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Deformed strings in the Heisenberg model

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Abstract

We investigate solutions to the Bethe equations for the isotropic $S = 1/2$ Heisenberg chain involving complex, string-like rapidity configurations of arbitrary length. Going beyond the traditional string hypothesis of undeformed strings, we describe a general procedure to construct eigenstates including strings with generic deformations, discuss general features of these solutions and provide a number of explicit examples including complete solutions for all wavefunctions of short chains. We finally investigate some singular cases and show from simple symmetry arguments that their contribution to zero-temperature correlation functions vanishes.

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1. Introduction

The problem of diagonalizing the Hamiltonian of a generic quantum system is too difficult to be carried out completely except in rather exceptional circumstances. For noninteracting models, this is easily done since multiparticle states are obtained from products of single particle ones. However, in the presence of interactions, finding the exact eigenstates and energy eigenvalues becomes a problem of dimensionality equal to that of the Hilbert space. A set of theories which stand out as an exception to this are so-called integrable models, the most fundamental of which is the Heisenberg spin-1/2 chain [1],

$$H = J \sum_{j=1}^{N} \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \left(S_j^z S_{j+1}^z - 1/4 \right) \right) - h \sum_{j=1}^{N} S_j^z, \tag{1}$$

where J is the magnetic exchange coupling constant and h is the external field. Throughout this paper, we will give results for the antiferromagnetic case $J = 1$ (the eigenstates are the same for $J < 0$, only their energies are reversed). Since the z-component of the total spin commutes with H, it is a good quantum number. Starting from a reference state with all spins pointing up,

$$|0\rangle = \otimes_{j=1}^{N} |\uparrow\rangle_j, \tag{2}$$

we can divide the Hilbert space into subsectors of fixed magnetization $\sigma = \frac{1}{N}\sum_j S_j^z$ spanned by the $\dim(N, M) = \binom{N}{M}$ basis states with $M = N(1/2 - \sigma)$ overturned spins at lattice positions $j_1, \ldots, j_M$,

$$|j_1, \ldots, j_M\rangle = S_{j_1}^- \cdots S_{j_M}^- |0\rangle. \tag{3}$$

The Schrödinger equation is solved by the Bethe Ansatz [2],

$$|\chi_M\rangle = \sum_{\{j\}} \chi_M(j_1, \ldots, j_M) |j_1, \ldots, j_M\rangle, \tag{4}$$

$$\chi_M(j_1, \ldots, j_M) = \prod_{M \geqslant a > b \geqslant 1} \mathrm{sgn}(j_a - j_b) \times \sum_P (-1)^{[P]} \mathrm{e}^{\mathrm{i}\sum_{a=1}^{M} k(\lambda_{P_a}) j_a + \frac{\mathrm{i}}{2}\sum_{M \geqslant a > b \geqslant 1} \mathrm{sgn}(j_a - j_b)\phi(\lambda_{P_a} - \lambda_{P_b})}, \tag{5}$$

with $\phi(\lambda) = 2\arctan\lambda$ and $k(\lambda) = \pi - 2\arctan 2\lambda$. The energy of an eigenstate is $E = E_0 - hN\sigma$, with $E_0 = \sum_j \frac{-2J}{1+4\lambda_j^2}$. The set of M rapidities λ are constrained by quantizing H through the imposition of periodic boundary conditions, yielding the Bethe equations

$$\left[\frac{\lambda_\alpha - \mathrm{i}/2}{\lambda_\alpha + \mathrm{i}/2}\right]^N = \prod_{\beta}^{\beta \neq \alpha} \frac{\lambda_\alpha - \lambda_\beta - \mathrm{i}}{\lambda_\alpha - \lambda_\beta + \mathrm{i}}, \qquad \alpha = 1, \ldots, M. \tag{6}$$

The correspondence between the number of distinct solutions to (6) for given M and the dimensionality of the sub-Hilbert space is known as the completeness problem, and is a highly nontrivial fact to verify. To classify the eigenstates, the standard strategy is to consider the logarithm of (6),

$$2\arctan 2\lambda_\alpha = 2\pi \frac{J_\alpha}{N} + \frac{1}{N} \sum_{\beta}^{\beta \neq \alpha} 2\arctan(\lambda_\alpha - \lambda_\beta) \qquad \mathrm{mod}\ 2\pi, \tag{7}$$

introducing a set of quantum numbers J (defined modulo N) which label the eigenstates (J are half-odd integers for $N - M$ even, and integers for $N - M$ odd). Since the Bethe wavefunctions formally vanish when two rapidities become equal, we could think that simply choosing M distinct quantum numbers among the set of N allowed possibilities, which we can clearly do in $\dim(N, M)$ ways, would allow us to reconstruct all the eigenstates in the subspace. This, as was known to Bethe himself, is too naive and simply fails[1]. The problem is that only some of the solutions to (7) are in terms of real rapidities; there also exist, as Bethe himself found, solutions involving groups of complex rapidities representing bound states of magnons. This led Bethe to investigate this problem rather extensively in his original paper, by attempting to explicitly construct all solutions. He realized that complex rapidities typically arrange themselves into regular patterns known as *strings*. More importantly, he also realized

[1] Interestingly, Bloch [41] studied the problem before Bethe but concluded that the wavefunction form now known as the Bethe Ansatz yielded *too many* solutions to the eigenvalue equation for $M = 2$. This illustrates the crucial importance of counting states: had Bloch done it correctly, we might not be speaking of Bethe's Ansatz.

that there exist states in which these strings get deformed back into extra real solutions with coinciding quantum numbers J for which the wavefunction is nonvanishing, meaning that the 'Pauli principle' of allowing only single occupancy of the J quantum numbers fails, and that counting states using these is invalid [2–4]. Bethe proposed a scenario wherein all eigenstates could be obtained from real solutions complemented by (deformed, possibly all the way back onto the real axis) string states, and showed that the counting of these solutions gives the correct number of eigenstates.

In the early 1970s, interest in general solutions to the Bethe equations was revived by Takahashi's fundamental work on the thermodynamics of the isotropic Heisenberg chain [5], making extensive use of the so-called string hypothesis in which only undeformed strings are assumed to be present. Gaudin [6] further considered the gapped anisotropic chain, while Takahashi extended his study to the gapless anisotropic chain [7]. While these papers used the simplest form of the string hypothesis, in which undeformed strings of arbitrary length were present, Takahashi's original treatment of the gapless case was shown by Johnson *et al* [8] to yield an incorrect high-temperature expansion. The reason for this discrepancy was that the states of a gapless anisotropic chain can only have strings of certain allowed lengths, and upon restricting the original equations to this set, Takahashi and Suzuki obtained the correct thermodynamics [9, 10]. As far as thermodynamics are concerned, the string hypothesis as expounded in the above papers is understood to give correct results as long as either the temperature or the magnetic field are not strictly vanishing [11]. Getting the thermodynamics right, however, in no way addresses the 'completeness' problem of the Bethe Ansatz. In fact, the successes of the thermodynamic Bethe Ansatz using the string hypothesis cast a long enduring shadow on the general awareness of Bethe's own understanding of the existence and characteristics of deformed string solutions, which were 'rediscovered' only decades later. There now exists a large literature on this subject for the particular case of the Heisenberg chains [3, 12–33].

The purpose of the present paper is to delve more deeply into the nature of Bethe eigenstates which deviate significantly from the traditional string hypothesis. As a starting point, we consider only the case of the isotropic antiferromagnet, but our main objective is to go beyond the usual case of only two downturned spins typically considered in the existing literature. The motivation for such a study comes in large part from recent work on dynamical correlation functions for large but finite chains [34, 35], to which such states can in principle contribute, and for which the string hypothesis is a good starting point but whose accuracy has to be confirmed state-by-state. Another important reason concerns the precise form of the finite-N corrections to various physical quantities within thermodynamic Bethe Ansatz: an accurate treatment of string deviations beyond the string hypothesis has to be performed to make hard, reliable statements on these. More formally, it is our opinion that the completeness problem is not properly addressed by arguments based exclusively on the string hypothesis: we believe that a true 'exact solution' of the Heisenberg chains requires providing an explicit scheme to recover *all* the eigenstates from solutions to the Bethe equations, and that proofs of completeness have to go hand in hand with a precise knowledge of what is being counted. Our objective is to make a step in this direction by proposing a scheme for states with deformed higher string-like complex rapidities.

The paper is organized as follows. In section 2, we set our notations and discuss basic aspects of complex solutions to the Bethe equations. In section 3, we derive the sets of equations for string deviations which are then used in section 4 to obtain and discuss explicit solutions in various cases and limits. Section 5 focuses on special degenerate cases and their form factors. Finally, after the conclusion, we give complete solutions to the Bethe equations for small chains in the appendix.

2. Strings in the Bethe equations

2.1. Pairs

It is easily seen that, if the set $\{\lambda\}$ is a solution to the Bethe equations, so is $\{\lambda^*\}$. A stronger statement was proven by Vladimirov [36], namely, that all solutions of the Bethe equations are self-conjugate, i.e. $\{\lambda\} = \{\lambda^*\}$. As a consequence, complex roots of the Bethe equations always come in pairs of conjugate roots, $\{\lambda_+, \lambda_-\}$ where $\mathrm{Im}\,\lambda_+ > 0$ and $\lambda_- := \lambda_+^*$.

Let us assume that the real parts of the various roots do not coincide, so $\mathrm{Re}\,\lambda_j \neq \mathrm{Re}\,\lambda_k$ if $j \neq k$, and that the pair is not centered on the origin. If the set $\{\lambda\}$ is symmetric, cases are possible where one or more pairs are in fact centered on the origin. Such cases are treated separately in section 5.

For the quantum numbers $\{J_+, J_-\}$ associated with the two conjugate roots, subtracting the Bethe equation associated with λ_- from that of λ_+ gives

$$2\pi\frac{J_+ - J_-}{N} = 2\arctan 2\lambda - 2\arctan 2\lambda^* - \frac{2}{N}[\arctan(\lambda - \lambda^*) - \arctan(\lambda^* - \lambda)]$$
$$- \frac{2}{N}\sum_k^{\lambda_k \neq \lambda_\pm} [\arctan(\lambda - \lambda_k) - \arctan(\lambda^* - \lambda_k)] \pmod{2\pi}. \qquad (8)$$

We choose the branch cut of the logarithm such that $-\pi < \mathrm{Im}\ln z \leqslant \pi$. Then the branch cuts of the inverse tangent are such that

$$\arctan z^* = \begin{cases} (\arctan z)^* + \pi & \text{if } z \in\,]-\mathrm{i}, -\mathrm{i}\infty[\\ (\arctan z)^* - \pi & \text{if } z \in\,]\mathrm{i}, \mathrm{i}\infty[\\ (\arctan z)^* & \text{elsewhere.} \end{cases} \qquad (9)$$

Taking the real part of the difference equation, taking into account the above branch cut and the fact that $\mathrm{Re}(\arctan\lambda - \arctan\lambda^*) = 0$ if $\mathrm{Re}\,\lambda \neq 0$, and that we work modulo π, the real part of the equation becomes

$$J_- - J_+ = \begin{cases} 1 & \text{if } \mathrm{Im}\,\lambda_+ > \frac{1}{2}, \\ 0 & \text{if } \mathrm{Im}\,\lambda_+ < \frac{1}{2}. \end{cases} \qquad (10)$$

In other words, there are two kinds of pairs: *narrow pairs* (also called *close pairs*), which are separated in the imaginary direction by less than i, and whose quantum numbers are equal; and *wide pairs*, which are separated by more than i and whose quantum numbers differ by one, where the higher quantum number is associated with the root in the negative half-plane. This distinction is found in, e.g. Destri and Löwenstein [15] and Babelon *et al* [16]. If $\mathrm{Im}\,\lambda_+ = \frac{1}{2}$, the Bethe equations become singular; we will study this important limit in more detail in the following sections.

The fact that solutions exist with repeated quantum numbers makes the counting of allowed states very complicated. This problem is addressed by the *string hypothesis* which, among other things, introduces a new type of quantum number meant to be strictly non-repeating.

2.2. The string hypothesis

If a root λ is complex with positive imaginary part and finite real part, the factor on the left-hand side of the Bethe equation (6) has a norm less than unity. This implies that for large N, the left-hand side will vanish exponentially. Therefore, the right-hand side must vanish exponentially as well. Likewise, if the imaginary part is negative, both sides must diverge. The only way for a factor on the right-hand side to vanish for fixed M as $N \to \infty$ is if there exists a root at a distance close to i below the root under consideration, where the difference is close to i. Since this is true for every complex root we choose on the left-hand side, all non-real roots should be arranged in strings of various length, in which the roots that make up the string are spaced by distances close to i. This is a loose statement of what is known as the *string hypothesis*.

The M roots of the Bethe equations are thus partitioned in a configuration of strings, where a j-string is a group of j roots such that

$$\lambda^j_{\alpha a} = \lambda^j_\alpha + \frac{\mathrm{i}}{2}(j+1-2a) + d^j_{\alpha a}, \qquad \text{with} \qquad a \in \{1, \ldots, j\}. \tag{11}$$

Here, j is the string length, λ^j_α is the string center and $d^j_{\alpha a} \equiv \epsilon^j_{\alpha a} + \mathrm{i}\delta^j_{\alpha a}$ is the deviation, with $\epsilon^j_{\alpha a}, \delta^j_{\alpha a} \in \mathbb{R}$. Furthermore, self-conjugacy dictates $d^j_{\alpha,a} = \left[d^j_{\alpha,j+1-a}\right]^*$. Note that every self-conjugate configuration of roots can be given in terms of a set of strings as above albeit with arbitrarily large deviations. The string hypothesis assumes that all deviations vanish in the thermodynamic limit.

Using the parametrization (11), let us now make our reasoning more precise. Consider the Bethe equations (6) for a root $\lambda^j_{\alpha a}$. Let A^j_α be the part of the product on the right-hand side pertaining to roots on other strings. We assume that A^j_α is of order unity. Furthermore, the quotient on the left-hand side is denoted $z^j_{\alpha a} \in \mathbb{C}$. We consider a root with positive imaginary part, so that $\left|z^j_{\alpha a}\right| < 1$. The Bethe equation can be written as

$$\left[z^j_{\alpha a}\right]^N = A^j_\alpha \prod_{b \neq a} \frac{d^j_{\alpha a} - d^j_{\alpha b} + \mathrm{i}(b-a-1)}{d^j_{\alpha a} - d^j_{\alpha b} + \mathrm{i}(b-a+1)}. \tag{12}$$

Our parametrization is such that $\mathrm{Im}\,\lambda^j_{\alpha a} > \mathrm{Im}\,\lambda^j_{\alpha a+1}$. Then, the positive-imaginary roots have $1 \leqslant a \leqslant \lfloor j/2 \rfloor$.

Let us start at $a = 1$. Since this is the top root,

$$\left[z^j_{\alpha a}\right]^N = A^j_\alpha \frac{d^j_{\alpha 1} - d^j_{\alpha 2}}{d^j_{\alpha 1} - d^j_{\alpha 2} + 2\mathrm{i}} \frac{d^j_{\alpha 1} - d^j_{\alpha 3} + \mathrm{i}}{d^j_{\alpha 1} - d^j_{\alpha 3} + 3\mathrm{i}} \cdots. \tag{13}$$

We now assume that the differences of δs are small enough for all but the first of the quotients on the right-hand side to be of order unity. Thus, we have

$$\left|d^j_{\alpha 1} - d^j_{\alpha 2}\right| \propto \left|z^j_{\alpha 1}\right|^N, \tag{14}$$

i.e., the difference must vanish exponentially with N.

Now consider the next root, $a = 2$. This time,

$$\left[z^j_{\alpha a}\right]^N = A^j_\alpha \frac{d^j_{\alpha 2} - d^j_{\alpha 1} - 2\mathrm{i}}{d^j_{\alpha 2} - d^j_{\alpha 1}} \frac{d^j_{\alpha 2} - d^j_{\alpha 3}}{d^j_{\alpha 2} - d^j_{\alpha 3} + 2\mathrm{i}} \frac{d^j_{\alpha 2} - d^j_{\alpha 4} + \mathrm{i}}{d^j_{\alpha 2} - d^j_{\alpha 4} + 3\mathrm{i}} \cdots, \tag{15}$$

and therefore we conclude

$$\left|\frac{d^j_{\alpha 2} - d^j_{\alpha 3}}{d^j_{\alpha 2} - d^j_{\alpha 1}}\right| \propto \left|z^j_{\alpha 2}\right|^N. \tag{16}$$

Multiplying by equation (14) gives

$$\left|d^j_{\alpha 2} - d^j_{\alpha 3}\right| \propto \left|z^j_{\alpha 2} z^j_{\alpha 1}\right|^N. \tag{17}$$

Continuing this reasoning until $a = \lfloor j/2 \rfloor$, we conclude that all differences of deviations vanish exponentially with N, while $\left|d^j_{\alpha,a} - d^j_{\alpha,a+1}\right| \gg \left|d^j_{\alpha,a+1} - d^j_{\alpha,a+2}\right|$. Furthermore, we know that for j even, $d^j_{\alpha,j/2} = -d^j_{\alpha,j/2+1}$ and $\mathrm{Re}\,d^j_{\alpha,j/2} = 0$; while for j odd, $d^j_{\alpha,\lfloor j/2 \rfloor} = 0$. Thus we conclude that all $d^j_{\alpha a}$ vanish exponentially with N, and their successive difference ratios as well, such that $\left|d^j_{\alpha,a}\right| \gg \left|d^j_{\alpha,a+1}\right|$. Note that during this derivation we have made a number of important assumptions, mainly that the factor A^j_α is of order unity and that the differences of consecutive δs are small. These assumptions do not necessarily hold at the same time: for instance, if many roots lie close to each other the derivation does not hold. In such cases, deviations may vanish more slowly. A more precise formulation of the string hypothesis is thus, that the deviations from string configurations as defined in (11), vanish exponentially with N if N is made large while all other parameters are kept constant.

Rewriting the Bethe equations under the assumption that the deviations vanish leads to the Bethe–Takahashi equations [5]

$$2\arctan\frac{2\lambda^j_\alpha}{j} = 2\pi\frac{I^j_\alpha}{N} + \frac{1}{N}\sum_{k=1}^{N_s}\sum_{\beta=1}^{M_k}\Theta_{jk}\left(\lambda^j_\alpha - \lambda^k_\beta\right) \qquad (\mathrm{mod}\ 2\pi), \tag{18}$$

with

$$\Theta_{jk}(\lambda) := 2(1-\delta_{jk})\arctan\frac{2\lambda}{|j-k|} + 4\arctan\frac{2\lambda}{|j-k|+2} + \cdots + 4\arctan\frac{2\lambda}{j+k-2} + 2\arctan\frac{2\lambda}{j+k}, \tag{19}$$

where the M roots are partitioned into M_j strings of length j such that $\sum_j jM_j = M$. All positive integers j are in principle allowed. For N even, I^j_α are half-odd integers for M_j even, and integers for M_j odd. The string hypothesis assumes that these equations have $\dim(N, M)$ distinct solutions in terms of the sets of real rapidities (allowing infinite ones).

2.3. Completeness

The Heisenberg Hamiltonian commutes with the total spin operator $S^2_{\mathrm{tot}} := \left(S^x_{\mathrm{tot}}\right)^2 + \left(S^y_{\mathrm{tot}}\right)^2 + \left(S^z_{\mathrm{tot}}\right)^2$ as well as with the total spin-z operator $S^z_{\mathrm{tot}} := \sum_{j=1}^N S^z_j$. States with $s = N/2 - M$, where s is the total-spin quantum number such that the eigenvalue of S^2_{tot} is $s(s+1)$, and $N/2-M$ is the S^z_{tot} eigenvalue, are highest-weight states. From these states, we can generate lower-weight states by repeatedly applying the total-spin lowering operator S^-_0. This corresponds to adding a particle with momentum $k = 0$ and therefore rapidity $\lambda = \infty$. In particular, looking at a fixed-M subspace with $M \leqslant N/2$, all solutions in the $M-1$ subspace are repeated with an extra infinite rapidity added. This means that in every M subspace we only have to solve for the $\binom{N}{M} - \binom{N}{M-1}$ solutions of highest weight.

It has been proposed [2, 5, 13, 37] that in the Heisenberg model, the Bethe–Takahashi quantum numbers of highest-weight states should be non-coinciding and bounded by

$$\left|I^j_\alpha\right| < I^j_\infty := \frac{1}{2}\left[N + 1 - \sum_{k\geqslant 1} M_k(2\min(n_j, n_k) - \delta_{j,k})\right]. \tag{20}$$

One can prove [2, 38] that the number of sets of quantum numbers that satisfy this constraint is $\binom{N}{M} - \binom{N}{M-1}$, exactly the number of highest-weight solutions with M down spins. Therefore, provided that for each of these quantum number choices a solution exists, is unique, and leads to an admissible solution of the Schrödinger equation, the Bethe Ansatz is complete.

In the analytically solvable case $M = 2$, it is known that indeed, for each of these quantum numbers a unique, admissible solution exists. However, some of the quantum numbers associated with two-strings do not lead to complex-pair solutions, as narrow pairs get narrower and eventually merge and split back onto the horizontal axis. Instead, in these cases, there are extra solutions with real roots. These extra real solutions can be connected one-to-one with the missing string solutions by way of the Bethe quantum numbers.

3. String deviations

In this section, we will derive equations for the exact string deviations. Determining these deviations is therefore completely equivalent to determining the exact roots of the Bethe equations in the complex plane. We will first establish the method by considering two- and three-strings, and then generalize to arbitrary string lengths.

3.1. Deviated two-strings

The Bethe–Takahashi equations (18) are found from the sum of the logarithmic Bethe equations, absorbing all contributions from branch cut crossings in the Bethe–Takahashi quantum numbers. To find the relation of these with the Bethe quantum numbers, let us carefully redo the derivation. We concentrate on the isotropic chain. Similar but more complicated derivations can be given for the anisotropic chain.

We use the relation

$$\arctan(a+\mathrm{i}b)+\arctan(a-\mathrm{i}b)=\xi(a,1+b)+\xi(a,1-b), \qquad \text{for } a,b\in\mathbb{R}, \tag{21}$$

where we defined

$$\xi(\epsilon,\delta):=\frac{1}{2\mathrm{i}}\left[\ln(\delta+\mathrm{i}\epsilon)-\ln(\delta-\mathrm{i}\epsilon)\right]=\arctan\frac{\epsilon}{\delta}+\pi\Theta(-\delta)\operatorname{sign}\epsilon. \tag{22}$$

We use $\operatorname{sign}0 = 0$ and Θ is the Heaviside step function with $\Theta(0) = \frac{1}{2}$. Note that $\xi(\epsilon,\delta) = \operatorname{Arg}(\delta+\mathrm{i}\epsilon)$ for $\epsilon \neq 0$, and $\xi(0,\delta) = 0$. A useful feature of $\xi(\epsilon,\delta)$ is that it is continuous on the line $\delta = 0$. Therefore, the value for zero deviations is well-defined, $\xi(\epsilon,0) = \frac{\pi}{2}\operatorname{sign}\epsilon$, and we need not keep track of the sign of δ in the limit.

Deviated two-strings are parametrized as $\lambda^{(2)}_{\alpha\pm} := \lambda^{(2)}_{\alpha} \pm \mathrm{i}\big(1+2\delta^{(2)}_{\alpha}\big)/2$, where $\lambda^{(2)}_{\alpha}$ and $\delta^{(2)}_{\alpha}$ are real numbers. The sum of the (log-) Bethe equations for $\lambda^{(2)}_{\alpha\pm}$ equals

$$\begin{aligned}\xi(\lambda,1+\delta)+\xi(\lambda,-\delta)=\pi\frac{J_++J_-}{N}&+\frac{1}{N}\sum_{\beta}^{k=1}\left[\xi\left(\lambda-\lambda^k_\beta,\delta+\frac{3}{2}\right)+\xi\left(\lambda-\lambda^k_\beta,-\delta+\frac{1}{2}\right)\right]\\&+\frac{1}{N}\sum_{\beta}^{k=2}\big[\xi\big(\lambda-\lambda^k_\beta,\delta+\delta^k_\beta+2\big)+\xi\big(\lambda-\lambda^k_\beta,-\delta-\delta^k_\beta\big)\\&+\xi\big(\lambda-\lambda^k_\beta,\delta-\delta^k_\beta+1\big)+\xi\big(\lambda-\lambda^k_\beta,-\delta+\delta^k_\beta+1\big)\big]\pmod{\pi},\end{aligned} \tag{23}$$

where, for legibility, we dropped the indices ${}^{(2)}_{\alpha}$. To compare with the Bethe–Takahashi equations, let us take all $\delta\to 0$,

$$\begin{aligned}\arctan\lambda+\frac{\pi}{2}=\pi\frac{J_++J_-}{N}&+\frac{1}{N}\sum_{\beta}^{k=1}\left[\arctan\frac{2}{3}\big(\lambda-\lambda^k_\beta\big)+\arctan 2\big(\lambda-\lambda^k_\beta\big)\right]\\&+\frac{1}{N}\sum_{\beta}^{k=2}\left[\arctan\frac{1}{2}\big(\lambda-\lambda^k_\beta\big)+\frac{\pi}{2}\operatorname{sign}\big(\lambda-\lambda^k_\beta\big)+2\arctan\big(\lambda-\lambda^k_\beta\big)\right]\pmod{\pi}.\end{aligned} \tag{24}$$

Comparing to the Bethe–Takahashi equations, we conclude for the relation between the quantum numbers

$$I^{(2)} - \frac{1}{2}\sum_{\beta}^{k=2} \mathrm{sign}\big(\lambda^{(2)} - \lambda_{\beta}^{(2)}\big) = \Theta(\delta) + 2J_{+} - \frac{N}{2} \pmod{N} \tag{25}$$

taking this equation modulo 2, we see that the criterion for a two-string with quantum number $I^{(2)}$ to be wide is

$$\Theta(\delta) = I^{(2)} + \frac{N}{2} - M + 1 - \frac{1}{2}\sum_{\beta}^{k=2} \mathrm{sign}\big(\lambda^{(2)} - \lambda_{\beta}^{(2)}\big) \pmod{2}. \tag{26}$$

The sum of the Bethe equations gives the equation for the string centers; therefore, we must look at the difference of the Bethe equations to find the deviations. The imaginary part of this equation can be written as

$$\left[\frac{1+\delta}{\delta}\right]^2 = \left[\frac{(1+\delta)^2+\lambda^2}{\delta^2+\lambda^2}\right]^N \prod_{\beta}^{k=1} \frac{(\delta-1/2)^2+\big(\lambda-\lambda_{\beta}^{k}\big)^2}{(\delta+3/2)^2+\big(\lambda-\lambda_{\beta}^{k}\big)^2}$$
$$\times \prod_{\beta}^{k=2} \frac{\big(\delta+\delta_{\beta}^{k}\big)^2+\big(\lambda-\lambda_{\beta}^{k}\big)^2}{\big(2+\delta+\delta_{\beta}^{k}\big)^2+\big(\lambda-\lambda_{\beta}^{k}\big)^2} \frac{\big(1-\delta+\delta_{\beta}^{k}\big)^2+\big(\lambda-\lambda_{\beta}^{k}\big)^2}{\big(1+\delta-\delta_{\beta}^{k}\big)^2+\big(\lambda-\lambda_{\beta}^{k}\big)^2}. \tag{27}$$

Together, equations (23), (27) and (26) determine the rapidity $\lambda_{\alpha}^{(2)}$ and deviation $\delta_{\alpha}^{(2)}$. It is of importance to note that the right-hand side of this equation is not strongly dependent on $\delta_{\alpha}^{(2)}$, as long as $\delta_{\alpha}^{(2)}$ is small compared to $\lambda_{\alpha}^{(2)}$, so that an iterative approach to solving these coupled equations can converge rapidly.

3.2. *Deviated three-strings*

Let us consider the equations for the deviation of a three-string in the presence of other strings of length not more than 2, which is enough to illustrate the general idea. In the presence of longer strings, terms will have to be added to these expressions but as these become quite unwieldy we defer this derivation to the treatment of the general case in the following section.

Parametrizing the three-string as

$$\lambda_{\alpha\pm}^{(3)} = \lambda_{\alpha}^{(3)} + \epsilon_{\alpha}^{(3)} \pm \mathrm{i}\big(1+\delta_{\alpha}^{(3)}\big), \qquad \lambda_{\alpha 0}^{(3)} = \lambda_{\alpha}^{(3)}, \tag{28}$$

we consider the sum over all three Bethe equations, writing $\lambda_{\alpha}^{(3)} = \lambda$

$$\arctan 2\lambda + \xi(2\lambda+2\epsilon, 3+2\delta) + \xi(2\lambda+2\epsilon, -1-2\delta) = \frac{\pi}{N}(J_{-}+J_{0}+J_{+}) \pmod{\pi}$$
$$+\frac{1}{N}\sum_{\beta}^{k=1}\left[\arctan\big(\lambda-\lambda_{\beta}^{k}\big) + \xi\big(\lambda+\epsilon-\lambda_{\beta}^{k}, 2+\delta\big) + \xi\big(\lambda+\epsilon-\lambda_{\beta}^{k}, -\delta\big)\right]$$
$$+\frac{1}{N}\sum_{\beta}^{k=2}\left[\xi\left(\lambda-\lambda_{\beta}^{k}, \frac{3}{2}+\delta_{\beta}^{k}\right) + \xi\left(\lambda-\lambda_{\beta}^{k}, \frac{1}{2}-\delta_{\beta}^{k}\right)\right.$$
$$+\xi\left(\lambda+\epsilon-\lambda_{\beta}^{k}, \frac{5}{2}+\delta+\delta_{\beta}^{k}\right) + \xi\left(\lambda+\epsilon-\lambda_{\beta}^{k}, -\frac{1}{2}-\delta-\delta_{\beta}^{k}\right)$$
$$\left.+\xi\left(\lambda+\epsilon-\lambda_{\beta}^{k}, \frac{3}{2}+\delta-\delta_{\beta}^{k}\right) + \xi\left(\lambda+\epsilon-\lambda_{\beta}^{k}, \frac{1}{2}-\delta+\delta_{\beta}^{k}\right)\right]. \tag{29}$$

Taking its limit for $\delta \to 0, \epsilon \to 0$,

$$\arctan\frac{2\lambda}{3} = \frac{\pi}{N}(J_- + J_0 + J_+) + \frac{1}{N}\sum_{\beta}^{k=1}\left[\arctan\left(\lambda - \lambda_\beta^k\right) + \arctan\frac{1}{2}\left(\lambda - \lambda_\beta^k\right) + \frac{\pi}{2}\mathrm{sign}\left(\lambda - \lambda_\beta^k\right)\right] \pmod{\pi} + \frac{1}{N}\sum_{\beta}^{k=2}\left[2\arctan\frac{2}{3}\left(\lambda - \lambda_\beta^k\right) + \arctan 2\left(\lambda - \lambda_\beta^k\right) + \arctan\frac{2}{5}\left(\lambda - \lambda_\beta^k\right) + \pi\,\mathrm{sign}\left(\lambda - \lambda_\beta^k\right)\right]. \tag{30}$$

Comparing to the Bethe–Takahashi equations, we find

$$J_- + J_0 + J_+ = I_\alpha^{(3)} - \frac{1}{2}\sum_{\beta}^{k=1}\mathrm{sign}\left(\lambda - \lambda_\beta^k\right) - \sum_{\beta}^{k=2}\mathrm{sign}\left(\lambda - \lambda_\beta^k\right) \pmod{N}. \tag{31}$$

The real part of the difference between the '+' and '−' logarithmic Bethe equations yields $J_+ - J_- = -1$. This leaves J_0 as of yet undetermined, but it turns out to be unnecessary to know this quantum number to be able to solve the equations.

The imaginary part of the difference between the '+' and '−' equations gives, when exponentiated,

$$\delta^2 + \epsilon^2 = r^2 := [(2+\delta)^2 + \epsilon^2]\left[\frac{3+2\delta}{1+2\delta}\right]^2\left[\frac{(1+2\delta)^2 + 4(\lambda+\epsilon)^2}{(3+2\delta)^2 + 4(\lambda+\epsilon)^2}\right]^N \times\prod_{\beta}^{k=1}\frac{(2+\delta)^2 + \left(\lambda+\epsilon-\lambda_\beta^k\right)^2}{\delta^2 + \left(\lambda+\epsilon-\lambda_\beta^k\right)^2} \times\prod_{\beta}^{k=2}\frac{\left(\frac{5}{2}+\delta+\delta_\beta^k\right)^2 + \left(\lambda+\epsilon-\lambda_\beta^k\right)^2}{\left(\frac{1}{2}+\delta+\delta_\beta^k\right)^2 + \left(\lambda+\epsilon-\lambda_\beta^k\right)^2}\,\frac{\left(\frac{3}{2}+\delta-\delta_\beta^k\right)^2 + \left(\lambda+\epsilon-\lambda_\beta^k\right)^2}{\left(\frac{1}{2}-\delta+\delta_\beta^k\right)^2 + \left(\lambda+\epsilon-\lambda_\beta^k\right)^2}. \tag{32}$$

The other independent equation is the Bethe equation for λ^0. However, for later generalization, it is more convenient to consider the sum of the '+' and '−' equations,

$$\xi(\epsilon, -\delta) = \theta := -\xi(\epsilon, 2+\delta) - \pi(J_+ + J_-) + N\left[\xi(2(\lambda+\epsilon), 3+2\delta) + \xi(2(\lambda+\epsilon), -1-2\delta)\right] - \sum_{\beta}^{k=1}\left[\xi\left(\lambda+\epsilon-\lambda_\beta^k, 2+\delta\right) + \xi\left(\lambda+\epsilon-\lambda_\beta^k, -\delta\right)\right] - \sum_{\beta}^{k=2}\left[\xi\left(\lambda+\epsilon-\lambda_\beta^k, \frac{5}{2}+\delta+\delta_\beta^k\right) + \xi\left(\lambda+\epsilon-\lambda_\beta^k, -\frac{1}{2}-\delta-\delta_\beta^k\right) + \xi\left(\lambda+\epsilon-\lambda_\beta^k, \frac{3}{2}+\delta-\delta_\beta^k\right) + \xi\left(\lambda+\epsilon-\lambda_\beta^k, \frac{1}{2}-\delta+\delta_\beta^k\right)\right]. \tag{33}$$

Both equations are written such that the terms on the right-hand side do not strongly depend on ϵ and δ. Now we can simply iterate

$$\delta = -|r|\cos\theta, \qquad \epsilon = |r|\sin\theta, \tag{34}$$

in order to find the exact roots.

3.3. Deviated strings of any length

Now that we know how to solve two- and three-strings, we are ready to generalize our approach to strings of any length. Consider a generic j-string,

$$\lambda^j_{\alpha a} = \lambda^j_\alpha + \epsilon^j_{\alpha a} + \frac{\mathrm{i}}{2}(j + 1 - 2a) + \mathrm{i}\delta^j_{\alpha a}, \tag{35}$$

where the deviations δ and ϵ are real and satisfy $\delta_a = -\delta_{j+1-a}$, $\epsilon_a = \epsilon_{j+1-a}$. Furthermore, for even j, $\epsilon_{j/2} = 0$; for odd j, $\epsilon_{\lfloor j/2\rfloor+1} = \delta_{\lfloor j/2\rfloor+1} = 0$.

Thus, for every j-string we have to find $\lfloor j/2\rfloor$ deviations $d = \epsilon + \mathrm{i}\delta$, as well as the string center λ. Following the logic of the three-string case, we will construct the sets of equations for the norms and arguments of the deviations separately. These equations are written in such a way that the right-hand side can be used to calculate a new guess for the left-hand side, of which we then take the inverse function. They are thus adapted to solution by an iterative procedure. For this to be successful, the equations are to be organized in such a way that the left-hand side varies strongly with the quantity under consideration (be it argument, norm or center), whereas the right-hand side varies only weakly. Let us start with the arguments.

3.3.1. Argument of deviations. First, we consider the sum of the Bethe equations for two conjugate roots. The sum equation reads (again, indices $^j_\alpha$ are suppressed to reduce the strain on the eye)

$$\pi(J_a + J_{j+1-a}) = \theta^a_{\mathrm{kin}} - \theta^a_{\mathrm{other}} - \theta^a_{\mathrm{self}} \pmod{N\pi}, \tag{36}$$

where

$$\begin{aligned}
\theta^a_{\mathrm{kin}} &:= N\big[\xi(2(\lambda+\epsilon_a), j+2-2a+2\delta_a) + \xi\big(2(\lambda+\epsilon_a), -j+2a-2\delta^j_{\alpha a}\big)\big],\\
\theta^a_{\mathrm{other}} &:= \sum_{k\beta}\sum_{1\leqslant b\leqslant k}^{(k,\beta)\neq(j,\alpha)} \xi\left(\lambda - \lambda^k_\beta + \epsilon_a - \epsilon^k_{\beta b}, 1 + (j-k)/2 - (a-b) + \left(\delta_a - \delta^k_{\beta b}\right)\right)\\
&\qquad + \xi\left(\lambda - \lambda^k_\beta + \epsilon_a - \epsilon^k_{\beta b}, 1 - (j-k)/2 + (a-b) - \left(\delta_a - \delta^k_{\beta b}\right)\right),\\
\theta^a_{\mathrm{self}} &:= \sum_{b=1}^{j} \xi\left(\epsilon_a - \epsilon_b, 1 - (a-b) + (\delta_a - \delta_b)\right) + \xi\left(\epsilon_a - \epsilon_b, 1 + (a-b) - (\delta_a - \delta_b)\right).
\end{aligned} \tag{37}$$

The self-scattering term θ^a_{self} contains a few terms that vary strongly with ϵ, δ, if these are small. Let us split these off as

$$\theta^a_{\mathrm{self}} = \theta^a_{\mathrm{residual}} + \xi(\epsilon_a - \epsilon_{a-1}, \delta_a - \delta_{a-1})\,[\text{if } a \neq 1] + \xi(\epsilon_a - \epsilon_{a+1}, -\delta_a + \delta_{a+1}) \quad [\text{if } a \neq j], \tag{38}$$

where the residual weakly-varying part is

$$\begin{aligned}
\theta^a_{\mathrm{residual}} &:= \xi(\epsilon_a - \epsilon_{a-1}, 2 - \delta_a + \delta_{a-1})\,[\text{if } a \neq 1] + \xi(\epsilon_a - \epsilon_{a+1}, 2 + \delta_a - \delta_{a+1}) \quad [\text{if } a \neq j]\\
&\quad + \sum_{\substack{1\leqslant b\leqslant a-2\\ a+2\leqslant b\leqslant j-a-1}} \xi(\epsilon_a - \epsilon_b, 1 - a + b + \delta_a - \delta_b) + \xi(\epsilon_a - \epsilon_b, 1 + a - b - \delta_a + \delta_b).
\end{aligned} \tag{39}$$

The strongly-varying terms are moved to the left-hand side in equation (36),

$$\begin{aligned}
&\xi(\epsilon_1 - \epsilon_2, -\delta_1 + \delta_2) = \theta_1 \pmod{2\pi}\\
&\xi(\epsilon_a - \epsilon_{a-1}, \delta_a - \delta_{a-1}) + \xi(\epsilon_a - \epsilon_{a+1}, -\delta_a + \delta_{a+1}) = \theta_a \pmod{2\pi} \quad \text{for } 1 < a < j\\
&\xi(\epsilon_j - \epsilon_{j-1}, \delta_j - \delta_{j-1}) = \theta_j \pmod{2\pi},
\end{aligned} \tag{40}$$

where

$$\theta_a := -\pi(J_a + J_{j+1-a}) + \theta^a_{\text{kin}} - \theta^a_{\text{other}} - \theta^a_{\text{residual}}. \tag{41}$$

Using $\xi(\epsilon,\delta) + \xi(-\epsilon,\delta) = 0$, we can sum equations (40) to

$$\xi(\epsilon_a - \epsilon_{a+1}, -\delta_a + \delta_{a+1}) = \sum_{b=1}^{a} \theta_b \quad (\text{mod } 2\pi). \tag{42}$$

Applying the inverse function of ξ on both sides, we determine $\epsilon_a - \epsilon_{a+1}$ and $\delta_a - \delta_{a+1}$ up to a common prefactor.

Note that, to be able to use equation (42), we need to determine $\pi(J_a + J_{j+1-a})$ modulo 2π. Here we use

$$J_a + J_{j+1-a} = 2J_a + 1 = M (\text{mod } 2) \quad \text{if } a \neq j/2 \tag{43}$$

$$J_{j/2} + J_{j/2+1} = 2J_{j/2} + (1+\sigma)/2 = M - (1+\sigma)/2 (\text{mod } 2) \quad \text{if } a = j/2, \tag{44}$$

where, for even j, we need to use a criterion such as (26) to determine the inner pair sign, $\sigma := \text{sign}\,\delta_{j/2}$. We will defer this derivation to the end of this section.

3.3.2. Norm of deviations. To find the latter, we must consider the difference between the Bethe equations. Writing this as

$$1 = r^2_{a,\text{kin}} r^{-2}_{a,\text{other}} r^{-2}_{a,\text{self}}, \tag{45}$$

with

$$\begin{aligned} r^2_{a,\text{kin}} &:= \left[\frac{(\lambda+\epsilon_a)^2 + (j/2 - a + \delta_a)^2}{(\lambda+\epsilon_a)^2 + (j/2 - a + 1 + \delta_a)^2}\right]^N, \\ r^2_{a,\text{other}} &:= \prod_{k\beta}^{(k,\beta)\neq(j,\alpha)} \prod_{1\leqslant b\leqslant k} \left[\frac{\left(\lambda - \lambda^k_\beta + \epsilon_a - \epsilon^k_{\beta b}\right)^2 + \left(-1 + \frac{j-k}{2} - a + b + \delta_a - \delta^k_{\beta b}\right)^2}{\left(\lambda - \lambda^k_\beta + \epsilon_a - \epsilon^k_{\beta b}\right)^2 + \left(1 + \frac{j-k}{2} - a + b + \delta_a - \delta^k_{\beta b}\right)^2}\right], \\ r^2_{a,\text{self}} &:= \prod_{1\leqslant b\leqslant j}^{b\neq a} \left[\frac{(\epsilon_a - \epsilon_b)^2 + (-1 - a + b + \delta_a - \delta_b)^2}{(\epsilon_a - \epsilon_b)^2 + (1 - a + b + \delta_a - \delta_b)^2}\right]. \end{aligned} \tag{46}$$

Again, we split up the self-scattering parts,

$$r^2_{a,\text{self}} = r^2_{a,\text{residual}} \frac{[(\epsilon_a - \epsilon_{a+1})^2 + (\delta_a - \delta_{a+1})^2]^{[\text{if } a\neq j]}}{[(\epsilon_a - \epsilon_{a-1})^2 + (\delta_a - \delta_{a-1})^2]^{[\text{if } a\neq 1]}}, \tag{47}$$

where the residual part of the self-scattering term is

$$\begin{aligned} r^2_{a,\text{residual}} &:= \frac{[(\epsilon_a - \epsilon_{a-1})^2 + (-2 + \delta_a - \delta_{a-1})^2]^{[\text{if } a\neq 1]}}{[(\epsilon_a - \epsilon_{a+1})^2 + (2 + \delta_a - \delta_{a+1})^2]^{[\text{if } a\neq j]}} \\ &\quad \times \prod_{1\leqslant b\leqslant j}^{b\notin\{a,a\pm 1\}} \frac{(\epsilon_a - \epsilon_b)^2 + (-1 - a + b + \delta_a - \delta_b)^2}{(\epsilon_a - \epsilon_b)^2 + (1 - a + b + \delta_a - \delta_b)^2}. \end{aligned} \tag{48}$$

Now we can write, in similar fashion as before,

$$\begin{aligned} &(\epsilon_1 - \epsilon_2)^2 + (\delta_1 - \delta_2)^2 = r_1^2, \\ &\left[\frac{(\epsilon_a - \epsilon_{a+1})^2 + (\delta_a - \delta_{a+1})^2}{(\epsilon_a - \epsilon_{a-1})^2 + (\delta_a - \delta_{a-1})^2}\right] = r_a^2, \\ &[(\epsilon_j - \epsilon_{j-1})^2 + (\delta_j - \delta_{j-1})^2]^{-1} = r_j^2, \end{aligned}$$

and we may multiply these equations out to get the norm we sought,

$$(\epsilon_a - \epsilon_{a+1})^2 + (\delta_a - \delta_{a+1})^2 = \prod_{b=1}^{a} r_b^2. \tag{49}$$

In these equations,

$$r_a^2 := r_{a,\mathrm{kin}}^2 r_{a,\mathrm{other}}^{-2} r_{a,\mathrm{residual}}^{-2}. \tag{50}$$

Equations (49) and (42) completely determine $\epsilon_a - \epsilon_{a+1}$ and $\delta_a - \delta_{a+1}$. For odd j, this sequence ends at $a = \lfloor j/2 \rfloor$, where $\epsilon_{a+1} = \delta_{a+1} = 0$. For even j, the endpoint is at $j/2$, where $\epsilon_a = \epsilon_{a+1} = 0$ and $\delta_a = -\delta_{a+1}$. In both cases, this allows us to find ϵ and δ themselves at the endpoint, after which all other deviations are found by summing the differences.

For odd j, therefore, the deviations are found from

$$\delta_a = -\sum_{b=a}^{\lfloor j/2 \rfloor} \cos\left[\sum_{c=1}^{b} \theta_c\right] \prod_{c=1}^{b} |r_c|, \qquad \epsilon_a = \sum_{b=a}^{\lfloor j/2 \rfloor} \sin\left[\sum_{c=1}^{b} \theta_c\right] \prod_{c=1}^{b} |r_c|. \tag{51}$$

For even j, the value $\theta_{j/2}$ cannot be determined as above; we must decide the width of the middle pair $\sigma := \operatorname{sign} \delta_{j/2}$ on the basis of a criterion such as (26), which we shall derive shortly. Here, the deviations are found from

$$\begin{aligned} \delta_a &= \frac{1}{2}\sigma \prod_{c=1}^{j/2} |r_c| - \sum_{b=a}^{j/2-1} \cos\left[\sum_{c=1}^{b} \theta_c\right] \prod_{c=1}^{b} |r_c|, \\ \epsilon_a &= \sum_{b=a}^{j/2-1} \sin\left[\sum_{c=1}^{b} \theta_c\right] \prod_{c=1}^{b} |r_c|. \end{aligned} \tag{52}$$

3.3.3. Rapidities. Finally, we need an equation for the rapidities. This is found from the total sum of the string Bethe equations, which becomes the Bethe–Takahashi equation for the string in the limit where the deviations vanish. Annoyingly, we need to pay attention to all branch cut terms to make the correct connection with the Bethe–Takahashi equation. The self-scattering terms all cancel, so that the total sum reads

$$\pi \sum_{a=1}^{j} J_{\alpha,a}^{j} = \sum_{a=1}^{j} \theta_{\mathrm{kin}}^a - \theta_{\mathrm{other}}^a. \tag{53}$$

The kinematic phases add up to

$$\begin{aligned} \sum_{a=1}^{j} \theta_{\mathrm{kin}}^a = N \Bigg[& \xi(2\lambda + 2\epsilon_1, j + 2\delta_1) + [\text{if } j \text{ even}]\, \xi(2\lambda, -2\delta_{j/2}) \\ & + \sum_{a=1}^{\lfloor (j-1)/2 \rfloor} \xi(2\lambda + 2\epsilon_{a+1}, j - 2a + 2\delta_{a+1}) + \xi(2\lambda + 2\epsilon_a, -j + 2a - 2\delta_a) \Bigg]. \end{aligned} \tag{54}$$

For the scattering phases, writing

$$\xi_{ab}^{\pm} := \xi\left(\lambda_\alpha^j - \lambda_\beta^k + \epsilon_{\alpha a}^j - \epsilon_{\beta b}^k, 1 \pm \left[(j-k)/2 + b - a + \delta_{\alpha a}^j - \delta_{\beta b}^k\right]\right) \tag{55}$$

and using

$$\sum_{b=1}^{k} \xi_{ab}^{+} + \xi_{ab}^{-} = \xi_{a1}^{-} + \xi_{a2}^{-} + \xi_{a,k-1}^{+} + \xi_{ak}^{+} + \sum_{b=1}^{k-2} \xi_{ab}^{+} + \xi_{a,b+2}^{-}, \tag{56}$$

we can group terms together as

$$\sum_{a=1}^{j} \theta^a_{\text{other}} = \sum_{k\beta}^{(k,\beta)\neq(j,\alpha)} \sum_{a=1}^{j} \left[\xi^-_{a1} + \xi^-_{a2} + \xi^+_{a,k-1} + \xi^+_{ak} + \sum_{b=1}^{k-2} \xi^+_{ab} + \xi^-_{a,b+2} \right]. \tag{57}$$

The iterative prescription for $\lambda \equiv \lambda^j_\alpha$ is then

$$\xi(2\lambda + 2\epsilon_1, j + 2\delta_1) + [\text{if } j \text{ even}]\, \xi(2\lambda, -2\delta_{j/2}) = \frac{\pi}{N} \sum_{a=1}^{j} J^j_{\alpha,a} + \frac{1}{N} \sum_{a=1}^{j} \theta^a_{\text{other}}$$
$$- \sum_{a=1}^{\lfloor (j-1)/2 \rfloor} \xi(2\lambda + 2\epsilon_{a+1}, j - 2a + 2\delta_{a+1}) + \xi(2\lambda + 2\epsilon_a, -j + 2a - 2\delta_a). \tag{58}$$

These equations take the place of the Bethe–Takahashi equations when solving for a deviated string. However, to make the connection with those, we need to establish a relationship between the various quantum numbers used. This we can do by taking the limit as $\delta, \epsilon \to 0$.

Using $\xi(\epsilon, \delta) + \xi(\epsilon, -\delta) = \pi \operatorname{sign} \epsilon$ and $\xi(\epsilon, 0) = (\pi/2) \operatorname{sign} \epsilon$, and taking the equation modulo $N\pi$, the kinetic phase goes to

$$\lim_{\substack{\epsilon\to 0\\ \delta\to 0}} \sum_{a=1}^{j} \theta^a_{\text{kin}} = N\left[\arctan \frac{2\lambda}{j} + \frac{j-1}{2} \pi \operatorname{sign} \lambda \right] \quad (\text{mod}\, N\pi). \tag{59}$$

For the scattering phase, we use

$$\lim_{\substack{\epsilon\to 0\\ \delta\to 0}} \sum_{a=1}^{j} \sum_{b=1}^{k-2} \xi^+_{ab} + \xi^-_{a,b+2} = j(k-2)\pi \operatorname{sign}\left(\lambda^j_\alpha - \lambda^k_\beta\right) \tag{60}$$

and

$$\lim_{\substack{\epsilon\to 0\\ \delta\to 0}} \left[\xi^-_{1,2} + \xi^+_{1,k} + \xi^-_{j,1} + \xi^+_{j,k-1} + \sum_{a=1}^{j-1} \left(\xi^-_{a,1} + \xi^-_{a+1,2} + \xi^+_{a,k-1} + \xi^+_{a+1,k} \right) \right]$$
$$= \xi\left(2\left(\lambda^j_\alpha - \lambda^k_\beta\right), |j-k|\right) + \xi\left(2\left(\lambda^j_\alpha - \lambda^k_\beta\right), j+k\right)$$
$$+ (j-k)\Theta(j-k)\pi \operatorname{sign}\left(\lambda^j_\alpha - \lambda^k_\beta\right) + 2 \sum_{c=|j-k|+2}^{j+k-2} \xi\left(2\left(\lambda^j_\alpha - \lambda^k_\beta\right), c\right)$$
$$= (1 - \delta_{j,k}) \arctan \frac{2\left(\lambda^j_\alpha - \lambda^k_\beta\right)}{|k-j|} + \arctan \frac{2\left(\lambda^j_\alpha - \lambda^k_\beta\right)}{k+j}$$
$$+ \left[(j-k)\Theta(j-k) + \frac{1}{2}\delta_{j,k} \right] \pi \operatorname{sign}\left(\lambda^j_\alpha - \lambda^k_\beta\right)$$
$$+ 2 \sum_{c=|k-j|+2}^{k+j-2} \arctan \frac{2\left(\lambda^j_\alpha - \lambda^k_\beta\right)}{c}, \tag{61}$$

where the sum over c is in steps of 2 and the Θ term derives from the cancellation of terms between $k - j$ and $j - k$, which occurs if $j > k$. The last equality follows because all remaining terms have positive values for the second argument of ξ.

Observing that $j(k-2)/2 + (j-k)\Theta(j-k) = jk/2 - \min(j,k)$, we may conclude that the relation between the Bethe and Bethe–Takahashi quantum numbers is, modulo N,

$$\sum_{a=1}^{j} J^j_{\alpha,a} = I^j_\alpha + N\frac{j-1}{2} - \sum_{k\beta}^{(k,\beta)\neq(j,\alpha)} \operatorname{sign}\left(\lambda^j_\alpha - \lambda^k_\beta\right) \left\{ \frac{jk}{2} - \min(j,k) + \tfrac{1}{2}\delta_{j,k} \right\}. \tag{62}$$

3.3.4. Width of the innermost pair. Given relation (10) between J_a and J_{j+1-a}, we can use expression (62) to determine the width of the innermost pair of an even string. Taking it modulo 2, we find

$$\Theta(\delta_{j/2}) = \frac{1}{2}\Bigg[2I_\alpha^j + N(j-1) - j(M+1) - j - 2 \\ - \sum_{k\beta}^{(k,\beta)\neq(j,\alpha)} \mathrm{sign}\big(\lambda_\alpha^j - \lambda_\beta^k\big)\{jk - 2\min(j,k) + \delta_{j,k}\}\Bigg] \pmod 2, \tag{63}$$

so that with $\sigma = 2\Theta(\delta_{j/2}) - 1$ we have found the last ingredient needed to find the deviations of even strings by equation (52).

3.4. Summary of the method

In the previous sections we have derived a number of equations for deviated strings, which can be solved by simple iteration. One starts from a solution of the Bethe–Takahashi equations (18), giving initial locations for the string centers. Naturally, these solutions have all deviations zero, $\epsilon_{\alpha a}^j = \delta_{\alpha a}^j = 0$. These values will be the initial guess. Equations (51) or (52) then give the next guess for the deviations $\epsilon_{\alpha a}^j$ and $\delta_{\alpha a}^j$, whereas equations (58) are used to obtain a new guess for the string centers λ_α^j. This procedure can be repeated until the desired level of convergence is achieved. Some results of this procedure are given in section A, where we present the complete solution of the Bethe Ansatz for the Heisenberg chains of $N = 8$ and $N = 10$ sites. Complete solutions up to $N = 6$ can be found elsewhere in the literature (see, e.g. [39]).

4. Structure of string solutions

Various authors have studied the fine structure of two-string solutions, starting with Bethe himself [2], and followed by Vladimirov [17], Essler *et al* [3] and Isler and Paranjape [4] (the latter providing also a discussion of string length greater that 2). It is found that there are two branches of two-strings: narrow and wide ones. The wide strings lie on a curve in the complex plane such that, with increasing real part, the imaginary part of the roots diverges with the asymptote $\mathrm{Im}\,\lambda = \pm\mathrm{Re}\,\lambda/\sqrt{N-1}$. The narrow strings get closer to the real line with increasing real part, and finally collapse onto it. This means that for high quantum numbers no narrow string solutions are available. Instead, extra solutions appear with two real roots. Motivated by these results, we study the three- and four-string case.

4.1. Fine structure for three-strings

Figure 1 shows the $\mathrm{Re}\,\lambda > 0$ solutions for a single three-string on a chain of 10^6 sites. The solutions separate into three branches, distinguished by their quantum number $I \pmod 3$. Two of the branches, with $I = 0 \pmod 3$ and $I = 1 \pmod 3$ are as good as indistinguishable for this value of N, although they are separately visible for smaller N.

Calculating the Bethe quantum numbers (J_+, J_0, J_-) from these solutions, it is found that they follow the pattern shown in figure 2. There are three branches of solutions, distinguished by the relations between the quantum numbers:

$$\begin{array}{ll} \text{branch 0} & J_0 + 1 = J_+ = J_- - 1, \\ \text{branch 1} & J_0 = J_+ = J_- - 1, \\ \text{branch 2} & J_0 - 1 = J_+ = J_- - 1. \end{array} \tag{64}$$

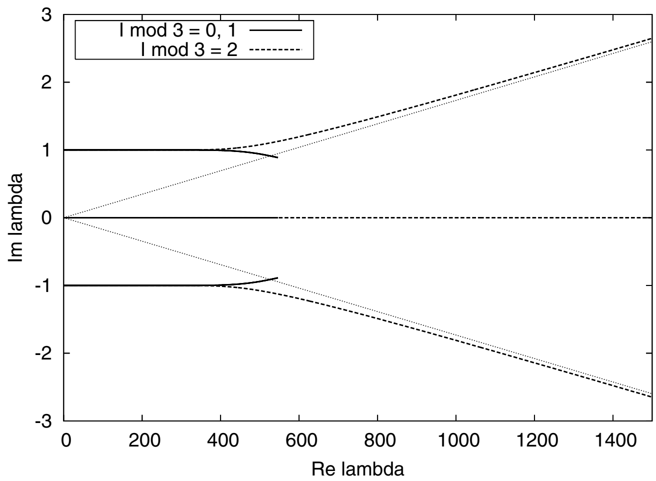

Figure 1. Locus of three-strings for a chain with $N = 10^6$ and $M = 3$. In this and all subsequent graphs, the rapidity complex plane is represented. The straight lines are the asymptotes (65) for the branch with all three quantum numbers distinct.

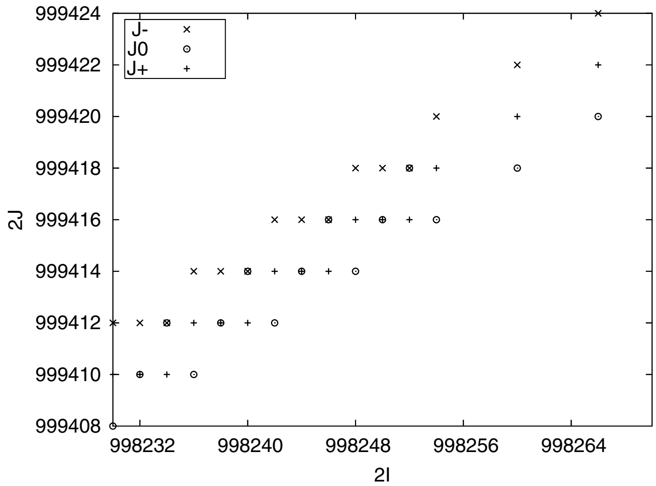

Figure 2. Bethe quantum numbers (J_-, J_0, J_+) for three-strings with increasing $I^{(3)}$.

Strings on the two branches for which $J_0 = J_+$ or $J_0 = J_-$ shrink with $\mathrm{Re}\,\lambda$. Beyond a certain point we can no longer find a deviated three-string solution for the given quantum numbers. We conjecture that further states are made up of a narrow string whose two roots have equal numbers, with the third quantum number corresponding to the real root. Further still, we expect the rapidities of states with yet higher quantum numbers to collapse onto the real axis yielding a purely real three-string, similar to what happens for two-strings. On the branch for which all quantum numbers are different, string solutions continue to exist with growing $\mathrm{Re}\,\lambda$, with increasing deviation. Assuming $\epsilon \ll \lambda$, we can derive the asymptotical relation

$$\mathrm{Im}\,\lambda = \frac{\pm\,\mathrm{Re}\,\lambda}{\sqrt{\frac{1}{3}(N-3)}}. \tag{65}$$

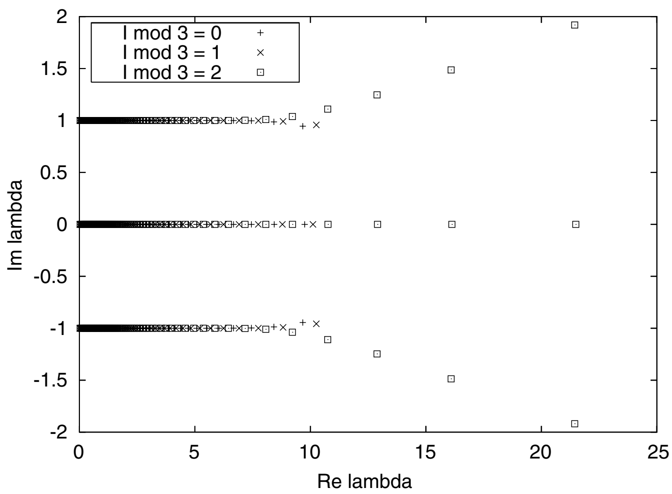

Figure 3. Three-strings for a chain with $N = 2000$ and $M/N = 0.4$.

The results given up until now studied configurations where the string under consideration was the only set of roots. In the large-N limit, this implies that we study a system very close to saturation field. To study a system at a magnetic field closer to zero, let us consider configurations with a single string accompanied by a number of real roots, such that $M/N = 0.4$. This is numerically much more intensive as a much larger set of equations must be solved. Therefore, only smaller systems can be considered here. Figure 3 shows the $\mathrm{Re}\,\lambda > 0$ solutions for a three-string in this case, on a chain of 2000 sites. It turns out that the overall structure is very similar to the lone-string case considered earlier.

4.2. Fine structure for four-strings

Figure 4 shows the $\mathrm{Re}\,\lambda > 0$ solutions for a single four-string on a chain of 10^6 sites. The solutions separate into four branches, distinguished by their quantum number $I\,(\mathrm{mod}\,4)$. Again, two of these branches ($I = 1, 3\,(\mathrm{mod}\,4)$) are nearly indistinguishable.

Calculating the Bethe quantum numbers $(J_{-2}, J_{-1}, J_{+1}, J_{+2})$ from these solutions, it is found that they follow the pattern shown in figure 5. There are four branches of solutions, again distinguished by the relations between the quantum numbers,

$$\begin{array}{ll} \text{branch 0} & J_{+1} = J_{-1} - 1 = J_{+2} - 2 = J_{-2} - 3, \\ \text{branch 1} & J_{+1} = J_{-1} = J_{+2} - 1 = J_{-2} - 2, \\ \text{branch 2} & J_{+1} = J_{-1} - 1 = J_{+2} + 1 = J_{-2}, \\ \text{branch 3} & J_{+1} = J_{-1} = J_{+2} + 2 = J_{-2} + 1. \end{array} \tag{66}$$

Assuming $\epsilon_0, \epsilon_1 \ll \lambda$, we can derive the asymptotical relation

$$\mathrm{Im}\,\lambda = \frac{\pm\,\mathrm{Re}\,\lambda}{\sqrt{N - 3 \pm \sqrt{\frac{2}{3}(N-3)(N-2)}}}. \tag{67}$$

Figure 6 shows the $\mathrm{Re}\,\lambda > 0$ solutions for a four-string accompanied by real roots such that $M/N = 0.4$, on a chain of 2000 sites.

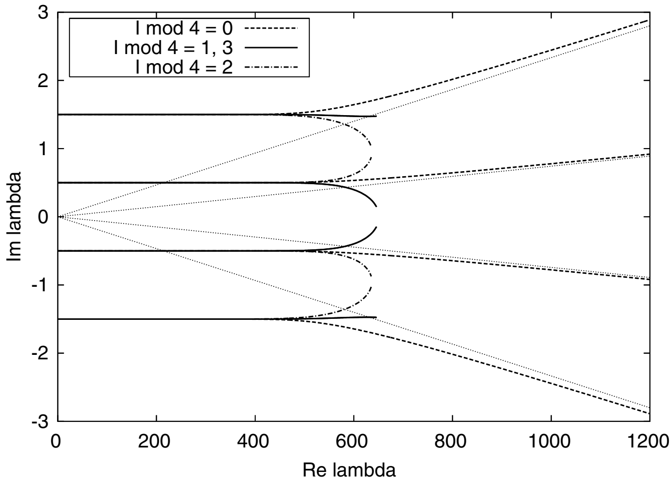

Figure 4. Locus of four-strings for a chain with $N = 10^6$ and $M = 4$. The straight lines are the asymptotes (67).

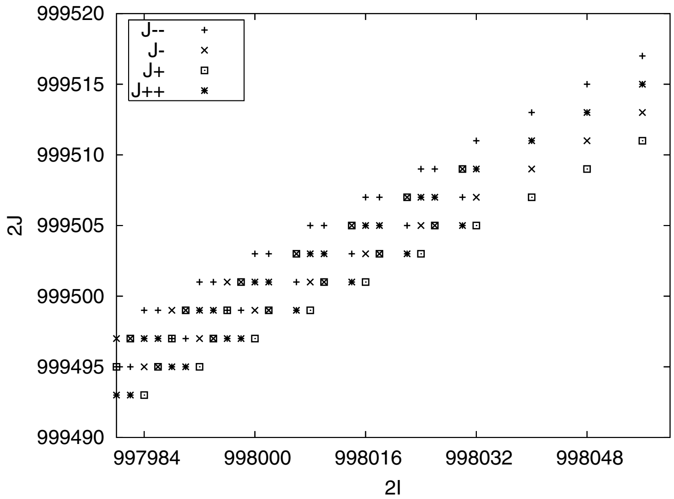

Figure 5. Bethe quantum numbers $(J_{-2}, J_{-1}, J_{+1}, J_{+2})$ for four-strings with increasing $I^{(4)}$.

4.3. Completeness

An interesting question is the fate of string-like solutions with increasing chain length N. The analytic solution is known only for the two-magnon sector $M = 2$; from $N = 22$ onward narrow two-strings 'collapse' and form pairs of roots on the real line, as described in [3]. The number of missing solutions equals

$$n_{\text{missing}}^{(M=2)} = \left\lfloor \frac{\sqrt{N}}{\pi} - \frac{1}{2} \right\rfloor. \tag{68}$$

The method described in this section can shed some light on this question, as we can try and find all solutions of the Bethe equations for a given number of magnons with increasing

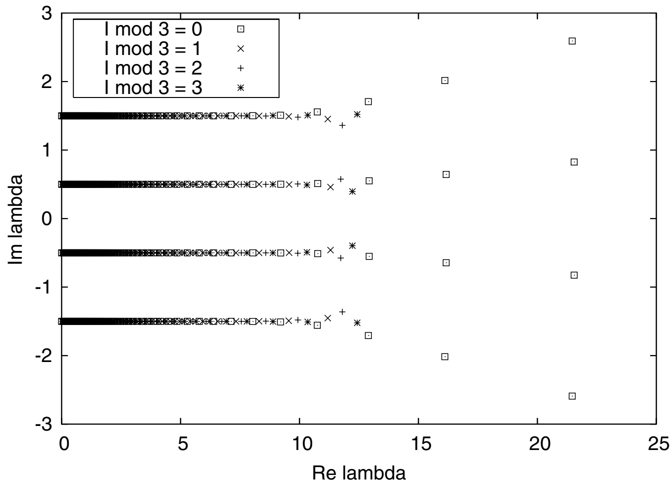

Figure 6. Four-strings for a chain with $N = 2000$ and $M/N = 0.4$.

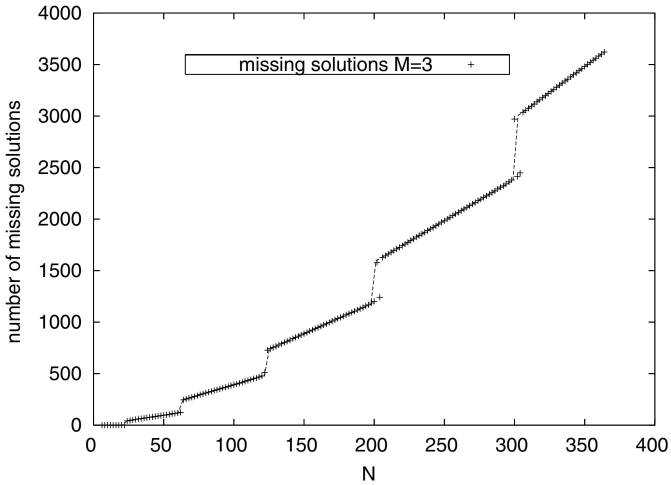

Figure 7. Missing solutions at $M = 3$. Around the jumps it sporadically happens that solutions are not found, or wrong solutions are found, depending on the convergence threshold set. The number of missing solutions turns out to fit to an empirical rule much like equation (68), namely $n^{(M=3)}_{\text{missing}} = 2(N-2)\lfloor \frac{\sqrt{N-1}}{\pi} - \frac{1}{2} \rfloor$.

chain length. The number of missing solutions then gives an upper bound to the number of non-string solutions. For $M = 3$, this is shown in figure 7. The situation for $M = 4$ is shown in figure 8. Note that, especially around the jumps in the graphs, the number of solutions found is rather sensitive to the degree of convergency required in iteration. This effect may shift the jumps a bit to the left and right but the overall shape of the function is not changed.

Finally, in figure 9 we show the number of missing solutions in a single log–log graph for M between 2 and 7. It can be seen from the plot that at every M, the number of missing solutions grows as $O(N^{M-3/2})$ and exhibits jumps on or very close to the locations dictated by

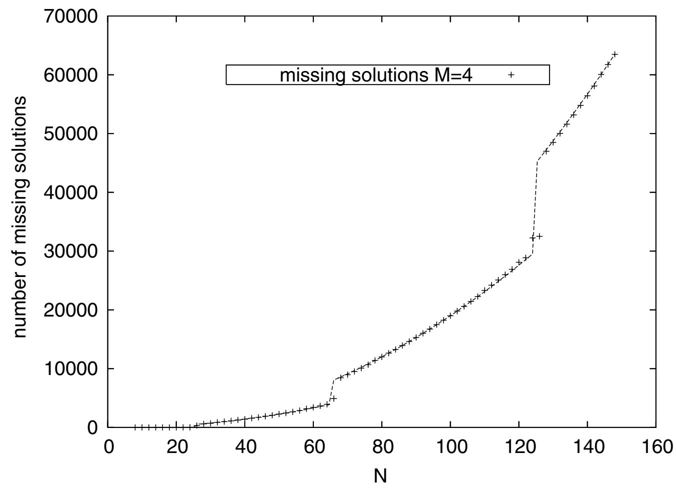

Figure 8. Missing solutions at $M = 4$. An empirical fit for the number of missing solutions is $n^{(M=4)}_{\text{missing}} = (N-2)(N-3)\lfloor \frac{\sqrt{N-4}}{\pi} - \frac{1}{2} \rfloor$.

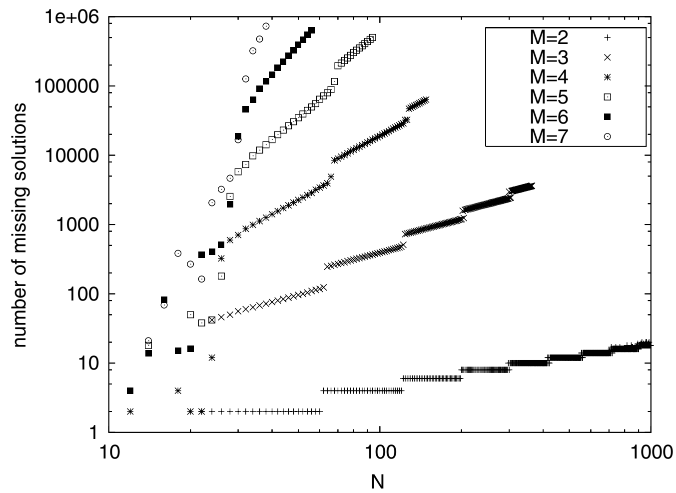

Figure 9. Log–log plot of the number of missing solutions at $M \in \{2 \dots 7\}$.

the $M = 2$ rule (68). These numbers fit in a picture where the collapse of narrow pairs—either only from two-strings or from higher strings as well—is the only aberration from the string hypothesis, if one allows for deviations in the strings themselves. Of course, it would be desirable to have a method to solve for the collapsed pairs as well, so that this statement can be checked. Since the number of higher strings is much lower than that of two-strings, a collapse of higher strings would not make a big difference in these graphs.

This also shows that, at least at the small numbers of magnons and chain lengths considered here, the method we describe captures the vast majority of solutions of the Bethe equations: the number of highest-weight solutions is $n^{(M)}_{\text{total}} = \binom{N}{M} - \binom{N}{M-1} = O\left(\frac{N^M}{M!}\right)$ so that the fraction of missing solutions scales as $\frac{n^{(M)}_{\text{missing}}}{n^{(M)}_{\text{total}}} = O\left(\frac{N^{-3/2}}{M!}\right)$.

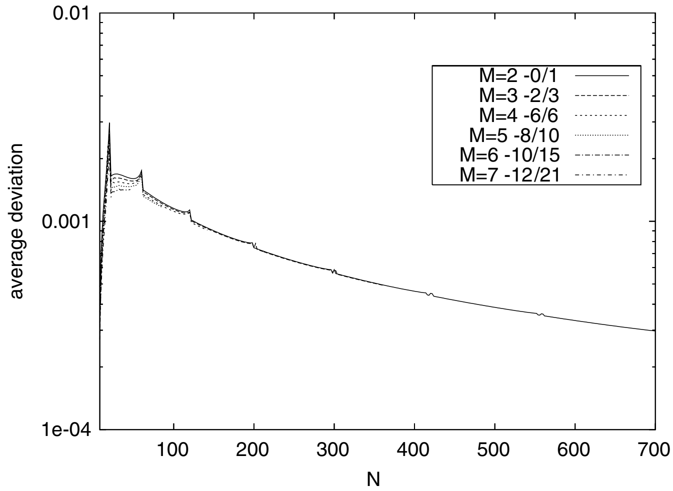

Figure 10. Scaling of deviations with increasing *N*, plotted against $N - 2M$. The vertical axis is logarithmic. The curves for $M > 2$ are divided by $3(M - 2)$ to show the collapse.

4.4. Scaling of deviations

The string hypothesis states that deviations should decrease with increasing chain length as $O(e^{-cN})$ for some constant c. In figure 10 the average deviation of string solutions is shown, where the average is taken over all solutions (including real roots) and the magnitude of deviation for a single string is given by

$$d := \sum_{a=1}^{n_j} \delta_a^2 + \epsilon_a^2. \tag{69}$$

Remarkably, the curves for all values of M collapse onto that of $M = 2$, if the average deviations are divided by $\sum_{l=1}^{n_j-1} l$. The string hypothesis suggests that such an average should decrease as a sum of exponentials; the curve is consistent with this.

We can also check the string hypothesis directly: if we keep λ approximately fixed (of course we are limited in our choice for λ, bounded as we are by having to find an actual solution of the Bethe equations), we see that the deviation δ indeed decreases exponentially with increasing *N*. This is shown in figure 11.

However, if we do not hold the string center constant but instead consider the behavior of the most outward string, we see that its deviation in fact increases with *N*, as shown in figure 12. This is because the string center of the peripheral string increases with *N* as well.

4.5. Deviation of peripheric strings

Let us parametrize the deviations as follows. For the roots in the j-string,

$$\lambda_a = \lambda + \frac{i}{2}(j + 1 - 2a) + d_a, \tag{70}$$

where $d_a := i\delta_a + \epsilon_a$. For the central root or pair,

$$\begin{aligned} &\delta_{(j+1)/2} = \epsilon_{(j+1)/2} = 0 &&\text{for } j \text{ odd,} \\ &\epsilon_{j/2} = 0 &&\text{for } j \text{ even.} \end{aligned} \tag{71}$$

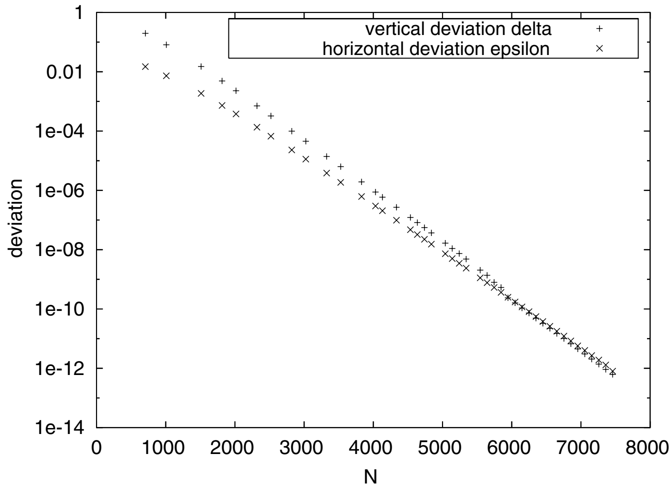

Figure 11. Exponential decrease with chain length N of the δ and ϵ of three-string solutions with $15.9925 < \mathrm{Re}\,\lambda < 15.9975$ at $M = 3$.

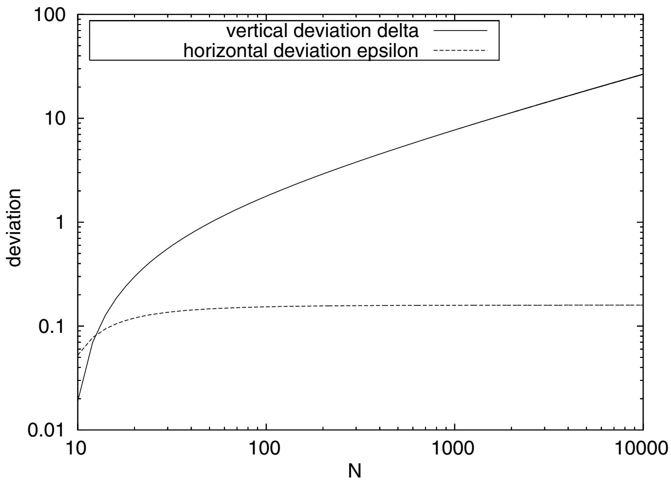

Figure 12. Increase with chain length N of the δ and ϵ of peripheral three-string solutions. The horizontal deviation ϵ, which appears to saturate, in fact keeps growing.

Furthermore, as the roots are grouped in pairs of conjugates,

$$d_{j-a} = d_a^*. \tag{72}$$

In the Bethe equation for a given root, the scattering phase features a product over the other roots of the string,

$$R_a := \prod_b^{b\neq a} \frac{d_a - d_b + (b-a+1)\,\mathrm{i}}{d_a - d_b + (b-a-1)\,\mathrm{i}}. \tag{73}$$

To lowest order in d, for $a \neq 1, j$,

$$R_a \approx -\left[\frac{d_a - d_{a-1}}{d_a - d_{a+1}}\right] \frac{\prod_b^{b\neq a-1}(b-a+1)\,\mathrm{i}}{\prod_b^{b\neq a+1}(b-a-1)\,\mathrm{i}} = \left[\frac{d_{a-1} - d_a}{d_a - d_{a+1}}\right] \frac{(j-a+1)(j-a)}{a(a-1)}. \tag{74}$$

For $a = 1$ or $a = j$,

$$R_1 \approx -\mathrm{i}\frac{j(j-1)}{d_1 - d_2}, \qquad R_j \approx -\mathrm{i}\frac{d_j - d_{j-1}}{-j(1-j)}. \tag{75}$$

Thus, starting from $a = 1$, we can successively construct the differences

$$d_{a+1} - d_a = -\mathrm{i}\frac{j(j-a)}{a}\left[\prod_{b=1}^{a} K_b\right]\left[\prod_{b=1}^{a-1}\frac{j-b}{b}\right]^2, \tag{76}$$

where K_a is given by the other factors in the Bethe equation,

$$K_a := \left[\frac{\lambda + (j+2-2a)\,\mathrm{i}/2}{\lambda + (j-2a)\,\mathrm{i}/2}\right]^{-N} \prod_{k\beta b}^{(k\beta)\neq(j\alpha)} \left[\frac{\lambda - \lambda_{\beta b}^k + (j+3-2a)\,\mathrm{i}/2}{\lambda - \lambda_{\beta b}^k + (j-1-2a)\,\mathrm{i}/2}\right]; \tag{77}$$

the product is understood to run over all complex roots *not* belonging to the same string.

For odd j, we can use $d_{(j+1)/2} = 0$ and sum over the differences to get

$$d_b = -\sum_{a=b}^{(j-1)/2} \frac{j(j-a)}{a}\binom{j-1}{a-1}^2 \prod_{c=1}^{a} K_c, \qquad \text{for} \qquad b \leqslant (j-1)/2. \tag{78}$$

For even j, we have $\mathrm{Re}\, d_{j/2} = 0$ and therefore $d_{j/2} = -d_{j/2+1}$. We now have, for $b \leqslant j/2 - 1$,

$$d_b = \frac{\mathrm{i}}{2}\left[j\binom{j-1}{j/2-1}^2 \prod_{c=1}^{j/2} K_c\right] - \mathrm{i}\sum_{a=b}^{j/2-1}\left[\frac{j(j-a)}{a}\binom{j-1}{a-1}^2 \prod_{c=1}^{a} K_c\right]. \tag{79}$$

The behavior of K_a for large N and λ depends on the order in which we take the limits. In particular, let us consider the limit for large λ, i.e. a string center far removed from the origin, while the other rapidities remain small. Then, $\lim_{\lambda\to\infty} K_a = 1$ and, for odd j,

$$\lim_{\lambda\to\infty} d_b = -\mathrm{i}\sum_{a=b}^{(j-1)/2} \frac{j(j-a)}{a}\binom{j-1}{a-1}^2. \tag{80}$$

Note that this number is of order unity and independent of the chain length N. This order of limits is relevant for instance when we consider the limit to large N at a fixed magnetization density M/N, as in that case the number of rapidities grows with N. Then, assuming a constant rapidity density, strings on the periphery will always be strongly deviated.

5. Symmetric and singular states

If the Bethe–Takahashi quantum numbers are distributed symmetrically around zero, then so are the rapidities. Such symmetric states merit special attention. The simplest example is the ground state, which has already been discussed. Since all the rapidities are then real, no problem is encountered. In the presence of bound states, the situation becomes more complicated. In a symmetric state, if the quantum number of a string is zero, then its center is also zero. Superimposing two higher strings of length differing by an even integer (e.g. a two-string and a four-string, or a three-string and a seven-string) means that pairs of rapidities coincide in the pure string hypothesis. String deformations, as we will see, regularize these situations and give allowable eigenstates. As we will discuss in this section, it turns out to distinguish two classes of symmetric states: those with only strings, and those which include even strings. Again, we concentrate on the isotropic chain, although similar issues exist also in the XXZ chain.

5.1. Multiple symmetric odd strings

In a symmetric state with more than one odd string at the origin, the solution of the Bethe–Takahashi equations is not a valid state: since there are two or more roots present at the origin, the exclusion principle is violated. However, if we take the deviations into account, this problem does not arise: the two roots that coincide in the limit are actually separated. As an example, we will show the solution for the simplest case where this problem arises: the symmetric state with one three-string and one real root at the origin, $I^{(3)} = 0$ and $I^{(1)} = 0$. Defining the rapidities $\lambda_{\pm \mathrm{i}} = \pm(\mathrm{i} + \delta)$, $\lambda_{-0} = -\lambda_{+0} > 0$, we find from the difference of Bethe equations that $J_{+\mathrm{i}} = -J_{-\mathrm{i}} = (N-1)/2$ (where also $J_{-\mathrm{i}} = J_{+\mathrm{i}} + 1 (\mathrm{mod}\, N)$). The quantum numbers for the real roots in the complex must be half-integer, opposite and as small as possible, leading to $J_{\pm 0} = \pm 1/2$.

The fixed points of the iterative equations for the deviations as given in section 3, however, are repulsive in this case; therefore, we need to either use another method (such as Newton–Raphson) or rewrite the iterative equations. An easy prescription that works is to take the sum of the equations for the positive-real and positive-imaginary root, which gives

$$\lambda' + \mathrm{i}(1+\delta') = \tan\left[\frac{N-1}{2}(\arctan 2\lambda + \mathrm{i}\,\mathrm{atanh}(2+2\delta)) - \frac{\theta_{\mathrm{other}}}{2}\right], \tag{81}$$

where, in the presence of other roots,

$$\theta_{\mathrm{other}} := \sum_{\beta}^{\lambda_\beta \notin \{\pm\lambda, \pm \mathrm{i}(1+\delta)\}} \arctan(\lambda - \lambda_\beta) + \arctan(\mathrm{i} + \mathrm{i}\delta - \lambda_\beta). \tag{82}$$

The full solution has no coinciding roots and the wavefunctions are the regular Bethe wavefunctions. The roots do, however, tend to grow very close as the chain length increases, leading to numerical problems: at more than 40 sites machine precision is too low to find an acceptable result (see figure 13). However, for smaller chains it is already clear that the values are exponentially decreasing. For large N, inserting the assumption $\lambda \ll 1$, $\delta \ll 1$ in the Bethe equation, we note that by symmetry of the set $\{\lambda_\beta\}$, the contribution of the other roots is the real number $0 < F < 1$ given by

$$F = \prod_{\beta}^{\lambda_\beta \notin \{\pm\lambda, \pm \mathrm{i}(1+\delta)\}} \frac{|\lambda_\beta|}{\sqrt{\lambda_\beta^2 + 1/4}}. \tag{83}$$

In this way, we get

$$\lambda = \sqrt{\frac{12}{F}} \cdot 3^{-N/2}, \qquad \delta = \frac{24(N-1)}{F} \cdot 3^{-N}\,\mathrm{e}^{-\mathrm{i}\Phi}, \tag{84}$$

proving that the opposite real roots are exponentially close to each other, but can be pushed further apart in the presence of a macroscopic number of down spins (i.e. at low magnetic fields).

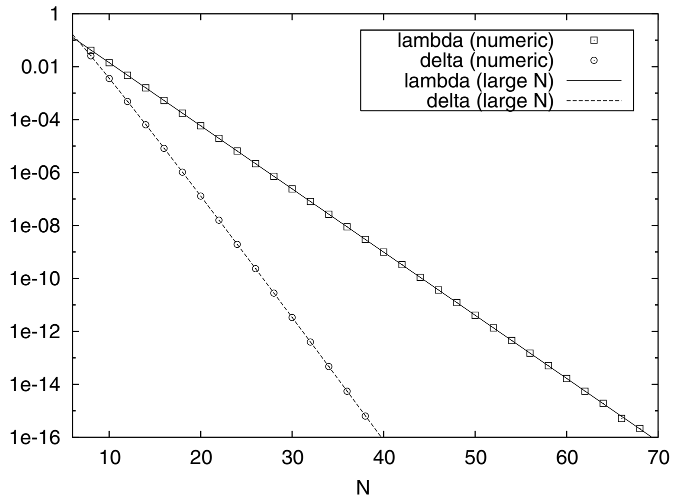

Figure 13. Comparison of the values λ (squares), δ (circles), in the absence of other roots, calculated by iteration of equation (81) and by the large-N approximation (84) (lines). The plot is limited to those values for which the iteration procedure remains within machine precision. It is seen that even for short chains, the large-N approximation yields very good results.

In this approximation, the reduced Bethe equations that must be satisfied by the remaining roots are

$$N \arctan 2\lambda_j - 2\arctan \lambda_j - \arctan \lambda_j/2 = \pi \left(J_j + \frac{1}{2}\right) + \sum_{k=1}^{M-4} \arctan(\lambda_j - \lambda_k) \quad (\mathrm{mod}\, \pi), \tag{85}$$

if we order the rapidities such that the last four are the set $\{\pm 0, \pm \mathrm{i}\}$.

The energy associated with the four roots $\{\pm 0, \pm \mathrm{i}\}$ equals, for large N,

$$E_{\{\pm 0, \pm \mathrm{i}\}} = -8/3. \tag{86}$$

5.2. Singular pair states at $M = 2$

Here, besides superimposing pairs of even-length strings at the origin (which we will not discuss here; their treatment would extend the present section, and could be addressed by adopting a similar logic to that used for superimposed odd-length strings in the previous section), we encounter a fundamentally different type of singular states, due to the presence of roots at the points $\pm \mathrm{i}/2$. At this point, the Bethe equations are singular; moreover, the singularity in the kinetic phase is stronger than in the usual case for a string, $(\mathrm{e}^{\mp N \log \delta})$ instead of $(\mathrm{e}^{\pm N})$. This would suggest that this divergence cannot be countered in the usual way by the divergence in the scattering phase. Yet, if we carefully consider the way in which we take the limit $\lambda_{\pm} \to \pm \mathrm{i}/2$, we shall see that we get a bona fide solution of the Bethe equations.

Note that the problem of singular states also arises in the XXZ model at 'root of unity' values for the anisotropy parameter, as was shown by Fabricius and McCoy [31, 32]: indeed, the exact complete N-strings of those articles correspond to the singular strings discussed here.

It was noted in [2, 3] that, in the $M = 2$ sector, the wavefunction corresponding to the roots $\pm\mathrm{i}/2$ is

$$\chi_{\pm\mathrm{i}/2}(j_1, j_2) = (-1)^{j_1}\delta_{j_1+1,j_2} + (-1)^{j_2}\delta_{j_1+N,j_2+1}. \tag{87}$$

Here we have made the periodicity of the chain explicit; note that it is essential that N is even for this state to exist. We shall see that if we take the limit $\lambda_\pm \to \pm\mathrm{i}/2$ along the path prescribed by the Bethe equations, we recover the wavefunction (87).

Consider $\lambda_\pm := \epsilon \pm \mathrm{i}(1+2\delta)/2$. We will take the limit $\epsilon \to 0, \delta \to 0$. As of yet, the signs of δ and ϵ are unspecified. To first order, the kinetic phase satisfies

$$\mathrm{e}^{\mathrm{i}k_+} = \mathrm{e}^{\mathrm{iRe}\,k_+}\,\mathrm{e}^{-\mathrm{Im}\,k_+} = \delta - \mathrm{i}\epsilon, \tag{88}$$

so that $\mathrm{e}^{-\mathrm{Im}\,k_+} = \sqrt{\delta^2+\epsilon^2}$, $\mathrm{e}^{\mathrm{iRe}\,k_+} = \sqrt{\frac{\delta-\mathrm{i}\epsilon}{\delta+\mathrm{i}\epsilon}}$. The scattering phase has (here, we denote $\Phi(k_+, k_-) = \phi(\lambda_+ - \lambda_-)$)

$$\tan\Phi(k_+, k_-)/2 = \mathrm{i}(1 - 2\,\mathrm{e}^{\mathrm{i}\Phi(k_+,k_-)}) = \lambda_+ - \lambda_- = \mathrm{i}(1+2\delta); \tag{89}$$

thus $\mathrm{e}^{\mathrm{i}\Phi} = -\delta$. Looking at the Bethe equations, we now see

$$\mathrm{e}^{\mathrm{i}k_+N} = -\mathrm{e}^{\mathrm{i}\Phi(k_+,k_-)} \Rightarrow (\delta - \mathrm{i}\epsilon)^N = \delta, \tag{90}$$

so that we must have $|\epsilon| \gg |\delta|$, from which we deduce

$$(-\mathrm{i})^N\epsilon^N = \delta, \qquad \mathrm{e}^{-\mathrm{Im}\,k_+} = |\epsilon|\,, \qquad \mathrm{e}^{\mathrm{iRe}\,k_+} = \mathrm{i}. \tag{91}$$

We see that, for both ϵ and δ to be real, we need N even. Furthermore,

$$\operatorname{sign}\delta = (-1)^{N/2}. \tag{92}$$

Let us turn our attention to the wavefunction. We write $\chi_{(\pm\mathrm{i}/2)}(j_1, j_2) = \chi^+_{\operatorname{sign}\delta} - \chi^-_{\operatorname{sign}\delta}$ where, for later convenience, we have defined

$$\chi^+_a(j_1, j_2) := \lim_{\substack{\delta\to 0}}^{|\epsilon|=(a\delta)^{1/N}} \mathrm{e}^{\mathrm{i}k_+j_1+\mathrm{i}k_-j_2}\,\mathrm{e}^{\mathrm{i}\Phi/2} \tag{93}$$

$$\chi^-_a(j_1, j_2) := \lim_{\substack{\delta\to 0}}^{|\epsilon|=(a\delta)^{1/N}} \mathrm{e}^{\mathrm{i}k_-j_1+\mathrm{i}k_+j_2}\,\mathrm{e}^{-\mathrm{i}\Phi/2}. \tag{94}$$

Inserting the first-order values just found,

$$\chi^\pm_a(j_1, j_2) = \mathrm{e}^{\mathrm{iRe}\,k(j_1+j_2)}\,\mathrm{e}^{\mp\mathrm{Im}\,k(j_1-j_2)}\,\mathrm{e}^{\mp\mathrm{i}\Phi/2} = \mathrm{i}^{j_1+j_2}(a\delta)^{\pm(j_1-j_2)/N}(-\delta)^{\pm 1/2},$$

so that

$$\chi^+_a(j_1, j_2) = -(a\delta)^{1/N}\delta^{-1/2}\left[a^{-1}(-1)^{N/2+j_2}\delta_{j_1+N,j_2+1} + O(\delta)\right], \tag{95}$$

$$\chi^-_a(j_1, j_2) = -(a\delta)^{1/N}\delta^{-1/2}\left[(-1)^{j_1}\delta_{j_1+1,j_2} + O(\delta)\right]. \tag{96}$$

We see that the prefactor, though divergent, is independent of position and therefore can be included in the normalization of the wavefunction $\chi^+_{\operatorname{sign}\delta} - \chi^-_{\operatorname{sign}\delta}$. Due to (92), it has the correct periodicity; we recover (87).

We did not have so specify the sign of ϵ in this derivation; it turns out that we can choose whether to approach the limit from the left or from the right half-plane.

We find the values of the quantum numbers when we consider the sum of the Bethe equations, namely,

$$\begin{aligned}\pi(J_+ + J_-) &= \lim_{\delta\to 0} N[\arctan(2\epsilon + \mathrm{i}(1+2\delta)) + \arctan(2\epsilon - \mathrm{i}(1+2\delta))] \\ &= N\operatorname{sign}\epsilon \lim_{\delta\to 0}\operatorname{sign}\delta\arctan|\delta|^{-1+1/N} = N\pi/2 \pmod{N\pi},\end{aligned} \tag{97}$$

so that the Bethe quantum numbers for the singular state at $M = 2$ are the half-integers

$$J_+ = \tfrac{1}{4}[\pm N - (2 - N \bmod 4)], \qquad J_- = \tfrac{1}{4}[\pm N + (2 - N \bmod 4)] \tag{98}$$

in agreement with (92). The sign of these quantum numbers is not uniquely determined: it equals the sign of ϵ we chose in the limiting procedure.

Naturally, the Bethe–Takahashi quantum number corresponding to a single two-string at the origin is $I^{(2)} = 0$.

5.3. Singular pair states at $M = 3$

For $M = 3$, one singular state is already known: the $M = 2$ state we just found, with an extra rapidity at infinity (i.e., momentum at zero). However, another choice for the momentum that respects the lattice inversion symmetry is $k_3 = \pi (\bmod 2\pi)$ (i.e., $\lambda_3 = 0$). Let us use $\lambda_\pm = \epsilon \pm \mathrm{i}(1 + 2\delta)/2$ and $|\epsilon| \gg |\delta|$ again.

The Bethe equation for λ_+ yields

$$\left[\frac{\epsilon + \mathrm{i}\delta}{\epsilon + \mathrm{i}(1+\delta)}\right]^N = -\mathrm{e}^{\mathrm{i}\Phi_{13}} \left[\frac{\delta}{1+\delta}\right]. \tag{99}$$

As $\lambda_3 \to 0, \lambda_+ \to \mathrm{i}/2$, we have $\mathrm{e}^{\mathrm{i}\Phi_{13}} = \mathrm{e}^{-\mathrm{i}\Phi_{23}} = 1/3$, so that, to first order, $(-\mathrm{i}\epsilon)^N = -\delta\, \mathrm{e}^{\mathrm{i}(\Phi_{13}-\Phi_{23})/2}$, and it turns out that we have to set $\operatorname{sign}\delta = (-1)^{1+N/2}$.

Given this limiting procedure, we can now write the wavefunction as

$$\begin{aligned}\chi(j_1, j_2, j_3) \propto{}& \left[\chi_a^+(j_1, j_2) - \chi_a^-(j_1, j_2)\right] \mathrm{e}^{\mathrm{i}k_3 j_3}\, \mathrm{e}^{\mathrm{i}(\Phi_{13}+\Phi_{23})/2} \\ &+ \left[\chi_a^+(j_2, j_3) - \chi_a^-(j_2, j_3)\right] \mathrm{e}^{\mathrm{i}k_3 j_1}\, \mathrm{e}^{-\mathrm{i}(\Phi_{13}+\Phi_{23})/2} \\ &+ \left[\chi_a^+(j_1, j_3)\, \mathrm{e}^{\mathrm{i}(\Phi_{13}-\Phi_{23})/2} - \chi_a^-(j_1, j_3)\, \mathrm{e}^{-\mathrm{i}(\Phi_{13}-\Phi_{23})/2}\right] \mathrm{e}^{\mathrm{i}k_3 j_2},\end{aligned} \tag{100}$$

where $a = (-1)^{1+N/2}\, \mathrm{e}^{\mathrm{i}(\Phi_{13}-\Phi_{23})/2}$.

Because the js are ordered, χ^+ is zero unless its arguments are j_1 and j_M, and χ^- vanishes in that case only. Using $\mathrm{e}^{\mathrm{i}k_3} = -1$ and the values from equations (95), (96), with the common prefactors divided out,

$$\begin{aligned}\chi_a^-(j_1, j_2) &= (-1)^{j_1} \delta_{j_1+1, j_2} \\ \chi_a^+(j_1, j_2) &= -\mathrm{e}^{-\mathrm{i}(\Phi_{13}-\Phi_{23})/2} (-1)^{j_2} \delta_{j_1+N, j_2+1},\end{aligned} \tag{101}$$

we find that the wavefunction equals

$$\begin{aligned}\chi_{(\pm \mathrm{i}/2, 0)}(j_1, j_2, j_3) &\propto (-1)^{j_3} \chi_1^-(j_1, j_2) + (-1)^{j_1} \chi_1^-(j_2, j_3) + (-1)^{j_2} \chi_1^+(j_1, j_3) \\ &\propto (-1)^{j_3+j_1} \delta_{j_1+1, j_2} + (-1)^{j_1+j_2} \delta_{j_2+1, j_3} + (-1)^{j_2+j_3} \delta_{j_1+N, j_3+1}.\end{aligned} \tag{102}$$

Note that this wavefunction can be formed by simply creating a down spin of momentum π on top of the $M = 2$ singular state.

The Bethe quantum numbers are

$$J_+ = \tfrac{1}{4}[\pm N - (N \bmod 4)], \qquad J_0 = 0, \qquad J_- = \tfrac{1}{4}[\pm N + (N \bmod 4)]. \tag{103}$$

The Bethe–Takahashi quantum numbers are

$$I^{(1)} = 0, \qquad I^{(2)} = 0. \tag{104}$$

Table 1. Highest-weight Bethe Ansatz solutions for $N = 8$, $M = 1$.

	$2J$	$2I_j$	λ	E_0
1.	0	0_1	0	−2
2.	−2	-2_1	−0.207 106 781 186 548	−1.707 106 781 186 55
3.	2	2_1	0.207 106 781 186 548	−1.707 106 781 18655
4.	−4	-4_1	−0.5	−1
5.	4	4_1	0.5	−1
6.	−6	-6_1	−1.207 106 781 186 55	−0.292 893 218 813 452
7.	6	6_1	1.207 106 781 186 55	−0.292 893 218 813 452

Table 2. Highest-weight Bethe Ansatz solutions for $N = 8$, $M = 2$. There are 15 states with all real solutions, and 5 with a single two-string.

	$2J$		$2I_j$		λ		E_0
1.	−1	1	-1_1	1_1	−0.114 121 737 195 075	0.114 121 737 195 075	−3.801 937 735 804 84
2.	−1	−3	-1_1	-3_1	−0.082 003 690 862 0831	−0.359 101 081 059 097	−3.267 035 098 361 37
3.	1	−3	1_1	-3_1	0.130 438 947 345 799	−0.378 439 593 963 216	−3.144 122 805 635 37
4.	−1	3	-1_1	3_1	−0.130 438 947 345 799	0.378 439 593 963 216	−3.144 122 805 635 37
5.	1	3	1_1	3_1	0.082 003 690 862 083	0.359 101 081 059 097	−3.267 035 098 361 37
6.	−1	−5	-1_1	-5_1	−0.053 960 768 395 4299	−0.914 799 098 278 114	−2.437 016 024 448 82
7.	1	−5	1_1	-5_1	0.155 070 403 217 499	−0.949 571 172 389 941	−2.258 652 022 504 15
8.	−1	5	-1_1	5_1	−0.155 070 403 217 499	0.949 571 172 389 941	−2.258 652 022 504 15
9.	1	5	1_1	5_1	0.053 960 768 395 4298	0.914 799 098 278 114	−2.4370 160 244 4882
10.	−3	3	-3_1	3_1	−0.398 736 694 441 202	0.398 736 694 441 202	−2.445 041 867 912 63
11.	−3	−5	-3_1	-5_1	−0.288 675 134 594 813	−0.866 025 403 784 438	−2
12.	−3	5	-3_1	5_1	−0.428 405 998 277 582	0.985 143 205 784 529	−1.562 983 975 551 18
13.	3	−5	3_1	-5_1	0.428 405 998 277 582	−0.985 143 205 784 529	−1.562 983 975 551 18
14.	3	5	3_1	5_1	0.288 675 134 594 813	0.866 025 403 784 438	−2
15.	−5	5	-5_1	5_1	−1.038 260 698 286 17	1.038 260 698 286 17	−0.753 020 396 282 533
16.	3	5	0_2		±0.5i		−1
17.	−5	−5	-2_2		−0.415 344 339 607 922 ± 0.499 530 117 286 392i		−0.855 877 194 364 632
18.	5	5	2_2		0.415 344 339 607 923 ± 0.499 530 117 286 392i		−0.855 877 194 364 631
19.	−7	−5	-4_2		−0.951 136 103 880 144 ± 0.544 496 295 465 675i		−0.474 312 879 134 482
20.	5	7	4_2		0.951 136 103 880 144 ± 0.544 496 295 465 675i		−0.474 312 879 134 482

5.4. Singular pair states at $M = 4$

Consider $M = 4$ and $\lambda_\pm := \epsilon \pm \mathrm{i}(1 + 2\delta)$. Apart from the solutions we just found, extended with the appropriate number of infinite rapidities, we can find a few more.

Note that for finite nonzero lambda, by symmetry, $\lambda_3 = -\lambda_4 =: \lambda$. The Bethe equation for λ_+ now gives

$$\delta = (-1)^{N/2}\,\mathrm{e}^{-\mathrm{i}(\Phi_{13}+\Phi_{14})}\epsilon^N. \tag{105}$$

By symmetry, $\Phi_{13} + \Phi_{14} = -\Phi_{23} - \Phi_{24} =: \Phi/2$, and the wavefunction can be written as

$$\begin{aligned}\chi(j_1, j_2, j_3, j_4) = {} & \chi^-_{(-1)^{N/2}\,\mathrm{e}^{\mathrm{i}\Phi}}(j_1, j_2)[\mathrm{e}^{\mathrm{i}k(j_3-j_4)}\,\mathrm{e}^{\mathrm{i}\Phi_{34}/2} - \mathrm{e}^{\mathrm{i}k(j_4-j_3)}\,\mathrm{e}^{-\mathrm{i}\Phi_{34}/2}] \\ & + \mathrm{e}^{\mathrm{i}\Phi}\chi^+_{(-1)^{N/2}\,\mathrm{e}^{\mathrm{i}\Phi}}(j_1, j_4)[\mathrm{e}^{\mathrm{i}k(j_2-j_3)}\,\mathrm{e}^{\mathrm{i}\Phi_{34}/2} - \mathrm{e}^{\mathrm{i}k(j_3-j_2)}\,\mathrm{e}^{-\mathrm{i}\Phi_{34}/2}] \\ & + \chi^-_{(-1)^{N/2}\,\mathrm{e}^{\mathrm{i}\Phi}}(j_3, j_4)[\mathrm{e}^{\mathrm{i}k(j_1-j_2)}\,\mathrm{e}^{\mathrm{i}\Phi_{34}/2} - \mathrm{e}^{\mathrm{i}k(j_2-j_1)}\,\mathrm{e}^{-\mathrm{i}\Phi_{34}/2}] \\ & + \chi^-_{(-1)^{N/2}\,\mathrm{e}^{\mathrm{i}\Phi}}(j_2, j_3)[\mathrm{e}^{\mathrm{i}k(j_1-j_4)}\,\mathrm{e}^{\mathrm{i}\Phi_{34}/2}\,\mathrm{e}^{\mathrm{i}\Theta} - \mathrm{e}^{\mathrm{i}k(j_4-j_1)}\,\mathrm{e}^{-\mathrm{i}\Phi_{34}/2}\,\mathrm{e}^{-\mathrm{i}\Theta}],\end{aligned} \tag{106}$$

Table 3. Highest-weight Bethe Ansatz solutions for $N = 8$, $M = 3$. There are 10 solutions with all reals, 15 with one two-string and 3 with a single three-string. We give both Bethe J and Bethe–Takahashi I quantum numbers. The latter are subscripted by the length of the string for which they are quantum numbers.

1.	0	−2	2	0_1	-2_1	2_1	0	−0.263 913 376 890 051	0.263 913 376 890 051	−5.128 419 063 844 58
2.	0	−2	−4	0_1	-2_1	-4_1	0.053 719 221 868 1322	−0.193 583 000 298 505	−0.650 848 824 168 377	−4.458 738 508 894 83
3.	0	2	−4	0_1	2_1	-4_1	0.023 817 698 135 0052	0.288 834 213 916 909	−0.720 503 071 221 302	−4.145 148 373 920 72
4.	−2	2	−4	-2_1	2_1	-4_1	−0.209 705 666 535 535	0.306 323 520 147 911	−0.681 661 096 925 392	−3.854 637 679 718 46
5.	0	−2	4	0_1	-2_1	4_1	−0.023 817 698 135 0052	−0.288 834 213 916 909	0.720 503 071 221302	−4.145 148 373 92072
6.	0	2	4	0_1	2_1	4_1	−0.053 719 221 868 1322	0.193 583 000 298 505	0.650 848 824 168 377	−4.458 738 508 894 83
7.	−2	2	4	-2_1	2_1	4_1	−0.306 323 520 147 911	0.209 705 666 535 536	0.681 661 096 925 392	−3.854 637 679 71846
8.	0	−4	4	0_1	-4_1	4_1	0	−0.763 017 839 489 689	0.763 017 839 489 689	−3.201 639 675 723 41
9.	−2	−4	4	-2_1	-4_1	4_1	−0.232 643 790 002 621	−0.723 239 730 965 897	0.793 819 433 881 308	−2.858 923 549 710 26
10.	2	−4	4	2_1	-4_1	4_1	0.232 643 790 002 621	−0.793 819 433 881 308	0.723 239 730 965 896	−2.858 923 549 710 26
11.	0	4	4	0_1		0_2	0	±0.5i		−3
12.	0	−6	−4	0_1		-2_2	0.088 835 948 519 7147	−0.620 939 972 021 564 ± 0.511 033 534 711 325i		−2.628 378 426 883 06
13.	0	4	6	0_1		2_2	−0.088 835 948 519 7147	0.620 939 972 021 564 ± 0.511 033 534 711 325i		−2.628 378 426 883 06
14.	−2	4	4	-2_1		0_2	−0.278 658 967 238 795	0.116 265 462 834 909 ± 0.499 999 922 966 273i		−2.512 683 203 063 87
15.	2	−4	−4	2_1		0_2	0.278 658 967 238 795	−0.116 265 462 834 909 ± 0.499 999 922 966 273i		−2.512 683 203 063 87
16.	−4	4	4	-4_1		0_2	−0.771 265 809 851 148	0.213 409 859 292 069 ± 0.499 994 150 006 002i		−1.548 394 037 044 22
17.	4	−4	−4	4_1		0_2	0.771 265 809 851 148	−0.213 409 859 292 069 ± 0.499 994 150 006 002i		−1.548 394 037 044 22
18.	−2	−6	−4	-2_1		-2_2	−0.139 811 316 778 799	−0.550 392 917 633 605 ± 0.506 870 069 123 91i		−2.596 968 283 237 32
19.	2	−6	−4	2_1		-2_2	0.347 810 384 779 931	−0.673 905 192 389 966 ± 0.514 426 127 068 346i		−2
20.	−4	−6	−4	-4_1		-2_2	−0.595 672 174 122 518	−0.314 924 940 488 343 ± 0.500 176 262 487 235i		−1.734 547 288 424 51
21.	4	−6	−4	4_1		-2_2	0.865 745 241 274 482	−0.740 655 728 477 336 ± 0.519 219 952 109 156i		−1.107 306 642 344 78
22.	−2	4	6	-2_1		2_2	−0.347 810 384 779 931	0.673 905 192 389 965 ± 0.514 426 127 068 346i		−2
23.	2	4	6	2_1		2_2	0.139 811 316 778 799	0.550 392 917 633 605 ± 0.506 870 069 123 91i		−2.596 968 283 237 31
24.	−4	4	6	-4_1		2_2	−0.865 745 241 274 482	0.740 655 728 477 336 ± 0.519 219 952 109 156i		−1.107 306 642 344 78
25.	4	4	6	4_1		2_2	0.595 672 174 122 519	0.314 924 940 488 342 ± 0.500 176 262 487 235i		−1.734 547 288 424 51
26.	6	0	10		0_3		±1.000 922 821141 08i		0	−0.669 941 260 432 018
27.	−8	−4	−6		-2_3		−0.615 758 454 071 295 ± 0.988 145 332 430 968i		−0.631 196 681 886 563	−0.554 274 006 757 972
28.	6	4	8		2_3		0.615 758 454 071 295 ± 0.988 145 332 430 968i		0.631 196 681 886 563	−0.554 274 006 757 972

where an extra phase factor has to be introduced for the terms in which the sites associated with λ_3, λ_4 surround the sites associated with the string,

$$\Theta := \tfrac{1}{2}(\Phi_{13} + \Phi_{23} - \Phi_{14} - \Phi_{24}) = 2\arctan\tfrac{2}{3}\lambda + 2\arctan 2\lambda. \qquad (107)$$

The Bethe equation for λ can be reduced, using symmetry and the values $\lambda_\pm = \pm\,\mathrm{i}/2$, to

$$(N-2)\arctan 2\lambda - \arctan\tfrac{2}{3}\lambda = \pi J_3. \qquad (108)$$

For $J_3 < (N-3)/2$, the solutions of (108) are real and the Bethe–Takahashi quantum numbers are $I^{(2)} = 0$ and $I_2^{(1)} = -I_1^{(1)} = J_3$. For $J_3 = (N-2)/2$, λ is imaginary; this configuration can be identified as a *deviated four-string* with $I^{(4)} = 0$.

The Bethe quantum numbers associated with $\lambda_\pm$ are the same as in the $M = 2$ cases.

5.5. Singular pair states at general M

We will now generalize the approach of the last sections. Again, we only consider highest-weight states. Consider a configuration of M roots, two of which form a singular two-string, $\lambda\pm := \epsilon \pm \frac{\mathrm{i}}{2}(1-2\delta)$. The other roots must be distributed symmetrically; the total momentum is π for even M, and 0 for odd M. For ease of notation, let the number of non-singular nonzero roots be $\tilde{M} := M - 2 - (M \bmod 2)$; we will indicate the particle at $k_0 = \pi$ with the index 0, and the two singular roots with $\pm$. The set is ordered $+, -, 0, 1, \ldots, \tilde{M}$, such that we always have $k_a = -k_{\tilde{M}-a+1}$ for $a > 0$.

Table 4. Highest-weight Bethe Ansatz solutions for $N = 8$, $M = 4$. There is 1 state with all real solutions, 6 with one two-string, 5 with one three-string, 1 single four-string and 1 with two two-strings.

	$2J$				$2I_j$				λ				E_0
1.	−1	1	−3	3	-1_1	1_1	-3_1	3_1	−0.129 472 946 374 929	0.129 472 946 374 929	−0.525 012 102 223 667	0.525 012 102 223 667	−5.651 093 408 937 18
2.	−1	1	3	5	-1_1	1_1	0_2		−0.142 469 067 830 567	0.142 469 067 830 566	±0.5i		−4.699 628 148 275 32
3.	−1	−3	3	5	-1_1	-3_1	0_2		−0.147 012 611 196 141	−0.557 070 238 574 442	0.352 041 424 885 292 ± 0.500 558 169 643 331i		−3.618 033 988 749 89
4.	1	−3	3	5	1_1	-3_1	0_2		0.121 186 177 969 172	−0.571 611 177 186 439	0.225 212 499 608 634 ± 0.500 028 862 163 533i		−3.707 106 781 186 55
5.	−1	3	−5	−3	-1_1	3_1	0_2		−0.121 186 177 969 172	0.571 611 177 186 439	−0.225 212 499 608 634 ± 0.500 028 862 163 533i		−3.707 106 781 18655
6.	1	3	−5	−3	1_1	3_1	0_2		0.147 012 611 196 141	0.557 070 238 574 442	−0.352 041 424 885 292 ± 0.500 558 169 643 331i		−3.618 033 988 749 89
7.	−3	3	3	5	-3_1	3_1	0_2		−0.563 825 262 393 496	0.563 825 262 393 496	±0.5i		−2.760 876 721 743 45
8.	1	7	−1	−7	0_1	0_3			−0.041 309 127 524 556	±1.025 705 081 230 74i		0.041 309 127 524 556	−2.726 109 445 035 78
9.	−1	7	−1	9	-2_1	0_3			−0.244 333 193 771 166	0.080 273 043 189 8699 ± 1.005 588 273 959 93i		0.083 787 107 391 4291	−2.292 893 218 813 45
10.	1	−9	1	−7	2_1	0_3			0.244 333 193 771 166	−0.080 273 043 189 8705 ± 1.005 588 273 959 93i		−0.083 787 107 391 4297	−2.292 893 218 813 45
11.	−3	5	3	7	-4_1	0_3			−0.669 122 922 881 511	0.224 281 457 794 713 ± 1.002 247 276 506 61i		0.220 560 007 292 084	−1.381 966 011 250 11
12.	3	−7	−3	−5	4_1	0_3			0.669 122 922 881 511	−0.224 281 457 794 714 ± 1.002 247 276 506 61i		−0.220 560 007 292 085	−1.381 966 011 250 11
13.	5	3	5	7	0_4				±1.556 126 503 577 05i		±0.5i		−0.539 495 129 981 236
14.	−5	−3	3	5	-1_2	1_2			−0.463 264 727 589 031 ± 0.502 293 853 569 903i		0.463 264 727 589 031 ± 0.502 293 853 569 903i		−1.622 797 146 027 04

Table 5. Highest-weight Bethe Ansatz solutions for $N = 10$, $M = 1$.

	$2J$	$2I_j$	λ	E_0
1.	0	0_1	0	−2
2.	−2	-2_1	−0.162 459 848 116 453	−1.809 016 994 374 95
3.	2	2_1	0.162 459 848 116 453	−1.809 016 994 374 95
4.	−4	-4_1	−0.363 271 264 002 68	−1.309 016 994 374 95
5.	4	4_1	0.363 271 264 002 68	−1.309 016 994 374 95
6.	−6	-6_1	−0.688 190 960 235 587	−0.690 983 005 625 053
7.	6	6_1	0.688 190 960 235 587	−0.690 983 005 625 053
8.	−8	-8_1	−1.538 841 768 587 63	−0.190 983 005 625 053
9.	8	8_1	1.538 841 768 587 63	−0.190 983 005 625 053

Table 6. Highest-weight Bethe Ansatz solutions for $N = 10$, $M = 2$. There are 28 states with only real roots and 7 two-strings.

	$2J$		$2I_j$		λ		E_0
1.	−1	1	-1_1	1_1	−0.088 163 490 354 2325	0.088 163 490 354 2325	−3.879 385 241 571 82
2.	−1	−3	-1_1	-3_1	−0.069 203 328 842 458	−0.267 198 865 360 809	−3.518 124 245 139 35
3.	1	−3	1_1	-3_1	0.097 718 323 279 698	−0.277 820 084 547 718	−3.454 611 568 467 11
4.	−1	3	-1_1	3_1	−0.097 718 323 279 698	0.277 820 084 547 718	−3.454 611 568 467 11
5.	1	3	1_1	3_1	0.069 203 328 842 4579	0.267 198 865 360 809	−3.518 124 245 139 35
6.	−1	−5	-1_1	-5_1	−0.055 907 937 962 4147	−0.547 952 407 065 598	−2.883 978 033 174 47
7.	1	−5	1_1	-5_1	0.109 874 636 222 197	−0.563 039 149 833 424	−2.789 683 340 115 66
8.	−1	5	-1_1	5_1	−0.109 874 636 222 197	0.563 039 149 833 424	−2.789 683 340 115 66
9.	1	5	1_1	5_1	0.055 907 937 962 4146	0.547 952 407 065 598	−2.883 978 033 174 47
10.	−1	−7	-1_1	-7_1	−0.034 695 289 328 3356	−1.239 447 329 308 34	−2.270 335 251 605 37
11.	1	−7	1_1	-7_1	0.128 695 417 975 475	−1.265 055 001 1227	−2.145 949 713 911 79
12.	−1	7	-1_1	7_1	−0.128 695 417 975 475	1.265 055 001 1227	−2.145 949 713 911 79
13.	1	7	1_1	7_1	0.034 695 289 328 3355	1.239 447 329 308 34	−2.270 335 251 605 37
14.	−3	3	-3_1	3_1	−0.288 675 134 594 813	0.288 675 134 594 813	−3
15.	−3	−5	-3_1	-5_1	−0.237 111 858 893 408	−0.529 263 808 491 695	−2.575 984 523 886 96
16.	−3	5	-3_1	5_1	−0.302 031 547 9501	0.577 921 130 897 795	−2.321 492 052 079 01
17.	−3	−7	-3_1	-7_1	−0.207 106 781 186 548	−1.207 106 781 186 55	−2
18.	−3	7	-3_1	7_1	−0.322 476 279 501 619	1.290 419 240 201 93	−1.673 537 303 6666
19.	3	−5	3_1	-5_1	0.302 031 547 9501	−0.577 921 130 897 795	−2.321 492 052 079 01
20.	3	5	3_1	5_1	0.237 111 858 893 408	0.529 263 808 491 695	−2.575 984 523 886 96
21.	3	−7	3_1	-7_1	0.322 476 279 501 619	−1.290 419 240 201 93	−1.673 537 303 6666
22.	3	7	3_1	7_1	0.207 106 781 186 548	1.207 106 781 186 55	−2
23.	−5	5	-5_1	5_1	−0.595 876 796 297 105	0.595 876 796 297 105	−1.652 703 644 666 14
24.	−5	−7	-5_1	-7_1	−0.441 763 667 008 89	−1.152 038 878 385 51	−1.440 222 720 585 52
25.	−5	7	-5_1	7_1	−0.623 646 218 099 693	1.321 786 200 3247	−1.032 913 373 828 82
26.	5	−7	5_1	-7_1	0.623 646 218 099 693	−1.321 786 200 3247	−1.032 913 373 828 82
27.	5	7	5_1	7_1	0.441 763 667 008 89	1.152 038 878 385 51	−1.440 222 720 585 52
28.	−7	7	-7_1	7_1	−1.373 738 709 727 31	1.373 738 709 727 31	−0.467 911 113 762 044
29.	5	5		0_2	±0.5i		−1
30.	−7	−5		-2_2	−0.324 895 275 386 474 ± 0.500 007 934 154 676i		−0.904 440 509 547 209
31.	5	7		2_2	0.324 895 275 386 474 ± 0.500 007 934 154 676i		−0.904 440 509 547 209
32.	−7	−7		-4_2	−0.733 883 240 086 612 ± 0.494 583 435 259 682i		−0.661 055 258 538 801
33.	7	7		4_2	0.733 883 240 086 612 ± 0.494 583 435 259 683i		−0.661 055 258 538 801
34.	−9	−7		-6_2	−1.308 874 184 404 64 ± 0.581 686 455 906 516i		−0.327 672 105 453 332
35.	7	9		6_2	1.308 874 184 404 64 ± 0.581 686 455 906 516i		−0.327 672 105 453 333

Table 7. Highest-weight Bethe Ansatz solutions for $N = 10$, $M = 3$. There are 35 states with only real roots, 35 states with 1 two-string and 5 three-strings.

	$2J$			$2I_j$			λ			E_0
1.	0	−2	2	0_1	-2_1	2_1	0	−0.194 145 912 742 908	0.194 145 912 742 908	−5.475 931 869 054 44
2.	0	−2	−4	0_1	-2_1	-4_1	0.030 448 405 969 0835	−0.158 812 988 572 359	−0.417 525 851 428 647	−4.987 662 857 976 36
3.	0	2	−4	0_1	2_1	-4_1	0.011 905 285 767 2312	0.206 226 507 953 237	−0.446 703 652 043 529	−4.820 334 627 141 44
4.	−2	2	−4	-2_1	2_1	-4_1	−0.168 609 880 330 85	0.216 339 433 204 765	−0.431 009 948 231 322	−4.627 803 961 483 96
5.	0	−2	4	0_1	-2_1	4_1	−0.011 905 285 767 2312	−0.206 226 507 953 237	0.446 703 652 043 529	−4.820 334 627 141 44
6.	0	2	4	0_1	2_1	4_1	−0.030 448 405 969 0835	0.158 812 988 572 359	0.417 525 851 428 647	−4.987 662 857 976 36
7.	−2	2	4	-2_1	2_1	4_1	−0.216 339 433 204 765	0.168 609 880 330 85	0.431 009 948 231 322	−4.627 803 961 483 96
8.	0	−2	−6	0_1	-2_1	-6_1	0.048 699 965 731 3438	−0.134 805 852 072 197	−0.959 436 831 888 961	−4.272 836 485 948 63
9.	0	2	−6	0_1	2_1	-6_1	0.030 800 784 679 8048	0.224 751 050 748 26	−1.012 966 828 840 85	−4.048 078 795 262 54
10.	−2	2	−6	-2_1	2_1	-6_1	−0.144 039 928 514 148	0.234 610 332 664 757	−0.984 119 425 039 908	−3.896 201 216 260 45
11.	0	−2	6	0_1	-2_1	6_1	−0.030 800 784 679 8048	−0.224 751 050 748 26	1.012 966 828 840 85	−4.048 078 795 262 54
12.	0	2	6	0_1	2_1	6_1	−0.048 699 965 731 3438	0.134 805 852 072 197	0.959 436 831 888 961	−4.272 836 485 948 63
13.	−2	2	6	-2_1	2_1	6_1	−0.234 610 332 664 757	0.144 039 928 514 148	0.984 119 425 039 908	−3.896 201 216 260 45
14.	0	−4	4	0_1	-4_1	4_1	0	−0.462 305 603 179 552	0.462 305 603 179 552	−4.156 443 643 217 49
15.	−2	−4	4	-2_1	-4_1	4_1	−0.180 394 151 048 265	−0.446 405 368 876 987	0.476 104 810 318 311	−3.931 476 369 392 98
16.	2	−4	4	2_1	-4_1	4_1	0.180 394 151 048 265	−0.476 104 810 318 311	0.446 405 368 876 987	−3.931 476 369 392 98
17.	0	−4	−6	0_1	-4_1	-6_1	0.058 435 206 208 11	−0.354 182 982 563 82	−0.915 295 996 328 78	−3.764 458 978 647 18
18.	−2	−4	−6	-2_1	-4_1	-6_1	−0.114 921 044 163 806	−0.342 596 892 874 812	−0.888 703 120 312 034	−3.741 527 388 711 19
19.	2	−4	−6	2_1	-4_1	-6_1	0.245 193 616 721 327	−0.365 361 975 424 906	−0.939 028 346 244 647	−3.357 880 903 404 88
20.	0	−4	6	0_1	-4_1	6_1	−0.018 885 646 061 2995	−0.485 909 456 596 173	1.040 982 063 899 09	−3.400 641 477 087 66
21.	−2	−4	6	-2_1	-4_1	6_1	−0.198 436 860 763 52	−0.469 682 684 730 587	1.065 257 638 598 04	−3.151 387 818 866
22.	2	−4	6	2_1	-4_1	6_1	0.155 381 755 8101	−0.499 539 838 699 096	1.012 130 460 854 51	−3.217 122 142 309 02
23.	0	4	−6	0_1	4_1	-6_1	0.018 885 646 061 2995	0.485 909 456 596 173	−1.040 982 063 899 09	−3.400 641 477 087 66
24.	−2	4	−6	-2_1	4_1	-6_1	−0.155 381 755 8101	0.499 539 838 699 096	−1.012 130 460 854 51	−3.217 122 142 309 02
25.	2	4	−6	2_1	4_1	-6_1	0.198 436 860 763 52	0.469 682 684 730 587	−1.065 257 638 598 04	−3.151 387 818 866
26.	0	4	6	0_1	4_1	6_1	−0.058 435 206 208 11	0.354 182 982 563 82	0.915 295 996 328 78	−3.764 458 978 647 18
27.	−2	4	6	-2_1	4_1	6_1	−0.245 193 616 721 327	0.365 361 975 424 906	0.939 028 346 244 646	−3.357 880 903 404 87
28.	2	4	6	2_1	4_1	6_1	0.114 921 044 163 806	0.342 596 892 874 812	0.888 703 120 312 033	−3.741 527 388 711 19
29.	0	−6	6	0_1	-6_1	6_1	0	−1.085 060 280 531 22	1.085 060 280 531 22	−2.700 596 159 221 18
30.	−2	−6	6	-2_1	-6_1	6_1	−0.172 721 676 586 505	−1.056 154 427 580 59	1.108 590 697 4044	−2.491 030 131 662 12
31.	2	−6	6	2_1	-6_1	6_1	0.172 721 676 586 505	−1.108 590 697 4044	1.056 154 427 580 59	−2.491 030 131 662 12
32.	−4	4	−6	-4_1	4_1	-6_1	−0.378 554 526 037 619	0.513 602 776 922 909	−0.966 214 460 382 166	−2.666 897 738 135 68
33.	−4	4	6	-4_1	4_1	6_1	−0.513 602 776 922 909	0.378 554 526 037 619	0.966 214 460 382 166	−2.666 897 738 135 68
34.	−4	−6	6	-4_1	-6_1	6_1	−0.398 349 213 977 874	−1.008 908 397 017 14	1.132 684 969 007	−1.943 962 027 256 95
35.	4	−6	6	4_1	-6_1	6_1	0.398 349 213 977 874	−1.132 684 969 007	1.008 908 397 017 14	−1.943 962 027 256 95
36.	0	4	6	0_1		0_2	0	±0.5i		−3
37.	0	−6	−6	0_1		-2_2	0.056 530 871 633 5665	−0.455 413 212 774 007 ± 0.499 668 130 106 944i		−2.804 762 479 918 06
38.	0	6	6	0_1		2_2	−0.056 530 871 633 5665	0.455 413 212 774 007 ± 0.499 668 130 106 944i		−2.804 762 479 918 06
39.	0	−8	−6	0_1		-4_2	0.090 425 155 129 218	−1.000 335 208 475 08 ± 0.542 526 961 485 32i		−2.393 642 470 327 58
40.	0	6	8	0_1		4_2	−0.090 425 155 129 218	1.000 335 208 475 08 ± 0.542 526 961 485 32i		−2.393 642 470 327 59
41.	−2	4	6	-2_1		0_2	−0.200 172 585 679 199	0.066 743 480 945 816 ± 0.500 000 000 004 612i		−2.719 292 485 021 54
42.	2	−6	−4	2_1		0_2	0.200 172 585 679 199	−0.066 743 480 945 8161 ± 0.500 000 000 004 612i		−2.719 292 485 021 54
43.	−4	4	6	-4_1		0_2	−0.468 771 675 793 569	0.125 508 670 454 143 ± 0.500 000 001 863 501i		−2.048 894 760 084 65
44.	4	−6	−4	4_1		0_2	0.468 771 675 793 569	−0.125 508 670 454 143 ± 0.500 000 001 863 501i		−2.048 894 760 084 65
45.	−6	4	6	-6_1		0_2	−1.063 399 255 453 41	0.191 077 192 208 424 ± 0.500 000 078 520 713i		−1.326 877 555 121 63
46.	6	−6	−4	6_1		0_2	1.063 399 255 453 41	−0.191 077 192 208 424 ± 0.500 000 078 520 713i		−1.326 877 555 121 63
47.	−2	−6	−6	-2_1		-2_2	−0.124 984 311 180 819	−0.403 681 825 206 182 ± 0.499 855 904 311 68i		−2.743 229 696 234 72
48.	2	−6	−6	2_1		-2_2	0.246 221 603 057 244	−0.493 540 317 657 487 ± 0.499 458 237 714 188i		−2.416 275 404 445 73
49.	−4	−6	−6	-4_1		-2_2	−0.378 918 428 348 842	−0.302 793 293 395 104 ± 0.499 987 591 712 302i		−2.186 553 388 207 35
50.	4	−6	−6	4_1		-2_2	0.516 773 005 230 149	−0.532 034 316 797 688 ± 0.499 172 688 023 818i		−1.749 685 891 892 08
51.	−6	−6	−6	-6_1		-2_2	−0.964 650 865 110 933	−0.165 525 974 819 192 ± 0.499 999 975 680 385i		−1.396 863 680 357 72
52.	6	−6	−6	6_1		-2_2	1.137 888 360 120 54	−0.586 251 077 568 763 ± 0.498 594 420 799 957i		−1.072 488 255 3555
53.	−2	6	6	-2_1		2_2	−0.246 221 603 057 244	0.493 540 317 657 487 ± 0.499 458 237 714 188i		−2.416 275 404 445 73
54.	2	6	6	2_1		2_2	0.124 984 311 180 819	0.403 681 825 206 181 ± 0.499 855 904 311 68i		−2.743 229 696 234 72
55.	−4	6	6	-4_1		2_2	−0.516 773 005 230 149	0.532 034 316 797 688 ± 0.499 172 688 023 818i		−1.749 685 891 892 08
56.	4	6	6	4_1		2_2	0.378 918 428 348 842	0.302 793 293 395 103 ± 0.499 987 591 712 302i		−2.186 553 388 207 35
57.	−6	6	6	-6_1		2_2	−1.137 888 360 120 54	0.586 251 077 568 763 ± 0.498 594 420 799 957i		−1.072 488 255 3555
58.	6	6	6	6_1		2_2	0.964 650 865 110 933	0.165 525 974 819 191 ± 0.499 999 975 680 385i		−1.396 863 680 357 72
59.	−2	−8	−6	-2_1		-4_2	−0.076 805 033 077 0082	−0.966 512 713 944 059 ± 0.539 831 327 733 351i		−2.427 272 732 829 41
60.	2	−8	−6	2_1		-4_2	0.278 433 506 109 15	−1.030 969 147 7318 ± 0.544 998 433 128 15i		−1.969 281 144 0996
61.	−4	−8	−6	-4_1		-4_2	−0.269 027 874 024 561	−0.915 978 266 911 757 ± 0.535 574 531 367 297i		−2.050 427 292 7206
62.	4	−8	−6	4_1		-4_2	0.556 876 840 014 352	−1.066 553 398 1297 ± 0.548 034 324 702 444i		−1.319 265 616 907 09
63.	−6	−8	−6	-6_1		-4_2	−0.656 499 569 607 335	−0.739 985 156 258 925 ± 0.515 757 553 318 274i		−1.348 612 181 134
64.	6	−8	−6	6_1		-4_2	1.210 119 861 365 82	−1.122 760 285 1135 ± 0.553 479 313 376 483i		−0.693 750 215 378 979
65.	−2	6	8	-2_1		4_2	−0.278 433 506 109 15	1.030 969 147 7318 ± 0.544 998 433 128 149i		−1.969 281 144 0996
66.	2	6	8	2_1		4_2	0.076 805 033 077 0082	0.966 512 713 944 059 ± 0.539 831 327 733 351i		−2.427 272 732 829 41
67.	−4	6	8	-4_1		4_2	−0.556 876 840 014 352	1.066 553 398 1297 ± 0.548 034 324 702 444i		−1.319 265 616 907 09

Table 7. (Continued.)

	$2J$			$2I_j$		λ		E_0
68.	4	6	8	4_1	4_2	0.269 027 874 024 561	0.915 978 266 911 757 ± 0.535 574 531 367 297i	−2.050 427 292 7206
69.	−6	6	8	-6_1	4_2	−1.210 119 861 365 82	1.122 760 285 1135 ± 0.553 479 313 376 483i	−0.693 750 215 378 979
70.	6	6	8	6_1	4_2	0.656 499 569 607 335	0.739 985 156 258 924 ± 0.515 757 553 318 274i	−1.348 612 181 134
71.	8	0	−8		0_3	±1.000 101 739 815 03i	0	−0.667 028 328 506 892
72.	−10	−4	−8		-2_3	−0.484 820 589 178 045 ± 0.999 766 941 293 111i	−0.486 503 017 249 458	−0.600 209 427 262 533
73.	8	4	10		2_3	0.484 820 589 178 044 ± 0.999 766 941 293 111i	0.486 503 017 249 457	−0.600 209 427 262 534
74.	−10	−6	−8		-4_3	−1.026 228 172 4686 ± 1.018 929 711 044 93i	−1.078 725 362 067 45	−0.413 312 403 154 196
75.	8	6	10		4_3	1.026 228 172 4686 ± 1.018 929 711 044 93i	1.078 725 362 067 45	−0.413 312 403 154 196

The Bethe equation for λ_+ gives

$$\delta = \epsilon^N (-1)^{N/2} (-1)^M \prod_{\beta=0}^{\tilde{M}} \mathrm{e}^{-\mathrm{i}\Phi_{1\beta}}, \tag{109}$$

where Φ_{10} is understood to be zero if M is even.

Consider the Bethe wavefunction (5). There will be one nonzero term with χ^+: the one involving $\chi^+(j_1, j_M)$. This term has a nontrivial scattering with the singular string, equal to $\mathrm{e}^{-\mathrm{i}(\sum_{\beta=0}^{M} \Phi_{+\beta} - \Phi_{-\beta})}$; again, this cancels against the factor that arises taking the limit as above.

Another nontrivial scattering phase occurs when the sites j_p, $j_{p+1} = j_p + 1$ are surrounded by a pair of sites associated with opposite momenta, yielding a phase

$$\begin{aligned} \Theta_\beta &:= \Phi(k_+, k_\beta) + \Phi(k_-, k_\beta) - \Phi(k_+, -k_\beta) - \Phi(k_-, -k_\beta) \\ &= -2[\Phi(k_+, |k_\beta|) + \Phi(k_-, |k_\beta|)], \end{aligned} \tag{110}$$

for $b \leqslant \tilde{M}/2$.

Moreover, only such permutations need to be retained in the sum as to make it possible for the sites involved in the singular complex to be adjacent. With these considerations, the Bethe wavefunction becomes

$$\begin{aligned} \chi_{\pm \mathrm{i}/2,\{k\}}(\{j\}) \propto \sum_{\mathcal{P}} &(-1)^{[\mathcal{P}]} \big[(-1)^{j_{\mathcal{P}(+)}} \delta_{\mathcal{P}(-),1+\mathcal{P}(+)} \delta_{j_{\mathcal{P}(+)}+1, j_{1+\mathcal{P}(+)}} \\ &+ (-1)^{j_{1+\mathcal{P}(+)}} \delta_{1+\mathcal{P}(-), M+\mathcal{P}(+)} \delta_{j_{\mathcal{P}(+)}+N, j_{1+\mathcal{P}(+)}+1} \big] \\ &\times \mathrm{e}^{\mathrm{i} \sum_{n=0}^{\tilde{M}} [k_n j_{\mathcal{P}n} + \frac{1}{2} \sum_{0 \leqslant m \leqslant \tilde{M}}^{\mathcal{P}m > \mathcal{P}n} \Phi_{mn}]} \\ &\times \mathrm{e}^{\mathrm{i} \sum_{n=1}^{\tilde{M}/2} [\Phi(k_+, |k_n|) + \Phi(k_-, |k_n|)][1 + \mathrm{sign}(\mathcal{P}(+) - \mathcal{P}n) \mathrm{sign}(\mathcal{P}(\tilde{M} - n + 1) - \mathcal{P}(-))]}. \end{aligned} \tag{111}$$

Note that, for convenience, the permutations $\mathcal{P}$ are the inverse of those in the earlier expression for the Bethe wavefunction (5). The permutation $\mathcal{P}$ is understood to be a map from $\{+, -, 0, 1, \ldots, \tilde{M}\}$ to $\{1, \ldots, M\}$.

We can make this expression slightly less ugly by splitting up the permutation $\mathcal{P}$ such that $\mathcal{P} = \mathcal{P}_{+,a} \mathcal{P}_{-,(a+1)} \mathcal{Q}_a$, where the permutation $\mathcal{Q}_a$ maps $\{0, 1, \ldots, \tilde{M}\}$ to $\{1, \ldots, a-1, a+2, \ldots, M\}$. Note that $[\mathcal{Q}_a] = [\mathcal{P}]$; this separation is possible because the Kronecker symbols in the sum select only those permutations that map $+, -$ onto the neighbors $a, a+1$. Thus, the general Bethe wavefunction in the presence of a singular string reads

$$\begin{aligned} \chi_{\pm \mathrm{i}/2,\{k\}}(\{j\}) \propto \sum_{a}^{1\ldots N} &\big[(-1)^{j_a} \delta_{j_a+1, j_{a+1}} + (-1)^{j_{a+1}} \delta_{j_a+N, j_{a+1}+1} \big] \\ &\times \sum_{\mathcal{Q}_a} (-1)^{[\mathcal{Q}_a]} \, \mathrm{e}^{\mathrm{i} \sum_{n=1}^{\tilde{M}} [k_n j_{\mathcal{Q}n} + \frac{1}{2} \sum_{0 \leqslant m \leqslant \tilde{M}}^{\mathcal{Q}m > \mathcal{Q}n} \Phi_{mn}]} \\ &\times \mathrm{e}^{\frac{\mathrm{i}}{2} \sum_{n=1}^{\tilde{M}} [\Phi(k_+, |k_n|) + \Phi(k_-, |k_n|)][1 - \mathrm{sign}(a - \mathcal{Q}n) \, \mathrm{sign}(a - \mathcal{Q}(\tilde{M} - n + 1))]}. \end{aligned} \tag{112}$$

Table 8. Highest-weight Bethe Ansatz solutions for $N = 10$, $M = 4$. Real: 15; one two-string: 45; one three-string: 21; one four-string: 3; two two-strings: 6.

	$2J$				$2I_j$				λ				E_0
1.	−1	1	−3	3	-1_1	1_1	-3_1	3_1	−0.098 282 545 025 1129	0.098 282 545 025 1129	−0.338 864 450 851 479	0.338 864 450 851 479	−6.592 207 346 738 67
2.	−1	1	−3	−5	-1_1	1_1	-3_1	-5_1	−0.048 434 606 508 8534	0.147 273 674 497 013	−0.267 004 842 580 402	−0.708 181 369 437 459	−6.043 279 374 312 69
3.	−1	1	3	−5	-1_1	1_1	3_1	-5_1	−0.078 404 059 108 8991	0.114 862 714 354 582	0.358 219 857 377 605	−0.789 251 476 492 64	−5.746 164 916 732 58
4.	−1	−3	3	−5	-1_1	-3_1	3_1	-5_1	−0.059 307 110 145 4481	−0.279 010 526 458 747	0.384 540 608 668 618	−0.731 224 480 925 44	−5.391 236 100 350 74
5.	1	−3	3	−5	1_1	-3_1	3_1	-5_1	0.124 662 932 656 233	−0.289 919 038 880 709	0.370 868 294 394 876	−0.754 237 921 414 972	−5.280 490 100 407 69
6.	−1	1	−3	5	-1_1	1_1	-3_1	5_1	−0.114 862 714 354 582	0.078 404 059 108 8991	−0.358 219 857 377 605	0.789 251 476 492 64	−5.746 164 916 732 58
7.	−1	1	3	5	-1_1	1_1	3_1	5_1	−0.147 273 674 497 013	0.048 434 606 508 8534	0.267 004 842 580 402	0.708 181 369 437 459	−6.043 279 374 312 69
8.	−1	−3	3	5	-1_1	-3_1	3_1	5_1	−0.124 662 932 656 233	−0.370 868 294 394 876	0.289 919 038 880 709	0.754 237 921 414 972	−5.280 490 100 407 69
9.	1	−3	3	5	1_1	-3_1	3_1	5_1	0.059 307 110 145 4481	−0.384 540 608 668 618	0.279 010 526 458 747	0.731 224 480 925 441	−5.391 236 100 350 74
10.	−1	1	−5	5	-1_1	1_1	-5_1	5_1	−0.094 645 832 237 1602	0.094 645 832 237 1602	−0.823 618 580 352 116	0.823 618 580 352 116	−4.938 815 320 515 82
11.	−1	−3	−5	5	-1_1	-3_1	-5_1	5_1	−0.076 019 055 326 4982	−0.296 621 171 920 812	−0.764 638 821 190 912	0.871 015 356 775 104	−4.528 913 482 004 07
12.	1	−3	−5	5	1_1	-3_1	-5_1	5_1	0.104 000 967 219 518	−0.307 340 634 433 945	−0.787 564 796 334 875	0.846 060 353 422 945	−4.460 851 356 605 23
13.	−1	3	−5	5	-1_1	3_1	-5_1	5_1	−0.104 000 967 219 518	0.307 340 634 433 945	−0.846 060 353 422 945	0.787 564 796 334 875	−4.460 851 356 605 23
14.	1	3	−5	5	1_1	3_1	-5_1	5_1	0.076 019 055 326 4981	0.296 621 171 920 812	−0.871 015 356 775 105	0.764 638 821 190 913	−4.528 913 482 004 07
15.	−3	3	−5	5	-3_1	3_1	-5_1	5_1	−0.318 235 743 727 828	0.318 235 743 727 828	−0.809 117 991 678 027	0.809 117 991 678 027	−3.952 153 757 713 84
16.	−1	1	5	5	-1_1	1_1		0_2	−0.103 959 905 180 572	0.103 959 905 180 572	±0.5i		−4.834 243 184 313 92
17.	−1	1	−7	−5	-1_1	1_1		-2_2	−0.021 382 497 255 0719	0.172 323 757 485 452	−0.674 008 166 064 223 ± 0.510 017 815 173 942i		−4.446 986 451 037 64
18.	−1	1	5	7	-1_1	1_1		2_2	−0.172 323 757 485 452	0.021 382 497 255 072	0.674 008 166 064 223 ± 0.510 017 815 173 942i		−4.446 986 451 037 64
19.	−1	−3	5	5	-1_1	-3_1		0_2	−0.104 593 798 656 92	−0.351 866 035 802 539	0.193 485 140 955 241 ± 0.499 999 653 215 326i		−4.217 653 267 780 04
20.	1	−3	5	5	1_1	-3_1		0_2	0.100 445 470 478 524	−0.355 902 075 708 872	0.106 594 005 665 624 ± 0.499 999 998 762 673i		−4.238 617 145 721 44
21.	−1	3	−5	−5	-1_1	3_1		0_2	−0.100 445 470 478 524	0.355 902 075 708 872	−0.106 594 005 665 624 ± 0.499 999 998 762 673i		−4.238 617 145 721 44
22.	1	3	−5	−5	1_1	3_1		0_2	0.104 593 798 656 92	0.351 866 035 802 539	−0.193 485 140 955 241 ± 0.499 999 653 215 326i		−4.217 653 267 780 04
23.	−1	−5	5	5	-1_1	-5_1		0_2	−0.090 879 829 229 5147	−0.825 164 324 699 012	0.269 621 291 144 371 ± 0.499 994 479 999 762i		−3.405 467 971 253 45
24.	1	−5	5	5	1_1	-5_1		0_2	0.105 307 215 882 061	−0.840 529 106 899 276	0.200 904 512 017 877 ± 0.499 999 589 7702i		−3.399 010 220 550 47
25.	−1	5	−5	−5	-1_1	5_1		0_2	−0.105 307 215 882 061	0.840 529 106 899 276	−0.200 904 512 017 878 ± 0.499 999 589 7702i		−3.399 010 220 550 47
26.	1	5	−5	−5	1_1	5_1		0_2	0.090 879 829 229 5148	0.825 164 324 699 012	−0.269 621 291 144 371 ± 0.499 994 479 999 762i		−3.405 467 971 253 45
27.	−1	−3	−7	−5	-1_1	-3_1		-2_2	−0.008 834 550 939 13665	−0.216 546 030 703 974	−0.559 928 758 547 488 ± 0.504 167 423 522 695i		−4.429 852 545 466 26
28.	1	−3	−7	−5	1_1	-3_1		-2_2	0.179 550 441 244 362	−0.221 778 574 218 436	−0.610 279 423 709 261 ± 0.506 397 643 535 308i		−4.152 074 687 116 64
29.	−1	3	−7	−5	-1_1	3_1		-2_2	−0.030 745 086 985 637	0.415 901 726 387 514	−0.715 074 371 644 748 ± 0.512 539 811 338 883i		−3.809 016 994 374 95
30.	1	3	−7	−5	1_1	3_1		-2_2	0.151 468 882 544 502	0.403 051 723 790 563	−0.753 368 073 442 49 ± 0.515 025 027 845 51i		−3.652 937 811 398 61
31.	−1	−5	−7	−5	-1_1	-5_1		-2_2	−0.012 708 972 240 1682	−0.668 797 728 861 12	−0.311 850 280 472 64 ± 0.500 036 029 910 984i		−3.626 741 380 447 43
32.	1	−5	−7	−5	1_1	-5_1		-2_2	0.181 053 532 776 174	−0.665 228 176 436 887	−0.380 087 206 678 755 ± 0.500 181 023 771 475i		−3.362 546 978 039 28

Table 8. (Continued).

	2J				2I_j			λ	E_0		
33.	−1	5	−7	−5	-1_1	5_1	-2_2	−0.045 767 907 357 4631	0.926 870 273 170 173	−0.771 539 863 055 997 ± 0.516 523 606 824 117i	−3.030 629 520 714 67
34.	1	5	−7	−5	1_1	5_1	-2_2	0.131 048 065 042 65	0.903 369 533 501 862	−0.806 958 457 457 649 ± 0.518 952 616 044 813i	−2.914 491 123 839 54
35.	−1	−3	5	7	-1_1	-3_1	2_2	−0.151 468 882 544 502	−0.403 051 723 790 563	0.753 368 073 442 489 ± 0.515 025 027 845 51i	−3.652 937 811 398 61
36.	1	−3	5	7	1_1	-3_1	2_2	0.030 745 086 985 6371	−0.415 901 726 387 514	0.715 074 371 644 748 ± 0.512 539 811 338 882i	−3.809 016 994 374 95
37.	−1	3	5	7	-1_1	3_1	2_2	−0.179 550 441 244 362	0.221 778 574 218 436	0.610 279 423 709 26 ± 0.506 397 643 535 308i	−4.152 074 687 116 64
38.	1	3	5	7	1_1	3_1	2_2	0.008 834 550 939 13666	0.216 546 030 703 974	0.559 928 758 547 488 ± 0.504 167 423 522 695i	−4.429 852 545 466 26
39.	−1	−5	5	7	-1_1	-5_1	2_2	−0.131 048 065 042 65	−0.903 369 533 501 862	0.806 958 457 457 648 ± 0.518 952 616 044 813i	−2.914 491 123 839 54
40.	1	−5	5	7	1_1	-5_1	2_2	0.045 767 907 357 4631	−0.926 870 273 170 173	0.771 539 863 055 997 ± 0.516 523 606 824 117i	−3.030 629 520 714 67
41.	−1	5	5	7	-1_1	5_1	2_2	−0.181 053 532 776 174	0.665 228 176 436 887	0.380 087 206 678 755 ± 0.500 181 023 771 475i	−3.362 546 978 039 28
42.	1	5	5	7	1_1	5_1	2_2	0.012 708 972 240 1683	0.668 797 728 861 12	0.311 850 280 472 639 ± 0.500 036 029 910 984i	−3.626 741 380 447 43
43.	−3	3	5	5	-3_1	3_1	0_2	−0.355 553 222 914 862	0.355 553 222 914 862	±0.5i	−3.656 620 431 047 11
44.	−3	−5	5	5	-3_1	-5_1	0_2	−0.310 549 149 731 366	−0.794 689 770 857 56	0.318 574 905 734 768 ± 0.499 979 423 585 762i	−2.918 521 798 836 65
45.	−3	5	−5	−5	-3_1	5_1	0_2	−0.360 233 082 912 354	0.848 576 145 478 809	−0.100 183 195 816 955 ± 0.499 999 999 566 872i	−2.822 077 454 947 37
46.	3	−5	5	5	3_1	-5_1	0_2	0.360 233 082 912 354	−0.848 576 145 478 809	0.100 183 195 816 955 ± 0.499 999 999 566 872i	−2.822 077 454 947 37
47.	3	5	−5	−5	3_1	5_1	0_2	0.310 549 149 731 366	0.794 689 770 857 56	−0.318 574 905 734 769 ± 0.499 979 423 585 762i	−2.918 521 798 836 65
48.	−5	5	5	5	-5_1	5_1	0_2	−0.866 025 403 784 439	0.866 025 403 784 439	±0.5i	−2
49.	−3	3	−7	−5	-3_1	3_1	-2_2	−0.229 462 592 190 66	0.426 266 635 315 86	−0.655 832 149 701 775 ± 0.508 800 262 277 932i	−3.486 587 516 207 92
50.	−3	−5	−7	−5	-3_1	-5_1	-2_2	−0.234 437 566 036 966	−0.674 991 138 847 386	−0.201 786 696 383 639 ± 0.500 000 627 189 207i	−3.309 016 994 374 95
51.	−3	5	−7	−5	-3_1	5_1	-2_2	−0.241 939 901 843 868	0.945 314 592 864 266	−0.716 718 680 744 767 ± 0.512 695 832 917 007i	−2.690 983 005 625 05
52.	3	−5	−7	−5	3_1	-5_1	-2_2	0.431 363 705 914 735	−0.665 169 819 698 726	−0.438 143 619 787 821 ± 0.500 516 359 010 736i	−2.704 629 576 417 68
53.	3	5	−7	−5	3_1	5_1	-2_2	0.348 365 993 887 336	0.865 789 319 383 562	−0.839 188 217 545 887 ± 0.521 200 974 010 199i	−2.401 041 297 5903
54.	−5	5	−7	−5	-5_1	5_1	-2_2	−0.667 531 693 785 548	0.956 294 518 754 508	−0.511 704 574 367 563 ± 0.501 490 757 455 866i	−1.934 282 851 005 86
55.	−3	3	5	7	-3_1	3_1	2_2	−0.426 266 635 315 859	0.229 462 592 190 66	0.655 832 149 701 775 ± 0.508 800 262 277 932i	−3.486 587 516 207 93
56.	−3	−5	5	7	-3_1	-5_1	2_2	−0.348 365 993 887 336	−0.865 789 319 383 562	0.839 188 217 545 887 ± 0.521 200 974 010 199i	−2.401 041 297 5903
57.	−3	5	5	7	-3_1	5_1	2_2	−0.431 363 705 914 735	0.665 169 819 698 726	0.438 143 619 787 821 ± 0.500 516 359 010 736i	−2.704 629 576 417 68
58.	3	−5	5	7	3_1	-5_1	2_2	0.241 939 901 843 868	−0.945 314 592 864 266	0.716 718 680 744 767 ± 0.512 695 832 917 007i	−2.690 983 005 625 05
59.	3	5	5	7	3_1	5_1	2_2	0.234 437 566 036 966	0.674 991 138 847 386	0.201 786 696 383 639 ± 0.500 000 627 189 207i	−3.309 016 994 374 95
60.	−5	5	5	7	-5_1	5_1	2_2	−0.956 294 518 754 508	0.667 531 693 785 548	0.511 704 574 367 562 ± 0.501 490 757 455 866i	−1.934 282 851 005 86

Table 8. (Continued.)

	2*J*				2I_j		λ			E_0
61.	−1	−9	9	1	0_1	0_3	0.014 144 950 160 5988	−0.014 144 950 160 5988	±1.003 573 875 8841i	−2.676 077 387 013 89
62.	−1	−9	−7	−5	0_1	-2_3	0.046 815 761 134 9673	−0.660 708 959 251 844	−0.648 455 956 153 308 ± 0.986 949 821 429 771i	−2.535 488 627 431 38
63.	1	9	7	5	0_1	2_3	−0.046 815 761 134 9673	0.660 708 959 251 843	0.648 455 956 153 307 ± 0.986 949 821 429 771i	−2.535 488 627 431 38
64.	−1	11	9	−1	-2_1	0_3	−0.181 833 282 738 665	0.050 498 718 072 9406	0.049 835 909 276 2097 ± 1.000 653 005 273 71i	−2.434 042 307 755 88
65.	1	−9	−11	1	2_1	0_3	0.181 833 282 738 665	−0.050 498 718 072 9411	−0.049 835 909 276 2102 ± 1.000 653 005 273 71i	−2.434 042 307 755 88
66.	−3	9	7	3	-4_1	0_3	−0.424 655 812 460 341	0.113 760 000 185 94	0.113 844 394 809 84 ± 1.000 484 504 750 88i	−1.826 327 433 840 95
67.	3	−7	−9	−3	4_1	0_3	0.424 655 812 460 341	−0.113 760 000 185 94	−0.113 844 394 809 841 ± 1.000 484 504 750 88i	−1.826 327 433 840 95
68.	−5	9	7	3	-6_1	0_3	−0.934 591 285 924 601	0.207 542 904 757 138	0.207 955 858 346 555 ± 1.000 024 229 008 46i	−1.100 194 426 716 94
69.	5	−7	−9	−3	6_1	0_3	0.934 591 285 924 601	−0.207 542 904 757 138	−0.207 955 858 346 556 ± 1.000 024 229 008 46i	−1.100 194 426 716 94
70.	−3	−7	−9	−5	-2_1	-2_3	−0.126 704 456 844 59	−0.615 682 260 875 608	−0.605 806 378 341 122 ± 0.984 707 473 508 637i	−2.446 312 073 084 19
71.	1	−7	−9	−5	2_1	-2_3	0.229 951 158 944 146	−0.701 127 655 052 017	−0.686 505 224 914 291 ± 0.988 444 451 913 007i	−2.190 983 005 625 05
72.	−5	−7	−9	−5	-4_1	-2_3	−0.352 172 387 161 592	−0.542 873 778 627 496	−0.537 259 991 040 618 ± 0.974 848 447 561 115i	−1.929 727 591 6029
73.	3	−7	−9	−5	4_1	-2_3	0.486 092 018 830 097	−0.747 279 186 877 142	−0.729 659 118 346 677 ± 0.990 097 903 104 581i	−1.553 641 958 169 63
74.	−5	−9	−11	−3	-6_1	-2_3	−0.778 299 777 225 231	−0.387 696 439 691 344	−0.384 618 695 188 188 ± 1.002 505 246 832 33i	−1.203 070 374 708 31
75.	5	−7	−9	−5	6_1	-2_3	1.044 950 259 323 46	−0.818 684 030 062 762	−0.795 754 579 948 182 ± 0.993 172 728 900 323i	−0.874 817 198 903 749
76.	−1	9	7	5	-2_1	2_3	−0.229 951 158 944 146	0.701 127 655 052 017	0.686 505 224 914 291 ± 0.988 444 451 913 007i	−2.190 983 005 625 05
77.	3	9	7	5	2_1	2_3	0.126 704 456 844 59	0.615 682 260 875 607	0.605 806 378 341 122 ± 0.984 707 473 508 637i	−2.446 312 073 084 19
78.	−3	9	7	5	-4_1	2_3	−0.486 092 018 830 097	0.747 279 186 877 141	0.729 659 118 346 677 ± 0.990 097 903 104 581i	−1.553 641 958 169 63
79.	5	9	7	5	4_1	2_3	0.352 172 387 161 592	0.542 873 778 627 496	0.537 259 991 040 618 ± 0.974 848 447 561 115i	−1.929 727 591 6029
80.	−5	9	7	5	-6_1	2_3	−1.044 950 259 323 46	0.818 684 030 062 761	0.795 754 579 948 182 ± 0.993 172 728 900 323i	−0.874 817 198 903 749
81.	5	11	9	3	6_1	2_3	0.778 299 777 225 231	0.387 696 439 691 344	0.384 618 695 188 188 ± 1.002 505 246 832 33i	−1.203 070 374 708 31
82.	7	5	5	9	0_4		±1.512 357 681 307 67i		±0.5i	−0.509 136 384 638 968
83.	−9	−9	−7	−7	-2_4		−0.698 286 762 160 898 ± 1.456 971 241 011 82i		−0.686 425 305 832 397 ± 0.500 238 343 641 787i	−0.450 548 494 320 44
84.	7	7	9	9	2_4		0.698 286 762 160 898 ± 1.456 971 241 011 82i		0.686 425 305 832 396 ± 0.500 238 343 641 787i	−0.450 548 494 320 44
85.	−5	−5	5	5	-1_2	1_2	−0.305 442 823 093 657 ± 0.499 984 508 292 436i		0.305 442 823 093 657 ± 0.499 984 508 292 436i	−1.829 687 501 998 33
86.	·	·	−7	−5	-1_2	-3_2	0.003 384 795 565 84607 ± 0.5i		−0.714 116 912 834 429 ± 0.512 421 220 515 184i	−1.635 213 925 035 11
87.	−5	−5	5	7	-1_2	3_2	−0.414 435 314 220 941 ± 0.499 872 871 440 981i		0.829 575 920 907 195 ± 0.519 831 244 766 274i	−1.415 530 659 646 27
88.	5	5	−7	−5	1_2	-3_2	0.414 435 314 220 941 ± 0.499 872 871 440 981i		−0.829 575 920 907 195 ± 0.519 831 244 766 274i	−1.415 530 659 646 27
89.	·	·	5	7	1_2	3_2	−0.003 384 795 565 84617 ± 0.5i		0.714 116 912 834 429 ± 0.512 421 220 515 184i	−1.635 213 925 035 11
90.	−7	−5	5	7	-3_2	3_2	−0.924 494 699 244 798 ± 0.527 627 690 529 573i		0.924 494 699 244 797 ± 0.527 627 690 529 573i	−1.011 058 686 019 45

Table 9. Highest-weight Bethe Ansatz solutions for $N = 10$, $M = 5$. Real: 1; one two-string: 10; one three-string: 14; one four-string: 7; one five-string: 1; two two-strings: 5; one two- and one three-string: 3. This table gives the quantum numbers and energy, the following one are the rapidities.

	$2J$					$2I_j$					E_0
1.	0	−2	2	−4	4	0_1	-2_1	2_1	-4_1	4_1	−7.015 446 354 492 04
2.	0	−2	2	4	6	0_1	-2_1	2_1	0_2		−6.270 597 435 408 44
3.	0	−2	−4	4	6	0_1	-2_1	-4_1	0_2		−5.267 634 884 835 57
4.	0	2	−4	4	6	0_1	2_1	-4_1	0_2		−5.386 286 924 5099
5.	−2	2	−4	4	6	-2_1	2_1	-4_1	0_2		−5.014 299 479 211 23
6.	0	−2	4	−6	−4	0_1	-2_1	4_1	0_2		−5.386 286 924 5099
7.	0	2	4	−6	−4	0_1	2_1	4_1	0_2		−5.267 634 884 835 57
8.	−2	2	4	−6	−4	-2_1	2_1	4_1	0_2		−5.014 299 479 211 23
9.	0	−4	4	4	6	0_1	-4_1	4_1	0_2		−4.519 120 444 134 79
10.	−2	−4	4	4	6	-2_1	-4_1	4_1	0_2		−4.176 925 752 574 98
11.	2	−4	4	−6	−4	2_1	-4_1	4_1	0_2		−4.176 925 752 574 98
12.	0	0	8	2	10	-1_1	1_1	0_3			−4.596 212 934 879 07
13.	0	−2	8	0	10	-1_1	-3_1	0_3			−4.041 811 226 150 61
14.	0	−2	8	2	10	1_1	-3_1	0_3			−4.038 532 763 3764
15.	0	2	−10	−2	−8	-1_1	3_1	0_3			−4.038 532 763 3764
16.	0	2	−10	0	−8	1_1	3_1	0_3			−4.041 811 226 150 61
17.	0	−4	6	4	8	-1_1	-5_1	0_3			−3.255 825 970 618 85
18.	2	−4	6	4	8	1_1	-5_1	0_3			−3.218 507 956 874 06
19.	−2	4	−8	−4	−6	-1_1	5_1	0_3			−3.218 507 956 874 06
20.	0	4	−8	−4	−6	1_1	5_1	0_3			−3.255 825 970 618 85
21.	−2	2	8	2	10	-3_1	3_1	0_3			−3.487 419 453 5884
22.	−2	−4	6	4	8	-3_1	-5_1	0_3			−2.829 371 661 775 33
23.	−2	4	−10	−2	−8	-3_1	5_1	0_3			−2.676 892 101 261 16
24.	2	−4	8	2	10	3_1	-5_1	0_3			−2.676 892 101 261 15
25.	2	4	−8	−4	−6	3_1	5_1	0_3			−2.829 371 661 775 33
26.	−4	4	8	0	12	-5_1	5_1	0_3			−1.894 226 038 299 81
27.	2	6	4	6	8	0_1	0_4				−2.548 943 069 875 17
28.	0	10	2	4	12	-2_1	0_4				−2.318 069 837 212 12
29.	0	−12	−4	−2	−10	2_1	0_4				−2.318 069 837 212 12
30.	−2	10	2	4	12	-4_1	0_4				−1.729 874 550 169 92
31.	2	−12	−4	−2	−10	4_1	0_4				−1.729 874 550 169 92
32.	−4	6	6	8	8	-6_1	0_4				−1.018 583 147 5762
33.	4	−8	−8	−6	−6	6_1	0_4				−1.018 583 147 5762
34.	−8	−14	−2	−10	−6	0_5					−0.441 081 772 978 35
35.	0	−6	−4	4	6	0_1	-1_2	1_2			−3.565 613 445 762 33
36.	−2	−6	−4	4	6	-2_1	-1_2	1_2			−3.284 575 135 362 44
37.	2	−6	−4	4	6	2_1	-1_2	1_2			−3.284 575 135 362 44
38.	−4	−6	−4	4	6	-4_1	-1_2	1_2			−2.453 462 784 563 56
39.	4	−6	−4	4	6	4_1	-1_2	1_2			−2.453 462 784 563 56
40.	4	6	−12	0	−8	0_2	0_3				−1.661 339 050 581 59
41.	−6	−4	6	4	8	-2_2	0_3				−1.289 345 823 927 68
42.	4	6	−8	−4	−6	2_2	0_3				−1.289 345 823 927 68

Table 10. Same situation as for Table 9. Here, only the rapidities are given, using the same ordering of states.

	λ				
1.	0	−0.216 201 306 054 532	0.216 201 306 054 532	−0.598 086 994 989 324	0.598 086 994 989 324
2.	0	−0.236 123 983 535 462	0.236 123 983 535 459	±0.5*i*	
3.	−0.012 782 837 434 4248	−0.230 841 400 083 837	−0.623 492 239 903 063	0.433 558 238 710 663 ± 0.500 715 214 079 799*i*	
4.	−0.012 708 381 262 3862	0.214 599 696 433 234	−0.648 132 093 473 336	0.223 120 389 151 246 ± 0.500 003 412 060 902*i*	
5.	−0.234 423 274 285 998	0.207 588 644 710 284	−0.633 319 866 543 208	0.330 077 248 059 462 ± 0.500 093 388 279 514*i*	
6.	0.012 708 381 262 3863	−0.214 599 696 433 234	0.648 132 093 473 336	−0.223 120 389 151 246 ± 0.500 003 412 060 902*i*	
7.	0.012 782 837 434 4248	0.230 841 400 083 837	0.623 492 239 903 063	−0.433 558 238 710 663 ± 0.500 715 214 079 799*i*	
8.	−0.207 588 644 710 284	0.234 423 274 285 998	0.633 319 866 543 208	−0.330 077 248 059 462 ± 0.500 093 388 279 514*i*	
9.	0	−0.638 964 515 019 459	0.638 964 515 019 459	±0.5*i*	
10.	−0.228 987 307 383 963	−0.630 868 659 689 258	0.635 640 354 199 363	0.112 107 806 436 93 ± 0.500 000 003 071 323*i*	
11.	0.228 987 307 383 964	−0.635 640 354 199 363	0.630 868 659 689 258	−0.112 107 806 436 93 ± 0.500 000 003 071 323*i*	
12.	−0.119 171 105 521 438	0.119 171 105 521 438	0	±1.044 606 753 806 32*i*	
13.	−0.085 023 961 997 9459	−0.312 113 477 180 648	0.136 030 459 567 589	0.130 553 489 805 505 ± 1.002 604 732 923 15*i*	
14.	0.124 189 013 936 543	−0.322 858 035 179 365	0.053 663 951 609 9222	0.072 502 534 816 4504 ± 1.018 710 022 129 22*i*	
15.	−0.124 189 013 936 543	0.322 858 035 179 365	−0.053 663 951 609 922	−0.072 502 534 816 4508 ± 1.018 710 022 129 22*i*	
16.	0.085 023 961 997 946	0.312 113 477 180 648	−0.136 030 459 567 59	−0.130 553 489 805 506 ± 1.002 604 732 923 15*i*	
17.	−0.075 721 769 694 6456	−0.725 740 545 465 692	0.265 501 628 544 808	0.267 980 343 307 763 ± 1.003 390 889 988 26*i*	
18.	0.102 266 631 391 811	−0.740 483 055 440 971	0.212 680 977 755 452	0.212 767 723 146 853 ± 1.009 823 401 696 68*i*	
19.	−0.102 266 631 391 811	0.740 483 055 440 972	−0.212 680 977 755 453	−0.212 767 723 146 853 ± 1.009 823 401 696 68*i*	
20.	0.075 721 769 694 6456	0.725 740 545 465 692	−0.265 501 628 544 809	−0.267 980 343 307 764 ± 1.003 390 889 988 26*i*	
21.	−0.326 130 791 413 012	0.326 130 791 413 012	0	±1.004 146 531 850 27*i*	
22.	−0.283 793 613 238 617	−0.703 591 333 579 051	0.326 773 853 208 772	0.330 305 546 804 447 ± 1.000 979 243 895 75*i*	
23.	−0.327 889 355 169 58	0.748 388 659 872 212	−0.138 122 396 549 785	−0.141 188 454 076 423 ± 0.997 955 113 962 176*i*	
24.	0.327 889 355 169 58	−0.748 388 659 872 212	0.138 122 396 549 784	0.141 188 454 076 422 ± 0.997 955 113 962 176*i*	
25.	0.283 793 613 238 617	0.703 591 333 579 051	−0.326 773 853 208 773	−0.330 305 546 804 447 ± 1.000 979 243 895 75*i*	
26.	−0.752 714 822 086 133	0.752 714 822 086 133	0	±1.000 828 082 942 51*i*	
27.	0	±1.570 673 436 609 84*i*		±0.5*i*	

Table 10. (Continued).

	λ		
28.	−0.178 607 041 441 292	0.041 494 752 806 2553 ± 1.5652371254888i	0.047 808 767 914 3884 ± 0.500 000 000 000 016i
29.	0.178 607 041 441 292	−0.041 494 752 806 257 ± 1.5652371254888i	−0.047 808 767 914 3897 ± 0.500 000 000 000 016i
30.	−0.409 691 857 045 755	0.100 174 313 634 614 ± 1.551 938 999 806 67i	0.104 671 614 888 266 ± 0.500 000 000 024 36i
31.	0.409 691 857 045 755	−0.100 174 313 634 615 ± 1.551 938 999 806 67i	−0.104 671 614 888 267 ± 0.500 000 000 024 36i
32.	−0.866 745 085 071 927	0.222 386 370 713 988 ± 1.534 601 783 486 48i	0.210 986 171 821 974 ± 0.500 000 011 478 703i
33.	0.866 745 085 071 927	−0.222 386 370 713 989 ± 1.534 601 783 486 48i	−0.210 986 171 821 975 ± 0.500 000 011 478 703i
34.	±2.163 766 883 029 61i	0	±1.000 014 800 380 88i
35.	0	−0.514 132 157 874 231 ± 0.501 914 843 963 61i	0.514 132 157 874 23 ± 0.501 914 843 963 61i
36.	−0.212 520 120 352 343	−0.442 421 739 397 568 ± 0.500 726 824 292 104i	0.548 681 799 573 739 ± 0.502 727 368 457 053i
37.	0.212 520 120 352 343	−0.548 681 799 573 739 ± 0.502 727 368 457 053i	0.442 421 739 397 568 ± 0.500 726 824 292 104i
38.	−0.637 971 552 680 178	−0.243 549 292 697 093 ± 0.500 003 577 484 99i	0.562 535 069 037 181 ± 0.503 130 323 501 314i
39.	0.637 971 552 680 178	−0.562 535 069 037 182 ± 0.503 130 323 501 314i	0.243 549 292 697 092 ± 0.500 003 577 484 99i
40.	±0.5i	0	±0.998 506 455 954 561i
41.	−0.675 004 371 842 435 ± 0.506 526 446 939 028i	0.448 002 978 170 04	0.451 002 882 757 414 ± 0.996 924 681 444 35i
42.	0.675 004 371 842 435 ± 0.506 526 446 939 028i	−0.448 002 978 170 041	−0.451 002 882 757 415 ± 0.996 924 681 444 35i

The reduced Bethe equations that must be satisfied by the remaining roots are

$$(N-1)\arctan 2\lambda_j - \arctan \frac{2}{3}\lambda_j = \pi J_j + \sum_{k=1}^{\tilde{M}} \arctan(\lambda_j - \lambda_k) \quad (\mathrm{mod}\,\pi). \tag{113}$$

The Bethe quantum numbers J_+, J_- are those of the $M = 2$ case (for M even) or the $M = 3$ case (for M odd).

5.6. Energy of singular pair

In computing the energy contribution of the singular pair $\pm\,\mathrm{i}/2$, we have to be careful to take the correct limit (109) arising from the Bethe equations. In this limit, the imaginary deviation is negligible compared to the real deviation, so that we may set $\lambda_\pm = \epsilon \pm \mathrm{i}/2$. The energy contribution of the singular pair is then always

$$E_{\{\mathrm{i}/2,-\mathrm{i}/2\}} = -1. \tag{114}$$

5.7. Validity of singular pair states

It has been argued by Siddharthan [28] (on the basis of numerically calculated energies) and Noh *et al* [30] (by symmetry considerations) that singular pair states such as we just discussed, though they are the solutions to the Bethe equations, do not (or not always) represent eigenstates of the Heisenberg model. However, we have shown above that they are valid solutions; moreover, we have checked the solutions of states found in this way against complete diagonalization at $N = 6$, $N = 8$ and $N = 10$, and find perfect agreement.

As for the former article, the author finds six singular states for $N = 6$, $M = 3$, where only two are allowed by symmetry; it is therefore not surprising that four of those states are not eigenstates. The author fails to take the Bethe equations for the singular roots themselves correctly into account, and therefore finds too many solutions. Considering the latter article, the situation with parity and translation symmetry is somewhat more subtle. It is considered in the following section, where it is used to prove that matrix elements of local operators with respect to the ground state and a singular pair state vanish.

5.8. Form factors for singular pair states vanish

In the case of singular pair states, the reduced determinant expressions for correlators [35] become degenerate. However, we can show that the form factors must vanish in this case with the following simple argument, based on their symmetry properties under lattice shifts and inversion.

5.8.1. Translation symmetry. All singular states have a symmetric rapidity distribution, which implies their total momentum must be either 0 or π. The former implies symmetry under lattice shifts, and corresponds to the case with an odd number of finite roots aside from $\pm\,\mathrm{i}/2$. The latter implies antisymmetry when shifting the lattice by one site, and corresponds to the case where there is an even number of such roots.

5.8.2. Parity symmetry. Let us now turn our attention to the symmetry properties under lattice inversion (the parity operation). Under parity, the wavefunction $\chi_{\{\lambda\}}(j_1 \ldots j_M)$ is taken to $\chi_{\{\lambda\}}(N - j_M + 1 \ldots N - j_1 + 1)$. Inserting this in the Bethe wavefunction, we get

$$\chi_{\{k\}}(N - j_M + 1 \ldots N - j_1 + 1) = \mathrm{e}^{\mathrm{i}\sum_\alpha k_\alpha (N+1)} A_0 \sum_{\mathcal{P}} (-1)^{[\mathcal{P}]} \mathrm{e}^{\frac{1}{2}\mathrm{i}\sum_{\alpha<\beta}\Phi(k_{\mathcal{P}\alpha},k_{\mathcal{P}\beta})} \mathrm{e}^{\mathrm{i}\sum_\alpha -k_{\mathcal{P}\alpha} j_{M-\alpha}}$$
$$= \mathrm{e}^{\mathrm{i}\sum_\alpha k_\alpha (N+1)} A_0 \sum_{\mathcal{P}} (-1)^{[\mathcal{P}]} \mathrm{e}^{\frac{1}{2}\mathrm{i}\sum_{\alpha<\beta}\Phi(-k_{\mathcal{P}(M-\alpha)},-k_{\mathcal{P}(M-\beta)})} \mathrm{e}^{\mathrm{i}\sum_\alpha -k_{\mathcal{P}(M-\alpha)} j_\alpha}. \tag{115}$$

Now let us set $k'_{M-\alpha} := -k_\alpha$, so that

$$\chi_{\{k\}}(N - j_M + 1 \ldots N - j_1 + 1) = \mathrm{e}^{\mathrm{i}\sum_\alpha k_\alpha (N+1)} A_0 \sum_{\mathcal{P}} (-1)^{[\mathcal{P}]} \mathrm{e}^{\frac{1}{2}\mathrm{i}\sum_{\alpha<\beta}\Phi(k'_{\mathcal{VPV}},k'_{\mathcal{VPV}})} \mathrm{e}^{\mathrm{i}\sum_\alpha k'_{\mathcal{VPV}} j_\alpha}, \tag{116}$$

where $\mathcal{V}$ is the inversion permutation, such that $\mathcal{VPV} = M - \mathcal{P}(M - \alpha)$. Realizing that $[\mathcal{VPV}] = [\mathcal{P}]$, we see that we recover the Bethe wavefunction for the set of momenta $\{k'\}$, with a prefactor $\mathrm{e}^{\mathrm{i}\sum_\alpha k_\alpha (N+1)} = \mathrm{e}^{\mathrm{i}\sum_\alpha k_\alpha}$. Therefore, a Bethe wavefunction with $\{k\} = \{-k\}$ is either symmetric (if $\sum_\alpha k_\alpha = 0$) or antisymmetric (if $\sum_\alpha k_\alpha = \pi$) under parity; conversely, if a state $\chi_{\{k\}}$ is an eigenfunction of parity at eigenvalue v, we must have $\chi_{\{k\}} = v\chi_{\{-k\}}$.

Consider, however, a singular Bethe wavefunction; take for instance $\chi_{\pm \mathrm{i}/2}(j_1, j_2) = (-1)^{j_1}\delta_{j_1,j_2} + (-1)^{j_2}\delta_{j1+N,j2+1}$. It is easily seen that this state is symmetric under parity, but antisymmetric under a single-site shift. In [30] this is taken to be a contradiction, implying that singular states cannot be Bethe states. However, even though $\{\lambda\} = \{-\lambda\}$, the momenta for the singular pair are $k_\pm = \pi/2 \pm \mathrm{i}\infty$; the limit that needs to be taken to arrive as this point is such that at no point $\lambda_- = -\lambda_+$ except at the limit itself. The opposite momenta $k_\pm = -\pi/2 \pm \mathrm{i}\infty$ yield, in the limit, the same wavefunction; but $\{k\} \neq \{-k\}$ and therefore the assumption leading to the symmetry relation above is not satisfied for singular Bethe states.

Applying the above argument to the singular-state wavefunction of (112), we see that lattice inversion takes the *finite* momenta to their opposites; but the part of the wavefunction corresponding to the singular pair is taken to itself. (Note that the extra scattering factor for opposite momenta surrounding a pair does not change, as the property of surrounding something is invariant under parity). Thus the eigenvalue under parity from a singular state is $-\mathrm{e}^{\mathrm{i}\sum_\alpha k_\alpha}$. Indeed, for a general singular state, symmetry under shifts implies antisymmetry under parity and vice versa.

5.8.3. Symmetry and form factors. For the general study of dynamics using all important excited states [34, 35, 40], it is essential to be able to determine all required matrix elements of local spin operators (form factors). It is easy to show that form factors of singular states with the ground state vanish. Consider an even singular state, i.e. of momentum π. The ground state for even M has momentum 0. Therefore, the only possibly nonvanishing form factor operates at momentum π,

$$F_\pi^\alpha(\mathrm{GS}, \{\pm \mathrm{i}/2, \lambda\}) = \langle \mathrm{GS}| \sum_j (-1)^j S_j^\alpha \,|\{\pm \mathrm{i}/2, \lambda\}\rangle\,. \tag{117}$$

As we have shown, the state $|\{\pm \mathrm{i}/2, \lambda\}\rangle$ is symmetric under parity. Since N is even, the state $\sum_j (-1)^j S_j^\alpha \,|\{\pm \mathrm{i}/2, \lambda\}\rangle$ is antisymmetric under parity. But the ground state $|\mathrm{GS}\rangle$ is symmetric; therefore, their overlap (which is the form factor) must be zero. The converse argument holds when we consider odd singular states; again, the form factor is zero.

6. Conclusion

In this paper, we have discussed a method allowing us to find an extended class of solutions of the Bethe equations in the complex plane, by calculating deviations to the string-hypothesis solution. For fixed M at increasing N, the fraction of solutions that cannot be found decreases algebraically with the number of sites and factorially with the number of magnons. The behavior of the number of missing solutions suggests that collapsing pairs are the only source of failure of the string picture in this regime. The average deviation of the string hypothesis is found to decrease with N, but it is not exponential in all cases. If the number of magnons becomes macroscopic, i.e. when the field becomes small, we expect that the method becomes more difficult to implement, as can be expected from general arguments (see, e.g. [11]).

We have also shown that singular states exist whenever a symmetric configuration includes an even string at the origin, leading to a singularity in the Bethe equations. These states are generalizations of the $M = 2$ singular state that had been known for a long time. We also show that, in contrast to what is claimed in the literature, these states can be seen as legitimate solutions to the Bethe equations, as long as the limit is taken in the correct way. We have also shown that all states in this class have zero form factors for local spin operators, and can therefore be ignored in the calculation of zero-temperature correlation functions of local spins. We have not yet investigated cases in which either a four or higher even string is present at the origin in a symmetric state, nor the case of superimposed pairs of even or odd strings at the origin. Yet another class of special solutions arises when a symmetric configuration includes two odd-length strings at the origin. Both of these last two situations lead to solutions with pairs of roots that are exponentially close to each other as N becomes large, without violating the exclusion principle. Form factors and norms for these states exist and are nonzero, but are hard to calculate due to the exponential degeneracy. We leave all of these for future work.

In summary, we have presented the sets of equations allowing to obtain eigenstates of the Heisenberg chain beyond the traditional string hypothesis. These results are of importance in particular for the calculation of dynamical correlation functions of finite chains, where form factors depend sensitively on deviations from pure strings. Although we have not pushed this direction here, the influence of the size-dependent string deviations on finite-size corrections to the thermal equilibrium expectation values of various quantities would be a further line of investigation worth pursuing. On a more formal level, although the state counting can be categorized using partitioning of rapidities in pure strings, the actual solutions to the Bethe equations can differ substantially from the string hypothesis, and can do so in very elaborate ways (especially for the higher strings which we consider here). We hope that the present work will provide stimulation for an eventually more faithful and representative classification of solutions to the Bethe equations.

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Appendix. Complete Bethe Ansatz solutions of finite chains

In tables 1–4, we give the rapidities for all highest-weight eigenstates of the isotropic Heisenberg chain at eight sites, except the reference state (which has no rapidities). Lower-weight states can be formed by adding the appropriate number of infinite rapidities. Similarly, tables 5–10 contain the results for ten sites.

At this size, the model is easily completely diagonalizable and therefore we do not need the Bethe Ansatz to solve it. However, while constructing the complete solution from the Bethe Ansatz solutions is easy for this number of particles, mapping the exactly diagonalized wavefunctions to solutions of the Bethe equations is not. Therefore, we believe it valuable to have an exhaustive list at hand. The solutions are found by the methods of section 3. The quantum numbers are determined from the rapidities, thereby providing a valuable check on their accuracy as solutions to the Bethe equations. We have also checked these solutions against a complete diagonalization, and found full agreement. One thing one can easily see is that these solutions neatly satisfy the classification in terms of the string hypothesis: the states can be associated one-to-one with string states, with small but significant deviations, and with quantum numbers that satisfy the bound (20).

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