Singularities in the Bethe solution of the XXX and XXZ Heisenberg spin chains

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Abstract

We examine the question of whether Bethe’s ansatz reproduces all states in the periodic Heisenberg XXZ and XXX spin chains. As was known to Bethe himself, there are states for which the Bethe momenta \( k_n \) diverge: these are in fact the simplest examples of “string” solutions. The coefficients of the Bethe wavefunction, too, diverge. When there are only two down spins in the system (the case considered by Bethe), we can renormalize these coefficients to get a sensible (and correct) wavefunction. We show that this is not always possible when there are more than two down spins. The Bethe equations have several such divergent solutions, and some of these correspond to genuine eigenfunctions of the Hamiltonian, but several do not. Nor do they reproduce the correct energy eigenvalues. Moreover, we point out that the algebraic Bethe ansatz, an alternative way to construct the wavefunctions proposed by Faddeev, Takhtajan et al., leads to vanishing wavefunctions for all these solutions. Thus, the Bethe ansatz solution of the Heisenberg model must be regarded as either incomplete, or inaccurate.

1 Introduction

The XXZ spin-half Heisenberg Hamiltonian for \( N \) interacting spins, on a one-dimensional chain with periodic boundary conditions \( (n + N \equiv n) \), is

\[
H = -2 \sum_{n=1}^{N} \left( S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z \right)
\]  

(1)

where \( \Delta \) is the anisotropy parameter, 0 for the XY model, 1 for the isotropic ferromagnet. \( \Delta = -1 \) can be mapped to the isotropic antiferromagnet. We have put the overall factor of 2 for convenience. In terms of the Pauli spin matrices,

\[
H = -\sum_{n=1}^{N} \left( \sigma_n^+ \sigma_{n+1}^- + \sigma_n^- \sigma_{n+1}^+ + \frac{\Delta}{2} \sigma_n^z \sigma_{n+1}^z \right)
\]  

(2)

where \( \sigma^\pm \equiv (\sigma^x \pm i\sigma^y)/2 \). This was among the first many-body quantum problems to be solved exactly. Bethe solved the isotropic model (the “XXX model”, \( \Delta = 1 \)) in 1931, and the XXZ Hamiltonian can be solved similarly with little additional effort. The form of wavefunction which he used has become known as the Bethe Ansatz and has been applied to a wide variety of other problems.

The Bethe ansatz, however, is a guess, and while one can generally verify whether or not it works, there is no easy way to tell whether it is “complete”, that is, whether all the energy eigenstates are of this form.

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There are actually two versions of the Bethe ansatz—the original method of Bethe, and the “algebraic Bethe ansatz” developed by Takhtajan, Faddeev and others based on the work of Baxter on vertex models. Though they start from very different ideas, the two approaches lead to the same equations and (apart from normalization) the same wavefunctions. Some concrete statements on completeness have been made in the case of the XXX model, namely that the algebraic Bethe ansatz reproduces only the states of “highest weight” with respect to the underlying SU(2) symmetry (which has been proved) and that it reproduces all such states (which has not been shown strictly). By “highest weight” is meant a state with the maximum allowed value of $S^z$ (the total $z$ component of the spin) for given total spin $S$; such a state is annihilated by the total spin raising operator $S^+$. The proof that all Bethe states are of highest weight, however, depends on a change of variables from Bethe’s $k_n$ to new variables $\lambda_n$ which arise more naturally in the algebraic method (besides being convenient in other ways), and the subsequent restriction that these variables must be finite-valued and distinct. The original ansatz of Bethe, in terms of the $k$’s, reproduces many non-highest-weight states without trouble. Moreover, this doesn’t answer the question of completeness in the anisotropic (XXZ) case where there is no underlying SU(2) symmetry. The arguments for completeness even in the XXX chain are not rigorous: Essler et al. show that the usual state-counting argument is not quite correct, but they view this as a reorganization of states and suggest that the ansatz for the XXX chain is SU(2) complete anyway.

Here, after a quick review of the Bethe ansatz, coordinate and algebraic, mainly to fix the notation, we look into these questions. We find that a number of states correspond to Bethe $k$’s which diverge to $\pm i\infty$, and these include states which are of highest weight at the isotropic point. The variables $\lambda_n$ which one usually uses in the algebraic Bethe ansatz are well-behaved, but the coefficients of the Bethe wavefunction are singular. The algebraic method offers an alternative way to produce a wavefunction, but this construction produces a vanishing wavefunction.

To handle this situation, one can consider only the ratios of the Bethe coefficients, rather than the coefficients themselves (which is reasonable since the wavefunctions are not normalized). These turn out to be finite, but we then find that some of the states thus produced are not eigenstates of the Hamiltonian at all. In fact, the energies predicted by the Bethe equations also turn out to be wrong.

In short, the equations of Bethe, written in terms of the variables $\lambda_n$, have a number of solutions with finite, well-behaved $\lambda_n$ which (depending on one’s viewpoint) either do not reproduce the corresponding eigenstates, or produce too many states including some which are not eigenstates.

Finally, we also point out that one can formally get rid of these singularities by introducing an Aharonov-Bohm flux through the ring, that is, associating different phases with the forward and backward spin hopping amplitudes. But for certain special values of the phase (namely, the $N$ roots of unity—corresponding to a total flux of a multiple of $2\pi$ through the ring) the singularities reappear, and for values of the flux close to zero or to any of these points the Bethe equations become numerically ill-behaved and any rootfinder would have severe problems converging to a solution.

## 2 The coordinate Bethe ansatz

Since the Hamiltonian commutes both with the total spin and with $\sigma_z = \sum_n \sigma^z_n$, we can work with an Ising basis with fixed $\sigma^z$. Suppose the number of down-spins is $l$ ($\leq N/2$; the other states can be reached by symmetry), and for a given Ising state, suppose the positions of the down-spins are $x_1, x_2,$ $\ldots, x_l$, and call this basis state $|x_1x_2\ldots x_l\rangle$. A general wavefunction can then be written in this basis as

$$|\Psi\rangle = \sum_{x_1 < x_2 < \ldots < x_l} \psi(x_1, x_2, \ldots, x_l) |x_1, x_2, \ldots, x_l\rangle. \quad (3)$$

Bethe suggested the following form for the expansion coefficients,

$$\psi(x_1, x_2, \ldots, x_l) = \sum_P A(P) \exp \left( i \sum_{n=1}^l k_{P_n} x_n \right) \quad (4)$$

where $P$ is a permutation of the integers $1, 2, \ldots, l$, the sum is over all permutations with amplitudes $A(P)$, and the $k$’s are some as yet undetermined quantities.
One can show that such a wavefunction solves the Hamiltonian (2) if the amplitude for exchange of two neighbouring particles is

\[ A_{mn} = \frac{A(\ldots, m, n, \ldots)}{A(\ldots, n, m, \ldots)} = \frac{e^{i(k_m + k_n)} - 2\Delta e^{ik_m} + 1}{e^{i(k_m + k_n)} - 2\Delta e^{ik_n} + 1} \]  

(5)

In addition, periodic boundary conditions imply that

\[ e^{ik_mN} = \prod_{n \neq m} A_{mn} = (-1)^{l-1} \prod_{n \neq m} e^{i(k_m + k_n)} - 2\Delta e^{ik_m} + 1 \]  

(6)

Equations (6) can be solved for \( k_n \), and each solution \( \{k_n\} \) gives us an eigenstate of (2), with associated energy

\[ E = -N\Delta/2 + 2l\Delta - 2 \sum_{n=1}^{l} \cos(k_n). \]  

(7)

For notational simplicity, we will often use

\[ z_n = e^{ik_n} \]  

(8)

so that the Bethe equations become

\[ z_m^N = (-1)^{l-1} \prod_{n \neq m} \frac{z_m z_n - 2\Delta z_m + 1}{z_m z_n - 2\Delta z_n + 1} \]  

(9)

3 The Algebraic Bethe Ansatz

The same equations can be derived rather differently, by diagonalizing the transfer matrix of the “six vertex model”, in which the Heisenberg XXZ Hamiltonian is embedded. Here we will concern ourselves only with the XXX model, where the algebra is much simpler. We will not describe this method (see [3], for instance) but only mention the change of variables involved, and how the eigenvectors are constructed.

In the case of the XXX model, we define new variables \( \lambda_n \) as follows:

\[ z_n = \frac{\lambda_n + i/2}{\lambda_n - i/2}, \]  

\[ \lambda_n = \frac{i}{2} \frac{z_n + 1}{z_n - 1} = \frac{1}{2} \cot(k_n/2). \]  

(10)

(11)

These variables arise very naturally in the algebraic approach. In terms of these, the Bethe equations (8) become

\[ \left( \frac{\lambda_m + i/2}{\lambda_m - i/2} \right)^N = \prod_{n \neq m} \frac{\lambda_m - \lambda_n + i}{\lambda_m - \lambda_n - i}, \]  

(12)

and the energy of the corresponding state is

\[ E = -\frac{N}{2} + \sum_n \frac{4}{1 + 4\lambda_n^2}. \]  

(13)

The commuting family of transfer matrices for the six vertex model, \( T(\lambda) \), embed the Heisenberg Hamiltonian, and the eigenvectors of the former are the eigenvectors of the latter. \( T(\lambda) \) is the trace of the monodromy matrix

\[ \tau(\lambda) = L_N(\lambda)L_{N-1}(\lambda) \ldots L_1(\lambda) \]  

(14)

where \( L_n(\lambda) \) is the “local \( L \) operator”

\[ L_n(\lambda) = \begin{pmatrix} \lambda + (i/2)\sigma_n^+ & i\sigma_n^- \\ i\sigma_n^+ & \lambda - (i/2)\sigma_n^+ \end{pmatrix}. \]  

(15)
Writing the monodromy matrix as
\[
\tau(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}, \tag{16}
\]

it can be shown that the vector
\[
\{|\lambda_n\rangle\} = \left( \prod_{n=1}^{i} B(\lambda_n) \right) \uparrow \uparrow \uparrow \ldots \tag{17}
\]
is an eigenvector of the transfer matrix \(T\), and therefore of \(H\), if the \(\{\lambda_n\}\) satisfy the equations (12).

## 4 Completeness

Since the Hamiltonian (2) is translationally invariant, a useful classification of the energy eigenstates is in terms of eigenstates of the translation operator \(T\) which shifts all spins by one lattice site to the left. All eigenstates of \(H\) can be chosen to be eigenstates of \(T\) (non-degenerate eigenstates are necessarily so anyway) with eigenvalues \(\phi\) such that \(\phi^N = 1\). The Bethe ansatz does this automatically: for given \(\{z_n\}\),
\[
\phi = \prod z_n.
\]

There is a limit where the Bethe method does reproduce all states without trouble: that of \(\Delta = 0\), or the XY model, which is equivalent to a free Fermi system. The exchange amplitudes \(A_{mn}\) in (4) each become \(-1\), and the \(k\)'s are \(2\pi i/N\) times an integer (for odd \(l\)) or a half-integer (for even \(l\)), all distinct (otherwise the wavefunction vanishes). We then have exactly as many states as we need. Some of these states evolve smoothly as one turns on \(\Delta\), but some don’t, and it’s interesting to see why not.

It turns out that the \(\Delta = 0\) states are sometimes degenerate, but the degeneracy is lifted for any finite \(\Delta\). The states, if chosen correctly, do evolve continuously as \(\Delta\) is changed from zero, but the \(\Delta = 0\) Bethe ansatz gives superpositions of these which are no longer eigenstates for any finite \(\Delta\). We see concrete examples of this below. This also suggests a way around the problem: introduce an Aharonov-Bohm flux, which does not change the eigenstates at \(\Delta = 0\) but lifts the degeneracies in energy. We discuss this later.

### 4.1 Four sites

The generic Bethe Ansatz wavefunction for two down-spins is
\[
|\psi\rangle = \sum_{x_1, x_2} \left( z_1^{x_1} z_2^{x_2} + \frac{1}{A} z_2^{x_1} z_1^{x_2} \right) |x_1, x_2\rangle \tag{18}
\]

with \(x_1 < x_2\); and we also have
\[
z_1^4 = A, \tag{19}
\]
\[
z_2^4 = 1/A, \tag{20}
\]
\[
A = -\frac{z_1 z_2 - 2\Delta z_1 + 1}{z_1 z_2 - 2\Delta z_2 + 1}. \tag{21}
\]

We will number sites starting from 0, to ease the algebra.

Let us follow the convention of denoting a down-spin by 1 and an up-spin by 0. In the case of four sites and two down-spins, we can write down the eigenvectors of \(T\), with corresponding eigenvalues \(\phi\), immediately:

\[
\phi = 1 : \quad |\psi_1\rangle = |1100\rangle + |0110\rangle + |0011\rangle + |1001\rangle
\]
\[
|\psi_2\rangle = |1010\rangle + |0101\rangle
\]
\[
\phi = i : \quad |\psi_3\rangle = |1100\rangle + i|0110\rangle - |0011\rangle - i|1001\rangle
\]
\[
|\psi_4\rangle = |1100\rangle - |0110\rangle + |0011\rangle - |1001\rangle
\]
\[
|\psi_5\rangle = |1010\rangle - |0101\rangle
\]
\[
\phi = -1 : \quad |\psi_6\rangle = |1100\rangle - i|0110\rangle - |0011\rangle + i|1001\rangle
\]
\[
|\psi_7\rangle = |1100\rangle + i|0110\rangle - |0011\rangle - i|1001\rangle
\]
\[
|\psi_8\rangle = |1100\rangle - |0110\rangle - i|0011\rangle + i|1001\rangle
\]
\[
|\psi_9\rangle = |1100\rangle + |0110\rangle + i|0011\rangle - i|1001\rangle
\]
Now, for $\phi = 0$ one has to further diagonalize $H$ in the subspace of $|\psi_1\rangle$ and $|\psi_2\rangle$; but it turns out that all the rest are already eigenstates of $H$. Moreover, $\psi_4$ and $\psi_5$ at $\Delta = 0$ are degenerate, and the Bethe ansatz gives us some superposition of these; but the degeneracy is lifted for arbitrarily small finite $\Delta$. This is one reason the completeness question is nontrivial: it is not obvious that new well-behaved solutions of the Bethe equations will emerge for finite $\Delta$, and if they do, they must be ill-behaved as $\Delta \to 0$ since we already have all the solutions there.

In fact, $|\psi_5\rangle$ is reproduced with the choice $(z_1, z_2) = \pm 1$. This solution works for all $\Delta$ except 0. We now demonstrate that there is no well-behaved solution for $|\psi_4\rangle$.

From the generic Bethe wavefunction in this case (18), we see that $z_1 z_2 = -1$. On the other hand, the coefficient of $|1010\rangle$ should be zero, so we have $z_2^2 + (1/A)z_1^2 = 0$. Combining these conditions gives us $z_1^4 = -A$ which contradicts (14) unless $z_1 = 0$, which implies $A = 0, z_2 = \infty$.

All the other states evolve smoothly as $\Delta$ is turned up from zero; however, singularities occur at particular values for $\Delta$. At $\Delta = 1$, the upper of the two $\phi = 0$ states corresponds to $z_1 = z_2 = 1$ so the Bethe wavefunction is singular (or zero). The same thing happens to the $\phi = \pm i$ states at $\Delta = \sqrt{2}$. Generally this “collision” of $z$’s or $k$’s occurs at the point where the $k$’s go complex. One can make sense of it, however, by considering the limit of the wavefunction as $\Delta$ approaches the critical value.

In terms of the algebraic Bethe ansatz (we confine ourselves here to the XXX point), things are a little different: if we require that the $\lambda$’s, rather than the $k$’s or the $z$’s, be finite, the value $z = 1$ is forbidden. Then the states $|\psi_3\rangle, |\psi_5\rangle$ and $|\psi_6\rangle$ (which are not highest weight states) are not reproduced. It may appear that the situation is saved for the highest-weight state $|\psi_4\rangle$: the values 0 and $\infty$ for $z$ translate to the nicer values $\pm i/2$ for $\lambda$. The energy (13) appears to be divergent, but if we take the $\lambda$’s to be $(-i/2 + \epsilon, i/2 + \epsilon)$ and let $\epsilon$ vanish, we do get the correct value. Unfortunately, these $\lambda$ values don’t produce an eigenstate: $B(i/2)B(-i/2)|\uparrow\uparrow\uparrow\uparrow\rangle = 0$, which is easy to verify.

So there exists at least one state, $|\psi_4\rangle$, which is not reproduced by the algebraic Bethe ansatz at the isotropic point. In fact a similar singularity exists with the state

$$\sum (-1)^n \sigma_n^- \sigma_{n+1}^- |\uparrow\uparrow\cdots\rangle,$$

for all even $N$. This state was actually known to Bethe [1], who remarks that the $k$’s must diverge to accommodate it.

4.2 Six sites

Here things get a little more complicated and we have many more states to contend with. But classification of states in terms of $\phi$, the eigenvalue of the translation operator $T$, can still be done. In case of a real translation eigenvalue $\phi$ ($\pm 1$) we can further consider the parity operator, which reverses the order of the spins. (If $\phi$ is not real, this doesn’t commute with $T$, but one can generalize the definition to take care of that.) So consider the state

$$|\psi\rangle = |110110\rangle + |011010\rangle + |001101\rangle + \ldots$$

$$-|101100\rangle - |010110\rangle - \ldots$$

(22)

which is the only state with $\phi = 1$ and parity $-1$, and is therefore an eigenstate of $H$ for arbitrary $\Delta$ (also, as one can verify, a highest weight state). Consider also the state

$$|\psi'\rangle = |110100\rangle - |011010\rangle + |001101\rangle + \ldots$$

$$+|101100\rangle - |010110\rangle + |001011\rangle - \ldots$$

(23)

which is also an eigenstate of $H$ (the only one with $\phi = -1$ and parity 1), and a lowering of a state analogous to $|\psi_4\rangle$ in the previous section. Neither of these states can be reproduced unless either two of the $z$’s are equal, or one of them vanishes (and, therefore, another diverges). Since the proof is not as compact as in the four site case, we leave it for appendix [4]. These states, too, are degenerate with other states at the XY point, and some superpositions of these are reproduced by the Bethe ansatz.

In appendix [4], we present the values of $A$ which produce these states at the isotropic point if we take appropriate limits for the divergent Bethe coefficients. As predicted, the corresponding values of $k$ are divergent.
4.3 Adding a flux

The XY degeneracies can be lifted by passing an Aharonov-Bohm flux through the ring. This modifies the forward and backward hopping amplitudes by phase factors:

\[ H = \sum_{n=1}^{N} \left( \alpha^* \sigma_n^+ \sigma_{n+1}^- + \alpha \sigma_n^- \sigma_{n+1}^+ + \frac{\Delta}{2} \sigma_n^z \sigma_{n+1}^z \right), \]  

(24)

where \( \alpha \) is a complex number of unit modulus. For \( \alpha = 1 \) we recover the original Hamiltonian. For most other values of \( \alpha \), the ground state degeneracies are lifted and the states evolve smoothly when one turns on \( \Delta \). But the singularities reappear when one removes the flux. Moreover, certain other values of \( \alpha \) also prove to be singular. This is an example of the fact, noted by Byers and Yang [8], that the energy levels of a quantum system on a ring are periodic in the flux through the ring. To see it in this case, we carry out a Bethe ansatz solution and get the analogue of (9):

\[ z_m^N = (-1)^{l-1} \prod_{n \neq m} \frac{\alpha^* z_m z_n - 2\Delta z_m + \alpha}{\alpha^* z_m z_n - 2\Delta z_n + \alpha}, \]  

(25)

which, if we define \( w_n = \alpha z_n \), becomes

\[ w_m^N \alpha^N = (-1)^{l-1} \prod_{n \neq m} \frac{w_m w_n - 2\Delta w_m + 1}{w_m w_n - 2\Delta w_n + 1}. \]  

(26)

These are identical to the Bethe equations if \( \alpha^N = 1 \), so for these values of \( \alpha \) the singularities will persist.

The exact solution of the \( \phi = -1 \) sector for four sites with flux is given in appendix B, and its behaviour as the flux is made to vanish can be seen explicitly there.

4.4 Longer chains

The common thing to the above examples is the divergence of one of the \( z \)'s, or of the \( k \)'s to \( \pm i\infty \). In fact for any system size and any number of overturned spins, if one of the \( z \)'s diverges at \( \Delta = 1 \), the algebraic Bethe ansatz fails to reproduce the corresponding state. To see this in the XXX case, note that if one \( z \) diverges, another must vanish; the \( \lambda \)'s corresponding to these are \( \pm i/2 \). Consider the general algebraic Bethe state:

\[ |\{\lambda_n\} = \prod B(\lambda_n) \uparrow\uparrow\uparrow \cdots \]  

Choosing the argument of the last \( B \) operator to be \( i/2 \), we can easily convince ourselves (from the definition of \( B \) in terms of the \( L \) matrices in sec. 3) that the action of this on the ferromagnetic state is merely to flip the first spin. If we choose the next \( B \) operator to have the argument \(-i/2\) that state is killed entirely. The values of the other \( \lambda \) variables then don’t matter.

It is also quite clear that such solutions will in general exist for all lattice lengths. To see this, plug the values \( \lambda_l = i/2, \lambda_{l-1} = -i/2 \) into eq. (12). These equations are immediately satisfied for \( m = l \) and \( m = l - 1 \). For the rest, they now become

\[ \left( \frac{\lambda_m + i/2}{\lambda_m - i/2} \right)^{N-1} \frac{\lambda_m - 3i/2}{\lambda_m + 3i/2} = \prod_{n \neq m} \frac{\lambda_m - \lambda_n + i}{\lambda_m - \lambda_n - i}, \]  

(27)

and any solution of these for \( \lambda_1, \ldots, \lambda_{l-2} \) combined with the above values for \( \lambda_{l-1}, \lambda_l \) is a solution of (12).

This, by the way, is the simplest sort of “string” solution—such solutions, of groups of complex \( \lambda_n \) with a common real part and the imaginary parts separated by \( i \), arranged symmetrically about the real axis, are generic in the thermodynamic limit. This particular string exists for all system sizes.

Therefore for any lattice length \( N \) and spin sector \( l \) there exist several solutions for the equations (12) for which the algebraic Bethe ansatz gives a vanishing wavefunction and the coordinate Bethe ansatz a singular one. How to handle these singularities, and whether they can give us meaningful wavefunctions, are discussed later.
Though we have discussed only the XXX model above, the same is true of the XXZ model. The variables \( \lambda_n \) are defined a little differently here (the earlier ones are related to these by a scale factor) and the Bethe equations are

\[
\left( \frac{\sin(\lambda_m + \eta)}{\sin(\lambda_m - \eta)} \right)^N = \prod_{m \neq n} \frac{\sin(\lambda_m - \lambda_n + 2\eta)}{\sin(\lambda_m - \lambda_n - 2\eta)}.
\]  

(28)

Here \( \Delta = \cos 2\eta \). These have the singular solution \( \lambda_{l-1}, \lambda_l = \pm \eta \) with \( l - 2 \) equations for the remaining \( \lambda_m \). The \( L \) matrix in this case is

\[
L_n(\lambda) = \begin{pmatrix}
\frac{w_4(\lambda) + w_3(\lambda)\sigma_n^z}{(\sin 2\eta)\sigma_n^+} & \frac{\sin 2\eta\sigma_n^-}{w_4(\lambda) - w_3(\lambda)\sigma_n^z}
\end{pmatrix}
\]  

(29)

with \((w_4 + w_3)(\lambda) = \sin(\lambda + \eta)\) and \((w_4 - w_3)(\lambda) = \sin(\lambda - \eta)\). The \( B \) operator is defined as before, and one can convince oneself that this choice of \( \lambda_n \) annihilates the reference state, just as in the XXX case.

Unfortunately our proofs regarding the specific singular states are not readily generalized to longer chains, so other than the one example at the end of sec. 4.1, and the states suggested at the end of appendix C, we have no rigorous examples to give. But the above examples involve states with \( \delta \)-independent coefficients, which are degenerate with other states at \( \delta = 0 \), and such states certainly exist for larger lattices as well, so it is entirely conceivable that they too could pose problems for the Bethe ansatz.

We can be a little more specific. In the XY limit, the \( k \)'s are the “bare” momenta \( 2\pi I_n/N \), where \( I_n \) are distinct integers (for odd \( l \)) or half-integers (for even \( l \)). Consider the sector \( \phi = 1 \) (\( \phi \) being, as above, the eigenvalue of \( T \)); this is the same as saying \( \sum k_n = 0 \). This can happen in two ways: either the \( k_n \)'s are symmetrically distributed around 0, or they are not. If they are not, the solution corresponding to \( -k_n \) is distinct from this solution but degenerate in energy with it. However, these two solutions, generally, do not evolve into well-behaved solutions as one turns on \( \Delta \): the solutions at finite \( \Delta \) correspond to superpositions of these, which are no longer degenerate. The same problem occurs in the \( \sum k_n = \pi \) sector.

Numerically, we investigated several such states. The idea was to solve equations (28) using a Newton-Raphson rootfinder (capable of finding complex roots: a simple modification of the standard method). For this method to work, one needs a good starting guess. So a possible method is to keep a finite flux \( \Phi \), start the rootfinder from the XY point where the solution is known (and not affected, except in energy, by the flux), evolve \( \Delta \) forward to some desired value and then evolve the flux down to zero. In every case, the last step failed to converge, yielding divergent \( z \)'s or \( k \)'s or else hitting some spurious solution which has two \( k \)'s equal and therefore yields a vanishing wavefunction.

It seems therefore that such singularities are very common, at least in the \( \phi = 1 \) and \( \phi = -1 \) sectors, possibly in the other sectors too.

5 Handling the singularities

Thus, for several eigenstates of the Heisenberg model the Bethe ansatz becomes ill-behaved and the coefficients of the wavefunction, diverge (in the coordinate Bethe ansatz) or vanish (in the algebraic method). For the coordinate method, one can handle the divergence by considering only the ratios of the coefficients, rather than the coefficients themselves. For the algebraic method, since the problem values of \( \lambda \) are \( \pm i/2 \), one can let them approach these values and consider the limiting ratios of the coefficients of the wavefunction. While this should work in principle, it would be rather messy and we don’t pursue it further: the algebraic BA is valuable more as a formal elegant unifying tool than as a practical calculational aid.

For the four site, two spin down case, if we take \( \lambda_1 = i/2, \lambda_2 = -i/2 \), this works fine and we reproduce the state \( |\psi_4 \rangle \) of sec. 4.1. This is demonstrated in appendix C. However, consider the six site case with three down spins. If we choose \( \lambda_2 \) and \( \lambda_3 \) to be \( \pm i/2 \), we are left with one Bethe equation for \( \lambda_1 \) which turns out to be a fifth degree equation with six solutions if one includes \( \lambda_1 = \infty \) (or \( z_1 = 1 \)). That, and \( \lambda_1 = 0 \), do lead to valid eigenstates which are precisely the problematic eigenstates discussed in sec. 4.2.
But the other four solutions for $\lambda_1$, though perfectly valid solutions of the Bethe equations (12), do not lead to correct wavefunctions (nor, indeed, to correct energies). This is further discussed in appendix 4.

For any even lattice length with three down spins, the Bethe equations have $N$ such singular solutions of which two yield genuine eigenstates and the rest are spurious. This presumably happens for all spin sectors, but we don’t have good estimates on what fraction of the total number of states is so affected.

Another possible way to handle these singularities (when solving the equations numerically) is to introduce a finite flux, and slowly turn it down to zero. It turns out that the equations are so ill-behaved that this does not help. A rootfinder such as the Newton-Raphson method, which is based on the Taylor series and requires smoothly varying functions, behaves very badly in the neighbourhood of such singularities.

Other kinds of singular Bethe states are possible—for instance, at certain special values of $\Delta$, two $k$ values may collide. If the corresponding Bethe state has a well-defined limit as $\Delta \to \Delta_0$, where $\Delta_0$ is the value where the $k$’s coincide, then there is no problem. This happens for instance with the $\phi = \pm i$ and one of the $\phi = 1$ states in sec. 4.1 at $\delta = \sqrt{2}$ and $\delta = 1$ respectively. And then again, the $k$’s may be well-behaved but the $\lambda$’s singular, as in the state $|1010\rangle - |0101\rangle$. Here, if one just works with the $k$’s, no problems arise. In particular, the Bethe coefficients are well-behaved.

6 Conclusion

The Bethe ansatz is a particular guess for a wavefunction and substituting it in the Hamiltonian, and applying periodic boundary conditions, leads to certain conditions on the parameters of the wavefunction, the $k$’s or the $\lambda$’s as one may prefer. We find that though Bethe’s equations for the $\lambda$’s by themselves have a large number of solutions, some of these solutions lead to singular, ill-defined wavefunctions. These problems arise from divergences in Bethe’s original quasimomenta $k_n$, though the $\lambda_n$ to which they can be transformed are well behaved.

We give explicit examples of this for four and six site lattices, but show that such solutions of the Bethe equations should occur for all lattice sizes. The question then is whether to allow such solutions or not. If we do not allow them, the Bethe ansatz is incomplete. If we do allow them, we get vanishing wavefunctions with the algebraic Bethe ansatz, and divergent ones with the coordinate method. If we attempt to make sense of these by considering only ratios of the Bethe coefficients, we get well-defined wavefunctions but not all of these are eigenstates of the Hamiltonian. Indeed, even without calculating the wavefunctions, we can check that the energies are wrong.

Earlier arguments for completeness have been based on counting of solutions to the Bethe equations (12), using the string hypothesis. But as we have seen, not every solution to the Bethe equations produces an eigenstate of the Hamiltonian. Therefore, even if the Bethe equations themselves have as many solutions as we require, it does not imply completeness of the method.

In the case of two down-spins, however, the Bethe ansatz is complete if one normalizes the divergent wavefunctions appropriately. This was known to Bethe [1], as was the fact that the $k$’s and the amplitudes for the wavefunction diverge for one state in this case. There are no incorrect solutions in this case.

One question to be answered is how many incorrect solutions do we obtain in the thermodynamic limit. In the case of three down spins, we get $N - 2$ wrong answers, which is a vanishing fraction of the total number of states in the thermodynamic limit. It will probably remain a vanishing fraction if the number of down spins is finite, but if a finite fraction of the spins are down—if $S^z = 0$, for instance—we haven’t formed an estimate.

One way to get around this, in principle, is to add a small flux to the system; but this helps only in a formal sense. The equations are very ill behaved near these singularities and any rootfinder would have a great deal of trouble converging to a solution.

Finally, some remarks on why all this is important. One reason is a matter of principle—it is good to know to what extent a given method solves a problem. Another is that the question could be relevant to other problems too—for instance, the Hubbard model, which becomes the Heisenberg antiferromagnet in one limit, may also exhibit similar singularities in its Bethe ansatz solution. This incompleteness will probably not matter much in calculations of thermodynamic properties, since the singular states may then be a vanishing fraction of the total number of states. However, when considering small systems, or systems with very few overturned spins such as low-lying excitations above the ferromagnetic state,
perhaps one should keep the completeness question in mind. And finally, the above considerations are very important indeed if one wants to use the Bethe ansatz for numerical calculations on a finite sized lattice. This should not be a common difficulty since other methods, such as exact diagonalization, can easily be used in one dimension.

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A Singular states in the six site lattice

For six sites and three down-spins, we have three $z$ variables and three two-particle scattering amplitudes $A_{nm}$ (since $A_{nm} = 1/A_{nm}$). Let $A_{123} = 1$; then we have

\[ A_{132} = \frac{1}{A_{23}}, \quad A_{213} = \frac{1}{A_{12}}, \quad A_{231} = \frac{1}{A_{12}A_{13}}, \]
\[ A_{312} = \frac{1}{A_{23}A_{13}}, \quad A_{321} = \frac{1}{A_{23}A_{13}A_{12}}. \] (30)

Also, from the Bethe ansatz equations we have

\[ z_1^6 = A_{12}A_{13}, \quad z_2^6 = \frac{A_{23}}{A_{12}}, \quad z_3^6 = \frac{1}{A_{13}A_{23}} \] (31)

Let us define $A_{23} = A$ and rewrite $A_{12}, A_{13}$ in terms of this and the $z$'s. Using all these in the formula (4) for the Bethe wavefunction, we get for $\psi(x_1, x_2, x_3)$ the formula

\[ \psi(x_1, x_2, x_3) = z_1 x_1 z_2 x_2 z_3 x_3 + \frac{1}{A} z_1 x_1 z_2 x_2 z_3 x_3 + \frac{1}{A} z_2 x_1 + 6 z_1 x_2 z_3 x_3 + \frac{1}{A} z_3 x_1 x_2 z_1 x_3 - 6 \] (32)

Now consider the state (22) in sec. 4.2. To reproduce this state, we require that

\[ \psi(0, 1, 2) = 0, \] (33)
\[ \psi(0, 2, 4) = 0. \] (34)

Each of these, together with $z_1 z_2 z_3 = 1$, can be used to solve for $A$. Using (14), we get

\[ A = -\frac{z_2^2}{z_3^2} \] (35)

and using (33),

\[ A = -\frac{z_1^3 z_2 + z_1^3 z_2^4 + z_2}{z_1^3 z_3 + z_1^3 z_3^4 + z_3} \] (36)

Unless $z_2$ or $z_3$ is zero, we can equate these, and after cancelling a common $z_2/z_3$ factor, rearranging and using $z_1 z_2 z_3 = 1$, we get

\[ z_1^3 (z_2 - z_3) - z_1^2 (z_2^2 - z_3^2) + (z_2 - z_3) = 0 \] (37)

and if we multiply the last term by $z_1 z_2 z_3$, this can be factorized as

\[ z_1 (z_2 - z_3) (z_3 - z_1) (z_1 - z_2) = 0. \] (38)

Thus, if the variables $z_1$, $z_2$, $z_3$ are all distinct, one of them must vanish (and consequently another must diverge).

A precisely analogous proof goes through for the state (23) using the condition $z_1 z_2 z_3 = -1$. 

9
B Some exact solutions in the four site case

Here, as in section 4, we work with states labelled by \( \phi \), the eigenvalue of the translation operator \( T \) which shifts all spins by one lattice site to the left.

B.1 Sector \( \phi = -1 \) with flux \( \alpha \)

We have two solutions in this sector, given by

\[
(z_1, z_2) = \frac{-\gamma \pm \sqrt{\gamma^2 + 4}}{2}
\]

where \( \gamma \) has the two possible values

\[
\gamma = \frac{\Lambda \pm \sqrt{\Lambda^2 - 8}}{2},
\]

\[
\Lambda = \frac{2\Delta}{\alpha - \alpha^*}.
\]

Note that as \( \alpha \to 1 \), \( \Lambda \) diverges, and consequently one solution for \( z_1, z_2 \) diverges, while the other approaches \( \pm 1 \).

B.2 Sector \( \phi = -1 \) with no flux

The state \( |1010\rangle - |0101\rangle \) is readily reproduced with \( z = \pm 1 \). To reproduce the other state, we need \( z_1 \to 0 \), \( z_2 \to \infty \). Now the Bethe coefficient of the state \( |1010\rangle \) is \( z_2^2 + z_1^2/A \), which on using \( z_1 z_2 = -1 \) and \( z_1^2 = A \) becomes \( 2z_2^2 \). The Bethe coefficient of \( |1100\rangle \), similarly, is \( z_2 - z_2^3 \). Both of these diverge as \( z_2 \to \infty \), but if we take their ratio, this vanishes. (It also vanishes, as it should, if \( z_2 \to 0 \).) So for this state, we can conclude that the \( |1010\rangle \) basis state is of zero weight compared to \( |1100\rangle \), and we do reproduce the correct eigenstate.

B.3 Sector \( \phi = 1 \) with no flux

There are two solutions in this sector, given by

\[
(z_1, z_2) = \frac{-\gamma \pm \sqrt{\gamma^2 - 4}}{2}
\]

for each of the two values of \( \gamma \)

\[
\gamma = \frac{\Delta \pm \sqrt{\Delta^2 + 8}}{2}.
\]

As \( \Delta \to 1 \), one of the \( \gamma \) solutions tends to \( 2 \), for which the \( z \) values collide at the value \( 1 \). At this point,

\[
A = \frac{z_1 z_2 - 2\Delta z_1 + 1}{z_1 z_2 - 2\Delta z_2 + 1}
\]

also becomes ill-defined. If it weren’t so, the wavefunction would vanish. Now, as before, we can consider the coefficients of \( |1010\rangle \) and \( |1100\rangle \) and eliminate the ill-behaved \( A \) from them, before taking the \( \Delta \to 1 \) limit. The former, as before, can be written solely in terms of \( z_2 \) as \( 2z_2^2 \) and the latter as \( z_2 + z_2^3 \). Both of these have well defined limits as \( z_2 \to 1 \), and the correct wavefunction is reproduced.

C Six sites: exact solutions for the singular states

Here again we confine ourselves to the XXX model. Let us look for a solution of the equations for \( \lambda_m \), for six sites and three down spins, with \( \lambda_1 = -i/2 \) and \( \lambda_3 = i/2 \). Then we only have to find \( \lambda_2 \), which we will call \( \lambda \). Equations [12] are already satisfied for \( \lambda_1 \) and \( \lambda_3 \), while for \( \lambda_2 = \lambda \) they become

\[
\left( \frac{\lambda + i/2}{\lambda - i/2} \right)^6 = \left( \frac{\lambda + 3i/2}{\lambda - i/2} \right) \left( \frac{\lambda + i/2}{\lambda - 3i/2} \right)
\]
which have solutions \( \lambda = \infty \) (which we will not disallow), \( \lambda = 0 \) and the four roots of

\[
16\lambda^4 + 40\lambda^2 - 7 = 0. \tag{45}
\]

For now, we will not specify which root we are considering; for all of these, the Bethe equations (12) are satisfied. The \( z \) values corresponding to these are \( z_1 = 0, z_3 = \infty \) with various finite values of \( z_2 \): +1 for \( \lambda = \infty, -1 \) for \( \lambda = 0 \), and other values for the other four solutions of \( \lambda \).

Our Bethe wavefunction (32) is then singular because of the singular values of the \( z \)'s. Let us, however, assume

\[
(z_1, z_2, z_3) = \left( \frac{1}{\beta}, z, \phi \beta / z \right) \tag{46}
\]

and take the limit of this as \( \beta \to \infty \). Here \( \phi \) is, as before, the eigenvalue of the translation operator: \( \phi^6 = 1 \). In that case, to leading order in \( \beta \), the coefficients of various Ising states in the Bethe wavefunction are

\[
|111000\rangle : \beta^5 \left( \frac{\phi}{z} + \frac{1}{z^4} \right)
\]

\[
|110100\rangle : \beta^3 \frac{1}{z^3}
\]

\[
|101100\rangle : \beta^5 \frac{\phi^2}{z^2}
\]

\[
|101010\rangle : \beta^4 \frac{1 + \phi^2 + \phi^4}{z^2}
\]

with coefficients of other Ising states being the above multiplied by appropriate powers of \( z_1z_2z_3 \). As \( \beta \to \infty \), the coefficient of \( |101010\rangle \) becomes insignificant. First consider the case \( z_2 = z = \pm 1 \), or \( \lambda = 0, \infty \). If we choose \( \phi = \pm 1 \) as appropriate, the coefficient of \( |111000\rangle \) can also be made to vanish (to order \( \beta^5 \)) and we recover precisely the two states discussed in appendix A.

But now consider the other four possible values of \( z \). In all eigenstates, the coefficients of \( |101100\rangle \) and \( |110100\rangle \) differ by a factor of \( \phi \) (or a power of it): \( \phi \), remember, is a sixth root of unity. Here they differ by a factor \( \phi^4 / z \), which is not a power of \( \phi \) since the four values of \( z \) other than \( \pm 1 \) are not sixth roots of unity. So for these values of \( z \), the states (which are in any case singular) are not eigenstates of the Hamiltonian even in a limiting sense.

In fact we have checked the parentage of all the exact eigenstates in the six site case, and apart from the two discussed above, all are reproduced with finite \( z \), with at worst a collision of two values. So there is no room for the remaining four solutions. Moreover, if one uses the values of \( \lambda \) calculated in this appendix to calculate the energy by equation (13), using a limiting method as in sec. 4.1 to handle the divergence for \( \lambda_1, \lambda_3 = \pm 2 \), one gets the correct answers for \( \lambda_2 = 0, \infty \) but wrong answers for the other four solutions for \( \lambda_2 \)—as one can verify with exact diagonalization. (For this calculation, all we need to assume is that

\[
\frac{4}{1 + 4(i/2)^2} + \frac{4}{1 + 4(-i/2)^2} = 2, \tag{47}
\]

which as a limit is justified in sec. 4.1, and which produces the correct energy when the wavefunction is correct). So there exist solutions of the Bethe equations (12) which do not correspond to actual eigenstates of the problem.

In the case of three down spins, the above generalizes quite readily to any even number of sites: for \( N \) sites, we get \( N - 2 \) spurious solutions, and two solutions for \( \lambda \) which correspond to genuine eigenstates. One of these is a lowering of the two down spin state given at the end of sec. 4.1; both remain eigenstates for all \( \Delta \). Thus, for eight sites, we get for \( \phi = 1 \)

\[
|\psi_1\rangle = |11010000\rangle - |10110000\rangle - |11001000\rangle + |10011000\rangle + \text{translations with } \phi = 1 \tag{48}
\]

and for \( \phi = -1 \)

\[
|\psi_2\rangle = |11010000\rangle + |10110000\rangle + |11001000\rangle - |10011000\rangle + \text{translations with } \phi = -1. \tag{49}
\]
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