Singular eigenstates in the even(odd) length Heisenberg spin chain

Pulak Ranjan Giri and Tetsuo Deguchi

Department of Physics, Graduate School of Humanities and Sciences, Ochanomizu University, Ohtsuka 2-1-1, Bunkyo-ku, Tokyo, 112-8610, Japan

E-mail: pulakgiri@gmail.com and deguchi@phys.ocha.ac.jp

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Abstract
We study the implications of the regularization for the singular solutions on the even(odd) length spin-$1/2$ XXX chains in some specific down-spin sectors. In particular, the analytic expressions of the Bethe eigenstates for three down-spin sector have been obtained along with their numerical forms in some fixed length chains. For an even-length chain if the singular solutions $\lambda_\alpha^\{\}\{}$ are invariant under the sign changes of their rapidities $\lambda_\alpha = -\lambda_\alpha^{}$, then the Bethe ansatz equations are reduced to a system of $M - 1/2$ equations in an even (odd) sector. For an odd $N$ length chain in the three down-spin sector, it has been analytically shown that there exist singular solutions in any finite length of the spin chain of the form $N = 3(2k + 1)$ with $k = 1, 2, 3, \cdots$. It is also shown that there exist no singular solutions in the four down-spin sector for some odd-length spin-$1/2$ XXX chains.

Keywords: Bethe ansatz, singular solutions, Heisenberg spin chain

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

1. Introduction

More than eight decades ago, Bethe solved [1] the spin-$1/2$ isotropic Heisenberg chain, i.e. the spin-$1/2$ XXX chain, by a method, known as the Bethe ansatz. In the algebraic Bethe ansatz [2–7], the eigenvalues and the eigenstates are expressed in terms of the rapidities $\lambda_\alpha$, known as the Bethe roots. These $\lambda_\alpha$ are the solutions of the Bethe ansatz equations, which are a set of polynomial equations, emerge as conditions for the eigenvalue equation of the transfer matrix of the spin-$1/2$ XXX chain. Numerical methods, such as, the Newton–Raphson, homotopy continuations and iterations are usually deployed to solve the Bethe ansatz equations. The
distinct and self-conjugate solutions [8] of the Bethe ansatz equations produce the Bethe eigenstates of the spin-1/2 XXX chain which are of highest weight. For the higher spin chains, however, there are repeated rapidities [9] in some solutions, which produce the Bethe eigenstates. The complex solutions present more challenges numerically as opposed to the real solutions, which are easier to evaluate.

Nonetheless, there has been growing interest in the solutions of the spin-1/2 XXX chain in recent years [10–13]. Although making use of the string hypothesis [14] one can estimate the total number of Bethe eigenstates, its certain assumptions do not always hold for any given finite length spin chain. For example, as the length of the chain increases, some of the two string solutions deform back to form two real distinct rapidities [15–17] and some of the two strings have much larger rapidities [18] for very large length spin chains, which is a violation of the string hypothesis. It is therefore necessary to look into the detailed analysis of the Bethe ansatz solutions. Moreover effects of the complex solutions on quantities such as the correlation functions [19, 20], form factors and fidelity are also important, while we need complete knowledge of the complex solutions beforehand in order to investigate them explicitly. It is also worth to mention that some types of solutions of the Bethe ansatz equations in the anisotropic Heisenberg spin chains are studied in [21–25].

The sets of rapidities associated with the spectrum of the spin-1/2 XXX chain are of two classes. One is regular solutions, for which both the Bethe eigenstates and the eigenvalues are finite and well-defined. The other is the singular sets of rapidities [26, 27], which have one pair of rapidities of the form \( \lambda_1 = \pm \frac{i}{2}, \lambda_2 = -\frac{i}{2} \). As the name suggests, the Bethe eigenstates and the eigenvalues are ill-defined because of the pair \( \lambda_1 = \frac{i}{2}, \lambda_2 = -\frac{i}{2} \). If one straight-forwardly plugs the singular solutions into the formula for the Bethe eigenstates in the algebraic Bethe ansatz method or into the eigenvalues, then the states vanish and the eigenvalues diverge. Singular solutions, nevertheless, are an essential part of the spectrum, because, without them the solutions are not complete. It is therefore imperative to devise a regularization scheme [7, 9, 12, 28–32, 40] to make the singular solutions viable such that both the eigenvectors and the eigenvalues become finite and well-defined. Recently, a detailed investigation is carried out by Nepomechie and Wang [31] and extended to higher spin chains [32], where the authors first solve the pole free form of the Bethe ansatz equations for the singular solutions and then introduce the regularization scheme to obtain a consistency condition, which is satisfied only by the physical singular solutions (i.e. the solutions which do produce the Bethe eigenstates and their corresponding eigenvalues). We note that in the standard approach for solving the algebraic Bethe ansatz there is an implicit assumption that no Bethe roots contain rapidities of the form \( \pm \frac{i}{2} \). As mentioned above, the presence of \( \pm \frac{i}{2} \) reduce the Bethe eigenstates to null states, making the eigenvalue equation trivial.

The purpose of this paper is to study the implications of the already developed regularization scheme on the even(odd) length spin chains in some specific down-spin sectors. For an even length spin-1/2 XXX chain, the singular solutions which are invariant under the change of sign of each of the rapidities, i.e. \( \{\lambda_a\} = \{-\lambda_a\} \), simplify the Bethe ansatz equations significantly such that they can be handled easily in the numerical process. For example, in our previous work [13] on non self-conjugate strings, singular strings and rigged configurations [33–38] of the spin-1/2 XXX chain, it helped us obtain the singular solutions in specific cases easily. We analytically show that the singular solutions \( \{\lambda_1 = \frac{i}{2}, \lambda_2 = -\frac{i}{2}, \lambda_3 = \pm \frac{i}{2}\} \) are present for any odd-length chain of the form of \( N = 3(2k + 1) \) with \( k = 1, 2, 3, \ldots \). The repetition of these singular solutions with such a periodicity of 6 in \( N \) has already been confirmed numerically in [12] for some values of the length of the spin chain. Analytically explicit expressions of the Bethe eigenstates for \( M = 3 \) have been obtained for even and odd-
length spin chains and the numerical forms of these states are also obtained for some fixed lengths. A graphical method is provided to search for any singular solution present, if at all, for the $M = 4$ sector in some finite odd-length spin chains.

We organize this paper in the following fashion: in the next section, we briefly discuss the algebraic Bethe ansatz method for the spin-1/2 XXX chain, which sets the basis for the subsequent sections. In section 3, we review the regularization for the singular solutions, which has been studied recently in [31]. In section 4 we show for the even-length spin-1/2 XXX chain that the Bethe ansatz equations for the singular solutions such that they are symmetrically distributed in the complex plane of rapidities, i.e. $\{\lambda_\alpha\} = \{-\lambda_\alpha\}$, can be written in a significantly reduced form. The explicit expression of the three down-spin singular Bethe eigenstate for even-length chains has been obtained and a derivation of the formulae for the Bethe eigenstate with two down-spins and that of three down-spins in the even-length chain have been provided in appendices A and B, respectively. In section 5 it is analytically shown that there exist singular solutions of the form $\{\lambda_1 = \frac{1}{2}, \lambda_2 = -\frac{1}{2}, \lambda_3 = \pm \frac{i}{\sqrt{2}}\}$ in any odd-length chain of the form $N = 3(2k + 1)$ with $k = 1, 2, 3, \ldots$. It is shown in appendix C. The corresponding Bethe eigenstates are derived in appendix D. A graphical method is also suggested for the odd $N$ cases to search for any possible singular solutions in the $M = 4$ down-spin sector and we show that for $N = 15, M = 4$ there is no singular solutions. Finally we conclude in section 6.

2. Algebraic Bethe ansatz

The spin-1/2 XXX chain on a one-dimensional periodic lattice of length $N$ is given by the Hamiltonian

$$H = J \sum_{i=1}^{N} \left( S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z - \frac{1}{4} \right),$$

(1)

where $J$ is the coupling constant and $S_i^j (j = x, y, z)$ is the spin-1/2 operator at the $i$th lattice site and in $j$-direction. The eigenstates and eigenvalues of this Hamiltonian can be obtained in the algebraic Bethe ansatz formulation in the following way. Let us consider the Lax operator as

$$L_\gamma (\lambda) = \begin{pmatrix} \lambda - iS_\gamma^z & -iS_\gamma^+ \\ -iS_\gamma^- & \lambda + iS_\gamma^z \end{pmatrix},$$

(2)

where $S_\gamma^\pm = S_\gamma^x \pm iS_\gamma^y$ and each element of $L_\gamma (\lambda)$ is a matrix of dimension $2^N \times 2^N$, which acts nontrivially on the $\gamma$th lattice site. The monodromy matrix, $T (\lambda)$, is then given by the direct product of the Lax matrices at each site

$$T (\lambda) = L_N (\lambda) L_{N-1} (\lambda) \cdots L_1 (\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix},$$

(3)

The Hamiltonian (1) can be obtained from the transfer matrix

$$t(\lambda) = A(\lambda) + D(\lambda),$$

(4)

by taking its logarithm at $\lambda = -\frac{L}{2}$ as

$$H = \frac{J}{2} \left( -i \left[ \frac{d}{d\lambda} \log t(\lambda) \right]_{\lambda=-\frac{L}{2}} - N \right).$$

(5)
In terms of the rapidities $\lambda_\alpha$, the Bethe state in the $M$ down-spin sector is expressed as

$$|\lambda_1, \lambda_2, \ldots, \lambda_M\rangle = \prod_{a=1}^{M} B(\lambda_a)|\Omega\rangle,$$

(6)

where $|\Omega\rangle$ is the reference eigenstate with all spins up and $B(\lambda_a)$ is an element of the monodromy matrix $T(\lambda_a)$ obtained from equation (3). The Bethe state (6) can explicitly be written as [39]

$$\prod_{\alpha=1}^{M} B(\lambda_{\alpha})|\Omega\rangle = (-i)^M \prod_{j<k}^{M} (\lambda_j - \lambda_k + i) \prod_{j=1}^{M} \left( \frac{\lambda_j - i/2}{\lambda_j + i/2} \right)^{N}$$

$$\times \sum_{1 \leq j_1 < j_2 < \cdots < j_N \leq M} \prod_{j \in \mathcal{P}} \prod_{j \in \mathcal{P}} \left( \frac{\lambda_{j_1} - \lambda_{j_2}}{\lambda_{j_1} + \lambda_{j_2} + i} \right)^{H(j-k)} \prod_{j=1}^{M} S^{\alpha}_{\mathcal{P}} |\Omega\rangle,$$

(7)

where $\mathcal{P}$ are elements of the permutation group $S_M$ of $M$ numbers and $H(x)$ is the Heaviside step function $H(x) = 1$ for $x > 0$ and $H(x) = 0$ for $x \leq 0$.

The action of the transfer matrix (4) on the Bethe state (6) is given by

$$t(\lambda) \prod_{a=1}^{M} B(\lambda_a)|\Omega\rangle = \Lambda(\lambda, \{\lambda_a\}) \prod_{a=1}^{M} B(\lambda_a)|\Omega\rangle$$

$$+ \sum_{k=1}^{M} \Lambda_k(\lambda, \{\lambda_a\}) B(\lambda) \prod_{a \neq k}^{M} B(\lambda_a)|\Omega\rangle,$$

(8)

where

$$\Lambda(\lambda, \{\lambda_a\}) = \left( \lambda + \frac{i}{2} \right)^{M} \prod_{a=1}^{M} \frac{\lambda - \lambda_a - i}{\lambda - \lambda_a} + \left( \lambda - \frac{i}{2} \right)^{M} \prod_{a=1}^{M} \frac{\lambda - \lambda_a + i}{\lambda - \lambda_a},$$

(9)

is the eigenvalue of the transfer matrix and the unwanted terms are

$$\Lambda_k(\lambda, \{\lambda_a\}) = \frac{i}{\lambda - \lambda_k} \left[ \left( \lambda_k + \frac{i}{2} \right)^{M} \prod_{a \neq k}^{M} \frac{\lambda_k - \lambda_a - i}{\lambda_k - \lambda_a} \right.$$

$$- \left. \left( \lambda_k - \frac{i}{2} \right)^{M} \prod_{a \neq k}^{M} \frac{\lambda_k - \lambda_a + i}{\lambda_k - \lambda_a} \right], \quad k = 1, 2, \ldots, M.$$  

(10)

Note that (8) becomes an eigenvalue equation when the unwanted terms (10) vanish, which give us the well known Bethe ansatz equations.
In terms of solutions $\lambda_\alpha$ of (11), known as the Bethe roots, the eigenvalue of the Hamiltonian $H$ for the $M$ down-spin state is expressed as
\[
E = \frac{J}{2} \left( -i \left[ \frac{d}{d \lambda} \log A(\lambda, \{ \lambda_\alpha \}) \right] \bigg|_{\lambda = -\frac{j}{2}} - N \right) = -\frac{J}{2} \sum_{\alpha = 1}^{M} \frac{1}{(\lambda_\alpha^2 + \frac{1}{4})}. \tag{12}
\]
To characterize the state in terms of the Bethe quantum numbers, $\beta$, $\alpha = 1, 2, \ldots, M$, one takes the logarithm of equation (11) as
\[
\sum_{\lambda} \pi_\lambda = -\sum \alpha_\beta \frac{1}{(\lambda_\alpha^2 + \frac{1}{4})}, \tag{13}
\]
The Bethe quantum numbers take integral (half integral) values if $N - M$ is odd (even) respectively. $\beta$ are in general repetitive and therefore are not much useful to count the total number of states of a spin chain. However, strictly non-repetitive quantum numbers can also be obtained. According to the string hypothesis, the rapidities for the $M$ down spin sector are typically arranged in a set of strings as,
\[
\lambda_{\alpha a}^j = \lambda_{\alpha a}^1 + \frac{1}{2}(j + 1 - 2\alpha) + \Delta_{\alpha a}^j, \quad a = 1, 2, \ldots, j, \quad \alpha = 1, 2, \ldots, M, \quad \text{mod } 2\pi. \tag{14}
\]
where the string center $\lambda_{\alpha a}^1$ for a length $j$-string is real, $\alpha$ represents the number of $j$-strings $M_j$ and the string deviations are given by $\Delta_{\alpha a}^j$. In the limit that the deviations vanish, $\Delta_{\alpha a}^j \to 0$, equations (13) reduce to the equations
\[
\arctan \left( \frac{2\lambda_{\alpha a}^j}{j} \right) = \frac{\pi I_{\alpha}^j}{N} + \frac{1}{N} \sum_{k=1}^{N} \sum_{\beta} \Theta_{jk} \left( \lambda_{\alpha a}^j - \lambda_{\beta b}^j \right), \quad \text{mod } \pi,
\]
\[
\Theta_{jk}(\lambda) = (1 - \delta_{jk}) \arctan \frac{2j}{|j - k|} + 2 \arctan \frac{2j}{|j - k| + 2} + \cdots + 2 \arctan \frac{2j}{j + k}, \tag{15}
\]
where $M_k$ is the number of $k$-strings present in a state such that $\sum k M_k = M$. The Takahashi quantum numbers, $I_{\alpha}^j$, which are strictly non-repetitive, are then given by
\[
|I_{\alpha}^j| \leq \frac{1}{2} \left( N - 1 - \sum_{k=1}^{kM} \left[ 2 \min(j, k) - \delta_{j,k} \right] M_k \right). \tag{16}
\]

3. Regularization for the singular solutions

In this section we review the regularization of the singular solutions, which was introduced in [9] and later pursued in detail in [7, 12, 30–32, 40], as these results are essential in our study. As mentioned in the introduction, the singular sets of rapidities make the eigenvalues and the eigenvectors ill-defined. It is manifest from the expression that the Bethe eigenstate (7)
vanishes and the eigenvalue equation (12) diverges. By considering typical singular solutions for the $M$ down-spins as
\[
\{ \lambda_1 = \frac{i}{2}, \lambda_2 = -\frac{i}{2}, \lambda_3, \lambda_4, \ldots, \lambda_M \},
\]
(17)
it can be easily seen that the presence of $\pm \frac{i}{2}$ in the singular solutions are responsible for the pathology in the expression of the Bethe eigenstate and the eigenvalue. To handle this situation the following regularization are used
\[
\hat{\lambda}_1 = ae + \frac{i}{2} \left( 1 + 2\epsilon^N \right),
\]
\[
\hat{\lambda}_2 = ae - \frac{i}{2} \left( 1 + 2\epsilon^N \right),
\]
(18)
where $a$ is a complex constant and $\epsilon$ is a complex parameter, whose $\epsilon \to 0$ limit gives the singular solutions. A rescaling of $\epsilon$ by $a$ reduces equation (18) to the one considered and extensively discussed in [31]. In this respect see also equation (31) of [9] and equation (3.4) of [7], where the same regularization has been considered.

To obtain the conditions for $\{ \lambda_1, \lambda_2, \ldots, \lambda_M \}$, a well-defined Bethe state with $M$ rapidities $\{ \tilde{\lambda}_a \} = \{ \hat{\lambda}_1, \hat{\lambda}_2, \hat{\lambda}_3, \hat{\lambda}_4, \ldots, \hat{\lambda}_M \}$ of the form
\[
\{ \tilde{\lambda}_1, \tilde{\lambda}_2, \lambda_3, \lambda_4, \ldots, \lambda_M \} = \frac{1}{\left( \hat{\lambda}_1 - \frac{1}{2i} \right)^N} \prod_{a=1}^{M} B(\tilde{\lambda}_a)|\Omega>,
\]
(19)
is necessary. Action of $t(\tilde{\lambda})$ on (19) in $\epsilon \to 0$ limit is given by
\[
\lim_{\epsilon \to 0} \left( \frac{1}{\hat{\lambda}_1 - \frac{1}{2i}} \right)^N \prod_{a=1}^{M} B(\tilde{\lambda}_a)|\Omega> = \lim_{\epsilon \to 0} \left( \frac{1}{\hat{\lambda}_1 - \frac{1}{2i}} \right)^N \prod_{a=1}^{M} B(\tilde{\lambda}_a)|\Omega>
\]
\[
+ \lim_{\epsilon \to 0} \sum_{k=1}^{M} \mathcal{A}_k \left( \lambda, \{ \tilde{\lambda}_a \} \right) \quad \times \left( \frac{\tilde{\lambda}_k - \frac{1}{2i}}{\hat{\lambda}_1 - \frac{1}{2i}} \right)^N B(\tilde{\lambda}) \prod_{a=1}^{M} B(\tilde{\lambda}_a)|\Omega>,
\]
(20)
where
\[
\lim_{\epsilon \to 0} \left( \frac{1}{\hat{\lambda}_1 - \frac{1}{2i}} \right)^N \prod_{a=1}^{M} B(\tilde{\lambda}_a)|\Omega> = \left( \lambda + \frac{i}{2} \right)^{N-1} \left( \lambda - \frac{3}{2}i \right) \prod_{a=3}^{M} \frac{\lambda - \tilde{\lambda}_a - i}{\lambda - \tilde{\lambda}_a}
\]
\[
+ \left( \lambda - \frac{i}{2} \right)^{N-1} \left( \lambda + \frac{3}{2}i \right) \prod_{a=3}^{M} \frac{\lambda - \tilde{\lambda}_a + i}{\lambda - \tilde{\lambda}_a},
\]
(21)
is the eigenvalue of the transfer matrix for the singular solutions and the unwanted terms are
\[
\lim_{\epsilon \to 0} \mathcal{A}_k \left( \lambda, \{ \tilde{\lambda}_a \} \right) = \lim_{\epsilon \to 0} \frac{i}{\lambda - \tilde{\lambda}_k}
\]
Here we remark that both sides of (20) have finite and well-defined limit and most importantly the Bethe eigenstate is finite in the limit and not a null state. Note that (20) becomes the eigenvalue equation corresponding to the singular solutions if the unwanted terms (22) vanish, i.e. in the $\epsilon \to 0$ limit the following equations can be obtained

\[
\prod \lambda = \alpha + \beta, \quad \alpha = a_i, \quad \beta = (1), \quad a = 3, 4, \ldots, M. \tag{23}
\]

\[
\prod \lambda = - \alpha + \beta, \quad \alpha = a_i, \quad \beta = (1), \quad a = 3, 4, \ldots, M. \tag{24}
\]

Equating the two expressions (23) and (24) one obtains

\[
\prod \lambda = \alpha + \beta, \quad \alpha = a_i, \quad \beta = (1). \tag{26}
\]

Note that equation (23) was obtained in [26, 31] and equation (26) was obtained in [31]. One can regard the set of equations (25)–(26) as the Bethe ansatz equations for the singular solutions, as the distinct and self-conjugate solutions produce the well-defined Bethe eigenstates and the eigenvalues for the singular solutions of the transfer matrix and for the Hamiltonian $H$. They are in agreement with the statement in [8] that the distinct and self-conjugate solutions of the Bethe equations are physical solutions. For our purpose we consider equations (25)–(26) to study the singular solutions for the even(odd) length chains.

Taking the product of all the Bethe equations in (25) one obtains

\[
\prod \lambda = (-1)^N \prod \lambda = (1). \tag{27}
\]

Dividing both sides of equation (27) by the both sides of equation (26) the condition [31]

\[
\left( \prod_{i=3}^{M} \left( \frac{\lambda_i + \frac{1}{2}}{\lambda_i - \frac{1}{2}} \right) \right)^N = 1, \tag{28}
\]

can be obtained, as also pointed out by Nepomechie in a private commutation. The set of equations (25) and (28) have been considered in [12] to obtain the physical singular solutions.

Here we remark that in [7] it is has been addressed that the singular solutions of even-length spin chains in odd down-spin sectors satisfy a trace condition (see equation (2.4) and the
related discussion after equation (3.4) of [7]) in the $\epsilon \to 0$ limit

$$\lim_{\epsilon \to 0} \prod_{i=1}^{M} \frac{\lambda_i + \frac{i}{2}}{\lambda_i - \frac{i}{2}} = \prod_{i=3}^{M} \frac{\lambda_i + \frac{i}{2}}{\lambda_i - \frac{i}{2}} = 1, \quad (29)$$

The authors assumed that the singular solutions satisfying the trance condition (29) are invariant under the sign changes of their rapidities. In the odd-down spin sectors the singular solutions then can be written in the form $\{\lambda_1 = \frac{i}{2}, \lambda_2 = -\frac{i}{2}, \lambda_3 = 0, \lambda_4, -\lambda_4, \ldots, \lambda_{M-1}, -\lambda_{M-1}\}$. Now note that $\{\lambda_3 = 0, \lambda_4, -\lambda_4, \ldots, \lambda_{M-1}, -\lambda_{M-1}\}$ automatically satisfy the trace condition (29).

As evident from equations (23)–(24), the parameter $a$ is a function of the rapidities $\{\lambda_{\alpha}, \alpha = 3, 4, \ldots, M\}$, in general. To obtain the singular Bethe eigenstates for $M$ down-spins we need to use

$$\tilde{\lambda}_1 = i\sqrt{\prod_{\alpha=3}^{M} \frac{\lambda_{\alpha} + \frac{1}{2}}{\lambda_{\alpha} - \frac{1}{2}} e^{\frac{i}{2} \left( 1 + 2e^N \right)},}$$

$$\tilde{\lambda}_2 = i\sqrt{\prod_{\alpha=3}^{M} \frac{\lambda_{\alpha} + \frac{1}{2}}{\lambda_{\alpha} - \frac{1}{2}} e^{-\frac{i}{2} \left( 1 + 2e^N \right)},} \quad (30)$$

in the Bethe state (19) and take the $\epsilon \to 0$ limit

$$|\lambda_1, \lambda_2, \ldots, \lambda_M\rangle = \lim_{\epsilon \to 0} \frac{1}{\tilde{\lambda}_1 - \frac{1}{2}} B(\tilde{\lambda}_1) B(\tilde{\lambda}_2) \prod_{\alpha=3}^{M} B(\lambda_{\alpha}) |\Omega\rangle. \quad (31)$$

The eigenvalue of the Hamiltonian $H$ for the singular solution $\{\frac{i}{2}, -\frac{i}{2}, \lambda_3, \lambda_4, \ldots, \lambda_M\}$ can be obtained from the eigenvalue equation (21) of the transfer matrix for the singular solutions as [40]

$$E = \frac{J}{2} \left( -i \left[ \frac{d}{d\lambda} \log \lim_{\epsilon \to 0} \lambda \left( \{\tilde{\lambda}_1\} \right) \right]_{\lambda = \frac{1}{2}} \right) - N = -J \left[ 1 + \frac{1}{2} \sum_{\alpha=3}^{M} \left( \frac{1}{\lambda_{\alpha}} + \frac{1}{\lambda_{\alpha}} \right) \right], \quad (32)$$

4. Even length spin chain

Numerically the even length spin-1/2 chain has been investigated for some finite values of the length $N$ [11, 12]. It has been observed numerically that for the singular solutions the rapidities are distributed symmetrically [11]. Alternatively, in the language of rigged configurations the singular solutions of an even-length spin chain are flip invariant [37]. Based on these, we in our previous work [13] assumed that the sum of the rapidities for the singular solutions of an even length spin-1/2 chain vanishes. Here, we discuss this assumption in the light of regularization as well as the singular solutions in general. To start with, let us consider the lowest down-spin sector for a singular solution to exist, i.e., $M = 2$. In this case equation (30) reduces to
The Bethe eigenstate, in this case, takes a simple form \[12, 15\] (see appendix A for the derivation)

\[
\sum_{\Omega} \left( \begin{array}{c} i \frac{1}{2} \\
\frac{i}{2} 
\end{array} \right) \equiv \sum_{j=1}^{N} (-1)^{s_j} S_j S_{j+1} |\Omega\rangle,
\]

with the eigenvalue \( E = -J \). We numerically confirmed up to some lengths of the spin chain that equation (34) is indeed the highest weight singular state. For \( N = 6 \), it takes the form

\[
\left( \begin{array}{c} i \frac{1}{2} \\
\frac{i}{2} 
\end{array} \right) \equiv (0, -1, 0, 2, 1, 0, -1, 0, 1, 0, 8, 1, 0, 1, -1, 0, 13),
\]

where \( 0_m \) is the short form of \( m \) consecutive 0’s, for example \( 0_3 = 0, 0, 0 \). For the three down spin sector, \( M = 3 \), equation (26) reads as

\[
\frac{\lambda_3 + \frac{i}{2} i}{\lambda_3 - \frac{i}{2} i} = \frac{\lambda_3 - \frac{i}{2} i}{\lambda_3 + \frac{i}{2} i} = 0,
\]

whose only solution is \( \lambda_3 = 0 \) and it is also a solution of equation (25), which means \( \{ \lambda_1 = \frac{i}{2}, \lambda_2 = -\frac{i}{2}, \lambda_3 = 0 \} \) is the only solution of the Bethe ansatz equations for the singular solutions (25)–(26). The regularization in this case becomes

\[
\tilde{\lambda}_1 = i \sqrt{-\frac{1}{3} e + \frac{i}{2} (1 + 2 e^X)},
\]

\[
\tilde{\lambda}_2 = i \sqrt{-\frac{1}{3} e - \frac{i}{2} (1 + 2 e^X)}.
\]

The Bethe eigenstate, in this case, becomes (see appendix B for the derivation)

\[
\left( \begin{array}{c} i \frac{1}{2} \\
\frac{i}{2} 
\end{array} \right) \equiv \sum_{j=1}^{N} (-1)^{s_j} S_j S_{j+1} \left( \sum_{k=1}^{N} (-1)^k S_k \right) |\Omega\rangle,
\]

with the eigenvalue \( E = -3J \). We numerically confirmed up to some lengths that equation (38) is indeed the highest weight singular Bethe eigenstate. For \( N = 6 \), it takes the form

\[
\left( \begin{array}{c} i \frac{1}{2} \\
\frac{i}{2} 
\end{array} \right) \equiv (0, 0, 1, 0, 0, -1, 0, 2, 1, 0, 2, 1, -1, 0, 10, 1, -1, 0, 2),
\]

\[
-1, 0, 2, 1, 0, 5, 1, 0, -1, 0, 13). \]

(39)

Analytic calculation for \( M > 4 \) becomes more difficult, but we can still proceed to find a symmetry, which the rapidities for the singular solutions follow. For general values of \( M \) equation (26) reads as

\[
\prod_{a=3}^{M} \frac{\lambda_a + \frac{i}{2} i}{\lambda_a - \frac{i}{2} i} - \prod_{a=3}^{M} \frac{\lambda_a - \frac{i}{2} i}{\lambda_a + \frac{i}{2} i} = 0.
\]

(40)
If a set of rapidities satisfy the conditions
\[ \lambda_\alpha + \lambda_{\alpha+1} = 0, \quad \text{for } \alpha = 3, 5, \cdots, M - 1, \] (41)
for even \( M \), then they satisfy equation (40). Similarly, if a set of rapidities satisfy the conditions
\[ \lambda_3 = 0, \]
\[ \lambda_\alpha + \lambda_{\alpha+1} = 0, \quad \text{for } \alpha = 4, 6, \cdots, M - 1. \] (42)
for odd \( M \), then they satisfy equation (40). It follows that the singular solutions \( \{\lambda_\alpha\} = \{\lambda_1, \lambda_2, \cdots, \lambda_M\} \), which satisfy the conditions (41) or (42), are invariant under the sign changes of each of their rapidities i.e. \( \{\lambda_\alpha\} = \{-\lambda_\alpha\} \). It implies that the sum of rapidities of such a singular solution for even \( N \) vanishes [13], i.e.
\[ \sum_{\alpha=1}^{M} \lambda_\alpha = 0. \] (43)
In the language of rigged configurations the conditions (41) and (42) or the condition (43) is equivalent to the flip invariance of the riggings, which has to be satisfied by singular solutions according to a conjecture in [37]. Note that the conditions (41) reduce the Bethe ansatz equations for the singular solutions in an even down-spin sector to a system of equations of \( (M - 2)/2 \) rapidities \( \{\lambda_3, \lambda_5, \cdots, \lambda_{M-1}\} \)
\[
\left( \frac{\lambda_\alpha - \frac{1}{2} i}{\lambda_\alpha + \frac{1}{2}} \right)^{N-2} = \frac{\lambda_\alpha - \frac{3}{2} i}{\lambda_\alpha + \frac{3}{2}} \prod_{\beta \neq \alpha} \frac{\lambda_\alpha - \lambda_\beta - i \lambda_\alpha + \lambda_\beta - i}{\lambda_\alpha - \lambda_\beta + i \lambda_\alpha + \lambda_\beta + i}, \quad \alpha \in [3, 5, \cdots, M - 1]. \] (44)
Similarly the conditions (42) reduce the Bethe ansatz equations for the singular solutions in an odd down-spin sector to a system of equations of \( (M - 3)/2 \) rapidities \( \{\lambda_4, \lambda_6, \cdots, \lambda_{M-1}\} \)
\[
\left( \frac{\lambda_\alpha - \frac{1}{2} i}{\lambda_\alpha + \frac{1}{2}} \right)^{N-2} = \frac{\lambda_\alpha - \frac{3}{2} i}{\lambda_\alpha + \frac{3}{2}} \prod_{\beta \neq \alpha} \frac{\lambda_\alpha - \lambda_\beta - i \lambda_\alpha + \lambda_\beta - i}{\lambda_\alpha - \lambda_\beta + i \lambda_\alpha + \lambda_\beta + i}, \quad \alpha \in [4, 6, \cdots, M - 1]. \] (45)
One can numerically show that apart from solutions of the form (43) there are no other solutions for even length chains up to, for instance \( N = 14 \).

5. Odd length spin chain

Singular solutions for the odd length chain is not much discussed in the literature until very recently [12, 31]. For two down-spins, \( M = 2 \), left-hand side of equation (26) is given by +1, while the right-hand side is given by −1. The disagreement between both sides implies that there is no singular solution. For three down-spins, \( M = 3 \), we obtain from equation (26)
\[
\frac{\lambda_3 + \frac{i}{2}}{\lambda_3 - \frac{i}{2}} + \frac{\lambda_3 - \frac{i}{2}}{\lambda_3 + \frac{i}{2}} = 0,
\]
(46)
whose solutions are \(\lambda_3 = \pm \frac{\sqrt{3}}{2}\). In order for them to become the Bethe roots they also have to satisfy (25), which in this case becomes
\[
\left( \frac{\lambda_3 - \frac{i}{2}}{\lambda_3 + \frac{i}{2}} \right)^{N-1} = \frac{\lambda_3 - \frac{i}{2}}{\lambda_3 + \frac{i}{2}}.
\]
(47)
In appendix C we derive from (47) the following equation for the singular solutions
\[
\left( \frac{\lambda_3 - \frac{3}{4}}{\lambda_3 + \frac{3}{4}} \right)^{\frac{N}{4}} \left( \lambda_3 - \frac{i}{2} \right)^{\frac{N}{4}} \left( \lambda_3 + \frac{i}{2} \right)^{\frac{N}{4}} + 4i\lambda_3^2 \sum_{r=0}^{\frac{N-1}{2}} \lambda_3^{N-3-2r} \times \left( \frac{3}{4} \right)^{\frac{N}{4}} \left( \sum_{r=0}^{\frac{N}{4}} \left( -\frac{i}{3} \right)^{r} N C_2 \right) = 0,
\]
(48)
for \(N\) satisfying
\[
N = 3(2k + 1), \quad k = 1, 2, 3, \ldots.
\]
(49)
We see that \(\lambda_3 = \pm \frac{\sqrt{3}}{2}\) are indeed solutions of equation (48), provided the length \(N\) of the chain satisfies equation (49). Note that numerical evidence for (49) has already been found in [12]. The regularization in this case becomes
\[
\tilde{\lambda}_1 = i\sqrt{\frac{1}{\sqrt{3}}} e + \frac{i}{2} \left( 1 + 2 e^N \right),
\]
\[
\tilde{\lambda}_2 = i\sqrt{\frac{1}{\sqrt{3}}} e - \frac{i}{2} \left( 1 + 2 e^N \right),
\]
(50)
where \(\pm\) correspond to the regularization of the two roots \(\lambda_3 = \pm \frac{\sqrt{3}}{2}\) respectively. The Bethe eigenstates, in this case, become (see appendix D for the derivation)
\[
\exp \left( \frac{\pi k i}{3} \right) S_1 \sum_{j=1}^{N} (-1)^{j+k} H^{j-k} S_j S_{j+1}^{-1} \right) |\Omega\rangle,
\]
(51)
with the eigenvalue \(E = -1.5J\). For \(N = 9\), numerically we obtain the singular eigenstates for \(\lambda_3 = \pm \frac{\sqrt{3}}{2}\) as
\[
\left( \frac{i}{2}, -\frac{i}{2}, \frac{\sqrt{3}}{2} \right) \equiv (0, 1, 0, 3, 1, 0, a, 0, a^*, 0, 4, -1, 0, 2, 1, 0, 2, 0, a, 0, 0, a, 0, a^*, 0, 2, -a^*, 0, 5, a^*, 0, 4, -1, 0, a^*, 0, 3, 1, 0, -a, 0, 2, a, 0, -a, 0, 1, a, 0, 8, -a, 1, 0, -a^*, 0, 3, a, 0, a^*, 0, 18, 1, 0, 2, -1, 0, a^*, 0, 1, 0, 1, -1, 0, 23, 1, 0, 16, a, -1, 0, a^*, 0, 3, 0, 1, -1, 0, 15, a, 0, 34, 0, 0, a^*, a^*, 0, 2, -a, 0, 2, -a^*, 0, 4, 0, 4),
\]
where $a = -\exp(\frac{\pi}{3}i)$.

In the four down-spin sector, it is more difficult to analytically search for any possible singular solutions. One possible method is to thoroughly look for all numerical roots of the spin-1/2 XXX chain, as done in [12], who obtained no singular solutions for odd lengths up to $N = 13$. However, a more efficient way would be just to concentrate on singular solutions. Here we just plot the graph associated with the Bethe ansatz equations for the singular solutions and look for any possible intersections of the curves. As an example we consider the $N = 15$ case but it can also be extended to other values of $N$. There are two possible situations, either $\lambda_3$ and $\lambda_4$ are real or they are complex conjugate to each other. Let us first discuss the complex rapidity case. Replacing $\lambda_3 = a + ib$, $\lambda_4 = a - ib$ in (26) we obtain

$$a^4 + b^4 + 2a^2b^2 - \frac{11}{2}a^2 - \frac{5}{2}b^2 + \frac{9}{16} = 0,$$

which is plotted in figure 1. The other two equations (25) are just the complex conjugate to each other, so we equate the real part and the imaginary part of both the sides

$$\text{Re} \left\{ \frac{a + (b - \frac{1}{2}i)}{a + (b + \frac{1}{2}i)} \right\}^{N-1} = \text{Re} \left\{ \frac{a + (b - \frac{1}{2}i)}{a + (b + \frac{1}{2}i)} \right\}^{2b - 1} = \frac{2b - 1}{2b + 1},$$

$$\text{Im} \left\{ \frac{a + (b - \frac{1}{2}i)}{a + (b + \frac{1}{2}i)} \right\}^{N-1} = \text{Im} \left\{ \frac{a + (b - \frac{1}{2}i)}{a + (b + \frac{1}{2}i)} \right\}^{2b - 1} = \frac{2b - 1}{2b + 1}.$$

Equations (55) and (56) are plotted for $N = 15$ in figures 2 and 3 respectively. In order to have a solution, the three curves (54)–(56) have to coincide at complex conjugate points. From figure 4, we see that these curves indeed coincide at $(a = 0, b = \pm \frac{1}{2})$, but they are not physical solutions, since the physical solutions for the spin-1/2 chain have to be distinct. For
Figure 1. Plot of equation (54). We assign $a$ in the horizontal axis and $b$ in the vertical axis.

Figure 2. Plot equation (55) for $N = 15$. 

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Figure 3. Plot equation (56) for $N = 15$.

Figure 4. Plots of equations (54) (blue curves), (55) (red curves) and (56) (green curves) for $N = 15$. 

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Although it seems from Figure 4 that there are intersections of the curves but they actually do not intersect. Because, although \( a = 0, b = \pm \frac{3}{2} \) are solutions of equation (54), they are not solutions of (55) or (56). It can be easily seen that the right-hand side of both the equations either vanish or become infinity while the left-hand side is finite.

Let us now consider the case when the two rapidities \( \lambda_3, \lambda_4 \) are real. From equation (26) we obtain

\[
\lambda_3^2 \lambda_4^2 - \frac{3}{4} \left( \lambda_3^2 + \lambda_4^2 \right) + \frac{9}{16} - 4\lambda_3 \lambda_4 = 0, \tag{57}
\]

which does not have any real solutions of the form \( \lambda_3 = -\lambda_4 \), which is also evident from Figure 5. The other two equations obtained from (25) are

\[
\left( \lambda_3 - \frac{3}{2} \right) \left( \lambda_3 + \frac{3}{2} \right) (\lambda_3 - \lambda_4 + i) - \left( \lambda_3 + \frac{1}{2} \right)^{N-1} \left( \lambda_3 - \lambda_4 - i \right) = 0, \tag{58}
\]

\[
\left( \lambda_4 - \frac{3}{2} \right) \left( \lambda_4 + \frac{3}{2} \right) (\lambda_4 - \lambda_3 + i) - \left( \lambda_4 + \frac{1}{2} \right)^{N-1} \left( \lambda_4 - \frac{3}{2} \right) \left( \lambda_4 - \lambda_3 - i \right) = 0, \tag{59}
\]

where the real part of the first term cancels with the real part of the second term in the left-hand side of both the above equations, while the imaginary part survives. In Figures 6 and 7...
we plot equations (58) and (59), respectively. In figure 8 the equations (57)–(59) have been plotted to see if there are any intersection of the three plots. The two regions inside the solid and dashed circles seem to have intersection points. However, the region inside the solid circle plotted in figure 9 and the region inside the dashed circle plotted figure 10 clearly show that there is no intersection point at all.

6. Conclusions

It is known that the singular solutions of the Bethe ansatz equations produce ill-defined Bethe eigenstates and eigenvalues in the standard approach. Therefore, one needs to properly regularize the solutions. We in this paper are particularly interested in the implications of this regularization on the Bethe eigenstates for the even(odd) length spin chains in some fixed down-spin sectors. Specifically, the analytic forms of the Bethe eigenstates for three down-spin sector of even and odd length spin chains have been obtained and their numerical forms in some fixed length chains are given. For the singular solutions if the rapidities are symmetrically distributed in the complex plane i.e. \( \{ \lambda_1 \} = \{ -\lambda_2 \} \) \( \text{for an even length spin-1/2 XXX chain} \) then the Bethe equations are expressed in a significantly reduced form. These equations can be handled easily in the numerical process. We have analytically shown that in the three down-spin sector of the odd-length chain, there exist singular solutions for any finite length of the spin chain of the form of \( N = 3(2k + 1) \) with \( k = 1, 2, 3, \ldots \). Searching for any possible singular solutions for the four down-spin sector of an odd-length chain is more difficult. However, we have shown with an example of \( N = 15 \) that it can be done easily by simply plotting the Bethe ansatz equations for the singular solutions and looking for any
Figure 7. Plot of equation (59) for $N = 15$.

Figure 8. Plot of equations (57) (blue curves), (58) (red curves) and (59) (green curves) for $N = 15$. 

Figure 9. Plot of the region inside solid circle in figure 8.

Figure 10. Plot of the region inside dashed circle in figure 8.
possible intersections of the three curves. For \( N = 15 \) case we found no singular solutions. Our approach can also be tested for higher values of the length of the spin chain.

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Appendix A. Two down-spin singular state for even \( N \)

Here, up to a proportionality constant, we show equation (34) with the help of equations (7), (31) and (33). Let us start with the definition of the singular Bethe state (31) for two down spins

\[
| \frac{i}{2}, -\frac{i}{2} \rangle = \frac{1}{\epsilon^{\frac{N}{2}}} \text{lim}_{\epsilon \to 0} \left( \frac{\tilde{\lambda}_1}{\tilde{\lambda}_1 - \frac{i}{2}} \right)^{N} B\left( \tilde{\lambda}_1 \right) B\left( \tilde{\lambda}_2 \right) |\Omega\rangle. \tag{A.1}
\]

Substituting explicit expression for the two down spin Bethe eigenstate, obtained from (7), in the above equation, we obtain

\[
| \frac{i}{2}, -\frac{i}{2} \rangle = -\frac{1}{\epsilon^{\frac{N}{2}}} \text{lim}_{\epsilon \to 0} \left( \frac{\tilde{\lambda}_1}{\tilde{\lambda}_1 - \frac{i}{2}} \right)^{N} \times \frac{\tilde{\lambda}_1 - \tilde{\lambda}_2 + i}{\tilde{\lambda}_1 - \tilde{\lambda}_2} \left( \frac{\tilde{\lambda}_1 - \frac{i}{2}}{\tilde{\lambda}_1 + \frac{1}{2}} \right)^{N} \left( \frac{\tilde{\lambda}_2 - \frac{i}{2}}{\tilde{\lambda}_2 + \frac{1}{2}} \right)^{N} \sum_{1 \leq \ell_1 < \ell_2 \leq N} \left( \frac{\tilde{\lambda}_1}{\tilde{\lambda}_1 - \frac{1}{2}} \right)^{N} \left( \frac{\tilde{\lambda}_2}{\tilde{\lambda}_2 - \frac{1}{2}} \right)^{N} \prod_{j=1}^{2} S_{\ell_j}^{-} |\Omega\rangle. \tag{A.2}
\]

Replacing \( \tilde{\lambda}_1, \tilde{\lambda}_2 \) of equation (33) in (A.2) we obtain

\[
| \frac{i}{2}, -\frac{i}{2} \rangle = 2(-1)^{N/2} \text{lim}_{\epsilon \to 0} \sum_{1 \leq \ell_1 < \ell_2 \leq N} \left[ (-1)^{x_2} e^{x_2 - x_1 - 1} (1 + o(\epsilon) + h. o(\epsilon)) + (-1)^{x_1} e^{x_1 - x_2 - 1} (1 + o(\epsilon) + h. o(\epsilon)) \right] \prod_{j=1}^{2} S_{\ell_j}^{-} |\Omega\rangle, \tag{A.3}
\]

where \( o(\epsilon) \) and \( h. o(\epsilon) \) are the order \( \epsilon \) and higher order terms respectively. Taking the \( \epsilon \to 0 \) limit in (A.3) we observe that the first term survives for \( x_2 = x_1 + 1 \) and in second term survives for \( x_1 = 1, x_2 = N \). Finally we obtain
\[ \left| \frac{1}{2}, \frac{-1}{2}, 0 \right\rangle = 2(-1)^{N/2+1} \sum_j (-1)^j S_j^+ S_{j+1}^- |\Omega\rangle. \quad (A.4) \]

**Appendix B. Three down-spin singular state for even \( N \)**

We now prove, up to a proportionality constant, equation (38). Let us start with the definition of the singular Bethe eigenstate (31) for \( N \) even and three down spins

\[ \left| \frac{1}{2}, \frac{-1}{2}, 0 \right\rangle = \lim_{c \to 0} \frac{1}{\left( \hat{\lambda}_1 - \frac{1}{2} \right)^N} B(\hat{\lambda}_1) B(\hat{\lambda}_2) B(0) |\Omega\rangle. \quad (B.1) \]

Substituting explicit form of equation (7) and because the third rapidity of a singular solution for an even length chain vanishes, setting \( \lambda_3 = 0 \) in the above equation we obtain

\[ \left| \frac{1}{2}, \frac{-1}{2}, 0 \right\rangle = i \lim_{c \to 0} \frac{1}{\left( \hat{\lambda}_1 - \frac{1}{2} \right)^N} \frac{\hat{\lambda}_1 - \hat{\lambda}_2 + i \hat{\lambda}_1 + i \hat{\lambda}_2 + i}{\hat{\lambda}_1 - \frac{1}{2}} \]

\[ \times \left( \hat{\lambda}_1 - \frac{1}{2} \right)^N \left( \hat{\lambda}_2 - \frac{1}{2} \right)^N \left( -\frac{1}{2} \right)^N \]

\[ \times \sum_{1 \leq j_1, j_2, j_3 \leq N} \left[ \left( \frac{\hat{\lambda}_1 + \frac{1}{2}}{\hat{\lambda}_1 - \frac{1}{2}} \right)^{j_3} \left( \frac{\hat{\lambda}_2 + \frac{1}{2}}{\hat{\lambda}_2 - \frac{1}{2}} \right)^{j_2} (-1)^{j_1} \right] \]

\[ + \frac{\hat{\lambda}_1 - \hat{\lambda}_2 - i \hat{\lambda}_1 - i}{\hat{\lambda}_1 - \frac{1}{2}} \left( \frac{\hat{\lambda}_2 + i}{\hat{\lambda}_2 - \frac{1}{2}} \right)^{j_3} \left( \frac{\hat{\lambda}_1 + i}{\hat{\lambda}_1 - \frac{1}{2}} \right)^{j_2} (-1)^{j_1} \]

\[ + \frac{\hat{\lambda}_1 - i \hat{\lambda}_2 - i}{\hat{\lambda}_1 + \frac{1}{2}} \left( \frac{\hat{\lambda}_2 - i}{\hat{\lambda}_2 - \frac{1}{2}} \right)^{j_3} \left( \frac{\hat{\lambda}_1 + \frac{1}{2}}{\hat{\lambda}_1 - \frac{1}{2}} \right)^{j_2} \]

\[ \times (-1)^{j_3} \left( \frac{\hat{\lambda}_2 + \frac{1}{2}}{\hat{\lambda}_2 - \frac{1}{2}} \right)^{j_2} \]

\[ + \frac{\hat{\lambda}_1 - \hat{\lambda}_2 - i}{\hat{\lambda}_1 - \frac{1}{2}} \left( \frac{\hat{\lambda}_2 + \frac{1}{2}}{\hat{\lambda}_2 - \frac{1}{2}} \right)^{j_3} \left( \frac{\hat{\lambda}_1 + \frac{1}{2}}{\hat{\lambda}_1 - \frac{1}{2}} \right)^{j_2} (-1)^{j_1} \]

\[ + \frac{\hat{\lambda}_1 - \hat{\lambda}_2 - i \hat{\lambda}_1 - \hat{\lambda}_2 - i}{\hat{\lambda}_1 + \frac{1}{2}} \left( \frac{\hat{\lambda}_1 + \frac{1}{2}}{\hat{\lambda}_1 - \frac{1}{2}} \right)^{j_3} \left( \frac{\hat{\lambda}_2 + \frac{1}{2}}{\hat{\lambda}_2 - \frac{1}{2}} \right)^{j_2} (-1)^{j_1} \]

\[ + \frac{\hat{\lambda}_1 - \hat{\lambda}_2 - i \hat{\lambda}_1 - \hat{\lambda}_2 - i}{\hat{\lambda}_1 + \frac{1}{2}} \left( \frac{\hat{\lambda}_1 + \frac{1}{2}}{\hat{\lambda}_1 - \frac{1}{2}} \right)^{j_3} \left( \frac{\hat{\lambda}_2 + \frac{1}{2}}{\hat{\lambda}_2 - \frac{1}{2}} \right)^{j_2} (-1)^{j_1} \]
Replacing the explicit form (37) in equation (B.2) and expanding in powers \( \epsilon \) we obtain

\[
\left( \frac{1}{2}, -\frac{i}{2}, 0 \right) = 3 \times 2^{2-N} i^{N-1} \lim_{\epsilon \to 0} \sum_{1 \leq s_1 < s_2 < s_3 \leq N} \left( \sqrt[3]{-\frac{1}{3} \epsilon} \right)^{s_2-s_3-1} (-1)^{s_2+s_3} (1 + h. o)
+ \left( \sqrt[3]{-\frac{1}{3} \epsilon} \right)^{s_2-s_1-1} (-1)^{s_2+s_1} (1 + h. o) + \left( \sqrt[3]{-\frac{1}{3} \epsilon} \right)^{s_1-s_2-1} (-1)^{s_1+s_2} (1 + h. o)
\times (-1)^{s_1+s_2} e^{N} (1 + h. o)
+ 3 \left( \sqrt[3]{-\frac{1}{3} \epsilon} \right)^{s_2-s_1-1} (-1)^{s_2+s_1+1} (1 + h. o) + \left( \sqrt[3]{-\frac{1}{3} \epsilon} \right)^{s_1-s_2-1} (-1)^{s_1+s_2} \prod_{j=1}^{3} S^{-}_{s_j} |\Omega\rangle,
\]  

(B.3)

where \( h. o \) represents terms of order \( o(\epsilon) + h. o(\epsilon) \). Taking the \( \epsilon \to 0 \) limit in (B.3) we see that the first term survives for \( s_2 = s_1 + 1 \), the second term survives for \( s_1 = 1, s_3 = N \), the third term survives for \( s_3 = s_2 + 1 \) and the remaining last three terms vanish. We therefore obtain

\[
\left( \frac{i}{2}, -i, 0 \right) = 3 \times 2^{2-N} i^{N+1} \left[ \sum_{1 \leq s_1 < s_2 < s_3 \leq N} (-1)^{s_1+s_3} S^{-}_{s_3} S^{-}_{s_2} S^{-}_{s_1}
+ \sum_{2 \leq s_2 < s_3 \leq N} (-1)^{s_2} S^{-}_{s_2} S^{-}_{s_3} \right] \prod_{j=1}^{3} S^{-}_{s_j} |\Omega\rangle.
\]  

(B.4)

Finally we obtain the simplified form of the singular state for three down spins

\[
\left( \frac{i}{2}, -i, 0 \right) = 3 \times 2^{2-N} i^{N+1} \left( \sum_{k=1}^{N} (-1)^{k} S^{-}_{k} \right) \sum_{j=1}^{N} (-1)^{j} S^{-}_{j} S^{-}_{j+1} |\Omega\rangle.
\]  

(B.5)

**Appendix C. Condition for the three down-spin singular states for odd** \( N \)

In this appendix we prove equation (48) and its corresponding condition equation (49). Let is start with equation (47)
\[ 0 = \left( \lambda_3 - \frac{1}{2} \right)^N \left( \lambda_3 + \frac{1}{2} \right) - \left( \lambda_3 + \frac{1}{2} \right)^N \left( \lambda_3 - \frac{3}{2} \right) \]

\[ = \left( \lambda_3 - \frac{1}{2} \right)^N \left( \lambda_3^2 + 2i\lambda_3 - \frac{3}{4} \right) - \left( \lambda_3 + \frac{1}{2} \right)^N \left( \lambda_3^2 - 2i\lambda_3 - \frac{3}{4} \right) \]

\[ = \left( \lambda_3^2 - \frac{3}{4} \right) \left( \lambda_3 - \frac{1}{2} \right)^N - \left( \lambda_3 + \frac{1}{2} \right)^N \left[ \lambda_3^2 - 2i\lambda_3 + \left( \lambda_3 - \frac{1}{2} \right)^N + \left( \lambda_3 + \frac{1}{2} \right)^N \right]. \quad \text{(C.1)} \]

The first term of equation (C.1) already has the desired factor \( \lambda_3^2 - 3/4 \). To find out the same factor in the second term let us consider

\[ \left( \lambda_3 - \frac{1}{2} \right)^N + \left( \lambda_3 + \frac{1}{2} \right)^N = \sum_{p=0}^{N} C_p \lambda_3^{-2p} \left( \frac{1}{2} \right)^p \left[ (-1)^p + 1 \right] \]

\[ = 2 \sum_{r=0}^{\frac{N-1}{2}} C_{2r} \lambda_3^{-N-2r} \left( \frac{1}{2} \right)^{2r}, \quad p = 2r \]

\[ = 2\lambda_3 \sum_{r=0}^{\frac{N-1}{2}} \frac{1}{4} C_{2r} (-1)^r \lambda_3^{N-1-2r} \]

\[ = 2\lambda_3 \left[ \frac{1}{4} N C_0 \lambda_3^{-N-1} + \frac{1}{4} N C_2 \lambda_3^{-N-3} \right. \]

\[ \left. + \cdots + \frac{1}{4} N C_{N-1} \lambda_3^{-N-1} \right] \]

\[ = 2\lambda_3 \left[ \frac{1}{4} N C_0 \left( -1 \right)^0 \lambda_3^{-N-3} \right. \]

\[ \left. + \frac{1}{4} N C_2 \left( -1 \right)^1 + \frac{3}{4} \frac{1}{4} N C_0 \left( -1 \right)^1 \lambda_3^{-N-5} \right] \lambda_3^2 \left( \lambda_3 - \frac{3}{4} \right) + \cdots \]

\[ \left. + \frac{1}{4} N C_{N-1} \lambda_3^{-N-1} \right] \lambda_3^{N-5} \left( \lambda_3 - \frac{3}{4} \right) \]

\[ = 2\lambda_3 \left( \lambda_3^2 - \frac{3}{4} \right) \sum_{r=0}^{\frac{N-1}{2}} \lambda_3^{-N-2r} \left( \frac{3}{4} \right)^r \sum_{s=0}^{r} \left( \frac{1}{3} \right)^s C_{2s} \right], \quad \text{(C.2)} \]

where \( \binom{N}{k} \) is the binomial coefficient. Substituting the last expression of (C.2) back in equation (C.1) we obtain equation (48). In order to arrive at the last expression of (C.2) we need a matching condition at the end of the series expansion, which is given by

\[ 0 = -3 \sum_{s=0}^{\frac{N-1}{2}} \left( -\frac{1}{3} \right)^s C_{2s} - N \left( -1 \right)^{\frac{N-1}{2}} \]

\[ = -3 \sum_{s=0}^{\frac{N-1}{2}} \left( -\frac{1}{3} \right)^s C_{2s} \quad \text{(C.3)} \]

\[ = -3 \sum_{s=0}^{\frac{N-1}{2}} C_{2s} \left( -\frac{N}{2}, \frac{1-N}{2}, \frac{1}{2}, -\frac{1}{3} \right). \quad \text{(C.4)} \]
\[ = -\frac{2^N}{\sqrt{3}} \cos \left( \frac{\pi}{6} N \right) \]  \hspace{1cm} (C.5)

To arrive at expression (C.4) from (C.3) we have used the relation 15.4.1 of [41]. Note that \( a \) or \( b \) of \( \sum \) \((a, b, c, z)\) has to be negative in order to hold the relation. In our case since \( N \geq 9 \) is odd, \( b = (1 - N)/2 \) is always a negative integer. To obtain (C.5) from (C.4) we have used the relation 15.1.19 of [41]. Equation (C.5) is satisfied when the length, \( N \), of the spin chain is given by equation (49).

**Appendix D. Three down-spin singular states for odd \( N \)**

We now prove, up to a proportionality constant, equation (51). Let us start with the definition of the singular Bethe eigenstate (31) for odd-\( N \) and three down spins

\[
\left( i/2 \right) \left( -i/2 \right) \left( \pm \sqrt{3}/2 \right) = \lim_{\epsilon \to 0} \frac{1}{(\lambda_1 - \frac{1}{2})^N B(\lambda_1)B(\lambda_2)B(\pm \sqrt{3}/2)} N \Omega. \]  \hspace{1cm} (D.1)

Substituting explicit form of equation (7) and setting \( \lambda_3 = \pm \sqrt{3}/2 \) in the above equation we obtain

\[
\times \left( \frac{\pm \sqrt{3}/2 - i/2}{\lambda_1 - \frac{1}{2}} \right)^N \sum_{1 \leq \lambda_1 < \lambda_2 < \lambda_3 \leq N} \left( \frac{\lambda_1 - \frac{1}{2}}{\lambda_1 - \frac{1}{2}} \right)^{\lambda_1} \left( \frac{\lambda_2 - \frac{1}{2}}{\lambda_2 - \frac{1}{2}} \right)^{\lambda_2} \left( \frac{\lambda_3 - \frac{1}{2} + i}{\lambda_3 - \frac{1}{2}} \right)^{\lambda_3} \]  \hspace{1cm} (D.1)

\[
\times \left( \exp \left( \pm \frac{\pi i}{3} \right) \right)^{\lambda_1} \left( \frac{\lambda_1 + \frac{i}{2}}{\lambda_1 - \frac{1}{2}} \right)^{\lambda_1} \left( \frac{\lambda_2 - \frac{1}{2} + i}{\lambda_2 - \frac{1}{2}} \right)^{\lambda_2} \left( \frac{\lambda_3 - \frac{1}{2} + i}{\lambda_3 - \frac{1}{2}} \right)^{\lambda_3} + \text{other terms} \]
Replacing the explicit form (50) in equation (D.2) and expanding in powers of $\epsilon$ we obtain

$$\lim_{\epsilon \to 0} \frac{1}{2} \left[ \prod_{j=1}^{N} S_{j} \right] \epsilon^{N}$$

where $h, o$ represents terms of order $o(\epsilon) + h, o(\epsilon)$. Taking the $\epsilon \to 0$ limit in (D.3) we see that the first term survives for $x_{2} = x_{1} + 1$, the second term survives for $x_{1} = 1, x_{3} = N$, the third term survives for $x_{3} = x_{2} + 1$ and the remaining last three terms vanish. We therefore obtain
\[ \left( \frac{i}{2}, \frac{-i}{2}, \frac{\sqrt{3}}{2} \right) = \mp 2\sqrt{3} (-1)^{\ell_{k+1}} \exp \left( \mp \frac{\pi}{6} (N + 1) \right) \sum_{1 \leq k_1 < k_2 < k_3 < N} (-1)^{\ell_{k_1}} \]
\[ \times \left( \exp \left( \pm \frac{\pi}{3} i \right) \right)^{\ell_{k_1}} S_{k_1}^- S_{k_2}^- S_{k_3}^- \]
\[ + \sum_{2 \leq k_2 \leq N-1} \left( \exp \left( \pm \frac{\pi}{3} i \right) \right)^{\ell_{k_2}} S_{k_1}^- S_{k_2}^- S_{k_N}^- + \sum_{1 \leq k_1 < k_2 + 1 \leq N} (-1)^{\ell_{k_2}+1} \]
\[ \times \left( \exp \left( \pm \frac{\pi}{3} i \right) \right)^{\ell_{k_2}} S_{k_1}^- S_{k_2}^- S_{k_2+1}^- \right) \Omega. \] (D.4)

Finally we obtain the simplified form of (D.4) for the singular states of three down spins
\[ \left( \frac{i}{2}, \frac{-i}{2}, \frac{\pm \sqrt{3}}{2} \right) = \mp 2\sqrt{3} (-1)^{\ell_{k+1}} \exp \left( \mp \frac{\pi}{6} (N + 1) \right) \sum_{k=1}^{N} \]
\[ \times \left( \exp \left( \pm \frac{\pi}{3} k i \right) S_{k}^- \sum_{j=1}^{N} (-1)^{j+H(j-k)} S_{j}^- S_{j+1}^- \right) \right) \Omega. \] (D.5)

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