Some Remarks On Nepomechie–Wang Eigenstates For Spin 1/2 XXX Model

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To Professor Boris Feigin on the occasion of his sixtieth anniversary

Abstract

We compute the energy eigenvalues of Nepomechie–Wang's eigenstates for the spin 1/2 isotropic Heisenberg chain.

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1 Introduction

The Bethe ansatz [B] allows us to construct eigenvectors for Hamiltonians of a wide range of integrable systems. In our paper we are basically interested in the spin $\frac{1}{2}$ isotropic Heisenberg chain (also known as the XXX model) with the periodic boundary condition which is the subject of the original Bethe's paper. According to the algebraic Bethe ansatz [FT] (see also the book [KBI]), the essence of the construction can be thought in the following way. We start from a family of mutually commuting operators $\{B_N(\lambda)\}_{\lambda\in\mathbb{C}}$, $[B_N(\lambda), B_N(\mu)] = 0$, and the ground state vector $|0\rangle_N$ where N is the length of the chain. Suppose that a collection of mutually distinct complex numbers $\lambda = (\lambda_1, \lambda_2, \dots, \lambda_\ell)$ satisfies the following system of algebraic equations, commonly known as the Bethe ansatz equations,

$$\left(\frac{\lambda_k + \frac{i}{2}}{\lambda_k - \frac{i}{2}}\right)^N = \prod_{\substack{j=1\\ j\neq k}}^{\ell} \frac{\lambda_k - \lambda_j + i}{\lambda_k - \lambda_j - i}, \qquad (k = 1, \cdots, \ell), \tag{1}$$

then the vector

$$\Psi_N(\lambda_1, \dots, \lambda_\ell) = \Psi_{\lambda,N} = B_N(\lambda_1)\cdots B_N(\lambda_\ell)|0\rangle_N \tag{2}$$

is an eigenvector of the spin $\frac{1}{2}$ isotropic Heisenberg chain if the vector is non-zero.

Recall that a solution $\lambda = (\lambda_1, \lambda_2, \dots, \lambda_\ell)$ to the equation (1) is called regular if the corresponding vector is non-zero $\Psi_{\lambda,N} \neq 0$. It had been observed by H. Bethe that the number of regular solutions to the system (1) is strictly smaller than the number of eigenvectors of the spin $\frac{1}{2}$ Heisenberg chain Hamiltonian even for $N = 4$ and $\ell = 2$ case. The problem to construct "missing" eigenstates has been investigated by many authors, and partially solved by [EKS, Eq.(26)]. The most natural way to characterize and construct "missing" eigenstates has been developed by Nepomechie–Wang [NW]. Recall that for $N = 4$ and $\ell = 2$, a "missing solution" corresponds to solutions $(\lambda_1, \lambda_2) = (\frac{i}{2}, -\frac{i}{2})$ in which case we have $B_4(\frac{i}{2})B_4(-\frac{i}{2})|0\rangle_4 = 0$. The similar phenomena appears for general singular solutions to the Bethe ansatz equations of the form

$$\lambda = \left\{\frac{i}{2}, -\frac{i}{2}, \lambda_3, \dots, \lambda_\ell\right\}. \tag{3}$$

The problem treated and partially solved in [NW] is to find a selection rule which guarantee that we can achieve $\Psi_{\lambda,N} \neq 0$ under certain regularization. Singular solutions of the form (3) such that one can make $\Psi_{\lambda,N} \neq 0$ is called physical singular solutions. For $N \leq 14$, Nepomechie–Wang's rule is confirmed by an extensive numerical computation [HNS1]. Also, the paper [KS] reveals that the set of solutions which satisfy Nepomechie–Wang's rule has a deep mathematical structure called the rigged configurations (see Section 4.1). The main purpose of the present paper is to give an explicit formula for the energy eigenvalues of the Bethe vectors constructed from the physical singular solutions (Theorem 6). We also provide an alternative proof of results of [NW] at Proposition 3.

2 Bethe vectors and Bethe ansatz equations

To start with let us recall that the Bethe ansatz method is a device to produce eigenvectors of an integrable system in question. In the present paper we apply the Bethe ansatz method to the spin $\frac{1}{2}$ isotropic Heisenberg model under the periodic boundary condition. The space of states $\mathfrak{H}_N$ of our model is

$$\mathfrak{H}_N = \bigotimes_{j=1}^{N} V_j, \quad V_j \simeq \mathbb{C}^2. \tag{4}$$

Then the Hamiltonian $\mathcal{H}_N$ is

$$\mathcal{H}_N = \frac{J}{4}\sum_{k=1}^{N}(\sigma_k^1\sigma_{k+1}^1 + \sigma_k^2\sigma_{k+1}^2 + \sigma_k^3\sigma_{k+1}^3 - \mathbb{I}_N), \qquad \sigma_{N+1}^a = \sigma_1^a, \tag{5}$$

where σ^a $(a = 1, 2, 3)$ are the Pauli matrices

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{6}$$

and the operators σ_k^a $(a = 1, 2, 3)$ act on $\mathfrak{H}_N$ as

$$\sigma_k^a = I \otimes \cdots \otimes \underbrace{\sigma^a}_{k} \otimes \cdots \otimes I, \tag{7}$$

that is, they act non trivially only on the space V_k. Here I is the 2×2 identity matrix and $\mathbb{I}_N$ is the identity matrix on the space of states; $\mathbb{I}_N = I^{\otimes N}$.

Let us consider the L-operators

$$L_k(\lambda) = \lambda I \otimes \mathbb{I}_N + \frac{i}{2}\sum_{a}^{3}\sigma^a \otimes \sigma_k^a \tag{8}$$

which acts on $\mathbb{C}^2 \otimes \mathfrak{H}_N$. Then we define the transfer matrix

$$T_N(\lambda) = L_N(\lambda)L_{N-1}(\lambda)\cdots L_1(\lambda). \tag{9}$$

The basic property of the L-operator (8) is that it satisfies the quantum Yang–Baxter relations, i.e.,

$$R(\lambda-\mu)\,(L_k(\lambda)\otimes L_k(\mu)) = (L_k(\mu)\otimes L_k(\lambda))\,R(\lambda-\mu) \tag{10}$$

where

$$R(\lambda) = \frac{1}{\lambda+i}\left(\left(\frac{\lambda}{2}+i\right) I \otimes I + \frac{\lambda}{2}\sum_{a=1}^{3}\sigma^a\otimes\sigma^a\right). \tag{11}$$

As a corollary of the quantum Yang–Baxter equation (10), one can show that the transfer matrices $T_N(\lambda)$ and $T_N(\mu)$ commute for any parameters λ and μ. It is clear from the definition of L-operator $L_k(\lambda)$, see (8), that the transfer matrix can be treated as 2×2 matrix

$$T_N(\lambda) = \begin{pmatrix} A_N(\lambda) & B_N(\lambda) \\ C_N(\lambda) & D_N(\lambda) \end{pmatrix}, \tag{12}$$

where $A_N(\lambda)$, $B_N(\lambda)$, $C_N(\lambda)$ and $D_N(\lambda)$ are operators acting on the space of states $\mathfrak{H}_N$. The fundamental consequence of the fact that the transfer matrix $T_N(\lambda)$ also satisfies the quantum Yang–Baxter equation is that the operators $B_N(\lambda)$ and $B_N(\mu)$ commute for any parameters $\lambda \in \mathbb{C}$ and $\mu \in \mathbb{C}$.

Let $\tau_N(\lambda)$ be the trace of the transfer matrix $T_N(\lambda)$ on the auxiliary space:

$$\tau_N(\lambda) = A_N(\lambda) + D_N(\lambda). \tag{13}$$

Then the main observation of the algebraic Bethe ansatz analysis of the XXX model is the following relation (see [FT]):

Theorem 1. *We have*

$$\mathcal{H}_N = \frac{iJ}{2}\frac{d}{d\lambda}\log \tau_N(\lambda)\Big|_{\lambda=\frac{i}{2}} - \frac{NJ}{2}\mathbb{I}_N \tag{14}$$

■

Now it is time to consider the local vectors $v_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \in V_k \simeq \mathbb{C}^2$ $(k = 1, \cdots N)$ and the global one

$$|0\rangle_N = v_+ \otimes \cdots \otimes v_+ \in \mathfrak{H}_N. \tag{15}$$

It is well-known that the vector $|0\rangle_N$ is an eigenvector of the operators $A_N(\lambda)$, $D_N(\lambda)$ and $C_N(\lambda)$, namely,

$$A_N(\lambda)|0\rangle_N = \left(\lambda + \frac{i}{2}\right)^N |0\rangle_N, \tag{16}$$

$$D_N(\lambda)|0\rangle_N = \left(\lambda - \frac{i}{2}\right)^N |0\rangle_N, \tag{17}$$

$$C_N(\lambda)|0\rangle_N = 0. \tag{18}$$

Definition 2. Define the Bethe vector corresponding to a collection of pairwise distinct complex numbers $\lambda = (\lambda_1, \ldots, \lambda_\ell)$ as

$$\Psi_N(\lambda_1, \ldots, \lambda_\ell) = B_N(\lambda_1) \cdots B_N(\lambda_\ell)|0\rangle_N. \tag{19}$$

■

The basic property of the Bethe vectors is that $\Psi_N(\lambda_1, \ldots, \lambda_\ell)$ is an eigenvector of the operator $\tau_N(\lambda)$, and thus of the Hamiltonian $\mathcal{H}_N$ (see Theorem 1) if and only if

1. the parameters $\lambda_1, \ldots, \lambda_\ell$ satisfy the system of the Bethe ansatz equations

$$\left(\frac{\lambda_k + \frac{i}{2}}{\lambda_k - \frac{i}{2}}\right)^N = \prod_{\substack{j=1 \\ j\neq k}}^{\ell} \frac{\lambda_k - \lambda_j + i}{\lambda_k - \lambda_j - i}, \qquad (k = 1, \cdots, \ell), \tag{20}$$

2. and $\Psi_N(\lambda_1,\ldots,\lambda_\ell)\neq 0$.

This result is derived from the action of $\tau_N(\lambda)$ on the Bethe vectors $\Psi_N(\lambda_1,\ldots,\lambda_\ell)$. More precisely, according to the standard argument (see, e.g., [FT]), we have the following expressions:

$$\begin{aligned}
&\{A_N(\lambda)+D_N(\lambda)\}B_N(\lambda_1)\cdots B_N(\lambda_\ell)|0\rangle_N \\
&=\Lambda(\lambda;\lambda_1,\cdots,\lambda_\ell)\prod_{j=1}^{\ell}B_N(\lambda_j)|0\rangle_N+\sum_{k=1}^{\ell}\left\{\Lambda_k(\lambda;\lambda_1,\cdots,\lambda_\ell)B_N(\lambda)\prod_{\substack{j=1\\ j\neq k}}^{\ell}B_N(\lambda_j)|0\rangle_N\right\},
\end{aligned} \tag{21}$$

where

$$\Lambda(\lambda;\lambda_1,\cdots,\lambda_\ell)=\left(\lambda+\frac{i}{2}\right)^N\prod_{j=1}^{\ell}\frac{\lambda-\lambda_j-i}{\lambda-\lambda_j}+\left(\lambda-\frac{i}{2}\right)^N\prod_{j=1}^{\ell}\frac{\lambda_j-\lambda-i}{\lambda_j-\lambda} \tag{22}$$

and for $k=1,2,\ldots,k$ we have

$$\Lambda_k(\lambda;\lambda_1,\cdots,\lambda_\ell)=\frac{i}{\lambda-\lambda_k}\left\{\left(\lambda_k+\frac{i}{2}\right)^N\prod_{\substack{j=1\\ j\neq k}}^{\ell}\frac{\lambda_k-\lambda_j-i}{\lambda_k-\lambda_j}-\left(\lambda_k-\frac{i}{2}\right)^N\prod_{\substack{j=1\\ j\neq k}}^{\ell}\frac{\lambda_j-\lambda_k-i}{\lambda_j-\lambda_k}\right\}. \tag{23}$$

We remark that combining the identity (21) and Theorem 1, we deduce that the energy eigenvalue $\mathcal{E}$ of the Hamiltonian $\mathcal{H}_N$ corresponding to the eigenvector $\Psi_N(\lambda_1,\ldots,\lambda_\ell)$ is

$$\mathcal{E}=-\frac{J}{2}\sum_{j=1}^{\ell}\frac{1}{\lambda_j^2+\frac{1}{4}} \tag{24}$$

if $\lambda_j\neq\pm\frac{i}{2}$ for all $j=1,2,\ldots,\ell$. It is well known that the Hamiltonian $\mathcal{H}_N$ commutes with the action of the algebra $\mathfrak{sl}_2$ which acts on $\mathfrak{H}_N$. In particular, the energy eigenvalue is constant for all eigenvectors belonging to the same irreducible $\mathfrak{sl}_2$-module. To be more precise, let $\mathbf{m}$ be the m-dimensional irreducible $\mathfrak{sl}_2$-module. Suppose that we have a non-zero Bethe vector $\Psi_N(\lambda_1,\ldots,\lambda_\ell)$ constructed from the solutions $\lambda_1,\ldots,\lambda_\ell$ to the Bethe ansatz equations. Then it is known that the vector $\Psi_N(\lambda_1,\ldots,\lambda_\ell)$ is the highest weight vector of the module $\mathbf{m}$ where $m=N-2\ell+1$.

Now it is time to recall the definition of the Nepomechie–Wang eigenstates. To begin with, recall that a solution to the Bethe ansatz equation is called singular, if it has the form

$$\lambda=\left\{\frac{i}{2},-\frac{i}{2},\lambda_3,\ldots,\lambda_\ell\right\}. \tag{25}$$

Note that since $B_N(\frac{i}{2})B_N(-\frac{i}{2})=0$ in this case, we have

$$\Psi_\lambda=B_N\left(\frac{i}{2}\right)B_N\left(-\frac{i}{2}\right)B_N(\lambda_3)\cdots B_N(\lambda_\ell)|0\rangle_N=0,$$

and the energy eigenvalue $\mathcal{E}$ of the state Ψ_λ is divergent. To resolve this problem, i.e., to construct a non-zero eigenvector of the Hamiltonian (5), following [NW] we define the perturbed version of (25) as follows:

$$\lambda_1 = \frac{i}{2} + \epsilon + c\,\epsilon^N, \qquad \lambda_2 = -\frac{i}{2} + \epsilon. \tag{26}$$

We note that a similar regularization method is described in [BMSZ, Eq.(3.4)].

Let

$$\Psi_\lambda^{(\epsilon)} := \frac{1}{\epsilon^N} B_N\left(\frac{i}{2} + \epsilon + c\,\epsilon^N\right) B_N\left(-\frac{i}{2} + \epsilon\right) B_N(\lambda_3)\cdots B_N(\lambda_\ell)|0\rangle_N. \tag{27}$$

Then we need to prove the following statement.

Proposition 3. *Suppose that c is given by (28) and (30).*

(1) The vector $\lim_{\epsilon\to 0}\Psi_\lambda^{(\epsilon)} = \Psi_\lambda$ is well-defined.

(2) Ψ_λ is an eigenvector of $\mathcal{H}_N$. ■

Remark 4. From the compatibility condition of c in (28) and (30), [NW] deduce a criterion for the singular solutions to provide non-zero Bethe vectors. Their criterion is verified up to the case of $N \le 14$ by an extensive numerical computation [HNS1]. ■

Although these assertions are essentially proved in [NW], their normalization of $B_N(\lambda)$ is different from the standard normalization used in the present paper. Since this difference of the normalizations changes the structure of the proof, we include some of the details of an alternative proof here.

Our proof of (1) is similar to the proof of $B_N(\frac{i}{2}+\epsilon)B_N(-\frac{i}{2}+\epsilon) \sim \epsilon^N$ given in Appendix A of [NW].[1] On the other hand, the proof of the statement corresponding to (1) given in [NW] is simpler.[2]

For the proof of the statement (2), we prepare the following lemma. Note that the following behaviors are different from the corresponding ones of [NW] since we are using a different normalization.

Lemma 5. *We use the regularization of equation (26).*

(a) If we take

$$c = -\frac{2}{i^{N+1}} \prod_{j=3}^{\ell} \frac{\lambda_j - \frac{3i}{2}}{\lambda_j + \frac{i}{2}}, \tag{28}$$

then we have

$$\Lambda_1(\lambda; \lambda_1, \cdots, \lambda_\ell) \sim \frac{\epsilon^{N+1}}{\lambda - \frac{i}{2} - \epsilon - c\,\epsilon^N}. \tag{29}$$

[1] In [NW], our $B_N(\lambda)$ is denoted by $\tilde{B}_N(\lambda)$.

[2] However their proof seems slightly incomplete since we have $\tilde{B}_N(\lambda_1)\tilde{B}_N(\lambda_2)|0\rangle_N \neq \tilde{B}_N(\lambda_1)|0\rangle_N \times \tilde{B}_N(\lambda_2)|0\rangle_N$. Here $\tilde{B}_N(\lambda)$ stands for the B_N operator in the normalization of [NW].

(b) If we take

$$c = 2i^{N+1} \prod_{j=3}^{\ell} \frac{\lambda_j + \frac{3i}{2}}{\lambda_j - \frac{i}{2}}, \tag{30}$$

then we have

$$\Lambda_2(\lambda; \lambda_1, \cdots, \lambda_\ell) \sim \frac{\epsilon^{N+1}}{\lambda + \frac{i}{2} - \epsilon}. \tag{31}$$

Proof. (a) We have

$$\begin{aligned}
\Lambda_1 &= \frac{i}{\lambda - \lambda_1} \left\{ \left(\lambda_1 + \frac{i}{2}\right)^N \prod_{j=2}^{\ell} \frac{\lambda_1 - \lambda_j - i}{\lambda_1 - \lambda_j} - \left(\lambda_1 - \frac{i}{2}\right)^N \prod_{j=2}^{\ell} \frac{\lambda_j - \lambda_1 - i}{\lambda_j - \lambda_1} \right\} \\
&= \frac{i}{\lambda - \lambda_1} \left\{ i^N \cdot \frac{c\,\epsilon^N}{i} \prod_{j=3}^{\ell} \frac{\frac{i}{2} - \lambda_j - i}{\frac{i}{2} - \lambda_j} - \epsilon^N \cdot \frac{-2i}{-i} \prod_{j=3}^{\ell} \frac{\lambda_j - \frac{i}{2} - i}{\lambda_j - \frac{i}{2}} \right\} \\
&= \frac{i\,\epsilon^N}{\lambda - \lambda_1} \left\{ c \cdot i^{N-1} \prod_{j=3}^{\ell} \frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}} - 2 \prod_{j=3}^{\ell} \frac{\lambda_j - \frac{3i}{2}}{\lambda_j - \frac{i}{2}} \right\}.
\end{aligned}$$

Therefore if we take c as in (28), we see that $\Lambda_1 \sim \epsilon^{N+1}/(\lambda - \lambda_1)$.

(b) We have

$$\begin{aligned}
\Lambda_2 &= \frac{i}{\lambda - \lambda_2} \left\{ \left(\lambda_2 + \frac{i}{2}\right)^N \prod_{\substack{j=1 \\ j \neq 2}}^{\ell} \frac{\lambda_2 - \lambda_j - i}{\lambda_2 - \lambda_j} - \left(\lambda_2 - \frac{i}{2}\right)^N \prod_{\substack{j=1 \\ j \neq 2}}^{\ell} \frac{\lambda_j - \lambda_2 - i}{\lambda_j - \lambda_2} \right\} \\
&= \frac{i}{\lambda - \lambda_2} \left\{ \epsilon^N \cdot \frac{-2i}{-i} \prod_{j=3}^{\ell} \frac{-\frac{i}{2} - \lambda_j - i}{-\frac{i}{2} - \lambda_j} - (-i)^N \frac{c\,\epsilon^N}{i} \prod_{j=3}^{\ell} \frac{\lambda_j + \frac{i}{2} - i}{\lambda_j + \frac{i}{2}} \right\} \\
&= \frac{i\,\epsilon^N}{\lambda - \lambda_2} \left\{ 2 \prod_{j=3}^{\ell} \frac{\lambda_j + \frac{3i}{2}}{\lambda_j + \frac{i}{2}} - \frac{c}{i^{N+1}} \prod_{j=3}^{\ell} \frac{\lambda_j - \frac{i}{2}}{\lambda_j + \frac{i}{2}} \right\}.
\end{aligned}$$

Therefore if we take c as in (30), we see that $\Lambda_1 \sim \epsilon^{N+1}/(\lambda - \lambda_2)$. ∎

Applying the statements (a) and (b) of Lemma 5 to identity (21), we come to a proof of Proposition 3 (2).

3 Energy eigenvalues for the Nepomechie–Wang states

Now we derive the energy eigenvalues for the Nepomechie–Wang states. The main result is Theorem 6.

1) Let $\mathcal{E}$ be the energy eigenvalue corresponding to the solutions $\{\lambda_1, \lambda_2, \ldots, \lambda_\ell\}$ of the Bethe ansatz equations. From Theorem 1, we see that it is enough to compute

$$\mathcal{E} = \frac{J}{2}\left\{ i\frac{d}{d\lambda}\log\Lambda(\lambda;\lambda_1,\cdots,\lambda_\ell)\Big|_{\lambda=\frac{i}{2}} - N \right\} \tag{32}$$

where

$$\Lambda(\lambda;\lambda_1,\cdots,\lambda_\ell) = \left(\lambda+\frac{i}{2}\right)^N \prod_{j=1}^{\ell}\frac{\lambda-\lambda_j-i}{\lambda-\lambda_j} + \left(\lambda-\frac{i}{2}\right)^N \prod_{j=1}^{\ell}\frac{\lambda_j-\lambda-i}{\lambda_j-\lambda} \tag{33}$$

as in (22). Thus it is enough to compute

$$\varepsilon = i\frac{d}{d\lambda}\log\Lambda\Big|_{\lambda=\frac{i}{2}} = \frac{i\frac{d\Lambda}{d\lambda}}{\Lambda}\Big|_{\lambda=\frac{i}{2}}. \tag{34}$$

2) Let us compute the denominator of ε:

$$\varepsilon_{\mathrm{deno}} := \Lambda\left(\frac{i}{2};\lambda_1,\cdots,\lambda_\ell\right) = i^N\prod_{j=1}^{\ell}\frac{\lambda_j+\frac{i}{2}}{\lambda_j-\frac{i}{2}}. \tag{35}$$

By using the regularizations (26), we obtain

$$\varepsilon_{\mathrm{deno}} := i^N\cdot\frac{i+\epsilon+c\,\epsilon^N}{\epsilon+c\,\epsilon^N}\cdot\frac{\epsilon}{\epsilon-i}\prod_{j=3}^{\ell}\frac{\lambda_j+\frac{i}{2}}{\lambda_j-\frac{i}{2}} = i^N\cdot\frac{i+\epsilon+c\,\epsilon^N}{(1+c\,\epsilon^{N-1})(\epsilon-i)}\prod_{j=3}^{\ell}\frac{\lambda_j+\frac{i}{2}}{\lambda_j-\frac{i}{2}}. \tag{36}$$

3) By using the identity

$$\frac{d}{d\lambda}\frac{\lambda-\lambda_j-i}{\lambda-\lambda_j} = \frac{d}{d\lambda}\left(1-\frac{i}{\lambda-\lambda_j}\right) = \frac{i}{(\lambda_j-\lambda)^2},$$

we have

$$\begin{aligned} i\frac{d\Lambda}{d\lambda} &= A_0(\lambda)+\sum_{j=1}^{\ell}A_j(\lambda) \\ &\quad + \text{terms containing at least one}\left(\lambda-\frac{i}{2}\right) \end{aligned} \tag{37}$$

where

$$A_0(\lambda) = iN\left(\lambda+\frac{i}{2}\right)^{N-1}\prod_{j=1}^{\ell}\frac{\lambda-\lambda_j-i}{\lambda-\lambda_j}$$

and for $j = 1, 2, \ldots, \ell$,

$$A_j(\lambda) = i\left(\lambda+\frac{i}{2}\right)^N\frac{\lambda-\lambda_1-i}{\lambda-\lambda_1}\cdots\frac{\lambda-\lambda_{j-1}-i}{\lambda-\lambda_{j-1}}\cdot\frac{i}{(\lambda_j-\lambda)^2}\cdot\frac{\lambda-\lambda_{j+1}-i}{\lambda-\lambda_{j+1}}\cdots\frac{\lambda-\lambda_\ell-i}{\lambda-\lambda_\ell}.$$

Below we compute the contribution from each term one by one.

4) Let us consider $A_0(\lambda)$:

$$A_0\left(\frac{i}{2}\right) = i^N N \cdot \frac{\frac{i}{2} - (\frac{i}{2} + \epsilon + c\,\epsilon^N) - i}{\frac{i}{2} - (\frac{i}{2} + \epsilon + c\,\epsilon^N)} \cdot \frac{\frac{i}{2} - (-\frac{i}{2} + \epsilon) - i}{\frac{i}{2} - (-\frac{i}{2} + \epsilon)} \prod_{j=3}^{\ell} \frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}}$$
$$= i^N N \cdot \frac{i + \epsilon + c\,\epsilon^N}{(1 + c\,\epsilon^{N-1})(\epsilon - i)} \prod_{j=3}^{\ell} \frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}}.$$

Therefore we obtain

$$\frac{1}{\varepsilon_{\mathrm{deno}}} \cdot A_0\left(\frac{i}{2}\right) = N.$$

5) Let us consider $A_1(\lambda)$ and $A_2(\lambda)$.

$$A_1\left(\frac{i}{2}\right) = i^{N+1} \frac{i}{\{\frac{i}{2} - (\frac{i}{2} + \epsilon + c\,\epsilon^N)\}^2} \cdot \frac{\frac{i}{2} - (-\frac{i}{2} + \epsilon) - i}{\frac{i}{2} - (-\frac{i}{2} + \epsilon)} \prod_{j=3}^{\ell} \frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}}$$
$$= -i^N \frac{1}{\epsilon\,(1 + c\,\epsilon^{N-1})^2(\epsilon - i)} \prod_{j=3}^{\ell} \frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}}.$$

On the other hand, we have

$$A_2\left(\frac{i}{2}\right) = i^{N+1} \frac{\frac{i}{2} - (\frac{i}{2} + \epsilon + c\,\epsilon^N) - i}{\frac{i}{2} - (\frac{i}{2} + \epsilon + c\,\epsilon^N)} \cdot \frac{i}{\{\frac{i}{2} - (-\frac{i}{2} + \epsilon)\}^2} \prod_{j=3}^{\ell} \frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}}$$
$$= -i^N \frac{i + \epsilon + c\,\epsilon^N}{\epsilon\,(1 + c\,\epsilon^{N-1})(\epsilon - i)^2} \prod_{j=3}^{\ell} \frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}}.$$

Thus we have

$$\begin{aligned}
&\lim_{\epsilon \to 0} \frac{1}{\varepsilon_{\mathrm{deno}}} \left\{ A_1\left(\frac{i}{2}\right) + A_2\left(\frac{i}{2}\right) \right\} \\
=& \lim_{\epsilon \to 0} \frac{1}{\varepsilon_{\mathrm{deno}}} \times \left(-i^N\right) \frac{(\epsilon - i) + (i + \epsilon + c\,\epsilon^N)(1 + c\,\epsilon^{N-1})}{\epsilon\,(1 + c\,\epsilon^{N-1})^2(\epsilon - i)^2} \prod_{j=3}^{\ell} \frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}} \\
=& -\lim_{\epsilon \to 0} \frac{(1 + c\,\epsilon^{N-1})(\epsilon - i)}{i + \epsilon + c\,\epsilon^N} \times \frac{2\epsilon + i\,c\,\epsilon^{N-1} + 2c\,\epsilon^N + c^2\epsilon^{2N-1}}{\epsilon\,(1 + c\,\epsilon^{N-1})^2(\epsilon - i)^2} \\
=& -\lim_{\epsilon \to 0} \frac{2\epsilon + i\,c\,\epsilon^{N-1} + 2c\,\epsilon^N + c^2\epsilon^{2N-1}}{\epsilon\,(1 + c\,\epsilon^{N-1})(\epsilon - i)(i + \epsilon + c\,\epsilon^N)} = -2.
\end{aligned}$$

6) Finally, for $j = 3, 4, \ldots, \ell$, we have

$$A_j\left(\frac{i}{2}\right) = i^{N+1} \frac{i + \epsilon + c\,\epsilon^N}{\epsilon + c\,\epsilon^N} \cdot \frac{\epsilon}{\epsilon - i} \cdot \frac{\lambda_3 + \frac{i}{2}}{\lambda_3 - \frac{i}{2}} \cdots \frac{\lambda_{j-1} + \frac{i}{2}}{\lambda_{j-1} - \frac{i}{2}} \cdot \frac{i}{(\lambda_j - \frac{i}{2})^2} \cdot \frac{\lambda_{j+1} + \frac{i}{2}}{\lambda_{j+1} - \frac{i}{2}} \cdots \frac{\lambda_\ell + \frac{i}{2}}{\lambda_\ell - \frac{i}{2}}.$$

Thus we have

$$\frac{1}{\varepsilon_{\mathrm{deno}}} \cdot A_j\left(\frac{i}{2}\right) = -\frac{\lambda_j - \frac{i}{2}}{\lambda_j + \frac{i}{2}} \cdot \frac{1}{(\lambda_j - \frac{i}{2})^2} = -\frac{1}{\lambda_j^2 + \frac{1}{4}}.$$

7) To summarize, we have

$$\varepsilon = N - 2 - \sum_{j=3}^{\ell} \frac{1}{\lambda_j^2 + \frac{1}{4}}.$$

Therefore we obtain the following result.

Theorem 6. *Suppose that we have the following physical singular solutions to the Bethe ansatz equations*

$$\left\{ \frac{i}{2}, -\frac{i}{2}, \lambda_3, \cdots, \lambda_\ell \right\}.$$

If we impose the regularization (26), the corresponding non-zero Bethe vector (i.e., the Nepomechie–Wang state) has the following energy eigenvalue:

$$\mathcal{E} = -J - \frac{J}{2} \sum_{j=3}^{\ell} \frac{1}{\lambda_j^2 + \frac{1}{4}}.$$

■

4 Examples

4.1 Rigged configurations

In our previous paper [KS], we pointed out that the rigged configurations (RC for short) provide a good parametrization for the combination of both regular solutions and physical singular solutions to the Bethe ansatz equations. In particular, we pointed out that the rigged configurations are essential for the description of the physical singular solutions and, as the result, we proposed conjectures on the total numbers of various classes of solutions to the Bethe ansatz equations.

In the spin $1/2$ XXX model case, a rigged configuration is comprised of a Young diagram ν (called a configuration) and integers (called riggings) attached to each row of ν. To be more specific, let $\nu = (\nu_1, \nu_2, \ldots, \nu_g)$ and let J_i $(1 \leq i \leq g)$ be the integer attached to the length ν_i row of ν. Then the set of rigged configurations is comprised of all ν and J_i $(1 \leq i \leq g)$ satisfying the following conditions. Suppose that the length of the state is N. Then the total number of the boxes of ν must not exceed $N/2$. We introduce the following integers which we call the vacancy numbers:

$$P_k(\nu) = N - 2\sum_{i=1}^{g} \min(k, \nu_i) \qquad (k \in \mathbb{Z}_{>0}). \tag{38}$$

Note that the second term is the number of boxes within the left k columns of ν. Suppose that the rigging J_i is attached to a length k row. Then it must satisfy $0 \leq J_i \leq P_k(\nu)$. Note that, as rigged configurations, we do not make distinction if the difference is only a reordering of riggings for the rows of the same length.

Below we provide labels of the solutions to the Bethe ansatz equations in terms of the rigged configurations. We refer the readers to [KS, Section 3.1] for the description of the correspondence between the rigged configurations and the solutions to the Bethe ansatz equations.

4.2 $N = 4$ case

Regular solutions to the Bethe ansatz equations. We refer the readers to [KS, Example 2] for additional information on this case. Since we consider regular solutions, we use (24) in order to determine the energy eigenvalue $\mathcal{E}$.

- The case $\ell = 0$. This case corresponds to the representation **5** which is generated by the vacuum vector $|0\rangle_4$. Then we have $\mathcal{E} = 0$.

- The case $\ell = 1$. The corresponding representation is **3**. Then we have the following three solutions:

λ_1	$\mathcal{E}$	RC
$\frac{1}{2}$	$-J$	$2\,\square\,2$
0	$-2J$	$2\,\square\,1$
$-\frac{1}{2}$	$-J$	$2\,\square\,0$

  Here, in order to display the rigged configurations, we put the vacancy numbers (resp. riggings) on the left (resp. right) of the corresponding rows of ν.

- The case $\ell = 2$. The corresponding representation is **1**. Then we have only one regular solution:

λ_1, λ_2	$\mathcal{E}$	RC
$\dfrac{1}{\sqrt{12}}, -\dfrac{1}{\sqrt{12}}$	$-3J$	$\begin{array}{c} 0\,\square\,0 \\ 0\,\square\,0 \end{array}$

To summarize, we have the following energy eigenvalues and their multiplicities

$$\left\{0^5, (-J)^6, (-2J)^3, (-3J)^1\right\}$$

from the regular solutions. Here we describe the multiplicities of the energy eigenvalues as in the following notation:

$$\{\text{eigenvalue}^{\text{multiplicity}}, \ldots\}.$$

Direct diagonalization. From the exact diagonalization of $\mathcal{H}_4$, we obtain the following multiplicities for the energy eigenvalues:

$$\left\{0^5, (-J)^7, (-2J)^3, (-3J)^1\right\}.$$

In conclusion, one eigenstate of eigenvalue $-J$ is missing from the list of regular solutions.

Nepomechie–Wang state. In the case of $\ell = 2$ we have the following physical singular solution:

λ_1, λ_2	RC
$\dfrac{i}{2}, -\dfrac{i}{2}$	$0\,\square\square\,0$

According to Theorem 6, the corresponding energy eigenvalue is $\mathcal{E} = -J$. Moreover the corresponding representation is **1** since $\ell = 2$. This result is compatible with the above observations.

4.3 $N = 6$ case

Regular solutions to the Bethe ansatz equations. We refer the readers to [KS, Example 11] for additional information on this case.

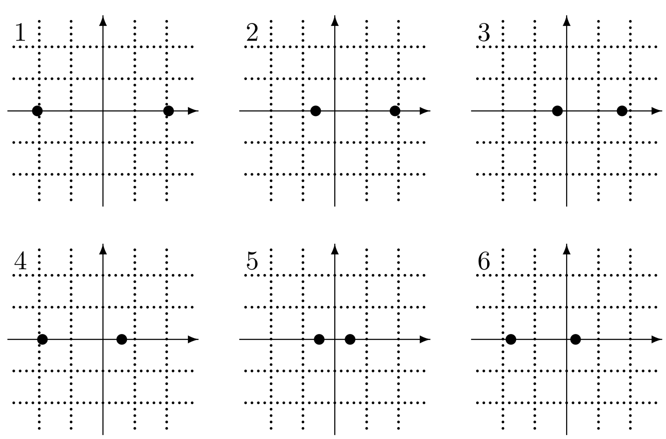
- The case $\ell = 0$. This case corresponds to the representation **7** which is generated by the vacuum vector $|0\rangle_6$. Then we have $\mathcal{E} = 0$.

- The case $\ell = 1$. The corresponding representation is **5**. Then we have the following five solutions:

λ_1	$\mathcal{E}$	RC
0.866025	$-0.5J$	4 $\square$ 4
0.288675	$-1.5J$	4 $\square$ 3
0	$-2J$	4 $\square$ 2
-0.288675	$-1.5J$	4 $\square$ 1
-0.866025	$-0.5J$	4 $\square$ 0

- The case $\ell = 2$. The corresponding representation is **3**. Then we have the following eight regular solutions:[3]

[3] In order to make the correspondence between the final six solutions and rigged configurations in a clearly visible form, we plot solutions (labeled by $1, 2, \ldots, 6$) on the complex plane.



Here the spacing of the dotted lines is 0.33 and solutions are arranged in the descending order of λ_1. According to [KS], we assume that the upper riggings specify the positions of λ_1 (the larger rigging corresponds to the larger value of λ_1). Next we specify λ_2 in the same manner. In fact, this kind of a clear relation is a typical behavior. See [KS, Section 4.1] for another example.

label	λ_1, λ_2	$\mathcal{E}$	RC
	$0.554592 \pm 0.512465i$	$-0.7192J$	2 □□ 2
	$-0.554592 \pm 0.512465i$	$-0.7192J$	2 □□ 0
1	$0.688190, -0.688190$	$-1.3819J$	2 □ 2 2 □ 0
2	$0.631084, -0.198071$	$-2.5J$	2 □ 2 2 □ 1
3	$0.582004, -0.094167$	$-2.7807J$	2 □ 2 2 □ 2
4	$0.198071, -0.631084$	$-2.5J$	2 □ 1 2 □ 0
5	$0.162459, -0.162459$	$-3.6180J$	2 □ 1 2 □ 1
6	$0.094167, -0.582004$	$-2.7807J$	2 □ 0 2 □ 0

- The case $\ell = 3$. The corresponding representation is $\mathbf{1}$. Then we have the following four regular solutions:

$\lambda_1, \lambda_2, \lambda_3$	$\mathcal{E}$	RC
$0, \pm 1.008757i$	$-0.6972J$	0 □□□ 0
$0.235900 \pm 0.500280i, -0.471800$	$-2J$	0 □□ 0 2 □ 0
$0.471800, -0.235900 \pm 0.500280i$	$-2J$	0 □□ 0 2 □ 2
$0, \pm 0.429253$	-4.3027	0 □ 0 0 □ 0 0 □ 0

To summarize, we have the following energy eigenvalues and their multiplicities

$$\big\{0^7, (-0.5J)^{10}, (-0.6972J)^1, (-0.7192J)^6, (-1.3819J)^3, (-1.5J)^{10},$$
$$(-2J)^7, (-2.5J)^6, (-2.7807J)^6, (-3.6180J)^3, (-4.3027J)^1\big\}$$

from the regular solutions.

Direct diagonalization. From the exact diagonalization of $\mathcal{H}_6$, we obtain the following multiplicities for the energy eigenvalues:

$$\left\{ 0^7, \left(-\frac{1}{2}J\right)^{10}, \left(-\frac{5-\sqrt{13}}{2}J\right)^{1}, \left(-\frac{7-\sqrt{17}}{4}J\right)^{6}, (-J)^3, \left(-\frac{5-\sqrt{5}}{2}J\right)^{3}, \left(-\frac{3}{2}J\right)^{10}, \right.$$
$$\left. (-2J)^7, \left(-\frac{5}{2}J\right)^{6}, \left(-\frac{7+\sqrt{17}}{4}J\right)^{6}, (-3J)^1, \left(-\frac{5+\sqrt{5}}{2}J\right)^{3}, \left(-\frac{5+\sqrt{13}}{2}J\right)^{1} \right\},$$

or, in order to facilitate the comparison, their numerical values are

$$\{0^7, (-0.5J)^{10}, (-0.6972J)^1, (-0.7192J)^6, (-J)^3, (-1.3819J)^3, (-1.5J)^{10},$$
$$(-2J)^7, (-2.5J)^6, (-2.7807J)^6, (-3J)^1, (-3.6180J)^3, (-4.3027J)^1\}.$$

In conclusion, the following energy eigenvalues (with multiplicities) are missing from the list of the regular solutions:

$$\{(-J)^3, (-3J)^1\}.$$

Nepomechie–Wang state. In the case of $\ell = 2$ we have the following physical singular solution which generates the representation **3**:

λ_1, λ_2	RC
$\frac{i}{2}, -\frac{i}{2}$	$2\ \boxed{}\boxed{}\ 1$

According to Theorem 6, the corresponding energy eigenvalue is $\mathcal{E} = -J$.

In the case of $\ell = 3$, we have the following physical singular solution which generates the representation **1**:

$\lambda_1, \lambda_2, \lambda_3$	RC
$0, \frac{i}{2}, -\frac{i}{2}$	$\begin{array}{lll} 0 & \boxed{}\boxed{} & 0 \\ 2 & \boxed{} & 1 \end{array}$

According to Theorem 6, the corresponding energy eigenvalue is $\mathcal{E} = -3J$.

Thus we have a perfect agreement with the above observations.

5 Conclusion

(a) We compute the energy of the Nepomechie–Wang eigenstates which correspond to the physical singular solutions to the Bethe ansatz equations (Theorem 6). Recall that in our previous paper [KS], we pointed out that the set of solutions to the Bethe ansatz equations which are either regular or physical singular in the sense of [NW] has a deep mathematical structure called the rigged configurations. Such property is apparent even for smaller values of the system size N. Therefore the present result provides yet another supporting evidence for the usefulness of Nepomechie–Wang's results.

We remark that in paper [EKS], the authors find examples where some of the string type solutions are replaced by pairs of real solutions. Therefore we expect that the correspondence between the rigged configurations and the set of regular and physical singular solutions to the Bethe ansatz equations requires extra modifications when N is large.

(b) We expect interesting connections between the physical singular solutions to the spin $\frac{1}{2}$ isotropic Heisenberg model and anomaly dimensions of certain generic gauge invariant operators in AdS$\times S^5$ theory studied in [BMSZ].

(c) In [HNS2], the authors considered the spin-s generalized Heisenberg chain. According to their numerical data, we propose the following conjecture.

Conjecture 7. *(1) If* $2s \equiv 1 \pmod 2$*, then the total number of states consists of either regular solutions or physical singular solutions (i.e., there are no strange solutions, i.e., solutions to the Bethe ansatz equations having some components equal, and therefore violate the Pauli principle), except possibly "sporadic physical states" to the Bethe ansatz equations*[4]

$$\lambda_0^{(\ell)} = (\underbrace{0, \ldots, 0}_{\ell}), \qquad \text{if } N \equiv \ell - 1 \pmod 2, \tag{40}$$

$$\lambda_{\pm}^{(\ell)} = (\underbrace{\pm s, \ldots, \pm s}_{\ell}), \qquad \text{if } N \equiv 2\ell - 2 \pmod 4. \tag{41}$$

As it has been shown in [HNS2, Table 5], the sporadic physical solutions really exist, namely, $\lambda_0^{(2)}$ *for* $N = 3$*, and* $\lambda_{\pm}^{(2)}$ *for* $N = 6$*.*

(2) If $2s \equiv 0 \pmod 2$*, then if* $\ell \equiv 1 \pmod 2$*, then total number of states is a union of regular solutions and physical singular solutions, and if* $\ell \equiv 0 \pmod 2$*, then the total number of solutions is a union of regular solutions and strange solutions.*

(3) Let $\mathcal{N}_{strange}(N, \ell)$ *(resp.* $\mathcal{N}_{sp}(N, \ell)$*) be the total number of strange (resp. physical singular) solutions corresponding to* N *and* ℓ*. Then, if* $2s \equiv 0 \pmod 2$*, we have*

$$\mathcal{N}_{strange}(2N, 2\ell) = \mathcal{N}_{sp}(2N - 1, 2\ell - 1). \tag{42}$$

■

An explicit, but still conjectural formula for the number $\mathcal{N}_{sp}(2N, 2\ell - 1)$ has been stated in [KS], Conjecture 14 (**B-b**), and we expect that the same conjecture is valid for the numbers $\mathcal{N}_{sp}(2N - 1, 2\ell - 1)$.

We would like to point out that this conjecture explains another difference between integer spin chains and half-integer spin chains which attracts great attention in the Haldane gap theory [H].

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[4] Indeed, the Bethe ansatz equations for spin s Heisenberg chain have the following form:

$$\left(\frac{\lambda_k + is}{\lambda_k - is}\right)^N = \prod_{\substack{j=1 \\ j \neq k}}^{\ell} \frac{\lambda_k - \lambda_j + i}{\lambda_k - \lambda_j - i}, \qquad (k = 1, \ldots, \ell). \tag{39}$$

Therefore, if $\lambda = \lambda_{\pm}^{(\ell)}$, then $\left(\frac{\pm 1 + i}{\pm 1 - i}\right)^N = (-1)^{\ell - 1}$, or equivalently, $(\mp i)^N = (-1)^{\ell - 1}$, so that, $N \equiv 2\ell - 2 \pmod 4$; In the case $\lambda = \lambda_0^{(\ell)}$, the Bethe ansatz equations take the form $(-1)^N = (-1)^{\ell - 1}$, i.e., $N \equiv \ell - 1 \pmod 2$.

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