

Note: The Bethe Ansatz

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May 31, 2026

Abstract

For the $M = 2$ sector of the antiferromagnetic XXX model, I derive the Bethe equations for periodic and open boundary conditions. For periodic boundary conditions, I also estimate the number of solutions.

For the XXX model, I derive the Bethe equations mostly following Bethe's original paper [1]. I also referred to [2, 3].

1 The XXX Model

Consider the following Hamiltonian on a circle with N lattice sites, namely the antiferromagnetic Heisenberg chain:

$$H = \frac{1}{2} \sum_{j=1}^N \boldsymbol{\sigma}_j \cdot \boldsymbol{\sigma}_{j+1} \quad (1)$$

$$= \sum_j (\sigma_j^+ \sigma_{j+1}^- + \sigma_j^- \sigma_{j+1}^+ + \frac{1}{2} \sigma_j^z \sigma_{j+1}^z) \quad (2)$$

$$= \sum_j (\sigma_{j+1}^- \sigma_j^+ + \sigma_{j-1}^- \sigma_j^+ + 2 \frac{1 - \sigma_j^z}{2} \frac{1 - \sigma_{j+1}^z}{2}) - 2 \sum_j \frac{1 - \sigma_j^z}{2} + \frac{N}{2}. \quad (3)$$

As a notational convention, set $\boldsymbol{\sigma}_{j+N} = \boldsymbol{\sigma}_j$. The Hamiltonian is $SU(2)$ invariant and translation invariant. Choose a basis that diagonalizes S^z . In the following, as a basis for wave functions, I take $|0\rangle = |\uparrow \uparrow \dots\rangle$ as the “vacuum” and write an M -particle state as

$$|f\rangle_M = \sum_{1 \leq x_1 < \dots < x_M \leq N} f(x_1, \dots, x_M) \sigma_{x_1}^- \dots \sigma_{x_M}^- |0\rangle \quad (4)$$

Note that the eigenfunction f is meaningful only on the domain $1 \leq x_1 < \dots < x_M \leq N$.

In the sector with particle number M , the term $-2 \sum_j \frac{1 - \sigma_j^z}{2} = -2M$ is a constant. Hence, in what follows I redefine

$$H = \sum_j (\sigma_{j+1}^- \sigma_j^+ + \sigma_{j-1}^- \sigma_j^+ + 2 \frac{1 - \sigma_j^z}{2} \frac{1 - \sigma_{j+1}^z}{2}) \quad (5)$$

and solve this Hamiltonian.

1.1 Translation Symmetry

(The content of this subsection will not be used later.)

By translation symmetry, the translation operator T defined by

$$T\sigma_j T^{-1} = \sigma_{j+1}, \quad T|0\rangle = |0\rangle, \quad (6)$$

and the Hamiltonian H can be diagonalized simultaneously. Since $T^N = 1$, the eigenvalues of T are quantized in \mathbb{Z}_N . In the eigenspace with $T = e^{iP}$, $P = \frac{2\pi p}{N}$, $p = 1, \dots, N-1$, the eigenfunction f satisfies

$$\sum_{1 \leq x_1 < \dots < x_M \leq N} f(x_1, \dots, x_M) \sigma_{x_1+1}^- \dots \sigma_{x_M+1}^- |0\rangle = e^{iP} \sum_{1 \leq x_1 < \dots < x_M \leq N} f(x_1, \dots, x_M) \sigma_{x_1}^- \dots \sigma_{x_M}^- |0\rangle. \quad (7)$$

In the sum on the left-hand side, the contribution with $x_M \leq N-1$ is

$$\sum_{1 \leq x_1 < \dots < x_M \leq N-1} f(x_1, \dots, x_M) \sigma_{x_1+1}^- \dots \sigma_{x_M+1}^- |0\rangle. \quad (8)$$

Comparing this with the contribution with $2 \leq x_1$ on the right-hand side,

$$e^{iP} \sum_{2 \leq x_1 < \dots < x_M \leq N} f(x_1, \dots, x_M) \sigma_{x_1}^- \dots \sigma_{x_M}^- |0\rangle = e^{iP} \sum_{1 \leq x_1 < \dots < x_M \leq N-1} f(x_1+1, \dots, x_M+1) \sigma_{x_1+1}^- \dots \sigma_{x_M+1}^- |0\rangle \quad (9)$$

we obtain

$$f(x_1, \dots, x_M) = e^{iP} f(x_1+1, \dots, x_M+1), \quad (x_M \leq N-1) \quad (10)$$

The contribution with $x_M = N$ in the sum on the left-hand side is

$$\sum_{1 \leq x_1 < \dots < x_{M-1} \leq N-1} f(x_1, \dots, x_{M-1}, N) \sigma_{x_1+1}^- \dots \sigma_{x_{M-1}+1}^- \sigma_1^- |0\rangle \quad (11)$$

$$= \sum_{1 \leq x_1 < \dots < x_{M-1} \leq N-1} f(x_1, \dots, x_{M-1}, N) \sigma_1^- \sigma_{x_1+1}^- \dots \sigma_{x_{M-1}+1}^- |0\rangle \quad (12)$$

and comparing this with the contribution with $x_1 = 1$ on the right-hand side,

$$e^{iP} \sum_{2 \leq x_2 < \dots < x_M \leq N} f(1, x_2, \dots, x_M) \sigma_1^- \sigma_{x_2}^- \dots \sigma_{x_M}^- |0\rangle \quad (13)$$

$$= e^{iP} \sum_{1 \leq x_2 < \dots < x_M \leq N-1} f(1, x_2+1, \dots, x_M+1) \sigma_1^- \sigma_{x_2+1}^- \dots \sigma_{x_M+1}^- |0\rangle \quad (14)$$

$$= e^{iP} \sum_{1 \leq x_1 < \dots < x_{M-1} \leq N-1} f(1, x_1+1, \dots, x_{M-1}+1) \sigma_1^- \sigma_{x_1+1}^- \dots \sigma_{x_{M-1}+1}^- |0\rangle \quad (15)$$

we obtain

$$f(x_1, \dots, x_{M-1}, N) = e^{iP} f(1, x_1+1, \dots, x_{M-1}+1) \quad (16)$$

1.2 Eigenvalue Equation

Let us examine the structure of the eigenvalue equation

$$H|f\rangle_M = E|f\rangle_M \quad (17)$$

1.2.1 $M = 1$

For $M = 1$, the third term drops out, and

$$H|f\rangle_1 = \sum_{j,x} (\delta_{jx}\sigma_{j+1}^- + \delta_{j,x}\sigma_{j-1}^-)f(x)|0\rangle \quad (18)$$

$$= \sum_j (f(j)\sigma_{j+1}^- + f(j)\sigma_{j-1}^-)|0\rangle \quad (19)$$

$$= \sum_j (f(j-1) + f(j+1))\sigma_j^-|0\rangle \quad (20)$$

therefore the eigenvalue equation is

$$\begin{cases} f(j-1) + f(j+1) = Ef(j) & j = 2, \dots, N-1, \\ f(N) + f(2) = Ef(1), \\ f(N-1) + f(1) = Ef(N), \end{cases} \quad (21)$$

The plane wave

$$f_k(x) = e^{ikx} \quad (22)$$

satisfies the first equation, and then $E_k = 2\cos k$. If $k = \frac{2\pi p}{N}$, $p = 0, \dots, N-1$, then e^{ikx} satisfies the second and third equations. Thus we have constructed N linearly independent solutions.

1.2.2 $M = 2$

For the hopping terms, when $x_1 \neq x_2$,

$$\sigma_{j\pm 1}^- \sigma_j^+ \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle = \delta_{jx_1} \sigma_{x_1\pm 1}^- \sigma_{x_2}^- |0\rangle + \delta_{jx_2} \sigma_{x_1}^- \sigma_{x_2\pm 1}^- |0\rangle \quad (23)$$

Notice the above relation. When two lowering operators act on the same site, set $\sigma_x^- \sigma_x^- = 0$. For the interaction term, we are using a diagonal basis, and

$$\sum_j \frac{1 - \sigma_j^z}{2} \frac{1 - \sigma_{j+1}^z}{2} \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle = \delta_{|x_1 - x_2|, 1} \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle. \quad (24)$$

$\delta_{|x_1 - x_2|, 1}$ returns 1 only when x_1 and x_2 are adjacent, and returns 0 otherwise. The action of the Hamiltonian on the wave function $|f\rangle_2$ is

$$H|f\rangle_2 = \sum_{1 \leq x_1 < x_2 \leq N} f(x_1, x_2) (\sigma_{x_1+1}^- \sigma_{x_2}^- |0\rangle + \sigma_{x_1}^- \sigma_{x_2+1}^- |0\rangle + \sigma_{x_1-1}^- \sigma_{x_2}^- |0\rangle + \sigma_{x_1}^- \sigma_{x_2-1}^- |0\rangle) + 2\delta_{|x_1 - x_2|, 1} \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle \quad (25)$$

Rewrite each term in order. The first term vanishes when $x_2 = x_1 + 1$, so

$$\text{1st.} = \sum_{2 \leq x_1 + 1 < x_2 \leq N} f(x_1, x_2) \sigma_{x_1+1}^- \sigma_{x_2}^- |0\rangle = \sum_{2 \leq x_1 < x_2 \leq N} f(x_1 - 1, x_2) \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle. \quad (26)$$

For the second term, separate the sum into the case $x_2 = N$ and the remaining cases. Also taking into account that the contribution with $x_1 = 1$ vanishes when $x_2 = N$, we have

$$\text{2nd.} = \sum_{1 \leq x_1 < x_2 \leq N-1} f(x_1, x_2) \sigma_{x_1}^- \sigma_{x_2+1}^- |0\rangle + \sum_{2 \leq x_1 \leq N-1} f(x_1, N) \sigma_{x_1}^- \sigma_1^- |0\rangle \quad (27)$$

$$= \sum_{1 \leq x_1 < x_2 - 1 \leq N-1} f(x_1, x_2 - 1) \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle + \sum_{2 \leq x_2 \leq N-1} f(x_2, N) \sigma_1^- \sigma_{x_2}^- |0\rangle. \quad (28)$$

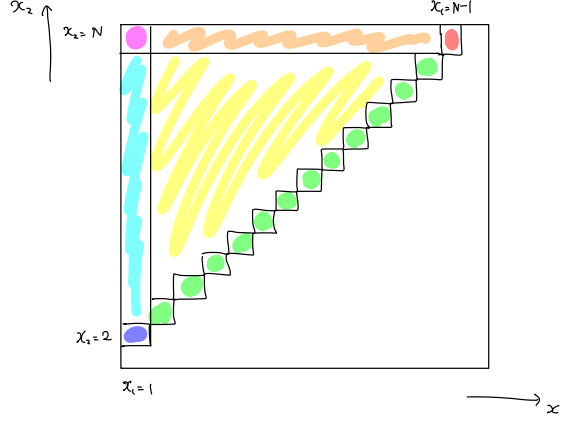


Figure 1

For the third term, separate the sum into the case $x_1 = 1$ and the remaining cases. Moreover, when $x_1 = 1$, the contribution with $x_2 = N$ vanishes, and hence

$$\text{3rd.} = \sum_{2 \leq x_1 < x_2 \leq N} f(x_1, x_2) \sigma_{x_1-1}^- \sigma_{x_2}^- |0\rangle + \sum_{2 \leq x_2 \leq N-1} f(1, x_2) \sigma_N^- \sigma_{x_2}^- |0\rangle \quad (29)$$

$$= \sum_{1 \leq x_1 < x_2-1 \leq N-1} f(x_1+1, x_2) \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle + \sum_{2 \leq x_1 \leq N-1} f(1, x_1) \sigma_{x_1}^- \sigma_N^- |0\rangle. \quad (30)$$

The fourth term vanishes when $x_2 = x_1 + 1$, so

$$\text{4th.} = \sum_{2 \leq x_1+1 < x_2 \leq N} f(x_1, x_2) \sigma_{x_1}^- \sigma_{x_2-1}^- |0\rangle = \sum_{1 \leq x_1 < x_2 \leq N-1} f(x_1, x_2+1) \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle. \quad (31)$$

The fifth term contributes only when the two points are adjacent on the circle, and

$$\text{5th.} = \sum_{1 \leq x \leq N-1} f(x, x+1) 2\sigma_x^- \sigma_{x+1}^- |0\rangle + f(1, N) 2\sigma_1^- \sigma_N^- |0\rangle. \quad (32)$$

The case distinction in the sums is illustrated in Figure 1. Let us look at the eigenvalue equation in each region.

- For $2 \leq x_1, x_1+1 \leq x_2 \leq N-1$ (yellow),

$$(A): \quad f(x_1-1, x_2) + f(x_1, x_2-1) + f(x_1+1, x_2) + f(x_1, x_2+1) = Ef(x_1, x_2). \quad (33)$$

- For $x_1 = 1, 3 \leq x_2 \leq N-1$ (cyan),

$$(B): \quad f(x_2, N) + f(1, x_2-1) + f(2, x_2) + f(1, x_2+1) = Ef(1, x_2). \quad (34)$$

- For $2 \leq x_1 \leq N-2, x_2 = N$ (orange),

$$(C): \quad f(x_1-1, N) + f(x_1, N-1) + f(x_1+1, N) + f(1, x_1) = Ef(x_1, N). \quad (35)$$

- For $2 \leq x_1 = x, x_2 = x+1, 2 \leq x \leq N-2$ (green),

$$(D): \quad f(x-1, x+1) + f(x, x+2) + 2f(x, x+1) = Ef(x, x+1). \quad (36)$$

- For $x_1 = 1, x_2 = 2$ (blue),

$$(E) : f(2, N) + f(1, 3) + 2f(1, 2) = Ef(1, 2). \quad (37)$$

- For $x_1 = N - 1, x_2 = N$ (red),

$$(F) : f(N - 2, N) + f(1, N - 1) + 2f(N - 1, N) = Ef(N - 1, N). \quad (38)$$

- For $x_1 = 1, x_2 = N$ (pink),

$$(G) : f(1, N - 1) + f(2, N) + 2f(1, N) = Ef(1, N). \quad (39)$$

Now, looking at the equations, it is convenient to extend the domain $1 \leq x_1 < x_2 \leq N$ of $f(x_1, x_2)$ so that it includes $0, N + 1, N + 2$, and to introduce boundary conditions for the extra degrees of freedom of $f(x_1, x_2)$. Introduce the following $2N - 1$ new variables:

$$f(0, x_2), \quad x_2 = 1, \dots, N - 1, \quad (40)$$

$$f(x_1, N + 1), \quad x_1 = 2, \dots, N, \quad (41)$$

$$f(N, N + 2), \quad (42)$$

Furthermore, impose the following “boundary conditions”:

$$\begin{cases} f(0, x_2) = f(x_2, N), & x_2 = 1, \dots, N - 1, \\ f(x_1, N + 1) = f(1, x_1), & x_1 = 2, \dots, N, \\ f(N, N + 2) = f(2, N). \end{cases} \quad (43)$$

These are natural relations for a function on the circle. Under these boundary conditions, the equations (A,B,C) can be combined as

$$(Eq.1) : f(x_1 - 1, x_2) + f(x_1, x_2 - 1) + f(x_1 + 1, x_2) + f(x_1, x_2 + 1) = Ef(x_1, x_2), \quad (|x_1 - x_2| \geq 2). \quad (44)$$

and similarly (D,E,F,G) can be rewritten as

$$(Eq.2) : f(x - 1, x + 1) + f(x, x + 2) + 2f(x, x + 1) = Ef(x, x + 1), \quad (x = 1, \dots, N), \quad (45)$$

For the extension of variables, it is equivalently possible to introduce infinitely many variables

$$f(x_1, x_2), \quad x_1, x_2 \in \mathbb{Z}, \quad x_1 < x_2 < x_1 + N, \quad (46)$$

and impose the boundary condition

$$(B.C.) : f(x_1, x_2) = f(x_2, x_1 + N) = f(x_2 - N, x_1) \quad (47)$$

instead. Thus the problem is to solve the eigenvalue equations (Eq.1, Eq.2), under the boundary condition (B.C.), for variables $f(x_1, x_2)$ satisfying $x_1 < x_2 < x_1 + N$.

Following Bethe [1], we find eigenfunctions. Since (Eq.1) has no interaction term, one expects a “two-particle plane-wave state” to be a solution. For example, for arbitrary complex numbers k_1, k_2 ,

$$e^{ik_1 x_1} e^{ik_2 x_2}, \quad e^{ik_2 x_1} e^{ik_1 x_2} \quad (48)$$

are both solutions of (Eq.1) with $E = 2 \cos k_1 + 2 \cos k_2$. However,

$$f(x_2, x_1 + N) = e^{ik_2 N} e^{ik_1 x_2} e^{ik_2 x_1} \quad (49)$$

so the boundary condition cannot be satisfied for general (k_1, k_2) . Therefore, for $k_1 \neq k_2$, assume a solution of the form

$$g_{\mathbf{k}}(x_1, x_2) = c_1 e^{i(k_1 x_1 + k_2 x_2)} + c_2 e^{i(k_2 x_1 + k_1 x_2)}, \quad x_1 < x_2 < x_1 + N, \quad (50)$$

and determine $\mathbf{k} = (k_1, k_2)$ and the relative ratio of c_1, c_2 from (Eq.2) and (B.C.). Substituting $g_{\mathbf{k}}(x_1, x_2)$ into (Eq.2), we get

$$g_{\mathbf{k}}(x-1, x+1) + g_{\mathbf{k}}(x, x+2) + 2g_{\mathbf{k}}(x, x+1) = E_{\mathbf{k}}g_{\mathbf{k}}(x, x+1) \quad (51)$$

We reinterpret this equation as follows. First introduce the function

$$h_{\mathbf{k}}(x) (= "g_{\mathbf{k}}(x, x)") := c_1 e^{i(k_1 x + k_2 x)} + c_2 e^{i(k_2 x + k_1 x)} = e^{i(k_1 + k_2)x} (c_1 + c_2) \quad (52)$$

Note that $g_{\mathbf{k}}(x_1, x_2)$ satisfies (Eq.1) for arbitrary (x_1, x_2) outside the original domain. Then the relation

$$g_{\mathbf{k}}(x-1, x+1) + h_{\mathbf{k}}(x) + h_{\mathbf{k}}(x+1) + g_{\mathbf{k}}(x, x+2) = E_{\mathbf{k}}g_{\mathbf{k}}(x, x+1) \quad (53)$$

holds. Using this, equation (51) is equivalent to

$$h_{\mathbf{k}}(x) + h_{\mathbf{k}}(x+1) - 2g_{\mathbf{k}}(x, x+1) = 0, \quad (54)$$

namely

$$(1 + e^{i(k_1 + k_2)})c_1 + (1 + e^{i(k_1 + k_2)})c_2 - 2c_1 e^{ik_2} - 2c_2 e^{ik_1} = 0 \quad (55)$$

Solving this, we obtain the relative ratio

$$\frac{c_1}{c_2} = -\frac{1 + e^{i(k_1 + k_2)} - 2e^{ik_1}}{1 + e^{i(k_1 + k_2)} - 2e^{ik_2}} \quad (56)$$

Here I assumed $c_2 \neq 0$.

The boundary condition (B.C.), $g_{\mathbf{k}}(x_2, x_1 + N) = g_{\mathbf{k}}(x_1, x_2)$, gives

$$(c_1 - c_2 e^{ik_1 N}) e^{i(k_1 x_1 + k_2 x_2)} + (c_2 - c_1 e^{ik_2 N}) e^{i(k_1 x_2 + k_2 x_1)} = 0, \quad x_1 < x_2 < x_1 + N. \quad (57)$$

Taking into account the assumption $k_1 \neq k_2$, the condition for this to hold for arbitrary $x_1 < x_2 < x_1 + N$ is

$$\begin{cases} c_1 = c_2 e^{ik_1 N}, \\ c_2 = c_1 e^{ik_2 N}, \end{cases} \quad (58)$$

Thus we obtain two equations, the Bethe equations, that determine the unknown variables (k_1, k_2) :

$$e^{ik_1 N} = -\frac{1 + e^{i(k_1 + k_2)} - 2e^{ik_1}}{1 + e^{i(k_1 + k_2)} - 2e^{ik_2}}, \quad (59)$$

$$e^{ik_2 N} = -\frac{1 + e^{i(k_1 + k_2)} - 2e^{ik_2}}{1 + e^{i(k_1 + k_2)} - 2e^{ik_1}}, \quad (60)$$

Here one should keep in mind that $k_1 \neq k_2$.

Because of $\varphi_{\mathbf{k}}$, k_1, k_2 do not take the usual wavenumber form. However, noting that

$$e^{i(k_1 + k_2)N} = 1 \quad (61)$$

we find for the sum that

$$k_1 + k_2 = \frac{2\pi(\lambda_1 + \lambda_2)}{N} \quad (62)$$

holds. The quantity $k_1 + k_2$ is nothing but the eigenvalue of the translation operator.

1.2.3 The Case $k_1 = k_2$

When $k_1 = k_2 = k$, if we take the ansatz

$$g_{k,k}(x_1, x_2) = e^{ik(x_1+x_2)} \quad (63)$$

then (Eq.1) and (Eq.2) give, respectively,

$$E = 4 \cos k, \quad 2 \cos k + 2 = E, \quad (64)$$

and hence we obtain $k = 0$, namely the constant solution $f(x_1, x_2) = \text{const.}$. Note that the $k = 0$ solution is special to the $SU(2)$ -symmetric case. If, in the XXZ model, the coefficient of $\sigma_j^z \sigma_{j+1}^z$ is multiplied by Δ , then the equation becomes

$$\cos k = \Delta \quad (65)$$

and the behavior is as follows:

- For $\Delta < -1$, there is no solution.
- For $\Delta = -1$, there is the single solution $k = \pi$.
- For $-1 < \Delta < 1$, there are two real solutions $k = \pm \cos^{-1}(\Delta)$.
- For $\Delta = 1$, there is the single solution $k = 0$.
- For $\Delta > 1$, there are two purely imaginary solutions $k = \pm \cosh^{-1}(\Delta)$.

On the other hand, the boundary condition (B.C.) gives

$$e^{ikN} = 1 \quad (66)$$

and therefore the purely imaginary solutions are not realized. For $-1 \leq \Delta \leq 1$, a solution exists only for special values of Δ determined by N .

For the XXX model ($\Delta = 1$),

- there is one constant solution with $k = 0$, independently of N .

1.2.4 Symmetries of the Bethe Equations

Let us record several properties of the Bethe equations.

$$e^{i\varphi_k} = \frac{c_1}{c_2} = -\frac{1 + e^{i(k_1+k_2)} - 2e^{ik_1}}{1 + e^{i(k_1+k_2)} - 2e^{ik_2}}, \quad k_1 \neq k_2, \quad (67)$$

$$e^{i\varphi_{k_2, k_1}} = e^{-i\varphi_{k_1, k_2}}, \quad (68)$$

$$e^{i\varphi_{-k_1, -k_2}} = e^{i\varphi_{k_2, k_1}} = e^{-i\varphi_{k_1, k_2}}, \quad (69)$$

$$[e^{i\varphi_{k_1, k_2}}]^* = e^{i\varphi_{k_2^*, k_1^*}} = e^{-i\varphi_{k_1^*, k_2^*}}, \quad (70)$$

$$e^{i\varphi_{k, k}} = -1, \quad (71)$$

$$e^{i\varphi_{0, k_2}} = e^{i\varphi_{k_1, 0}} = 1, \quad (72)$$

Note these identities. Also note that the function $e^{i\varphi_{k, k}}$ as a function of k is discontinuous at $k = 0$.

$$f_1(k_1, k_2) = e^{ik_1 N - \varphi_{k_1, k_2}}, \quad f_2(k_1, k_2) = e^{ik_2 N + \varphi_{k_1, k_2}} \quad (73)$$

If we set the above, the Bethe equations are

$$f_1(k_1, k_2) = f_2(k_1, k_2) = 1. \quad (74)$$

Since $f_1(k_2, k_1) = f_2(k_1, k_2)$ and $f_2(k_2, k_1) = f_1(k_1, k_2)$,

- the equations are symmetric under the interchange $(k_1, k_2) \rightarrow (k_2, k_1)$. In other words, (k_1, k_2) is a solution if and only if (k_2, k_1) is a solution. After all, the Bethe ansatz solution $g_{\mathbf{k}}$ was specified by a pair of two distinct wavenumbers (k_1, k_2) .

Since $f_1(-k_1, -k_2) = f_1(k_1, k_2)^{-1}$ and $f_2(-k_1, -k_2) = f_2(k_1, k_2)^{-1}$,

- the equations are symmetric under $(k_1, k_2) \rightarrow (-k_1, -k_2)$. In other words, (k_1, k_2) is a solution if and only if $(-k_1, -k_2)$ is a solution. This presumably comes from inversion symmetry of the system.

Since $f_1(k_1, k_2)^* = f_1(k_1^*, k_2^*)^{-1}$ and $f_2(k_1, k_2)^* = f_2(k_1^*, k_2^*)^{-1}$,

- the equations are symmetric under $(k_1, k_2) \rightarrow (k_1^*, k_2^*)$. In other words, (k_1, k_2) is a solution if and only if (k_1^*, k_2^*) is a solution.
- Note that the solutions have the character of ‘‘PT-symmetry breaking’’. That is, if one extends the XXX model to a parameter-dependent model while preserving this symmetry, complex solutions are generated by the collision of two real solutions.

Since $f_1(k, k) = f_2(k, k) = -1$,

- $k_1 = k_2 = \frac{2\pi(n-1/2)}{N}$, $n = 1, \dots, N$, are solutions.

Since $f_1(0, k_2) = 1$ and $f_2(0, k_2) = e^{ik_2 N}$,

- $(k_1, k_2) = (0, \frac{2\pi n}{N})$, $n = 0, \dots, N - 1$, are solutions.

1.2.5 Real Solutions

Following Bethe [1], let us count the number of independent solutions when k_1, k_2 are real.

$$e^{i\varphi_{\mathbf{k}}} = -\frac{e^{-i(k_1+k_2)/2} + e^{i(k_1+k_2)/2} - 2e^{i(k_1-k_2)/2}}{e^{-i(k_1+k_2)/2} + e^{i(k_1+k_2)/2} - 2e^{-i(k_1-k_2)/2}} = -\frac{\cos \frac{k_1+k_2}{2} - e^{-i(k_2-k_1)/2}}{\cos \frac{k_1+k_2}{2} - e^{i(k_2-k_1)/2}} \quad (75)$$

As is clear from this rewriting, if k_1, k_2 are real, then $\varphi_{\mathbf{k}}$ is also real. The Bethe equations can be rewritten as

$$\begin{cases} Nk_1 - \varphi_{\mathbf{k}} = 0 & \text{mod } 2\pi, \\ Nk_2 + \varphi_{\mathbf{k}} = 0 & \text{mod } 2\pi, \end{cases} \quad (76)$$

Let us examine the properties of $\varphi_{\mathbf{k}}$:

$$\varphi_{\mathbf{k}} = \pi + 2\arg\left(\cos \frac{k_1+k_2}{2} - e^{-i(k_2-k_1)/2}\right) \quad (77)$$

$$= \pi + 2\arg\left(-2\sin \frac{k_1}{2} \sin \frac{k_2}{2} + i \sin \frac{k_2-k_1}{2}\right) \quad (78)$$

$$= \pi + 2\arg\left(2\sin \frac{k_1}{2} \sin \frac{k_2}{2} - i \sin \frac{k_2-k_1}{2}\right) \pmod{2\pi}, \quad (79)$$

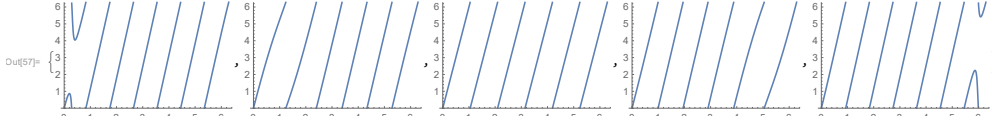


Figure 2: The function $Nk_1 - \varphi_{\mathbf{k}} \bmod 2\pi$, with $N = 7$. From left to right, $k_2 = \pi/10, \pi/2, \pi, 3\pi/2, 2\pi - \pi/10$.

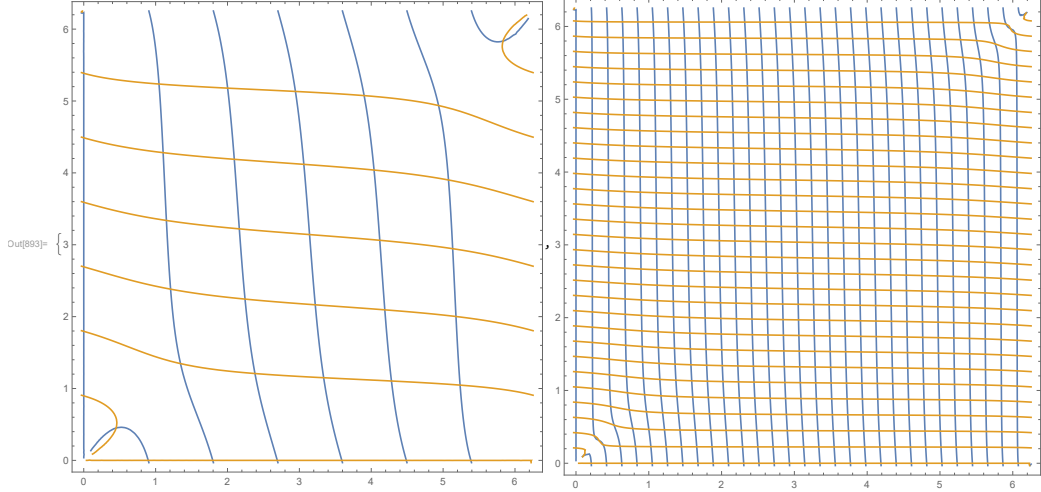


Figure 3: Solution curves for $Nk_1 - \varphi_{\mathbf{k}} \equiv 0$ (blue) and $Nk_2 + \varphi_{\mathbf{k}} \equiv 0$ (yellow). The horizontal axis is k_1 , and the vertical axis is k_2 . The precision is MachinePrecision. Solutions (k_1, k_2) are obtained as intersections of the two solution curves. The two panels are for $N = 7, 30$, respectively.

Thus, when k_1 is varied from 0 through k_2 to 2π , $\varphi_{\mathbf{k}}$ increases monotonically as $\varphi_{0,k_2} = 0 \rightarrow \varphi_{k_2,k_2} = \pi \rightarrow \varphi_{2\pi,k_2} = 2\pi$. Therefore, for any k_2 , the function $Nk_1 - \varphi_{\mathbf{k}}$ has winding number $N - 1$ as k_1 winds once from 0 to 2π . Hence the equation $Nk_1 - \varphi_{\mathbf{k}} \equiv 0$ for k_1 has at least $N - 1$ solutions, independently of k_2 . Note that, in general, there may also be an even number of additional solutions that are unstable under deformations of k_2 . Figure 2 shows plots of the function $Nk_1 - \varphi_{\mathbf{k}}$ for several choices of k_2 in the case $N = 7$. From Figure 2, one sees that multiple solutions in k_1 tend to appear when k_2 is close to $0 = 2\pi$.

Do the unstable solutions not protected by the winding number contribute to solutions of the Bethe equations? To check this, Figure 3 shows the zeros of $Nk_1 - \varphi_{\mathbf{k}}$ and $Nk_2 + \varphi_{\mathbf{k}}$. From the figure, one sees that the smallest point $(k_1 = 0, k_2^{\min})$ with $k_2 > 0$ at $k_1 = 0$ arises from an unstable zero not fixed by the winding number. Moreover, considering the stability of the existence of this solution $(0, k_2^{\min})$ with respect to N , since $(k_1, k_2) = (\frac{\pi}{N}, \frac{\pi}{N})$ is a solution, the solution $(0, k_2^{\min})$ is expected to remain for arbitrary N .

Assume that intersections such as those near $k_1 = k_2 = \frac{2\pi(2-1/2)}{N}$ in the right panel of Figure 3 are not true solutions because of numerical precision (this will later turn out to be wrong). Then the number of solutions satisfying $0 \leq k_1 < k_2 < 2\pi$ is

$$\left(\sum_{n=1}^{N-2} n \right) + 1 = \frac{(N-1)(N-2)}{2} + 1 \quad (80)$$

This differs from Bethe's estimate [1], $\frac{(N-1)(N-2)}{2}$, only by the contribution from the unstable zero. Below I also record Bethe's argument.

1.2.6 Bethe's Estimate of the Number of Real Solutions

Let us follow the argument in [1].

The solutions are

$$k_1 = \frac{2\pi\lambda_1}{N} + \frac{\varphi_{\mathbf{k}}}{N}, \quad (81)$$

$$k_2 = \frac{2\pi\lambda_2}{N} - \frac{\varphi_{\mathbf{k}}}{N}, \quad (82)$$

$$\lambda_1, \lambda_2 = 0, \dots, N-1. \quad (83)$$

$\varphi_{\mathbf{k}}$ may be taken to satisfy

$$-\pi \leq \varphi_{\mathbf{k}} \leq \pi \quad (84)$$

$$k_2 - k_1 = \frac{2\pi(\lambda_2 - \lambda_1)}{N} - \frac{2\varphi_{\mathbf{k}}}{N} \quad (85)$$

Therefore, for $\lambda_1 = 0, \dots, \lambda_2 - 2$, the inequality $0 \leq k_1 < k_2$ is satisfied. However, when $\lambda_1 = \lambda_2 - 1$, $k_1 < k_2$ may fail. Indeed, if one formally solves the Bethe equations $e^{i(k_1 N - \varphi_{\mathbf{k}})} = e^{i(k_2 N + \varphi_{\mathbf{k}})} = 1$ for the case $k_1 = k_2$, one obtains the solution $\varphi_{\mathbf{k}} = \pi$, $\lambda_1 = \lambda_2 - 1$. If the Bethe equation $e^{ik_1 N} = e^{i\varphi_{k_1, k_2}}$ is regarded as an equation determining k_1 for fixed k_2 , the monotonicity of $\varphi_{\mathbf{k}}$ on $0 \leq k_1 \leq k_2$ shows that, for a fixed branch λ_1 , there is at most one solution. Hence $\lambda_1 = \lambda_2 - 1$ is inappropriate as a solution. Thus the number of independent ansatz solutions $g_{\mathbf{k}}(x_1, x_2)$ is

$$\sum_{\lambda_2=2}^{N-1} \sum_{\lambda_1=0}^{\lambda_2-2} = \sum_{\lambda_2=2}^{N-1} (\lambda_2 - 1) = \frac{(N-1)(N-2)}{2}. \quad (86)$$

This argument misses the fact that, due to the singular behavior of $\varphi_{\mathbf{k}}$ at $k_1 = 0$, a solution with $\lambda_1 = 0$ may exist when $\lambda_2 = 1$. Indeed, if $k_1 = 0$ and $k_1 < k_2$, then the Bethe equations give $\lambda_1 = 0$ and

$$k_2 = \frac{2\pi\lambda_2}{N}. \quad (87)$$

This has solutions for $\lambda_2 = 1, \dots, N-1$.

1.2.7 Complex-Conjugate Solutions

The number of real solutions is $\frac{(N-1)(N-2)}{2} + 1$, and the number of constant solutions is one when N is even and zero when N is odd. Since the dimension of the $M = 2$ Hilbert space is $\frac{N(N-1)}{2}$, the number of solutions is short by $N-2$ when N is even and by $N-3$ when N is odd.

Since the total momentum $k_1 + k_2$ is real, we may set

$$\begin{cases} k_1 = u + k, \\ k_2 = u - k, \end{cases} \quad (88)$$

Following [1], first look for solutions in which k_1, k_2 are complex conjugates. That is, set $k = iv$ with v real. It is enough to study $v > 0$.

$$e^{i\varphi_{\mathbf{k}}} = -\frac{\cos \frac{k_1+k_2}{2} - e^{-i(k_2-k_1)/2}}{\cos \frac{k_1+k_2}{2} - e^{i(k_2-k_1)/2}} = -\frac{\cos u - e^{-v}}{\cos u - e^v} \quad (89)$$

Then the Bethe equations become

$$\begin{cases} e^{iuN-vN} = e^{i\varphi_k} = -\frac{\cos u - e^{-v}}{\cos u - e^v}, \\ e^{iuN+vN} = e^{-i\varphi_k} = -\frac{\cos u - e^v}{\cos u - e^{-v}}. \end{cases} \quad (90)$$

Thus, introducing the function

$$F(u, v) := \frac{e^v - \cos u}{e^{-v} - \cos u} \quad (91)$$

we have

$$e^{iuN} = -\text{Sign}F(u, v), \quad (92)$$

$$Nv = \log |F(u, v)|. \quad (93)$$

The second equation (93) can be rewritten as

$$\frac{e^v - \cos u}{e^{-v} - \cos u} = e^{2v} \frac{e^{-v} - \cos u e^{-2v}}{e^{-v} - \cos u} \quad (94)$$

From this, when $-\cos u \geq 0$ and $N > 2$, there is no solution other than $v = 0$. Therefore it is enough to consider the region $\cos u > 0$. Also, when $\cos u = 1$, $\log |F(u, v)| = v$, so for $N > 1$ there is no solution. Thus it remains to consider only $0 < \cos u < 1$. In this case, the function $\log |F(u, v)|$ diverges to $+\infty$ at $v = -\log \cos u$ and is asymptotic to $v + \text{const.}$. Moreover,

$$\partial_v \log F(u, v) = \frac{e^v(e^{-v} - \cos u) + (1 - e^{-v} \cos u)}{(e^v - \cos u)(e^{-v} - \cos u)} > 0, \quad (0 < v < -\log \cos u), \quad (95)$$

$$\partial_v^2 \log F(u, v) = \frac{e^v(e^{2v} - 1) \cos u \sin^2 u}{(e^v - \cos u)^2 (e^v \cos u - 1)^2} > 0, \quad (0 < v < -\log \cos u), \quad (96)$$

so it is convex and monotonically increasing for $0 < v < -\log \cos u$. The slope at $v = 0$ is $\frac{2}{1 - \cos u}$, and hence

- if $N < \frac{2}{1 - \cos u}$, there is one intersection for $v \gtrsim -\log \cos u$.
- if $N > \frac{2}{1 - \cos u}$, there is one intersection each for $v \lesssim -\log \cos u$ and $v \gtrsim -\log \cos u$.

Next determine u from the first equation (92). Since $e^{2iuN} = 1$, a necessary condition is

$$u = \frac{\pi n}{N}, \quad n \in \mathbb{Z} \quad (97)$$

At this value, $e^{iuN} = (-1)^n$, so if (u, v) is a solution then $(-u, v)$ is also a solution. Since $e^v - \cos u > 0$, the sign change on the right-hand side of (92) occurs at $v = -\log \cos u$, which is the divergence point of the right-hand side of (93). From the condition $0 < \cos u < 1$,

- when N is odd, the candidates are $u_n = \pm \frac{\pi n}{N}$, $n = 1, \dots, \frac{N-1}{2}$;
- when N is even, the candidates are $u_n = \pm \frac{\pi n}{N}$, $n = 1, \dots, \frac{N-2}{2}$.

Figure 4 plots the functions Nv and $\log |F(u, v)|$ for $u = u_n$, $n = 1, \dots, \text{Floor}[\frac{N-1}{2}]$, for $N = 7, 20$. Equation (92) is

$$(-1)^n = \begin{cases} -1 & (0 < v < -\log \cos u_n), \\ 1 & (-\log \cos u_n < v), \end{cases} \quad (98)$$

and hence

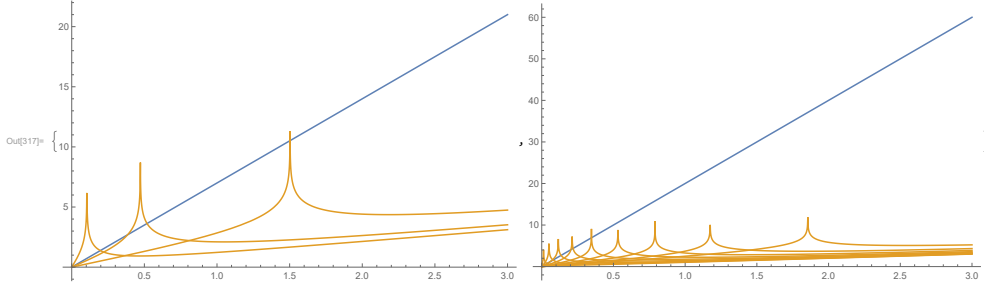


Figure 4: Plots of Nv (blue) and $\log |F(u, v)|$ (yellow) for $u = u_n$, $n = 1, \dots, \text{Floor}(\frac{N-1}{2})$, for $N = 7$ (left) and $N = 20$ (right).

- for odd n , the condition for a solution is $0 < v < -\log \cos u_n$;
- for even n , the condition for a solution is $-\log \cos u_n < v$.

Taking this into account,

- if n is odd and $N > \frac{2}{1-\cos u_n}$ is satisfied, there is one solution for $v \lesssim -\log \cos u_n$.
- if n is odd and $N < \frac{2}{1-\cos u_n}$ is satisfied, there is no solution.
- if n is even, there is one solution for $v \gtrsim -\log \cos u_n$.

The condition $N < \frac{2}{1-\cos u_n}$ is equivalent to

$$n < \frac{2N}{\pi} \sin^{-1}\left(\frac{1}{\sqrt{N}}\right) \quad (99)$$

The number of odd integers $n = 2m - 1$, $m = 1, 2, \dots$, satisfying this condition is M_N , where M_N is the largest integer not exceeding $\frac{N}{\pi} \sin^{-1}\left(\frac{1}{\sqrt{N}}\right) + \frac{1}{2}$. For $N \gg 1$,

$$M_N \sim \frac{\sqrt{N}}{\pi} \quad (100)$$

Computing M_N , one obtains

$$M_N = \begin{cases} 1 & (N \leq 21) \\ 2 & (22 \leq N \leq 61) \\ 3 & (62 \leq N \leq 120) \\ 4 & (121 \leq N \leq 199) \\ 5 & (200 \leq N \leq 298) \\ 6 & (299 \leq N \leq 416) \\ \vdots & \end{cases} \quad (101)$$

and so on. As examples, Figure 5 shows the functions $\log |F(u, v)|$ for $u = u_1, u_3$ at $N = 10, 21, 40$.

Therefore, the number of complex-conjugate solutions is, with a factor of two from the contributions of $u = u_n$ and $-u_n$,

- when N is odd, $N - 1 - 2M_N$.
- when N is even, $N - 2 - 2M_N$.

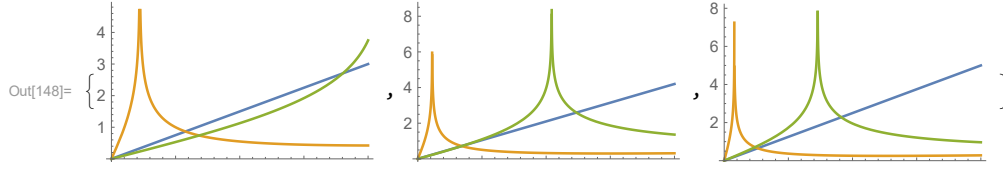


Figure 5: The functions Nv (blue), $\log |F(u_1, v)|$ (yellow), and $\log |F(u_3, v)|$ (green) for $N = 10, 21, 40$.

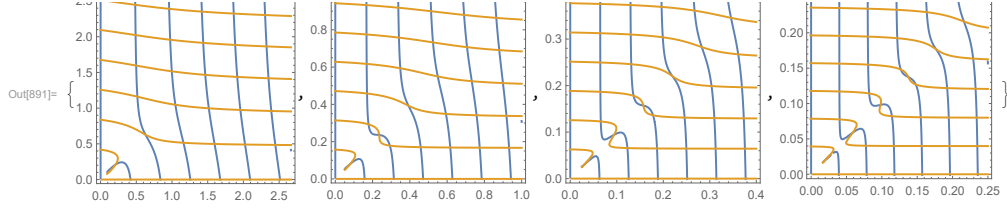


Figure 6: Solution curves for $Nk_1 - \varphi_{\mathbf{k}} \equiv 0$ (blue) and $Nk_2 + \varphi_{\mathbf{k}} \equiv 0$ (yellow). The horizontal axis is k_1 , and the vertical axis is k_2 . Only the neighborhood of $(k_1, k_2) = (0, 0)$ is shown. From left to right, $N = 15, 40, 100, 160$.

1.2.8 Real Solutions with Close Wavenumbers

Compared with the Hilbert-space dimension $N(N - 1)/2$, the number of solutions is short by approximately $2M_N \sim \frac{2\sqrt{N}}{\pi}$ for large N . Looking at [3, 4] and related references, it seems that additional real solutions exist. In Section 1.2.5, I ignored intersections with close wavenumbers near $(k_1, k_2) = \frac{2\pi(2-1/2)}{N}, \frac{2\pi(N-1-1/2)}{N}$ for $N = 20$, but these are in fact solutions. See Figure 6.

By plotting neighborhoods of $k_1 = k_2 = \frac{2\pi(n-1/2)}{N}$, $n = 1, 2, 3, \dots$, and checking by eye when such solutions appear, I find:

- For $N = 22$, they appear near $k_1 = k_2 = \pm \frac{2\pi(2-1/2)}{N}$.
- For $N = 62$, they appear near $k_1 = k_2 = \pm \frac{2\pi(3-1/2)}{N}$.
- For $N = 121$, they appear near $k_1 = k_2 = \pm \frac{2\pi(4-1/2)}{N}$.
- For $N = 200$, they appear near $k_1 = k_2 = \pm \frac{2\pi(5-1/2)}{N}$.
- For $N = 299$, they appear near $k_1 = k_2 = \pm \frac{2\pi(6-1/2)}{N}$.
- For $N = 417$, they appear near $k_1 = k_2 = \pm \frac{2\pi(7-1/2)}{N}$.

The values of N at which new solutions appear agree exactly with $M_N - 1$ in the previous subsection. Therefore, the number of real solutions with close wavenumbers is

$$2(M_N - 1) \tag{102}$$

I leave a rigorous computation of the number of close-wavenumber solutions for later.

1.2.9 Counting Bethe-Ansatz Solutions

Summarizing the above,

- there is one constant solution.
- the number of real solutions with separated wavenumbers is $\frac{(N-1)(N-2)}{2} + 1$.
- the number of complex-conjugate solutions is
 - for odd N , $N - 1 - 2M_N$.
 - for even N , $N - 2 - 2M_N$.
- the number of real solutions with close wavenumbers is $2(M_N - 1)$.

Thus the number of Bethe-ansatz solutions is

- for odd N , $\frac{N(N-1)}{2}$.
- for even N , $\frac{N(N-1)}{2} - 1$.

Therefore, when N is even, one solution is missing.

1.2.10 The Case $N = 3$

For $N = 3$, there are two real solutions, $(k_1, k_2) = (0, 2\pi/3), (0, 4\pi/3)$, and one constant solution. Let us solve the eigenvalue equation directly and compare with the Bethe-ansatz solutions. There are variables $\mathbf{f} = (f(1, 2), f(1, 3), f(2, 3))^T$, and the eigenvalue equation is

$$\begin{cases} f(2, 3) + f(1, 3) + 2f(1, 2) = Ef(1, 2), \\ f(1, 2) + f(2, 3) + 2f(1, 3) = Ef(1, 3), \\ f(1, 3) + f(1, 2) + 2f(2, 3) = Ef(2, 3). \end{cases} \quad (103)$$

that is,

$$\begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix} \mathbf{f} = E\mathbf{f}. \quad (104)$$

Solving this, we obtain the following three solutions:

$$\mathbf{f} = (1, 1, 1)^T, \quad E = 4, \quad (105)$$

$$\mathbf{f} = (1, 0, -1)^T, \quad E = 1, \quad (106)$$

$$\mathbf{f} = (1, -1, 0)^T, \quad E = 1. \quad (107)$$

These correspond to the constant solution and the Bethe-ansatz solutions. ¹

1

$$g_{0, \frac{2\pi}{3}}(x_1, x_2) = e^{\frac{2\pi i}{3}x_1} + e^{\frac{2\pi i}{3}x_2} = (-1, e^{\pi i/3}, e^{-\pi i/3}), \quad (108)$$

$$g_{0, \frac{4\pi}{3}}(x_1, x_2) = e^{\frac{2\pi i}{3}x_1} + e^{\frac{2\pi i}{3}x_2} = (-1, e^{-\pi i/3}, e^{\pi i/3}). \quad (109)$$

Linear combinations of these.

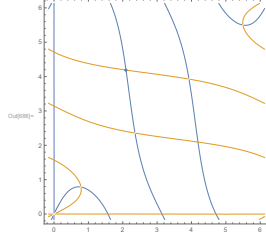


Figure 7: Real solutions of the Bethe equations for $N = 4$. The point $(\frac{2\pi}{3}, \frac{4\pi}{3})$ is also plotted.

1.2.11 The Case $N = 4$

On the other hand, for $N = 4$, the above argument gives four real solutions, $(k_1, k_2) = (0, 2\pi/4), (0, 4\pi/4), (0, 6\pi/4), (2\pi/3, \frac{4\pi}{3})$, and one constant solution. Since the Hilbert-space dimension is 6, one solution is missing. See Figure 7 for the real solutions of the Bethe equations. Let us solve the eigenvalue equation directly and compare with the Bethe-ansatz solutions.

There are variables $\mathbf{f} = (f(1, 2), f(1, 3), f(1, 4), f(2, 3), f(2, 4), f(3, 4))^T$, and the eigenvalue equation is

$$\begin{cases} f(2, 4) + f(1, 3) + 2f(1, 2) = Ef(1, 2), \\ f(3, 4) + f(1, 2) + f(2, 3) + f(1, 4) = Ef(1, 3), \\ f(1, 3) + f(2, 4) + 2f(1, 4) = Ef(1, 4), \\ f(1, 3) + f(2, 4) + 2f(2, 3) = Ef(2, 3), \\ f(1, 4) + f(2, 3) + f(3, 4) + f(1, 2) = Ef(2, 4), \\ f(2, 4) + f(1, 3) + 2f(3, 4) = Ef(3, 4), \end{cases} \quad (110)$$

that is,

$$\begin{pmatrix} 2 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 2 & 0 & 1 & 0 \\ 0 & 1 & 0 & 2 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 2 \end{pmatrix} \mathbf{f} = E\mathbf{f}. \quad (111)$$

Solving this, we obtain the following six solutions:

$$\mathbf{f} = (1, 1, 1, 1, 1, 1)^T, \quad E = 4, \quad (112)$$

$$\mathbf{f} = (1, -2, 1, 1, -2, 1)^T, \quad E = -2, \quad (113)$$

$$\mathbf{f} = (0, -1, 0, 0, 1, 0)^T, \quad E = 0, \quad (114)$$

$$\mathbf{f} = (-1, 0, 0, 0, 0, 1)^T, \quad E = 2, \quad (115)$$

$$\mathbf{f} = (-1, 0, 0, 1, 0, 0)^T, \quad E = 2, \quad (116)$$

$$\mathbf{f} = (-1, 0, 1, 0, 0, 0)^T, \quad E = 2. \quad (117)$$

On the other hand,

$$\text{constant solution : } \mathbf{f} = (1, 1, 1, 1, 1, 1), \quad E = 4, \quad (118)$$

$$(k_1, k_2) = (\frac{2\pi}{3}, \frac{4\pi}{3}) : \mathbf{f} = (1, -2, 1, 1, -2, 1), \quad E = -2, \quad (119)$$

$$(k_1, k_2) = (0, \pi) : \mathbf{f} = (0, -1, 0, 0, 1, 0), \quad E = 0, \quad (120)$$

$$(k_1, k_2) = (0, \frac{\pi}{2}) : \mathbf{f} = (1, 0, -i, i, 0, -1), \quad E = 2, \quad (121)$$

$$(k_1, k_2) = (0, \frac{3\pi}{2}) : \mathbf{f} = (1, 0, i, -i, 0, -1), \quad E = 2 \quad (122)$$

Thus one solution with $E = 2$ is indeed missing.

In general, when the number of sites is even, the following solution of the eigenvalue equation exists.²

$$|\psi\rangle = \sum_{j=1}^N (-1)^j \sigma_j^- \sigma_{j+1}^- |0\rangle. \quad (123)$$

Indeed, substituting the above $|\psi\rangle$ into the eigenvalue equation confirms that it is a solution with eigenvalue $E = 2$. The missing solution seems to be due to having neglected the case in which the denominator in (56) vanishes, but I am not fully satisfied with this explanation. For example, [5] contains a discussion. I record a note on this in the next subsection.

1.2.12 “Singular Solutions” of the Bethe Equations

$$e^{ik_j} = \frac{\lambda_j + i}{\lambda_j - i}, \quad j = 1, 2, \quad (124)$$

and introduce λ_j . Then

$$1 + e^{i(k_1+k_2)} - 2e^{ik_1} = \frac{-2i(\lambda_2 - \lambda_1 - 2i)}{(\lambda_1 - i)(\lambda_2 - i)}, \quad (125)$$

$$1 + e^{i(k_1+k_2)} - 2e^{ik_2} = \frac{-2i(\lambda_1 - \lambda_2 - 2i)}{(\lambda_1 - i)(\lambda_2 - i)} \quad (126)$$

Using these identities, the Bethe equations become

$$\left(\frac{\lambda_1 + i}{\lambda_1 - i}\right)^N = -\frac{\lambda_2 - \lambda_1 - 2i}{\lambda_1 - \lambda_2 - 2i}, \quad (127)$$

$$\left(\frac{\lambda_2 + i}{\lambda_2 - i}\right)^N = -\frac{\lambda_1 - \lambda_2 - 2i}{\lambda_2 - \lambda_1 - 2i} \quad (128)$$

The case in which the denominator vanishes is singular, so after clearing denominators,

$$(\lambda_1 + i)^N (\lambda_1 - \lambda_2 - 2i) = -(\lambda_1 - i)^N (\lambda_2 - \lambda_1 - 2i), \quad (129)$$

$$(\lambda_2 + i)^N (\lambda_2 - \lambda_1 - 2i) = -(\lambda_2 - i)^N (\lambda_1 - \lambda_2 - 2i) \quad (130)$$

we obtain the solution

$$\lambda_1 = i, \lambda_2 = -i \quad (131)$$

It is known that, under a suitable regularization, the corresponding eigenvalue and eigenvector give $|\psi\rangle$ and $E = 2$ [5].

1.2.13 The Solutions Are Given by Complex-Conjugate Pairs

From the symmetry of the Bethe equations under complex conjugation, if $\{k_1, k_2\}$ is a solution, then $\{k_1^*, k_2^*\}$ is also a solution. In fact, as sets one has $\{k_1, k_2\} = \{k_1^*, k_2^*\}$. For general M , this was proved using the transfer matrix in [7]. Also, [6] states only that, by the symmetry of the Bethe equations under complex conjugation, one may take $k_2 = k_1^*$ for complex solutions. Is that really sufficient?

²I learned this from Hoshio Katsura. I thank him.

For $M = 2$, one can prove this as follows using the fact that momentum and energy are real.³ Since $k_1 + k_2$ is the total momentum, it is real; in particular, $\text{Im } k_1 + \text{Im } k_2 = 0$. When $\text{Im } k_1 = -\text{Im } k_2 \neq 0$, we want to show $\text{Re } k_1 = \text{Re } k_2$. The energy is

$$E_{\mathbf{k}} = 2 \cos k_1 + 2 \cos k_2 = 4 \cos \frac{k_1 + k_2}{2} \cos \frac{k_1 - k_2}{2} \quad (132)$$

and its imaginary part is

$$\text{Im } E_{\mathbf{k}} = -4 \cos \frac{k_1 + k_2}{2} \sin \frac{\text{Re}(k_1 - k_2)}{2} \sinh \frac{\text{Im}(k_1 - k_2)}{2}. \quad (133)$$

Since the Hamiltonian is Hermitian, $\text{Im } E_{\mathbf{k}} = 0$. Under the assumption $\text{Im } k_1 = -\text{Im } k_2 \neq 0$, this implies either $k_1 + k_2 = \pi \pmod{2\pi}$, or $\text{Re}(k_1 - k_2) = 0$. Thus the claim is proved when $k_1 + k_2 \neq \pi \pmod{2\pi}$.

Now consider the case $k_1 + k_2 = \pi$. In this case the Bethe equations are

$$e^{ik_1 N} = -\frac{1 + e^{i(k_1+k_2)} - 2e^{ik_1}}{1 + e^{i(k_1+k_2)} - 2e^{ik_2}} = e^{2ik_1}, \quad (134)$$

$$e^{ik_2 N} = -\frac{1 + e^{i(k_1+k_2)} - 2e^{ik_2}}{1 + e^{i(k_1+k_2)} - 2e^{ik_1}} = e^{2ik_2}, \quad (135)$$

Solutions exist when N is even, and they are

$$(k_1, k_2) = \left(\frac{2\pi n}{N-2}, \pi - \frac{2\pi n}{N-2} \right), \quad n = 0, \dots, N-3 \quad (136)$$

Thus, in the case $k_1 + k_2 = \pi$, there are no complex solutions.

1.2.14 Comparison with Existing Results

[6] points out the shortage of M_N complex-conjugate solutions discussed in Sections 1.2.7 and 1.2.8, together with the accompanying appearance of real solutions with close wavenumbers. The calculation in this note agrees with the calculation in [6].

1.2.15 Spectrum of Complex-Conjugate Solutions

Let us compute the spectrum of the complex-conjugate solutions for large N . Ignoring the $2M \sim \frac{2\sqrt{N}}{\pi}$ exceptional solutions, and further taking $(u, v) = (u_n, -\log \cos u_n)$ as an approximate solution, the solution (k_1, k_2) is roughly

$$k_1 = k - i \log \cos k, \quad (137)$$

$$k_2 = k + i \log \cos k, \quad (138)$$

$$k = \frac{\pi n}{N}, \quad n = -\frac{N}{2}, -\frac{N}{2} + 1, \dots, \frac{N}{2}, \quad (139)$$

The energy eigenvalue is

$$E(k_1, k_2) = 2 \cos k_1 + 2 \cos k_2 = e^{ik_1} + e^{-ik_1} + e^{ik_2} + e^{-ik_2} \quad (140)$$

$$= e^{ik} \cos k + e^{-ik} (\cos k)^{-1} + e^{ik} (\cos k)^{-1} + e^{-ik} \cos k \quad (141)$$

$$= 2 \cos^2 k + 2 = \cos 2k + 4, \quad -\frac{\pi}{2} < k < \frac{\pi}{2}. \quad (142)$$

³I also learned this proof from Hosho Katsura.

1.2.16 Backup Calculation

Let us consider complex solutions. I follow the argument in [1]. First rewrite the Bethe equations slightly.

$$e^{i\varphi_{\mathbf{k}}} = -\frac{\cos \frac{k_1+k_2}{2} - e^{-i(k_2-k_1)/2}}{\cos \frac{k_1+k_2}{2} - e^{i(k_2-k_1)/2}} = -\frac{\cos \frac{k_1+k_2}{2} - \cos \frac{k_1-k_2}{2} - i \sin \frac{k_1-k_2}{2}}{\cos \frac{k_1+k_2}{2} - \cos \frac{k_1-k_2}{2} + i \sin \frac{k_1-k_2}{2}} \quad (143)$$

From this,

$$\cot \frac{\varphi_{\mathbf{k}}}{2} = \frac{1}{\tan \frac{\varphi_{\mathbf{k}}}{2}} = \frac{\sin \varphi_{\mathbf{k}}}{1 - \cos \varphi_{\mathbf{k}}} = \frac{1}{i} \frac{e^{i\varphi_{\mathbf{k}}} - e^{-i\varphi_{\mathbf{k}}}}{2 - e^{i\varphi_{\mathbf{k}}} - e^{-i\varphi_{\mathbf{k}}}} = \frac{\sin \frac{k_1-k_2}{2}}{\cos \frac{k_1+k_2}{2} - \cos \frac{k_1-k_2}{2}} = \frac{1}{2} \left(\cot \frac{k_1}{2} - \cot \frac{k_2}{2} \right), \quad (144)$$

namely,

$$2 \cot \frac{\varphi_{\mathbf{k}}}{2} = \cot \frac{k_1}{2} - \cot \frac{k_2}{2} \quad (145)$$

$$k_1 = u + iv, \quad k_2 = u - iv \quad (146)$$

With this parametrization, since the total momentum $k_1 + k_2$ is real, u is real. The variable v is complex in general.

$$\cot \frac{k_1}{2} = \frac{\cos \frac{u+iv}{2}}{\sin \frac{u+iv}{2}} = \frac{\cos \frac{u}{2} \cos \frac{iv}{2} - \sin \frac{u}{2} \sin \frac{iv}{2}}{\sin \frac{u}{2} \cos \frac{iv}{2} + \cos \frac{u}{2} \sin \frac{iv}{2}} = \frac{\cos \frac{u}{2} \cosh \frac{v}{2} - i \sin \frac{u}{2} \sinh \frac{v}{2}}{\sin \frac{u}{2} \cosh \frac{v}{2} + i \cos \frac{u}{2} \sinh \frac{v}{2}} \quad (147)$$

$$= \frac{(\cos \frac{u}{2} \cosh \frac{v}{2} - i \sin \frac{u}{2} \sinh \frac{v}{2})(\sin \frac{u}{2} \cosh \frac{v}{2} - i \cos \frac{u}{2} \sinh \frac{v}{2})}{\sin^2 \frac{u}{2} \cosh^2 \frac{v}{2} + \cos^2 \frac{u}{2} \sinh^2 \frac{v}{2}} \quad (148)$$

$$= \frac{\cos \frac{u}{2} \sin \frac{u}{2} - i \cosh \frac{v}{2} \sinh \frac{v}{2}}{\sin^2 \frac{u}{2} \cosh^2 \frac{v}{2} + \cos^2 \frac{u}{2} \sinh^2 \frac{v}{2}} \quad (149)$$

$$= \frac{2 \sin u - 2i \sinh v}{(1 - \cos u)(1 + \cosh v) + (1 + \cos u)(\cosh v - 1)} \quad (150)$$

$$= \frac{\sin u - i \sinh v}{\cosh v - \cos u}. \quad (151)$$

Replacing v by $-v$, we get

$$\cot \frac{k_2}{2} = \frac{\sin u + i \sinh v}{\cosh v - \cos u}. \quad (152)$$

Although v is complex in general, in the following I take v to be real. Thus k_1, k_2 are assumed to be complex conjugates. It is enough to consider $v > 0$.

$$\varphi_{\mathbf{k}} = \psi_{\mathbf{k}} + i\chi_{\mathbf{k}} \quad (153)$$

and separate real and imaginary parts. Then the Bethe equations become

$$\psi_{\mathbf{k}} \equiv -\psi_{\mathbf{k}} \pmod{2\pi}, \quad (154)$$

$$Nv = \chi_{\mathbf{k}} \quad (155)$$

2 Open Boundary Conditions

Since the Bethe ansatz is obtained by connecting free-field solutions for $|x_2 - x_1| > 1$ to the region $|x_2 - x_1| = 1$, one might naively expect it to apply also to open boundary conditions. For open boundary

conditions, the Hamiltonian is

$$H = \sum_{j=1}^{N-1} (\sigma_{j+1}^- \sigma_j^+ + \sigma_j^- \sigma_{j+1}^+ + 2 \frac{1 - \sigma_j^z}{2} \frac{1 - \sigma_{j+1}^z}{2}). \quad (156)$$

Let us examine the structure of the eigenvalue equation

$$H |f\rangle_M = E |f\rangle_M \quad (157)$$

2.1 $M = 1$

For $M = 1$, the third term drops out, and

$$H |f\rangle_1 = \sum_{j=1}^{N-1} \sum_{x=1}^N (\delta_{jx} \sigma_{j+1}^- + \delta_{j+1,x} \sigma_j^-) f(x) |0\rangle \quad (158)$$

$$= \sum_{j=1}^{N-1} (f(j) \sigma_{j+1}^- + f(j+1) \sigma_j^-) |0\rangle \quad (159)$$

$$= \sum_{j=2}^N f(j-1) \sigma_j^- |0\rangle + \sum_{j=1}^{N-1} f(j+1) \sigma_j^- |0\rangle. \quad (160)$$

This gives the eigenvalue equation

$$\begin{cases} f(j-1) + f(j+1) = Ef(j) & j = 2, \dots, N-1, \\ f(2) = Ef(1), \\ f(N-1) = Ef(N), \end{cases} \quad (161)$$

If $f(0)$ and $f(N+1)$ are added as variables, this is equivalent to

$$f(j-1) + f(j+1) = Ef(j), \quad j = 1, \dots, N, \quad (162)$$

$$f(0) = f(N+1) = 0. \quad (163)$$

The N linearly independent solutions are

$$f_k(x) = \sin \frac{\pi p x}{N+1}, \quad p = 1, \dots, N. \quad (164)$$

2.2 $M = 2$

For the hopping terms, when $x_1 \neq x_2$,

$$\sigma_{j+1}^- \sigma_j^+ \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle = \delta_{jx_1} \sigma_{x_1+1}^- \sigma_{x_2}^- |0\rangle + \delta_{jx_2} \sigma_{x_1}^- \sigma_{x_2+1}^- |0\rangle, \quad (165)$$

$$\sigma_j^- \sigma_{j+1}^+ \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle = \delta_{j+1,x_1} \sigma_{x_1-1}^- \sigma_{x_2}^- |0\rangle + \delta_{j+1,x_2} \sigma_{x_1}^- \sigma_{x_2-1}^- |0\rangle, \quad (166)$$

Notice these relations. When two lowering operators act on the same site, set $\sigma_x^- \sigma_x^- = 0$. From this,

$$\sum_{j=1}^{N-1} \sigma_{j+1}^- \sigma_j^+ |f\rangle_2 = \sum_{1 \leq x_1 < x_2 \leq N} \sum_{j=1}^{N-1} f(x_1, x_2) (\delta_{jx_1} \sigma_{x_1+1}^- \sigma_{x_2}^- |0\rangle + \delta_{jx_2} \sigma_{x_1}^- \sigma_{x_2+1}^- |0\rangle) \quad (167)$$

$$= \sum_{1 \leq x_1 < x_2 - 1 \leq N-1} f(x_1, x_2) \sigma_{x_1+1}^- \sigma_{x_2}^- |0\rangle + \sum_{1 \leq x_1 < x_2 \leq N-1} f(x_1, x_2) \sigma_{x_1}^- \sigma_{x_2+1}^- |0\rangle \quad (168)$$

$$= \sum_{2 \leq x_1 < x_2 \leq N} f(x_1 - 1, x_2) \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle + \sum_{1 \leq x_1 < x_2 - 1 \leq N-1} f(x_1, x_2 - 1) \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle, \quad (169)$$

$$\sum_{j=1}^{N-1} \sigma_j^- \sigma_{j+1}^+ |f\rangle_2 = \sum_{1 \leq x_1 < x_2 \leq N} \sum_{j=1}^{N-1} f(x_1, x_2) (\delta_{j+1, x_1} \sigma_{x_1-1}^- \sigma_{x_2}^- |0\rangle + \delta_{j+1, x_2} \sigma_{x_1}^- \sigma_{x_2-1}^- |0\rangle) \quad (170)$$

$$= \sum_{2 \leq x_1 < x_2 \leq N} f(x_1, x_2) \sigma_{x_1-1}^- \sigma_{x_2}^- |0\rangle + \sum_{1 \leq x_1 < x_2-1 \leq N-1} f(x_1, x_2) \sigma_{x_1}^- \sigma_{x_2-1}^- |0\rangle \quad (171)$$

$$= \sum_{1 \leq x_1 < x_2-1 \leq N-1} f(x_1+1, x_2) \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle + \sum_{1 \leq x_1 < x_2 \leq N-1} f(x_1, x_2+1) \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle. \quad (172)$$

For the interaction term,

$$\sum_{j=1}^{N-1} \frac{1-\sigma_j^z}{2} \frac{1-\sigma_{j+1}^z}{2} \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle = \delta_{x_1+1, x_2} \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle \quad (173)$$

and therefore

$$\sum_{1 \leq x_1 < x_2 \leq N} \sum_{j=1}^{N-1} 2 \frac{1-\sigma_j^z}{2} \frac{1-\sigma_{j+1}^z}{2} |f\rangle_2 = \sum_{1 \leq x_1 < x_2 \leq N} f(x_1, x_2) 2 \delta_{x_1+1, x_2} \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle \quad (174)$$

$$= \sum_{x=1}^{N-1} f(x, x+1) 2 \sigma_x^- \sigma_{x+1}^- |0\rangle. \quad (175)$$

Thus the action of the Hamiltonian on the wave function $|f\rangle_2$ is

$$H |f\rangle_2 = \sum_{2 \leq x_1 < x_2 \leq N} f(x_1-1, x_2) \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle + \sum_{1 \leq x_1 < x_2-1 \leq N-1} f(x_1, x_2-1) \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle \quad (176)$$

$$+ \sum_{1 \leq x_1 < x_2-1 \leq N-1} f(x_1+1, x_2) \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle + \sum_{1 \leq x_1 < x_2 \leq N-1} f(x_1, x_2+1) \sigma_{x_1}^- \sigma_{x_2}^- |0\rangle \quad (177)$$

$$+ \sum_{x=1}^{N-1} f(x, x+1) 2 \sigma_x^- \sigma_{x+1}^- |0\rangle \quad (178)$$

The eigenvalue equation is

- For $2 \leq x_1, x_1+1 \leq x_2 \leq N-1$ (yellow),

$$(A): \quad f(x_1-1, x_2) + f(x_1, x_2-1) + f(x_1+1, x_2) + f(x_1, x_2+1) = Ef(x_1, x_2). \quad (179)$$

- For $x_1=1, 3 \leq x_2 \leq N-1$ (cyan),

$$(B): \quad f(1, x_2-1) + f(2, x_2) + f(1, x_2+1) = Ef(1, x_2). \quad (180)$$

- For $2 \leq x_1 \leq N-2, x_2=N$ (orange),

$$(C): \quad f(x_1-1, N) + f(x_1, N-1) + f(x_1+1, N) = Ef(x_1, N). \quad (181)$$

- For $x_1=x, x_2=x+1, 2 \leq x \leq N-2$ (green),

$$(D): \quad f(x-1, x+1) + f(x, x+2) + 2f(x, x+1) = Ef(x, x+1). \quad (182)$$

- For $x_1=1, x_2=2$ (blue),

$$(E): \quad f(1, 3) + 2f(1, 2) = Ef(1, 2). \quad (183)$$

- For $x_1=N-1, x_2=N$ (red),

$$(F): \quad f(N-2, N) + 2f(N-1, N) = Ef(N-1, N). \quad (184)$$

- For $x_1 = 1, x_2 = N$ (pink),

$$(G) : \quad 0 = Ef(1, N). \quad (185)$$

As in the periodic-boundary case, it is convenient to extend the domain $1 \leq x_1 < x_2 \leq N$ of $f(x_1, x_2)$ and introduce boundary conditions for the extra degrees of freedom. Introduce the following $2N + 1$ variables:

$$f(0, x_2), \quad x_2 = 1, \dots, N + 1, \quad (186)$$

$$f(x_1, N + 1), \quad x_1 = 0, \dots, N, \quad (187)$$

and impose the following boundary conditions:

$$(B.C.) \quad \begin{cases} f(0, x_2) = 0, & x_2 = 1, \dots, N + 1, \\ f(x_1, N + 1) = 0, & x_1 = 0, \dots, N. \end{cases} \quad (188)$$

Then the equations (A,B,C) can be combined as

$$(Eq.1) : \quad f(x_1 - 1, x_2) + f(x_1, x_2 - 1) + f(x_1 + 1, x_2) + f(x_1, x_2 + 1) = Ef(x_1, x_2), \quad |x_2 - x_1| > 1, \quad (189)$$

Moreover, (D,E,F,G) can also be rewritten as

$$(Eq.2) : \quad f(x - 1, x + 1) + f(x, x + 2) + 2f(x, x + 1) = Ef(x, x + 1), \quad (x = 1, \dots, N - 1), \quad (190)$$

We want to solve the eigenvalue equations (Eq.1, Eq.2, G) under the boundary conditions (B.C.). (Eq.1) has the following eight free-field solutions:

$$e^{ik_1 x_1} e^{ik_2 x_2}, e^{ik_1 x_2} e^{ik_2 x_1}, e^{-ik_1 x_1} e^{ik_2 x_2}, e^{-ik_1 x_2} e^{ik_2 x_1}, \quad (191)$$

$$e^{ik_1 x_1} e^{-ik_2 x_2}, e^{ik_1 x_2} e^{-ik_2 x_1}, e^{-ik_1 x_1} e^{-ik_2 x_2}, e^{-ik_1 x_2} e^{-ik_2 x_1}, \quad (192)$$

$$E_{\mathbf{k}} = 2 \cos k_1 + 2 \cos k_2 \quad (193)$$

Thus write the solution as

$$g_{\mathbf{k}}(x_1, x_2) = c_1^{++} e^{ik_1 x_1} e^{ik_2 x_2} + c_2^{++} e^{ik_1 x_2} e^{ik_2 x_1} + c_1^{-+} e^{-ik_1 x_1} e^{ik_2 x_2} + c_2^{-+} e^{-ik_1 x_2} e^{ik_2 x_1} \quad (194)$$

$$+ c_1^{+-} e^{ik_1 x_1} e^{-ik_2 x_2} + c_2^{+-} e^{ik_1 x_2} e^{-ik_2 x_1} + c_1^{--} e^{-ik_1 x_1} e^{-ik_2 x_2} + c_2^{--} e^{-ik_1 x_2} e^{-ik_2 x_1} \quad (195)$$

The function $g_{\mathbf{k}}(x_1, x_2)$ again satisfies the relation

$$g_{\mathbf{k}}(x - 1, x + 1) + g_{\mathbf{k}}(x, x) + g_{\mathbf{k}}(x + 1, x + 1) + g_{\mathbf{k}}(x, x + 2) = E_{\mathbf{k}} g_{\mathbf{k}}(x, x + 1) \quad (196)$$

so substituting $g_{\mathbf{k}}(x)$ into (Eq.2), the condition for $g_{\mathbf{k}}(x_1, x_2)$ to be a solution is

$$g_{\mathbf{k}}(x, x) + g_{\mathbf{k}}(x + 1, x + 1) - 2g_{\mathbf{k}}(x, x + 1) = 0 \quad (197)$$

This equation has a solution, and for $c_1^{\sigma\sigma'}, c_2^{\sigma\sigma'}$ we obtain

$$\frac{c_1^{\sigma\sigma'}}{c_2^{\sigma\sigma'}} = -\frac{1 + e^{i(\sigma k_1 + \sigma' k_2)} - 2e^{i\sigma k_1}}{1 + e^{i(\sigma k_1 + \sigma' k_2)} - 2e^{i\sigma' k_2}} =: e^{i\varphi_{\sigma\sigma'}}, \quad \sigma, \sigma' \in \{+, -\}, \quad (198)$$

Since the equation is linear, we are taking a linear combination of the solutions for each $(\pm k_1, \pm k_2)$. Noting that $e^{i\varphi_{--}} = e^{-i\varphi_{++}}$ and $e^{i\varphi_{+-}} = e^{-i\varphi_{-+}}$, the ansatz solution satisfying (Eq.1, Eq.2) is, with coefficients a, b, c, d ,

$$g_{\mathbf{k}}(x_1, x_2) = a(e^{i(k_1 x_1 + k_2 x_2 + \frac{\alpha}{2})} + e^{i(k_1 x_2 + k_2 x_1 - \frac{\alpha}{2})}) + b(e^{-i(k_1 x_1 + k_2 x_2 + \frac{\alpha}{2})} + e^{-i(k_1 x_2 + k_2 x_1 - \frac{\alpha}{2})}) \quad (199)$$

$$+ c(e^{i(k_1 x_1 - k_2 x_2 + \frac{\beta}{2})} + e^{i(k_1 x_2 - k_2 x_1 - \frac{\beta}{2})}) + d(e^{-i(k_1 x_1 - k_2 x_2 + \frac{\beta}{2})} + e^{-i(k_1 x_2 - k_2 x_1 - \frac{\beta}{2})}) \quad (200)$$

where

$$e^{i\alpha} = -\frac{1 + e^{i(k_1+k_2)} - 2e^{ik_1}}{1 + e^{i(k_1+k_2)} - 2e^{ik_2}}, \quad (201)$$

$$e^{i\beta} = -\frac{1 + e^{i(k_1-k_2)} - 2e^{ik_1}}{1 + e^{i(k_1-k_2)} - 2e^{-ik_2}} = -\frac{e^{ik_1} + e^{ik_2} - 2e^{i(k_1+k_2)}}{e^{ik_1} + e^{ik_2} - 2} \quad (202)$$

Next solve the boundary conditions (B.C.). From $f(0, x_2) = 0$,

$$a(e^{i(k_2x_2 + \frac{\alpha}{2})} + e^{i(k_1x_2 - \frac{\alpha}{2})}) + b(e^{-i(k_2x_2 + \frac{\alpha}{2})} + e^{-i(k_1x_2 - \frac{\alpha}{2})}) \quad (203)$$

$$+ c(e^{i(-k_2x_2 + \frac{\beta}{2})} + e^{i(k_1x_2 - \frac{\beta}{2})}) + d(e^{-i(-k_2x_2 + \frac{\beta}{2})} + e^{-i(k_1x_2 - \frac{\beta}{2})}) \quad (204)$$

$$= (ae^{-i\alpha/2} + ce^{-i\beta/2})e^{ik_1x_2} + (be^{i\alpha/2} + de^{i\beta/2})e^{-ik_1x_2} \quad (205)$$

$$+ (ae^{i\alpha/2} + de^{-i\beta/2})e^{ik_2x_2} + (be^{-i\alpha/2} + ce^{i\beta/2})e^{-ik_2x_2}. \quad (206)$$

Thus, assuming $k_1 \neq k_2$,

$$\begin{cases} ae^{-i\alpha/2} + ce^{-i\beta/2} = 0, \\ be^{i\alpha/2} + de^{i\beta/2} = 0, \\ ae^{i\alpha/2} + de^{-i\beta/2} = 0, \\ be^{-i\alpha/2} + ce^{i\beta/2} = 0, \end{cases} \quad (207)$$

Solving these equations gives

$$b = ae^{i\beta}, \quad c = -ae^{-i(\alpha-\beta)/2}, \quad d = -ae^{i(\alpha+\beta)/2} \quad (208)$$

and therefore the ansatz solution is determined as

$$g_{\mathbf{k}}(x_1, x_2) = (e^{i(k_1x_1 + k_2x_2 + \frac{\alpha}{2})} + e^{i(k_1x_2 + k_2x_1 - \frac{\alpha}{2})})e^{-i\beta/2} + (e^{-i(k_1x_1 + k_2x_2 + \frac{\alpha}{2})} + e^{-i(k_1x_2 + k_2x_1 - \frac{\alpha}{2})})e^{i\beta/2} \quad (209)$$

$$- (e^{i(k_1x_1 - k_2x_2 + \frac{\beta}{2})} + e^{i(k_1x_2 - k_2x_1 - \frac{\beta}{2})})e^{-i\alpha/2} - (e^{-i(k_1x_1 - k_2x_2 + \frac{\beta}{2})} + e^{-i(k_1x_2 - k_2x_1 - \frac{\beta}{2})})e^{i\alpha/2}. \quad (210)$$

The condition that the boundary condition $f(x_1, N+1) = 0$ hold for arbitrary x_1 gives equations for k_1, k_2 . Set $L = N+1$. Then

$$f(x_1, L) = (e^{i(k_1x_1 + k_2L + \frac{\alpha}{2})} + e^{i(k_1L + k_2x_1 - \frac{\alpha}{2})})e^{-i\beta/2} + (e^{-i(k_1x_1 + k_2L + \frac{\alpha}{2})} + e^{-i(k_1L + k_2x_1 - \frac{\alpha}{2})})e^{i\beta/2} \quad (211)$$

$$- (e^{i(k_1x_1 - k_2L + \frac{\beta}{2})} + e^{i(k_1L - k_2x_1 - \frac{\beta}{2})})e^{-i\alpha/2} - (e^{-i(k_1x_1 - k_2L + \frac{\beta}{2})} + e^{-i(k_1L - k_2x_1 - \frac{\beta}{2})})e^{i\alpha/2} \quad (212)$$

$$= (e^{i(k_2L + \frac{\alpha}{2})}e^{-i\beta/2} - e^{i(-k_2L + \frac{\beta}{2})}e^{-i\alpha/2})e^{ik_1x_1} + (e^{-i(k_2L + \frac{\alpha}{2})}e^{i\beta/2} - e^{-i(-k_2L + \frac{\beta}{2})}e^{i\alpha/2})e^{-ik_1x_1} \quad (213)$$

$$+ (e^{i(k_1L - \frac{\alpha}{2})}e^{-i\beta/2} - e^{-i(k_1L - \frac{\beta}{2})}e^{i\alpha/2})e^{ik_2x_1} + (e^{-i(k_1L - \frac{\alpha}{2})}e^{i\beta/2} - e^{-i(k_1L - \frac{\beta}{2})}e^{-i\alpha/2})e^{-ik_2x_1} \quad (214)$$

$$= 2i \sin(k_2L + \frac{\alpha - \beta}{2})e^{ik_1x_1} - 2i \sin(k_2L + \frac{\alpha - \beta}{2})e^{-ik_1x_1} \quad (215)$$

$$+ 2i \sin(k_1L - \frac{\alpha + \beta}{2})e^{ik_2x_1} - 2i \sin(k_1L - \frac{\alpha + \beta}{2})e^{-ik_2x_1} \quad (216)$$

$$= -4 \sin(k_2L + \frac{\alpha - \beta}{2}) \sin(k_1x_1) - 4 \sin(k_1L - \frac{\alpha + \beta}{2}) \sin(k_2x_1). \quad (217)$$

Thus, assuming $k_1 \neq k_2$, the boundary condition gives

$$\sin(k_2L + \frac{\alpha - \beta}{2}) = \sin(k_1L - \frac{\alpha + \beta}{2}) = 0, \quad (218)$$

or equivalently

$$e^{2ik_2(N+1)} = e^{-i\alpha}e^{i\beta} = \frac{1 + e^{i(k_1+k_2)} - 2e^{ik_2}}{1 + e^{i(k_1+k_2)} - 2e^{ik_1}} \times \frac{e^{ik_1} + e^{ik_2} - 2e^{i(k_1+k_2)}}{e^{ik_1} + e^{ik_2} - 2}, \quad (219)$$

$$e^{2ik_1(N+1)} = e^{i\alpha}e^{i\beta} = \frac{1 + e^{i(k_1+k_2)} - 2e^{ik_1}}{1 + e^{i(k_1+k_2)} - 2e^{ik_2}} \times \frac{e^{ik_1} + e^{ik_2} - 2e^{i(k_1+k_2)}}{e^{ik_1} + e^{ik_2} - 2} \quad (220)$$

These correspond to the Bethe equations for open boundary conditions. **Compare with existing results.**

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