Journal of Statistical Physics, Vol. 88, Nos. 3/4, 1997

Quasi-Bound States of Two Magnons in the Spin-$\frac{1}{2}$ *XXZ* Chain

Yoshifumi Morita,[1] Mahito Kohmoto,[1] and Tohru Koma[2]

Received January 23, 1996; final February 17, 1997

We study two-magnon Bethe states in the spin-1/2 *XXZ* chain. The string hypothesis assumes that complex rapidities of the bound states take special forms. It is known, however, that there exist "non-string states," which substantially disagrees with the string hypothesis. In order to clarify their nature, we study the large-N behavior of solutions of the Bethe-Ansatz equations to obtain explicit forms of typical Bethe states, where N is the length of the chain, and apply the scaling analysis (the multifractal analysis) to the Bethe states. It turns out that the non-string states contain "quasi-bound" states, which in some sense continuously interpolate between extended states and localized states. The "quasi-bound" states can be distinguished from known three types of states, i.e., extended, localized, and critical states. Our results indicate that there might be a need to reconsider the standard classification scheme of wavefunctions.

KEY WORDS: Quantum spin chains; *XXZ* chain; Bethe Ansatz; string hypothesis; non-string states; scaling analysis; multifractal analysis; characterization of wavefunctions.

1. INTRODUCTION

Consider the spin-1/2 *XXZ* chain. The Hamiltonian is given by

$$\mathscr{H} = -\frac{1}{2} \sum_{j=1}^{N} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z) \tag{1.1}$$

[1] Institute for Solid State Physics, University of Tokyo, 7-22-1 Roppongi Minato-ku, Tokyo 106, Japan; e-mail: morita@kodama.issp.u-tokyo.ac.jp.
[2] Department of Physics, Gakushuin University, Mejiro, Toshima-ku, Tokyo 171, Japan; e-mail: koma@riron.gakushuin.ac.jp.

0022-4715/97/0800-0745$12.50/0

with periodic boundary conditions

$$\sigma_{N+1}^{k}=\sigma_{1}^{k} \qquad \text{for} \quad k=x, y, z \tag{1.2}$$

where $\sigma_j^k(k=x, y, z)$ are the Pauli matrices acting at site j. The Heisenberg chain (the spin-1/2 XXZ chain with an isotropic coupling $\Delta=1$) is the first model treated by the Bethe's famous hypothesis i.e., the Bethe Ansatz (BA).[1] Thereby an eigenvalue problem of the Hamiltonian is reduced to solving the so-called Bethe-Ansatz equations (BAEs). Later the method was extended to the spin-1/2 XXZ chain with an anisotropic coupling ($|\Delta| \neq 1$).[2] Many unsolved problems, however, still remain in the BA method. Among them, the string hypothesis[1,3] may be most notorious, which assumes that complex solutions of the BAEs take special forms. The physical meaning of the complex solution is that the corresponding energy eigenstate includes "bound states of magnons". In fact, several authors[4] found evidence that the picture based on the string hypothesis fails. In particular, Vladimirov[5] obtained explicit solutions of the BAEs which substantially disagree with the string hypothesis in the two-magnon sector of the Heisenberg chain. The "non-string states" obtained by Vladimirov exhibit a somewhat strange behavior which is inbetween those of scattering states and bound states.[6] The nature of such solutions has not yet been revealed.

In this paper, we focus on the two-magnon Bethe states in the spin-1/2 XXZ chain including the non-string states. We characterize all these states by a "function"[3] $f(\alpha)$ in the scaling analysis (the multifractal analysis).[7] It turns out that the non-string states contain "quasi-bound" states, which are neither extended nor localized in a usual manner. The "quasi-bound" states should be distinguished from critical states which appear in the Harper equation[7] and the Fibonnaci lattice.[8,9] A critical state too is neither extended nor localized. The crucial difference between these two types of states is that, whereas the nature of a critical state is retained in a scaling limit for an infinite volume, the "quasi-bound" state looks as a localized state in the limit. But we stress again that the "quasi-bound" state is definitely characterized with the use of the scaling analysis, and is clearly distinguished from usual extended states and usual localized states.

The present paper is organized as follows. In Section 2, we briefly review the Bethe Ansatz for two magnon states. Section 3 is devoted to usual two-magnon scattering states. In Section 4, we treat two-magnon

[3] We should note that $f(\alpha)$ is not necessarily a usual function of α, although the notation $f(\alpha)$ is often used. The right object to be studied is a pair of exponents α and f which characterizes the multifractality of a wavefunction. In the following, we write (α, f) instead of $f(\alpha)$. The precise definition will be given in Section 5.

bound states, which are classified into the so-called string states and the non-string states. In order to get explicit forms of typical non-string states, we study large-N behavior of solutions of the BAEs. The non-string states thus obtained are characterized by a set of pairs (α, f) of exponents with the use of the scaling analysis in Section 5. In Appendix A, we count the number of all the two-magnon bound states including the non-string states. Appendix B is devoted to a proof of Theorem 5 which gives a mathematical foundation of a numerical multifractal analysis of wavefunctions.

2. BETHE ANSATZ FOR TWO MAGNONS

We begin with a brief review of the Bethe Ansatz (BA) for two magnons. By using the BA method, the eigenvalue problem of the spin-1/2 *XXZ* Hamiltonian (1.1) is reduced to solving a set of algebraic equations called the Bethe-Ansatz equations (BAEs). Some of the solutions of the BAEs must be obtained by a delicate limiting procedure.[4] For treating this problem, it is convenient to impose twisted boundary conditions[11,12] instead of the periodic boundary conditions (1.2) as follows:

$$\mathscr{H}^{(\varepsilon)} = -\frac{1}{2} \sum_{j=1}^{N-1} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z) \\ -\frac{1}{2} \Delta \sigma_N^z \sigma_1^z - e^{i\varepsilon} \sigma_N^+ \sigma_1^- - e^{-i\varepsilon} \sigma_N^- \sigma_1^+ \tag{2.1}$$

where $\sigma_j^{\pm} = (\sigma_j^x \pm i\sigma_j^y)/2$, and ε is a small positive parameter.[5] Clearly, in the limit $\varepsilon \downarrow 0$, we recover the Hamiltonian (1.1) with the periodic boundary conditions (1.2).

We focus on the two-magnon states given by linear combinations of the base vectors

$$|y_1, y_2\rangle = \sigma_{y_1}^- \sigma_{y_2}^- \,|\uparrow \cdots \uparrow\rangle \tag{2.2}$$

for $1 \leqslant y_1 < y_2 \leqslant N$, where $|\uparrow \cdots \uparrow\rangle$ stands for the state with all the spins up. The Bethe states are given by

$$\Phi(z_1, z_2) = \sum_{1 \leqslant y_1 < y_2 \leqslant N} \phi(z_1, z_2; y_1, y_2)\,|y_1, y_2\rangle \tag{2.3}$$

with

$$\phi(z_1, z_2; y_1, y_2) = z_1^{y_1} z_2^{y_2} + A(z_1, z_2)\, z_2^{y_1} z_1^{y_2} \tag{2.4}$$

[4] See Remark 6 at the end of Appendix A, and refs. 1, 10, and 11.

[5] Our results about "quasi-bound" states are valid also for $\varepsilon = 0$.

and with the two-magnon scattering amplitude

$$A(z_1, z_2) = -\frac{z_1 z_2 - 2\Delta z_2 + 1}{z_1 z_2 - 2\Delta z_1 + 1} \tag{2.5}$$

The complex numbers z_1 and z_2 are determined by the BAEs

$$z_1^N e^{i\varepsilon} = -\frac{z_1 z_2 - 2\Delta z_1 + 1}{z_1 z_2 - 2\Delta z_2 + 1} \tag{2.6}$$

$$z_2^N e^{i\varepsilon} = -\frac{z_1 z_2 - 2\Delta z_2 + 1}{z_1 z_2 - 2\Delta z_1 + 1} \tag{2.7}$$

The energy eigenvalue is given by

$$E = -(\tfrac{1}{2}N - 4)\,\Delta - z_1 - z_1^{-1} - z_2 - z_2^{-1} \tag{2.8}$$

The completeness of the two-magnon Bethe states (2.3) was proved in ref. 11.

Since the Bethe state (2.3) satisfies $\Phi(z_2, z_1) = A(z_2, z_1)\,\Phi(z_1, z_2)$, we can take $|z_1| \geqslant |z_2|$ without loss of generality. From (2.6) and (2.7), one has

$$z_1 z_2 = e^{i2\pi n/N} e^{-2i\varepsilon/N} \tag{2.9}$$

with $n = 0, 1,..., (N-1)$. Therefore we can classify all the roots of the BAEs for finite N as

$$\text{type I:} \quad |z_1| = |z_2| = 1 \tag{2.10}$$

$$\text{type II:} \quad |z_1| > 1 > |z_2| \tag{2.11}$$

3. TYPE-I STATES: SCATTERING STATES

Let us consider the type-I roots, which lead to two-magnon scattering states. The complex numbers z_1 and z_2 of type I can be written

$$z_1 = e^{ik_1}, \qquad z_2 = e^{ik_2} \tag{3.1}$$

in terms of real quasi-wavenumbers k_1 and k_2. The scattering amplitude (2.5) can be written

$$A(z_1, z_2) = -\frac{\cos(K/2) - \Delta e^{ik/2}}{\cos(K/2) - \Delta e^{-ik/2}} = -e^{-2i\delta} \tag{3.2}$$

where $K=(k_2+k_1)$ and $k=(k_2-k_1)$, and δ is the phase shift, which is real. By substituting (3.1) and (3.2) into (2.4), we have

$$\begin{aligned}\phi(y_1, y_2; z_1, z_2) &= e^{iK(y_1+y_2)/2} e^{ik(y_2-y_1)/2} - e^{-2i\delta} e^{iK(y_1+y_2)/2} e^{-ik(y_2-y_1)/2} \\ &= 2ie^{-i\delta} e^{iK(y_1+y_2)/2} \sin[k(y_2-y_1)/2+\delta] \qquad (3.3)\end{aligned}$$

Clearly this state is a scattering state of two magnons. We define the wavefunction of the scattering state by

$$\psi_s(y) = \sin[ky/2+\delta] \qquad (3.4)$$

for $1 \leqslant y < N$.

As is well known, all the roots of the BAEs for the XY model with $\Delta=0$ are of type-I. In fact, we get $|z_1|=|z_2|$ from the BAEs (2.6) and (2.7) with $\Delta=0$. More generally all the energy eigenstates are scattering states. This is a consequence of the equivalence between the XY chain and a one-dimensional free fermion model.

Let us give concrete examples of the type-I roots, which we will use for a demonstration in Section 5. Take $\varepsilon=0$, $\Delta=1$ and $N=4m+1$ with $m=1, 2,\ldots$. Then we get the solution

$$(z_1, z_2) = (-\exp[-i\pi\ell/(2m)], -\exp[i\pi\ell/(2m)]) \qquad (3.5)$$

where ℓ is an integer. The corresponding wavefunction is

$$\psi_s(y) = \sin\left[\frac{\pi\ell}{2m}y - \frac{\pi\ell}{4m}\right] \qquad (3.6)$$

To show this, we introduce the so-called rapidities

$$\lambda_j = \cot(k_j/2) \qquad \text{for} \quad j=1, 2 \qquad (3.7)$$

Then the BAEs (2.6) and (2.7) are written

$$\left(\frac{\lambda_1+i}{\lambda_i}\right)^N = \frac{\lambda_1-\lambda_2+2i}{\lambda_1-\lambda_2-2i} \qquad (3.8)$$

$$\left(\frac{\lambda_2+i}{\lambda_2-i}\right)^N = \frac{\lambda_2-\lambda_1+2i}{\lambda_2-\lambda_1-2i} \qquad (3.9)$$

By taking logarithm, we have

$$2N\arctan(\lambda_1) = 2\pi I_1 + 2\arctan[(\lambda_1-\lambda_2)/2] \qquad (3.10)$$

$$2N\arctan(\lambda_2) = 2\pi I_2 + 2\arctan[(\lambda_2-\lambda_1)/2] \qquad (3.11)$$

with integers I_1 and I_2. We choose $I_1 = -I_2 = \ell$. Then we can take $\lambda_1 = -\lambda_2 = \lambda$. As a result, the equations (3.10) and (3.11) become

$$2N \arctan(\lambda) = 2\pi\ell + 2 \arctan(\lambda) \tag{3.12}$$

Consequently we get the solutions $\lambda = \tan[\pi\ell/(N-1)]$, which are identical to the desired solutions (3.5), with (3.1) and (3.7).

4. TYPE-II STATES: BOUND STATES

Next we consider the type-II roots of the BAEs, which lead to two-magnon bound states. These states are further classified into the so-called "string states", and "non-string states". The latter contains "quasi-bound" states, and "quasi-scattering" states, which are of main interest in the present paper. The following lemma is useful for studying these type-II states.

Lemma 1. A root (z_1, z_2) satisfying the type-II condition $|z_1| > 1 > |z_2|$ can be expressed as $(z_1, z_2) = (\exp[iu + v], \exp[iu - v])$ in terms of $v > 0$ and $u = (\pi r - \varepsilon)/N(r = 0, 1,..., (2N-1))$.

Proof. From (2.9), we can set $z_1 = \exp[iu_1 + v]$ and $z_2 = \exp[iu_2 - v]$ with $v > 0$ and $u_1 \in [0, 2\pi)$, $u_2 \in [0, 2\pi)$. The energy (2.8) must be real and $\mathrm{Im}(z_1 + z_1^{-1} + z_2 + z_2^{-1}) = 0$. Combining this with the above parametrization, we get $\sin u_1 = \sin u_2$. This implies $u_1 = u_2 = u$, $u_1 + u_2 = \pi$ or $u_1 + u_2 = 3\pi$. But, from (2.9), $z_1 z_2 \neq -1$ for a small ε, and we have $u_1 = u_2 = u$. Further, combining this with (2.9), we obtain the desired result $u = (\pi r - \varepsilon)/N(r = 0, 1,..., 2N-1)$. ∎

Note that for a type-II root (z_1, z_2), we get

$$\frac{z_1 z_2 - 2\Delta z_2 + 1}{z_1 z_2 - 2\Delta z_1 + 1} = \mp e^{-Nv} \tag{4.1}$$

by using Lemma 1 for the left-hand side of the BAE (2.7). Here the signs $\mp$ correspond to $r =$ even and odd in Lemma 1, respectively. Substitute (4.1) into (2.4) with (2.5), then we get

$$\begin{aligned}\phi(y_1, y_2; z_1, z_2) &= [e^{iu(y_1+y_2)} e^{-v(y_2-y_1)} \pm e^{-Nv} e^{iu(y_1+y_2)} e^{v(y_2-y_1)}] \\ &= 2e^{-Nv/2} e^{iu(y_1+y_2)} \times \begin{cases} \cosh v\left[\dfrac{N}{2} - (y_2 - y_1)\right] \\ \sinh v\left[\dfrac{N}{2} - (y_2 - y_1)\right] \end{cases}\end{aligned} \tag{4.2}$$

These states are nothing but the bound states obtained approximately by Bethe.[1] We define the wavefunction of the bound state by

$$\psi_{\rm b}(y) = 2e^{-Nv/2} \times \begin{cases} \cosh v \left[\dfrac{N}{2} - y\right] & \text{for} \quad r = \text{even} \\ \sinh v \left[\dfrac{N}{2} - y\right] & \text{for} \quad r = \text{odd} \end{cases} \tag{4.3}$$

and for $1 \leqslant y \leqslant N/2$. Here we have restricted the range of y to half of the whole range, because the wavefunctions (4.3) are symmetric or antisymmetric under the reflection $y \to y' = N - y$. All the wavefunctions decay exponentially as $\psi_{\rm b}(y) \sim e^{-vy}$ for large distances $y \leqslant N/2$ between two magnons under the following assumption.

Standard Assumption 2. The parameter v for the type-II roots is bounded from below by a positive constant v_0 which is independent of the number of the sites N.

Under this assumption, one gets the well-known string solutions (4.6) below for two-magnon bound states.[1, 3] The assumption, however, does not necessarily hold as Vladimirov[5] pointed out. In this paper, we do not assume the above Standard Assumption 2.

4.1. String States

We briefly review the relation between Standard Assumption 2 and the string hypothesis.[1, 3] For simplicity, we treat only the case with $\Delta = 1$.

Consider a type-II root $(z_1, z_2) = (e^{iu+v}, e^{iu-v})$. Clearly $z_1 = (z_2^*)^{-1}$ holds. Combining this with the representation

$$z_j = \frac{\lambda_j + i}{\lambda_j - i} \tag{4.4}$$

in terms of the rapidities $\lambda_j (j = 1, 2)$, we have

$$\lambda_1 = \lambda_2^* \tag{4.5}$$

On the other hand, under Standard Assumption 2 and with (4.1), we have[6] $z_1 z_2 - 2z_2 + 1 = O(e^{-cN})$ with a positive constant c which is independent of

[6] Below we use the symbol O for expressing the order of a number.

the number of the sites N. This can be written as $\lambda_1 - \lambda_2 - 2i = O(e^{-cN})$. From this and (4.5), we have

$$\lambda_1 = \lambda' + i + O(e^{-cN}), \qquad \lambda_2 = \lambda' - i + O(e^{-cN}) \tag{4.6}$$

where λ' is a real number. This is nothing but the string hypothesis for the two-magnon Bethe states. Thus we have the string solutions (4.6) under Standard Assumption 2.

Theorem 3. Let $|\Delta| > 1$. Then all the type-II roots (2.11) are of the string form (4.6).

Proof. BAEs (2.6) and (2.7) for type-II roots (2.11) can be written

$$\Delta^{-1} \cos u = \frac{e^{(N-1)v} \pm e^{v}}{e^{Nv} \pm 1} \tag{4.7}$$

in terms of the parameters u and in Lemma 1, where the signs $\pm$ correspond to $r =$ even, and odd, respectively. For the right-hand side, one can easily get the bounds

$$e^{-v} \leqslant \frac{e^{(N-1)v} + e^{v}}{e^{Nv} + 1} \leqslant 1 \tag{4.8}$$

and

$$e^{-v} - \frac{2}{N} \leqslant \frac{e^{(N-1)v} - e^{v}}{e^{Nv} - 1} \leqslant e^{-v} \tag{4.9}$$

Therefore, if $v \to 0$ as $N \to \infty$, then the right-hand side of (4.7) tends to one. But, for the left-hand side of (4.7), we have $|\Delta^{-1} \cos u| < 1$ from the assumption $|\Delta| > 1$. This implies that Standard Assumption 2 holds. As we showed in the above, Standard Assumption 2 leads to the string form (4.6). ∎

4.2. Non-String States

Consider the case where some type-II solutions do not satisfy Standard Assumption 2. In general one cannot distinguish a bound state from scattering states for a finite system. Because of a similar reason, one cannot distinguish a non-string state from string states for a finite N. In the following, we consider only a large-N behavior of solutions (u, v) of (4.7).

Table I. The Large-*N* Behavior of the Solutions (u, v) of (4.7) for the Non-string Bound States[a]

	Δ	u	range of γ
(i)	$\Delta = 1$	$\sim bN^{-\gamma/2}$	$0 < \gamma < 1$
(ii)	$0 < \Delta < 1$	$\sim \arccos \Delta + b'N^{-\gamma}$	$0 < \gamma < 1$
(iii-a) ($r = \text{even}$)	$\Delta = 1$	$\sim bN^{-(\gamma - 1/2)}$	$1 < \gamma \leqslant 3/2$
(iii-b) ($r = \text{even}$)	$\Delta = 1$	$\sim bN^{-1/2}$	$\gamma = 1$
(iv-a) ($r = \text{odd}$)	$\Delta = 1$	$\sim 2N^{-1/2} + b'N^{-2(\gamma - 3/4)}$	$1 < \gamma \leqslant 5/4$
(iv-b) ($r = \text{odd}$)	$\Delta = 1$	$\sim bN^{-1/2}$	$\gamma = 1$
(v)	$0 < \Delta < 1$	$\sim \arccos \Delta + b'N^{-1}$	$\gamma = 1$

[a] We express $v \sim aN^{-\gamma}$ in terms of γ with a positive constant a. The classification is the same as in Section 4.2. b and b' are constants.

From Lemma 1, the parameter u takes an order between $O(1/N)$ and $O(1)$. For a given order of u, the corresponding order of v is determined by (4.7). Then, if $v \to O$ as $N \to \infty$, we call such pairs (u, v) of solutions as "non-string solutions," and the corresponding Bethe states as "non-string states". Moreover we restrict u to those having asymptotic forms[7] $u \sim bN^{-\beta}$, where b is a real constant, and $\beta \in [0, 1]$. Of course, there exists a different type of asymptotic forms, such as $u \sim bN^{-\beta} \log N$. But such corrections to the power law *do not* affect results of the scaling analysis as we will show in Section 5.2.1. Thus the scaling property of all the non-string states are represented by those of the solutions (u, v) with the power law.

From the well-known results[8] for the XY model ($\Delta = 0$) and Theorem 3, non-string solutions appear only in the cases with $0 < |\Delta| \leqslant 1$. In addition we have only to consider the cases with a positive Δ because the left-hand side of (4.7) changes the sign as $-\Delta^{-1} \cos u'$ under the transformation $u = \pi + u' = \pi + (\pi r' - \varepsilon)/N$ with $r' = 0, 1,..., (2N-1)$. Thus we will consider only the cases with $0 < \Delta \leqslant 1$. The existence of the non-string solutions gives a caution to the string hypothesis. The non-string states can be further classified into the two types of classes, "quasi-bound" and "quasi-scattering" states as we shall show below. All the results in this section are summarized in Table I.

[7] Below we use the symbol $\sim$ for expressing an asymptotic behavior.
[8] See Section 3.

4.2.1. "Quasi-Bound" States. Consider non-string solutions (u, v) satisfying the conditions $v \to 0$ and $Nv \to \infty$ as $N \to \infty$. Then the corresponding wavefunction (4.3) becomes

$$\psi_{\text{qb}}(y) \sim e^{-vy} \tag{4.10}$$

for a large N, and $1 \leqslant y \leqslant N/2$. When we restrict u to those with $u \sim bN^{-\beta}$ as mentioned above, all the corresponding solutions v can be expressed as $v \sim aN^{-\gamma}$ with a positive constant a and $\gamma \in (0, 1)$ as we will show below. Then the wavefunction (4.10) is extended over a range y less than or equal to the order of N^{γ}. But the wavefunction decays rapidly in the outside of the range. Thus the wavefunction is *unnormalizable* in the thermodynamic limit $N \to \infty$, but it is *not extended over the whole range*. In this sense, we say that the wavefunction is a "quasi-bound state".

Let us obtain these typical "quasi-bound" solutions which give the complete list of the scaling indices α and f for all the quasi-bound states. For this purpose we divide the range of Δ into the following two cases; (i) $\Delta = 1$, and (ii) $0 < \Delta < 1$.

Case (i): $\Delta = 1$. The left-hand side of (4.7) can be expanded as

$$\cos u \sim 1 - \tfrac{1}{2} u^2 \tag{4.11}$$

because u must satisfy the condition that $u \to 0$ as $N \to \infty$, which can be seen in the proof of Theorem 3.

On the other hand, the right-hand side of (4.7) can be expanded as[9]

$$\frac{e^{(N-1)v} \pm e^{v}}{e^{Nv} \pm 1} \cong e^{-v} \sim 1 - v \tag{4.12}$$

from the assumption $Nv \to \infty$ as $N \to \infty$. Combining this with (4.11), we have $v \sim u^2/2$. Therefore we get $v \sim aN^{-\gamma}$ and $u \sim bN^{-\gamma/2}$ with $\gamma \in (0, 1)$ from the assumptions that $v \to 0$ and $Nv \to \infty$ as $N \to \infty$.

Case (ii): $0 < \Delta < 1$. We write u in Lemma 1 as $u = u_0 + u_1$, where

$$u_0 = \frac{\pi r_0 - \varepsilon}{N} + \delta u, \quad \text{and} \quad u_1 = \frac{\pi r_1}{N} - \delta u \tag{4.13}$$

Here r_0 and r_1 are integers, and we choose r_0 and δu such that $\Delta^{-1} \cos u_0 = 1$ and $\delta u = O(1/N)$. As in the above Case (i), u_1 must satisfy

[9] Below we use the symbol $\cong$ when an expression is an approximation, but gives a correct asymptotic behavior.

the condition $\lim_{N\to\infty} u_1 = 0$. Then the left-hand side of (4.7) can be expanded as

$$\Delta^{-1}\cos u = \Delta^{-1}(\cos u_0 \cos u_1 - \sin u_0 \sin u_1) \sin 1 - \frac{\sqrt{1-\Delta^2}}{\Delta} u_1 \qquad (4.14)$$

Therefore we have $v \sim \sqrt{\Delta^{-2}-1}\, u_1 = \sqrt{\Delta^{-2}-1}(u - \arccos \Delta)$ in the same way as in the case (i) above. Since we can assume $u_1 \sim b'N^{-\beta}$ with a real constant b' and $\beta \in [0, 1]$ as well as u, we obtain $v \sim aN^{-\gamma}$ and $u \sim \arccos \Delta + b'N^{-\gamma}$ with $\gamma \in (0, 1)$.

In both of the above two cases we obtain $v \sim aN^{-\gamma}$ with $\gamma \in (0, 1)$ and a positive constant a, although u has the different ranges of the orders.

4.2.2. "Quasi-Scattering" States. Next we consider solutions (u, v) satisfying $Nv \to 0$ as $N \to \infty$ or $v \sim aN^{-1}$ with a positive constant a. The corresponding states are classified into four types of states (4.15), (4.18), (4.21), and (4.26) below. Although all of these states are extended in the usual sense, we call them "quasi-scattering" states to distinguish them from the usual two-magnon scattering states (3.4). In order to get all these quasi-scattering states, we divide the present case into the following five cases; (iii-a), (iii-b), (iv-a), (iv-b), and (v). Here the cases iii) and (iv) are devoted to $\Delta = 1$, and (v) to $0 < \Delta < 1$. The difference between (iii) and (iv) is due to r = even and odd. We further have subdivided the cases (iii) and (iv) into the two cases (a) and (b), by using a difference between asymptotic behaviors of v. These five cases yield the complete list of all the quasi-scattering states.

Case (iii-a): $\Delta = 1$ and r = even. Consider first the case that $Nv \to 0$ as $N \to \infty$. Clearly the corresponding wavefunction (4.3) becomes

$$\psi_{\text{qs}}(y) \sim 2 \qquad (4.15)$$

for a large N, and $1 \leqslant y \leqslant N/2$. Thus the wavefunction becomes homogeneous in the large-N limit.

Next consider the equation (4.7) with r even. For the right-hand side, we use a large-N expansion as

$$\frac{e^{(N-1)v} + e^{v}}{e^{Nv}+1} = e^{-v} + \frac{e^{v} - e^{-v}}{e^{Nv}+1}$$

$$\sim 1 - v + v\left(1 - \frac{1}{2}Nv\right) = 1 - \frac{1}{2}Nv^2 \qquad (4.16)$$

Combining this with the expansion (4.11) for the left-hand side, we get $v \sim N^{-1/2}u$. Assuming $u \sim bN^{-\beta}$ with $\beta \in [0, 1]$, we obtain $v \sim aN^{-\gamma}$ and $u \sim bN^{-(\gamma-1/2)}$ with $\gamma \in (1, 3/2]$. For $\gamma \in [1/2, 1]$, there is no solution v ratifying $Nv \to 0$ as $N \to \infty$.

Case (iii-b): $\Delta = 1$ and $r =$ even. Next we consider the case that $v \sim aN^{-1}$. Then the corresponding wavefunction (4.3) becomes

$$\psi_{qs}(y) \sim 2e^{-a/2} \times \cosh\{aN^{-1}[(N/2) - y]\} \tag{4.17}$$

$$= 2e^{-a/2} \times \cosh[a(1-x)/2] \tag{4.18}$$

for a large N, and $1 \leqslant y \leqslant N/2$. Here $x = 2y/N \in [0, 1]$ for a large N. This wavefunction is also extended over the whole range.

To show this, it is sufficient to prove that there exists a corresponding solution u of (4.7) with r even. For this purpose we expand the right-hand side of (4.7) with r even as

$$\begin{aligned} \frac{c^{(N-1)v} + e^{v}}{e^{Nv} + 1} &= e^{-v} + \frac{e^{v} - e^{-v}}{e^{Nv} + 1} \\ &\cong 1 - v + \frac{2v}{e^{a} + 1} \\ &= 1 - v \times \tanh(a/2) \end{aligned} \tag{4.19}$$

Thus we can find a solution $u \sim bN^{-1/2}$ from the expansion (4.11) for a small u.

Case (iv-a): $\Delta = 1$ and $r =$ odd. Consider first the case that $Nv \to 0$ as $N \to \infty$. Then the corresponding wavefunction (4.3) becomes

$$\psi_{qs}(y) = 2e^{-Nv/2} \times \sinh\{v[(N/2) - y]\} \tag{4.20}$$

$$\cong 2v[N/2 - y] = Nv(1-x) \tag{4.21}$$

for a large N, and $1 \leqslant y \leqslant N/2$. Here $x = 2y/N \in [0, 1]$ for a large N. Although this wavefunction is extended over the whole range, it exhibits the strange behavior for large y.

Consider the equation (4.7) with r odd to find the corresponding solutions (u, v) to the result (4.21). Note that

$$\begin{aligned} \frac{e^{(N-1)v} - e^{v}}{e^{Nv} - 1} &= e^{-v} - \frac{e^{v} - e^{-v}}{e^{Nv} - 1} \cong 1 - v - \frac{2v}{Nv + N^2v^2/2 + N^3v^3/6} \\ &\sim 1 - v - \frac{2}{N}\left(1 - \frac{1}{2}Nv + \frac{1}{12}N^2v^2\right) = 1 - \frac{2}{N} - \frac{1}{6}nv^2 \end{aligned} \tag{4.22}$$

for the right-hand side of (4.7) with r odd. For the left-hand side of (4.7), we recall the expression $u = u_0 + u_1$ with

$$u_0 = \frac{\pi r_0 - \varepsilon}{N} + \delta u \qquad \text{and} \qquad u_1 = \frac{\pi r_1}{N} - \delta u \tag{4.23}$$

We choose r_0 and δu such that $\cos u_0 = 1 - 2/N$ and $\delta u = O(1/N)$. Then the left-hand side of (4.7) with $\Delta = 1$ can be expanded as

$$\begin{aligned} \cos u &= \cos u_0 \cos u_1 - \sin u_0 \sin u_1 \\ &\cong \left(1 - \frac{2}{N}\right)\left(1 - \frac{1}{2} u_1^2\right) - \frac{2}{\sqrt{N}} u_1 \\ &\sim 1 - \frac{2}{N} - \frac{2}{\sqrt{N}} u_1 - \frac{1}{2u_1^2} \end{aligned} \tag{4.24}$$

for a small u_1. From (4.22) and (4.24), we have

$$\frac{1}{6} Nv^2 \sim \frac{2}{\sqrt{N}} u_1 + \frac{1}{2} u_1^2 \tag{4.25}$$

Similar to Case (ii), we can assume $u_1 \sim b'N^{-\beta}$ with $\beta \in [0, 1]$. Combining this with (4.25), we obtain $v \sin aN^{-\gamma}$ and $u \sin 2N^{-1/2} + b'N^{-2(\gamma - 3/4)}$ with $\gamma \in (1, 5/4]$. For $\gamma \in [3/4, 1]$, there is no solution satisfying $Nv \to 0$ as $N \to \infty$.

Case (iv-b): $\Delta = 1$ and $r = \text{odd}$. Next we consider the case with $v \sim aN^{-1}$. Clearly the corresponding wavefunction (4.3) becomes

$$\begin{aligned} \psi_{\text{qs}}(y) &\sim 2e^{-a/2} \times \sinh\{aN^{-1}[(N/2) - y]\} \\ &= 2e^{-a/2} \times \sinh[a(1 - x)/2] \end{aligned} \tag{4.26}$$

for a large N, and $1 \leqslant y \leqslant N/2$. Here $x = 2y/N \in [0, 1]$ for a large N. This wavefunction is also extended over the whole range.

Similar to Case (iii-b), it is sufficient to show that there exists a corresponding solution u. We expand the right-hand side of (4.7) with r odd as

$$\begin{aligned} \frac{e^{(N-1)v} - e^{v}}{e^{Nv} - 1} &= e^{-v} - \frac{e^{v} - e^{-v}}{e^{Nv} - 1} \\ &\cong 1 - v - \frac{2v}{e^{a} - 1} \\ &= 1 - v \times \coth(a/2) \end{aligned} \tag{4.27}$$

Thus we can find a solution $u \sim bN^{-1/2}$ from the expansion (4.11) for a small u.

Case (v): $0 < \Delta < 1$ and $r =$ even, or odd. In the same way as in Case (ii), one can easily show that there appears only one type of solutions $v \sin aN^{-1}$ and $u \sin \arccos \Delta + b'N^{-1}$. Therefore the corresponding wavefunctions are (4.18), and (4.26) for $r =$ even, and odd, respectively.

Consequently we obtained all the typical non-string states which give the complete list of all the scaling indices α and f for all the non-string states.

5. SCALING ANALYSIS FOR THE WAVEFUNCTIONS

Let us characterize the Bethe states by using the scaling analysis (the multifractal analysis).[7, 13] Our main interest in this section is how the non-string states, in particular, the quasi-bound states, are distinguished from other usual scattering and usual bound states (string states). We begin with a brief review of the scaling analysis for wavefunctions.

5.1. GENERAL CONSIDERATIONS

Usually *infinite-volume* states are classified into localized, extended and critical states. Whereas localized states are normalizable, both extended and critical states are not. The corresponding energy spectra are, respectively, point-like, absolutely continuous, and singular continuous.[14] The scaling analysis is a very powerful method to characterize a wavefunction. Actually the method has been proved to be very successful in the elucidation of wavefunction structures and spectral properties in one-dimensional quasi-periodic systems.[7] In the language of the scaling analysis, the above three types of states are distinguished clearly by the set $\{(\alpha, f)\}$ of pairs of the scaling indices α and f, which we will introduce in this section. In the present context, we focus on the question how the wavefunctions of the spin-1/2 XXZ chain are classified by the scaling analysis.

Consider a wavefunction defined on a one-dimensional lattice Λ with a periodic boundary condition. We take a scaling limit of a sequence of the lattices $\{\Lambda_n\}$ so that the wavefunctions we consider are defined on a continuous interval $[0, 1]$ in the limit $n \to \infty$. In the nth step of the scaling, the system is periodic with a period $N_n = |\Lambda_n|$. Consider a probability measure

$$p_i = |\psi_i|^2 \tag{5.1}$$

for a wavefunction ψ_i at site $i \in \Lambda_n$, and with a normalization

$$\sum_{i=1}^{N_n} p_i = \sum_{i=1}^{N_n} |\psi_i|^2 = 1 \tag{5.2}$$

Assign a uniform Lebesgue measure $l_n = N_n^{-1}$ to all the sites in the lattice Λ_n. Then the whole Lebesgue measure of the system Λ_n is normalized to unity. In the limit $n \to \infty$, the probability measure is defined on the interval [0, 1], and one can discuss its singularities and scaling properties.

For an example, see Fig. 1 where a probability measure p_i for a normalized wavefunction is shown in each step of the scaling.[10] Let us fix a sequence of lattice sizes N_n by the relation $N_n = e^{n\varepsilon_n}$ for $n = 1, 2, 3, \ldots$. Then the Lebesgue measure l_n can be written in the scaling form

$$l_n = \exp(-n\varepsilon_n) \tag{5.3}$$

where ε_n is usually called scaling index. We take ε_n to be constant in the merical analysis[11] for the Bethe wavefunctions in Section 5.3.

Before introducing our strategy for calculating the indices α and f, we explain a standard strategy, although the standard one is not well-defined and not useful for a numerical analysis. Let us define the scaling index α_i by

$$p_i = l_n^{\alpha_i} \tag{5.4}$$

Further we define by $\Omega_n(\alpha)\, d\alpha$ the number of sites having index $\alpha_i \in [\alpha, \alpha + d\alpha)$ with a small positive $d\alpha$. Then one can expect that there exist an index $f(\alpha)$ and a measure $\rho(\alpha)$ such that

$$\Omega_n(\alpha) \cong l_n^{-f(\alpha)} \rho(\alpha) \tag{5.5}$$

for a sufficiently large system size n. If the measure $\rho(\alpha)$ is non-zero and non-singular, then one can define the entropy function $S(\alpha)$ in the thermodynamic limit as

$$S(\alpha) = \lim_{n \to \infty} \frac{1}{n} \log \Omega_n(\alpha) = \varepsilon f(\alpha) \tag{5.6}$$

Here we have used (5.3), and written $\varepsilon = \lim_{n \to \infty} \varepsilon_n$ under the assumption of the existence of the limit. But we cannot justify the above assumption

[10] See, for details, Section 5.3.

[11] In general ε_n is not necessarily constant [7].

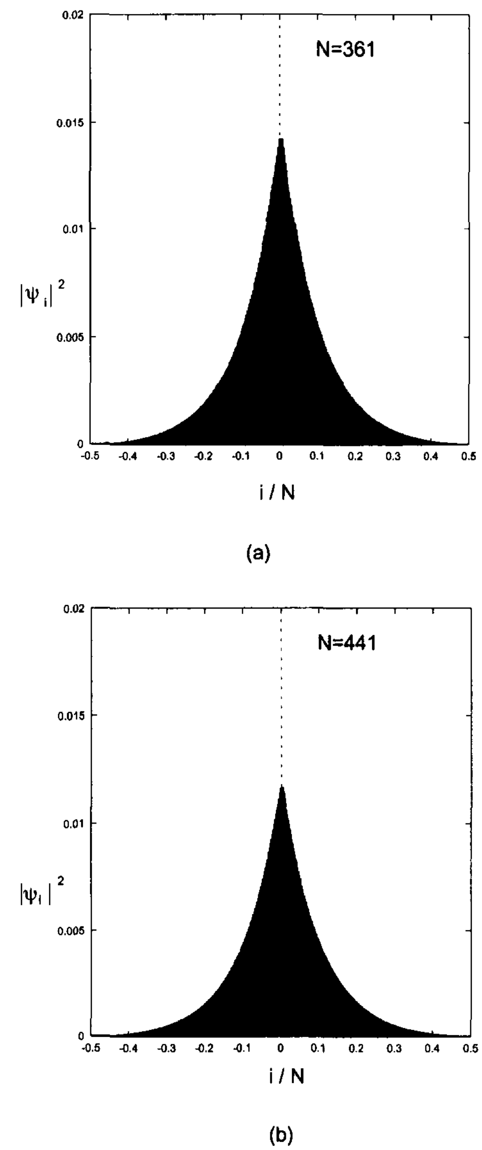
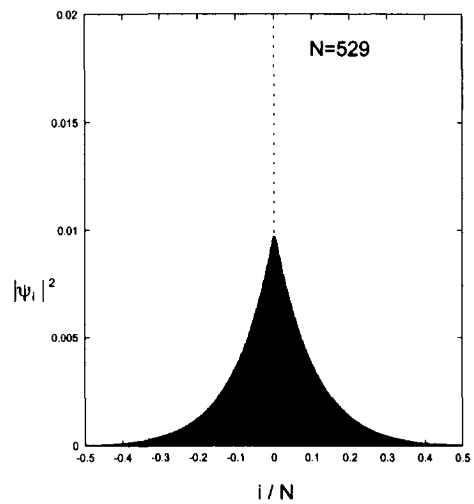
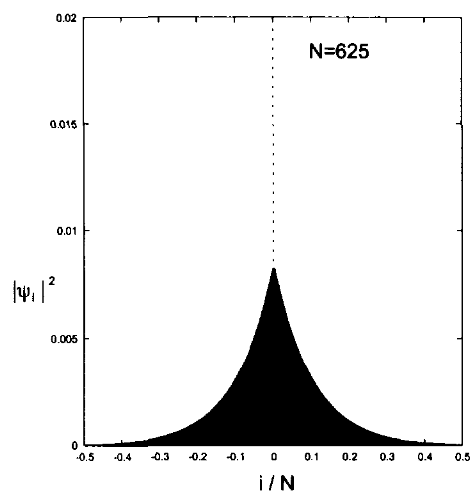


Fig. 1. Probability distribution for the normalized wavefunctions of Example B [(4.26) in Case (iv-b) in Section 4.2].



(c)



(d)

Fig. 1 (*Continued*)

that $\rho(\alpha)$ is non-singular. The simplest counter-example is the homogeneous wavefunction $\psi_i = \text{const.}$ for all the sites i. In fact we have

$$p_i = l_n, \qquad \Omega_n(\alpha) = l_n^{-1}\,\delta(\alpha - 1) \tag{5.7}$$

for the wavefunction, where $\delta(\alpha)$ is the Dirac's delta measure. Thus the formula (5.6) is not necessarily useful for calculating an index $f(\alpha)$.

In order to avoid the difficulty, we introduce an analogue of the thermodynamic formalism in statistical mechanics for many-body systems. The method is more useful for numerically computing scaling indices α and f.

Let us define the "partition function" by

$$Z_n(Q) = \sum_i w_i(q) \tag{5.8}$$

with

$$w_i(q) = p_i^q \tag{5.9}$$

and the free energy[12]

$$G(q) = \lim_{n \to \infty} G_n(q) \tag{5.10}$$

with

$$G_n(q) = \frac{1}{n} \ln Z_n(q) \tag{5.11}$$

We define the index $\alpha = \alpha(q)$ as

$$\alpha(q) = -\frac{1}{\varepsilon}\frac{dG(q)}{dq} \tag{5.12}$$

with $\varepsilon = \lim_{n \to \infty} \varepsilon_n$, and define the entropy $S(q)$ as

$$S(q) = \lim_{n \to \infty} S_n(q) \tag{5.13}$$

[12] The function D_q,[15] which is often used by the authors, is related to our free energy $G(q)$ by $D_q = -G(q)/[\varepsilon(q-1)]$. Since $D_q|_{q=0}$ is equal to the Hausdorff dimension of the space, the D_q is often called the generalized Hausdorff dimension. Of course, the formalism with D_q is equivalent to ours.

with

$$S_n(q) = -\frac{1}{n} \sum_i P_i(q) \log P_i(q) \tag{5.14}$$

where the probability $P_i(q)$ is given by

$$P_i(q) = \frac{1}{Z_n(q)} w_i(q) = \frac{1}{Z_n(q)} \exp[-n\varepsilon_n \alpha_i q] \tag{5.15}$$

The index $f = f(q)$ is defined by

$$f(q) = S(q)\, \varepsilon \tag{5.16}$$

Clearly the index $\alpha(q)$ (5.12) is the expectation of α_i with respect to the "Gibbs measure" at the "temperature" q^{-1}, and $S(q)$ (5.813) is corresponding to the entropy at the "temperature". Thus the indices $\alpha(q)$ and $f(q)$ can be interpreted as smeared indices α and f with "thermal fluctuation". Varying the value of the inverse temperature q, one can get all the pairs $\{(\alpha(q), f(q))\}$ of indices for a given wavefunction ψ. For example, we can get the desired pair $(\alpha, f) = (1, 1)$ for the above homogeneous wavefunction $\psi_i = \text{const.}$ without any difficulty from the definitions (5.12), (5.13) and (5.16).

We should remark the following: One may think that the definition (5.13) of the entropy $S(q)$ is equivalent to

$$S(q) = G(q) + \varepsilon\alpha(q)\, q \tag{5.17}$$

with (5.12). This is *not* true. The second term $\varepsilon\alpha(q)\, q$ in the right-hand side of (5.17) is ill-defined when $\alpha = \infty$ at $q = 0$. In fact we encounter such a situation for the Bethe wavefunctions in the present spin-1/2 *XXZ* chain. We shall discuss this point again in Section 5.2.1. In order to avoid this difficulty, we introduced the definition (5.13) for the entropy $S(q)$. Starting from the definition (5.13), the entropy (5.17) can be *fomally* rederived in the following way:

$$\begin{aligned} S_n(q) &= -\frac{1}{n} \sum_i P_i(q) \log P_i(q) \\ &= \frac{1}{n} \sum_i P_i(q) \log Z_n(q) - \frac{1}{n} \sum_i P_i(q) \log\{\exp[-n\varepsilon_n q \alpha_i]\} \\ &= G_n(q) + \varepsilon_n \left(\sum_i P_i(q)\, \alpha_i \right) \cdot q \end{aligned} \tag{5.18}$$

Thus we *formally* get (5.17) in the limit $n \to \infty$ because we have

$$\frac{d}{dq} G_n(q) = -\varepsilon_n \sum_i P_i(q)\, \alpha_i \tag{5.19}$$

from the definitions of the partition function (5.8) with (5.9), and of the free energy (5.11). But much care has to be taken since there often appears a situation such that[13]

$$q \frac{d}{dq} \lim_{n \to \infty} G_n(q) \neq \lim_{n \to \infty} q \frac{d}{dq} G_n(q) \tag{5.20}$$

A wavefunction is clearly characterized by the set

$$\{(\alpha, f)\} = \{(\alpha(q), f(q)) \mid q \text{ in the whole range}\} \tag{5.21}$$

For example, an extended wavefunction has $\{(\alpha, f)\}$ containing a single point $(\alpha, f) = (1, 1)$, and a localized wavefunction has $\{(\alpha, f)\}$ consisting of two points; $(\alpha, f) = (0, 0)$ and $(\infty, 1)$. For a critical wavefunction, the set $\{(\alpha, f)\}$ forms a smooth curve with a finite range $[\alpha^{\min}, \alpha^{\max}]$ of α in the $\alpha - f$ plane and the maximum value of f is not at $\alpha = 1$. Before applying the scaling analysis to the Bethe wavefunctions of the spin-1/2 *XXZ* chain, we emphasize the following point. The scaling analysis is often applied to a *finite* system, and the set "$\{(\alpha, f)\}$" for a *finite* system is obtained. The result necessarily shows a smooth curve without an extrapolation. But the set $\{(\alpha, f)\}$ in the thermodynamic limit $n \to \infty$ *does not necessarily* gives a smooth curve. Thus one must carefully extrapolate data of finite systems to the infinite volume in order to obtain the set $\{(\alpha, f)\}$ numerically. We will discuss this point again in Section 5.3, where numerical demonstrations are performed in order to clarify the point.

5.2. Scaling Analysis for the Non-String States of Two Magnons

Now we apply the scaling analysis to the non-string states obtained in Section 4.2. The main results are as follows: we obtain that the set $\{(\alpha, f)\}$ for the quasi-bound states (4.10) consists of two points, $(\alpha, f) = (\gamma, \gamma)$ and $(\infty, 1)$, with $\gamma \in (0, 1)$. Clearly the set $\{(\alpha, f)\}$ is different from those for extended and localized wavefunctions. But all the sets $\{(\alpha, f)\}$ for the quasi-scattering states in Section 4.2.2 are the same as that for a usual extended wavefunction as we already expected.

[13] See Remark 4(ii) below.

5.2.1. (α, f) for the Quasi-Bound States. Consider first the quasi-bound states (4.10). In the following, we consider only the leading order for a sufficiently large lattice size N, because one can show that higher orders are all negligible.

Note that

$$\sum_{y=1}^{N/2} |\psi_{\text{qb}}(y)|^2 \cong \sum_{y=1}^{N/2} \exp[-2vy] \sim \frac{1}{2v} \tag{5.22}$$

from (4.10). Since $v \to 0$ as $N \to \infty$ from the definition of the quasi-bound states (4.10), the wavefunction is *unnormalizable in the thermodynamic limit.* The normalized wavefunction is

$$\psi_{\text{qb}}(y) \sim \sqrt{2v}\, e^{-vy} \tag{5.23}$$

The partition function (5.8) is

$$\begin{aligned} Z_n(q) &= \sum_{y=1}^{N_n/2} |\psi_{\text{qb}}(y)|^{2q} \\ &\cong (2v)^q \sum_{y=1}^{N_n/2} e^{-2qvy} = (2v)^q \times \frac{1-e^{-N_n qv}}{e^{2qv}-1} \end{aligned} \tag{5.24}$$

For $q=0$, we have

$$\frac{1}{n} Z_n(q=0) = \frac{1}{n} \log \frac{N_n}{2} \sim \varepsilon \tag{5.25}$$

Here we have used $N_n = e^{n\varepsilon_n}$ and $\varepsilon = \lim_{n\to\infty} \varepsilon_n$. On the other hand, for $q \neq 0$,

$$\frac{1}{n} Z_n(q) \cong \frac{q}{n} \log v - \frac{1}{n} \log v = \frac{q-1}{n} \log v \tag{5.26}$$

From these observations, the free energy is

$$G(q) = \lim_{n\to\infty} \frac{1}{n} \ln Z_n(q) = \begin{cases} \gamma(1-q)\,\varepsilon & \text{for } q>0 \\ \varepsilon & \text{for } q=0 \end{cases} \tag{5.27}$$

where we have used the result $v \sim aN^{-\gamma} \times \{\text{correction}\}$ with a positive constant a and $\gamma \in (0, 1)$ in Section 4.2.1. Here we stress that corrections to the power law $v \sim aN^{-\gamma}$, such as logarithm, do not affect the result of $G(q)$.

Further we have

$$\alpha(q) = -\frac{1}{\varepsilon}\frac{d}{dq}G(q) = \begin{cases} \gamma & \text{for } q>0 \\ \infty & \text{for } q=0 \end{cases} \tag{5.28}$$

where we have defined the derivative at $q=0$ as

$$\left.\frac{d}{dq}G(q)\right|_{q=0} = \lim_{q\downarrow 0}\frac{G(q)-G(0)}{q} \tag{5.29}$$

In a similar way we get

$$\lim_{n\to\infty} q\frac{d}{dq}G_n(q) = \lim_{n\to\infty} q\frac{d}{dq}\frac{1}{n}\ln Z_n(q) = -q\varepsilon\gamma \tag{5.30}$$

Combining this with (5.18) and (5.19), we have

$$S(q) = \lim_{n\to\infty} S_n(q) = \begin{cases} \varepsilon\gamma & \text{for } >0 \\ \varepsilon & \text{for } q=0 \end{cases} \tag{5.31}$$

This implies

$$f(q) = \begin{cases} \gamma & \text{for } q>0 \\ 1 & \text{for } q=0 \end{cases} \tag{5.32}$$

from (5.16). Combining this with (5.28), we conclude that $\{(\alpha, f)\}$ for the quasi-bound states (4.10) with $\gamma\in(0, 1)$ consists of two points, $(\alpha, f) = (\gamma, \gamma)$ and $(\infty, 1)$.

Remark 4. (i) There is no need to consider a negative q because α is a decreasing function of q satisfying[14] $\alpha=\infty$ at $q=0$.

(ii) Clearly, from the result (5.28), the present case is a non-trivial example such that the definition (5.17) of the entropy function is ill-defined. Thus $q=0$ is a singular point, and one must carefully treat it. The discontinuity of the free energy $G(q)$ at $q=0$ leads to $\alpha=\infty$, not $\alpha=\gamma$! from (5.30).

5.2.2. (α, f) for the Quasi-Scattering States. Next consider the quasi-scattering states obtained in Section 4.2.2. One can easily show that the set $\{(\alpha, f)\}$ of the wavefunction (4.15) consists of a single point

[14] But indices α from negative q usually appear for critical states.[7]

$(\alpha, f)=(1, 1)$. As we shall show, the same is true for the other wavefunctions in Section 4.2.2. All the wavefunctions can be written in the form

$$\psi_{\rm qs}(y)=g(y/N) \tag{5.33}$$

in terms of a smooth function g. Note that

$$\sum_{y=1}^{N/2} |\psi_{\rm qs}(y)|^{2s}=\sum_{y=1}^{N/2} |g(y/N)|^{2s} \sim NC_s \tag{5.34}$$

with

$$C_s=\int_0^{1/2} dt\, |g(t)|^{2s} \tag{5.35}$$

Here s is a real number such that the free energy $G(s)$ is well-defined. Hence the normalized wavefunction becomes

$$\psi_{\rm qs}(y)\cong\frac{1}{\sqrt{C_1 N}}\, g(y/N) \tag{5.36}$$

The partition function (5.8) is

$$\begin{aligned} Z_n(q) &= \sum_{y=1}^{N_n/2} |\psi_{\rm qs}(y)|^{2q} \\ &\cong \frac{1}{(C_1 N_n)^q} \sum_{y=1}^{N_n/2} |g(y/N_n)|^{2q} \\ &\sim \frac{1}{(C_1 N_n)^q}\, N_n \int_0^{1/2} dt\, |g(t)|^{2q} \\ &= \frac{C_q}{(C_1)^q} N_n^{1-q} = \frac{C_q}{(C_1)^q} \exp[n\varepsilon_n(1-q)] \end{aligned} \tag{5.37}$$

Then the free energy is

$$G(q)=\lim_{n\to\infty}\frac{1}{n}\ln Z_n(q)=\varepsilon(1-q) \tag{5.38}$$

and

$$\alpha(q)=-\frac{1}{\varepsilon}\frac{d}{dq}G(q)=1 \tag{5.39}$$

Further we have

$$\lim_{n\to\infty} \frac{d}{dq} G_n(q) = \lim_{n\to\infty} \frac{1}{n}\frac{d}{dq} \ln Z_n(q) = -\varepsilon \tag{5.40}$$

where we have used the fact that g defined in (5.33) is a smooth function. Combining this with (5.18) and (5.19), we get the entropy function

$$S(q) = \lim_{n\to\infty} S_n(q) = \varepsilon \tag{5.41}$$

This implies $f(q) = 1$ from (5.16). With (5.39), we have that $\{(\alpha, f)\}$ for the quasi-scattering states consists of a single point $(\alpha, f) = (1, 1)$.

5.3. Scaling Analysis for the Two-Magnon States: Numerical Demonstrations

As shown in Section 5.2, the free energies $G(q)$ (S.27) for the quasi-bound states are singular at $q = 0$. In such a situation, a numerical analysis often yields enormous errors. One must carefully extrapolate data of finite systems to an infinite volume. In this section, we make numerical demonstrations for the two-magnon Bethe states, and compare the numerical results with the exact results in Section 5.2. We consider such a demonstration is instructive and gives useful informations for future studies where quasi-bound state appears but analytic results can not be obtained.

Before proceeding to concrete examples, we explain our numerical method in a general setting. Consider first the index α given by (5.12). But it is very hard to compute numerically the right-hand side of (5.12). In fact, a numerical analysis often yields enormous errors. We take another way. Define

$$\alpha_n(q) = -\frac{1}{\varepsilon_n}\frac{d}{dq} G_n(q) \tag{5.42}$$

Below we fix $\varepsilon_n = \log 2$ for all n. The $\alpha_n(q)$ is a smooth function of q for a finite n. We further define

$$\hat{\alpha}(q) = \lim_{n\to\infty} \alpha_n(q) \tag{5.43}$$

The following theorem is useful for a numerical analysis.

Theorem 5. Suppose the existence of the scaling index $\alpha(q)$ at an interier point q in a range of q. Then the limit $\hat{\alpha}(q)$ of (5.43) exists, and

$$\alpha(q) = -\frac{1}{\varepsilon}\frac{d}{dq}G(q) = \hat{\alpha}(q) \tag{5.44}$$

In Appendix B, we prove the statement of the theorem by using an analogy between the present system and a system for statistical mechanics for many-body systems[16] But such an analogy is not necessarily complete. In fact, the free energies $G(q)$ (5.27) for the quasi-bound states is discontinuous at $q=0$. We further remark that α exists everywhere except for a countable number of points q, because of the convexity of the free energy $G(q)$.[16, 17] In other words, the discontinuities of α form a set of the Lebesgue measure zero on the range of q.

Relying on Theorem 5, we calculate $\alpha(q)$. Namely we first compute $\alpha_n(q)$ (5.42) for finite n, and extrapolate $\alpha_n(q)$ to $\hat{\alpha}(q)$ in the limit $n \to \infty$. We calculate the corresponding values of $f(q)$ as follows. First we compute $f_n(q) = S_n(q)/\varepsilon_n$ for finite systems, where $S_n(q)$ is given by (5.18). The set (α_n, f_n) is always smooth for finite n. By extrapolating $n \to +\infty$, we get (α, f). Our extrapolation method is as follows. Examples of the finite-size effect on (α_n, f_n) can be seen in Fig. 2, where we have plotted the minimum value $\alpha_n^{\min}$ of $\alpha_n(q)$, the corresponding value $f_n^{\min}$ of $f_n(q)$, the maximum value $\alpha_n^{\max}$ of $\alpha_n(q)$, and the corresponding $f_n^{\max}$ of $f_n(q)$ versus $1/n$ for the wavefunction (3.6) with $l/m = 0.9$. Since the finite-size corrections seem to be $O(1/n)$, we determine the extrapolated values by using a least squares fitting the form $a + b/n$ to the data. Here a and b are parameters to be determined.

Having the results in Sections 3 and 4 in mind, we have calculated numerically $\{(\alpha, f)\}$ for the following four examples of wavefunctions. Example A is a type-I wavefunction having (2.10), and Examples B, C and D are type-II wavefunction having (2.11). The data and the results are summarized in Table II. Let us proceed to the details of the four examples.

Example A: Usual Scattering States (Section 3)

For the scattering state (3.4), we treated the wavefunction $\psi_s(y)$ (3.6). We fixed $l/m = 0.9$ so that the corresponding wavenumber k is constant.

Figure 3 shows the probability distribution $|\psi_s(y)|^2$ for the wavefunction. As shown in Fig. 4, the set $\{(\alpha_n, f_n)\}$ for a finite n always gives a smooth curve. As shown in Fig. 5, $\alpha_n(q)$ seems to converge to $\alpha(y) = 1$

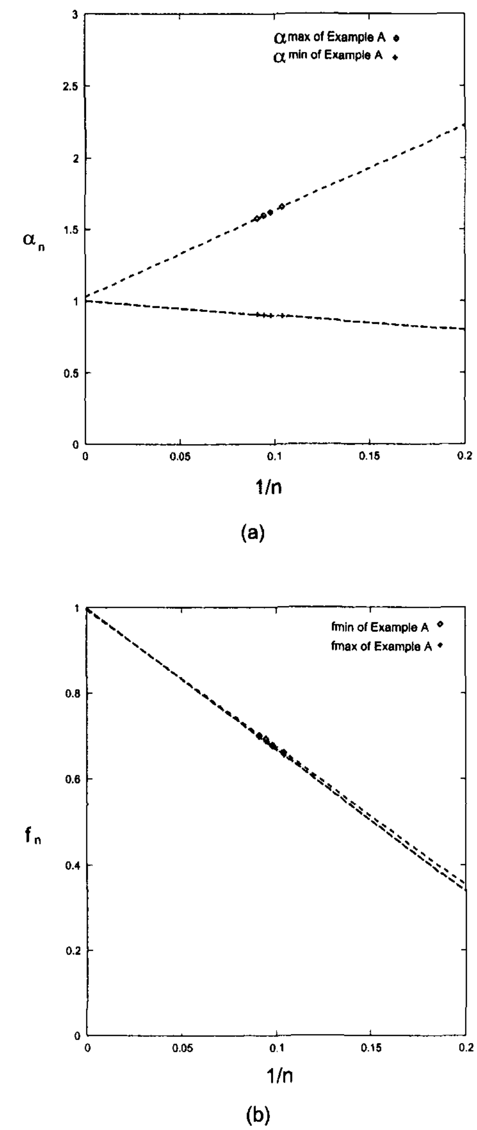


Fig. 2. The minimum value $\alpha_n^{\min}$ of $\alpha_n(q)$, the corresponding value $f_n^{\min}$ of $f_n(q)$, the maximum value $\alpha_n^{\max}$ of $\alpha_n(q)$, and the corresponding $f_n^{\max}$ of $f_n(q)$ versus $1/n$ for the wavefunctions (3.6) with $l/m = 0.9$ (Example A below). $N = 2^n = 401, 801, 1201, 1601$. Straight lines are determined by using a least square fitting.

Table II. The Data and the Numerical Results for the Scaling Properties of the Wavefunctions when $\Delta = 1$

	System size $N = 2^n$	character of wavefunction (α, f)
A: scattering state	401, 801, 1201, 1601	extended
[(3.6) with $l/m = 0.9$]		$(1, 1)$
B: quasi-scattering state	361, 441, 529, 625	extended
[(4.26) in Case (iv-b)]		$(1, 1)$
C: string bound state	365, 445, 525, 605	localized
[(4.3) with $v \sim$ const., and r odd]		$(0, 0)$, $(\infty, 1)$
D: quasi-bound state	256, 625, 1296	quasi bound
[(4.10) with $\gamma = 1/2$, and r odd]		$(0.5, 0.5)$, $(\infty, 1)$

for all q as $n \to \infty$. Actually the maximum and the minimum values of a converge to $\alpha = 1$, and the corresponding $\{(\alpha, f)\}$ becomes a single point as shown in Fig. 2. Thus we conclude that $\{(\alpha, f)\}$ consists of the single point $(\alpha, f) = (1, 1)$. This result $\{(\alpha, f)\}$ agrees with the fact that the wavefunction is extended as clearly seen in Fig. 3.

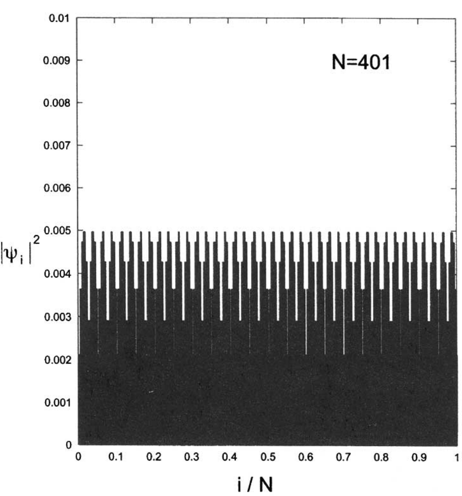


Fig. 3. Probability distribution for the normalized wavefunctions of Example A.

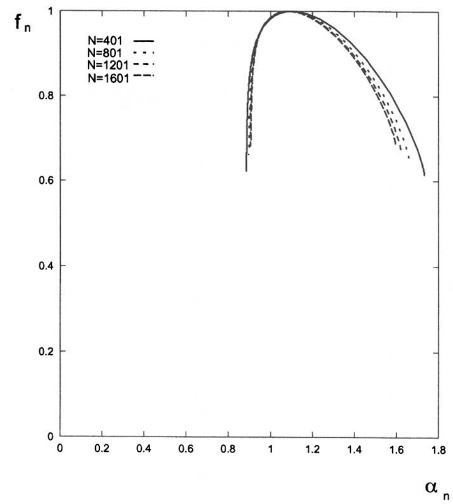


Fig. 4. (α_n, f_n) for Example A.

Example B: Quasi-Scattering States [Case (iv-b) in Section 4.2.2]

Figure 1 shows the probability distribution for the wavefunction (4.26) in Case (iv-b). Whether the wavefunction is extended or notes is not clear from the figure. Similar to Example A, we found that $\{(\alpha, f)\}$ consists of the single point $(\alpha, f) = (1, 1)$, although (α_n, f_n) for a finite n is also

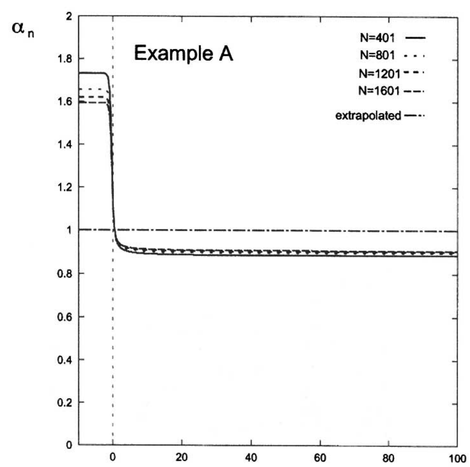


Fig. 5. $\alpha_n(q)$ for Example A.

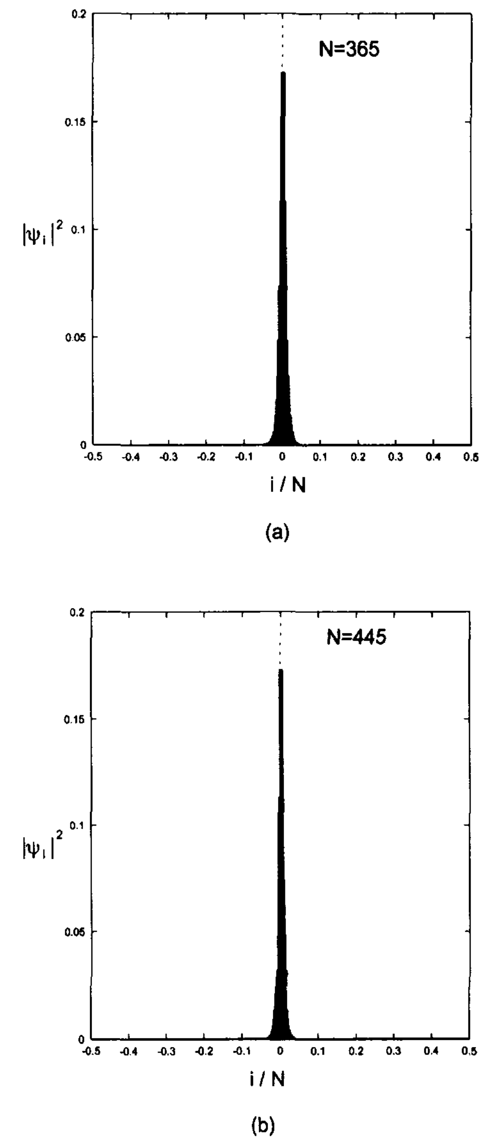
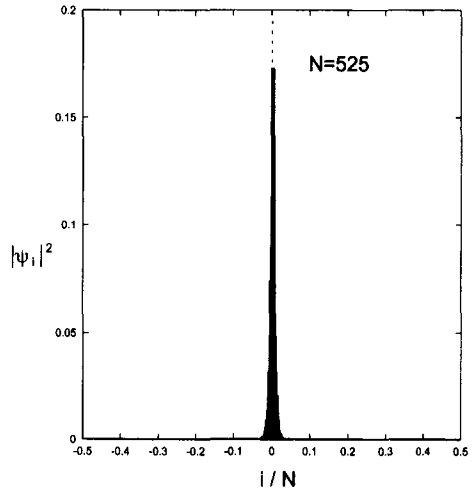
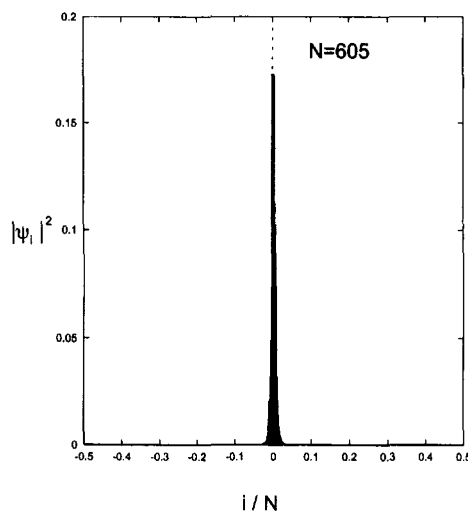


Fig. 6. Probability distribution for the normalized wavefunctions of Example C [(4.3) with $v \sim$ const., and r odd].



(c)



(d)

Fig. 6 (*Continued*)

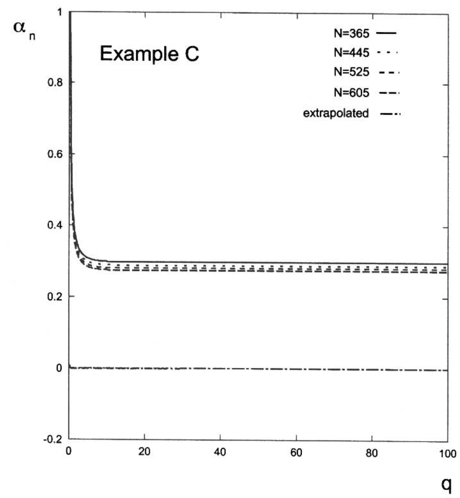


Fig. 7. $\alpha_n(q)$ for Example C.

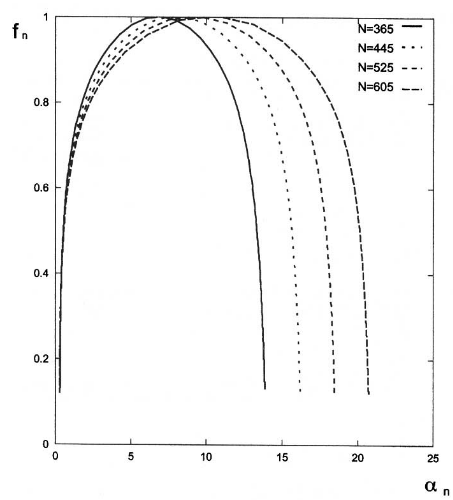


Fig. 8. (α_n, f_n) for Example C.

smooth. This agrees with the anaytic result in Section 5.2.2. Namely the wavefunction is extended.

Example C: String Bound States (Section 4.1)

Figure 6 shows the probability distribution $|\psi_{sb}(y)|^2$ for the wavefunction (4.3) with $v \sim$ const. and r odd.

As shown in Fig. 7, $\alpha_n(q)$ converges to $\alpha(q) = 0$ for $0 < q < \infty$ and the point $q = 0$ is singular. The corresponding $\alpha_n(q)$ at $q = 0$ diverges to $+\infty$. This singularity is reflected in the behavior of (α_n, f_n) for finite n as seen in Fig. 8.

Namely the maximum value of α diverges to $+\infty$. We also found $f(q) = 0$ for $0 < q < \infty$. These results agree with the fact that the wavefunction is localized as clearly seen in Fig. 6.

Example D: Quasi-Bound States [Case (i) in Section 4.2.1]

We choose $\gamma = 1/2$ for the wavefunction (4.10) with r odd. Similar to Example C, we obtain $(\alpha, f) = (0.5, 0.5)$ for $0 < q < \infty$. The point $q = 0$ is singular as seen in Fig. 9.

The corresponding $\alpha_n(q)$ at $q = 0$ diverges to $+\infty$. This singularity is reflected in the behavior of (α_n, f_n) for finite n as seen in Fig. 10.

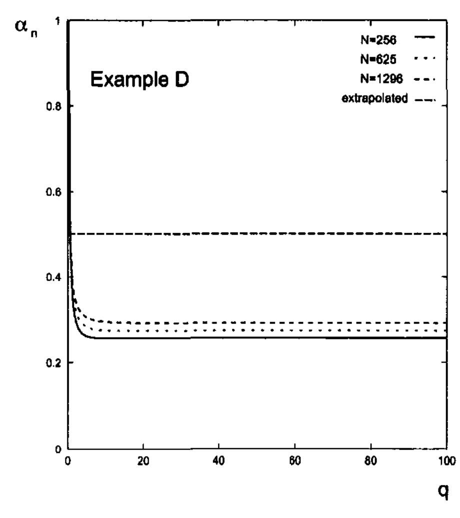


Fig. 9. $\alpha_n(q)$ for Example D [(4.10) with $\gamma = 1/2$, and r odd].

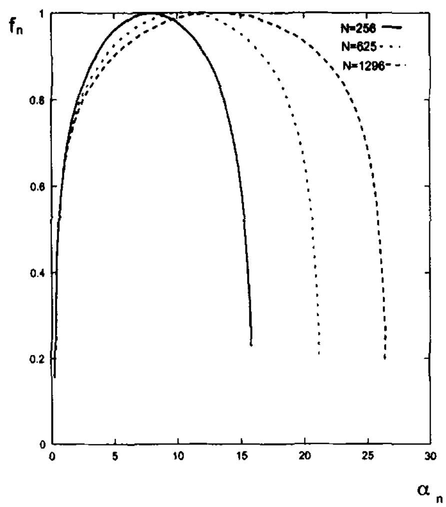


Fig. 10. (α_n, f_n) for Example D.

These results agree with the anaytic result for quasi-bound state in Section 5.2.1.

APPENDIX A. STATE COUNTING

We shall count the number of all the type-II states, i.e., the number of the solutions (u, v) of (4.7). Note that the right-hand side of (4.7) is a monotonically decreasing function with respect to v for a fixed N. The function is vanishing as $v \to \infty$, and satisfies

$$\lim_{v \downarrow 0} \frac{e^{(N-1)v} \pm e^{v}}{e^{Nv} \pm 1} = \begin{cases} 1 & \text{for } r \text{ even} \\ 1 - \dfrac{2}{N} & \text{for } r \text{ odd} \end{cases} \tag{A.1}$$

Therefore a solution (u, v) of (4.7) is uniquely determined for a fixed r in the range

$$0 < \Delta^{-1} \cos\left(\frac{\pi}{N} r - \frac{\varepsilon}{N}\right) < \begin{cases} 1 & \text{for } r \text{ even} \\ 1 - \dfrac{2}{N} & \text{for } r \text{ odd} \end{cases} \tag{A.2}$$

Since $\Delta^{-1} \cos[(\pi r - \varepsilon)/N]$ changes the sign as $-\Delta^{-1} \cos u'$ under the transformation $u = \pi + u' = \pi + (\pi r' - \varepsilon)/N$ with $r' = 0, 1, ..., 2N-1$, we have only to consider the case with $\Delta \geqslant 0$. From these observations the number $n_b^{(e)}(\Delta)$ of the type-II states for r even is

$$n_b^{(e)}(\Delta) \sim \begin{cases} \dfrac{N}{2} & (|\Delta| > 1) \\ \dfrac{N}{2} - \dfrac{N}{\pi} \arccos \Delta & (0 < |\Delta| \leqslant 1) \\ 0 & (\Delta = 0) \end{cases} \tag{A.3}$$

For r odd, the number $n_b^{(o)}(\Delta)$ of the type-II states is

$$n_b^{(o)}(\Delta) \sim \begin{cases} \dfrac{N}{2} & (|\Delta| > 1) \\ \dfrac{N}{2} - \dfrac{N}{\pi} \arccos \left[\Delta \left(1 - \dfrac{2}{N} \right) \right] & (0 < |\Delta| \leqslant 1) \\ 0 & (\Delta = 0) \end{cases} \tag{A.4}$$

Thus the total number of the type-II states is

$$n_b(\Delta) \sim \begin{cases} N & (|\Delta| > 1) \\ N - \dfrac{N}{\pi} \arccos \Delta - \dfrac{N}{\pi} \arccos \left[\Delta \left(1 - \dfrac{2}{N} \right) \right] & (0 < |\Delta| \leqslant 1) \\ 0 & (\Delta = 0) \end{cases} \tag{A.5}$$

As we showed in Theorem 3, when $|\Delta| > 1$, all the bound states are string states. Thus the number $n_b(\Delta)$ for $|\Delta| > 1$ is equal to the number of the string states. When $0 < |\Delta| \leqslant 1$, both of the string and the non-string states appear as a bound state. The result (A.5) for $\Delta = 0$ agrees with the result for the XY chain.

Remark 6. When $N =$ even and $\varepsilon = 0$, the equation (4.7) has the "solution" $u = \pi/2$ and $v = \infty$. Clearly the corresponding Bethe state (2.3) with $(z_1, z_2) = (e^{iu+v}, e^{iu-v})$ becomes ill-defined. Therefore the "solution" is often excluded from the set of the Bethe states [18]. However the two-magnon Bethe states without the "solution" is not complete. To avoid this difficulty, use have introduced the small positive ε into the Hamiltonian of the spin-1/2 XXZ chain. Thereby there appear no such a singular "solution", and the system of the Behte states is complete. See, for details, ref. 11.

APPENDIX B. PROOF OF THEOREM 5

We first show that the free energy $G_n(q)$ (5.11) for a finite volume is convex with respect to q. The free energy $G(q)$ in the infinite-volume limit is also convex because the convexity is retained for any limit. It can be shown that

$$\frac{d^2}{dq^2} G_n(q) = \frac{1}{n} [\langle u_i^2 \rangle - \langle u_i \rangle^2] \geqslant 0 \tag{B.1}$$

where $u_i = n\varepsilon_n \alpha_i$, and

$$\langle \cdots \rangle = \frac{1}{Z_n(q)} \sum_i (\cdots) e^{-qu_i} \tag{B.2}$$

Thus $G_n(q)$ is convex. Using this convexity, we have

$$\frac{d}{dq} G_n(q) = \inf_{\Delta q' > 0} \frac{G_n(q + \Delta q') - G_n(q)}{\Delta q'} \leqslant \frac{G_n(q + \Delta q) - G_n(q)}{\Delta q} \tag{B.3}$$

for any positive Δq. Here we have used the assumption that q is an interier point. In the limit $n \to \infty$, we get

$$\lim_{k \to \infty} \sup_{n \geqslant k} \frac{d}{dq} G_n(q) \leqslant \frac{G(q + \Delta q) - G(q)}{\Delta q} \tag{B.4}$$

from the assumption of Theorem 5. Further we take the limit $\Delta q \downarrow 0$. Then we have

$$\lim_{k \to \infty} \sup_{n \geqslant k} \frac{d}{dq} G_n(q) \leqslant \frac{d}{dq} G(q) \tag{B.5}$$

For a negative Δq,

$$\frac{d}{dq} G_n(q) = \inf_{\Delta q' < 0} \frac{G_n(q + \Delta q') - G_n(q)}{\Delta q'} \geqslant \frac{G_n(q + \Delta q) - G_n(q)}{\Delta q} \tag{B.6}$$

In the same way, we get

$$\lim_{k \to \infty} \inf_{n \geqslant k} \frac{d}{dq} G_n(q) \geqslant \frac{d}{dq} G(q) \tag{B.7}$$

Combining this with (B.5), we have

$$\frac{d}{dq} G(q) \geqslant \lim_{k \to \infty} \sup_{n \geqslant k} \frac{d}{dq} G_n(q) \geqslant \lim_{k \to \infty} \inf_{n \geqslant k} \frac{d}{dq} G_n(q) \geqslant \frac{d}{dq} G(q) \tag{B.8}$$

Thus,

$$\lim_{n \to \infty} \frac{d}{dq} G_n(q) = \frac{d}{dq} G(q) \tag{B.9}$$

This implies (5.44), with the definitions (5.42) and (5.43). ▮

ACKNOWLEDGMENTS

We wish to thank Hal Tasaki for many useful suggestions. Y.M. thanks Kenichi Asano for helpful suggestions about numerical techniques.

REFERENCES

1. H. Bethe, *Z. Phys.* **71**:205, (1931).
2. R. Orbach, *Phys. Rev.* **112**:309, (1958).
3. M. Takahashi, *Prog. Theor. Phys.* **46**:401 (1971); M. Gaudin, *Phys. Rev. Lett.* **26**:1301 (1971); M. Takahashi, and M. Suzuki, *Prog. Theor. Phys.* **46**:2187 (1972).
4. F. Woynarovich, *J. Phys.* **A15**:2985, (1982); C. Destri, and J. H. Lowenstein, *Nucl. Phys. B* **205**[FS5]:369 (1982); O. Babelon, H. J. de Vega, and C. M. Viallet, *Nucl. Phys. B* **220**[FS8]:13, (1983).
5. A. A. Vladimirov, *Phys. Lett.* **105A**:418 (1984).
6. F. H. L. Essler, V. E. Korepin, and K. Schoutens, *J. Phys. A* **25**:4115 (1992); K. Isler, and M. B. Paranjape, *Phys. Lett.* **319B**:209 (1993); G. Jüttner and B. D. Dörfel, *J. Phys. A* **26**:3105 (1993).
7. See, for a review, H. Hiramoto, and M. Kohmoto, *Int. J. Mod. Phys. B* **6**:281 (1992).
8. M. Kohmoto, L. P. Kadanoff, and C. Tang, *Phys. Rev. Lett.* **50**:1870 (1983).
9. S. Ostlund, R. Pandit, D. Rand, H. J. Schellhuber, and E. D. Siggia, *Phys. Rev. Lett.* **50**:1873 (1983).
10. S. Katsura, *Ann. Phys.* **31**:325 (1965).
11. T. Koma, and H. Ezawa, *Prog. Theor. Phys.* **78**:1009 (1987).
12. F. C. Alcaraz, M. N. Barber, and M. T. Batchelor, *Phys. Rev. Lett.* **58**:771 (1987).
13. T. C. Halsey, M. H. Jensen, L. Kadanoff, I. Procaccia, and B. Shraiman, *Phys. Rev. A* **33**:1141 (1986).
14. See, for example, M. Reed, and B. Simon, *Methods of Modern Mathematical Physics I, Functional Analysis*, (Academic Press, New York, 1972), Chapter VII.
15. B. Huckstein, and L. Schweitzer, *Phys. Rev. Lett.* **72**:713 (1994).
16. R. B. Griffiths, *J. Math. Phys.* **5**:1215 (1964).
17. R. B. Griffiths, in *Phase Transition and Critical Phenomena*, Vol. 1, C. Domb and M. S. Green, eds., (Academic Press, New York, 1972).
18. Y. Kato, N. Mugibayashi, and K. Sekine, in RIMS Kôkyûroku No. 159, 1972, *The Hamiltonian, its definition and spectrum*, p. 69, (Research Institute for Mathematical Sciences, Kyoto Unversity, Kyoto), [in Japanese].