

Thermal Bethe-Ansatz Method for the Spin-1/2 XXZ Heisenberg Chain^{*)}

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A new method is proposed for calculating the free energy of the one-dimensional spin-1/2 XXZ Heisenberg model. The partition function is written in terms of the transfer matrix for a two-dimensional Ising system, whose maximum eigenvalue is obtained by the Bethe-ansatz method leading to the free energy in the thermodynamic limit. This method uses no such assumption as the completeness of the Bethe states that has been proved only partially and yields better results than the previous methods do.

§ 1. Introduction

The Bethe-ansatz method^{1)~6)} has been widely used to study thermal properties of the one-dimensional spin-1/2 XXZ Heisenberg model, e.g., the specific heat, magnetic susceptibilities, etc.^{7)~9)} However, these calculations depend on the string conjecture,^{10)~12)} or more basically on the assumption of the completeness of the Bethe states that has been proved only partially.¹³⁾ In other words, these calculations require the complete knowledge of all the eigenvalues of the Hamiltonian of the model.

In this paper, we propose a new method for the statistical mechanics of the one-dimensional spin-1/2 XXZ Heisenberg model, which we call the thermal Bethe-ansatz method.¹⁴⁾ This method is free from the unproven assumptions mentioned above, because it is sufficient to obtain only the maximum eigenvalue of the transfer matrix of an Ising system. It consists in (i) using the path integral idea to transform the partition function of the model into the one of a two-dimensional Ising system,^{15)~22),25)} and (ii) applying the Bethe-ansatz method to find the maximum eigenvalue of the transfer matrix of the Ising system. Then, the standard procedure gives the free energy of the model in the thermodynamic limit.^{19)~22)}

Thus, in § 2, we use the Trotter formula to carry out the transformation (i) mentioned above. The partition function of the Ising system so obtained is rewritten in terms of the transfer matrix in the "space" direction in § 3. In § 4, we shall analyze the eigenvalue problem of the transfer matrix by the Bethe-ansatz method and obtain a set of the eigenvalues which is determined by the solutions to the system of the Bethe-ansatz equations. In particular, one of the Bethe-ansatz eigenvalues equals the maximum eigenvalue of the transfer matrix as is proved in § 5. Then, the maximum eigenvalue leads to the free energy of the model in the thermodynamic limit.

Thus, for calculating the free energy of the one-dimensional spin-1/2 XXZ Heisenberg model, it is sufficient to solve analytically or numerically only the Bethe-ansatz equations corresponding to the maximum eigenvalue of the transfer

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matrix. In fact, the free energy of the isotropic XY model is obtained analytically in § 6. As is well-known, this special case was solved analytically by Lieb et al. in 1961²³⁾ and by Katsura in 1962.²⁴⁾ Their methods are different from ours. Quite recently, Inoue and Suzuki²⁵⁾ diagonalized the transfer matrix of this special case by the method of the Jordan-Wigner transformation. Further, in § 7, we calculate the zero-field free energy and the susceptibility of the isotropic ferromagnetic model by solving the system of the Bethe-ansatz equations numerically, and obtain better results than those obtained by the previous methods.^{7)~9), 26)~32)}

§ 2. Path integral form of the partition function

The Hamiltonian of the one-dimensional spin-1/2 XXZ Heisenberg model is given by^{*)}

$$\widehat{H}_{N,B} := \sum_{j=1}^N \widehat{H}_{N;j,j+1}, \quad (2.1)$$

$$\widehat{H}_{N;j,j+1} := 2^{-1}(1 - \widehat{\sigma}_{N;j} \cdot \widehat{\sigma}_{N;j+1} + \Delta \widehat{\sigma}_{N;j}^z \widehat{\sigma}_{N;j+1}^z) - 2^{-1}h(\widehat{\sigma}_{N;j}^z + \widehat{\sigma}_{N;j+1}^z), \quad (2.2)$$

where B in (2.1) stands for the boundary condition,

$$B = \begin{cases} P & : \text{periodic,} & \widehat{\sigma}_{N;N+1} = \widehat{\sigma}_{N;1}, \\ F & : \text{free,} & \widehat{H}_{N;N,N+1} = 0 \end{cases} \quad (2.3)$$

and $\widehat{\sigma}_{N;j}$ is the spin operator for the site j ($j=1, \dots, N$),

$$\widehat{\sigma}_{N;j} := 1 \otimes \cdots \otimes 1 \otimes \widehat{\sigma} \otimes 1 \otimes \cdots \otimes 1,$$

an N -fold tensor product having the Pauli matrix $\widehat{\sigma}$ at the j th place; Δ and h are the anisotropy parameter and the external field, respectively. Our free boundary condition is different from the standard one $\widehat{\sigma}_{N;N+1} = 0$. It is convenient for the following calculation.

By using the path integral idea, we transform the partition function of the model with an even number of spins,

$$Z_{2n,B} = \text{Tr} \exp[-\beta \widehat{H}_{2n,B}] \quad (n=1, 2, \dots) \quad (2.4)$$

into a partition function of a two-dimensional Ising model in the following way, where β is the inverse temperature and Tr denotes the trace of a matrix.

We follow Suzuki,^{15)~17), 19), 20)} to begin with, dividing the Hamiltonian (2.1) with an even number of spins into two parts such that each one is a sum of operators all commuting with each other:

$$\widehat{H}_{2n}^{(1)} = \sum_{j=1}^n \widehat{H}_{2n;2j-1,2j} \quad (2.5)$$

and

$$\widehat{H}_{2n,B}^{(2)} = \sum_{j=1}^n \widehat{H}_{2n;2j,2j+1} \quad (2.6)$$

*) The symbol $:=$ signifies definition.

to write

$$Z_{2n,B} = \lim_{M \uparrow \infty} Z_{2n,B}^{(M)} \tag{2.7}$$

by invoking the Trotter formula,

$$\exp[\widehat{H} + \widehat{H}'] = \lim_{M \uparrow \infty} \{\exp[\widehat{H}/M] \exp[\widehat{H}'/M]\}^M, \quad (\widehat{H}, \widehat{H}': \text{ matrices})$$

in terms of the approximate finite- M partition function,

$$Z_{2n,B}^{(M)} = \text{Tr} \left\{ \exp \left[-\frac{\beta}{M} \widehat{H}_{2n}^{(1)} \right] \exp \left[-\frac{\beta}{M} \widehat{H}_{2n,B}^{(2)} \right] \right\}^M. \tag{2.8}$$

We call M the Trotter number.

Let us first put (2.8) into a path integral form,

$$\begin{aligned} Z_{2n,B}^{(M)} = \sum_{\Omega} & \langle \omega_{2n}^1 | \exp \left[-\frac{\beta}{M} \widehat{H}_{2n}^{(1)} \right] | \omega_{2n}^2 \rangle \langle \omega_{2n}^2 | \exp \left[-\frac{\beta}{M} \widehat{H}_{2n,B}^{(2)} \right] | \omega_{2n}^3 \rangle \dots \\ & \dots \langle \omega_{2n}^{2M} | \exp \left[-\frac{\beta}{M} \widehat{H}_{2n,B}^{(2)} \right] | \omega_{2n}^1 \rangle, \end{aligned} \tag{2.9}$$

where $\omega_{2n}^k := (\sigma_1^k, \dots, \sigma_{2n}^k)$ and

$$| \omega_{2n} \rangle := | \sigma_1 \rangle \otimes \dots \otimes | \sigma_{2n} \rangle \tag{2.10}$$

with

$$| \sigma \rangle := \begin{cases} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, & (\sigma = +1) \\ \begin{pmatrix} 0 \\ 1 \end{pmatrix} & (\sigma = -1) \end{cases}$$

and the summation runs over all the “paths” $\Omega := (\omega_{2n}^1, \dots, \omega_{2n}^{2M})$, that is, over all the configurations ω_{2n}^k for each “time” k ($k=1, \dots, 2M$). The matrix elements in (2.9) are easy to write down because the summand either in (2.5) or (2.6) all commutes with each other. Thus,

$$\langle \omega_{2n}^{2l-1} | \exp \left[-\frac{\beta}{M} \widehat{H}_{2n}^{(1)} \right] | \omega_{2n}^{2l} \rangle = \prod_{j=1}^n \tau(\sigma_{2j-1}^{2l-1}, \sigma_{2j}^{2l-1}; \sigma_{2j-1}^{2l}, \sigma_{2j}^{2l}) \tag{2.11}$$

and

$$\begin{aligned} & \langle \omega_{2n}^{2l} | \exp \left[-\frac{\beta}{M} \widehat{H}_{2n,B}^{(2)} \right] | \omega_{2n}^{2l+1} \rangle \\ &= \begin{cases} \prod_{j=1}^n \tau(\sigma_{2j}^{2l}, \sigma_{2j+1}^{2l}; \sigma_{2j}^{2l+1}, \sigma_{2j+1}^{2l+1}), & (B=P) \\ \delta_F^{2l} \prod_{j=1}^{n-1} \tau(\sigma_{2j}^{2l}, \sigma_{2j+1}^{2l}; \sigma_{2j}^{2l+1}, \sigma_{2j+1}^{2l+1}) & (B=F) \end{cases} \\ & \quad (l=1, \dots, M) \end{aligned} \tag{2.12}$$

with periodic boundary conditions, namely, one in the “time” direction,

$$\sigma_j^{2M+1} = \sigma_j^1, \quad (j=1, \dots, 2n)$$

and the other in the “space” direction,

$$\sigma_{2n+1}^k = \sigma_1^k, \quad (k=1, \dots, 2M)$$

where

$$\tau(\sigma_i^k, \sigma_j^k; \sigma_i^l, \sigma_j^l) := \langle \sigma_i^k, \sigma_j^k | \exp \left[-\frac{\beta}{M} \widehat{H}_{2; i, j} \right] | \sigma_i^l, \sigma_j^l \rangle \tag{2.13}$$

and

$$\delta_F^k := 4^{-1} (1 + \sigma_{2n}^k \sigma_{2n}^{k+1}) (1 + \sigma_1^k \sigma_1^{k+1}). \tag{2.14}$$

The expression (2.9) has the form^{15)~17),19),20)} of the partition function of a two-dimensional $2n \times 2M$ Ising spin system with its substates in the k th row specified by ω_{2n}^k ($k=1, \dots, 2M$) and with the Boltzmann weight for each state $\Omega = (\omega_{2n}^1, \dots, \omega_{2n}^{2M})$ given by the corresponding term in (2.9). In other words, one may think of (2.13) as a Boltzmann factor for a four-spin interaction. Then, each term in (2.9) is represented by such an assembly of the interaction “paths”.

§ 3. Transfer matrix in the “space” direction

The free energy per spin of the present model (2.1) in the thermodynamic limit is given by

$$f(B) := -\beta^{-1} \lim_{n \uparrow \infty} (2n)^{-1} \log Z_{2n, B}. \tag{3.1}$$

THEOREM 3.1. For any $(\beta, \Delta, h) \in \mathbf{R}^3$, the limit $n \uparrow \infty$ in (3.1) exists and is independent of the boundary condition B of (2.3).

This theorem can be proved³³⁾ by using an inequality related to Peierls’s. Then, (2.7) gives the free energy per spin in the thermodynamic limit,

$$f := -\beta^{-1} \lim_{n \uparrow \infty} \lim_{M \uparrow \infty} (2n)^{-1} \log Z_{2n, B}^{(M)}. \tag{3.2}$$

THEOREM 3.2. Let $(\beta, \Delta, h) \in \mathbf{R}^3$. Then, the limit

$$f^{(M)} := -\beta^{-1} \lim_{n \uparrow \infty} (2n)^{-1} \log Z_{2n, B}^{(M)} \tag{3.3}$$

exists and is independent of the boundary condition B of (2.3). Further, the free energy per spin of the model (2.1) in the thermodynamic limit can be written as

$$f = \lim_{M \uparrow \infty} f^{(M)},$$

i.e., the order of limits in (3.2) can be interchanged.^{19)~22)} A rigorous proof along the line of Suzuki and Inoue^{21),22)} is given in Appendix A.

In order to calculate the limit $n \uparrow \infty$ in (3.3), we rewrite (2.9) in terms of the transfer matrix in the “space” direction.

Note that

$$\tau(-\sigma_i^k, \sigma_j^k: \sigma_i^l, -\sigma_j^l) = \langle \sigma_i^k, \sigma_i^l | \widehat{V}_{2; i, j} | \sigma_j^k, \sigma_j^l \rangle, \tag{3.4}$$

where

$$\widehat{V}_{2; i, j} := \exp\left[-\frac{\beta h}{4M}(\sigma_{2; i^z} - \sigma_{2; j^z})\right] \widehat{V}_{2; i, j}^{(0)} \exp\left[\frac{\beta h}{4M}(\sigma_{2; i^z} - \sigma_{2; j^z})\right] \tag{3.5}$$

and

$$\widehat{V}_{2; i, j}^{(0)} := (2D)^{-1} [D^2 + \sigma_{2; i^x} \sigma_{2; j^x} + \sigma_{2; i^y} \sigma_{2; j^y} + D^2(1-2c) \sigma_{2; i^z} \sigma_{2; j^z}] \tag{3.6}$$

with

$$D = \exp[\beta\Delta/2M] \quad \text{and} \quad c = \exp[-\beta/M] \cosh(\beta/M). \tag{3.7}$$

Therefore, from (2.11), (2.12) and (2.14), the finite- M partition function (2.9) can be rewritten as

$$Z_{2n, B}^{(M)} = \begin{cases} \text{Tr}(\widehat{R}'_{2M} \widehat{R}_{2M})^n, & (B=P) \\ \sum_{\omega_{2M}, \omega'_{2M}} \langle \omega_{2M} | \widehat{\delta}_F (\widehat{R}'_{2M} \widehat{R}_{2M})^{n-1} \widehat{R}'_{2M} \widehat{\delta}_F | \omega'_{2M} \rangle, & (B=F) \end{cases} \tag{3.8}$$

using the transfer matrices in the “space” direction,

$$\widehat{R}_{2M} := \prod_{j=1}^M \widehat{V}_{2M; 2j-1, 2j} \quad \text{and} \quad \widehat{R}'_{2M} := \prod_{j=1}^M \widehat{V}_{2M; 2j, 2j+1},$$

where

$$\widehat{\delta}_F := \prod_{j=1}^M 2^{-1} (1 - \sigma_{2M; 2j-1^z} \sigma_{2M; 2j^z}) \tag{3.9}$$

and $\widehat{V}_{2M; i, j}$ is a $2M$ -fold tensor product $1 \otimes \dots \otimes 1$ with two 1’s at the i and j th places replaced by the matrix $\widehat{V}_{2; i, j}$ with the periodic boundary condition,

$$\widehat{V}_{2M; 2M, 2M+1} = \widehat{V}_{2M; 2M, 1}.$$

Further, we rewrite (3.8) into the form (3.12) below which is more convenient for the purpose of applying the Bethe-ansatz method to the eigenvalue problem of the transfer matrix.

Note, to begin with, that the matrices \widehat{R}_{2M} and \widehat{R}'_{2M} have the following properties:

$$\widehat{R}'_{2M} = \widehat{T}_{2M}^{-1} \widehat{R}_{2M} \widehat{T}_{2M}, \quad [\widehat{R}_{2M}, (\widehat{T}_{2M})^2] = 0,$$

where

$$\widehat{T}_{2M} := \widehat{S}_{2M; 1, 2M} \widehat{S}_{2M; 2, 2M} \dots \widehat{S}_{2M; 2M-1, 2M}$$

with

$$\widehat{S}_{2M; j, 2M} := 2^{-1} (1 + \widehat{\sigma}_{2M; j} \cdot \widehat{\sigma}_{2M; 2M}). \quad (j=1, \dots, 2M-1)$$

The operator \widehat{T}_{2M} shifts any periodic array of the spin states by one lattice unit backwards in the “time” direction. Clearly, $(\widehat{T}_{2M})^{2M} = 1$. Therefore, for any integer $L > 0$, we obtain

$$\begin{aligned}
 (\widehat{R}'_{2M}\widehat{R}_{2M})^{ML} &= (\widehat{T}_{2M}^{-1}\widehat{R}_{2M}\widehat{T}_{2M}\widehat{R}_{2M}\widehat{T}_{2M}^{-2})^{ML} \\
 &= (\widehat{T}_{2M}^{-1}\widehat{R}_{2M}\widehat{T}_{2M}^{-1}\widehat{R}_{2M})^{ML} \\
 &= (\widehat{U}_{2M})^{2ML},
 \end{aligned} \tag{3.10}$$

where

$$\widehat{U}_{2M} := \widehat{T}_{2M}^{-1}\widehat{R}_{2M}. \tag{3.11}$$

Let us now restrict n to multiples of M , that is to say, $n = ML$ ($L = 1, 2, \dots$). Then, (3.8) can be rewritten as

$$Z_{2ML,B}^{(M)} = \begin{cases} \text{Tr}(\widehat{U}_{2M})^{2ML}, & (B=P) \\ \sum_{\omega_{2M}, \omega'_{2M}} \langle \omega_{2M} | \widehat{\delta}_F (\widehat{U}_{2M})^{2ML-1} \widehat{T}_{2M}^{-1} \widehat{\delta}_F | \omega'_{2M} \rangle. & (B=F) \end{cases} \tag{3.12}$$

Therefore, by Theorem 3.2 and the first line of (3.12), we obtain:

THEOREM 3.3. The finite- M free energy of our system with $B = P$ can be written as

$$f^{(M)} = -\beta^{-1} \log \Lambda_{2M}^{\max}$$

in terms of the maximum eigenvalue Λ_{2M}^{\max} of the transfer matrix \widehat{U}_{2M} in the “space” direction of our Ising model.

The second line of (3.12) will be used in the proof of Theorem 5.3 below.

§ 4. Thermal Bethe ansatz

In order to obtain the maximum eigenvalue Λ_{2M}^{\max} of the transfer matrix \widehat{U}_{2M} , we assume that the eigenstates of \widehat{U}_{2M} have the Bethe-ansatz form,^{1),34),35)}

$$|B_k\rangle = \sum_{1 \leq y_1 < \dots < y_k \leq 2M} \sum_P A_P F(z_{P1}, y_1) \dots F(z_{Pk}, y_k) |y_1, \dots, y_k\rangle \quad (k=0, 1, \dots, 2M) \tag{4.1}$$

with

$$F(z_j, y) = \begin{cases} a_j z_j^{(y+1)/2} & (y = \text{odd}) \\ z_j^{y/2} & (y = \text{even}), \end{cases} \quad (j=1, \dots, k) \tag{4.2}$$

where $|y_1, \dots, y_k\rangle$ is the state with all the spins up except those k spins at the sites y_1, \dots, y_k ; the summation runs over all the possible distributions of the k down spins, and over all the permutations P of $(1, \dots, k)$. $\{z_k, a_k\}$ and $\{A_P\}$ are complex numbers to be determined as follows.

As in the original Bethe ansatz (see Appendix B for the details), the eigenvalue equation leads to the conditions,

$$z_j = \frac{D^{-1}E\lambda_j - D^{-2} + (DC)^2}{\lambda_j(\lambda_j - D^{-1}E^{-1})}, \quad a_j = (DC)^{-1}(\lambda_j - D^{-1}E^{-1}), \quad (j=1, \dots, k) \tag{4.3}$$

$$\frac{A_{(P_1, \dots, P(j+1), P_j, \dots, P_k)}}{A_{(P_1, \dots, P_j, P(j+1), \dots, P_k)}} = -\frac{\lambda_{P_j} \lambda_{P(j+1)} - 2DsE^{-1} \tilde{\Delta} \lambda_{P_j} + (DsE^{-1})^2}{\lambda_{P_j} \lambda_{P(j+1)} - 2DsE^{-1} \tilde{\Delta} \lambda_{P(j+1)} + (DsE^{-1})^2} \quad (j=1, \dots, k-1) \tag{4.4}$$

and to the eigenvalue,

$$\Lambda_{2M; k} = (Ds)^{M-k} \lambda_1 \dots \lambda_k, \tag{4.5}$$

where

$$s = 1 - c, \quad E = \exp[\beta h / M], \quad \tilde{\Delta} = D^2 - s^{-1} \sinh(\beta \Delta / M) \tag{4.6}$$

and $\lambda_1, \dots, \lambda_k$ are determined by the system of the Bethe-ansatz equations,

$$\left[\frac{D^{-1} E \lambda_j - D^{-2} + (Dc)^2}{\lambda_j (\lambda_j - D^{-1} E^{-1})} \right]^M = (-1)^{k-1} \prod_{l=1}^k \frac{\lambda_j \lambda_l - 2DsE^{-1} \tilde{\Delta} \lambda_l + (DsE^{-1})^2}{\lambda_j \lambda_l - 2DsE^{-1} \tilde{\Delta} \lambda_j + (DsE^{-1})^2} \quad (j=1, \dots, k) \tag{4.7}$$

In particular, for the isotropic XY-case, $\Delta=1$, we have $\tilde{\Delta}=0$. Therefore, we obtain :

Remark 4.1. For $\Delta=1$, the Bethe-ansatz equations (4.7) can be rewritten as

$$\lambda_j^2 - D^{-1} (E z_j^{-1} + E^{-1}) \lambda_j - (Ds)^2 z_j^{-1} = 0 \tag{4.8}$$

with

$$z_j^M = (-1)^{k-1} \quad (j=1, \dots, k) \tag{4.9}$$

Similarly, we have the following remark.

Remark 4.2. In the high temperature limit, $\beta=0$, the Bethe-ansatz equations (4.7) can be rewritten as

$$\lambda_j [\lambda_j - (z_j^{-1} + 1)] = 0 \tag{4.10}$$

with

$$z_j^M = (-1)^{k-1} \quad (j=1, \dots, k) \tag{4.11}$$

We define K^{XY} to be the set of all the solution vectors $\lambda = (\lambda_1, \dots, \lambda_k)$ ($k=0, 1, \dots, 2M$) to the system of the Bethe-ansatz equations in Remark 4.1 such that the z 's in (4.9) satisfy the condition,

$$z_i \neq z_j \quad (i \neq j) \tag{4.12}$$

Further, we define

$$\mathbf{R}_P := \{x \mid x > 0\}.$$

Lemma 4.3. Let $\lambda^{XY} \in K^{XY}$. Then, for any $(\beta_0, h_0) \in \mathbf{R}_P \times \mathbf{R}$, there exists a solution λ to the system of the Bethe-ansatz equations (4.7) analytic in a neighborhood $\mathcal{D} \subset \mathbf{C}^3$ of $(\beta, \Delta, h) = (\beta_0, 1, h_0)$ such that $\lambda = \lambda^{XY}$ for $(\beta, \Delta, h) = (\beta_0, 1, h_0)$ and that the Bethe state (4.1) constructed from the solution λ is non-vanishing.

Proof First, we show the existence of λ . For this purpose, let

$$g_j := M \log \left[\frac{D^{-1}E\lambda_j - D^{-2} + (Dc)^2}{\lambda_j(\lambda_j - D^{-1}E^{-1})} \right] - 2\pi i n_j - i\pi(k-1) \\ - \sum_{i=1}^k \log \left[\frac{\lambda_j \lambda_i - 2DsE^{-1}\tilde{\Delta}\lambda_i + (DsE^{-1})^2}{\lambda_j \lambda_i - 2DsE^{-1}\tilde{\Delta}\lambda_j + (DsE^{-1})^2} \right] \quad (j=1, \dots, k)$$

with integer n_j ($j=1, \dots, k$). Then, the Bethe-ansatz equations (4.7) can be rewritten as $g_j=0$ ($j=1, \dots, k$). Therefore, by the well-known theorem on implicit functions, it is sufficient to show that the Jacobian determinant,

$$\frac{D(g_1, \dots, g_k)}{D(\lambda_1, \dots, \lambda_k)}$$

is non-vanishing for $\lambda=\lambda^{XY}$ and $(\beta, \Delta, h)=(\beta_0, 1, h_0)$. Since $\Delta=1$, it is easily shown that the Jacobian matrix becomes diagonal with the diagonal element being given by

$$J_{jj} = M \left[\frac{D^{-1}E}{D^{-1}E\lambda_j^{XY} + (Ds)^2} - \frac{1}{\lambda_j^{XY}} - \frac{1}{\lambda_j^{XY} - D^{-1}E^{-1}} \right].$$

Therefore, it is sufficient to show that $J_{jj} \neq 0$ ($j=1, \dots, k$). By the Bethe-ansatz equations (4.8), J_{jj} can be rewritten as

$$J_{jj} = -M \frac{2\lambda_j^{XY} - D^{-1}[E(z_j^{XY})^{-1} + E^{-1}]}{\lambda_j^{XY}(\lambda_j^{XY} - D^{-1}E^{-1})},$$

where z_j^{XY} ($j=1, \dots, k$) are those determined by (4.9). Clearly, the numerator equals the derivative of the left-hand side of (4.8) with respect to λ_j except for the factor $(-M)$. This implies that if J_{jj} vanishes, then the discriminant of (4.8),

$$D^{-2}[E(z_j^{XY})^{-1} + E^{-1}]^2 + 4(Ds)^2(z_j^{XY})^{-1}$$

must vanish. However, from the definitions of (s, D, E) and (4.9), it is easily shown that the discriminant is non-vanishing. Thus, all the diagonal elements J_{jj} of the Jacobian are non-vanishing. Therefore, the Jacobian determinant is non-vanishing also.

Next, we show that the Bethe state (4.1) constructed from the solution λ is non-vanishing for $(\beta, \Delta, h)=(\beta_0, 1, h_0)$.

Note that for $\Delta=1$, (4.4) becomes

$$A_P = \text{sgn}(P) A_{(1, \dots, k)},$$

where sgn denotes the signature of the permutation P . In particular,

$$\langle 2, 4, \dots, 2k | B_k \rangle = A_{(1, \dots, k)} \sum_P \text{sgn}(P) z_{P1}^{XY} (z_{P2}^{XY})^2 \dots (z_{Pk}^{XY})^k \\ = A_{(1, \dots, k)} z_1^{XY} \dots z_k^{XY} \prod_{i < j} (z_j^{XY} - z_i^{XY}),$$

where the second equality is obtained by the Vandermonde determinant. This implies that the Bethe state is non-vanishing because of the condition (4.12). Thus, the proof of the lemma is complete. \square

Lemma 4.4. Let $\lambda=(\lambda_1, \dots, \lambda_k)$ be a solution to the system of the Bethe-ansatz equations (4.7). Then, there exists a polynomial \mathcal{P} of λ_j ($j=1, \dots, k$) and the parameters (s, D, E) such that

$$\mathcal{P}(\lambda_j, s, D, E)=0. \quad (j=1, \dots, k) \tag{4.13}$$

Proof From the definitions of the parameters $(s, D, E, c, \tilde{\Delta})$, the Bethe-ansatz equations (4.7) can be rewritten as the algebraic equations with k unknowns $(\lambda_1, \dots, \lambda_k)$ and the parameters (s, D, E) . In addition, the statement of Lemma 4.3 implies that the Bethe-ansatz equations (4.7) are regular, i.e., these have a finite number of solutions. Therefore, by applying the elimination method to (4.7), we obtain (4.13). \square

We wish to treat similarly the solutions to the system of the Bethe-ansatz equations in Remark 4.2. However, if some of the elements of the solution λ to (4.10) vanish, then the Jacobian matrix corresponding to the one in Lemma 4.3 has an indeterminate form 0/0. In the following, we consider only those solutions to (4.10) other than λ such that some of the elements of λ vanish, the latter being unnecessary for calculating the free energy as will be shown in the next section.

We define K^0 to be the set of all the solutions $\lambda=(\lambda_1, \dots, \lambda_k)$ ($k=0, 1, \dots, 2M$) to the system of the Bethe-ansatz equations for $\beta=0$ (see Remark 4.2) such that $\lambda_j \neq 0$ ($j=1, \dots, k$) and the z 's in (4.11) satisfy the condition (4.12).

Lemma 4.5. Let $\lambda^0 \in K^0$. Then, for any $(\Delta_0, h_0) \in \mathbb{C}^2$, there exists a solution λ to the system of the Bethe-ansatz equations (4.7) analytic in a neighborhood $\mathcal{D} \subset \mathbb{C}^3$ of $(\beta, \Delta, h)=(0, \Delta_0, h_0)$ such that $\lambda=\lambda^0$ for $(\beta, \Delta, h)=(0, \Delta_0, h_0)$ and that the Bethe state (4.1) constructed from the solution λ is non-vanishing.

§ 5. Maximum eigenvalue of the transfer matrix

In order to show that one of the Bethe-ansatz eigenvalues (4.5) equals the maximum eigenvalue Λ_{2M}^{\max} of the transfer matrix \hat{U}_{2M} , we study the properties of these eigenvalues.

Lemma 5.1. For any $(\beta, \Delta, h) \in \mathbb{R}_p \times \mathbb{R}^2$, the maximum eigenvalue $\Lambda_{2M; k}^{\max}$ of $\hat{U}_{2M; k}$ is positive and simple, where the subscript k denotes the restriction to the k -down-spin subspace.

Proof In the foregoing basis system (2.10), the matrices \hat{R}_{2M} and \hat{R}'_{2M} have positive diagonal elements and non-negative off-diagonal elements. Further, non-vanishing off-diagonal elements connect every two spin arrangements with one pair of neighboring opposite spins flipped. Therefore, any two basis vectors with k down spins can be connected with a positive matrix element by sufficiently many applications of $\hat{R}'_{2M}\hat{R}_{2M}$, but two basis vectors with different numbers of down spins can never be connected. Thus, the lemma follows from (3.10) and the Perron-Frobenius theorem. \square

Since the eigenvalue $\Lambda_{2M; k}^{\max}$ is a root of the characteristic equation of the matrix $\hat{U}_{2M; k}$, we obtain:

Corollary 5.2. For given $(\beta, \Delta, h) \in \mathbb{R}_p \times \mathbb{R}^2$, there exists a neighborhood $\mathcal{D} \subset \mathbb{C}^3$

of (β, Δ, h) such that the eigenvalue $\Lambda_{2M; k}^{\max}$ is simple and analytic in the three complex variables (β, Δ, h) .

THEOREM 5.3.

$$\Lambda_{2M}^{\max} = \Lambda_{2M; M}^{\max}. \tag{5.1}$$

Proof For any state $|\omega_{2M}\rangle$, $\delta_F|\omega_{2M}\rangle$ is an M -down-spin or zero vector by (3.9). Therefore, from Theorem 3.2 and (3.12), we obtain (5.1). \square

Next, we study the properties of the Bethe-ansatz eigenvalues (4.5) in the $\Delta=1$ case, i.e., the case of the isotropic XY model.

Lemma 5.4. For $\Delta=1$, the limit $L \uparrow \infty$ of

$$\widehat{R}_{2M}^{(L)} := [(2/D)^{2M} \widehat{R}'_{2M} \widehat{R}_{2M}]^{ML}$$

with

$$\exp(-\beta/M) = (2ML)^{-1} \gamma_1 \quad \text{and} \quad \beta h = L^{-1} \gamma_2 \quad (\gamma_1, \gamma_2 = \text{const}) \tag{5.2}$$

becomes the density matrix of the isotropic XY model, i.e.,

$$\lim_{L \uparrow \infty} \widehat{R}_{2M}^{(L)} = \exp[2^{-1} \gamma_1 \sum_{j=1}^{2M} (\delta_{2M; j^x} \delta_{2M; j+1^x} + \delta_{2M; j^y} \delta_{2M; j+1^y})]. \tag{5.3}$$

Proof Since the matrix (3.6) can be rewritten as

$$\widehat{V}_{2; i, j}^{(0)} = 2^{-1} D [1 + (\gamma_1/2ML) (\delta_{2; i^x} \delta_{2; j^x} + \delta_{2; i^y} \delta_{2; j^y}) - (\gamma_1/2ML)^2 \delta_{2; i^z} \delta_{2; j^z}],$$

we obtain (5.3) from the definitions of the matrices. \square

We define $\mu^{(k)} = (\mu_1, \dots, \mu_k)$ ($k=0, 1, \dots, 2M$) by

$$\mu_j = 2^{-1} \left[D^{-1} (E z_j^{-1} + E^{-1}) + \sqrt{D^{-2} (E z_j^{-1} + E^{-1})^2 + 4(Ds)^2 z_j^{-1}} \right]$$

with

$$z_j = \exp(2\pi i I_j / M), \tag{5.4}$$

where

$$I_j := -2^{-1}(k-1) + j - 1. \quad (j=1, \dots, k)$$

Further, we define

$$\Lambda_{2M; k}(\mu) := (Ds)^{M-k} \mu_1 \dots \mu_k. \quad (k=0, 1, \dots, 2M)$$

Then, from the definitions of the sets K^{XY} and K^0 , we have:

Lemma 5.5.

$$\mu^{(k)} \in K^{XY}$$

and

$$\mu^{(k)} \in K^0 \text{ for } \beta = 0. \quad (k=0, 1, \dots, 2M)$$

Lemma 5.6. Let $\Delta=1$. Then, for any $(\beta, h) \in \mathbf{R}_{NN} \times \mathbf{R}$, the maximum eigenvalue $\Lambda_{2M; k}^{\max}$ equals $\Lambda_{2M; k}(\mu)$, where \mathbf{R}_{NN} is the set of non-negative numbers.

Proof We consider first the case $\beta > 0$. From Lemmas 4.3 and 5.5, $\Lambda_{2M; k}(\mu)$ becomes the Bethe-ansatz eigenvalue of the transfer matrix \hat{U}_{2M} . Therefore, by (3.10),

$$\Lambda_{2M; k}^{(L)} := [(2/D)^M \Lambda_{2M; k}(\mu)]^{2ML}$$

becomes an eigenvalue of the matrix $\hat{R}_{2M}^{(L)}$ in Lemma 5.4. Further, we consider the limit $L \uparrow \infty$ in Lemma 5.4 so that from the definition of $\Lambda_{2M; k}(\mu)$ and (5.2), we obtain

$$\lim_{L \uparrow \infty} \Lambda_{2M; k}^{(L)} = \exp\left\{\gamma_1 \sum_{j=1}^k [(z_j)^{1/2} + (z_j)^{-1/2}]\right\}. \tag{5.5}$$

The right-hand side equals the well-known maximum and simple eigenvalue²⁴⁾ of the density matrix of the isotropic XY model (5.3) in the k -down-spin space.

We prove the statement of the lemma by deducing a contradiction from the assumption that $\Lambda_{2M; k}^{\max} \neq \Lambda_{2M; k}(\mu)$ for β and h as determined by (5.2) for a certain L_0 .

Since $\Lambda_{2M; k}^{\max}$ is simple and analytic as shown in Corollary 5.2, $\Lambda_{2M; k}^{\max}$ with $L = L_0 + 1$ is not equal to $\Lambda_{2M; k}(\mu)$ with $L = L_0 + 1$. The same results holds for the maximum eigenvalue of $\hat{R}_{2M; k}^{(L)}$. Therefore, the limit $L \uparrow \infty$ of $\Lambda_{2M; k}^{(L)}$ is not the maximum one, or is degenerate. This contradicts the above result (5.5). Thus, the case $\beta > 0$ has been proved. In the case $\beta = 0$, consider the limit $\beta \downarrow 0$. \square

For the $\Delta \neq 1$ case, we consider the analytic continuation of the solutions to the system of the Bethe-ansatz equations (4.7) and the corresponding eigenvalues (4.5) with respect to β or Δ .

Lemma 5.7. For any $(\Delta, h) \in \mathbf{R}^2$, there exists $\varepsilon > 0$ such that for $\beta \in [0, \varepsilon]$, the Bethe-ansatz equations with k unknowns in (4.7) have the unique solution λ such that for $\beta = 0, \lambda = \mu^{(k)}(\beta = 0)$ and that the corresponding Bethe-ansatz eigenvalue (4.5) equals the maximum eigenvalue $\Lambda_{2M; k}^{\max}$ of the transfer matrix $\hat{U}_{2M; k}$.

Proof From Lemmas 4.3, 4.5 and 5.5, there exists a solution λ to the Bethe-ansatz equations with k unknowns in (4.7) analytic in a neighborhood $\mathcal{D} \subset \mathbf{C}^3$ of $(\beta, \Delta, h) = (0, 1, h)$ such that for $(\beta, \Delta, h) = (0, 1, h), \lambda = \mu^{(k)}$. Therefore, the corresponding eigenvalue $\Lambda_{2M; k}$ of (4.5) is an analytic function of (β, Δ, h) in \mathcal{D} . Further, from Corollary 5.2 and Lemma 5.6, there exists a domain $\mathcal{D}' \subset \mathcal{D}$ such that $\Lambda_{2M; k} = \Lambda_{2M; k}^{\max}$ in \mathcal{D}' . Therefore, from Lemma 4.5 and Corollary 5.2, one can find the analytic continuation of the solution λ and the corresponding eigenvalue $\Lambda_{2M; k}$ with respect to (β, Δ, h) along the path,

$$\gamma_t := (0, 1 - t + t\Delta, h). \quad (0 \leq t \leq 1)$$

Thus, we obtain the statement of the lemma. \square

THEOREM 5.8. For any given $(\beta_0, \Delta_0, h_0) \in \mathbf{R}_{NN} \times \mathbf{R}^2$, the maximum eigenvalue $\Lambda_{2M; k}^{\max}$ of the transfer matrix \hat{U}_{2M} can be constructed from the Bethe-ansatz eigenvalue (4.5) with a solution to the Bethe-ansatz equations with k unknowns in (4.7), where \mathbf{R}_{NN} is defined in Lemma 5.6.

Proof Let λ be the solution to the Bethe-ansatz equations which is obtained by the analytic continuation in Lemma 5.7. Then, from Lemma 4.4, λ is a vector-valued algebraic function of the complex variable β for fixed $(\Delta, h) = (\Delta_0, h_0)$. Therefore, if β_0 is not a singular point of λ , then one can find the analytic continuation of β and the corresponding eigenvalue $\Lambda_{2M; k}$ with respect to β along the path γ such that

$$\gamma \subset \{\beta \in \mathbf{C} \mid \Lambda_{2M; k}^{\max} \text{ is simple and analytic in } \beta\}$$

from Corollary 5.2 and Lemma 5.7. If β_0 is a singular point of λ , then we consider the limit $\beta \rightarrow \beta_0$ in addition to the above procedure. \square

Remark As another proof of the theorem, one can also use the analytic continuation with respect to Δ for fixed $(\beta, h) = (\beta_0, h_0)$.

This theorem combined with Theorem 5.3 gives :

THEOREM 5.9. For calculating the free energy per spin of the model (2.1) in the thermodynamic limit, it is sufficient to find only one solution λ to the Bethe-ansatz equations with $k=M$ unknowns in (4.7) which leads to the maximum eigenvalue Λ_{2M}^{\max} of the transfer matrix \hat{U}_{2M} . In fact, the free energy is determined by the Bethe-ansatz eigenvalue (4.5) as will be shown in the following sections.

To conclude this section, we emphasize the following. One can also apply the Bethe ansatz directly to the eigenvalue problem of the Hamiltonian (2.1) following the original way.¹⁾ However, for calculating the free energy, one needs the assumption of completeness of the system of the Bethe states; this assumption has been proved only partially.¹³⁾ If this assumption is correct, one must notice that not all the solutions to the system of the Bethe-ansatz equations give the eigenvectors of the Hamiltonian;¹³⁾ we have to examine each solution to select the right ones. In our thermal Bethe-ansatz method, it is sufficient to find only one solution to the Bethe-ansatz equations as shown in Theorem 5.9.

§ 6. Isotropic XY case

In this section, we calculate the free energy per spin of the isotropic ($\Delta=1$) XY model in the thermodynamic limit as an example. In the following, we restrict β and h to non-negative numbers, respectively.

From Lemmas 5.3, 5.6 and the definition of $\Lambda_{2M; M}(\mu)$, we have

$$\log \Lambda_{2M}^{\max} = -2^{-1}\beta + J_M$$

with

$$J_M = \sum_{j=1}^M \log \{ 2^{-1} [(Ez_j^{-1} + E^{-1}) + \sqrt{(Ez_j^{-1} + E^{-1})^2 + 4 \sinh^2(\beta/M) z_j^{-1}}] \}.$$

Thus, for a sufficiently small β ,

$$J_M = \frac{1}{\pi} \sum_{j=1}^M \int_0^\pi dx \log [Ez_j^{-1} + E^{-1} + 2iz_j^{-1/2} \sinh(\beta/M) \cos x]$$

by the formula,

$$\int_0^\pi \log [a + b \cos x] dx = \pi \log [2^{-1} (a + \sqrt{a^2 - b^2})]. \quad (a \geq |b|)$$

But, by Corollary 5.2, this holds for all $\beta \in \mathbf{R}$. The limit $M \uparrow \infty$ can be calculated by using the properties of the z 's of (5.4) as shown in Appendix C. Thus, we obtain

$$\lim_{M \uparrow \infty} \log \Lambda_{2M}^{\max} = -\frac{\beta}{2} + \frac{1}{\pi} \int_0^\pi dx \log \{ 2 \cosh \beta [\cos x + h] \}.$$

Therefore, by Theorems 3.2 and 3.3, we obtain the well-known result for the free energy of the isotropic XY model,^{23),24)}

$$f(\beta, h) = \frac{1}{2} - \frac{1}{\beta\pi} \int_0^\pi dx \log \{ 2 \cosh \beta [\cos x + h] \}.$$

Recently, Inoue and Suzuki²⁵⁾ obtained the same result by diagonalizing the transfer matrix of this special case by the method of the Jordan-Wigner transformation.

§ 7. Isotropic ferromagnetic case

As a second example, we calculate the low temperature limit of the zero-field free energy and the susceptibility of the model (2.1) with the anisotropy parameter $\Delta=0$. Here, we have to resort to numerical calculations to solve the system of the Bethe-ansatz equations.

For the purpose of studying the properties of the Bethe-ansatz equations (4.7) for $\Delta=0$ and the state with M -down spins, it is convenient to apply the transformation $\lambda \leftrightarrow q$,

$$E\lambda_j = [(2c)^{-1} - iq_j]^{-1} + s, \quad (j=1, \dots, M) \tag{7.1}$$

where E, c and s are defined in (3.7) and (4.6). Then, we have

Remark 7.1. The solution $\mu^{(M)}(\beta=0)$ in Lemmas 5.5 and 5.6 transforms into

$$g_j^{(0)} := -2^{-1} \tan \left[\frac{\pi}{2M} (2j - M - 1) \right]. \quad (j=1, \dots, M) \tag{7.2}$$

Therefore, upon taking the logarithm, the system of the Bethe-ansatz equations (4.7) for $\Delta=0$ whose solution satisfies the condition,

$$\lambda_j(\beta=0) = \mu_j^{(M)}(\beta=0) \quad (j=1, \dots, M) \tag{7.3}$$

can be rewritten as

$$\begin{aligned} & -2i\beta h/M + 2[\tan^{-1}(Aq_j) - \tan^{-1}(2cq_j)] \\ & = \frac{\pi}{M}(2j - M - 1) + \frac{2}{M} \sum_{i=1}^M \tan^{-1}[s(q_j - q_i)], \quad (j=1, \dots, M) \end{aligned} \quad (7.4)$$

where we take the principal value of \tan^{-1} and

$$A := 2cs/(1+c). \quad (7.5)$$

From Theorem 5.3, Lemma 5.7 and Remark 7.1, we obtain:

Lemma 7.2. Let $h \in \mathbf{R}$. Then, there exists $\varepsilon > 0$ such that for any $\beta \in [0, \varepsilon]$, the system of the Bethe-ansatz equations (7.4) has the unique solution q_j ($j=1, \dots, M$) which gives the maximum eigenvalue $\Lambda_{2M}^{\max} = \Lambda_{2M; M}^{\max}$ of the transfer matrix \hat{U}_{2M} .

We rewrite the maximum eigenvalue Λ_{2M}^{\max} in terms of the solution q_j ($j=1, \dots, M$). By (7.1) and (7.5), we have

$$\begin{aligned} \log \lambda_j &= -\beta h/M + \log(1+c) + 2^{-1} \log[1 + (Aq_j)^2] \\ & \quad - 2^{-1} \log[1 + (2cq_j)^2] - i \tan^{-1}(Aq_j) + i \tan^{-1}(2cq_j), \quad (j=1, \dots, M) \end{aligned}$$

where we take the principal value of \tan^{-1} and \log . Therefore, by (4.5) and (7.4), the maximum eigenvalue can be rewritten as

$$\log \Lambda_{2M}^{\max} = M \log(1+c) + 2^{-1} \sum_{j=1}^M \{ \log[1 + (Aq_j)^2] - \log[1 + (2cq_j)^2] \} \quad (7.6)$$

in terms of the solution q_j ($j=1, \dots, M$) in Lemma 7.2.

To calculate the maximum eigenvalue (7.6), we prepare the following two lemmas.

Lemma 7.3. Let $h \in \mathbf{R}$. Then, the unique solution q_j ($j=1, \dots, M$) for the state with $M=2m$ down spins ($m=1, 2, \dots$) in Lemma 7.2 satisfies

$$q_{m+j} = -q_j^*. \quad (j=1, \dots, m) \quad (7.7)$$

Therefore, the system of the Bethe-ansatz equations (7.4) can be written as

$$\begin{aligned} & -i\beta h/m + 2[\tan^{-1}(Ap_j) - \tan^{-1}(2cp_j)] \\ & = \pi(2j-1)/(2m) + m^{-1} \sum_{i=1}^m \{ \tan^{-1}[s(p_j - p_i)] + \tan^{-1}[s(p_j + p_i^*)] \}, \quad (j=1, \dots, m) \end{aligned} \quad (7.8)$$

where

$$p_j = q_{m+j}. \quad (j=1, \dots, m) \quad (7.9)$$

Proof From the assumption $h \in \mathbf{R}$ and the form of the system of the Bethe-ansatz equations (4.7) for $\Delta=0$, we know that if $(\lambda_1, \dots, \lambda_M)$ is a solution, then $(\lambda_1^*, \dots, \lambda_M^*)$ is also a solution. Therefore, (7.7) follows from the positivity of the maximum eigenvalue $\Lambda_{2M; M}^{\max}$ (see Lemma 5.1), the uniqueness of the solution which gives the maximum eigenvalue and the transformation (7.1). \square

Lemma 7.4. There exists $\varepsilon > 0$ such that for any $\beta \in [0, \varepsilon)$, the solution p_j ($j=1, \dots, m$) in Lemma 7.3 can be written as a power of series in $h \in \mathbf{R}$ if h is sufficiently small,

$$p_j = \rho_j^{(0)} + ih\rho_j^{(1)} + h^2\rho_j^{(2)} + ih^3\rho_j^{(3)} + \dots, \quad (j=1, \dots, m)$$

where $\rho_j^{(l)}$ ($l=0, 1, \dots$) are real numbers determined by the system of the Bethe-ansatz equations (7.8).

Proof Let $q_j(h)$ ($j=1, \dots, M$) be the unique solution in Lemma 7.2. Then, by applying the transformation $h \rightarrow -h$ and taking the complex conjugate of (7.4), we obtain

$$q_j(h) = q_j(-h)^* \quad (j=1, \dots, M)$$

This property combined with Lemma 4.5 and (7.9) gives the statement of the lemma. \square

By Theorem 3.3 and the above two lemmas, the finite- M free energy can be written as

$$f^{(M)} = f^{(M)}(h=0) - 2^{-1}h^2\chi^{(M)} + \dots,$$

where the finite- M zero-field free energy $f^{(M)}(h=0)$ and the finite- M susceptibility $\chi^{(M)}$ are given by

$$f^{(M)}(h=0) = -M\beta^{-1}\log(1+c) + \beta^{-1}\sum_{j=1}^m \{ \log[1+(2c\rho_j^{(0)})^2] - \log[1+(A\rho_j^{(0)})^2] \} \tag{7.10}$$

and

$$\begin{aligned} \chi^{(M)} = & 2\beta^{-1}\sum_{j=1}^m \left[(\rho_j^{(1)})^2 \left\{ \frac{(2c)^2[1-(2c\rho_j^{(0)})^2]}{[1+(2c\rho_j^{(0)})^2]^2} - \frac{A^2[1-(A\rho_j^{(0)})^2]}{[1+(A\rho_j^{(0)})^2]^2} \right\} \right. \\ & \left. + 2\rho_j^{(0)}\rho_j^{(2)} \left[\frac{A^2}{1+(A\rho_j^{(0)})^2} - \frac{(2c)^2}{1+(2c\rho_j^{(0)})^2} \right] \right], \end{aligned} \tag{7.11}$$

respectively; $\rho_j^{(0)}$, $\rho_j^{(1)}$ and $\rho_j^{(2)}$ ($j=1, \dots, m$) are determined by the system of the Bethe-ansatz equations,

$$\begin{aligned} & 2[\tan^{-1}(A\rho_j^{(0)}) - \tan^{-1}(2c\rho_j^{(0)})] \\ & = \pi(2j-1)/(2m) + m^{-1}\sum_{l=1}^m \{ \tan^{-1}[s(\rho_j^{(0)} - \rho_l^{(0)})] + \tan^{-1}[s(\rho_j^{(0)} + \rho_l^{(0)})] \}, \end{aligned} \tag{7.12}$$

$$\begin{aligned} & -\beta/(2m) + \frac{A\rho_j^{(1)}}{1+(A\rho_j^{(0)})^2} - \frac{2c\rho_j^{(1)}}{1+(2c\rho_j^{(0)})^2} \\ & = (2m)^{-1}\sum_{l=1}^m s(\rho_j^{(1)} - \rho_l^{(1)}) \left[\frac{1}{1+s^2(\rho_j^{(0)} - \rho_l^{(0)})^2} + \frac{1}{1+s^2(\rho_j^{(0)} + \rho_l^{(0)})^2} \right] \end{aligned} \tag{7.13}$$

and

$$\begin{aligned} & \frac{A\rho_j^{(2)}}{1+(A\rho_j^{(0)})^2} - \frac{2c\rho_j^{(2)}}{1+(2c\rho_j^{(0)})^2} + \frac{A\rho_j^{(0)}(A\rho_j^{(1)})^2}{[1+(A\rho_j^{(0)})^2]^2} - \frac{2c\rho_j^{(0)}(2c\rho_j^{(1)})^2}{[1+(2c\rho_j^{(0)})^2]^2} \\ &= (2m)^{-1} \sum_{l=1}^m \left\{ \frac{s(\rho_j^{(2)} - \rho_l^{(2)})}{1+s^2(\rho_j^{(0)} - \rho_l^{(0)})^2} + \frac{s(\rho_j^{(2)} + \rho_l^{(2)})}{1+s^2(\rho_j^{(0)} + \rho_l^{(0)})^2} \right. \\ & \quad \left. + \frac{s^3(\rho_j^{(0)} - \rho_l^{(0)})(\rho_j^{(1)} - \rho_l^{(1)})^2}{[1+s^2(\rho_j^{(0)} - \rho_l^{(0)})^2]^2} + \frac{s^3(\rho_j^{(0)} + \rho_l^{(0)})(\rho_j^{(1)} - \rho_l^{(1)})^2}{[1+s^2(\rho_j^{(0)} + \rho_l^{(0)})^2]^2} \right\}. \end{aligned} \tag{7.14}$$

(j=1, ..., m)

We solve the system of the Bethe-ansatz equations (7.12)~(7.14) for $\rho_j^{(0)}, \rho_j^{(1)}$ and $\rho_j^{(2)}$ (j=1, ..., m) numerically by iteration method. We consider first (7.12). For given $X_j(i)$, we define

$$\rho_j^{(0)}(i) = -(2c)^{-1} \tan[\pi(2j-1)/(2m) + X_j(i)]$$

and proceed to the (i+1)th iteration by

$$\begin{aligned} X_j(i+1) &= (1-a)X_j(i) + \alpha m^{-1} \sum_{l=1}^m \{ \tan^{-1}[s(\rho_j^{(0)}(i) - \rho_l^{(0)}(i))] \\ & \quad + \tan^{-1}[s(\rho_j^{(0)}(i) + \rho_l^{(0)}(i))] - 2 \tan^{-1}(A\rho_j^{(0)}(i)) \}, \\ & \quad (j=1, \dots, m; \quad i=0, 1, \dots) \end{aligned}$$

thus repeating the process, where the acceleration factor α is determined by numerical experiment for small m to minimize the number of times of the iteration for desired accuracy. The initial values $X_j(0)$ (j=1, ..., m) are chosen as follows. We recall, to begin with, that at $\beta=0$ the solution to (7.12) is unique and is guaranteed by Lemma 7.2 to give the maximum eigenvalue Λ_{2M}^{\max} . Then, we proceed with a decreasing sequence of temperatures $0 = \beta_0 < \beta_1 < \dots < \beta_i < \dots$, taking the iteration limit $X_j(i_{\max})$ for β_k as the initial value for the iteration for β_{k+1} . The initial value for the highest temperature β_0 is taken to be $X_j(0) = 0$ (j=1, ..., m). From the iteration limits for each temperature, we can obtain the finite- M free energy $f^{(M)}(\beta, h=0)$ of (7.10).

Similarly, we can find the solutions $\rho_j^{(1)}$ and $\rho_j^{(2)}$ (j=1, ..., m) of the system of the Bethe-ansatz equations (7.13) and (7.14). Then, the finite- M susceptibility $\chi^{(M)}$ is obtained from (7.11) and the solution $\rho_j^{(0)}$ (j=1, ..., m) so obtained.

Now we have to take the limit $M \uparrow \infty$. For this purpose, we prepare two lemmas.

Lemma 7.5.^{17)~19),36)} The finite- M partition function (2.8) can naturally be extended to negative integers M . The function $Z_{2n,B}^{(M)}$ ($M = \pm 1, \pm 2, \dots$) so obtained is even with respect to M , i.e.,

$$Z_{2n,B}^{(-M)} = Z_{2n,B}^{(M)},$$

where B denotes the boundary condition (2.3).

Proof From (2.8), we have¹⁹⁾

$$Z_{2n,B}^{(-M)} = \text{Tr} \left\{ \exp \left[\frac{\beta}{M} \hat{H}_{2n}^{(1)} \right] \exp \left[\frac{\beta}{M} \hat{H}_{2n,B}^{(2)} \right] \right\}^{-M}$$

$$\begin{aligned}
 &= \text{Tr} \left\{ \exp \left[-\frac{\beta}{M} \hat{H}_{2n,B}^{(2)} \right] \exp \left[-\frac{\beta}{M} \hat{H}_{2n}^{(1)} \right] \right\}^M \\
 &= Z_{2n,B}^{(M)}. \quad \square
 \end{aligned}$$

This combined with Theorem 3.2 gives:

Lemma 7.6.^{17)~19),36)}

$$f^{(-M)} = f^{(M)}.$$

This implies that if $f^{(M)}$ can be expanded in powers of M^{-1} , then there appear only even powers. Thus, approximately for sufficiently large M ,

$$f^{(M)} \sim \sum_{l=0}^k c_l M^{-2l}. \tag{7.15}$$

Then, by Theorem 3.2, the free energy equals the coefficient c_0 approximately. In order to find the coefficient c_0 we determine the expansion (7.15) by the least-squares fitting at several M 's to the calculated $f^{(M)}$ with the degree k being chosen by the AIC method³⁷⁾ based on the consideration that the fit would not be good enough for smaller k while numerical errors would be disturbing at larger k . We remark in passing that one may try an expansion in powers of M^{-1} in the same way, but it results in worse fitting than the one from (7.15) in our numerical experiment.

We solve the system of the Bethe-ansatz equations (7.12)~(7.14) of

$$M = 2m = 1000, 1100, 1200, 1400, 1600, 1800, 2000, 2400$$

for each of the temperatures as given by

$$(J\beta)^{-1/2} = 0.02, 0.04, 0.06, 0.08, 0.10, 0.12, 0.14, 0.16, 0.18, 0.20$$

and of

$$M = 4000 \quad \text{for} \quad (J\beta)^{-1/2} = 0.02$$

using the desk-top computer NEC PC-9801F, where J is the exchange integral, whose value we have taken to be 2 so far. Then, the zero-field free energy $f(\beta, h=0)$ is obtained from (7.10) and the numerical extrapolation discussed above.

For the susceptibility χ , we have not been able to prove a theorem corresponding to Theorem 3.2 for the free energy that permits one to interchange the order of the thermodynamic limit and the limit $M \uparrow \infty$ of the Trotter number. In the calculation of the susceptibility χ , therefore, we assume the interchangeability leaving its justification for future studies. Thus, we write the susceptibility χ as

$$\chi = \lim_{M \uparrow \infty} \chi^{(M)}, \tag{7.16}$$

using $\chi^{(M)}$, the finite- M (7.11) in the thermodynamic limit. In this way, the susceptibility χ is obtained by the same procedure as above.

The M^{-2} dependence of $-f^{(M)}(\beta, h=0) \times \beta^{3/2} J^{1/2}$ and $\chi^{(M)} \beta^{-2} J^{-1}$ at fixed temperature $(J\beta)^{-1} = 4 \times 10^{-4}$ are shown in Figs. 7.1 and 7.2, respectively. The temperature dependence of the zero-field free energy $f(\beta, h=0)$ multiplied by $\beta^{3/2}$ and the suscep-

tibility χ by β^{-2} are given in Figs. 7.3 and 7.4, respectively. It is observed that the curves in Figs. 7.3 and 7.4 approach non-zero and finite values with well-defined gradients as $(J\beta)^{-1} \downarrow 0$, implying that the critical exponents of the specific heat and the susceptibility are given by $\alpha = -0.5$ and $\gamma = 2$, respectively. These results agree with Takahashi and Yamada's (see Table 7.1),⁷⁾ the best so far available, which were obtained by Takahashi and Suzuki's integral equation method⁵⁾ based on the Bethe ansatz for the eigenvalue problem of the Hamiltonian.

We remark in passing the following. By using the same integral equation method combined with the finite-string-size scaling, Schlottmann obtained⁹⁾

$$\chi \sim 0.84 \times J\beta^2 / \log(J\beta). \quad (\beta \uparrow \infty)$$

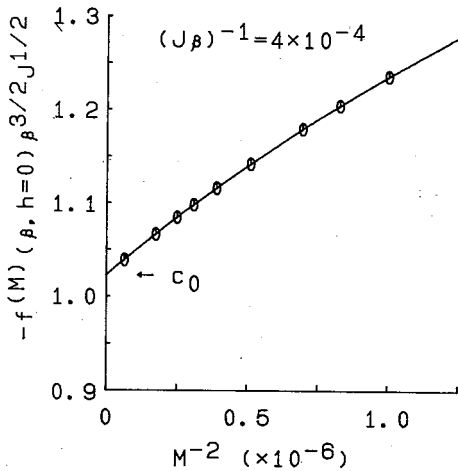


Fig. 7.1. $-f^{(M)}(\beta, h=0) \times \beta^{3/2} J^{1/2}$ versus M^{-2} at temperature $(J\beta)^{-1} = 4 \times 10^{-4}$.

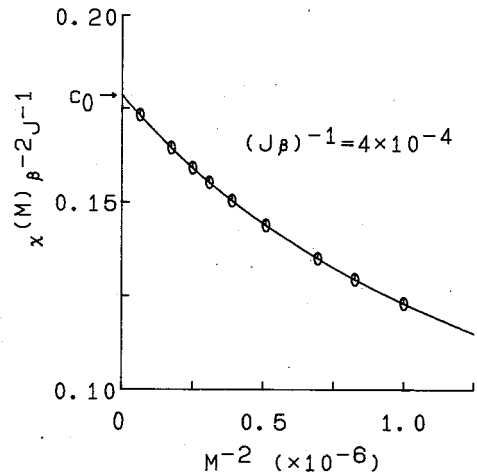


Fig. 7.2. $\chi^{(M)} \beta^{-2} J^{-1}$ versus M^{-2} at temperature $(J\beta)^{-1} = 4 \times 10^{-4}$.

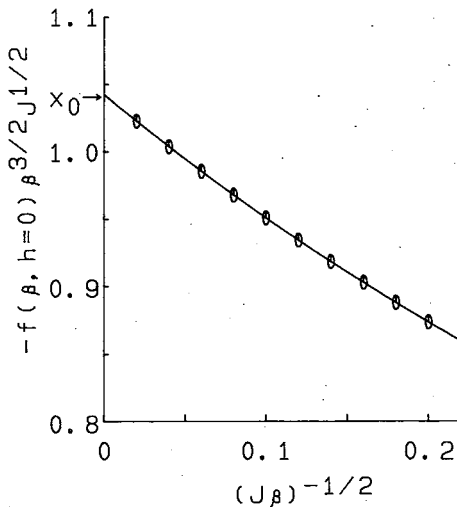


Fig. 7.3. $-f(\beta, h=0) \times \beta^{3/2} J^{1/2}$ versus $(J\beta)^{-1/2}$. As temperature $(J\beta)^{-1} \downarrow 0$, it approaches the critical amplitude x_0 .

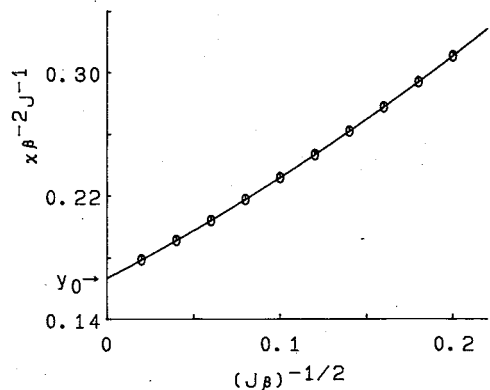


Fig. 7.4. $\chi \beta^{-2} J^{-1}$ versus $(J\beta)^{-1/2}$. As temperature $(J\beta)^{-1} \downarrow 0$, it approaches the critical amplitude y_0 .

Table 7.1. The critical exponents α and γ obtained using various methods.

Authors	Methods	α	γ
Baker et al. (1964)	High temperature series expansion and Padé approximation	—	1.66 ± 0.07
Bonner and Fisher (1964)	Numerical diagonalization of the Hamiltonian	-0.45 ~ -0.5	1.8
Kondo and Yamaji (1972)	Green function decoupling approximation	-1/2	2
Lyklema (1983)	Handscomb and Monte Carlo method	-0.3 ± 0.1	1.75 ± 0.02
Cullen and Landau (1983)	Trotter formula and Monte Carlo method	—	1.32
Takahashi and Yamada (1985)	Original Bethe-ansatz method	-1/2	2
Schlottmann (1985)	Original Bethe-ansatz method	-0.49 ± 0.02	2.00 ± 0.02
Inoue and Suzuki (1986)	Pair-product approximation and renormalization group method	—	2
Takahashi (1986)	Spin wave approximation	-1/2	2
Present author	Thermal Bethe-ansatz method	-1/2	2

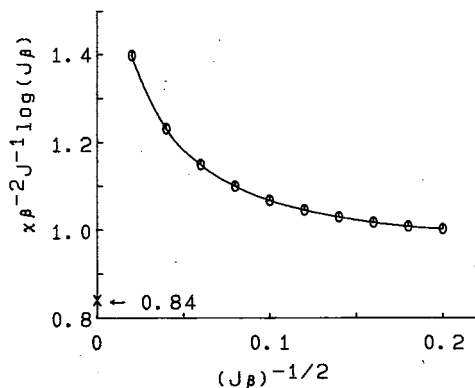


Fig. 7.5. $\chi\beta^{-2}J^{-1}\log(J\beta)$ versus $(J\beta)^{-1/2}$. The curve does not approach a finite value as temperature $(J\beta)^{-1} \downarrow 0$.

However, it is incorrect as Takahashi pointed out.²⁶⁾ To see this, we plot our values of $\chi\beta^{-2}J^{-1}\log(J\beta)$ as a function of $(J\beta)^{-1/2}$ in Fig. 7.5. Clearly, it is observed that the curve diverges as $(J\beta)^{-1/2} \downarrow 0$. Thus, there is no such logarithmic correction in the susceptibility χ as was proposed by Schlottmann.

The results from other approximations^{27)~32)} are also given in Table 7.1. To compare our results with Takahashi and Yamada's⁷⁾ in detail, we assume that, in the low temperature limit, the zero-field free energy and the susceptibility can be expand-

Table 7.2. The coefficients of the low-temperature expansion of the zero-field free energy. The numbers in the brackets give the errors in the last digit.

Methods and authors	x_0	x_1	x_2
Green function decoupling approximation Kondo and Yamaji (1972)	$\frac{5}{6}$ $\times 1.0421869\dots$	$-7/3$	$6.581\dots$
Original Bethe-ansatz method Takahashi and Yamada (1985)	$1.042(1)$	$-1.00(2)$	$0.9(1)$
Spin wave approximation Takahashi (1986)	$1.0421869\dots$	-1	$1.2320919\dots$
Thermal Bethe-ansatz method Present author	$1.042186(2)$	$-0.9999(1)$	$0.952(3)$

Table 7.3. The coefficients of the low-temperature expansion of the susceptibility.

Methods and authors	y_0	y_1	y_2
Green function decoupling approximation Kondo and Yamaji (1972)	$1/6$	—	—
Original Bethe-ansatz method Takahashi and Yamada (1985)	$0.1667(5)$	$0.586(9)$	$0.7(1)$
Spin wave approximation Takahashi (1986)	$1/6$	$0.582597\dots$	$0.678839\dots$
Thermal Bethe-ansatz method Present author	$0.1666666(8)$	$0.58259(2)$	$0.6789(2)$

ed in powers of $w = (J\beta)^{-1/2}$ such that

$$-f(\beta, h=0) = Jw^3 \sum_{l=0}^{\infty} x_l w^l \quad (7.17)$$

and

$$\chi = J^{-1} w^{-4} \sum_{l=0}^{\infty} y_l w^l$$

as proposed by Takahashi and Yamada.⁷⁾ We approximate $-f(\beta, h=0) \times J^{-1} w^{-3}$ and $\chi \times Jw^4$ by polynomials in w and determine their coefficients by the least-squares fitting used above. As shown in Tables 7.2 and 7.3, our results are consistent with Takahashi and Yamada's⁷⁾ which they obtained by computing $f(\beta, h=0)$ and χ down to $(J\beta)^{-1} = 4 \times 10^{-3}$ using the supercomputer HITAC S-810. Our results are in fact more precise than theirs. Further, we notice that the results from the spin wave approximation²⁶⁾ deviate from the value of the third term in the zero-field free energy (7.17).

We remark:

- (a) Takahashi and Yamada used the Takahashi-Suzuki integral equations⁵⁾ which depend on the string conjecture,^{*} or more basically on the unproven assumption of the completeness of the system of the Bethe-eigenstates of the Hamiltonian (2·1).
- (b) Our results reconfirm that the spin wave approximation cannot be justified in the one-dimensional isotropic ferromagnetic model because of the disagreement mentioned above in the third term in the zero-field free energy (7·17). We recall that the spin-wave approximation as applied to the one-dimensional isotropic ferromagnetic model results in diverging zero-field magnetization per site, which Takahashi²⁶⁾ had to suppress by imposing an ad hoc constraint of zero-magnetization without reasonable ground. Nevertheless, it is remarkable that the coefficients of the first and the second term in (7·17) agree surprisingly well with those of ours.

In conclusion, we emphasize that our thermal Bethe-ansatz method uses no such assumption as the completeness of the system of the Bethe states that has been proved only partially and that it yields the better results than the previous methods do. It has to be noticed, however, that, for calculating the susceptibility, we used the assumption (7·16), namely, that the large Trotter number limit and the thermodynamic limit can be exchanged. Its proof is left for future studies.

Finally, we note that our thermal Bethe-ansatz method can be applied also to the one-dimensional Hubbard model. The detailed results will be reported in the near future.

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Appendix A

— Proof of Theorem 3.2^{19)~22)} —

First, we prepare the following lemma along the line of Suzuki and Inoue.^{21),22)}

Lemma A.1. Let $\hat{H}^{(1)}$, $\hat{H}^{(2)}$ and \hat{H}' be three Hermitian matrices satisfying $[\hat{H}^{(2)}, \hat{H}'] = 0$. Then,

$$|\log \text{Tr}\{\exp[\hat{H}^{(1)}]\exp[\hat{H}^{(2)}]\exp[\hat{H}']\}^M - \log \text{Tr}\{\exp[\hat{H}^{(1)}]\exp[\hat{H}^{(2)}]\}^M| \leq M\|\hat{H}'\|. \tag{A·1}$$

Proof Note that the left-hand side of (A·1) equals

$$\left| \int_0^1 dx \frac{d}{dx} \log \text{Tr}\{\exp[\hat{H}^{(1)}]\exp[\hat{H}^{(2)}]\exp[x\hat{H}']\}^M \right| = \left| \int_0^1 dx \frac{M \text{Tr}(\hat{H}'\hat{A}^\dagger\hat{A})}{\text{Tr}(\hat{A}^\dagger\hat{A})} \right|,$$

^{*}) Non-string solutions were found by Woynarovich in 1982,¹⁰⁾ by Babelon et al. in 1983¹¹⁾ and by Vladimirov in 1984.¹²⁾

where

$$\hat{A} := \begin{cases} \hat{Q}^{M/2} & (M = \text{even}) \\ \exp[2^{-1}\hat{H}^{(1)}]\exp[2^{-1}(\hat{H}^{(2)} + x\hat{H}')] \hat{Q}^{(M-1)/2}, & (M = \text{odd}) \end{cases}$$

with

$$\hat{Q} := \exp[2^{-1}(\hat{H}^{(2)} + x\hat{H}')] \exp[\hat{H}^{(1)}] \exp[2^{-1}(\hat{H}^{(2)} + x\hat{H}')].$$

The numerator of the integrand can be rewritten as

$$\text{Tr}(\hat{H}' \hat{A}^\dagger \hat{A}) = \sum_i E_i \langle e_i | \hat{A}^\dagger \hat{A} | e_i \rangle,$$

where $|e_i\rangle$ and E_i are the system of the orthonormal eigenvectors and the corresponding eigenvalues of the matrix \hat{H}' . Therefore, by $\langle e_i | \hat{A}^\dagger \hat{A} | e_i \rangle \geq 0$, we obtain

$$|\text{Tr}(\hat{H}' \hat{A}^\dagger \hat{A})| \leq \max_i (|E_i|) |\text{Tr}(\hat{A}^\dagger \hat{A})|,$$

and the statement of the lemma follows. \square

By putting

$$\hat{H}^{(1)} = -\frac{\beta}{M} \hat{H}_{2n}^{(1)}, \quad \hat{H}^{(2)} = -\frac{\beta}{M} \hat{H}_{2n,F}^{(2)} \quad \text{and} \quad \hat{H}' = -\frac{\beta}{M} \hat{H}_{2n;2n,1}$$

in Lemma A.1, we obtain

$$|f^{(M)}(2n, P) - f^{(M)}(2n, F)| \leq (2n)^{-1} \|\hat{H}_{2;1,2}\|,$$

where

$$f^{(M)}(2n, B) := (2n\beta)^{-1} \log Z_{2n,B}^{(M)}$$

and F and P denote the boundary condition B in (2.3). Therefore, it is sufficient to show the existence of the double limit in (3.3) in the free boundary case $B = F$ of (2.3).

The finite- M free energy $f^{(M)}(2n, F)$ with free boundary condition shall be abbreviated as $f^{(M)}(2n)$, whenever there is no confusion.

Next we show that the sequence $f^{(M)}(2n)$ ($n = 1, 2, \dots$) converges uniformly with respect to M . For this purpose, we use arguments similar to Griffith's on the thermodynamic limit.^{19),33)}

First, we divide the Hamiltonian $-(\beta/M)\hat{H}_{2n,F}$ into three parts

$$\begin{aligned} \hat{H}^{(1)} &= -\frac{\beta}{M} \hat{H}_{2n}^{(1)}, \\ \hat{H}^{(2)} &= \sum_{l=0}^{L-1} \sum_{j=1}^{K-1} \left(-\frac{\beta}{M} \hat{H}_{2n;2lK+2j,2lK+2j+1} \right) \end{aligned}$$

and

$$\hat{H}' = \sum_{l=1}^{L-1} \left(-\frac{\beta}{M} \hat{H}_{2n;2lK,2lK+1} \right).$$

Then, Lemma A.1 gives the following lemma.

Lemma A.2. Let $n = KL$ ($K, L = 1, 2, \dots$). Then,

$$|f^{(M)}(2n) - f^{(M)}(2K)| \leq (2K)^{-1} \|\widehat{H}_{2;1,2}\|.$$

In the particular case $n = 2^p 2^q$ ($p, q = 1, 2, \dots$) of Lemma A.2, we obtain

$$|f^{(M)}(2 \cdot 2^{p+q}) - f^{(M)}(2 \cdot 2^p)| \leq 2^{-p-1} \|\widehat{H}_{2;1,2}\|.$$

This implies that $f^{(M)}(2 \cdot 2^p)$ is a Cauchy sequence in p and possesses a well-defined limit $f^{(M)}$. Further, as $q \uparrow \infty$, we have

$$|f^{(M)} - f^{(M)}(2 \cdot 2^p)| \leq 2^{-p-1} \|\widehat{H}_{2;1,2}\|.$$

The limit $f^{(M)}$ thus obtained for the particular sequence $\{n = 2^p\}$ is also obtained for an arbitrary sequence increasing to infinity. To see this, let $n = 2^p K$ ($p, K = 1, 2, \dots$). Then, in the same way as above,

$$\begin{aligned} |f^{(M)} - f^{(M)}(2K)| &\leq |f^{(M)} - f^{(M)}(2 \cdot 2^p)| + |f^{(M)}(2 \cdot 2^p) - f^{(M)}(2n)| + |f^{(M)}(2n) - f^{(M)}(2K)| \\ &\leq \|\widehat{H}_{2;1,2}\| [2^{-p-1} + 2^{-p-1} + (2K)^{-1}]. \end{aligned}$$

Thus, as $p \uparrow \infty$, we obtain

$$|f^{(M)} - f^{(M)}(2K)| \leq (2K)^{-1} \|\widehat{H}_{2;1,2}\|. \tag{A.2}$$

This implies that $f^{(M)}(2n)$ converges uniformly with respect to M as we wished to show.

We can now prove the statement of Theorem 3.2. For this purpose, we use the standard argument for the interchangeability of double limits.^{19),21),22)} The inequality (A.2) combined with Theorem 3.1 shows that for any given $\epsilon > 0$ and for any M , one can find n such that

$$|f^{(M)} - f^{(M)}(2n)| \leq \epsilon/3$$

and

$$|f - f(2n)| \leq \epsilon/3.$$

On the other hand, the Trotter formula (2.7) implies that for given n , there exists M such that

$$|f^{(M)}(2n) - f(2n)| \leq \epsilon/3.$$

These inequalities give

$$\begin{aligned} |f - f^{(M)}| &\leq |f - f(2n)| + |f(2n) - f^{(M)}(2n)| + |f^{(M)}(2n) - f^{(M)}| \\ &\leq \epsilon. \end{aligned}$$

Thus, the proof of Theorem 3.2 is complete. \square

Appendix B

— Bethe Ansatz^{1),34),35)} for the Transfer Matrix \widehat{U}_{2M} —

In this appendix, we show that

$$\widehat{U}_{2M}|B_k\rangle = \Lambda_{2M;k}|B_k\rangle. \quad (k=0, 1, \dots, 2M) \tag{B.1}$$

Note that from the definition of the matrix $\widehat{V}_{2; i,j}$ in (3.5), we have

$$\begin{aligned} &\langle \sigma_i^k, \sigma_j^k | \widehat{V}_{2; i,j} | \sigma_i^l, \sigma_j^l \rangle \\ &= \begin{cases} Ds & \text{(all the spins up, or down),} \\ Dc & (\sigma_i^k = \sigma_i^l, \sigma_j^k = \sigma_j^l, \sigma_i^k \neq \sigma_j^k), \\ E^{-1}D^{-1} & (\sigma_i^k = \sigma_j^l = +1, \sigma_j^k = \sigma_i^l = -1), \\ ED^{-1} & (\sigma_i^k = \sigma_j^l = -1, \sigma_j^k = \sigma_i^l = +1), \\ 0 & \text{otherwise.} \end{cases} \end{aligned} \tag{B.2}$$

Lemma B.1. Let

$$|z_j; k, k+1\rangle := F(z_j, k)|-1, +1\rangle + F(z_j, k+1)|+1, -1\rangle. \quad (k=1, \dots, 2M)$$

Then,

$$\widehat{V}_{2; i,j}|z_j; 2l-1, 2l\rangle = \lambda_j|z_j; 2l, 2l+1\rangle. \quad (l=1, \dots, M) \tag{B.3}$$

Proof From the definitions (4.2) and (4.3), we have

$$\begin{pmatrix} Dc & E^{-1}D^{-1} \\ ED^{-1} & Dc \end{pmatrix} \begin{pmatrix} F(z_j, 2l-1) \\ F(z_j, 2l) \end{pmatrix} = \lambda_j \begin{pmatrix} F(z_j, 2l) \\ F(z_j, 2l+1) \end{pmatrix}. \quad (l=1, \dots, M)$$

This implies (B.3) by (B.2). \square

Lemma B.2. Let

$$\begin{aligned} &|z_{P_j}, z_{P(j+1)}; k, k+1\rangle \\ &:= \sum^{(j,j+1)} A_P F(z_{P_j}, k) F(z_{P(j+1)}, k+1) |-1, -1\rangle, \quad (k=1, \dots, 2M) \end{aligned}$$

where the summation $\sum^{(j,j+1)}$ runs over two permutations, (P_1, \dots, P_k) and $(P_1, \dots, P(j+1), P_j, \dots, P_k)$. Then,

$$\begin{aligned} &\widehat{V}_{2; i,j}|z_{P_j}, z_{P(j+1)}; 2l-1, 2l\rangle \\ &= (Ds)^{-1} \lambda_{P_j} \lambda_{P(j+1)} |z_{P_j}, z_{P(j+1)}; 2l, 2l+1\rangle. \quad (l=1, \dots, M) \end{aligned} \tag{B.4}$$

Proof From the definitions (4.2)~(4.4), we have

$$\begin{aligned} &(Ds)^2 \sum^{(i,j+1)} A_P F(z_{P_j}, 2l-1) F(z_{P(j+1)}, 2l) \\ &= \lambda_{P_j} \lambda_{P(j+1)} \sum^{(j,j+1)} A_P F(z_{P_j}, 2l) F(z_{P(j+1)}, 2l+1). \quad (l=1, \dots, M) \end{aligned}$$

This implies (B.4) by (B.2). \square

Further, from the system of the Bethe-ansatz equations (4.7) and the definitions (4.2)~(4.4), we obtain:

Lemma B.3.

$$A_{(P_1, \dots, P_k)} F(z_{P_k}, 2M+1) = A_{(P_k, P_1, \dots, P(k-1))} F(z_{P_k}, 1).$$

We now prove (B.1). First, Lemmas B.1 and B.2 combined with the definitions

of \widehat{R}_{2M} , (4.1) and (4.5) give

$$\begin{aligned} \widehat{R}_{2M}|B_k\rangle &= \sum_{1 \leq y_1 < \dots < y_k \leq 2M} \sum_P (DS)^{M-k} \lambda_{P_1} \dots \lambda_{P_k} A_P F(z_{P_1}, y_1+1) \dots \\ &\quad \dots F(z_{P_k}, y_k+1) |y_1, \dots, y_k\rangle \\ &= \Lambda_{2M; k} \sum_{1 \leq y_1 < \dots < y_k \leq 2M} \sum_P A_P F(z_{P_1}, y_1+1) \dots F(z_{P_k}, y_k+1) |y_1, \dots, y_k\rangle. \end{aligned}$$

($k=0, 1, \dots, 2M$)

Therefore, by (3.11) and Lemma B.3, we obtain

$$\begin{aligned} \widehat{U}_{2M}|B_k\rangle &= \Lambda_{2M; k} \left[\sum_{1 \leq y_1 < \dots < y_k \leq 2M-1} \sum_P A_P F(z_{P_1}, y_1+1) \dots F(z_{P_k}, y_k+1) |y_1+1, \dots, y_k+1\rangle \right. \\ &\quad + \sum_{1 \leq y_1 < \dots < y_{k-1} \leq 2M-1} \sum_P A_P F(z_{P_1}, y_1+1) \dots F(z_{P_{k-1}}, y_{k-1}+1) \\ &\quad \times F(z_{P_k}, 2M+1) |1, y_1+1, \dots, y_{k-1}+1\rangle \Big] \\ &= \Lambda_{2M; k} \left[\sum_{2 \leq y_1 < \dots < y_k \leq 2M} \sum_P A_P F(z_{P_1}, y_1) \dots F(z_{P_k}, y_k) |y_1, \dots, y_k\rangle \right. \\ &\quad + \sum_{2 \leq y_2 < \dots < y_k \leq 2M} \sum_P A_P F(z_{P_1}, 1) F(z_{P_2}, y_2) \dots F(z_{P_k}, y_k) |1, y_2, \dots, y_k\rangle \Big] \\ &= \Lambda_{2M; k} |B_k\rangle. \quad (k=0, 1, \dots, 2M) \quad \square \end{aligned}$$

Appendix C

— Calculation of the Limit $M \uparrow \infty$ of J_M —

For simplicity, we restrict M to even integers, $M=2m$ ($m=1, 2, \dots$). Then, J_M can be written as

$$J_M = J_m^{(0)} + \sum_{k=1}^2 \sum_{j=1}^m J_{m,j}^{(k)}(\sin \varphi_j),$$

where

$$J_m^{(0)} := 2 \sum_{j=1}^m \log [2 \cosh(\beta h/M) \cos \varphi_j],$$

$$J_{m,j}^{(k)} := \frac{1}{\pi} \int_{E^{(k)}} dx \log L_j(w), \quad (E^{(1)} = [0, \pi/2], \quad E^{(2)} = [\pi/2, \pi])$$

$$L_j(w) := 1 + \left[\frac{\sinh(\beta h/M)w + \sinh(\beta/M) \cos x}{\cosh(\beta h/M) \cos \varphi_j} \right]^2$$

and

$$\varphi_j := \frac{\pi}{M}(j-1/2). \quad (j=1, 2, \dots)$$

From the definitions, one can easily obtain the following lemmas.

Lemma C.1. Let A and B be two complex numbers. Then,

$$\prod_{j=1}^m [A(\cos \varphi_j)^2 + B] = (\alpha_+)^M + (\alpha_-)^M,$$

where

$$\alpha_{\pm} = \frac{\sqrt{A+B} \pm \sqrt{B}}{2}.$$

Lemma C.2. For any $\varepsilon > 0$,

$$\begin{aligned} \min(\sum^{(\varepsilon)} J_{m,j}^{(k)}(1-\varepsilon), \sum^{(\varepsilon)} J_{m,j}^{(k)}(1)) &\leq \sum^{(\varepsilon)} J_{m,j}^{(k)}(\sin \varphi_j) \\ &\leq \max(\sum^{(\varepsilon)} J_{m,j}^{(k)}(1-\varepsilon), \sum^{(\varepsilon)} J_{m,j}^{(k)}(1)), \end{aligned}$$

where the summation $\sum^{(\varepsilon)}$ runs over integer j satisfying $1-\varepsilon \leq \sin \varphi_j \leq 1$.

Lemma C.3. If $\{w_j\}$ is bounded, then, for any $\varepsilon > 0$,

$$\lim_{m \uparrow \infty} (\sum_{j=1}^m - \sum^{(\varepsilon)} J_{m,j}^{(k)}(w_j)) = 0.$$

By Lemma C.1, we obtain

$$\begin{aligned} \lim_{m \uparrow \infty} J_m^{(0)} &= \log 2 + \lim_{M \uparrow \infty} 2^{-1} M \log [\cosh(\beta h/M)] \\ &= \log 2 \end{aligned}$$

and

$$\begin{aligned} 2^{-1} J_m^{(0)} + \sum_{j=1}^m J_{m,j}^{(k)}(w) \\ = \pi^{-1} \int_{E^{(k)}} dx \log \{ [\alpha_+^{(M)}(x)]^M + [\alpha_-^{(M)}(x)]^M \}, \quad (k=1, 2; w = \text{const}) \end{aligned} \tag{C.1}$$

where

$$\begin{aligned} \alpha_{\pm}^{(M)}(x) &:= \sqrt{\cosh^2(\beta h/M) + [\sinh(\beta h/M) + \sinh(\beta/M) \cos x]^2} \\ &\quad \pm [\sinh(\beta h/M) + \sinh(\beta/M) \cos x]. \end{aligned}$$

It is easily shown that the integrand of (C.1) is bounded on $E^{(1)} \cup E^{(2)}$. Therefore, by the Lebesgue convergence theorem, we obtain

$$\lim_{m \rightarrow \infty} [2^{-1} J_m^{(0)} + \sum_{j=1}^m J_{m,j}^{(k)}(w)] = \pi^{-1} \int_{E^{(k)}} dx \log \{2 \cosh \beta [\cos x + hw]\}.$$

($k=1, 2; w=\text{const}$)

Therefore, by Lemmas C.2 and C.3, we obtain

$$\begin{aligned} \lim_{M \rightarrow \infty} J_M &= \pi^{-1} \lim_{\varepsilon \downarrow 0} \int_0^\pi dx \log \{2 \cosh \beta [\cos x + (1-\varepsilon)h]\} \\ &= \pi^{-1} \int_0^\pi dx \log \{2 \cosh \beta [\cos x + h]\}. \end{aligned}$$

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