (filled black circles) on site $n = 1$ and end at one of two points indicated by filled circles at $n = N$. The allowed paths representing the basis states (11) lie entirely inside the filled region, including the boundaries. The black and red trajectories are examples of two states from (11): $\langle 1, 3, 4, 5, 8|$ and $\langle 0, 0, 3, 8, N|$, respectively. Lower panel: Illustration of the full set of states entering the chiral coordinate Bethe ansatz (77). Directed paths start at one of $M + 1$ filled circles on site $n = 1$ and end at one of $M + 1$ filled circles at $n = N$. The blue line represents a state $\langle 4, N, N, N, N|$ which belongs to the extra set of auxiliary states (12), whereas the black and the red line "belong" to the original set of basis states, see the upper panel.

For our purpose it is convenient to enlarge the basis by adding to (11) extra chiral states of the form (10) with

$$m_0 + k + m_N = M,$$
$$m_0 = 0, 1, \dots, M, \qquad m_N = 2, \dots M, \quad (12)$$

rendering the enlarged set of states,

$$m_0, m_N = 0, 1, \dots, M, \qquad m_0 + k + m_N = M, \qquad (13)$$

completely symmetric, see Fig. 1, lower panel. For $M = 0$ and $M = 1$, the basis vector set (11) coincides with the enlarged set (13). For $M > 1$ the number of auxiliary vectors increases monotonically with M. For $M = 2, 3, 4$, the number of auxiliary vectors is $1, N + 1, \frac{N^2+N+4}{2}$, respectively. For arbitrary $M \geqslant 2$, the number of additional vectors can be calculated on combinatorial grounds and is equal to

$$d_+^{\text{add}}(M) = \sum_{j=0}^{M-2} \sum_{k=0}^{j} \binom{N-1}{k}. \qquad (14)$$

It can be proved (see Appendix B) that all auxiliary vectors are linear combinations of the $d_+(M)$ basis vectors. The full generating set (13) contains in total,

$$d_+^{\text{total}}(M) = \sum_{j=0}^{M} \sum_{k=0}^{j} \binom{N-1}{k}, \qquad (15)$$

vectors. Each vector from the set corresponds to a directed path in Fig. 1, lower panel.

Note that in the G_M^+ case, we deal with the bra vectors. In the following we show how to construct the auxiliary vectors for the ket G_M^- basis.

Adding auxiliary ket vectors to the basis of G_M^-

Analogously, introduce the local ket states,

$$\tilde{\phi}_n(x) = \begin{pmatrix} 1 \\ e^{-\theta_- - \alpha_- - \beta_- + (2x-n+1)\eta} \end{pmatrix}, \qquad (16)$$

and construct factorized states out of them,

$$|\underbrace{0, \dots, 0}_{m_0}, \underbrace{n_1, \dots, n_k}_{k}, \underbrace{N, \dots, N}_{m_N}\rangle\rangle,$$

obtainable from bra vectors (10) via the replacement $\phi \to \tilde{\phi}$. Analogousy to (11), the above ket states with

$$m_0 + k + m_N = \widetilde{M},$$
$$m_0 = 0, 1, \dots, \widetilde{M}, \qquad m_N = 0, 1, \qquad (17)$$

where $\widetilde{M} = N - 1 - M$, form a basis of the invariant subspace G_M^- [14]. Adding additional ket states in analogy to (12), we get another fully symmetric set of ket vectors with

$$m_0, m_N = 0, 1, \dots, \widetilde{M}, \qquad m_0 + k + m_N = \widetilde{M}, \qquad (18)$$

and their total number is

$$d_-^{\text{total}}(M) = \sum_{j=0}^{\widetilde{M}} \sum_{k=0}^{j} \binom{N-1}{k}. \qquad (19)$$

IV. PHANTOM BETHE EIGENSTATES IN G_M^+ FOR $M = 0$–2

A. $M = 0$ case

When $M = 0$, the invariant subspace G_0^+ consists of just one state, a spin-helix state (SHS) [19–21],

$$\langle \Psi_0| = \phi_1(0) \cdots \phi_N(0), \qquad (20)$$

with

$$\langle \Psi_0|H = \langle \Psi_0|E_0, \qquad (21)$$

$$E_0 = -\sinh(\eta)[\coth(\alpha_-) + \tanh(\beta_-) + \coth(\alpha_+) + \tanh(\beta_+)], \qquad (22)$$

see Refs. [14,15]. In the factorized state $\langle\Psi_0|$, the qubit phase grows linearly, implying underlying chiral properties of the state. Indeed, for a Hermitian Hamiltonian in the easy-plane regime, the SHS $\langle\Psi_0|$ for $\beta_\pm = 0$ carries the magnetic current,

$$j^z = \frac{\langle\Psi_0|\mathbf{j}_k^z|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} = 2\,\sin\gamma, \qquad (23)$$
$$\mathbf{j}_k^z = 2\big(\sigma_k^x\sigma_{k+1}^y - \sigma_k^y\sigma_{k+1}^x\big).$$

For a Hermitian system in the easy axis regime (7), the SHS $\langle\Psi_0|$ carries no magnetic current, i.e., $j^z = 0$. Remarkably, the SHS (20) has been produced experimentally in a system of cold atoms where the z-axis anisotropy of the Heisenberg interaction can be controlled by Feshbach resonance [22,23].

B. $M = 1$ case

Define the following factorized states:

$$\langle n| = e^{n\eta}\phi_1(0)\cdots\phi_n(0)\phi_{n+1}(1)\cdots\phi_N(1). \qquad (24)$$

The states $\langle 0|, \langle 1|, \dots, \langle N|$ span the subspace G_1^+ [14]. Consequently, there exist $N+1$ Bethe eigenstates which are linear combinations of the basis vectors,

$$\big\langle\Psi_1^{(\alpha)}\big| = \sum_{n=0}^{N}\langle n|f_n^{(\alpha)}, \qquad \alpha = 0, 1, \dots, N, \qquad (25)$$

where the greek upper index α enumerates the states of the G_1^+ multiplet.

Define the boundary parameters,

$$a_\pm = \frac{\sinh(\alpha_\pm + \eta)}{\sinh(\alpha_\pm)}, \qquad b_\pm = \frac{\cosh(\beta_\pm + \eta)}{\cosh(\beta_\pm)}. \qquad (26)$$

The coefficients $\{f_n^{(\alpha)}\}$ can be written in the following coordinate Bethe ansatz form [14]

$$f_n^{(\alpha)} = g_n\big(A_+^{(\alpha)}e^{inp(\alpha)} + A_-^{(\alpha)}e^{-inp(\alpha)}\big), \qquad 0 \leqslant n \leqslant N,$$
$$g_0 = \frac{1}{1 - a_-b_-}, \qquad g_N = \frac{1}{1 - a_+b_+}, \qquad (27)$$
$$g_1 = g_2 = \cdots = g_{N-1} = 1.$$

Note that writing $f_n^{(\alpha)}$ as a product of the listed g_n times a second factor allows this one to be a sum of plane waves for all sites n even at the ends with $n = 0$ and N. The quasimomentum $p(\alpha)$ is subject to Eq. (31) which is the consistency condition for the following relations for the amplitudes $A_\pm^{(\alpha)}$:

$$A_-^{(\alpha)} = S_L[p(\alpha)]A_+^{(\alpha)},$$
$$A_-^{(\alpha)} = e^{2iNp(\alpha)}S_R[p(\alpha)]A_+^{(\alpha)}, \qquad (28)$$

where $S_L(p)$ and $S_R(p)$ are the reflection matrices on the left and right boundaries [24], respectively, with

$$S_L(p) = -\frac{1 - a_-e^{ip}}{a_- - e^{ip}}\frac{1 - b_-e^{ip}}{b_- - e^{ip}}, \qquad (29)$$

$$S_R(p) = -\frac{a_+ - e^{ip}}{1 - a_+e^{ip}}\frac{b_+ - e^{ip}}{1 - b_+e^{ip}}. \qquad (30)$$

The compatibility condition of Eq. (28) is exactly the BAE for $M = 1$,

$$e^{2iNp}\prod_{\sigma=\pm}\frac{a_\sigma - e^{ip}}{1 - a_\sigma e^{ip}}\frac{b_\sigma - e^{ip}}{1 - b_\sigma e^{ip}} = 1. \qquad (31)$$

The solutions of BAE (31) are denoted by $p(\alpha)$ with $\alpha = 0, \dots, N$. The corresponding eigenvalue in terms of the Bethe root $p(\alpha)$ is given by

$$E(\alpha) = 4\,\cos[p(\alpha)] - 4\Delta + E_0. \qquad (32)$$

For a Hermitian system, the single quasimomentum $p(\alpha)$ can be real or purely imaginary. It has been proved in Ref. [14] that the invariant subspaces G_1^+ have additional internal structure when, at least, one of the additional constraints $a_\pm b_\pm = 1$ is satisfied.

Once the eigenstates are constructed, physical quantities can be calculated, e.g., the expectation value of the spin current. A qualitative analysis yields that the spin currents in the single-particle multiplet can differ from the SHS current $j_{\mathrm{SHS}}^z = 2\,\sin\gamma$ at most by $O(\frac{1}{N})$ corrections in the easy-plane regime. Consider a Hermitian Hamiltonian in the easy-plane regime with the boundary parameters,

$$\beta_+ = \beta_- = 0, \qquad \alpha_\pm = -i\gamma \pm i\frac{\pi}{2} \bmod 2\pi i,$$
$$\theta_- - \theta_+ = i(N-1)\gamma \quad \bmod\ 2\pi i. \qquad (33)$$

The explicit expressions of the current in the $N+1$ eigenstates are [14]

$$j^z(\alpha) = \frac{\big\langle\Psi_1^{(\alpha)}\big|\mathbf{j}_l^z\big|\Psi_1^{(\alpha)}\big\rangle}{\big\langle\Psi_1^{(\alpha)}\big|\Psi_1^{(\alpha)}\big\rangle}$$
$$= 2\,(\sin\gamma)\bigg(1 - \frac{4}{N}\frac{1 - \cos^2[p(\alpha)]}{1 + \Delta^2 - 2\Delta\,\cos[p(\alpha)]}\bigg), \qquad (34)$$

$$p(\alpha) = \frac{\pi\alpha}{N}, \qquad \alpha = 0, \dots, N.$$

It can be seen from the above that all phantom Bethe states are current carrying states: The upper and lower bounds for the current of the multiplet are of order of the SHS current j_{SHS},

$$j_{\mathrm{SHS}}\bigg(1 - \frac{4}{N}\bigg) \leqslant j^z(\alpha) \leqslant j_{\mathrm{SHS}} = 2\,\sin\gamma. \qquad (35)$$

The upper bound is saturated; indeed $j^z(0) = j^z(N) = j_{\mathrm{SHS}}$ since the respective Bethe states $\langle\Psi_1^{(\alpha)}|$ with $\alpha = 0, N$ are, in fact, spin-helix states, differing by an initial phase. The lower bound is approached most closely for $p(\alpha) \leqslant \gamma \leqslant p(\alpha+1)$, and it can be saturated if an α satisfies $p(\alpha) = \gamma$, i.e. for some root of unity anisotropies.

In the following we omit the upper index α enumerating the physical BAE solutions for brevity of notation.

C. $M = 2$ case

For $M = 2$, we follow the same procedure to construct the Bethe eigenstates, via a generating set (13), i.e., vectors $\langle 0, 0|, \langle 0, 1|, \dots, \langle 0, N|, \dots, \langle N, N|$.

Using convenient notations,

$$w_\pm = a_\pm + b_\pm, \tag{36}$$

the action of H on set $\langle n, m|$ is given by

$$\langle 0,0|H = (4\Delta\, a_- b_- - w_- - w_+)\langle 0,0| + 4\Delta\,(w_- - 2\Delta\; a_- b_-)\langle 0,1|, \tag{37}$$

$$\langle 0,1|H = (w_- - w_+ - 4\Delta\, a_- b_-)\langle 0,1| + 2\langle 0,2| + 2\, a_- b_- \langle 0,0|, \tag{38}$$

$$\langle 0,n|H = (w_- - w_+ - 4\Delta)\langle 0,n| + 2\langle 0,n-1| + 2\langle 0,n+1| + 2(1 - a_- b_-)\langle 1,n|, \quad 2 \leqslant n \leqslant N-1, \tag{39}$$

$$\langle 0,N|H = (w_- + w_+ - 4\Delta)\langle 0,N| + 2(1 - a_- b_-)\langle 1,N| + 2(1 - a_+ b_+)\langle 0,N-1|, \tag{40}$$

$$\begin{aligned}\langle n,m|H = &-(w_- + w_+ + 4\Delta)\langle n,m| + 2\langle n-1,m| + 2\langle n+1,m|\\ &+2\langle n,m+1| + 2\langle n,m-1|, \quad 1 \leqslant n < m \leqslant N-1, \quad m-n > 1,\end{aligned} \tag{41}$$

$$\langle n,n+1|H = -(w_- + w_+)\langle n,n+1| + 2\langle n-1,n+1| + 2\langle n,n+2|, \quad 1 \leqslant n \leqslant N-2, \tag{42}$$

$$\langle n,N|H = (w_+ - w_- - 4\Delta)\langle n,N| + 2\langle n-1,N| + 2\langle n+1,N| + 2(1 - a_+ b_+)\langle n,N-1|, \quad 1 \leqslant n \leqslant N-2, \tag{43}$$

$$\langle N-1,N|H = (w_+ - w_- - 4\Delta a_+ b_+)\langle N-1,N| + 2\langle N-2,N| + 2a_+ b_+ \langle N,N|, \tag{44}$$

$$\langle N,N|H = (4\Delta a_+ b_+ - w_+ - w_-)\langle N,N| + 4\Delta(w_+ - 2\Delta a_+ b_+)\langle N-1,N|. \tag{45}$$

Obviously, the factorized states $\langle n, m|$ span an invariant subspace G_2^+ of H. The respective phantom Bethe eigenstates belonging to G_2^+ can be written as a linear combination of $\langle n, m|$ as

$$\langle \Psi_2| = \sum_{0 \leqslant n_1 < n_2 \leqslant N} \langle n_1, n_2|\, f_{n_1,n_2} + \sum_{n=0,N} \langle n,n| f_{n,n}, \tag{46}$$

with yet unknown eigenvalue E. Later, for convenience, we extend the notation to a double sum over $0 \leqslant n_1 \leqslant n_2 \leqslant N$ with, however, $f_{n,n} \equiv 0$ for $n \neq 0, N$.

We write E as

$$E = 2\Lambda - 8\Delta + E_0, \tag{47}$$

where E_0 is defined in Eq. (22). The eigenvalue equation $\langle \Psi_2|H = \langle \Psi_2|E$ gives rise to the following recursive identities for the coefficients $f_{n,m}$,

$$(\Lambda - 2\Delta\delta_{n+1,m})f_{n,m} = f_{n+1,m} + f_{n-1,m} + f_{n,m+1} + f_{n,m-1}, \quad 2 \leqslant n < m \leqslant N-2, \tag{48}$$

$$(\Lambda - 2\Delta\delta_{n,N-2})f_{n,N-1} = f_{n+1,N-1} + f_{n-1,N-1} + f_{n,N-2} + (1 - a_+ b_+)f_{n,N}, \quad 2 \leqslant n \leqslant N-2, \tag{49}$$

$$(\Lambda - 2\Delta\delta_{2,m})f_{1,m} = f_{1,m+1} + f_{1,m-1} + f_{2,m} + (1 - a_- b_-)f_{0,m}, \quad 2 \leqslant m \leqslant N-2, \tag{50}$$

$$\Lambda\, f_{1,N-1} = f_{2,N-1} + f_{1,N-2} + (1 - a_+ b_+)f_{1,N} + (1 - a_- b_-)f_{0,N-1}, \tag{51}$$

$$(\Lambda - w_-)f_{0,m} = f_{0,m-1} + f_{0,m+1} + f_{1,m}, \qquad 2 \leqslant m \leqslant N-2, \tag{52}$$

$$(\Lambda - w_+)f_{n,N} = f_{n-1,N} + f_{n+1,N} + f_{n,N-1}, \quad 2 \leqslant n \leqslant N-2, \tag{53}$$

$$(\Lambda - w_-)f_{0,N-1} = (1 - a_+ b_+)f_{0,N} + f_{0,N-2} + f_{1,N-1}, \tag{54}$$

$$(\Lambda - w_+)f_{1,N} = (1 - a_- b_-)f_{0,N} + f_{2,N} + f_{1,N-1}, \tag{55}$$

$$(\Lambda - w_- - w_+)f_{0,N} = f_{0,N-1} + f_{1,N}, \tag{56}$$

$$(\Lambda + 2\Delta\, a_- b_- - w_- - 2\Delta)f_{0,1} = f_{0,2} + 2\Delta(w_- - 2\Delta\, a_- b_-)f_{0,0}, \tag{57}$$

$$(\Lambda + 2\Delta\, a_+ b_+ - w_+ - 2\Delta)f_{N-1,N} = f_{N-2,N} + 2\Delta(w_+ - 2\Delta\, a_+ b_+)f_{N,N}, \tag{58}$$

$$(\Lambda - 2\Delta\, a_- b_- - 2\Delta) f_{0,0} = a_- b_- f_{0,1}, \tag{59}$$

$$(\Lambda - 2\Delta\, a_+ b_+ - 2\Delta) f_{N,N} = a_+ b_+ f_{N-1,N}. \tag{60}$$

We propose the following ansatz:

$$f_{n,m} = g_{n,m} \sum_{\sigma_1,\sigma_2=\pm} \left(A^{1,2}_{\sigma_1,\sigma_2} e^{i\sigma_1 n p_1 + i\sigma_2 m p_2} + A^{2,1}_{\sigma_2,\sigma_1} e^{i\sigma_2 n p_2 + i\sigma_1 m p_1} \right), \tag{61}$$

where p_1, p_2 are quasimomenta and the coefficients $\{g_{n,m}\}$ are p independent. We impose $g_{n,m} \equiv 1$ for $n, m \neq 0, N$. Considering the bulk term Eq. (48) with $m \neq n+1$ and using the ansatz (61), we get the expression of Λ and energy,

$$\Lambda = 2\cos(p_1) + 2\cos(p_2), \tag{62}$$

$$E = 4\sum_{j=1}^{2} \cos(p_j) - 8\Delta + E_0. \tag{63}$$

To satisfy Eq. (48) with $m = n+1$, we get the two-body scattering matrix [24],

$$A^{2,1}_{\sigma_2,\sigma_1} = S_{1,2}(\sigma_1 p_1, \sigma_2 p_2) A^{1,2}_{\sigma_1,\sigma_2}, \tag{64}$$

where S has the following symmetry and explicit expression:

$$\begin{aligned} S_{1,2}(p,p') &= S_{2,1}(-p',-p) \\ &= -\frac{1 - 2\Delta e^{ip'} + e^{ip'+ip}}{1 - 2\Delta e^{ip} + e^{ip'+ip}}. \end{aligned} \tag{65}$$

The ansatz (61) allows us to get the following expressions from Eqs. (49) and (50):

$$g_{n,N} = \frac{1}{1 - a_+ b_+}, \qquad g_{0,n} = \frac{1}{1 - a_- b_-}, \qquad 2 \leqslant n \leqslant N-2. \tag{66}$$

The boundary dependent Eqs. (52) and (53) determine the following left and right reflection matrices, respectively:

$$A^{j,k}_{-,\sigma_k} = S_L(p_j) A^{j,k}_{+,\sigma_k}, \tag{67}$$

$$A^{j,k}_{\sigma_j,-} = e^{2iNp_k} S_R(p_k) A^{j,k}_{\sigma_j,+}, \tag{68}$$

where the reflection matrices $S_L(p)$ and $S_R(p)$ are given by Eqs. (29) and (30),

$$S_L(p) = -\frac{1 - a_- e^{ip}}{a_- - e^{ip}} \frac{1 - b_- e^{ip}}{b_- - e^{ip}}, \tag{69}$$

$$S_R(p) = -\frac{a_+ - e^{ip}}{1 - a_+ e^{ip}} \frac{b_+ - e^{ip}}{1 - b_+ e^{ip}}. \tag{70}$$

The scattering matrix in (65) and reflection matrices in (29) and (30) determine all amplitudes $A^{j,k}_{\sigma_j,\sigma_k}$. The consistency condition of our ansatz gives the BAE,

$$\begin{aligned} &e^{2iNp_j} S_{j,k}(p_j, p_k) S_R(p_j) S_{k,j}(p_k, -p_j) \\ &\times S_L(-p_j) = 1, \quad j,k = 1,2, \quad j \neq k. \end{aligned} \tag{71}$$

One can verify that our BAE in (71) is consistent with the one given by MABA [5] and the functional T-Q relation [6,9], see Appendix A. Letting m in (52) and n in (53) take values 2 and $N-2$, respectively, and using the reflection matrices (29) and (30), we have

$$g_{1,N} = g_{N-1,N} = \frac{1}{1 - a_+ b_+}, \qquad g_{0,1} = g_{0,N-1} = \frac{1}{1 - a_- b_-}, \tag{72}$$

extending the result (66) to $1 \leqslant n \leqslant N-1$. Substituting the result in (72) into Eq. (54), we get the expression of $g_{0,N}$,

$$g_{0,N} = \frac{1}{(1 - a_- b_-)(1 - a_+ b_+)}. \tag{73}$$

The remaining coefficients $f_{0,0}$ and $f_{N,N}$ are derived from Eqs. (57) and (58),

$$g_{0,0} = \frac{a_- b_-}{2\Delta(1 - a_- b_-)(w_- - 2\Delta a_- b_-)}, \qquad g_{N,N} = \frac{a_+ b_+}{2\Delta(1 - a_+ b_+)(w_+ - 2\Delta a_+ b_+)}. \tag{74}$$

Using Eqs. (C12)–(C14), we reparametrize the functions $\{g_{n,m}\}$ in terms of $\alpha_\pm$ and $\beta_\pm$ as

$$g_{n,m} = \begin{cases} 1, & n, m \neq 0, N, \\ F_-(1), & n = 0, \quad m \neq 0, N, \\ F_+(1), & n \neq 0, N, \quad m = N, \\ F_-(1)F_+(1), & n = 0, \quad m = N, \\ F_-(1)F_-(2), & n = m = 0, \\ F_+(1)F_+(2), & n = m = N, \end{cases} \tag{75}$$

where

$$F_\sigma(k) = \delta_{k,0} - (1 - \delta_{k,0}) \frac{\sinh[\alpha_\sigma + (k-1)\eta]}{\sinh(k\eta)} \times \frac{\cosh[\beta_\sigma + (k-1)\eta]}{\cosh(\alpha_\sigma + \beta_\sigma + k\eta)}, \qquad \sigma = \pm. \tag{76}$$

Note that for our further generalization (79) it is convenient to define $F_\sigma(0) = 1$ via (76), even though $F_\sigma(0)$ does not appear in (75). One can prove that our ansätze (61), (75) satisfy all the relations (48)–(60), see Appendix D.

Remark. In the generic case, the invariant subspace G_2^+ is irreducible. However, on special manifolds, further internal structures appear, leading to the existence of one or more sub-subspaces, which are invariant with respect to the action of the Hamiltonian. As an example, for $a_\pm b_\pm = 1$, three invariant subspaces of G_M^+ appear. The details of this further structuring and the consequences for the BAE sets are discussed in Appendix E.

V. GENERALIZATION FOR ARBITRARY M

On the basis of our findings we formulate the following hypothesis: phantom Bethe vectors, i.e., Bethe states with infinite rapidities, respectively, momenta $k_j = \pm\gamma$ are for general M given by a superposition of the states (10). We denote the vector $\langle 0,\dots,0,\tilde{n}_1,\dots,\tilde{n}_k,N,\dots,N|$ from (10) simply as $\langle n_1,\dots,n_M|$ where some of the first site labels n_j may be identical to 0 and some of the last ones identical to N.

We have seen in the $M=1,2$ cases, that writing f_n or $f_{n,m}$ as a product of certain prefactors g_n or $g_{n,m}$ times a second factor allows this one to be a sum of plane waves for all sites even at the ends with n or m equal to 0 or N. Analyzing the $M=1,2$ cases, we see that the prefactors g only depend on the number of site labels 0, respectively, N. This inspired us to formulate a general rule for the arbitrary M case with a certain prefactor $g_{n_1,\dots,n_M} \equiv C_{m_0,m_N}$ where m_0 and m_N denote the number of site labels equal to 0, respectively, N in the sequence $n_1,\dots,n_M$. Using this rule we find

$$\langle\Psi_M| = \sum_{n_1,\dots,n_M} \langle n_1,\dots,n_M| f_{n_1,\dots,n_M}, \tag{77}$$

$$f_{n_1,\dots,n_M} = C_{m_0,m_N} \sum_{r_1,\dots,r_M} \sum_{\sigma_1,\dots,\sigma_M=\pm} A^{r_1,\dots,r_M}_{\sigma_{r_1},\dots,\sigma_{r_M}} \times \exp\left(i\sum_{k=1}^{M} \sigma_{r_k} n_k p_{r_k}\right), \tag{78}$$

where in (77) we sum over all configurations $n_1,\dots,n_M$ allowed by (13). The first sum in (78) is over all permutations $r_1,\dots,r_M$ of $1,\dots,M$, whereas the coefficients C_{m_0,m_N} depend only on m_0, m_N and are given by remarkably simple expressions,

$$C_{m_0,m_N} = \prod_{k=0}^{m_0} F_-(k) \prod_{l=0}^{m_N} F_+(l), \tag{79}$$

where $F_\sigma(m)$'s are defined by Eq. (76). The amplitudes $A^{r_1,\dots,r_M}_{\sigma_{r_1},\dots,\sigma_{r_M}}$ are determined by the two-body scattering matrix S in (65) and the reflection matrices S_L, S_R in (29) and (30),

$$A^{\dots,r_{n+1},r_n,\dots}_{\dots,\sigma_{r_{n+1}},\sigma_{r_n},\dots} = S_{r_n,r_{n+1}}(\sigma_{r_n} p_{r_n}, \sigma_{r_{n+1}} p_{r_{n+1}}) \times A^{\dots,r_n,r_{n+1},\dots}_{\dots,\sigma_{r_n},\sigma_{r_{n+1}},\dots}, \tag{80}$$

$$A^{r_1,\dots}_{-,\dots} = S_L(p_{r_1}) A^{r_1,\dots}_{+,\dots}, \tag{81}$$

$$A^{\dots,r_M}_{\dots,-} = e^{2Nip_{r_M}} S_R(p_{r_M}) A^{\dots,r_M}_{\dots,+}. \tag{82}$$

The compatibility of the whole scheme is guaranteed by a set of transcendental equations for the quasimomenta, the BAE,

$$e^{2iNp_{r_1}} S_{r_1,r_2}(p_{r_1},p_{r_2}) \cdots S_{r_1,r_M}(p_{r_1},p_{r_M}) S_R(p_{r_1}) \times S_{r_M,r_1}(p_{r_M},-p_{r_1}) \cdots S_{r_2,r_1}(p_{r_2},-p_{r_1}) S_L(-p_{r_1}) = 1, \quad r_1 = 1,\dots,M. \tag{83}$$

The BAE (83) coincide with those obtained by other approaches [5,6]. The corresponding eigenvalue in terms of quasimomenta $\{p_1,\dots,p_M\}$ is

$$E = 4\sum_{j=1}^{M}[\cos(p_j) - \Delta] + E_0. \tag{84}$$

Analogously we construct the other set of eigenstates $|\Psi_M\rangle\rangle$ belonging to G_M^-. The substitutions,

$$\alpha_\pm \to -\alpha_\pm, \quad \beta_\pm \to -\beta_\pm, \quad \theta_\pm \to i\pi + \theta_\pm, \tag{85}$$

leave the Hamiltonian invariant and give the following replacements:

$$M \to \widetilde{M}, \quad a_\pm \to \tilde{a}_\pm, \quad b_\pm \to \tilde{b}_\pm, \tag{86}$$

where

$$\tilde{a}_\pm = \frac{\sinh(\alpha_\pm - \eta)}{\sinh(\alpha_\pm)}, \quad \tilde{b}_\pm = \frac{\cosh(\beta_\pm - \eta)}{\cosh(\beta_\pm)}. \tag{87}$$

The vectors in (13) and (18) and the fundamental relations (C1)–(C10) all show the symmetry (85) and (86). This is sufficient to prove that the eigenstates $|\Psi_M\rangle\rangle$ can be constructed in analogy to (77). Following (77), we make the ansatz,

$$|\Psi_M\rangle\rangle = \sum_{n_1,\dots,n_{\widetilde{M}}} \tilde{f}_{n_1,\dots,n_{\widetilde{M}}} |n_1,\dots,n_{\widetilde{M}}\rangle\rangle, \tag{88}$$

with

$$\tilde{f}_{n_1,\dots,n_{\widetilde{M}}} = \widetilde{C}_{m_0,m_N} \sum_{r_1,\dots,r_{\widetilde{M}}} \sum_{\sigma_1,\dots,\sigma_{\widetilde{M}}=\pm} \widetilde{A}^{r_1,\dots,r_{\widetilde{M}}}_{\sigma_{r_1},\dots,\sigma_{r_{\widetilde{M}}}} \times \exp\left(i\sum_{k=1}^{\widetilde{M}} \sigma_{r_k} n_k \tilde{p}_{r_k}\right). \tag{89}$$

Substituting $A^{\dots}_{\dots}$, C_{m_0,m_N} and $\{p_1,\dots,p_M\}$ in Eqs. (79)–(84) with $\widetilde{A}^{\dots}_{\dots}$, $\widetilde{C}_{m_0,m_N}$ and $\{\tilde{p}_1,\dots,\tilde{p}_{\widetilde{M}}\}$, respectively, and then using the substitutions (85) and (86), we get another chiral coordinate Bethe ansatz, now for the G_M^- Bethe eigenvectors.

The chiral coordinate Bethe ansatz in Eqs. (77)–(83) and (88) and (89) are the main result of this paper. Equations (77)–(83) give the full set of Bethe vectors for the G_M^+ invariant subspace and the dual Eqs. (88) and (89) give the full set of Bethe vectors for the G_M^- invariant subspace, in total, all 2^N phantom Bethe vectors.

At present, it is difficult to prove our hypotheses in (78) and (89) completely. However, there are many arguments that corroborate our hypotheses. On one hand, we retrieve the same BAE which have been obtained by other approaches. On the other hand, the correctness of our conjecture for, at least, a part of the coefficients $f_{n_1,\dots,n_M}$ in (78) can be proved for arbitrary M.

VI. SPIN-HELIX EIGENSTATES

Among the vectors constituting the G_M^+ basis plus the auxiliary vectors, there are $M+1$ linearly independent SHS of the form

$$\langle \mathrm{SHS}; m| = \bigotimes_{n=1}^{N} \phi_n(m) \propto \langle\underbrace{0,\dots,0}_{m},\underbrace{N,\dots,N}_{M-m}|, \quad m = 0,\dots,M, \tag{90}$$

which have the same chirality but a different initial qubit phase.

Below we look for conditions under which these SHSs become eigenstates of the Hamiltonian. Acting by the Hamiltonian H on these SHSs and using Eqs. (C1)–(C4), we find

$$\langle \text{SHS}; m|H = -\left(\frac{\sinh\eta\cosh(\alpha_- + \beta_- + 2m\eta)}{\sinh(\alpha_-)\cosh(\beta_-)} + \frac{\sinh\eta\cosh[\alpha_+ + \beta_+ + 2(M-m)\eta]}{\sinh(\alpha_+)\cosh(\beta_+)}\right)\langle \text{SHS}; m| + \frac{2\sinh\eta\sinh[(M-m)\eta]\cosh[\alpha_+ + \beta_+ + (M-m)\eta]}{\sinh(\alpha_+)\cosh(\beta_+)}\langle \text{SHS}; m|\sigma_N^z - \frac{2\sinh\eta\sinh(m\eta)\cosh(\alpha_- + \beta_- + m\eta)}{\sinh(\alpha_-)\cosh(\beta_-)}\langle \text{SHS}; m|\sigma_1^z. \tag{91}$$

It is clear from the above that the SHS $\langle \text{SHS}; m|$ becomes an eigenstate of H if one or two additional conditions are satisfied, namely:

(i) when $\cosh(\alpha_- + \beta_- + M\eta) = 0$, $\langle \text{SHS}; M|$ is an eigenstate of H,

(ii) when $\cosh(\alpha_+ + \beta_+ + M\eta) = 0$, $\langle \text{SHS}; 0|$ is an eigenstate of H,

(iii) when $\cosh[\alpha_+ + \beta_+ + (M-m)\eta] = 0$, $\cosh(\alpha_- + \beta_- + m\eta) = 0$, $m \neq 0, M$, $\langle \text{SHS}; m|$ is an eigenstate of H,

and the corresponding eigenvalues are given by Eq. (91).

VII. DISCUSSION

We have analyzed the integrable open XXZ spin-$\frac{1}{2}$ chain satisfying the PRC,

$$\eta = \frac{\alpha_- + \beta_- + \alpha_+ + \beta_+ + \theta_- - \theta_+ + 2im\pi}{N - 2M - 1}, \tag{92}$$

where m is an arbitrary integer and the integer M has the range $0 \leqslant M \leqslant N-1$. For a Hamiltonian under the PRC (5), when $N - 2M - 1 \neq 0$, the crossing parameter η can only take $N - 2M - 1$ discrete values with relative positions equidistant on the complex plane [9]. When $N - 2M - 1 = 0$, the crossing parameter η can take arbitrary value and the two boundaries satisfy a certain constraint. Under this condition, the Hilbert space splits into two invariant subspaces [14], and remarkable singular peaks in the magnetization current of the associated dissipative quantum system occur [25], which can now be related to the existence of spin-helix eigenstates and their generalizations in the spectrum of the effective Hamiltonian.

Under the PRC, two conventional BAE with M and $\widetilde{M} = N - M - 1$ regular Bethe roots appear, which correspond to two invariant subspaces G_M^+ and G_M^- with the dimensions $\dim G_M^+ = \sum_{k=0}^{M}\binom{N}{k}$ and $\dim G_M^- = \sum_{k=M+1}^{N}\binom{N}{k} = 2^N - \dim G_M^+$. We conjecture that the number of independent Bethe states corresponding to the full set of solutions to the Bethe ansatz equations is identical to the dimensions of the respective invariant subspaces rendering the set of Bethe states complete. The existence of specific invariant subspaces and the homogeneity of Bethe equations imply that the system may have a certain discrete symmetry, which would be interesting to formulate explicitly.

Our proposed chiral coordinate Bethe ansatz allows to construct the full set of Bethe eigenstates, separately for G_M^+ and G_M^- as a linear combination over a symmetric set of vectors, spanning the respective chiral invariant subspace. The set of vectors contains spin-helix states with "kinks". Unlike in the periodic case, we have to treat the nondiagonal boundary fields which break the magnetization conservation, i.e., the $U(1)$ symmetry. The integer M determines the maximum number of kinks. An exciting result is that the expansion coefficients for the open spin chain in the chiral basis of SHS with kinks have a very simple analytic form. The Bethe equations are consistent with the ones resulting from MABA (see Appendices A and F), whose completeness has been discussed in Ref. [7].

We demonstrated that for small M, the Bethe eigenstates have some unusual chiral properties such as high magnetization currents.

It should be noted that in the isotropic case $\Delta = 1$, the chiral feature of our basis vectors disappears. In this case, the system can be solved by the conventional algebraic Bethe ansatz (see Appendix G).

Our method can be generalized to other integrable open systems, not necessarily of quantum origin, such as the asymmetric simple exclusion process (ASEP) with open boundaries [26,27], the spin-1 Fateev-Zamolodchikov model [28], and spin-s integrable systems [29]. Potentially, a generalization of our results to the XYZ spin-$\frac{1}{2}$ chain [30] might exist, which is a challenging open problem.

The formulation of the chiral coordinate Bethe ansatz has become possible due to the existence of phantom Bethe roots, which appear both in open and in periodically closed systems [15].

Another interesting question is how to obtain the eigenstates of non-Hermitian systems under PRC. Using our bases and the chiral coordinate Bethe ansatz method, we can always construct the left or right eigenstates which correspond to one subspace, whether the system is Hermitian or not. For a Hermitian system the dual states can be directly obtained. If the system is not Hermitian, the construction of the dual states is still challenging. A very intuitive example is the one-species ASEP with open boundary conditions, which belongs to the $M = 0$ case. The left steady state of the Markov matrix is a simple factorized state, whereas the right steady state has a very complicated structure, which, however, can be calculated exactly by other approaches, the matrix product approach [31], or the recursive approach [32].

Our results may lay the basis for further analytic studies and may possibly serve for a new understanding relevant for experimental applications, e.g., the experimental realization of the model and eigenstates by techniques presented in Refs. [22,23].

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APPENDIX A: BAE RESULTING FROM MABA

It has been proved under condition (5) there exists a conventional BAE [5,6,9],

$$\left[\frac{\sinh\left(x_j+\frac{\eta}{2}\right)}{\sinh\left(x_j-\frac{\eta}{2}\right)}\right]^{2N}\prod_{\sigma=\pm}\frac{\sinh\left(x_j-\alpha_\sigma-\frac{\eta}{2}\right)}{\sinh\left(x_j+\alpha_\sigma+\frac{\eta}{2}\right)}\frac{\cosh\left(x_j-\beta_\sigma-\frac{\eta}{2}\right)}{\cosh\left(x_j+\beta_\sigma+\frac{\eta}{2}\right)}$$
$$=\prod_{k\neq j}^{M}\frac{\sinh(x_j-x_k+\eta)}{\sinh(x_j-x_k-\eta)}\frac{\sinh(x_j+x_k+\eta)}{\sinh(x_j+x_k-\eta)},\quad j=1,\ldots,M. \tag{A1}$$

The above BAE, in terms of the single-particle quasimomentum p_j,

$$e^{ip_j}=\frac{\sinh\left(x_j+\frac{\eta}{2}\right)}{\sinh\left(x_j-\frac{\eta}{2}\right)}, \tag{A2}$$

take the form [14]

$$e^{2iNp_j}\prod_{\sigma=\pm}\frac{a_\sigma-e^{ip_j}}{1-a_\sigma e^{ip_j}}\frac{b_\sigma-e^{ip_j}}{1-b_\sigma e^{ip_j}}=\prod_{\sigma=\pm}\prod_{k\neq j}^{M}\frac{1-2\Delta e^{ip_j}+e^{ip_j+i\sigma p_k}}{1-2\Delta e^{i\sigma p_k}+e^{ip_j+i\sigma p_k}},\quad j=1,\ldots,M, \tag{A3}$$

where $a_\pm, b_\pm$ are defined in (26). Valid physical Bethe roots $\{p_1,\ldots,p_M\}$ satisfy the selection rules $e^{ip_j}\neq e^{\pm ip_k}$, $e^{ip_j}\neq\pm1$. We see that Eq. (A3) is identical to our BAE (83) in the main text. The invariance of the Hamiltonian H with respect to the substitution (85) under condition (5) allows to construct another set of homogeneous BAE by replacing $\alpha_\pm$, $\beta_\pm$, and M in (A3) with $-\alpha_\pm$, $-\beta_\pm$, and $\widetilde{M}=N-1-M$, respectively, see Ref. [14]. The second set of BAE, thus, reads

$$e^{2iN\tilde{p}_j}\prod_{\sigma=\pm}\frac{\tilde{a}_\sigma-e^{i\tilde{p}_j}}{1-\tilde{a}_\sigma e^{i\tilde{p}_j}}\frac{\tilde{b}_\sigma-e^{i\tilde{p}_j}}{1-\tilde{b}_\sigma e^{i\tilde{p}_j}}=\prod_{\sigma=\pm}\prod_{k\neq j}^{\widetilde{M}}\frac{1-2\Delta e^{i\tilde{p}_j}+e^{i\tilde{p}_j+i\sigma\tilde{p}_k}}{1-2\Delta e^{i\sigma\tilde{p}_k}+e^{i\tilde{p}_j+i\sigma\tilde{p}_k}},\quad j=1,\ldots,\widetilde{M}, \tag{A4}$$

where $\tilde{a}_\pm, \tilde{b}_\pm$ are defined in Eq. (87).

APPENDIX B: LINEAR DEPENDENCE OF THE AUXILIARY VECTORS

Here we show that all extra-auxiliary bra vectors participating in the CCBA are linear combinations of the basis vectors of G_M^+, and similarly, all extra-auxiliary ket vectors are linear combinations of the G_M^- basis vectors. For the proof, it is enough to demonstrate that any bra vector from the extended (symmetrized) bra set is orthogonal to any ket vector from the extended (symmetrized) ket set, i.e., (B5).

To this end, define the function $y(n, v_n, \tilde{v}_n)$ as

$$\phi_n(v_n)\tilde{\phi}_n(\tilde{v}_n)=1-e^{2y(n,v_n,\tilde{v}_n)\eta},$$
$$y(n,v_n,\tilde{v}_n)=v_n+\tilde{v}_n-n+1. \tag{B1}$$

When $y(n, v_n, \tilde{v}_n)=0$, the local vectors $\phi_n(v_n)$ and $\tilde{\phi}_n(\tilde{v}_n)$ are orthogonal. Introduce the inner products,

$$\langle n_1,\ldots,n_M|m_1,\ldots,m_{\widetilde{M}}\rangle\rangle=\exp\left(\eta\sum_{j=1}^{M}n_j+\eta\sum_{k=1}^{\widetilde{M}}m_k\right)\prod_{n=1}^{N}(1-e^{2y(n,v_n,\tilde{v}_n)\eta}), \tag{B2}$$

where $\langle n_1,\ldots,n_M|$ belongs to the extended G_M^+ set of vectors and $|m_1,\ldots,m_{\widetilde{M}}\rangle\rangle$ belongs to the extended G_M^+ set of vectors. Obviously,

$$0\leqslant v_1\leqslant v_2\leqslant\cdots\leqslant v_N\leqslant M,$$
$$0\leqslant\tilde{v}_1\leqslant\tilde{v}_2\leqslant\cdots\leqslant\tilde{v}_N\leqslant\widetilde{M},$$
$$v_{n+1}-v_n=0,1,\quad \tilde{v}_{n+1}-\tilde{v}_n=0,1, \tag{B3}$$

and

$$y(n+1,v_{n+1},\tilde{v}_{n+1})-y(n,v_n,\tilde{v}_n)=0,\pm1,\quad y(1,v_1,\tilde{v}_1)\geqslant0,\quad y(N,v_N,\tilde{v}_N)\leqslant0. \tag{B4}$$

So $y(n, v_n, \tilde{v}_n) = 0$ holds, at least, for one point $n\,(1 \leqslant n \leqslant N)$ which implies that any pair of vectors $\langle n_1, \ldots, n_M| \in G_M^+$ and $|m_1, \ldots, m_{\widetilde{M}}\rangle\rangle \in G_M^-$ are orthogonal,

$$\langle n_1, \ldots, n_M|m_1, \ldots, m_{\widetilde{M}}\rangle\rangle = 0. \tag{B5}$$

APPENDIX C: THE PROOF OF EQS. (37)–(45)

It is easy to prove the following identities:

$$\phi_n(x)\phi_{n+1}(x)h_{n,n+1} = \sinh\eta\phi_n(x)\phi_{n+1}(x)\sigma_n^z - \sinh\eta\,\phi_n(x)\,\phi_{n+1}(x)\,\sigma_{n+1}^z, \tag{C1}$$

$$\phi_n(x-1)\phi_{n+1}(x)h_{n,n+1} = \sinh\eta\phi_n(x-1)\,\phi_{n+1}(x)\sigma_{n+1}^z - \sinh\eta\phi_n(x-1)\phi_{n+1}(x)\sigma_n^z, \tag{C2}$$

$$\phi_1(x)h_1 = \frac{\sinh\eta}{\sinh(\alpha_-)\cosh(\beta_-)}[\cosh(\alpha_-)\sinh(\beta_-) - \sinh(\alpha_- + \beta_- + 2x\eta)]\phi_1(x)\sigma_1^z - \frac{\sinh\eta\cosh(\alpha_- + \beta_- + 2x\eta)}{\sinh(\alpha_-)\cosh(\beta_-)}\phi_1(x), \tag{C3}$$

$$\phi_N(x)h_N = \frac{\sinh\eta}{\sinh(\alpha_+)\cosh(\beta_+)}\{\sinh[\alpha_+ + \beta_+ + 2(M-x)\eta] - \cosh(\alpha_+)\sinh(\beta_+)\}\phi_N(x)\sigma_N^z - \frac{\sinh\eta\cosh[\alpha_+ + \beta_+ + 2(M-x)\eta]}{\sinh(\alpha_+)\cosh(\beta_+)}\phi_N(x), \tag{C4}$$

$$h_{n,n+1}\tilde{\phi}_n(x)\tilde{\phi}_{n+1}(x) = \sinh\eta\sigma_n^z\tilde{\phi}_n(x)\tilde{\phi}_{n+1}(x) - \sinh\eta\sigma_{n+1}^z\tilde{\phi}_n(x)\tilde{\phi}_{n+1}(x), \tag{C5}$$

$$h_{n,n+1}\tilde{\phi}_n(x-1)\tilde{\phi}_{n+1}(x) = \sinh\eta\sigma_{n+1}^z\tilde{\phi}_n(x-1)\tilde{\phi}_{n+1}(x) - \sinh\eta\sigma_n^z\tilde{\phi}_n(x-1)\,\tilde{\phi}_{n+1}(x), \tag{C6}$$

$$h_1\tilde{\phi}_1(x) = \frac{\sinh\eta}{\sinh(\alpha_-)\cosh(\beta_-)}[\cosh(\alpha_-)\sinh(\beta_-) - \sinh(\alpha_- + \beta_- - 2x\eta)]\sigma_1^z\tilde{\phi}_1(x) + \frac{\sinh\eta\cosh(\alpha_- + \beta_- - 2x\eta)}{\sinh(\alpha_-)\cosh(\beta_-)}\tilde{\phi}_1(x), \tag{C7}$$

$$h_N\tilde{\phi}_N(x) = \frac{\sinh\eta}{\sinh(\alpha_+)\cosh(\beta_+)}\{\sinh[\alpha_+ + \beta_+ - 2(\widetilde{M}-x)\eta] - \cosh(\alpha_+)\sinh(\beta_+)\}\sigma_N^z\tilde{\phi}_N(x) + \frac{\sinh\eta\,\cosh[\alpha_+ + \beta_+ - 2(\widetilde{M}-x)\eta]}{\sinh(\alpha_+)\cosh(\beta_+)}\tilde{\phi}_N(x). \tag{C8}$$

We note the useful identities,

$$\phi_n(x)\sigma_n^z = \pm\frac{\cosh\eta}{\sinh\eta}\phi_n(x) \mp \frac{e^{\mp\eta}}{\sinh\eta}\phi_n(x \pm 1), \tag{C9}$$

$$\sigma_n^z\tilde{\phi}_n(x) = \pm\frac{\cosh\eta}{\sinh\eta}\tilde{\phi}_n(x) \mp \frac{e^{\mp\eta}}{\sinh\eta}\tilde{\phi}_n(x \pm 1). \tag{C10}$$

Using Eqs. (C1)–(C4) and (C9) repeatedly, we get Eqs. (37)–(45). Some identities, used in our calculations, are as follows:

$$E_0 = -w_- - w_+ + 4\Delta, \tag{C11}$$

$$\frac{\sinh\eta\cosh(\alpha_\pm + \beta_\pm)}{\sinh(\alpha_\pm)\cosh(\beta_\pm)} = w_\pm - 2\Delta, \tag{C12}$$

$$\frac{\sinh\eta\cosh(\alpha_\pm + \beta_\pm + \eta)}{\sinh(\alpha_\pm)\cosh(\beta_\pm)} = a_\pm b_\pm - 1, \tag{C13}$$

$$\frac{\sinh\eta\cosh(\alpha_\pm + \beta_\pm + 2\eta)}{\sinh(\alpha_\pm)\cosh(\beta_\pm)} = 2a_\pm b_\pm\Delta - w_\pm. \tag{C14}$$

APPENDIX D: THE PROOF OF EQS. (48)–(60)

Define the auxiliary function,

$$W_{n,m} = \sum_{\sigma_1,\sigma_2=\pm}\left(A^{1,2}_{\sigma_1,\sigma_2}e^{i\sigma_1 np_1 + i\sigma_2 mp_2} + A^{2,1}_{\sigma_2,\sigma_1}e^{i\sigma_2 np_2 + i\sigma_1 mp_1}\right), \tag{D1}$$

where n, m are arbitrary integers. Using BAE (71), the scattering matrix in (65) and reflection matrices in (29) and (30), one can get the following properties of $W_{n,m}$:

$$\Lambda W_{n,m} = \sum_{\sigma=\pm1}(W_{n+\sigma,m} + W_{n,m+\sigma}), \tag{D2}$$

$$2\Delta W_{n,n+1} = W_{n+1,n+1} + W_{n,n}, \tag{D3}$$

$$w_- W_{0,n} = a_- b_- W_{1,n} + W_{-1,n}, \tag{D4}$$

$$w_+ W_{n,N} = a_+ b_+ W_{n,N-1} + W_{n,N+1}, \tag{D5}$$

$$(\Lambda - 2\Delta a_- b_- - 2\Delta)W_{0,0} = 2\Delta(w_- - 2\Delta a_- b_-)W_{0,1}, \tag{D6}$$

$$(\Lambda - 2\Delta a_+ b_+ - 2\Delta)W_{N,N} = 2\Delta(w_+ - 2\Delta a_+ b_+)W_{N-1,N}. \tag{D7}$$

With the help of Eqs. (D2)–(D7), we can prove that our ansatz satisfies all the relations (48)–(60). For instance, Eq. (55) can be proved as follows:

$$\begin{aligned}(\Lambda - w_- - w_+)f_{0,N} &= g_{0,N}(\Lambda - w_- - w_+)W_{0,N}\\ &= g_{0,N}[(1 - a_- b_-)W_{1,N} + (1 - a_+ b_+)W_{0,N-1}]\\ &= f_{1,N} + f_{0,N-1}.\end{aligned} \tag{D8}$$

APPENDIX E: POSSIBILITY OF A FURTHER PARTIONING OF THE INVARIANT SUBSPACES ON SPECIAL MANIFOLDS

Let us consider the special case: $a_\pm b_\pm = 1$. Under this specific condition, from Eq. (40) the SHS $\langle 0, N|$ is an eigenstate of H,

$$\langle 0, N|H = (w_- + w_+ - 4\Delta)\langle 0, N|. \tag{E1}$$

This SHS $\langle 0, N|$ corresponds to a special limiting case solution of BAE (71) with $p_1 = -i\ln(a_-)$, $p_2 = -i\ln(a_+)$. In fact, both numerator and denominator on the left-hand side of (71) become zero, but the ratio stays finite.

The bra vectors $\langle 0, n|$, $n = 0, \dots, N$ form another subsubspace as follows:

$$\begin{aligned}\langle 0, 0|H &= (4\Delta - w_- - w_+)\langle 0, 0| + 4\Delta(w_- - 2\Delta)\langle 0, 1|,\\ \langle 0, n|H &= (w_- - w_+ - 4\Delta)\langle 0, n| + 2\langle 0, n-1|\\ &\quad +2\langle 0, n+1|, \quad 1 \leqslant n \leqslant N-1,\\ \langle 0, N|H &= (w_- + w_+ - 4\Delta)\langle 0, N|.\end{aligned} \tag{E2}$$

The phantom Bethe states belonging to the above invariant subsubspace have the form $\langle\Psi_2| = \sum_{n=0}^{N}\langle 0, n|f_{0,n}$. Note that the coefficients $f_{0,n}$ are different from those appearing in Eq. (46). Guided by Eq. (E2) we propose $f_{0,n}$ to be a sum of plain waves,

$$f_{0,n} = A_+ e^{inp} + A_- e^{-inp}, \quad n = 1, \dots, N-1, \tag{E3}$$

whereas $f_{0,0}$, $f_{0,N}$ will be derived from the consistency conditions of (E2). Following Eqs. (E2) and (E3) we obtain

$$f_{0,0} = \frac{A_+ + A_-}{2\Delta\,(w_- - 2\Delta)}, \quad f_{0,N} = \frac{f_{0,N-1}}{2\cos(p) - w_+}, \tag{E4}$$

and

$$\frac{A_-}{A_+} = -\prod_{u=a_-,b_-}\frac{1 - 2\Delta e^{ip} + ue^{ip}}{1 - 2\Delta u + ue^{ip}} = -e^{2iNp}. \tag{E5}$$

The corresponding energy reads $E = 4\cos(p) + w_- - w_+ - 4\Delta$ where p satisfies the reduced BAE,

$$e^{2iNp} = \prod_{u=a_-,b_-}\frac{1 - 2\Delta e^{ip} + ue^{ip}}{1 - 2\Delta u + ue^{ip}}. \tag{E6}$$

We can also get the same BAE (E6) by letting p_1, p_2 in BAE (71) be $-i\ln(a_-)$ and p, respectively (note that for the Hermitian case the constants $a_\pm$, $b_\pm$ are real). Noting that $\pm p$ are equivalent solutions and excluding two trivial solutions $p = 0, \pi$, BAE (E6) has N-independent nontrivial solutions.

Analogously, the bra vectors $\langle n, N|$, $n = 0, \dots, N$ form another subsubspace. Suppose that $\langle\Psi_2| = \sum_{n=0}^{N}\langle n, N|f_{n,N}$. The coefficients $\{f_{n,N}\}$ can be obtained via the following transformation:

$$f_{n,N} \to f_{0,N-n}, \quad \text{with } a_\pm, b_\pm, w_\pm \to a_\mp, b_\mp, w_\mp.$$

The corresponding energy is $E = 4\cos(p) + w_+ - w_- - 4\Delta$ where the quasimomentum p is a solution of the following BAE:

$$e^{2iNp} = \prod_{u=a_+,b_+}\frac{1 - 2\Delta e^{ip} + ue^{ip}}{1 - 2\Delta u + ue^{ip}}. \tag{E7}$$

The remaining $\binom{N}{2} - N$ eigenstates span the full G_2^+ basis. The two reflection matrices in (29) and (30) become -1 and $-e^{2iNp}$, respectively. In this case, the "boundary terms" in Eq. (71) vanish, and the BAE (71) acquire a simple form

$$e^{2iNp_j} = \prod_{\sigma=\pm}\prod_{k\neq j}\frac{1 - 2\Delta e^{ip_j} + e^{ip_j + i\sigma p_k}}{1 - 2\Delta e^{i\sigma p_k} + e^{ip_j + i\sigma p_k}}, \quad j = 1, 2. \tag{E8}$$

To sum up, in the special case we consider, the set of Bethe root pairs $\{p_1, p_2\}$ in the original BAE (71) splits into four subsets:

(i) one pair $\{p_1, p_2\} = \{-i\ln(a_+), -i\ln(a_-)\}$ corresponding to SHS $\langle 0, N|$,

(ii) N pairs $\{p_1, p\}$ with $p_1 = -i\ \ln(a_-)$ and p given by the solution of (E6),

(iii) N pairs $\{p_1, p\}$ with $p_1 = -i\ \ln(a_+)$ and p given by the solution of (E7),

(iv) $\binom{N}{2} - N$ pairs $\{p_1, p_2\}$ given by the solution of BAE (E8).

In total, there are $1 + N + \binom{N}{2} = \dim G_2^+$ solutions, as expected.

Our example shows that there can be further partitionings of G_2^+, which for $a_\pm b_\pm = 1$ leads to three internal invariant subspaces of dimension $1, N, N$ within G_2^+ which are invariant with respect to the action of H. Likewise, if just one of the two conditions $a_\pm b_\pm = 1$ is satisfied, some internal invariant subspaces disappear, whereas others remain. Under other constraints (arising when the coefficients of some "unwanted" terms on the right-hand side of Eqs. (37)–(45) vanish) various internal invariant subspaces of G_2^+ can appear.

APPENDIX F: ON THE EQUIVALENCE OF CCBA WITH MABA

The algebraic form of Bethe vectors has been given by MABA [5,10,18], whereas little is known about their inner structures. In this Appendix we want to present an alternative basis natural for the work with MABA which, however, leads to involved expressions of the expansion coefficients. Still, this basis will be useful in the limit $\Delta \to 1$ which is considered in the next Appendix.

Let us introduce a different set of bra vectors on sites n,

$$\psi_n(x) = (1, e^{\alpha_+ + \beta_+ + \theta_+ + (2M - N + n - 2x)\eta}). \tag{F1}$$

Replacing ϕ_n in (10) with ψ_n on some sites, we construct an alternative set of factorized bra vectors for the quantum chain as follows:

$$\begin{aligned}
&{}_B\langle \underbrace{0, \dots, 0}_{m_0}, \underbrace{n_1, \dots, n_k}_{M-m_0} | \\
&= \bigotimes_{l_1=1}^{n_1-1} \phi_{l_1}(m_0) \bigotimes \psi_{n_1}(m_0+1) \bigotimes_{l_2=n_1+1}^{n_2-1} \phi_{l_2}(m_0+1) \\
&\quad \bigotimes \psi_{n_2}(m_0+2) \cdots \bigotimes \psi_{n_k}(M) \bigotimes_{l_{k+1}=n_k+1}^{N} \phi_{l_{k+1}}(M), \\
&\quad 0 < n_1 < n_2 < \cdots < n_k \leqslant N, \quad m_0, k \geqslant 0,
\end{aligned} \tag{F2}$$

where $\phi_n(x)$ and $\psi_n(x)$ are defined in (8) and (F1), respectively. This basis appeared in a natural way in unpublished work on various representations of MABA Bethe states. The vectors in (F2) form an alternative basis of G_M^+ and are equivalent to the basis (10), (11) in the main text.

By inspection, we found that the Bethe vectors constructed in Refs. [5,18] can be expanded as linear combinations of the basis (F2), however, with extremely unwieldy coefficients. In contrast, the chiral basis using our proposed trick of the basis extension yields explicit compact symmetric forms for the coefficients of the Bethe vectors.

APPENDIX G: THE $\Delta = 1$ CASE

When $\Delta = 1$, the system degenerates into an isotropic Heisenberg chain. Let $\eta \to 0$, $\alpha_\pm \to 0$, and

$$\lim_{\eta\to 0} \frac{\sinh(\alpha_\pm)}{\sinh\eta} = \frac{\kappa_\pm}{\cosh(\beta_\pm)},$$

we get an integrable XXX chain where the two boundary terms are

$$h_1 = \frac{1}{\kappa_-}\left[\cosh(\theta_-)\sigma_1^x + i\sinh(\theta_-)\sigma_1^y + \sinh(\beta_-)\sigma_1^z\right],$$

$$h_N = \frac{1}{\kappa_+}\left[\cosh(\theta_+)\sigma_N^x + i\sinh(\theta_+)\sigma_N^y - \sinh(\beta_+)\sigma_N^z\right].$$

Now our phantom Bethe roots criterion (5) degenerates into

$$\beta_- + \beta_+ + \theta_- - \theta_+ = 0 \mod 2i\pi, \tag{G1}$$

which is independent of the number of Bethe roots. With the help of the following gauge transformation:

$$U = \begin{pmatrix} -e^{\theta_+ + \beta_+} & e^{\theta_+ - \beta_+} \\ 1 & 1 \end{pmatrix},$$

on all sites we can diagonalize h_N and triangularize h_1,

$$\tilde{h}_N = U_N^{-1} h_N U_N = -\frac{\cosh(\beta_+)}{\kappa_+}\sigma_N^z,$$

$$\tilde{h}_1 = U_1^{-1} h_1 U_1 = -\frac{\cosh(\beta_-)}{\kappa_-}\sigma_1^z - \frac{\sinh(\beta_- + \beta_+)}{\kappa_- e^{-\beta_+}}\left(\sigma_1^x - i\sigma_1^y\right).$$

Due to the fact $[h_{n,n+1}, U_n U_{n+1}] = 0$, the conventional algebraic Bethe ansatz can now be used with the number of Bethe roots varying from 0 to N.

In the $\Delta = 1$ case, the crucial chiral feature disappears, and our vectors in (10) become indistinguishable. However, if we adopt the alternative basis in (F2), the limit will be simple. Both local states,

$$\phi = \lim_{\eta\to 0} \phi_n(x) = (1, -e^{\theta_+ - \beta_+}),$$

and

$$\psi = \lim_{\eta\to 0} \psi_n(x) = (1, e^{\theta_+ + \beta_+}),$$

are conserved and they act as "spin-up" and "spin-down" states, respectively. The state $\phi \otimes \phi \otimes \cdots \otimes \phi$ is a vacuum state and the replacement $\phi \to \psi$ on the vacuum state can be seen as a quasiparticle. The number of Bethe roots represents the maximum number of particles.

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