

## Completeness of solutions of Bethe's equations

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We consider the Bethe equations for the isotropic spin-1/2 Heisenberg quantum spin chain with periodic boundary conditions. We formulate a conjecture for the number of solutions with pairwise distinct roots of these equations, in terms of numbers of so-called singular (or exceptional) solutions. Using homotopy continuation methods, we find all such solutions of the Bethe equations for chains of length up to 14. The numbers of these solutions are in perfect agreement with the conjecture. We also discuss an indirect method of finding solutions of the Bethe equations by solving the Baxter T-Q equation. We briefly comment on implications for thermodynamical computations based on the string hypothesis.

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### I. INTRODUCTION

The Heisenberg quantum spin chain is a one-dimensional array of  $N$  quantum spin-1/2 spins with nearest-neighbor isotropic interactions and periodic boundary conditions. The Hamiltonian is given by

$$H = \frac{1}{4} \sum_{n=1}^N (\vec{\sigma}_n \cdot \vec{\sigma}_{n+1} - 1), \quad \vec{\sigma}_{N+1} \equiv \vec{\sigma}_1, \quad (1.1)$$

where  $\vec{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$  are the usual  $2 \times 2$  Pauli spin matrices, and  $\vec{\sigma}_n$  denotes the spin operators at site  $n$ . The vector space describing this system has dimension  $2^N$ , so the Hamiltonian is a  $2^N \times 2^N$  matrix. The basic problem is to determine the eigenvectors and eigenvalues of this matrix, which grows in size exponentially with  $N$ .

The Heisenberg spin chain is of fundamental importance in theoretical physics. It is a model of (anti)ferromagnetism, which is realized experimentally (e.g.,  $\text{KCuF}_3$  and  $\text{Sr}_2\text{CuO}_3$ ) [1]. It has many other applications and connections, including conformal field theory [2,3],  $\mathcal{N} = 4$  supersymmetric Yang-Mills theory, and string theory [4]. Moreover, it is the prototype of so-called quantum integrable models: one-dimensional many-body quantum systems that have many conserved quantities, and that therefore admit exact solutions [5–8].

An exact solution of the Heisenberg model was discovered by Hans Bethe [9]. In particular, the eigenvalues of the Hamiltonian Eq. (1.1) are given by

$$E = -\frac{1}{2} \sum_{k=1}^M \frac{1}{\lambda_k^2 + \frac{1}{4}}, \quad (1.2)$$

where  $\{\lambda_1, \dots, \lambda_M\}$  satisfy Bethe's celebrated equations

$$\begin{aligned} \left(\lambda_k + \frac{i}{2}\right)^N \prod_{\substack{j \neq k \\ j=1}}^M (\lambda_k - \lambda_j - i) \\ = \left(\lambda_k - \frac{i}{2}\right)^N \prod_{\substack{j \neq k \\ j=1}}^M (\lambda_k - \lambda_j + i), \\ k = 1, 2, \dots, M, \quad M = 0, 1, \dots, \frac{N}{2}. \end{aligned} \quad (1.3)$$

It is therefore customary to refer to the  $\lambda_k$ 's as “Bethe roots.” The solutions of other quantum integrable models entail generalizations of these equations.

For given values of  $N$  and  $M$ , the Bethe equations have various sets of solutions. Roughly speaking, for each such solution  $\{\lambda_1, \dots, \lambda_M\}$ , there is a corresponding energy level (1.2) and eigenvector (the construction of which will be sketched in Sec. II) of the Hamiltonian. However, ever since the time of Bethe's remarkable discovery, the nagging question of “completeness” has persisted: namely, whether the Bethe equations have too many, too few, or just the right number of solutions to account for all  $2^N$  eigenstates of the Hamiltonian.<sup>1</sup> The existence of so-called singular (or exceptional) solutions of the Bethe equations makes the completeness problem particularly confusing.<sup>2</sup> A related question is whether the set of Bethe roots characterizing any given state must be pairwise distinct, i.e., obey the “Pauli principle.” Although it is generally believed that the answer to this question is “yes,” there is no proof (to our knowledge) of this assertion [17].<sup>3</sup>

<sup>1</sup>Various completeness proofs have been proposed for the case  $N \rightarrow \infty$  [7,9–11]. However, these proofs rely on the so-called string hypothesis, which itself has not been proved; see also, e.g., Refs. [12–16].

<sup>2</sup>There has been considerable discussion in the literature about such solutions; see, e.g., Refs. [17–25].

<sup>3</sup>The coordinate Bethe ansatz wavefunction, which is proportional to the algebraic Bethe ansatz state, does vanish for coincident

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We formulate here a precise conjecture for the number of solutions with pairwise distinct roots of the Bethe equations, in terms of numbers of singular solutions. [See Eq. (2.12) below.] Its meaning is that the Bethe equations generally have “too many” solutions with pairwise distinct roots; but after appropriate culling, there remain exactly the right number of solutions to account for all  $2^N$  eigenstates of the Hamiltonian.

In order to check this conjecture, it is necessary to find *all* solutions with pairwise distinct roots of the Bethe equations. For certain energy levels, in particular for the ground state, which has  $N/2$  real Bethe roots, it is straightforward to compute numerically the Bethe roots for large values of  $N$  ( $\sim 10^3$ ) (see, e.g., Ref. [2]), and to compute analytically the energy in the  $N \rightarrow \infty$  limit [7]. However, finding all solutions of the Bethe equations is unfortunately a difficult problem even for modest values of  $N$  ( $\sim 10$ )—certainly much more difficult than directly diagonalizing the Hamiltonian. For example, on a desktop computer, the direct solution of Eq. (1.3) is not feasible for  $N = 8$  beyond  $M = 3$ .

We discuss two approaches for tackling this problem. Using homotopy continuation methods, which heretofore had not been applied to the Bethe equations, we find all solutions with pairwise distinct roots up to  $N = 14$ ,  $M = 7$ . We also discuss an indirect method of finding solutions of the Bethe equations by solving the Baxter T-Q equation.

Our results, summarized in Table II, are in precise agreement with the conjecture. These results also suggest that the naive prediction Eq. (2.8) for the number of solutions of the Bethe equations is incorrect not only for small values of  $N$ , but also for  $N \rightarrow \infty$ , in contradiction with several computations based on the string hypothesis.

The conjecture may also be of interest to mathematicians. Indeed, the Bethe equations are evidently a system of polynomial equations, and therefore belong to the realm of algebraic geometry. These equations have a finite number of solutions; i.e., the algebraic variety of the solutions has dimension 0. Nevertheless, the number of such solutions should be calculable *a priori*. (See also Refs. [12,16,26] and references therein.)

The outline of this paper is as follows. In Sec. II we formulate our conjecture for the number of solutions with pairwise distinct roots of the Bethe equations, in terms of numbers of singular solutions. In Sec. III we briefly describe the homotopy continuation method with references to some surveys on the method, and how we use it to solve the Bethe equations. In Sec. IV we discuss an indirect way of finding the Bethe roots by solving instead the T-Q equation. Finally, we present a summary and discussion of our results in Sec. V.

## II. THE COMPLETENESS-PAULI-PRINCIPLE CONJECTURE

For given values of  $N$  and  $M$ , let us denote by  $\mathcal{N}(N, M)$  the number of solutions of the Bethe Eqs. (1.3) with pairwise

rapidities. However, it is only the proportionality factor and not the algebraic Bethe ansatz state itself that vanishes for coincident rapidities. The corresponding coordinate Bethe ansatz wavefunction can therefore be made nonzero by a simple renormalization (of the sort required for physical singular states), the need for which cannot be precluded.

distinct Bethe roots (i.e.,  $\lambda_j \neq \lambda_k$  for  $j \neq k$ ). We always count solutions up to permutations of the Bethe roots: if  $\{\lambda_1, \dots, \lambda_M\}$  is a solution, then any permutation of these  $\lambda_k$ 's is not counted as a separate solution.

We would like to formulate a conjecture for  $\mathcal{N}(N, M)$ . To this end, it is necessary to review in a little more detail the solution of the model. Instead of following Bethe's original approach (which is now referred to as the coordinate Bethe ansatz), we find it easier to use the algebraic Bethe ansatz approach [6–8]. The main point is that the state with all spins up, which is called the “reference” state and which we denote by  $|0\rangle$ , is an eigenstate of the Hamiltonian (with eigenvalue 0); and additional eigenstates, called “Bethe states,” can be constructed by acting with certain creation operators  $B(\lambda)$  on the reference state:

$$|\lambda_1, \dots, \lambda_M\rangle = B(\lambda_1) \cdots B(\lambda_M)|0\rangle, \quad (2.1)$$

where  $\{\lambda_1, \dots, \lambda_M\}$  are (by assumption) pairwise distinct, and are solutions of the Bethe equations. Since the creation operators commute  $[B(\lambda), B(\lambda')] = 0$ , any permutation of the Bethe roots  $\{\lambda_1, \dots, \lambda_M\}$  evidently does not affect the state Eq. (2.1). The corresponding energy eigenvalue is given by Eq. (1.2).

The Hamiltonian Eq. (1.1) commutes with the total spin  $\vec{S}$ ,

$$[H, \vec{S}] = 0, \quad \vec{S} = \frac{1}{2} \sum_{n=1}^N \vec{\sigma}_n. \quad (2.2)$$

Hence,  $H$ ,  $\vec{S}^2$ , and  $S^z$  can all be simultaneously diagonalized,

$$\begin{aligned} H|E, s, m\rangle &= E|E, s, m\rangle, \\ \vec{S}^2|E, s, m\rangle &= s(s+1)|E, s, m\rangle, \\ S^z|E, s, m\rangle &= m|E, s, m\rangle. \end{aligned} \quad (2.3)$$

It can be further shown that the Bethe states Eq. (2.1) are highest-weight states,

$$S^+|\lambda_1, \dots, \lambda_M\rangle = 0, \quad S^\pm = S^x \pm iS^y, \quad (2.4)$$

so the spin quantum numbers are given by

$$s = m = \frac{N}{2} - M. \quad (2.5)$$

Although the Bethe ansatz can give only highest-weight ( $m = s$ ) eigenstates of the Hamiltonian, the eigenstates with  $m < s$  can easily be obtained by repeatedly acting with the spin-lowering operator  $S^-$  on the Bethe states.

It is now not difficult to determine, for a given value of  $N$ , the possible values of spin  $s$  (and hence the possible values of  $M$ ), and their multiplicities (which naively should be the number of solutions of the Bethe equations with  $M$  Bethe roots). Indeed, the Clebsch-Gordan theorem implies that the  $N$ -fold tensor product of spin-1/2 representations decomposes into a direct sum of (irreducible) spin- $s$  representations,

$$\underbrace{\frac{1}{2} \otimes \cdots \otimes \frac{1}{2}}_N = \bigoplus_{s=0}^{\frac{N}{2}} n_s s, \quad (2.6)$$

where  $n_s$ , the number of representations with spin- $s$ , is given by

$$n_s = \binom{N}{\frac{N}{2} - s} - \binom{N}{\frac{N}{2} - s - 1}. \quad (2.7)$$

Note from Eq. (2.6) that the values of  $s$  range from 0 to  $N/2$ ; hence, according to Eq. (2.5), the values of  $M$  also range from 0 to  $N/2$ , as already anticipated in Eq. (1.3).

It follows from Eqs. (2.5) and (2.7) that  $\mathcal{N}(N, M)$ , the number of solutions of the Bethe equations with  $M$  pairwise distinct roots, should naively be given by

$$\mathcal{N}(N, M) \stackrel{?}{=} \binom{N}{M} - \binom{N}{M-1}. \quad (2.8)$$

However, this is not correct. The flaw in the argument can be traced back to the incorrect assumption that every solution of the Bethe equations with pairwise distinct roots produces, via Eq. (2.1), an eigenstate of the Hamiltonian. Indeed, the Bethe equations admit so-called singular (or exceptional) solutions, one of whose roots is  $i/2$  and another of which is  $-i/2$ ; and only a subset of those solutions produces eigenstates of the Hamiltonian. Those singular solutions that produce eigenstates of the Hamiltonian we call “physical,” and those singular solutions that do not produce eigenstates of the Hamiltonian we call “unphysical.”

Fortunately, there exists a simple criterion for determining whether a given singular solution is physical or unphysical. Consider a general singular solution of the Bethe equations,

$$\left\{ \frac{i}{2}, -\frac{i}{2}, \lambda_3, \dots, \lambda_M \right\}, \quad (2.9)$$

where  $\lambda_3, \dots, \lambda_M$  are pairwise distinct and are not equal to  $\pm i/2$ . The Bethe Eqs. (1.3) imply that the last  $M-2$  roots  $\{\lambda_3, \dots, \lambda_M\}$  obey

$$\left( \frac{\lambda_k + \frac{i}{2}}{\lambda_k - \frac{i}{2}} \right)^{N-1} \left( \frac{\lambda_k - \frac{3i}{2}}{\lambda_k + \frac{3i}{2}} \right) = \prod_{\substack{j \neq k \\ j=3}}^M \frac{\lambda_k - \lambda_j + i}{\lambda_k - \lambda_j - i}, \quad k = 3, \dots, M. \quad (2.10)$$

This singular solution is physical if  $\{\lambda_3, \dots, \lambda_M\}$  also obey [25]

$$\left[ - \prod_{k=3}^M \left( \frac{\lambda_k + \frac{i}{2}}{\lambda_k - \frac{i}{2}} \right) \right]^N = 1. \quad (2.11)$$

We are finally ready to formulate a precise conjecture for  $\mathcal{N}(N, M)$  in terms of numbers of singular solutions. Let  $\mathcal{N}_s(N, M)$  denote the number of solutions of the Bethe Eqs. (1.3) that are singular [i.e., that have the form (2.9)]; and let  $\mathcal{N}_{\text{sp}}(N, M)$  denote the number of such singular solutions that satisfy Eq. (2.11) and hence are physical. We conjecture that

$$\mathcal{N}(N, M) - \mathcal{N}_s(N, M) + \mathcal{N}_{\text{sp}}(N, M) = \binom{N}{M} - \binom{N}{M-1}. \quad (2.12)$$

The physical meaning of this conjecture is that the Bethe equations generally have “too many” solutions with pairwise distinct roots; but after discarding the singular solutions

that do not satisfy Eq. (2.11), there remain exactly the right number of solutions to account for all  $\binom{N}{M} - \binom{N}{M-1}$  highest-weight eigenstates (and therefore all  $2^N$  eigenstates) of the Hamiltonian. Hence, Eq. (2.12) expresses the completeness—after appropriate culling—of the solutions of the Bethe equations with pairwise distinct roots. It is therefore natural to call it the “completeness–Pauli-principle conjecture.”<sup>4</sup> Unfortunately, we do not have conjectures for  $\mathcal{N}, \mathcal{N}_s, \mathcal{N}_{\text{sp}}$  separately for general values of  $N$  and  $M$ , but only for the combination  $\mathcal{N} - \mathcal{N}_s + \mathcal{N}_{\text{sp}}$ .

We emphasize the two-way nature of this conjecture:

(i) for every highest-weight eigenstate of the Hamiltonian, there is a solution of the Bethe equations with pairwise distinct roots; and

(ii) for every solution of the Bethe equations with pairwise distinct roots that (if it is singular) also satisfies Eq. (2.11), there is a highest-weight eigenstate of the Hamiltonian.

To our knowledge, previous studies of completeness have focused only on point (i), and therefore have not addressed the many unphysical singular solutions of the Bethe equations. A case in point is Ref. [23], which reports solutions of the Bethe equations for  $N = 8$  and  $N = 10$ , but the only singular solutions that are included are the physical ones.

In order to check the conjecture, it is necessary to find *all* the solutions with pairwise distinct roots of the Bethe equations. It is to this task that we now turn.

### III. HOMOTOPY CONTINUATION

Homotopy continuation (often called continuation) is the main numerical approach to find isolated roots of polynomial systems without regard to the dimension of the ambient space, restrictions on the systems, or the bounds on the size of the domain in Euclidean space where the solutions are sought. In this section we outline the method and its main features and mention the main software packages.

Some surveys of this material are Refs. [27–30]. The classic Ref. [31] is a good reference for many software implementation details. The methods apply more generally than systems of polynomials, but without many of the features we need, e.g., guarantees for finding solutions and accurate computation of singular solutions. The classic reference for continuation methods in this general situation (putting the case of polynomial systems in context) is Ref. [32].

Polynomial system solving has a long history of applications to widely diverse areas, e.g., kinematics, chemical

<sup>4</sup>We could generalize Eq. (2.12) to allow for violations of the Pauli principle by adding an extra term:

$$\begin{aligned} \mathcal{N}(N, M) - \mathcal{N}_s(N, M) + \mathcal{N}_{\text{sp}}(N, M) + \mathcal{N}_{\text{strange}}(N, M) \\ = \binom{N}{M} - \binom{N}{M-1}, \end{aligned}$$

where  $\mathcal{N}_{\text{strange}}(N, M)$  is the number of “strange” solutions of the Bethe equations whose roots are *not* pairwise distinct but which nevertheless produce, via Eq. (2.1), eigenstates of the Hamiltonian. However, as far as we have checked, there is no need for such a term, i.e.,  $\mathcal{N}_{\text{strange}}(N, M) = 0$ .

reaction systems, game theory, mathematical biology, systems of nonlinear differential equations, and physics. Applications to theoretical kinematics go back to the 19th Century. It is fair to say that the main application areas presented in Refs. [28,31] lie in kinematics and robotics; for more details, see the references in those books and the survey article [30]. Chemical reactions systems are treated in Ref. [31]; for more details, see the references there and in Refs. [28,33–35]. Game theory applications and some references may be found in Ref. [28]. Polynomial systems arise naturally in the discretization of systems of nonlinear differential equations; for more details, see the early Refs. [36,37], some more recent Refs. [38,39], and the references contained therein. For applications to a variety of models from mathematical biology, see Refs. [40–42]. For recent applications to physics, see, e.g., Refs. [43–53] and the references contained therein.

The continuation method to find the solutions of a polynomial system  $f$  starts with a polynomial system  $g$  (called the start system) and a set  $\mathcal{S}_g$  of nonsingular solutions of  $g$ , which are called start points. The method proceeds to deform the system  $g$  and  $\mathcal{S}_g$  to the system  $f$  and a set of solutions  $\mathcal{S}_f$  of  $f$ . We make this precise below. The references listed above detail many different possible choices of  $g$  for which homotopy continuation is guaranteed to find a set of solutions of  $f$ , which contain all isolated solutions of  $f$ . We use the total degree homotopy (explained below), which is the first homotopy that was shown to find all solutions of a polynomial system.

For Bethe’s Eqs. (1.3), we begin by introducing the polynomials  $f_k$  in the variables  $\lambda_1, \dots, \lambda_M$ , which we regard as specifying a variable point in  $\mathbb{C}^M$ ,

$$f_k(\vec{\lambda}) = \left(\lambda_k + \frac{i}{2}\right)^N \prod_{\substack{j \neq k \\ j=1}}^M (\lambda_k - \lambda_j - i) - \left(\lambda_k - \frac{i}{2}\right)^N \prod_{\substack{j \neq k \\ j=1}}^M (\lambda_k - \lambda_j + i), \quad (3.1)$$

where  $\vec{\lambda} = (\lambda_1, \lambda_2, \dots, \lambda_M)^T$ . Notice that the degrees of the polynomials  $f_k$  are  $N + M - 2$  after simplifying [since the top degree terms of the left-hand side and right-hand side of Eq. (1.3) are equal].

We then define the following homotopy function:

$$\vec{H}(\vec{\lambda}, t) = (1 - t)\vec{f}(\vec{\lambda}) + \gamma t \vec{g}(\vec{\lambda}), \quad (3.2)$$

where  $\vec{f} = (f_1, \dots, f_M)^T$ ,  $\vec{g} = (g_1, \dots, g_M)^T$ ,  $g_k = \lambda_k^{N+M-2} - 1$ . Moreover,  $t \in [0, 1]$  is a homotopy parameter, and  $\gamma$  is a random complex number. When  $t = 1$ , we have known solutions to  $\vec{g}(\vec{\lambda}) = 0$ , or equivalently,  $\vec{H}(\vec{\lambda}, 1) = 0$ . Specifically, the solutions of  $g_k = 0$  are

$$\lambda_k = \omega^{jk}, \quad \omega = e^{2\pi i / (N+M-2)}, \quad j_k = 0, 1, \dots, N + M - 3. \quad (3.3)$$

The solutions of  $\vec{g}(\vec{\lambda}) = 0$  therefore yield values for each  $\lambda_k$ . The known solutions are called start points, and the system  $\vec{H}(\vec{\lambda}, 1) = 0$  is called the start system. Such a start system with the degree  $d_k$  of  $g_k$  equal to the degree of  $f_k$  for all  $k$  and with the number of solutions of  $\vec{H}(\vec{\lambda}, 1) = 0$  equal to  $\prod_{k=1}^n d_k$  is called a *total degree start system*. (The number of

isolated solutions of a system of  $n$  polynomial equations  $f_k$  in  $n$  variables is always less than or equal to  $\prod_{i=1}^n \deg f_i$ .) Choosing a total degree start system and a random complex number  $\gamma$  guarantees finding all the solutions. The use of the random  $\gamma$ , which is called the  $\gamma$  trick, was introduced in Ref. [54]. A good discussion of a more general version of this trick is given in Ref. [28], Lemma 7.1.3].

However, as previously explained, we are interested in solutions  $(\lambda_1, \dots, \lambda_M)$  up to permuting the coordinates, and with no two  $\lambda$ ’s equal. Hence, we may restrict  $j_k$  in Eq. (3.3) to run over all  $M$ -tuples of integers

$$0 \leq j_1 < j_2 < j_3 < \dots < j_M \leq N + M - 3. \quad (3.4)$$

To see this, note that the equations  $H_1, \dots, H_M$  of the homotopy  $\vec{H}(\vec{\lambda}, t)$  are permuted by the symmetric group on the variables  $\lambda_1, \dots, \lambda_M$ . Indeed, under a permutation  $\sigma$  taking  $\lambda_j$  to  $\lambda_k$ ,  $H_j$  is taken to  $H_k$ . This has strong consequences for the homotopy [55]: we explain the consequence we need. The paths in  $\lambda, t$  space over the interval  $(0, 1]$ , are permuted by the action of the symmetric group. A start point has pairwise disjoint entries if and only if the orbit in the set of start points under the symmetric group consists of exactly  $M!$  points. Since there is one path for each of the start points, we see that the number of paths a given path over  $(0, 1]$  is taken to under the symmetric group is  $M!$  if and only if the start point has pairwise disjoint entries. The orbit of a root of  $\vec{H}(\vec{\lambda}, 0) = 0$ , which is a limit of a path  $p$ , equals the set of limits as  $t \rightarrow 0$  of the paths in the orbit of the path  $p$  under the symmetric group action. From this we see that a root of  $\vec{H}(\vec{\lambda}, 0) = 0$  can have pairwise disjoint entries only if it is the limit of some path with a start point having pairwise disjoint entries. Note that this does not preclude a path with start point having pairwise disjoint coordinates ending at a root of  $\vec{H}(\vec{\lambda}, 0) = 0$  without pairwise disjoint coordinates. Note also that the number of start points is only  $\binom{N+M-2}{M}$  since it equals the number of  $M$ -tuples of integers Eq. (3.4).

At  $t = 0$ , we evidently recover the Bethe equations. The problem of finding the solutions of the Bethe equations now reduces to tracking solutions of  $\vec{H}(\vec{\lambda}, t) = 0$  from  $t = 1$  where we know solutions to  $t = 0$ . The numerical method used in path tracking from  $t = 1$  to  $t = 0$  arises from solving the *Dauidenko differential equation*:

$$\frac{d\vec{H}(\vec{\lambda}(t), t)}{dt} = \frac{\partial \vec{H}(\vec{\lambda}(t), t)}{\partial \vec{\lambda}} \frac{d\vec{\lambda}(t)}{dt} + \frac{\partial \vec{H}(\vec{\lambda}(t), t)}{\partial t} = 0. \quad (3.5)$$

In particular, path tracking reduces to solving initial value problems numerically with the start points being the initial conditions. Since we also have an equation that vanishes along the path, namely  $\vec{H}(\vec{\lambda}, t) = 0$ , predictor and corrector methods, e.g., rkf45 as a predictor with the Newton-Rapson’s method as a corrector, are used to solve these initial value problems.

Continuation methods parallelize naturally, by sending different paths to different processors to track. Predictor and corrector methods combined with adaptive stepsize and adaptive precision algorithms [56,57] provide reliability without giving up efficiency. The major concerns for implementing a numerical path-tracking algorithm are to decide the number of digits used to provide reliable computation, which predictor or corrector method to employ, and the stepsize  $\Delta t$ ; see

TABLE I. Solutions with distinct roots of the Bethe equations for  $N = 8$ ,  $M = 4$ . Singular solutions that are unphysical are labeled by \*, and singular solutions that are physical are labeled by \*\*.

Number	Bethe roots $\{\lambda_k\}$		
1	$\pm 0.5250121022236669$	$\pm 0.1294729463749287$	
2	$0.5570702385744416$	$0.1470126111961413$	$-0.3520414248852914 \pm 0.5005581696433306I$
3*	$\pm 0.5I$	$-0.2930497652740115 \pm 0.5002695484553508I$	
4*	$\pm 0.5I$	$0.09053461122303935$	$0.4866819617430914$
5*	$\pm 0.5I$	$-0.04929340793103601 + 1.631134975618312I$	$-0.2430919428911911 - 0.06188079036780695I$
6*	$\pm 0.5I$	$0.6439488581706157 - 0.1197616885579488I$	$0.05986712277687283 + 1.57171694471433I$
7*	$\pm 0.5I$	$0.04929340793103601 + 1.631134975618312I$	$0.2430919428911911 - 0.06188079036780695I$
8**	$\pm 0.5I$	$\pm 0.5638252623934961$	
9	$0.2205600072920844$	$-0.6691229228815117$	$0.2242814577947136 \pm 1.002247276506607I$
10*	$\pm 0.5I$	$0.1695810016454493$	$-0.522716443014433$
11*	$\pm 0.5I$	$-0.05986712277687283 + 1.57171694471433I$	$-0.6439488581706157 - 0.1197616885579488I$
12*	$\pm 0.5I$	$1.653144833689466I$	$-0.050307293346599I$
13*	$\pm 0.5I$	$0.522716443014433$	$-0.1695810016454493$
14*	$\pm 0.5I$	$0.050307293346599I$	$-1.653144833689466I$
15*	$\pm 0.5I$	$-0.4866819617430914$	$-0.09053461122303935$
16*	$\pm 0.5I$	$0.04929340793103601 - 1.631134975618312I$	$0.2430919428911911 + 0.06188079036780695I$
17*	$\pm 0.5I$	$0.2930497652740115 \pm 0.5002695484553508I$	
18**	$\pm 0.5I$	$\pm 0.1424690678305666$	
19**	$\pm 0.5I$	$\pm 1.556126503577051I$	
20*	$\pm 0.5I$	$3.517084291308099I$	$1.508105736964082I$
21	$0.2443331937711654$	$-0.08378710739142802$	$-0.08027304318986867 \pm 1.005588273959932I$
22*	$\pm 0.5I$	$0.05986712277687283 - 1.57171694471433I$	$0.6439488581706157 + 0.1197616885579488I$
23	$0.1211861779691729$	$-0.5716111771864383$	$0.2252124996086327 \pm 0.5000288621635332I$
24		$\pm 0.4632647275890309 \pm 0.5022938535699026I$	
25	$-0.1470126111961413$	$-0.5570702385744416$	$0.3520414248852914 \pm 0.5005581696433306I$
26*	$\pm 0.5I$	$-0.05986712277687283 - 1.57171694471433I$	$-0.6439488581706157 + 0.1197616885579488I$
27	$0.08378710739142802$	$-0.2443331937711654$	$0.08027304318986867 \pm 1.005588273959932I$
28*	$\pm 0.5I$	$-0.2430919428911911 + 0.06188079036780695I$	$-0.04929340793103601 - 1.631134975618312I$
29	$\pm 1.025705081230743I$	$\pm 0.0413091275245562$	
30*	$\pm 0.5I$	$-1.508105736964082I$	$-3.517084291308099I$
31	$0.5716111771864383$	$-0.1211861779691729$	$-0.2252124996086327 \pm 0.5000288621635332I$
32	$-0.2205600072920844$	$0.6691229228815117$	$-0.2242814577947136 \pm 1.002247276506607I$

Refs. [28,57] for more details regarding the construction and implementation of a path tracking algorithm.

We mention that for polynomial systems, there are special path-tracking algorithms [58–60], often called endgames, to compute singular solutions. When the endpoint of a solution path is singular, there are several approaches that give highly accurate estimates of the endpoint. These methods use the fact that the homotopy continuation path  $\vec{\lambda}(t)$  approaching a solution of  $\vec{H}(\vec{\lambda}, t) = 0$  as  $t \rightarrow 0$  lies on a complex analytic curve, which may be locally uniformized near  $(\lambda, 0)$ , by an analytic disk. Many of these endgames are implemented in several sophisticated numerical packages such as Bertini [29], PHCpack [61], and HOMPACK [62]. Their binaries are all available as freeware from their respective research groups. We note also HOM4PS-2.0 [63], the leading homotopy continuation software using polyhedral methods: this software is not useful for us in this article because it does not allow the user to specify a homotopy and a set of start points.

We employed Bertini [29] with adaptive precision tracking [56,57]: due to the high degree of Bethe's equations, a precision of 2000 bits (roughly 600 digits) is needed to solve the system. We ran Bertini on a 64-bit Linux cluster with 13 dual Xeon 5410 nodes (each with 8 GB RAM and 8 cores) and 9 dual

Xeon E5520 nodes (each with 12 GB RAM and 8 cores). One node acted as manager with up to 22 computing nodes (giving a total of 176 cores).

The results for  $N = 2, \dots, 12$  are presented in a set of supplemental tables [64], an example of which is Table I. To give some perspective in computational effort, the case of  $(N, M) = (14, 7)$  took 4413.5 seconds of computation while the case of  $(N, M) = (12, 6)$  took 168.8 seconds of computation.

#### IV. SOLVING THE T-Q EQUATION

There is also a powerful indirect way of determining the Bethe roots based on the Baxter T-Q equation. By virtue of the model's integrability, one can construct the so-called transfer matrix  $t(\lambda)$ , a  $2^N \times 2^N$  matrix that is a function of an arbitrary parameter  $\lambda$ , which commutes with itself for different values of this parameter as well as with the Hamiltonian Eq. (1.1) [5–8]:

$$[t(\lambda), t(\lambda')] = 0, \quad [t(\lambda), H] = 0. \quad (4.1)$$

Furthermore, it can be shown that the eigenvalues of the transfer matrix, which we denote here by  $T(\lambda)$ , are polynomials in

$\lambda$  of degree  $N$ ,

$$T(\lambda) = \sum_{j=0}^N T_j \lambda^j, \quad (4.2)$$

where the coefficients  $T_j$  are independent of  $\lambda$ . Moreover, the transfer matrix eigenvalues satisfy the celebrated T-Q equation [5–8]

$$T(\lambda) Q(\lambda) = \left(\lambda + \frac{i}{2}\right)^N Q(\lambda - i) + \left(\lambda - \frac{i}{2}\right)^N Q(\lambda + i), \quad (4.3)$$

where  $Q(\lambda)$  is a polynomial in  $\lambda$  of degree  $M$ , whose zeros are the sought-after solutions of the Bethe Eqs. (1.3),

$$Q(\lambda) = \prod_{m=1}^M (\lambda - \lambda_m) = \sum_{j=0}^M Q_j \lambda^j, \quad Q_M = 1, \quad (4.4)$$

where the coefficients  $Q_j$  are independent of  $\lambda$ . Indeed, dividing both sides of Eq. (4.3) by  $Q(\lambda)$ , it appears that the right-hand side has poles at the zeros of  $Q(\lambda)$ , in contradiction with the fact the left-hand side is a polynomial in  $\lambda$  and must therefore be regular. The only way out of this paradox is for the poles to cancel, the condition for which is precisely the Bethe Eqs. (1.3).

Interestingly, it is possible to solve the T-Q Eq. (4.3) numerically for both  $T(\lambda)$  and  $Q(\lambda)$ ; and then, by finding the zeros of  $Q(\lambda)$ , determine all the solutions of the Bethe equations.<sup>5</sup> The basic idea is to substitute Eqs. (4.2) and (4.4) into the T-Q Eq. (4.3) and then equate coefficients with equal powers of  $\lambda$ . In other words, Eqs. (4.2) and (4.4) imply that

$$T(\lambda) Q(\lambda) - \left[ \left(\lambda + \frac{i}{2}\right)^N Q(\lambda - i) + \left(\lambda - \frac{i}{2}\right)^N Q(\lambda + i) \right] = \sum_{j=0}^{N+M} c_j \lambda^j, \quad (4.5)$$

where the coefficients  $c_j$  are independent of  $\lambda$ ; and the T-Q equation implies that

$$c_j = 0, \quad j = 0, 1, \dots, N + M. \quad (4.6)$$

Note that  $c_{M+1}, \dots, c_{M+N}$  are independent of  $T_0$  and are linear in  $T_1, \dots, T_N$ . Therefore, Eqs. (4.6) with  $j = M + 1, \dots, M + N$  can be solved uniquely for  $T_1, \dots, T_N$  in terms of  $Q_0, \dots, Q_{M-1}$ . Substituting this solution into the remaining coefficients  $c_0, \dots, c_M$ , we arrive at a system of  $M + 1$  nonlinear equations,

$$c_j = 0, \quad j = 0, 1, \dots, M, \quad (4.7)$$

for the  $M + 1$  unknowns  $Q_0, \dots, Q_{M-1}, T_0$ .<sup>6</sup> This system of equations is somewhat simpler than the corresponding  $M$

Bethe Eqs. (1.3). Indeed, the above procedure can easily be implemented on a desktop computer, which can perform the case  $N = 9$  in a few minutes but cannot manage higher values of  $N$ . The results agree with the corresponding results (up to  $N = 9$ ) obtained in Sec. III. We have not attempted to implement this procedure on better hardware.

A variation of the above procedure is to first determine the eigenvalues  $T(\lambda)$  by explicitly diagonalizing the transfer matrix  $t(\lambda)$ <sup>7</sup> and then solving the T-Q Eq. (4.3) for  $Q(\lambda)$ .<sup>8</sup> This approach has the advantage that solving the T-Q equation for only  $Q$  is a linear (albeit, overdetermined) problem; however, it has the disadvantage of requiring the diagonalization of a large matrix. This procedure can also be easily implemented on a desktop computer, which can again perform the case  $N = 9$  in a few minutes but cannot manage higher values of  $N$ . Unlike the former approach where one solves the T-Q equation for both  $T$  and  $Q$ , the only singular solutions that this method can generate are the physical ones. Hence, this method can check only point (i) of the two points listed below Eq. (2.12).

## V. SUMMARY AND DISCUSSION

Our results are summarized in Table II. For each set of values  $(N, M)$ , we report a set of four integers:

$$(\mathcal{N}, \mathcal{N}_s, \mathcal{N}_{\text{sp}}; \mathcal{N} - \mathcal{N}_s + \mathcal{N}_{\text{sp}}),$$

where  $\mathcal{N}$  is the number of solutions with pairwise distinct roots of the Bethe equations;  $\mathcal{N}_s$  is the number of singular solutions; and  $\mathcal{N}_{\text{sp}}$  is the number of singular solutions that are physical (see Sec. II for further details). These quantities can easily be read off from Table I and the supplemental tables [64] as follows:  $\mathcal{N}$  is the number of solutions listed in a given table;  $\mathcal{N}_s$  is the number of those solutions labeled with either a single \* or double \*\* star; and  $\mathcal{N}_{\text{sp}}$  is the number of those solutions labeled with a double star.

Remarkably, the quantities  $\mathcal{N} - \mathcal{N}_s + \mathcal{N}_{\text{sp}}$  in all the entries of Table II coincide with  $\binom{N}{M} - \binom{N}{M-1}$ , in perfect agreement with the conjecture Eq. (2.12). Although this conjecture was motivated from consideration of a physical model Eq. (1.1), it can be viewed solely as a statement about the solutions of the polynomial Eqs. (1.3) and (2.11), which begs for a proof.

It is easy to see that the number of solutions for  $M = 1$  is  $N - 1$ ,

$$\mathcal{N}(N, 1) = N - 1. \quad (5.1)$$

Moreover, for  $M = 2$ , we observe

$$\mathcal{N}(N, 2) = \frac{1}{2}[N^2 + 3N + 1 + (-1)^N]. \quad (5.2)$$

It would be interesting to formulate conjectures (not to mention proofs) for  $\mathcal{N}(N, M)$  for  $M \geq 3$ .

<sup>5</sup>This very nice approach does not seem to be widely known. To our knowledge, it was first published by Baxter [15], and it has recently been rediscovered in the context of Richardson-Gaudin models [65,66].

<sup>6</sup>Since  $c_0, \dots, c_M$  are linear in  $T_0$ , it is also possible to eliminate  $T_0$  in terms of  $Q_0, \dots, Q_{M-1}$ , and thereby arrive at a system of  $M$  nonlinear equations for  $M$  unknowns.

<sup>7</sup>In practice, one first computes the eigenvectors of the numerical matrix  $t(\lambda_0)$  (where  $\lambda_0$  is some generic numerical value), and then one acts with  $t(\lambda)$  on these eigenvectors to obtain the corresponding eigenvalues  $T(\lambda)$  as polynomials in  $\lambda$ .

<sup>8</sup>This approach for determining Bethe roots has been used many times in the past, e.g., Refs. [14,67,68].

TABLE II. The values  $(\mathcal{N}, \mathcal{N}_s, \mathcal{N}_{sp}; \mathcal{N} - \mathcal{N}_s + \mathcal{N}_{sp})$  for given values of  $N$  and  $M$ , where  $\mathcal{N}$  is the number of solutions with pairwise distinct roots of the Bethe equations;  $\mathcal{N}_s$  is the number of singular solutions; and  $\mathcal{N}_{sp}$  is the number of singular solutions that are physical.

N \ M	1	2	3	4	5	6	7
2	(1,0,0; 1)						
3	(2,0,0; 2)						
4	(3,0,0; 3)	(2, 1, 1; 2)					
5	(4,0,0; 4)	(6, 1, 0; 5)					
6	(5,0,0; 5)	(9, 1, 1; 9)	(9, 5, 1; 5)				
7	(6,0,0; 6)	(15, 1, 0; 14)	(20, 6, 0; 14)				
8	(7,0,0; 7)	(20, 1, 1; 20)	(34, 7, 1; 28)	(32, 21, 3; 14)			
9	(8,0,0; 8)	(28, 1, 0; 27)	(54, 8, 2; 48)	(69, 27, 0; 42)			
10	(9,0,0; 9)	(35, 1, 1; 35)	(83, 9, 1; 75)	(122, 36, 4; 90)	(122, 84, 4; 42)		
11	(10,0,0; 10)	(45, 1, 0; 44)	(120, 10, 0; 110)	(209, 44, 0; 165)	(252, 120, 0; 132)		
12	(11,0,0; 11)	(54, 1, 1; 54)	(163, 10, 1; 154)	(325, 55, 5; 275)	(456, 163, 4; 297)	(452, 330, 10; 132)	
13	(12, 0, 0; 12)	(66, 1, 0; 65)	(220, 12, 0; 208)	(494, 65, 0; 429)	(792, 220, 0; 572)	(919, 490, 0, 429)	
14	(13, 0, 0; 13)	(77, 1, 1; 77)	(285, 13, 1; 273)	(709, 78, 6; 637)	(1281, 286, 6; 1001)	(1701, 715, 15; 1001)	(1701, 1287, 15; 429)

Several remarks about the singular solutions are in order:

(i) Inspection of Table I and the supplemental tables [64] shows that many (but not all) of the unphysical singular solutions (i.e., those solutions labeled by a single star \*) are not self-conjugate. This does not violate any theorems, since only solutions corresponding to eigenstates of the Hamiltonian are required to be invariant under complex conjugation [69]. Such solutions definitely do *not* obey the string hypothesis, since string configurations are (by definition) self-conjugate.

(ii) For odd values of  $N$ , it appears from Table II that most singular solutions are unphysical; i.e.,  $\mathcal{N}_{sp}(N, M) = 0$  for most values of  $M$  if  $N$  is odd. An exception is the case  $N = 9, M = 3$ , for which  $\mathcal{N}_{sp}(9, 3) = 2$ ; and this repeats with a periodicity of 6:  $\mathcal{N}_{sp}(15, 3) = 2$ , etc. We expect that similar exceptions occur for higher values of  $M$ .

(iii) It appears from Table II that, among the singular solutions, relatively few are physical (i.e., generally  $\mathcal{N}_s \gg \mathcal{N}_{sp}$ ), with  $\mathcal{N}_{sp} \sim M$ .

(iv) For  $M \sim N/2$  and most values of  $N$ , it appears from Table II that the number of unphysical singular solutions  $\mathcal{N}_s - \mathcal{N}_{sp}$  is comparable to the number of highest-weight states of the Hamiltonian. This suggests that the naive formula Eq. (2.8) for the number of solutions of the Bethe equations is incorrect not only for small values of  $N$ , but also for  $N \rightarrow \infty$ . This, in turn, suggests that the computations claiming to prove this naive formula for  $N \rightarrow \infty$  [7,9–11] are also incorrect. These computations nevertheless manage to obtain the correct number of highest-weight states, perhaps because the assumption of the string hypothesis (which all of these

computations make) effectively projects out sufficiently many of these unphysical singular solutions (many of which, as noted above, do not obey the string hypothesis) in the thermodynamic limit. It would be interesting to understand this point better, given that the criterion for selecting the physical singular solutions is not that they obey the string hypothesis, but instead Eq. (2.11).

We have seen that, using appropriate computer resources, numerical homotopy methods are effective for solving the Bethe equations directly. It would be interesting to also implement the indirect approach based on the T-Q equation using similar computer resources and compare the effectiveness of these approaches.

As noted in the Introduction, the model that we have studied here is the prototype of an entire zoo of quantum integrable models, which have generalizations of the Bethe equations. We expect that the methods used here can also be used to study completeness in some of these other models.

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