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Correlation length and free energy of the $S=\frac{1}{2}$ XXZ chain in a magnetic field

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The correlation length and the free energy of the $S=\frac{1}{2}$ XXZ chain in a magnetic field in the z direction are calculated with use of a set of equations for a series of infinite numbers. These are derived by the Bethe-ansatz method for the quantum transfer matrix. The equations for free energy should be equivalent to the thermodynamic Bethe-ansatz nonlinear integral equations. A numerical method that calculates precisely the free energy and the correlation length is given.

I. INTRODUCTION

In a previous paper[1] the author proposed a set of equations that calculates the free energy and correlation length of the $S=\frac{1}{2}$ XYZ chain in zero magnetic field at arbitrary temperatures. Here a set of equations is given that calculates the free energy and correlation length of the $S=\frac{1}{2}$ XXZ chain in a magnetic field in the z direction. The Hamiltonian is as follows:

$$\mathcal{H}=-J\sum_{j=1}^{N}(S_j^xS_{j+1}^x+S_j^yS_{j+1}^y+\Delta S_j^zS_{j+1}^z)-2h_z\sum_{j=1}^{N}S_j^z,\quad J>0,\quad \infty>\Delta>-\infty\ . \tag{1}$$

About 20 years ago the thermodynamic Bethe-ansatz integral equations[2] had been proposed for the free energy of this system. Using these equations, the thermodynamic properties of this system were investigated in subsequent papers.[3-5]

The quantum transfer matrix of this model is equivalent to the diagonal-to-diagonal transfer matrix of the six-vertex model. The properties of the diagonal-to-diagonal transfer matrix were investigated by Truong and Schotte.[6] This is a special case of the inhomogeneous six-vertex model.[7] Koma[8] and Yamada[9] obtained the free energy and the correlation length for the $\Delta=1$ and $h_z=0$ case by taking the limit of the infinite Trotter number numerically. In this paper we give a set of equations by taking the limit of the infinite Trotter number analytically. So the equations become simpler than those for the finite Trotter number. The numerical method that is proposed in this paper is efficient in accurate calculations of the free energy and the correlation length at given temperature T, anisotropy Δ, and magnetic field h_z. The free energy and correlation length are given by a set of equations in an infinite number of unknowns. The set of equations for free energy should be equivalent to the set of nonlinear thermodynamic integral equations, which was given in the 1970's.[2] In the problem of the XYZ chain[1] the unknown numbers are all real numbers. But for the XXZ model in a nonzero magnetic field, the unknown numbers are complex numbers. Then the numerical iteration method is not as simple as for the XYZ model.

In Sec. II we consider the transfer matrix of the XXZ model in a magnetic field. We find that there are two correlation lengths ξ_{xx} and ξ_{zz}. We derive the equations for the free energy and ξ_{xx} in the limit of the infinite Trotter number. In Sec. III we show that our equations are solved exactly in some special cases such as the Ising limit ($\Delta\to\infty$), the XY limit ($\Delta=0$), and the $h_z=T=0$ case. In Sec. IV we give the numerical method, which is used to calculate our equations at given Δ, h_z, and temperature. We compare our results with experimental results on the organic ferromagnet p-NPNN. In Sec. V we consider ξ_{zz} in the $|\Delta|\geq 1$ and $h_z=0$ case. We discuss the relation with the correlation length of the XYZ model in Ref. 1.

II. FUNDAMENTAL EQUATIONS OF THE $S=\frac{1}{2}XXZ$ CHAIN IN A MAGNETIC FIELD

A. Quantum transfer matrix

The partition function Z of the XXZ model described by (1) is approximated as follows:

$$\begin{aligned}Z&=\mathrm{Tr}\{\exp[-\mathcal{H}_1/(MT)]\exp[-\mathcal{H}_2/(MT)]\}^M\ ,\\ \mathcal{H}_1&=-\sum_{j=\mathrm{odd}}J\{S_j^xS_{j+1}^x+S_j^yS_{j+1}^y+\Delta S_j^zS_{j+1}^z\}+h_z(S_j^z+S_{j+1}^z)\ ,\\ \mathcal{H}_2&=-\sum_{j=\mathrm{even}}J\{S_j^xS_{j+1}^x+S_j^yS_{j+1}^y+\Delta S_j^zS_{j+1}^z\}+h_z(S_j^z+S_{j+1}^z)\ .\end{aligned}\tag{2}$$

This is the same with the partition function of the six-vertex model with $2M\times N$ bonds:[10]

$$Z=\sum_{\{\sigma\}}\prod_{j=1}^{N}\prod_{i=1}^{M}B(\sigma_{2i+j,j}\sigma_{2i+j+1,j};\sigma_{2i+j,j+1}\sigma_{2i+j+1,j+1})\ .$$

Here $\sigma_{l,m}$; ($l=1,2,\ldots,2M$, $m=1,2,\ldots,N$) denotes the direction of bonds and takes values $+1$ or -1. **B** is given by the 4×4 matrix:

$$B(\sigma_1\sigma_2;\sigma_1'\sigma_2')=\begin{bmatrix} b & 0 & 0 & c\\ 0 & 0 & a & 0\\ 0 & a & 0 & 0\\ c & 0 & 0 & b'\end{bmatrix},$$

$$a=\exp(-J\Delta/4MT)\sinh(J/2MT),\quad b=\exp[(J\Delta+4h_z)/4MT],$$
$$b'=\exp[(J\Delta-4h_z)/4MT],\quad c=\exp(-J\Delta/4MT)\cosh(J/2MT). \tag{3}$$

If we put $\sigma_{l,m}\rightarrow(-1)^{l+m+1}\sigma_{l,m}$, Z is given by

$$Z=\sum_{\{\sigma\}}\prod_{j=1}^{N}\prod_{i=1}^{M}A(\sigma_{2i+j,j}\sigma_{2i+j+1,j};\sigma_{2i+j,j+1}\sigma_{2i+j+1,j+1}),\quad A(\sigma_1\sigma_2;\sigma_1'\sigma_2')=\begin{bmatrix} a & 0 & 0 & 0\\ 0 & c & b' & 0\\ 0 & b & c & 0\\ 0 & 0 & 0 & a\end{bmatrix}. \tag{4}$$

Then in the case $N=2M\times$integer, Z is given by the transfer matrix

$$\begin{aligned} Z=\mathrm{Tr}\mathbf{T}^N,\quad &\mathbf{T}(\sigma_1,\sigma_2,\ldots,\sigma_{2M};\sigma_1',\sigma_2',\ldots,\sigma_{2M}')\\ &\equiv A(\sigma_1\sigma_2;\sigma_{2M}'\sigma_1')\\ &\times A(\sigma_3\sigma_4;\sigma_2'\sigma_3')\cdots A(\sigma_{2M-1}\sigma_{2M};\sigma_{2M-2}'\sigma_{2M-1}'). \end{aligned} \tag{5}$$

This $2^{2M}\times 2^{2M}$ matrix is the diagonal-to-diagonal transfer matrix of the six-vertex model and different from the conventional row-to-row transfer matrix. Truong and Schotte[6] and Koma[8] treated the eigenvalue problem using the Bethe ansatz. The eigenvalue problem of this transfer matrix is the special case of the inhomogeneous six-vertex model on the square lattice, which was treated by Baxter.[7]

The number of down spins k in one row in a conserved quantity. A down spin behaves as a particle, and we can construct an eigenfunction and its eigenvalue using k parameters.

For the largest eigenvalue, k is equal to M. We write this eigenvalue as Λ_M^0 and corresponding eigenvector as $|0\rangle$. The exact free energy per site is given by the limiting value of Λ_M^0 as $M\rightarrow\infty$:

$$f=-T\ln(\lim_{M\rightarrow\infty}\Lambda_M^0). \tag{6}$$

Let us consider the two-point functions $S^{xx}(n)\equiv\langle S_l^xS_{l+n}^x\rangle$ and $S^{zz}(n)\equiv\langle S_l^zS_{l+n}^z\rangle$. $S^{yy}(n)\equiv\langle S_l^yS_{l+n}^y\rangle$ is the same with $S^{xx}(n)$. These are written as

$$S^{xx}(n)=\frac{\mathrm{Tr}(\mathbf{T}^{N-n}\mathbf{R}^n\mathbf{U}_x\mathbf{R}^{-n}\mathbf{T}^n\mathbf{U}_x)}{\mathrm{Tr}\mathbf{T}^N}, \tag{7}$$

$$S^{zz}(n)=\frac{\mathrm{Tr}(\mathbf{T}^{N-n}\mathbf{R}^n\mathbf{U}_z\mathbf{R}^{-n}\mathbf{T}^n\mathbf{U}_z)}{\mathrm{Tr}\mathbf{T}^N}. \tag{8}$$

Here **R** is the shift operator, and $\mathbf{U}_x$ and $\mathbf{U}_z$ are defined by

$$\begin{aligned} \mathbf{U}_x&\equiv\tfrac{1}{2}\delta_{\sigma_1,-\sigma_1'}\prod_{j=2}^{2M}\delta_{\sigma_j,\sigma_j'},\\ \mathbf{U}_z&\equiv\tfrac{1}{2}\sigma_1\delta_{\sigma_1,\sigma_1'}\prod_{j=2}^{2M}\delta_{\sigma_j,\sigma_j'},\\ \mathbf{R}&\equiv\delta_{\sigma_2,\sigma_1'}\delta_{\sigma_3,\sigma_2'}\cdots\delta_{\sigma_1,\sigma_{2M}'}. \end{aligned} \tag{9}$$

$\mathbf{R}^2$ and transfer matrix **T** commute. So we put the corresponding eigenvalue of $\mathbf{R}^2$ as $\exp(iK_j)$ of the eigenstate $|j\rangle$. K_j is the total momentum of the state j. It is given by $(2\pi/M)\times$integer. $S^{\alpha\alpha}(n)$ at $n=$even is given by

$$S^{\alpha\alpha}(n)=\sum_j\frac{\langle 0|\mathbf{U}_\alpha|j\rangle\langle j|\mathbf{U}_\alpha|0\rangle}{\langle 0|0\rangle\langle j|j\rangle}\times\left[\frac{\Lambda_j}{\Lambda_M^0}\right]^n\exp(-iK_jn/2), \tag{10a}$$

and at $n=$odd it is

$$S^{\alpha\alpha}(n)=\sum_j\frac{\langle 0|\mathbf{R}\mathbf{U}_\alpha\mathbf{R}^{-1}|j\rangle\langle j|\mathbf{U}_\alpha|0\rangle}{\langle 0|0\rangle\langle j|j\rangle}\left[\frac{\Lambda_j}{\Lambda_M^0}\right]^n\times\exp[-iK_j(n-1)/2]. \tag{10b}$$

Here $\langle 0|$ and $\langle j|$ are left eigenvectors corresponding to $|0\rangle$ and $|j\rangle$. Then if Λ_j is the next largest eigenvalue that satisfies $\langle 0|\mathbf{U}_\alpha|j\rangle\langle j|\mathbf{U}_\alpha|0\rangle\neq 0$ or $\langle 0|\mathbf{R}\mathbf{U}_\alpha\mathbf{R}^{-1}|j\rangle\langle j|\mathbf{U}_\alpha|0\rangle\neq 0$, the correlation length $\xi_{\alpha\alpha}$ is given by $1/\ln(\Lambda_M^0/|\Lambda_j|)$. ξ_{xx} is determined by the largest eigenvalue Λ_{M-1}^0 in the subspace $k=M\pm 1$, because the operator $\mathbf{U}_x$ changes the number of down arrows. While ξ_{zz} is determined by a second eigenvalue Λ_M^1 in subspace $k=M$, because $\mathbf{U}_z$ does not change the number of down arrows,

$$\xi_{xx}^{-1}=\lim_{M\to\infty}\ln(\Lambda_M^0/|\Lambda_{M-1}^0|)\ ,$$
$$\xi_{zz}^{-1}=\lim_{M\to\infty}\ln(\Lambda_M^0/|\Lambda_M^1|)\ . \tag{11}$$

Without loss of generality, we can put $k\le M$ because the case of $k>M$ is reduced to $k<M$ by reversing spin direction and putting $h_z\to -h_z$. As the matrix **T** is asymmetric, the eigenvalues are not necessarily real. But the largest eigenvalues Λ_M^0 and Λ_{M-1}^0 are real and positive because all the elements of matrix **T** are nonnegative. At $\Delta<1$, Λ_M^1 is not necessarily real. In this case the correlation function $S^{zz}(n)$ is oscillating depending on the phase of Λ_M^1 and damps exponentially with the correlation length ξ_{zz}. We have $|\Lambda_M^1|<|\Lambda_{M-1}^0|(\xi_{xx}>\xi_{zz})$ for $|\Delta|<1$ case. On the contrary $|\Lambda_M^1|>|\Lambda_{M-1}^0|(\xi_{xx}<\xi_{zz})$ if $|\Delta|>1$ and $|h_z|$ is sufficiently small.

B. Inhomogeneous six-vertex model

The inhomogeneous six-vertex model[7] is defined as follows:

$$\mathbf{T}=\mathrm{Tr}[\mathbf{R}_1(\sigma_1,\sigma_1')\mathbf{R}_2(\sigma_2,\sigma_2')\cdots\mathbf{R}_{2M}(\sigma_{2M},\sigma_{2M}')]\ ,$$
$$\mathbf{R}_l(++)=\begin{bmatrix}a_l & 0\\ 0 & b_l'\end{bmatrix},\quad \mathbf{R}_l(+-)=\begin{bmatrix}0 & 0\\ c_l & 0\end{bmatrix},\tag{12}$$
$$\mathbf{R}_l(-+)=\begin{bmatrix}0 & c_l\\ 0 & 0\end{bmatrix},\quad \mathbf{R}_l(--)=\begin{bmatrix}b_l & 0\\ 0 & a_l\end{bmatrix}.$$

Set $h(x)=\sin x$ and assume that parameters a_l,b_l,b_l',c_l are given by

$$a_l=\rho_l h(-v+v_l+\eta),\quad b_l=t\rho_l h(-v+v_l-\eta)\ ,$$
$$b_l'=t^{-1}\rho_l h(-v+v_l-\eta),\quad c_l=\rho_l h(2\eta)\ . \tag{13}$$

In this case we can construct the Bethe-ansatz eigenvector of $\mathbf{T}(v)$:

$$f(y_1,y_2,\ldots,y_k)=\sum_P^{k!}A(P)\prod_{j=1}^{k}\phi(w_{Pj},y_j)\ ,$$
$$\phi(w,y)=t^y\prod_{l=2}^{y}\frac{h(w-v_{l-1}+\eta)}{h(w-v_l-\eta)}\ , \tag{14}$$
$$A(P)=\epsilon(P)\prod_{1\le j<m\le k}h(w_{Pj}-w_{Pm}+2\eta)\ .$$

Parameters $w_1,\ldots,w_k$ should satisfy

$$\prod_{l=1}^{2M}\frac{h(w_m-v_l+\eta)}{h(w_m-v_l-\eta)}=-t^{2M}\prod_{j=1}^{k}\frac{h(w_m-w_j+2\eta)}{h(w_m-w_j-2\eta)}\ ,$$
$$m=1,2,\ldots,k\ . \tag{15}$$

The eigenvalue is

$$\Lambda(v)=\left[\prod_{l=1}^{2M}a_l\right]t^k\prod_{j=1}^{k}\frac{h(v-w_j+2\eta)}{h(v-w_j)}$$
$$+\left[\prod_{l=1}^{2M}b_l'\right]t^k\prod_{j=1}^{k}\frac{h(v-w_j-2\eta)}{h(v-w_j)}\ . \tag{16}$$

One can verify that this vector satisfies $\mathbf{T}(v)f=\Lambda(v)f$ after cumbersome but straightforward calculations.

C. Transcendental equations

If we choose v_l, ρ_l, t, η, and v so that

$$a_{2l}=c_{2l}=1,\quad b_{2l}=b_{2l}'=0$$

and

$$a_{2l-1}=a,\quad b_{2l-1}=b,\quad b_{2l-1}'=b',\quad c_{2l-1}=c\ , \tag{17}$$

the transfer matrices (5) and (12) are equivalent and eigenvalue problem of (5) is solved by the formula in Sec. II B. These are satisfied if we write

$$v=0,\quad v_{2l}=\eta,\quad \rho_{2l}=1/h(2\eta)\ ,$$
$$v_{2l-1}=v_1,\quad t=\exp\left[\frac{h_z}{MT}\right]\ , \tag{18a}$$

$$\frac{h(v_1+\eta)}{h(2\eta)}=\frac{a}{c},\quad \cos 2\eta=\tilde\Delta\ ,$$
$$\tilde\Delta\equiv\frac{a^2+bb'-c^2}{2a\sqrt{bb'}}=\frac{\sinh(J\Delta/2MT)}{\sinh(J/2MT)}\ . \tag{18b}$$

At $\Delta>1$ Eqs. (18b) are satisfied if we write

$$2\eta=i\cosh^{-1}\tilde\Delta,\quad \rho_{2l-1}=\frac{c}{i(\tilde\Delta^2-1)^{1/2}}\ ,$$
$$v_1+\eta=\pi-2\alpha,\quad 2\alpha=i\sinh^{-1}[a(\tilde\Delta^2-1)^{1/2}/c]\ . \tag{19a}$$

At $\Delta<-1$, Eqs. (18b) are satisfied if we write

$$2\eta=\pi-i\cosh^{-1}(-\tilde\Delta),\quad \rho_{2l-1}=\frac{c}{i(\tilde\Delta^2-1)^{1/2}}$$
$$v_1+\eta=2\alpha,\quad 2\alpha=i\sinh^{-1}[a(\tilde\Delta^2-1)^{1/2}/c]\ . \tag{19b}$$

At $1>\Delta>-1$ Eqs. (18b) are satisfied if we put

$$2\eta=\cos^{-1}\tilde\Delta,\quad \rho_{2l-1}=\frac{c}{(1-\tilde\Delta^2)^{1/2}}\ ,$$
$$v_1+\eta=\pi-2\alpha,\quad 2\alpha=\sin^{-1}[a(1-\tilde\Delta^2)^{1/2}/c]\ . \tag{19c}$$

Then Eqs. (15) and (16) become

$$\Lambda=a^Mt^k\prod_{j=1}^{k}\frac{h(w_j-2\eta)}{h(w_j)}\ , \tag{20}$$

$$\left[\frac{h(w_m)h(w_m-v_1+\eta)}{h(w_m-2\eta)h(w_m-v_1-\eta)}\right]^M=t^{2M}\prod_{j=1}^{k}\frac{h(w_m-w_j+2\eta)}{h(w_m-w_j-2\eta)}\ . \tag{21}$$

The eigenvalue of $\mathbf{R}^2$ is

$$e^{iK}=t^{2k}\prod_{m=1}^{k}\frac{h(w_m)h(w_m-v_1+\eta)}{h(w_m-2\eta)h(w_m-v_1-\eta)}\ . \tag{22}$$

At $1>\Delta>-1$ we put $h(x)=\sinh(x)$, $w_m\to iw_m$, $\alpha\to i\alpha$, $\eta\to i\eta$. The case $\Delta=1$ is special. In the limit

$\Delta \to 1+$, η, and α become zero if we use Eq. (19a). But w_m's also go to zero. Dividing all parameters by $-2i\eta$ we derive equations for the case $\Delta=1$. The case $\Delta=-1$ is also treated similarly. Putting $w_m=x_m-\alpha$ and using Eqs. (20)–(22) we have the following equations:

$$\Lambda e^{-iK/2}=\exp\left[\frac{J\Delta}{4T}\right]\left[\frac{h(2\alpha)}{h(2\alpha+2\eta)}\right]^M \times\left[\prod_{l=1}^{k}\frac{h(x_l+\alpha+2\eta)h(x_l-\alpha-2\eta)}{h(x_l-\alpha)h(x_l+\alpha)}\right]^{1/2}, \tag{23}$$

$$\left[\frac{h(x_l-\alpha)h(x_l+\alpha+2\eta)}{h(x_l+\alpha)h(x_l-\alpha-2\eta)}\right]^M = -\exp\left[\frac{2h_z}{T}\right]\prod_{j=1}^{k}\frac{h(x_l-x_j+2\eta)}{h(x_l-x_j-2\eta)}, \tag{24}$$

$l=1,2,\ldots,k$.

Here

$$h(x)=\sin x,\quad \eta=\frac{i}{2}\mathrm{sgn}(\Delta)\cosh^{-1}(|\tilde{\Delta}|)\ ,\quad \alpha=\frac{i}{2}\sinh^{-1}[a(\tilde{\Delta}^2-1)^{1/2}/c]\ , \tag{25a}$$

for $|\Delta|>1$,

$$h(x)=x,\quad \eta=\frac{i}{2}\mathrm{sgn}(\Delta),\quad \alpha=\frac{i}{2}\tanh\frac{J}{2MT}\ , \tag{25b}$$

for $\Delta=\pm 1$, and

$$h(x)=\sinh x,\quad \eta=\frac{i}{2}\cos^{-1}(\tilde{\Delta})\ ,\quad \alpha=\frac{i}{2}\sin^{-1}[a(1-\tilde{\Delta}^2)^{1/2}/c]\ , \tag{25c}$$

for $|\Delta|<1$.

D. Limit of $M\to\infty$

At $k=M$ Eqs. (24) are written as

$$M\ln\left[\frac{h(x_l-\alpha)h(x_l+\alpha+2\eta)h(x_l-2\eta)}{h(x_l+\alpha)h(x_l-\alpha-2\eta)h(x_l+2\eta)}\right]=-2\pi\left[l-\frac{1}{2}\right]i+\frac{2h_z}{T}+\sum_{j=1}^{M}\ln\left[\frac{h(x_l-x_j+2\eta)h(x_l-2\eta)}{h(x_l-x_j-2\eta)h(x_l+2\eta)}\right]. \tag{26a}$$

For the largest eigenvalue Λ_M^0 we have

$$\mathrm{Re}x_1>\mathrm{Re}x_2>\cdots>\mathrm{Re}x_M,\quad x_l=-\bar{x}_{M+1-l},\quad l=1,2,\ldots,M\ . \tag{26b}$$

We put the solution of (26a) as y_l's to discriminate from solutions of the largest eigenvalue. For Λ_{M-1}^0 the corresponding equation is

$$M\ln\left[\frac{h(y_l-\alpha)h(y_l+\alpha+2\eta)h(y_l-2\eta)}{h(y_l+\alpha)h(y_l-\alpha-2\eta)h(y_l+2\eta)}\right]=-2\pi li+\frac{2h_z}{T}+\ln\left[\frac{h(2\eta-y_l)}{h(2\eta+y_l)}\right] +\sum_{j=1}^{M-1}\ln\left[\frac{h(y_l-y_j+2\eta)h(y_l-2\eta)}{h(y_l-y_j-2\eta)h(y_l+2\eta)}\right], \tag{27a}$$

$$\mathrm{Re}y_1>\cdots>\mathrm{Re}y_{M-1},\quad y_l=-\bar{y}_{M-l},\quad l=1,2,\ldots,M-1\ . \tag{27b}$$

Thus we can calculate Λ_M^0 and Λ_{M-1}^0 using these equations and Eq. (23). The correct eigenvalue is obtained in the limit of infinite M. In the calculation of Koma[8] and Yamada[9] this limit is taken by the numerical extrapolation. In this paper we take the limit of $M\to\infty$ in Eqs. (23), (26) and (27) analytically. α is of the order of J/MT. Then in the limit of $M\to\infty$, Eqs. (26) become

$$\frac{2J_s}{T}g(x_l)=2\pi\left[l-\frac{1}{2}\right]+\frac{2h_zi}{T}+\frac{1}{i}\sum_{j=1}^{\infty}\ln[f(x_l,x_j)f(x_l,-\bar{x}_j)],\quad l=1,2,\ldots \tag{28}$$

for the largest eigenvalue Λ_M^0. Equations (27) become

$$\frac{2J_s}{T}g(y_l)=2\pi l+\frac{2h_zi}{T}+\frac{1}{i}\left[\ln\left[\frac{h(2\eta+y_l)}{h(2\eta-y_l)}\right]+\sum_{j=1}^{\infty}\ln[f(y_l,y_j)f(y_l,-\bar{y}_j)]\right],\quad l=1,2,3,\ldots \tag{29}$$

for Λ_{M-1}^0. Here

$$J_s=\begin{cases}\frac{J}{4}(\Delta^2-1)^{1/2} & \text{for } |\Delta|>1\\ \frac{J}{4} & \text{for } |\Delta|=1\\ \frac{J}{4}(1-\Delta^2)^{1/2} & \text{for } |\Delta|<1\ ,\end{cases} \tag{30}$$

$$g(x)\equiv\frac{h'(x)}{h(x)}-\frac{1}{2}\frac{h'(x+2\eta)}{h(x+2\eta)}-\frac{1}{2}\frac{h'(x-2\eta)}{h(x-2\eta)}=\begin{cases}\cot x-\dfrac{\sin 2x}{\cosh 2\theta-\cos 2x} & \text{for } |\Delta|>1\\ \dfrac{1}{x}-\dfrac{x}{x^2+1} & \text{for } |\Delta|=1\\ \coth x-\dfrac{\sinh 2x}{\cosh 2x-\cos 2\theta} & \text{for } |\Delta|<1\ ,\end{cases} \tag{31}$$

$$f(x,y)\equiv\frac{h(x-y-2\eta)h(x+2\eta)}{h(x-y+2\eta)h(x-2\eta)}\ . \tag{32}$$

In the limit $M\to\infty$, $\tilde{\Delta}$ is Δ. Using Eqs. (25) we have

$$2\eta=i\theta,\quad \theta=\begin{cases}\cosh^{-1}\Delta & \text{for } \Delta>1\\ \cos^{-1}\Delta & \text{for } 1>\Delta>-1\\ -\cosh^{-1}(-\Delta) & \text{for } \Delta<-1\ .\end{cases}$$

Infinite series $\{x_l\}$ and $\{y_l\}$ are determined by Eqs. (28) and (29). These series converge to zero.

When M becomes large, α becomes small as $O(J/(4MT))$. Then the form of Eq. (23) is not appropriate for taking the limit $M\to\infty$. For this purpose the following equations are useful:

$$\prod_{l=1}^{M}\left[h'(-2\eta)+\frac{h(-2\eta)}{\delta_l^+-\alpha}\right]=\left[\frac{h(2\eta)+2\alpha h'(2\eta)}{2\alpha}\right]^M+\left[\frac{h(2\eta)}{2\alpha}\right]^M ,$$
$$h'(-2\eta)\prod_{l=2}^{M}\left[h'(-2\eta)+\frac{h(-2\eta)}{\delta_l^--\alpha}\right]=\left[\frac{h(2\eta)+2\alpha h'(2\eta)}{2\alpha}\right]^M-\left[\frac{h(2\eta)}{2\alpha}\right]^M , \tag{33}$$

$$\delta_l^+\equiv -i\alpha\cot\left[\frac{\pi(l-\frac{1}{2})}{M}\right],\quad \delta_l^-\equiv -i\alpha\cot\left[\frac{\pi l}{M}\right]\ . \tag{34}$$

Using these we rewrite Eq. (23) as follows:

$$\Lambda_M^0=CD^+\left[\prod_{l=1}^{M}\frac{h(x_l-\alpha-2\eta)h(x_l+\alpha+2\eta)}{h(x_l-\alpha)h(x_l+\alpha)[h'(-2\eta)+h(-2\eta)/(\delta_l^+-\alpha)]^2}\right]^{1/2} , \tag{35}$$

$$\Lambda_{M-1}^0=\frac{CD^-}{h'(-2\eta)}\left[\prod_{l=1}^{M-1}\frac{h(y_l-\alpha-2\eta)h(y_l+\alpha+2\eta)}{h(y_l-\alpha)h(y_l+\alpha)[h'(-2\eta)+h(-2\eta)/(\delta_l^--\alpha)]^2}\right]^{1/2}\ . \tag{36}$$

Momentum K is zero for these states. Here we set

$$C=e^{J\Delta/4T}\left[\frac{h(2\alpha)[h(2\eta)+2\alpha h'(2\eta)]}{2\alpha h(2\eta+2\alpha)}\right]^M , \tag{37}$$

$$D^{\pm}=\left[1\pm\left[\frac{h(2\eta)}{h(2\eta)+2\alpha h'(2\eta)}\right]^M\right]\ . \tag{38}$$

In Eq. (35) the product of the lth and $(M+1-l)$th terms is $1+O(l^{-2})$ at $M/2\ge l\ge 1$. In the limit of infinite M, Eq. (35) becomes

$$\Lambda_M^0=2\cosh(J\Delta/4T)\prod_{l=1}^{\infty}\frac{|h(2\eta-x_l)h(2\eta+x_l)|J_s^2}{h(x_l)h(\bar{x}_l)|h^2(2\eta)|\{[T\pi(l-\frac{1}{2})]^2+(J\Delta/4)^2\}}\ . \tag{39}$$

Using $\cosh x=\prod_{l=1}^{\infty}(1+\{x/[\pi(l-\frac{1}{2})]\}^2)$, we have

$$\Lambda_M^0=2\prod_{l=1}^{\infty}\left|\frac{h(2\eta-x_l)h(2\eta+\bar{x}_l)}{h^2(x_l)h^2(2\eta)}\right|\left[\frac{J_s}{T\pi(l-\frac{1}{2})}\right]^2\ . \tag{40}$$

In the same way, Eq. (36) becomes

$$\Lambda_{M-1}^0=2\left[\frac{J}{4}\right]\prod_{l=1}^{\infty}\left|\frac{h(2\eta-y_l)h(2\eta+y_l)}{h^2(y_l)h^2(2\eta)}\right|\left[\frac{J_s}{T\pi l}\right]^2 . \tag{41}$$

Equations (28) and (29), and (40) and (41) do not contain the Trotter number M, and these are simpler than (26) and (27), and (23).

If we set

$$\begin{aligned}
&p_l=-i\tan 2\eta/\tan x_l,\quad q_l=-i\tan 2\eta/\tan y_l \quad \text{for } |\Delta|>1 ,\\
&p_l=\pm 1/x_l,\quad q_l=\pm 1/y_l \quad \text{for } \Delta=\pm 1 ,\\
&p_l=-i\tanh 2\eta/\tanh x_l,\quad q_l=-i\tanh 2\eta/\tanh y_l \quad \text{for } |\Delta|<1 ,
\end{aligned} \tag{42}$$

Eqs. (28) and (29) become

$$\frac{J\Delta}{2T}G(p_l)=\frac{2h_z i}{T}+2\pi\left[l-\frac{1}{2}\right]+\frac{1}{i}\sum_{j=1}^{\infty}\ln[L(p_l,p_j)L(p_l,-\bar{p}_j)] , \tag{43}$$

$$\frac{J\Delta}{2T}G(q_l)=\frac{2h_z i}{T}+2\pi l+\frac{1}{i}\left[\ln\left[\frac{q_l-i}{q_l+i}\right]+\sum_{j=1}^{\infty}\ln[L(q_l,q_j)L(q_l,-\bar{q}_j)]\right] , \tag{44}$$

where

$$G(x)\equiv x-\frac{\Delta^{-2}x}{x^2+1},\quad L(x,y)\equiv\frac{iy+[1-\Delta^{-2}/(1-ix)]}{-iy+[1-\Delta^{-2}/(1+ix)]}=\frac{x^2+1-\Delta^{-2}-ix\Delta^{-2}+iy(1+x^2)}{x^2+1-\Delta^{-2}+ix\Delta^{-2}-iy(1+x^2)} . \tag{45}$$

Equations (40) and (41) become

$$\Lambda_M^0=2\prod_{l=1}^{\infty}\left[\frac{J\Delta}{4\pi T(l-1/2)}\right]^2[(p_l^2+1)(\bar{p}_l^2+1)]^{1/2} , \tag{46}$$

$$\Lambda_{M-1}^0=2\left[\frac{J}{4T}\right]\prod_{l=1}^{\infty}\left[\frac{J\Delta}{4\pi Tl}\right]^2[(q_l^2+1)(\bar{q}_l^2+1)]^{1/2} . \tag{47}$$

These equations are convenient for numerical calculations. In the $|\Delta|<1$ and $h_z=0$ case, Eqs. (44) and (47) are equivalent to those for Λ_1 of the XYZ model if we put $J=J_z=J_y$, $J\Delta=J_x$ in Eqs. (40) and (41) of Ref. 1.

III. ANALYTICAL SOLUTIONS FOR SPECIAL CASES

A. Ising limit

In this limit we have

$$\Delta\to\infty,\quad J=J_z/\Delta,\quad \Delta^{-2}\to 0 . \tag{48}$$

Then Eq. (43) becomes

$$p_l=\frac{4\pi T(l-1/2)}{J_z}+\frac{(4h_z-2TD)i}{J_z} , \tag{49a}$$

$$D\equiv\ln\left[\prod_{j=1}^{\infty}\frac{(p_j-i)(\bar{p}_j+i)}{(p_j+i)(\bar{p}_j-i)}\right] . \tag{49b}$$

Substituting (49a) into (49b) we find that

$$e^D=\frac{\cosh[(J_z-4h_z+2TD)/(4T)]}{\cosh[(J_z+4h_z-2TD)/(4T)]} . \tag{50}$$

Solving this equation with respect to e^D we have

$$e^D=\exp\left[\frac{J_z+2h_z}{2T}\right]\left\{\left[\sinh^2\left[\frac{h_z}{T}\right]+e^{-J_z/T}\right]^{1/2}-\sinh\left[\frac{h_z}{T}\right]\right\} . \tag{51}$$

Using this and Eqs. (46) and (48) we have Λ_M^0 and free energy per site:

$$f=-T\ln\left[\exp\left[\frac{J_z}{4T}\right]\left\{\cosh\left[\frac{h_z}{T}\right]+\left[\sinh^2\left[\frac{h_z}{T}\right]+e^{-J_z/T}\right]^{1/2}\right\}\right]. \tag{52}$$

This is the well-known result for the Ising chain in a magnetic field.

B. $\Delta=0$ case (XY chain)

From (25c) we have $2\eta=\pi i/2$, $h(x)=\sinh x$. Then all logarithms in (28) and (29) vanish. Equation (28) gives

$$\frac{1}{\tanh x_l}-\tanh x_l=\frac{4\pi T(l-\frac{1}{2})}{J}+\frac{4h_z i}{J},$$

and therefore

$$\frac{1}{\tanh x_l}=\left[\frac{2\pi T(l-\frac{1}{2})+2h_z i}{J}\right]+\left[\left[\frac{2\pi T(l-\frac{1}{2})+2h_z i}{J}\right]^2+1\right]^{1/2}. \tag{53}$$

Substituting this into Eq. (40) and using the identity $\ln[a+(a^2-b^2)^{1/2}]=(2\pi)^{-1}\int_0^{2\pi}dx\,\ln(2a+2b\cos x)$ we have

$$\begin{aligned}\Lambda_M^0&=2\exp\left[\sum_{l=1}^{\infty}\frac{1}{2\pi}\int_0^{2\pi}dx\,\ln\left[1+\frac{(J\cos x+2h_z)^2}{[2\pi T(l-\frac{1}{2})]^2}\right]\right]\\&=\exp\left\{\frac{1}{2\pi}\int_0^{2\pi}dx\,\ln\left[2\cosh\left[\frac{J\cos x+2h_z}{2T}\right]\right]\right\}.\end{aligned} \tag{54}$$

Then free energy is

$$f=-\frac{T}{2\pi}\int_0^{2\pi}dx\,\ln\left[2\cosh\left[\frac{J\cos x+2h_z}{2T}\right]\right]. \tag{55}$$

In the same way we have

$$\frac{1}{\tanh y_l}=\left[\frac{2\pi Tl+2h_z i}{J}\right]+\left[\left[\frac{2\pi Tl+2h_z i}{J}\right]^2+1\right]^{1/2},$$

$$\Lambda_{M-1}^0=\frac{J}{2T}\exp\left[\frac{1}{2\pi}\int_0^{2\pi}dx\,\ln\left[\frac{\sinh[(J\cos x+2h_z)/2T]}{(J\cos x+2h_z)/2T}\right]\right].$$

The inverse of correlation length is

$$\xi_{xx}^{-1}=\frac{1}{2\pi}\int_0^{2\pi}dx\,\ln[\coth|(J\cos x+2h_z)/2T|], \tag{56a}$$

for $2|h_z|\le J$ and

$$\xi_{xx}^{-1}=\ln\left\{\left|\frac{2h_z}{J}\right|+\left[\left[\frac{2h_z}{J}\right]^2-1\right]^{1/2}\right\}+\frac{1}{2\pi}\int_0^{2\pi}dx\,\ln[\coth|(J\cos x+2h_z)/2T|], \tag{56b}$$

for $2|h_z|>J$. Results (55) and (56) agree with the known results.[11]

C. $T=h_z=0$ case

At very small T, the distribution of x_l's becomes dense. The mean distance is of the order of T/J_s. At $h_z=0$ all x_l's are on the real axis. Assume that $\rho(x)$ is the distribution function of x_l's. Equation (28) becomes

$$\frac{\pi T}{J_s}\int_x^K\rho(t)dt+\frac{T}{J_s}\int_0^K\frac{1}{2i}\ln[f(x,y)f(x,-y)]\rho(y)dy=g(x). \tag{57}$$

Here $K=\pi/2$ for $|\Delta|>1$ and $K=\infty$ for $|\Delta|\le 1$. We define function $F(x)$ as

$$F(x)\equiv\begin{cases}\dfrac{\pi T}{J_s}\displaystyle\int_x^K\rho(t)dt & \text{at } x>0\\ -F(-x) & \text{at } x<0.\end{cases} \tag{58}$$

By the partial differentiation of the second integral in Eq. (57), we have

$$F(x)-\int_{-K}^{K} q(x-y)F(y)dy = g(x) , \tag{59}$$

$$q(x)\equiv\frac{1}{2\pi i}\left[\frac{h'(x-2\eta)}{h(x-2\eta)}-\frac{h'(x+2\eta)}{h(x+2\eta)}\right]=\begin{cases}\dfrac{1}{\pi}\dfrac{\sinh 2\theta}{\cosh 2\theta-\cos 2x} & \text{for } |\Delta|>1\\ \dfrac{1}{\pi}\dfrac{\operatorname{sgn}(\Delta)}{x^2+1} & \text{for } |\Delta|=1\\ \dfrac{1}{\pi}\dfrac{\sin 2\theta}{\cosh 2x-\cos 2\theta} & \text{for } |\Delta|<1 .\end{cases} \tag{60}$$

We define the Fourier transform of a function $a(x)$ as follows:

$$\tilde{a}(n)\equiv\int_{-\pi/2}^{\pi/2} a(x)e^{-2inx}dx \quad \text{for } |\Delta|>1 ,$$

$$\tilde{a}(\omega)\equiv\int_{-\infty}^{\infty} a(x)e^{-i\omega x}dx \quad \text{for } |\Delta|\le 1 .$$

The Fourier transform of $g(x)$ and $q(x)$ are

$$\tilde{g}(n)=-\pi i\,\operatorname{sgn}(n)(1-e^{-|2n\theta|}) \quad \text{for } |\Delta|>1 , \tag{61a}$$

$$\tilde{g}(\omega)=-\pi i\,\operatorname{sgn}(\omega)(1-e^{-|\omega|}) \quad \text{for } |\Delta|=1 , \tag{61b}$$

$$\tilde{g}(\omega)=-\pi i\left[\coth\frac{\pi\omega}{2}-\frac{\cosh(\pi-2\theta)\omega/2}{\sinh\pi\omega/2}\right] \quad \text{for } |\Delta|<1 , \tag{61c}$$

$$\tilde{q}(n)=\operatorname{sgn}(\Delta)e^{-|2n\theta|} \quad \text{for } |\Delta|>1 , \tag{62a}$$

$$\tilde{q}(\omega)=\operatorname{sgn}(\Delta)e^{-|\omega|} \quad \text{for } |\Delta|=1 , \tag{62b}$$

$$\tilde{q}(\omega)=\frac{\sinh[(\pi-2\theta)\omega/2]}{\sinh(\pi\omega/2)} \quad \text{for } |\Delta|<1 . \tag{62c}$$

The function $g(x)$ has a pole at $x=0$. But we can define the Fourier integral by the principal part integral. One should note that the Fourier transform becomes discrete at $|\Delta|>1$ because the interval of integration is finite. Then we have the analytic solution of Eq. (59):

$$\tilde{F}(n)=-\pi i\,\operatorname{sgn}(n),\quad F(x)=\cot x \quad \text{for } \Delta>1 ; \tag{63a}$$

$$\tilde{F}(\omega)=-\pi i\,\operatorname{sgn}(\omega),\quad F(x)=\frac{1}{x} \quad \text{for } \Delta=1 ; \tag{63b}$$

$$\tilde{F}(\omega)=-\pi i\tanh\left[\frac{(\pi-\theta)\omega}{2}\right],\quad F(x)=\frac{\pi/(\pi-\theta)}{\sinh[\pi x/(\pi-\theta)]} \quad \text{for } |\Delta|<1 ; \tag{63c}$$

$$\tilde{F}(\omega)=-\pi i\tanh(\omega/2),\quad F(x)=\frac{\pi}{\sinh\pi x} \quad \text{for } \Delta=-1 ; \tag{63d}$$

$$\tilde{F}(n)=-\pi i\tanh n|\theta|,\quad F(x)=\sum_{n=-\infty}^{\infty}\frac{\pi\theta}{\sinh[\pi\theta(x-n\pi)]} \quad \text{for } \Delta<-1 . \tag{63e}$$

From Eq. (40) the ground-state energy per site e is

$$e=-\lim_{T\to 0} T\ln\Lambda_M^0=\frac{J_s}{\pi}\int_0^K \ln\left[\frac{h(2\eta-x)h(x+2\eta)}{F^2(x)h^2(x)h^2(2\eta)}\right]F'(x)dx . \tag{64}$$

Substituting Eq. (63), we have

$$
e=\begin{cases}-\dfrac{J\Delta}{4} \quad \text{for } \Delta\ge 1 & \text{(65a)}\\[2mm] -J\left[\dfrac{\Delta}{4}+(1-\Delta^2)^{1/2}\displaystyle\int_0^\infty \frac{\sinh(\theta\omega)}{\sinh(\pi\omega)\cosh[(\pi-\theta)\omega]}d\omega\right] \quad \text{for } |\Delta|<1 & \text{(65b)}\\[2mm] J(\tfrac{1}{4}-\ln 2) \quad \text{for } \Delta=-1 & \text{(65c)}\\[2mm] J\left[\dfrac{\Delta}{4}-(\Delta^2-1)^{1/2}\displaystyle\sum_{n=1}^{\infty} e^{-2n|\theta|}\tanh|n\theta|\right] \quad \text{for } \Delta<-1\ . & \text{(65d)}\end{cases}
$$

These results coincide with the known exact ground state energy per site of the *XXZ* model in zero field[12] as they should.

IV. NUMERICAL CALCULATIONS

In Eqs. (43) and (44) it is possible to calculate each term of the sum. We must use the logarithmic function many times because each term contains one. This procedure consumes a lot of computing time. It is very convenient if we can take the logarithm of the product. The logarithm is a multivalued function. In actual numerical calculation the imaginary part of $\ln x$ is fixed at $[\pi,-\pi]$, but there is no guarantee that this choice of branch is appropriate. So we transform Eqs. (43) and (44) as follows:

$$
\begin{aligned}
p_l &= V\left[\frac{4T}{J\Delta}\left[\frac{h_z i}{T}+\pi(l-1/2)+\frac{1}{2i}\ln X_l\right]\right],\\
X_l &= \exp\left[\frac{J\Delta i}{2T}[V^{-1}(p_l)-G(p_l)]\right]\prod_{j=1}^{\infty} L(p_l,p_j)L(p_l,-\bar{p}_j)\ ;
\end{aligned}
\tag{66a}
$$

$$
\begin{aligned}
q_l &= V\left[\frac{4T}{J\Delta}\left[\frac{h_z i}{T}+\pi l+\frac{1}{2i}\ln Y_l\right]\right],\\
Y_l &= \exp\left[\frac{J\Delta i}{2T}[V^{-1}(q_l)-G(q_l)]\right]\left[\frac{q_l-i}{q_l+i}\right]\prod_{j=1}^{\infty} L(q_l,q_j)L(q_l,-\bar{q}_j)\ .
\end{aligned}
\tag{66b}
$$

In this transformation function $V(x)$ is arbitrary if the branch of logarithm is taken appropriately. We choose function

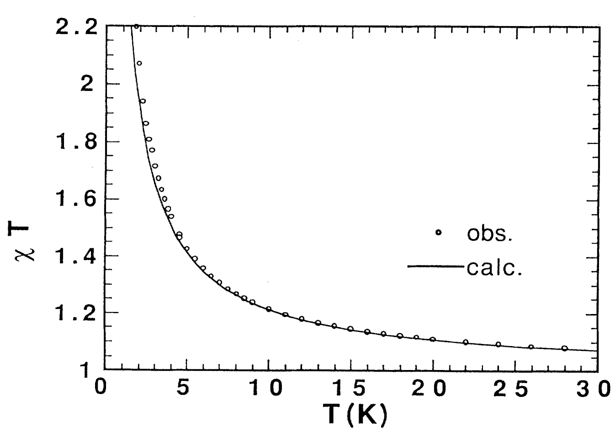

FIG. 1. Zero-field magnetic susceptibility multiplied by the temperature. The solid line is theoretical results for $\Delta=1$. The circles are the experimental results on *p*-NPNN. We put $J=4.3$ K.

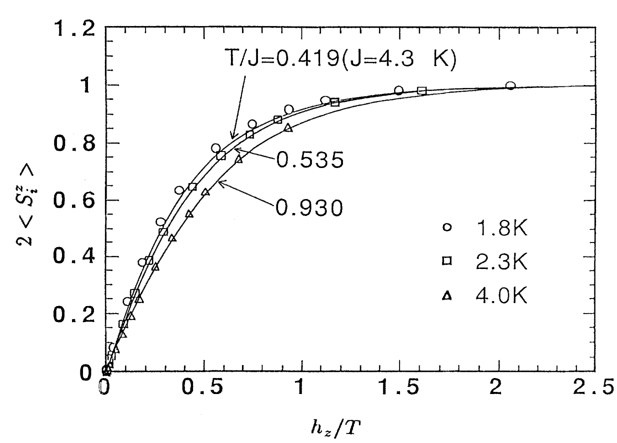

FIG. 2. The magnetization curve of Heisenberg ferromagnet $\Delta=1$. Solid lines are our theoretical results. Circles are experimental results on *p*-NPNN at 1.8 K. Squares are those at 2.3 K. Triangles are those at 4.0 K.

TABLE I. Free energy, magnetization, and correlation length ξ_{xx} for different anisotropy parameters Δ and temperatures. The zero-field magnetic susceptibility $\chi\equiv-\partial^2 f(T,h_z)/\partial h_z^2|_{h_x=0}$ is also given.

h_z/J	$f/J+\Delta/4$	$2\langle S_z\rangle$	ξ_{xx}	h_z/J	$f/J+\Delta/4$	$2\langle S_z\rangle$	ξ_{xx}
	$\Delta=1.5$ $T/J=0.2$ $J\chi=82.269$				$\Delta=1.5$ $T/J=0.4$ $J\chi=10.6370$		
0.0	−0.013 75	0.0	1.1644	0.0	−0.088 74	0.0	0.9813
0.2	−0.200 43	0.9955	0.7990	0.2	−0.214 93	0.9001	0.8100
0.4	−0.400 05	0.9994	0.6782	0.4	−0.404 56	0.9751	0.6818
0.6	−0.600 01	0.9999	0.6060	0.6	−0.601 59	0.9918	0.6070
0.8	−0.800 00	1.0000	0.5563	0.8	−0.800 57	0.9971	0.5566
1.0	−1.000 00	1.0000	0.5195	1.0	−1.000 21	0.9989	0.5196
1.2	−1.200 00	1.0000	0.4909	1.2	−1.200 08	0.9996	0.4909
1.4	−1.400 00	1.0000	0.4677	1.4	−1.400 03	0.9999	0.4677
1.6	−1.600 00	1.0000	0.4486	1.6	−1.600 01	0.9999	0.4486
1.8	−1.800 00	1.0000	0.4324	1.8	−1.800 00	1.0000	0.4324
2.0	−2.000 00	1.0000	0.4185	2.0	−2.000 00	1.0000	0.4185
	$\Delta=1.0$ $T/J=0.2$ $J\chi=14.1799$				$\Delta=1.0$ $T/J=0.4$ $J\chi=5.116 05$		
0.0	−0.064 96	0.0	1.9713	0.0	−0.162 63	0.0	1.1753
0.2	−0.205 27	0.9441	1.1394	0.2	−0.247 26	0.7225	1.0073
0.4	−0.400 68	0.9932	0.8375	0.4	−0.415 56	0.9172	0.8155
0.6	−0.600 09	0.9991	0.7015	0.6	−0.605 50	0.9719	0.6965
0.8	−0.800 01	0.9999	0.6213	0.8	−0.801 99	0.9899	0.6200
1.0	−1.000 00	1.0000	0.5673	1.0	−1.000 73	0.9963	0.5669
1.2	−1.200 00	1.0000	0.5278	1.2	−1.200 27	0.9987	0.5277
1.4	−1.400 00	1.0000	0.4974	1.4	−1.400 10	0.9995	0.4974
1.6	−1.600 00	1.0000	0.4731	1.6	−1.600 04	0.9998	0.4731
1.8	−1.800 00	1.0000	0.4531	1.8	−1.800 01	0.9999	0.4531
2.0	−2.000 00	1.0000	0.4362	2.0	−2.000 01	1.0000	0.4362
	$\Delta=0.5$ $T/J=0.2$ $J\chi=3.304 78$				$\Delta=0.5$ $T/J=0.4$ $J\chi=2.094 40$		
0.0	−0.183 57	0.0	2.7389	0.0	−0.271 43	0.0	1.3525
0.2	−0.247 60	0.6154	1.9890	0.2	−0.320 73	0.4728	1.2297
0.4	−0.407 87	0.9243	1.2145	0.4	−0.448 34	0.7709	1.0089
0.6	−0.601 10	0.9890	0.8839	0.6	−0.618 39	0.9099	0.8330
0.8	−0.800 15	0.9985	0.7279	0.8	−0.806 85	0.9660	0.7144
1.0	−1.000 02	0.9998	0.6382	1.0	−1.002 53	0.9874	0.6344
1.2	−1.200 00	1.0000	0.5791	1.2	−1.200 93	0.9953	0.5780
1.4	−1.400 00	1.0000	0.5367	1.4	−1.400 34	0.9983	0.5363
1.6	−1.600 00	1.0000	0.5044	1.6	−1.600 13	0.9994	0.5042
1.8	−1.800 00	1.0000	0.4787	1.8	−1.800 05	0.9998	0.4787
2.0	−2.000 00	1.0000	0.4577	2.0	−2.000 02	0.9999	0.4577
	$\Delta=-0.5$ $T/J=0.2$ $J\chi=0.777 26$				$\Delta=-0.5$ $T/J=0.4$ $J\chi=0.856 89$		
0.0	−0.516 83	0.0	3.0885	0.0	−0.572 83	0.0	1.5343
0.2	−0.532 56	0.1592	2.9956	0.2	−0.590 08	0.1736	1.4973
0.4	−0.582 16	0.3434	2.6793	0.4	−0.643 08	0.3589	1.3894
0.6	−0.673 81	0.5847	2.0949	0.6	−0.734 53	0.5565	1.2269
0.8	−0.818 19	0.8485	1.4289	0.8	−0.864 90	0.7417	1.0445
1.0	−1.002 92	0.9718	1.0036	1.0	−1.027 68	0.8754	0.8815
1.2	−1.200 41	0.9960	0.7924	1.2	−1.210 90	0.9478	0.7566
1.4	−1.400 06	0.9994	0.6776	1.4	−1.404 12	0.9797	0.6670
1.6	−1.600 01	0.9999	0.6060	1.6	−1.601 53	0.9924	0.6027
1.8	−1.800 00	1.0000	0.5563	1.8	−1.800 57	0.9972	0.5553
2.0	−2.000 00	1.0000	0.5195	2.0	−2.000 21	0.9990	0.5192

TABLE I. (*Continued*).

h_z/J	$f/J+\Delta/4$	$2\langle S_z\rangle$	ξ_{xx}	h_z/J	$f/J+\Delta/4$	$2\langle S_z\rangle$	ξ_{xx}
	$\Delta=-1.0$ $T/J=0.2$	$J\chi=0.48412$			$\Delta=-1.0$ $T/J=0.4$	$J\chi=0.55256$	
0.0	−0.706 96	0.0	2.9481	0.0	−0.752 87	0.0	1.5358
0.2	−0.716 76	0.0993	2.9323	0.2	−0.764 01	0.1123	1.5192
0.4	−0.747 58	0.2122	2.8511	0.4	−0.798 48	0.2351	1.4663
0.6	−0.803 47	0.3532	2.6247	0.6	−0.859 36	0.3776	1.3707
0.8	−0.892 39	0.5476	2.1708	0.8	−0.951 04	0.5423	1.2322
1.0	−1.026 69	0.7971	1.5540	1.0	−1.076 76	0.7131	1.0678
1.2	−1.204 70	0.9556	1.0801	1.2	−1.234 11	0.8520	0.9093
1.4	−1.400 67	0.9934	0.8323	1.4	−1.413 74	0.9353	0.7805
1.6	−1.600 09	0.9991	0.7009	1.6	−1.605 25	0.9743	0.6853
1.8	−1.800 01	0.9999	0.6213	1.8	−1.801 96	0.9903	0.6164
2.0	−2.000 00	1.0000	0.5673	2.0	−2.000 73	0.9964	0.5657
	$\Delta=-1.5$ $T/J=0.2$	$J\chi=0.29812$			$\Delta=-1.5$ $T/J=0.4$	$J\chi=0.36763$	
0.0	−0.909 45	0.0	2.6684	0.0	−0.947 32	0.0	1.4922
0.2	−0.915 54	0.0622	2.6931	0.2	−0.954 73	0.0748	1.4873
0.4	−0.935 17	0.1368	2.7350	0.4	−0.977 77	0.1574	1.4691
0.6	−0.971 44	0.2293	2.7244	0.6	−1.018 72	0.2552	1.4285
0.8	−1.028 58	0.3474	2.5855	0.8	−1.081 33	0.3750	1.3541
1.0	−1.113 44	0.5115	2.2388	1.0	−1.170 46	0.5204	1.2392
1.2	−1.237 85	0.7413	1.6831	1.2	−1.290 58	0.6813	1.0919
1.4	−1.407 46	0.9318	1.1694	1.4	−1.441 85	0.8252	0.9383
1.6	−1.601 09	0.9892	0.8788	1.6	−1.617 29	0.9201	0.8060
1.8	−1.800 15	0.9985	0.7273	1.8	−1.806 69	0.9676	0.7049
2.0	−2.000 02	0.9998	0.6381	2.0	−2.002 51	0.9876	0.6311

$V(x)$ as follows:

$$V(x)=V^{-1}(x)=x \quad \text{for } \Delta\geq 1\ ; \tag{67a}$$

$$V(x)=\tan\theta/\tanh\left[\frac{\pi-\theta}{\pi}\sinh^{-1}\frac{\pi}{(\pi-\theta)x}\right],$$
$$V^{-1}(x)=\frac{\pi/(\pi-\theta)}{\sinh\{[\pi/\pi-\theta)]\tanh^{-1}(\tan\theta/x)\}} \quad \text{for } |\Delta|<1\ ; \tag{67b}$$

$$V(x)=\pi/\sinh^{-1}(\pi/x),\quad V^{-1}(x)=\pi/\sinh(\pi/x) \quad \text{for } \Delta=-1\ ; \tag{67c}$$

$$V(x)=\tanh\theta/\tanh\left[\frac{2K(g)}{\pi}\text{tn}^{-1}\left[\frac{\pi}{2K(g)x},g\right]\right],$$
$$V^{-1}(x)=\frac{\pi/2K}{\text{tn}[(\pi/2K)\tanh^{-1}(\tanh|\theta|/x),g]},$$
$$K[(1-g^2)^{1/2}]/K(g)=|\theta|/\pi \quad \text{for } \Delta<-1\ . \tag{67d}$$

Here $\text{tn}(x,g)\equiv\text{sn}(x,g)/\text{cn}(x,g)$ is an elliptic function. $K(g)$ is a complete elliptic integral of the first kind with modulus g. In this choice of $V(x)$, the imaginary part of logarithm can be fixed at $[\pi,-\pi]i$. Functions $V(x)$ and $V^{-1}(x)$ are obtained from the distribution of roots (63) at zero temperature and zero field. In actual numerical calculation we treat p_l and q_l at $l\leq L$, where L is a certain integer. The p_j and q_j at $j>L$ are approximated by $p_j=4T\pi(j-1/2)/(J\Delta)+i\,\text{Im}(p_L)$ and $q_j=4T\pi j/(J\Delta)+i\,\text{Im}(q_L)$. The products in Eqs. (66) are estimated accurately.

Iterative calculation of Eqs. (66) converges very rapidly for arbitrary h_z, Δ, and T, and we get Λ_M^0 and Λ_{M-1}^0. The magnetization and magnetic susceptibility are given by differentiations of free energy with respect to h_z. So we need to calculate $\partial p_l/\partial h_z$ and $\partial^2 p_l/\partial h_z^2$. These are given by solutions of linear equations which are obtained by the differentiation of Eqs. (43).

In Fig. 1 the calculation of magnetic susceptibility at $\Delta=1$ is shown. The results are compared with the experimental results on the γ phase of p-NPNN ($C_{13}H_{16}N_3O_4$), which is an organic quasi-one-dimensional ferromagnet with $J=4.3$ K.[13] It is made of only carbon, nitrogen, hydrogen, and oxygen. In Fig. 2 the calculation of magnetization at finite field is compared with experimental result of this substance. The agreement is surprisingly good. The experimental details were published in Ref. 13. Of course, these calculations are possible by using the method of Bethe-ansatz integral equations,[2–5] but calculations become much simpler. In Table I, the free energy, ξ_{xx} and magnetization are given for several sets of temperature, Δ and h_z.

V. CORRELATION LENGTH ξ_{zz}

Here we consider ξ_{zz}, which is defined by Eq. (11). In the case $|\Delta|>1$ and $h_z=0$, ξ_{zz} is longer than ξ_{xx}, and the problem is very simple. In Eq. (24) we put $k=M$ and

$$z_1=\begin{cases}\pi/2 & \text{for } |\Delta|>1\\ \infty & \text{for } |\Delta|=1\ ,\end{cases}$$
$$z_2>z_3>\cdots>z_M,\quad z_{M+1-j}=-z_{j+1}\ . \tag{68}$$

We have the equation for $z_2,z_3,\ldots$ in the limit $M\to\infty$:

$$\frac{2J_s}{T}g(z_l)=2\pi(l-1)+\frac{1}{i}\left[\ln f(z_l,z_1)+\sum_{j=2}^{\infty}\ln[f(z_l,z_j)f(z_l,-z_j)]\right]\ , \tag{69}$$

$$\Lambda_M^1=2\left[\frac{J\Delta}{4}\right]\prod_{l=2}^{\infty}\frac{h(2\eta-z_l)h(2\eta+z_l)}{h^2(z_l)h^2(2\eta)}\left[\frac{J_s}{T\pi(l-1)}\right]^2\ . \tag{70}$$

These are transformed as

$$r_1=0\ ,$$
$$\frac{J\Delta}{2T}G(r_l)=2\pi(l-1)+\frac{1}{i}\left[\ln L(r_l,0)+\sum_{j=2}^{\infty}\ln[L(r_l,r_j)L(r_l,-r_j)]\right],\quad l=2,3,\ldots\ , \tag{71}$$

$$\Lambda_M^1=2\left[\frac{J\Delta}{4T}\right]\prod_{l=2}^{\infty}\left[\frac{J\Delta}{4\pi T(l-1)}\right]^2(r_l^2+1)\ . \tag{72}$$

This eigenvalue is the same with Λ_1 in Eqs. (40) and (41) of Ref. 1 at $J_z\ge J_y=|J_x|$ if we set $J=J_y$, $\Delta=\mathrm{sgn}(J_x)J_z/J_y$. The generalization of these equations to $h_z\neq 0$ or $|\Delta|<1$ is not simple. In these cases, z_1 is also variable, and Λ_M^1 is sometimes a complex number. Analyses of Λ_M^1 for these cases are remained in further investigations.

VI. SUMMARY AND DISCUSSION

In this paper we derived transcendental equations with an infinite number of unknowns, which give the free energy and correlation length ξ_{xx} of the one-dimensional XXZ model in a magnetic field. For this system the free energy has already been given by the thermodynamic nonlinear integral equations derived in the 1970's.[2] The equations for free energy (6), (43), and (46) should be equivalent to them, but the equations for the correlation lengths (11), (43)–(47), and (71) and (72) are completely different. One should note that the row-to-row transfer matrix for the homogeneous six-vertex model cannot give the transcendental equations for the finite-temperature XXZ chain. One must solve the eigenvalue problem of the diagonal-to-diagonal transfer matrix on a strip of finite width. This is solved as a special case of the inhomogeneous six-vertex model.

Our theory is applied to the organic ferromagnet p-NPNN. The agreement of magnetic susceptibility and magnetization with experiment is very good.

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