Progress of Theoretical Physics, Vol. 48, No. 6B, December 1972

One-Dimensional Anisotropic Heisenberg Model at Finite Temperatures

Minoru TAKAHASHI and Masuo SUZUKI*

Department of Physics, College of General Education
Osaka University, Toyonaka, Osaka
**Institute for Solid State Physics, University of Tokyo*
Roppongi, Minato-ku, Tokyo

(Received May 11, 1972)

The thermodynamics of the one-dimensional Heisenberg-Ising model for $|\Delta|<1$ as well as of the X-Y-Z model is reduced to a set of non-linear integral equations under some plausible assumptions. It is remarkable that the number of unknown functions involved in them becomes ***finite*** when $\pi/\cos^{-1}\Delta$ is a rational number for the Heisenberg-Ising model and when K_l/ζ is a rational number for the X-Y-Z model (where coupling constants J_x, J_y and J_z are parametrized by ζ, l, and J_z as $J_x=J_z\,\mathrm{cn}\,(2\zeta, l)$ and $J_y=J_z\,\mathrm{dn}\,(2\zeta, l)$; $1\geq l\geq 0$, $K_l\geq 2\zeta\geq 0$, and K_l is the complete elliptic integral of the first kind of modulus l). The validity of our theory has been confirmed by the high-temperature expansion of the free energy through the second term for a general value of Δ and through the fourth term for $\Delta=\frac{1}{2}$.

§ 1. Introduction

One of the authors[1] and Gaudin[2] have discussed the thermodynamics of the Heisenberg-Ising ring of spin $\frac{1}{2}$ with the anisotropy parameter Δ in the range $|\Delta|=1$ and $|\Delta|\geq 1$, respectively. These arguments have also been extended to the region $|\Delta|<1$ by one of the authors.[3] However, this extension has been criticized by Johnson, McCoy and Lai[4] with the use of the high-temperautre expansion.

In this paper, we make new propositions on the energy spectrum of the excited states for a large chain and derive non-linear integral equations for the thermodynamics of the anisotropic Heisenberg model (X-Y-Z model) as well as of the Heisenberg-Ising model for $|\Delta|<1$ in one dimension. The ground state of the Hamiltonian

$$\mathcal{H}=J\sum_{i=1}^{N}\{S_i^xS_{i+1}^x+S_i^yS_{i+1}^y+\Delta(S_i^zS_{i+1}^z-\tfrac{1}{4})\}-2\mu_0H\sum_{i=1}^{N}S_i^z;\quad S_{N+1}\equiv S_1, \tag{1·1}$$

has been discussed by many authors.[6),7)] In § 2, two assumptions on the distribution of parameters which determine the eigenvalues of (1·1) for $|\Delta|<1$ are proposed and consequently eigenvalue equations are reduced to more convenient ones for the real parts of these parameters. As the energy spectrum of this Hamiltonian is invariant under the transformation $(J, \Delta)\rightarrow(-J, -\Delta)$, we confine ourselves to the region $1>\Delta\geq 0$. In § 3, non-linear integral equations are derived for the free energy of the Heisenberg-Ising model (1·1) in the thermodynamic limit. In contrast to the case $|\Delta|\geq 1$, it is quite remarkable that the number of unknown functions involved in these non-linear equations becomes *finite* when $\pi/\cos^{-1}\Delta$ is a rational number for $|\Delta|<1$. In particular, the free energy calculated from the non-linear integral equations has been checked to agree with the well-known exact results obtained by the usual high-temperature expansion method, at least, through the second term in a power series of J/T for the general value of Δ in the range $|\Delta|<1$, and through the fourth term for $\Delta=\frac{1}{2}$. In § 4 we start with Baxter's equations[8] for eigenvalues of the X-Y-Z model and obtain non-linear integral equations for the free energy with the use of assumptions similar to those for the Heisenberg-Ising model. Summary and discussion will be given in the last section.

§ 2. Eigenstates and eigenvalues of a large Heisenberg-Ising system

In this section we discuss the eigenvalues of the Hamiltonian (1·1) for $1>\Delta\geq 0$. Now suppose that there are M down-spins and N-M up-spins. Following Bethe[6),7)] we write

$$\Psi=\sum_{z_1<z_2<\cdots<z_M}\Phi(z_1,z_2,\cdots,z_M)S_{z_1}^-S_{z_2}^-\cdots S_{z_M}^-|0\rangle \tag{2·1a}$$

and

$$\Phi(z_1,z_2,\cdots,z_M)=\sum_P\exp\{i(\sum_{j=1}^M k_{Pj}z_j+\tfrac{1}{2}\sum_{j<l}\phi_{Pj,Pl})\}\,. \tag{2·1b}$$

Here $k_1,k_2,\cdots,k_M$ are quasi-momenta, P denotes permutations of the integers $1,2,\cdots,m$, and the phases $\phi_{\alpha\beta}$ are defined by

$$\cot(\tfrac{1}{2}\phi_{\alpha\beta})=\cot\theta\,\mathrm{th}\{\tfrac{1}{2}\theta(x_\alpha-x_\beta)\}\,, \tag{2·2}$$

where x_α are introduced to parametrize the quasi-momenta k_α as follows:

$$\cot(\tfrac{1}{2}k_\alpha)=\cot(\tfrac{1}{2}\theta)\,\mathrm{th}(\tfrac{1}{2}\theta x_\alpha)\,, \tag{2·3}$$

$$\Delta=\cos\theta \quad\text{and}\quad \pi/2\geq\theta>0\,. \tag{2·4}$$

In the case $S^z=(N-2M)/2\geq 0$, the energy eigenvalue E and the momentum eigenvalue K are given by

$$\begin{aligned}E&=J\sum_{\alpha=1}^M(\cos k_\alpha-\Delta)-(N-2M)\mu_0H\\&=\sum_{\alpha=1}^M\{-2\pi J\theta^{-1}\sin\theta\, a_1(x_\alpha)+2\mu_0H\}-N\mu_0H\,,\end{aligned} \tag{2·5a}$$

$$K=\sum_{\alpha=1}^M k_\alpha=\sum_{\alpha=1}^M\frac{1}{i}\ln\frac{\mathrm{sh}\frac{1}{2}\theta(x_\alpha+i)}{\mathrm{sh}\frac{1}{2}\theta(x_\alpha-i)}\,; \tag{2·5b}$$

where

$$a_1(x)\equiv\frac{1}{2p_0}\frac{\sin(\pi/p_0)}{\mathrm{ch}(\pi x/p_0)-\cos(\pi/p_0)};\quad p_0\equiv\frac{\pi}{\theta}. \tag{2·6}$$

The periodic boundary condition

$$\Phi(z_1, z_2, \cdots, z_{M-1}, N+1)=\Phi(1, z_1, z_2, \cdots, z_{M-1}) \tag{2·7}$$

is expressed by the relation

$$\left\{\frac{\mathrm{sh}\,\frac{1}{2}\theta(x_\alpha+i)}{\mathrm{sh}\,\frac{1}{2}\theta(x_\alpha-i)}\right\}^N=-\prod_{\beta=1}^{M}\left\{\frac{\mathrm{sh}\,\frac{1}{2}\theta(x_\alpha-x_\beta+2i)}{\mathrm{sh}\,\frac{1}{2}\theta(x_\alpha-x_\beta-2i)}\right\};\quad \alpha=1, 2, \cdots M. \tag{2·8}$$

Here, it should be remarked that the coupled equations (2·2), (2·3) and (2·8) have a periodic property with respect to the M parameters x_α. Thus, at first sight it seems convenient to confine the region for x_α in the first zone $-\pi\theta^{-1}<\mathrm{Im}\,x_\alpha\leq\pi\theta^{-1}$. However, it will be found to be more convenient to make use of an "extended zone" in our problem and to identify such parameters x_α as coincide with one another if any of them is repeatedly shifted by the period $2\pi i\theta^{-1}$. Hereafter the symbol (mod $2p_0i$) implies the above feature of the periodicity, where $p_0\equiv\pi/\theta$. First, we discuss the case in which p_0 is an irrational number, and later we take a limiting process for the case in which p_0 is a rational number. In the limit of large N, the roots of (2·8) are grouped in a various strings characterized by a common real abscissa and an order n. The following two propositions play a main role in our theory. A reasoning for them will be discussed in § 5.

Assumption 1: A string of order n consists of the sets

$$x_{\alpha,+}^{n,k}\equiv x_\alpha^n+(n+1-2k)i+O(\exp-\delta N) \qquad (\mathrm{mod}\ 2p_0i)$$

and

$$x_{\alpha,-}^{n,k}\equiv x_\alpha^n+(n+1-2k)i+p_0i+O(\exp-\delta N), \quad (\mathrm{mod}\ 2p_0i) \tag{2·9}$$

where $\delta>0$, $k=1, 2, \cdots, n$, and x_α^n is real. We call these states the n-th-order bound states with $+$ and $-$ parities, respectively.

Assumption 2: The parity v and order n of a bound state should satisfy the following conditions:

$$\sin\{\pi(n-1)/p_0\}\geq0 \quad \text{for } v=+1, \tag{2·10a}$$

$$\sin\{\pi(n-1)/p_0\}\leq0 \quad \text{for } v=-1 \tag{2·10b}$$

and

$$2\sum_{j=1}^{n-1}[j/p_0]=(n-1)[(n-1)/p_0], \tag{2·11}$$

where $[x]$ denotes the maximum integer less than or equal to x (Gauss' symbol).

The requirement (2·11) comes from a plausible condition for the number of magnons in some special limit. (For details, see the discussion in § 5.)

Here we define series of real numbers p_i and series of integers ν_i, m_i, and y_i as follows:

$$p_0=\pi/\theta,\ p_1=1,\ \nu_i=[p_{i-1}/p_i],\ p_i=p_{i-2}-p_{i-1}\nu_{i-1},$$

$$m_0=0,\ m_i=\sum_{k=1}^{i}\nu_k,$$

$$y_{-1}=0,\ y_0=1,\ y_1=\nu_1,\ y_2=\nu_1\nu_2+1 \quad\text{and}\quad y_i=y_{i-2}+\nu_i y_{i-1}. \tag{2·12}$$

It is clear that p_0 is given by the continued fraction

$$\frac{1}{p_0}=\frac{1}{\nu_1+}\frac{1}{\nu_2+}\frac{1}{\nu_3+}\cdots. \tag{2·13}$$

The order and parity of all bound states which satisfy assumption 2 are expressed by

$$n_j=y_{i-1}+(j-m_i)y_i \quad\text{for } m_i\leq j<m_{i+1},\ j=1,2,\cdots,$$

$$v_1=+1,\ v_{m_1}=-1 \quad\text{and}\quad v_j=\exp(\pi i[(n_j-1)/p_0]) \quad\text{for } j\neq 1,\ m_1. \tag{2·14}$$

This will be proved in Appendix A. Now suppose that there are M_j bound states of parity v_j and order n_j. Taking the product of Eqs. (2·8) for n_j components of a string, we have the following equations for the real part $x_\alpha^{n_j}$ of (2·9) (hereafter we write $x_\alpha^{n_j}$ as $x_\alpha{}^j$):

$$\{e_j(x_\alpha{}^j)\}^N=-\prod_{k=1}^{\infty}\prod_{\beta=1}^{M_k}E_{jk}(x_\alpha{}^j-x_\beta{}^k), \tag{2·15a}$$

where

$$e_j(x)=g(x;\ n_j, v_j),$$

$$E_{jk}(x)=\begin{cases} g(x;\ 2n_j, v_jv_k)\prod_{l=1}^{n_j-1}g^2(x;\ 2l, v_jv_k) & \text{for } n_j=n_k,\\ g(x;\ (n_j+n_k), v_jv_k)\,g(x;\ |n_j-n_k|, v_jv_k) & \\ \times\prod_{l=1}^{\mathrm{Min}(n_j,n_k)-1}g^2(x;\ |n_j-n_k|+2l, v_jv_k) & \text{for } n_j\neq n_k, \end{cases}$$

$$g(x;\ n, +)=\frac{\mathrm{sh}\,\frac{1}{2}\theta(x+ni)}{\mathrm{sh}\,\frac{1}{2}\theta(x-ni)},\quad g(x;\ n, -)=-\frac{\mathrm{ch}\,\frac{1}{2}\theta(x+ni)}{\mathrm{ch}\,\frac{1}{2}\theta(x-ni)}. \tag{2·15b}$$

The logarithm of Eqs. (2·15a) yields

$$Nt_j(x_\alpha{}^j)=2\pi I_\alpha{}^j+\sum_{k=1}^{\infty}\sum_{\beta=1}^{M_k}\Theta_{jk}(x_\alpha{}^j-x_\beta{}^k),\quad \alpha=1,2,\cdots,M_j, \tag{2·16a}$$

where

$$t_j(x)=f(x;\ n_j, v_j),\ \Theta_{jk}(x)=f(x;\ |n_j-n_k|, v_jv_k)+f(x;\ n_j+n_k, v_jv_k)$$
$$+2\sum_{i=1}^{\mathrm{Min}(n_j,n_k)-1}f(x;\ |n_j-n_k|+2i, v_jv_k), \tag{2·16b}$$

and

$$f(x;\ n,v)\equiv\begin{cases}0 \quad \text{for } n/p_0=\text{integer},\\ \dfrac{1}{i}\ln\{-g(x;\ n,v)\}=2v\tan^{-1}\{(\cot(n\pi/2p_0))^v\,\text{th}(\pi x/2p_0)\}\\ \hfill\text{otherwise}.\end{cases}\tag{2·17}$$

The property that $f(x;\ n,v)=0$ for $n/p_0=$integer in (2·17), comes from the requirement that $\Theta_{jk}(x)$ do not contain any kind of step function. The quantity I_α^j is an integer (or half-odd integer) for M_j odd (or even), which is located in the region

$$|I_\alpha^j|<\frac{1}{2\pi}|Nf(\infty;\ n_j,v_j)-\sum_{k=1}^{\infty}M_k\Theta_{jk}(\infty)|.\tag{2·18}$$

Note that $f(x;\ n_j,v_j)$ is a monotonously increasing function for $r(j)$ odd, and a monotonously decreasing function for $r(j)$ even, when $r(j)$ is defined by

$$m_{r(j)}\leq j<m_{r(j)+1}.\tag{2·19}$$

§ 3. Non-linear integral equations for the free energy of the Heisenberg-Ising model in the thermodynamic limit

Following Yang and Yang,[9] we define particles and holes of bound states. From (2·15), we obtain integral equations for distribution functions ρ_j and ρ_j^h of particles and holes of bound states for the thermodynamic limit as follows:

$$a_j(x)=(-1)^{r(j)}(\rho_j+\rho_j^h)+\sum_{k=1}^{\infty}T_{jk}*\rho_k(x),\tag{3·1}$$

where $r(j)$ is defined in (2·19), and

$$T_{jk}(x)=(2\pi)^{-1}\frac{d}{dx}\Theta_{jk}(x)\quad\text{and}\quad a_j(x)=(2\pi)^{-1}\frac{d}{dx}t_j(x).\tag{3·2}$$

The symbol $a*b$ denotes the convolution of $a(x)$ and $b(x)$ as follows:

$$a*b(x)=\int_{-\infty}^{\infty}a(x-y)b(y)dy.\tag{3·3}$$

The energy and entropy are given by

$$E/N=\sum_{j=1}^{\infty}\int_{-\infty}^{\infty}(-Aa_j(x)+2n_j\mu_0H)\rho_j(x)dx-\mu_0H\tag{3·4}$$

and

$$S/N=\sum_{j=1}^{\infty}\int_{-\infty}^{\infty}\{(\rho_j+\rho_j^h)\ln(\rho_j+\rho_j^h)-\rho_j\ln\rho_j-\rho_j^h\ln\rho_j^h\}dx,\tag{3·5}$$

respectively, where $A\equiv2\pi J\theta^{-1}\sin\theta$. Minimizing the free energy $F=E-TS$ with respect to ρ_j, we obtain the following non-linear equations for $\eta_j=\rho_j^h/\rho_j$:

$$\ln \eta_j = (-Aa_j + 2n_j\mu_0 H)/T + \sum_{k=1}^{\infty} (-1)^{r(k)} T_{jk} * \ln(1+\eta_k^{-1}), \tag{3·6}$$

where $r(k)$ is defined in (2·19). In Appendix B, we prove the following relations:

$$\begin{aligned}
&T_{jk} - s_i*((1-2\delta_{m_{i-1},j})T_{j-1,k} + T_{j+1,k}) = (-1)^{i+1}(\delta_{j-1,k}+\delta_{j+1,k})s_i\,,\\
&a_j - s_i*((1-2\delta_{m_{i-1},j})a_{j-1} + a_{j+1}) = 0 \quad \text{for } m_{i-1} \le j \le m_i - 2\,,\\
&T_{jk} - (1-2\delta_{m_{i-1},j})s_i*T_{j-1,k} - d_i*T_{j,k} - s_{i+1}*T_{j+1,k}\\
&\qquad = (-1)^{i+1}(\delta_{j-1,k}s_i + \delta_{j,k}d_i - \delta_{j+1,k}s_{i+1})\,,\\
&a_j - (1-2\delta_{m_{i-1},j})s_i*a_{j-1} - d_i*a_j - s_{i+1}*a_{j+1} = 0 \quad \text{for } j = m_i - 1\,,
\end{aligned} \tag{3·7}$$

where

$$s_i(x) \equiv \frac{1}{4p_i}\operatorname{sech}\frac{\pi x}{2p_i}\,, \quad d_i(x) \equiv \int_{-\infty}^{\infty}\frac{dk}{2\pi}\cdot\frac{e^{ikx}\operatorname{ch}((p_i - p_{i+1})k)}{2\operatorname{ch}(p_i k)\operatorname{ch}(p_{i+1}k)}\,. \tag{3·8}$$

Using these relations we can rewrite (3·1) as follows:

$$\begin{aligned}
&\rho_j + \rho_j^h = s_i*(\rho_{j-1}^h + \rho_{j+1}^h) \quad \text{for } m_{i-1} \le j \le m_i - 2\,,\\
&\rho_j + \rho_j^h = s_i*\rho_{j-1}^h + d_i*\rho_j^h - s_{i+1}*\rho_{j+1}^h \quad \text{for } j = m_i - 1
\end{aligned} \tag{3·9}$$

with $\rho_0^h = \delta(x)$. Equations (3·6) are rewritten as

$$\begin{aligned}
&\ln(1+\eta_0) = -2\pi J \sin\theta\,\delta(x)/(\theta T)\,,\\
&\ln\eta_j = (1-2\delta_{m_{i-1},j})s_i*\ln(1+\eta_{j-1}) + s_i*\ln(1+\eta_{j+1}) \quad \text{for } m_{i-1} \le j \le m_i - 2\,,\\
&\ln\eta_j = (1-2\delta_{m_{i-1},j})s_i*\ln(1+\eta_{j-1}) + d_i*\ln(1+\eta_j) + s_{i+1}*\ln(1+\eta_{j+1})\\
&\qquad\qquad \text{for } j = m_i - 1
\end{aligned} \tag{3·10}$$

and

$$\lim_{j\to\infty}\frac{\ln\eta_j}{n_j} = \frac{2\mu_0 H}{T}\,. \tag{3·11}$$

The free energy of this system $F \equiv E - TS$ is given by

$$\frac{F}{N} = -2\pi J\theta^{-1}\sin\theta\int_{-\infty}^{\infty}a_1(x)s_1(x)dx - T\int_{-\infty}^{\infty}\ln(1+\eta_1(x))s_1(x)dx\,. \tag{3·12}$$

If $p_0 \equiv \pi/\theta$ is a rational number given by the continued fraction

$$\frac{1}{p_0} = \frac{1}{\nu_1 +}\,\frac{1}{\nu_2 +}\cdots\frac{1}{\nu_\alpha}\,; \quad \nu_1, \nu_\alpha \ge 2\,, \tag{3·13}$$

we take the limit $\nu_{\alpha+1} \to \infty$ in Eqs. (3·10). Then in this limit we have that $p_\alpha = 0+$ and $s_{\alpha+1} = d_\alpha = \frac{1}{2}\delta(x)$. Therefore, a partial set of the integral equations (3·10) (namely for $j \ge m_\alpha - 1$) can be reduced to the following simple difference equations:

$$\ln \eta_{m_\alpha-1}=\tfrac{1}{2}\ln\{(1+\eta_{m_\alpha})/(1+\eta_{m_\alpha-2})\}$$

and

$$\ln \eta_j=\tfrac{1}{2}\ln\{(1+\eta_{j-1})(1+\eta_{j+1})\} \quad \text{for } j\geq m_\alpha . \tag{3·14}$$

The general solution of these difference equations is given by

$$\eta_{m_\alpha-1}=\kappa^2+(a+a^{-1})\kappa$$

and

$$\eta_{m_\alpha+n}+1=\left(\frac{(a^{n+1}-a^{-n-1})\kappa+(a^{n+2}-a^{-n-2})}{a-a^{-1}}\right)^2\Big/(1+(a+a^{-1})\kappa+\kappa^2),\quad n\geq 0 . \tag{3·15}$$

Substituting (3·15) into (3·10) we can determine the parameters a and κ as

$$a=\exp(-y_\alpha\mu_0 H/T) \quad \text{and} \quad \ln\kappa(x)=s_\alpha*\ln(1+\eta_{m_\alpha-2}). \tag{3·16}$$

Thus, the set of Eqs. (3·10) has been reduced to that with a finite number of unknown functions $\eta_1, \eta_2, \cdots, \eta_{m_\alpha-2}$ and κ; i.e.,

$$\ln(1+\eta_0)=-2\pi J\sin\theta\delta(x)/(\theta T) ,$$

$$\ln\eta_j=(1-2\delta_{m_{i-1},j})s_i*\ln(1+\eta_{j-1})+s_i*\ln(1+\eta_{j+1})$$
$$\text{for } m_{i-1}\leq j\leq m_i-2,\quad 1\leq i<\alpha ,$$

$$\ln\eta_j=(1-2\delta_{m_{i-1},j})s_i*\ln(1+\eta_{j-1})+d_i*\ln(1+\eta_j)+s_{i+1}*\ln(1+\eta_{j+1})$$
$$\text{for } j=m_i-1,\quad 1\leq i<\alpha$$

and

$$\eta_{m_\alpha-1}=\kappa^2+(a+a^{-1})\kappa \quad \text{and} \quad \ln\kappa=s_\alpha*\ln(1+\eta_{m_\alpha-2}). \tag{3·17}$$

Especially when p_0 is an integer ν_1, the above equations (3·17) are reduced again to the following very simple ones:

$$\ln(1+\eta_0)=-2\pi J\theta^{-1}\sin\theta\delta(x)/T ,$$

$$\ln\eta_j=s_1*\ln\{(1+\eta_{j-1})(1+\eta_{j+1})\} \quad \text{for } j=1, 2, 3, \cdots, \nu_1-3 ,$$

$$\ln\eta_{\nu_1-2}=s_1*\ln\left\{(1+\eta_{\nu_1-3})\left(1+2\kappa\,\mathrm{ch}\frac{p_0\mu_0 H}{T}+\kappa^2\right)\right\}$$

and

$$\ln\kappa=s_1*\ln(1+\eta_{\nu_1-2}). \tag{3·18}$$

The high-temperature expansion of the free energy based on these equations is given in Appendix C. The results thus obtained agree with the well-known exact one at least up to the second term for a general value of Δ. In particular, it is easy to obtain more terms of the high-temperature expansion for $\Delta=\frac{1}{2}$. The free energy for this case is given by

$$F/N=-\tfrac{1}{2}J-T\ln\kappa(0), \tag{3·19}$$

where $\kappa(x)$ is the solution of the following coupled non-linear integral equations

$$\ln\eta_1(x)=-3\sqrt{3}(J/T)s_1(x)+s_1*\ln(1+\eta_2),$$
$$\eta_2(x)=\kappa^2(x)+2\kappa(x)\,\mathrm{ch}(3\mu_0 H/T)$$

and

$$\ln\kappa(x)=s_1*\ln(1+\eta_1). \tag{3·20}$$

The case $H=0$ is investigated in Appendix D. The free energy calculated from (3·20) agrees with that obtained by Katsura and Inawashiro[10] through the fourth term in the high-temperature expansion method.

In Appendix E it will be shown that for the limit $p_0\to 2$, Eqs. (3·10) are solved analytically and one obtains the exact free energy of the isotropic X-Y model.[11] In the limit $p_0\to\infty$, Eqs. (3·10) become equivalents to those for the isotropic Heisenberg model[1] as it should be.

§ 4. The one-dimensional X-Y-Z model

In recent papers,[8] Baxter obtained a set of transcendental equations to determine the energy spectrum of the one-dimensional X-Y-Z model, the Hamiltonian of which is given by

$$\mathcal{H}=\sum_{i=1}^{N}(J_x S_i^x S_{i+1}^x+J_y S_i^y S_{i+1}^y+J_z S_i^z S_{i+1}^z), \tag{4·1}$$

where $S_{N+1}\equiv S_1$, $N=$even and $1\geq J_y/J_z\geq J_x/J_z\geq 0$ (this restriction goes without loss of generality, since the eigenvalues are unaltered by changing the signs of any two of J_x, J_y and J_z). The coupling constants J_x and J_y are parametrized by ζ and l as

$$J_x=J_z\,\mathrm{cn}(2\zeta,l),\ J_y=J_z\,\mathrm{dn}(2\zeta,l);\quad 1\geq l\geq 0,\ K_l\geq 2\zeta\geq 0. \tag{4·2}$$

Here K_l denotes the complete elliptic integral of the first kind of modulus l. There appear $N/2$ parameters $x_1, x_2, \cdots$, and $x_{N/2}$ which satisfy

$$\left\{\frac{H(\zeta(x_\alpha+i))}{H(\zeta(x_\alpha-i))}\right\}^N=-\exp(2\pi\nu/Q)\prod_{\beta=1}^{N/2}\left\{\frac{H(\zeta(x_\alpha-x_\beta+2i))}{H(\zeta(x_\alpha-x_\beta-2i))}\right\}, \tag{4·3a}$$

$$\sum_{\alpha=1}^{N/2}\zeta x_\alpha=K_{l'}\nu'+iK_l\nu \tag{4·3b}$$

for $\alpha=1,2,\cdots,N/2$, where $Q=K_{l'}/\zeta$; ν and ν' are certain integers and $H(z)$ is Jacobi's elliptic theta function of modulus $l'=\sqrt{1-l^2}$. The function $H(z)$ is also related to the usual elliptic theta function as

$$H(z)\equiv\vartheta_1(z/2K_{l'};\ iK_l/K_{l'}). \tag{4·4}$$

The energy eigenvalue E and momentum eigenvalue K are given by

$$E=-J_z\pi\zeta^{-1}\,\mathrm{sn}(2\zeta)\sum_{\alpha=1}^{N/2}\boldsymbol{a}_1(x_\alpha)-NJ_zR \tag{4·5a}$$

and

$$e^{i\kappa}=\exp\left(-\frac{\pi\nu}{Q}\right)\prod_{\alpha=1}^{N/2}\frac{H(\zeta(x_\alpha+i))}{H(\zeta(x_\alpha-i))}, \tag{4·5b}$$

respectively, where

$$\boldsymbol{a}_1(x)\equiv\sum_{j=-\infty}^{\infty}a_1(x-2jQ), \tag{4·6a}$$

$$R\equiv\tfrac{1}{4}-\pi(4\zeta)^{-1}\,\mathrm{sn}(2\zeta)\{\boldsymbol{a}_1(0)+\boldsymbol{a}_1(Q)\}, \tag{4·6b}$$

and the parameter p_0 of $a_1(x)$ in (2·6) is now replaced by

$$p_0\equiv K_l/\zeta\,. \tag{4·7}$$

It should be noted that $\boldsymbol{a}_1(x)$ is expressed in terms of Jacobi's zeta function $Z(\zeta)$ with modulus l as follows:

$$\boldsymbol{a}_1(x)=\frac{\zeta}{\pi}\left\{Z(\zeta)+\frac{\mathrm{sn}\,\zeta\,\mathrm{cn}\,\zeta\,\mathrm{dn}\,\zeta}{\mathrm{sn}^2\zeta-\mathrm{sn}^2(i\zeta x)}\right\}, \tag{4·8}$$

and $Z(\zeta)$ denotes Jacobi's zeta function with modulus l. Now we assume that assumptions 1 and 2 are valid for the new parameters $x_1, x_2, \cdots,$ and $x_{N/2}$ in (4·3). In the same way as in §§ 2 and 3, we obtain integral equations for the thermodynamics of the X-Y-Z model. The differences are that the real parts of the new parameters shrink to the region $[-Q, Q]$ and that the number of parameters x is always $N/2$. We introduce new functions defined by

$$\boldsymbol{s}_i(x)=\sum_{j=-\infty}^{\infty}s_i(x+2jQ)$$

and

$$\boldsymbol{d}_i(x)=\sum_{j=-\infty}^{\infty}d_i(x+2jQ), \tag{4·9}$$

where the functions $s_i(x)$ and $d_i(x)$ are defined in (3·8). Then our non-linear integral equations for the X-Y-Z model are given by

$$\ln(1+\eta_0)=-J_z\pi\zeta^{-1}\,\mathrm{sn}(2\zeta)\delta(x)/T\,,$$

$$\ln\eta_j=(1-2\delta_{m_{i-1},j})\boldsymbol{s}_i*\ln(1+\eta_{j-1})+\boldsymbol{s}_i*\ln(1+\eta_{j+i})\qquad \text{for } m_{i-1}\le j\le m_i-2\,,$$

$$\ln\eta_j=(1-2\delta_{m_{i-1},j})\boldsymbol{s}_i*\ln(1+\eta_{j-1})+\boldsymbol{d}_i*\ln(1+\eta_j)+\boldsymbol{s}_{i+1}*\ln(1+\eta_{j+1})\qquad \text{for } j=m_i-1\,, \tag{4·10}$$

$$\lim_{j\to\infty}\frac{\ln\eta_j}{n_j}=\frac{2\lambda}{T}. \tag{4·11}$$

The convolution used here is defined in the range $[-Q, Q]$ as

$$f*g(x)\equiv\int_{-Q}^{Q}f(x-x')g(x')dx'\,. \tag{4·12}$$

When p_0 is a rational number (or integer), the integral equations (4·10) and (4·11) are reduced to those corresponding to (3·17) (or (3·18)), where $\mu_0 H$ is replaced by λ. It is clear that the solutions η_j of these equations are even functions of λ. The quantity λ is the Lagrange multiplier associated with the condition that $M(=$the number of the parameters $x)$ is $N/2$. To determine the value of λ, we start with the expression

$$F/N=\frac{1}{N}\Big(E-TS-\lambda(N-2M)\Big)=-J_zR-J_z\pi\zeta^{-1}\operatorname{sn}(2\zeta)$$
$$\times\int_{-Q}^{Q}\boldsymbol{a}_1(x)\boldsymbol{s}_1(x)dx-T\int_{-Q}^{Q}\ln(1+\eta_1(x))\boldsymbol{s}_1(x)dx. \tag{4·13}$$

Differentiating this equation with respect to λ, and using the relation

$$\partial(E-TS)/\partial M=-2\lambda\,, \tag{4·14}$$

we obtain

$$1-\frac{2M}{N}=T\int_{-Q}^{Q}(1+\eta_1(x))^{-1}\frac{\partial\eta_1(x)}{\partial\lambda}\boldsymbol{s}_1(x)dx\,. \tag{4·15}$$

The parameter λ should be chosen so that the right-hand side may vanish. In Appendix F we prove that this holds at $\lambda=0$. Thus, Eq. (4·11) is rewritten as

$$\lim_{j\to\infty}(\ln\eta_j)/n_j=0\,. \tag{4·16}$$

In Appendix G we solve Eqs. (4·10) and (4·16) for the limit $p_0\to 2$. The results thus obtained gives the exact free energy of the anisotropic X-Y model in zero magnetic field. In the limit $p_0\to\infty$, we obtain the non-linear integral equations of the Heisenberg-Ising model for $|\varDelta|>1$ in the zero field.[2] In the limit $l\to 0$, we obtain non-linear equations of the Heisenberg-Ising model for $|\varDelta|<1$ in the zero field. These are equivalent to the equations in § 3, if we put $H=0$ and $\theta=2\zeta$.

§ 5. Summary and discussion

Coupled non-linear integral equations for the free energy of the Heisenberg-Ising model with $|\varDelta|<1$ and in more general for the X-Y-Z model have been derived with the use of two plausible assumptions on the distribution of x_α's. The number of our coupled equations becomes finite, when π/θ is a rational number. The high-temperature expansion series has been checked to agree with the rigorous one, at least, through the second term for a general value of $\varDelta(=\cos\theta)$ and through the fourth term for $\varDelta=\frac{1}{2}$.

The plausibility of our assumptions 1 and 2 may be realized in the following discussion. In the limit of large N, we assume that the parameters x_α to satisfy (2·8) are grouped in various strings in the complex plane of these variables. To realize what character these strings have, let Im $x_\alpha \neq np_0$. Then the absolute value of the parenthesis on the left-hand side in Eq. (2·8) is less or larger than unity. Consequently the absolute value of the whole left-hand side in Eq. (2·8) goes to zero or infinity as N becomes infinite. So is the right-hand side in Eq. (2·8). Therefore we may expect that in a string there always exists, at least, one parameter x_β which satisfies one of the relations

$$x_\alpha - x_\beta = \pm 2i + 2p_0 im\,; \quad m = \text{integer}, \tag{5·1}$$

i.e.,

$$x_\alpha - x_\beta = \pm 2i \qquad (\text{mod}\ 2p_0 i) \tag{5·2}$$

for any α. For more detail, we have + (or −) sign in (5·2), if the imaginary part of x_α is located in the region $2mp_0 < \text{Im}\ x_\alpha < (2m+1)p_0$ (or $(2m-1)p_0 < \text{Im}\ x_\alpha < 2mp_0$). Furthermore, if $\{x_\alpha\}$ are solutions of (2·8), then the complex conjugates $\{\bar{x}_\alpha\}$ are also its solutions. This may yield symmetric distributions of the solutions $\{x_\alpha\}$ about the real axis in the complex plane. This symmetric situation is also valid with respect to the $p_0 i$-axis (mod $2p_0 i$). From these guiding principles, we have proposed the two assumptions.

In particular, it may be instructive to mention here why we propose Eq. (2·11) in assumption 2. Let us consider a special situation that all bound states have the same order n and parity v. Assume that the relation

$$\int_{-\infty}^{\infty} \rho_{n,v} dk = \frac{1}{2n} \tag{5·3}$$

holds when $\rho_{n,v}^h$ is zero. For this case, the integral equation corresponding to (3·1) becomes of the form

$$\frac{1}{2\pi}\frac{d}{dx}f(x;\ n, v) = \text{sign}\ a_n{}^v \cdot \rho_{n,v}(x) + \frac{1}{2\pi}\frac{d}{dx}\int_{-\infty}^{\infty}\{f(x-x';\ 2n, +)$$
$$+2\sum_{j=1}^{n-1} f(x-x';\ 2j, +)\}\rho_{n,v}(x')dx', \tag{5·4}$$

where

$$a_n{}^+ = 1 - \frac{n}{p_0} + 2\left[\frac{n}{2p_0}\right] \quad \text{and} \quad a_n{}^- = -\frac{n}{p_0} + 2\left[\frac{n}{2p_0} + \frac{1}{2}\right]. \tag{5·5}$$

Equation (5·3) is rewritten as

$$2na_n{}^v = \text{sign}\ a_n{}^v + a_{2n}^+ + 2\sum_{j=1}^{n-1} a_{2j}^+ . \tag{5·6}$$

Combining the above equation (5·6) with (2·10), we have

$$2\sum_{j=1}^{n-1}[j/p_0] = (n-1)[n-1/p_0]. \tag{5·7}$$

When p_0 is a rational number (of the form $\nu_1+\frac{1}{\nu_2+}\frac{1}{\nu_3+}\cdots\frac{1}{+\nu_\alpha}$), there is an alternative method to derive integral equations by assuming from the beginning that the order n of bound states is restricted to integers smaller than y_α for this case. The equations thus derived are equivalent to those obtained by taking the limit $\nu_{\alpha+1}\to\infty$ in § 3, as shown in Appendix H. In both derivations, the densities ρ_1 and $\rho_1{}^h$, at least, obey identical equations, and consequently we arrive at the identical expression of the free energy in the two methods. In particular when p_0 is an integer, the coupled integral equations proposed in a previous paper[3] are equivalent to Eqs. (3·18). Thus, the previous theory in Ref. 3) can be regarded as still valid at $\pi/\theta=p_0=$integer. A failure in that paper is to have applied illegally those assumptions which hold only for $p_0=$integer to the other general case $p_0=$non-integer.

In the limit $T\to 0$, Eqs. (3·10) and (3·11) are reduced to the linear integral equations obtained by Orbach,[7] and we have solved analytically Eqs. (4·10) and (4·11) to obtain the exact ground-state energy by Baxter.[8] (See Appendix I.)

Acknowledgments

The authors are grateful to Drs. Johnson, McCoy and Lai for sending the preprint of their paper[3] prior to publication. One of the authors (M.T.) acknowledges the financial support of the Sakkokai Foundation.

Appendix A

——*Proof of (2·14)*——

We should always remember through this Appendix that p_0 is assumed to be an irrational number. Equation (2·11) is rewritten as

$$\sum_{j=1}^{n-1}\left(\left[\frac{n}{p_0}\right]-\left[\frac{j}{p_0}\right]-\left[\frac{n-j}{p_0}\right]\right)=(n-1)\left(\left[\frac{n}{p_0}\right]-\left[\frac{n-1}{p_0}\right]\right). \tag{A·1}$$

It is clear that the right-hand side of (A·1) is zero or $n-1$. Using the simple relation

$$[\alpha+\beta]-[\alpha]-[\beta]=0 \quad \text{or} \quad 1, \tag{A·2}$$

we have

$$\left[\frac{j}{p_0}\right]+\left[\frac{n-j}{p_0}\right]=\left[\frac{n-1}{p_0}\right] \quad \text{for } j=1,2,\cdots,n-1. \tag{A·3}$$

Since p_0 is not an integer, this condition (A·3) is satisfied, if $n=1,2,\cdots,[p_0]+1$. When $n>[p_0]+1$, (A·3) is equivalent to the conditions

$$n_1-i=\left[\frac{n-[ip_0]}{p_0}\right]=\left[\frac{n-[ip_0]-1}{p_0}\right]+1 \quad \text{for } i=1,2,\cdots,n_1-1, \tag{A·4}$$

where

$$n_1 \equiv [(n-1)/p_0]+1\,. \tag{A·5}$$

After a simple manipulation, (A·4) are replaced by the equations

$$n=[ip_0]+[(n_1-i)p_0]+1=n_1\nu_1+[ip_2]+[(n_1-i)p_2]+1$$
$$\text{for } i=1, 2, \cdots, n_1-1\,. \tag{A·6}$$

Similarly, these conditions (A·6) are satisfied, if $n_1=2, 3, \cdots, [1/p_2]+1$. If $n_1>[1/p_2]+1$, it is required again that

$$n_1=n_2\nu_2+[ip_3/p_2]+[(n_2-i)p_3/p_2]+1 \quad \text{for } i=1, 2, \cdots, n_2-1 \tag{A·7}$$

with $n_2\equiv[1/p_2]+1$. Repeating this process, we obtain all integers that satisfy Eq. (2·11).

Appendix B

——*Derivation of (3·7)*——

It is convenient to introduce functions A_{jl} defined by

$$A_{jl}(x)=(-1)^{r(j)}\delta_{jl}\delta(x)+T_{jl}(x)\,. \tag{B·1}$$

The Fourier transformations $\hat{A}_{jl}(k)$ of the functions $A_{jl}(x)$ satisfy the symmetry property

$$\hat{A}_{jl}(k)=\hat{A}_{lj}(k) \tag{B·2}$$

and they are calculated as

$$\mathrm{sh}(p_0k)\hat{A}_{jl}=\mathrm{sh}\{((-1)^{i+1}p_0-q_j+q_l)k\}+\mathrm{sh}\{((-1)^{i}p_0+q_j+q_l)k\}$$
$$+2\sum_{h=1}^{n_j-1}\mathrm{sh}\{(-q_j+q_l+\alpha_h)k\} \quad \text{for } m_{i-1}<j<m_i,\ \ j\le l\ne m_i$$
$$\text{and} \quad j=m_{i-1},\ \ j\le l$$

and

$$\mathrm{sh}(p_0k)\hat{A}_{jm_i}=\mathrm{sh}\{((-1)^{i}p_0-q_{m_i}+q_j)k\}+\mathrm{sh}\{((-1)^{i}p_0+q_{m_i}+q_j)k\}$$
$$+2\sum_{l=1}^{\nu_{i-1}-1}\mathrm{sh}\{(-q_{m_i}+q_j+\alpha_l)k\} \quad \text{for } m_{i-1}+1\le j\le m_i-1\,, \tag{B·3}$$

where

$$\alpha_l=p_0-2l+2p_0[l/p_0]\,,$$
$$q_j=(-1)^i(p_i-(j-m_i)p_{i+1}) \quad \text{for } m_i\le j<m_{i+1}\,. \tag{B·4}$$

Fourier transformations of $a_j(x)$ are given by

$$\hat{a}_j(k)=\frac{\mathrm{sh}(q_jk)}{\mathrm{sh}(p_0k)}\,. \tag{B·5}$$

After a lengthy calculation, we have

$$\hat{A}_{j,l}-\{(1-2\delta_{j,m_{i-1}})\hat{A}_{j-1,l}+\hat{A}_{j+1,l}\}/2\,\mathrm{ch}(p_ik)=(-1)^{i+1}\delta_{jl}\,,$$

$$\hat{a}_j-\{(1-2\delta_{j,m_{i-1}})\hat{a}_{j-1}+\hat{a}_{j+1}\}/2\,\mathrm{ch}(p_ik)=0\quad \text{for } m_{i-1}\leq j\leq m_i-2\,,$$

$$\mathrm{ch}\{(p_i+p_{i+1})k\}\hat{A}_{j,l}-(1-2\delta_{j,m_{i-1}})\mathrm{ch}(p_{i+1}k)\hat{A}_{j+1,l}-\mathrm{ch}(p_ik)\hat{A}_{j-1,l}$$
$$=2(-1)^{i+1}\delta_{jl}\mathrm{ch}(p_ik)\mathrm{ch}(p_{i+1}k),$$

$$\mathrm{ch}\{(p_i+p_{i+1})k\}\hat{a}_j-(1-2\delta_{j,m_{i-1}})\mathrm{ch}(p_ik)\hat{a}_{j-1}-\mathrm{ch}(p_{i+1}k)\hat{a}_{j+1}=0$$
$$\text{for } j=m_i-1\,. \qquad (\mathrm{B\cdot 6})$$

These equations are equivalent to (3·7).

Appendix C

——High-temperature expansion for a general value of Δ——

At first we obtain the solution of the zeroth order, $\eta_j{}^{(0)}$ by putting $A/T=0$ in Eqs. (3·10). The integral equations (3·10) are reduced to the following difference equations:

$$\ln(1+\eta_0{}^{(0)})=0\,,$$

$$\ln\eta_j{}^{(0)}=\tfrac{1}{2}(1-2\delta_{m_{i-1},j})\ln(1+\eta_{j-1}^{(0)})+\tfrac{1}{2}\ln(1+\eta_{j+1}^{(0)}),\quad m_{i-1}\leq j\leq m_i-2\,,$$

$$\ln\eta_j{}^{(0)}=\tfrac{1}{2}(1-2\delta_{m_{i-1},j})\ln(1+\eta_{j-1}^{(0)})+\tfrac{1}{2}\ln(1+\eta_j{}^{(0)})+\tfrac{1}{2}\ln(1+\eta_{j+1}^{(0)}),$$
$$j=m_i-1$$

and

$$\lim_{j\to\infty}\frac{\ln\eta_j{}^{(0)}}{n_j}=\frac{2\mu_0H}{T}\,. \qquad (\mathrm{C\cdot 1})$$

The solution of the above difference equations (C·1) is given by

$$1+\eta_j{}^{(0)}=\frac{f^2(n_j+y_i-1)}{f^2(y_i-1)}\,,\quad f(n)=\frac{z^{n+1}-z^{-n-1}}{z-z^{-1}}$$
$$\text{and}\qquad z\equiv\exp(-\mu_0H/T)\,. \qquad (\mathrm{C\cdot 2})$$

In order to apply an iterative method to Eqs. (3·10), we expand $\ln(1+\eta_j(x))$ with respect to the parameter A/T as

$$\ln(1+\eta_j(x))=\ln(1+\eta_j{}^{(0)})+\sum_{n=1}^{\infty}\left(\frac{A}{T}\right)^n c_j{}^{(n)}(x),$$

$$1+\eta_j(x)=(1+\eta_j{}^{(0)})\exp\left(\sum_{n=1}^{\infty}\left(\frac{A}{T}\right)^n c_j{}^{(n)}(x)\right)$$

$$=(1+\eta_j{}^{(0)})\left\{1+\frac{A}{T}c_j{}^{(1)}+\left(\frac{A}{T}\right)^2\frac{(c_j{}^{(1)})^2}{2}+c_j{}^{(2)}\right\}+\cdots,$$

$$\eta_j(x)=\eta_j^{(0)}+(1+\eta_j^{(0)})\frac{A}{T}c_j^{(1)}+(1+\eta_j^{(0)})\left\{\frac{(c_j^{(1)})^2}{2}+c_j^{(2)}\right\}\left(\frac{A}{T}\right)^2+\cdots,$$

$$\ln\eta_j(x)=\ln\eta_j^{(0)}+\ln\left\{1+\left(\frac{1+\eta_j^{(0)}}{\eta_j^{(0)}}\right)c_j^{(1)}\left(\frac{A}{T}\right)+\left(\frac{1+\eta_j^{(0)}}{\eta_j^{(0)}}\right)\left\{c_j^{(2)}+\frac{(c_j^{(1)})^2}{2}\right\}\left(\frac{A}{T}\right)^2+\cdots\right\}$$

$$=\ln\eta_j^{(0)}+(1+(\eta_j^{(0)})^{-1})c_j^{(1)}\frac{A}{T}+\left\{(1+(\eta_j^{(0)})^{-1})\left(c_j^{(2)}+\frac{(c_j^{(1)})^2}{2}\right)\right.$$

$$\left.-\frac{\{(1+(\eta_j^{(0)})^{-1})c_j^{(1)}\}^2}{2}\right\}\left(\frac{A}{T}\right)^2+\cdots. \qquad (\mathrm{C}\cdot 3)$$

The equations for $c_j^{(1)}$ are written as

$$\sum_{l=1}^{\infty}[\delta_{jl}(1+(\eta_j^{(0)})^{-1})-D_{jl}*]c_l^{(1)}=-\delta_{j1}s_1(x), \qquad (\mathrm{C}\cdot 4)$$

where

$$D_{jl}=\begin{cases}(1-2\delta_{j,m_{i-1}})\delta_{j,l+1}s_i+\delta_{j,l-1}s_i & \text{for } m_{i-1}\le j\le m_i-2,\\ (1-2\delta_{j,m_{i-1}})\delta_{j,l+1}s_i+\delta_{j,l}d_i+\delta_{j,l-1}s_{i+1} & \text{for } j=m_i-1.\end{cases} \qquad (\mathrm{C}\cdot 5)$$

The solution of (C·4) is easily given by

$$\hat{c}_l^{(1)}=\frac{1}{f(1)f(y_i-1)f(n_l+y_i-1)}\left\{f(n_l+2y_i-1)\frac{\mathrm{sh}(q_lk)}{\mathrm{sh}(p_0k)}\right.$$

$$\left.-f(n_l-1)\frac{\mathrm{sh}\{(q_l-2(-1)^{i+1}p_i)k\}}{\mathrm{sh}(p_0k)}\right\} \quad \text{for } m_{i-1}\le l<m_i. \qquad (\mathrm{C}\cdot 6)$$

Thus, the high-temperature expansion of the free energy is obtained as

$$F/NT=-\frac{A}{T}\int_{-\infty}^{\infty}a_1(x)s_1(x)dx-\int_{-\infty}^{\infty}\ln(1+\eta_1(x))s_1(x)dx$$

$$=-\ln(z+z^{-1})-\frac{A}{T}\cdot\frac{1}{2\pi}\frac{1}{f^2(1)}\int_{-\infty}^{\infty}\frac{\mathrm{sh}\{(p_0-1)k\}+\mathrm{sh}\{(p_0-3)k\}}{\mathrm{sh}(p_0k)}\cdot\frac{dk}{2\,\mathrm{ch}\,k}+O\left(\left(\frac{A}{T}\right)^2\right)$$

$$=-\ln\left(2\,\mathrm{ch}\frac{\mu_0H}{T}\right)-\frac{J\Delta}{4T}\left(1-\tanh^2\frac{\mu_0H}{T}\right)+O\left(\left(\frac{J}{T}\right)^2\right) \qquad (\mathrm{C}\cdot 7)$$

up to the first order of J/T. This agrees with the well-known results obtained by the ordinary high-temperature expansion method.

Appendix D

——*High-temperature expansion for $\Delta=\frac{1}{2}$ through the fourth term*——

In order to confirm the validity of our treatment, we have performed the high-temperature expansion of the free energy for $\Delta=\frac{1}{2}$ in a power series of J/T up to the fourth term. Now the free energy for $\Delta=\frac{1}{2}$ is expressed as

$$\frac{F}{N}=-A\int_{-\infty}^{\infty}a_1(x)s_1(x)dx-T\int_{-\infty}^{\infty}\ln(1+\eta_1(x))s_1(x)dx$$
$$=-\frac{1}{2}J-T\ln\kappa(0). \qquad (\mathrm{D}\cdot1)$$

Here $\kappa(x)$ is the solution of the following non-linear integral equations:

$$\ln\eta_1(x)=-c(J/T)s_1(x)+2s_1*\ln(1+\kappa), \qquad (\mathrm{D}\cdot2)$$
$$\ln\kappa(x)=s_1*\ln(1+\eta_1), \qquad (\mathrm{D}\cdot3)$$

where

$$c=3\sqrt{3} \qquad \text{and} \qquad s_1(x)=\frac{1}{4}\operatorname{sech}\left(\frac{\pi x}{2}\right). \qquad (\mathrm{D}\cdot4)$$

As the solution for $J=0$ is given by $\eta_1(x)=3$ and $\kappa(x)=2$, we may find the solution for the general value of J in a power series of J/T as follows:

$$\eta_1(x)=3+b_1(x)(J/T)+b_2(x)(J/T)^2+b_3(x)(J/T)^3+\cdots$$

and

$$\kappa(x)=2+c_1(x)(J/T)+c_2(x)(J/T)^2+c_3(x)(J/T)^3+\cdots. \qquad (\mathrm{D}\cdot5)$$

Substituting (D·5) into (D·2) and (D·3), and expanding again the logarithmic functions there, we obtain the following linear integral equations for $b_n(x)$ and $c_n(x)$:

$$2c_n(x)-s_1*b_n(x)=B_n(x),$$
$$2s_1*c_n(x)-b_n(x)=C_n(x), \qquad (\mathrm{D}\cdot6)$$

where $B_n(x)$ and $C_n(x)$ are expressed by simple polynomials of the functions $\{b_k\}(k=1,\cdots,n-1)$ and $\{c_k\}(k=1,\cdots,n-1)$;

$$B_1(x)=0,\ C_1(x)=3cs_1(x),\ B_2(x)=\frac{1}{2}c_1^2-\frac{1}{8}s_1*b_1^2,\ C_2(x)=\frac{1}{3}s_1*c_1^2-\frac{1}{6}b_1^2,$$
$$B_3(x)=c_1c_2-\frac{1}{6}c_1^3-\frac{1}{4}s_1*(b_1b_2)+\frac{1}{48}s_1*b_1^3,$$
$$C_3(x)=-\frac{1}{3}b_1b_2+\frac{1}{27}b_1^3+\frac{2}{3}s_1*(c_1c_2)-\frac{2}{27}s_1*c_1^3, \quad \text{etc.} \qquad (\mathrm{D}\cdot7)$$

Now the coupled integral equations (D·6) are solved by the Fourier transform to give

$$\hat{b}_n(k)=\{\hat{s}_1(k)\}^{-1}\{\hat{q}(k)\hat{B}_n(k)-\hat{p}(k)\hat{C}_n(k)\},$$
$$\hat{c}_n(k)=\{2\hat{s}_1(k)\}^{-1}\{\hat{p}(k)\hat{B}_n(k)-\hat{q}(k)\hat{C}_n(k)\}, \qquad (\mathrm{D}\cdot8)$$

where $\hat{s}_1(k)$ denotes a Fourier transform of $s_1(x)$, and consequently it is given by $\hat{s}_1(k)=\frac{1}{2}\operatorname{sech} k$. The Fourier transforms $\hat{p}(k)$ and $\hat{q}(k)$ are defined by

$$\hat{p}(k)=\frac{\hat{s}_1(k)}{1-\{\hat{s}_1(k)\}^2}=\frac{\operatorname{sh} 2k}{\operatorname{sh} 3k}$$

and

$$\hat{q}(k)=\frac{\{\hat{s}_1(k)\}^2}{1-\{\hat{s}_1(k)\}^2}=\frac{\operatorname{sh}\ k}{\operatorname{sh} 3k}, \tag{D·9}$$

respectively. In this way it is possible, in principle, to obtain the solution in a power series of J/T up to an arbitrary order. In fact we have found the series expansions through the fourth term (i.e., $n=3$). The results thus obtained are summarized as

$$\hat{b}_1(k)=-3c\hat{p},\quad \hat{c}_1(k)=-(3c/2)\hat{q},$$

$$\hat{b}_2(k)=\frac{1}{24}\{4\hat{p}(\widehat{c_1^2})+4(\widehat{b_1^2})+\hat{q}(\widehat{b_1^2})\},\quad \hat{c}_2(k)=\frac{1}{48}\{\hat{p}(\widehat{b_1^2})+12(\widehat{c_1^2})+4\hat{q}(\widehat{c_1^2})\},$$

$$\hat{b}_3(k)=\left\{(12\hat{s}_1)^{-1}\hat{p}+\frac{1}{4}\right\}(\widehat{b_1b_2})\left\{-7/(3^3\times 4^2\times s_1)-\frac{1}{48}\right\}(\widehat{b_1^3})+\frac{1}{3}\hat{p}(\widehat{c_1c_2})$$
$$-\frac{5}{54}\hat{p}(\widehat{c_1^3}). \tag{D·10}$$

With use of the above results, the free energy is expressed by

$$\frac{F}{N}=-T\ln 2-\frac{J}{4}\left\{2-\frac{3c}{2\pi}\int_{-\infty}^{\infty}\hat{q}(k)dk\right\}-\frac{3c^2J^2}{32T}\int_{-\infty}^{\infty}\{p^3(x)+q^3(x)\}dx$$
$$-\frac{c^3J^3}{2^7T^2}\int_{-\infty}^{\infty}\{2(\widehat{p^2})^2+(\widehat{q^2})^2-3\hat{q}\{(\widehat{p^2})^2+(\widehat{q^2})^2\}-6\hat{p}\widehat{p^2}\widehat{q^2}\}dk+\cdots \tag{D·11}$$

$$=-T\ln 2-\frac{J}{8}-\frac{9}{2^7}\frac{J^2}{T}-\frac{1}{2^7}\frac{J^3}{T^2}+\cdots. \tag{D·11'}$$

Here, we have used the following formulae

$$\widehat{p^2}=\frac{1}{2\pi c}\frac{(kc)\operatorname{ch}(2k)+\pi\operatorname{sh}(2k)}{\operatorname{sh}(3k)}, \tag{D·12}$$

$$\widehat{q^2}=\frac{1}{2\pi c}\frac{(kc)\operatorname{ch} k-\pi\operatorname{sh} k}{\operatorname{sh}(3k)}, \tag{D·13}$$

$$I_3(a,b,c,)\equiv\int_{-\infty}^{\infty}\frac{\operatorname{sh}(ax)\operatorname{sh}(bx)\operatorname{sh}(cx)}{\operatorname{sh}^3 3x}dx$$
$$=\frac{\pi}{6}\{f(a+b-c)+f(a-b+c)+f(-a+b+c)-f(a+b+c)\};$$

$$f(x)=\left(\frac{x^2}{36}-\frac{1}{4}\right)\tan\frac{\pi x}{6} \tag{D·14}$$

for $|a|+|b|+|c|<9$, and in particular

$$I_2(a,b)\equiv I_3(a,b,3)=\frac{\pi}{18}\left\{(a-b)\cot\frac{\pi(a-b)}{6}-(a+b)\cot\frac{\pi(a+b)}{6}\right\} \qquad (\text{D}\cdot 15)$$

together with formulae derived by differentiating (D·14) and (D·15) with respect to a, b or c.

Appendix E

——Isotropic X-Y limit——

The isotropic X-Y Hamiltonian corresponds to the case $\nu_1=2$ and $\nu_2\to\infty$ in (2·13). Consequently, the coupled non-linear integral equations (3·10) for this limit are reduced to the simple equations:

$$\ln\eta_1=-\frac{A}{T}s_1(x)+\frac{1}{2}\ln\{(1+\eta_1)(1+\eta_2)\}, \qquad (\text{E}\cdot 1)$$

$$\ln\eta_2=\frac{1}{2}\ln\{(1+\eta_3)/(1+\eta_1)\}, \qquad (\text{E}\cdot 2)$$

$$\ln\eta_j=\frac{1}{2}\ln\{(1+\eta_{j-1})(1+\eta_{j+1})\},\quad j=3,4,\cdots \qquad (\text{E}\cdot 3)$$

and

$$\lim_{j\to\infty}(\ln\eta_j)/(2j-3)=\frac{2\mu_0 H}{T}. \qquad (\text{E}\cdot 4)$$

The general solution of the difference equation (E·3) is given by

$$1+\eta_j=f^2(j-1)\quad \text{for } j=2,3,\cdots, \qquad (\text{E}\cdot 5)$$

where

$$f(j)=\frac{az^{2j}-a^{-1}z^{-2j}}{z^2-z^{-2}},\quad z=\exp\left(-\frac{\mu_0 H}{T}\right).$$

Substituting (E·5) into (E·1), (E·2) and (E·4) we have

$$1+\eta_1=f^{-2}(0),\quad a=\left(\frac{z^2+\exp(-As_1(x)/T)}{z^{-2}+\exp(-As_1(x)/T)}\right)^{1/2}. \qquad (\text{E}\cdot 6)$$

Using the formula (3·12), we arrive at the well-known expression[11] in the form

$$\frac{F}{N}=-\mu_0 H-T\int_{-\infty}^{\infty}s_1(x)\ln(1+z^2\exp(T^{-1}As_1(x)))(1+z^2\exp(-T^{-1}As_1(x)))dx$$

$$=-\mu_0 H-T\int_{-\pi}^{\pi}\frac{dx}{2\pi}\ln\left\{1+z^2\exp\left(\frac{J}{T}\cos k\right)\right\}. \qquad (\text{E}\cdot 7)$$

Appendix F

——Proof of $\lambda=0$——

When p_0 is a rational number, it is clear that $\partial\eta_1/\partial\lambda$ vanishes at $\lambda=0$, because η_1 is a function of $\mathrm{ch}(y_\alpha\lambda/T)$.

When p_0 is an irrational number, we introduce functions $\eta_j^\alpha(x)$ satisfying a series of the following coupled integral equations:

$$\begin{cases} \ln(1+\eta_0{}^\alpha) = -\pi J_z\zeta^{-1}\,\mathrm{sn}(2\zeta)\delta(x)/T\,, \\ \ln\eta_j{}^\alpha = (1-2\delta_{m_{i-1},j})\boldsymbol{s}_i*\ln(1+\eta_{j-1}^\alpha)+\boldsymbol{s}_i*\ln(1+\eta_{j+1}^\alpha) \\ \qquad\qquad\qquad\qquad\qquad\qquad \text{for } m_{i-1}\leq j\leq m_i-2,\quad i\leq\alpha\,, \\ \ln\eta_j{}^\alpha = (1-2\delta_{m_{i-1},j})\boldsymbol{s}_i*\ln(1+\eta_{j-1}^\alpha)+\boldsymbol{d}_i*\ln(1+\eta_j{}^\alpha)+\boldsymbol{s}_{i+1}*\ln(1+\eta_{j+1}^\alpha) \\ \qquad\qquad\qquad\qquad\qquad\qquad \text{for } j=m_i-1,\quad i<\alpha\,, \\ \eta_{m_\alpha-1}^\alpha = \{\kappa^\alpha(x)\}^2+2\kappa^\alpha(x)\,\mathrm{ch}(y_\alpha\lambda/T)\,, \\ \ln\kappa^\alpha(x) = (1-2\delta_{m_\alpha-1,m_{\alpha-1}})\boldsymbol{s}*\ln(1+\eta_{m_\alpha-2}^\alpha)\,. \end{cases} \tag{F·1}$$

The functions $\eta_j\equiv\lim_{\alpha\to\infty}\eta_j{}^\alpha$ satisfies Eqs. (4·10) and (4·11). Differentiating (F·1) with respect to λ we have linear integral equations for $\partial\eta_j{}^\alpha/\partial\lambda$. At $\lambda=0$ it is clear that no inhomogeneous term appears in these equations. Therefore we have $\partial\eta_j{}^\alpha/\partial\lambda|_{\lambda=0}=0$ and $\partial\eta_1/\partial\lambda|_{\lambda=0}=0$. We arrive also at the same conclusion by using the high-temperature expansion method, because each term in the series is even with respect to λ as shown in Appendix C.

Appendix G

——Anisotropic X-Y limit——

The anisotropic *X-Y* Hamiltonian corresponds to the case $\nu_1=2$ and $\nu_2\to\infty$ in (4·10). The coupled equations (4·10) for this limit are reduced as follows:

$$\ln\eta_1 = -J_z\pi T^{-1}\zeta^{-1}\,\mathrm{sn}(2\zeta)\boldsymbol{s}_1(x)+\tfrac{1}{2}\ln\{(1+\eta_1)(1+\eta_2)\}\,, \tag{G·1}$$

$$\ln\eta_2 = \tfrac{1}{2}\ln\{(1+\eta_3)/(1+\eta_1)\}\,, \tag{G·2}$$

$$\ln\eta_j = \tfrac{1}{2}\ln\{(1+\eta_{j-1})(1+\eta_{j+1})\}\,;\quad j=3,4,\cdots\,, \tag{G·3}$$

$$\lim_{j\to\infty}\frac{\ln\eta_j}{(2j-3)}=0\,. \tag{G·4}$$

The solution of the above difference equations is given by

$$1+\eta_1=(a(x)+1)^{-2}\quad\text{and}\quad 1+\eta_j=(a(x)+j)^2;\quad j=2,3,\cdots\,, \tag{G·5}$$

where

$$a(x) = -\{1+\exp(As_1(x)/T)\}^{-1}; \quad A = J_z\pi\zeta^{-1}\operatorname{sn}(2\zeta) \quad \text{and} \quad \zeta = K_l/2\,. \tag{G·6}$$

Substituting this into (4·13) we have

$$\frac{F}{N} = -\frac{1}{4}(J_z - J_y) - T\int_{-Q}^{Q} s_1(x)\ln\left\{1+\exp\left(\frac{A}{T}s_1(x)\right)\right\}\left\{1+\exp\left(-\frac{A}{T}s_1(x)\right)\right\}dx\,. \tag{G·7}$$

We transform the variable x as follows:

$$q = \sin^{-1}\operatorname{cn}\left(\frac{K_l x}{1+k'}, k\right), \quad k' = (1-l')/(1+l'), \quad k' = \sqrt{1-k^2}, \quad l' = \sqrt{1-l^2}$$

and

$$\varepsilon(q) = As_1(x) = \frac{J_z}{1+k'}\operatorname{dn}\left(\frac{K_l x}{1+k'}, k\right) = \frac{J_z}{1+k'}\sqrt{1-k^2\cos^2 q}\,. \tag{G·8}$$

Finally we obtain

$$\frac{F}{N} = -\frac{1}{4}(J_z - J_y) - T\int_{-\pi/2}^{\pi/2}\frac{dq}{2\pi}\ln\left\{1+\exp\left(\frac{\varepsilon(q)}{T}\right)\right\}\left\{1+\exp\left(-\frac{\varepsilon(q)}{T}\right)\right\}. \tag{G·9}$$

Appendix H

——*Non-linear equations for a rational number* p_0——

Let p_0 be a rational number given in the form

$$p_0 = \frac{u}{v} = \nu_1 + \frac{1}{\nu_2 +}\frac{1}{\nu_3 +}\cdots\frac{1}{+\nu_\alpha} > 2; \quad \nu_\alpha \geq 2\,, \tag{H·1}$$

where u and v are integer and prime to each other. In this case we add to Assumption 2 another condition that $n_j < u$. Since $u = y_\alpha$ in our previous notation, we have only to consider bound states with parity v_j and order n_j for $j=1, 2, \cdots, m_\alpha$. (These notations are defined in (2·12) and (2·14).) It must be remarked that at $j=m$ and $k=m_\alpha-1$, the second term of r. h. s. of (2·16) for $\theta_{jk}(x)$ is zero, because $(n_j+n_k)/p_0 = v =$ integer. Thus, we obtain a set of integral equations slightly different from (3·10) as follows:

$$\ln(1+\eta_0) = -2\pi J\theta^{-1}\sin\theta\delta(x)/T\,,$$

$$\ln\eta_j = (1-2\delta_{m_{i-1},j})s_i * \ln(1+\eta_{j-1}) + s_i * \ln(1+\eta_{j+1})$$

$$\text{for } m_{i-1} \leq j \leq m_i - 2, \quad j < m_\alpha - 2, \quad i \leq \alpha\,,$$

$$\ln\eta_j = (1-2\delta_{m_{i-1},j})s_i * \ln(1+\eta_{j-1}) + d_i * \ln(1+\eta_j) + s_{i+1} * \ln(1+\eta_{j+1})$$

$$\text{for } j = m_i - 1, \quad j < \alpha\,,$$

$$\ln \eta_{m_\alpha-2}=(1-2\delta_{m_{\alpha-1},m_\alpha-2})s_i*\ln(1+\eta_{m_\alpha-3})+s_i*\ln\{(1+\eta_{m_\alpha-1})(1+\eta_{m_\alpha}^{-1})\},$$

$$\ln \eta_{m_\alpha-1}=\frac{y_\alpha\mu_0 H}{T}+s_\alpha*\ln(1+\eta_{m_\alpha-2})$$

and

$$\ln \eta_{m_\alpha}=\frac{y_\alpha\mu_0 H}{T}-s_\alpha*\ln(1+\eta_{m_\alpha-2}). \tag{H·2}$$

It is clear that this set of equations is equivalent to (3·17). The above arguments are applied also to the *X-Y-Z* model in a quite similar way.

Appendix I

——The limit $T\to 0$——

In this limit we put $\varepsilon_j(x)=T\ln\eta_j(x)$. Equations (3·10) and (3·11) are written as follows:

$$\varepsilon_j(x)=(1-2\delta_{m_{i-1},j})s_i*\varepsilon_{j-1}^+ + s_i*\varepsilon_{j+1}^+ \quad \text{for } m_{j-1}\le j\le m_i-2,$$

$$\varepsilon_j(x)=(1-2\delta_{m_{i-1},j})s_i*\varepsilon_{j-1}^+ + d_i*\varepsilon_j^+ + s_{i+1}*\varepsilon_{j+1}^+ \quad \text{for } j=m_i-1,$$

$$\varepsilon_0^+=-A\delta(x),\quad \lim_{j\to\infty}\frac{\varepsilon_j}{n_j}=2\mu_0 H,\quad A\equiv 2\pi J\theta^{-1}\sin\theta, \tag{I·1}$$

where

$$\varepsilon_j^+(x)\equiv\begin{cases}\varepsilon_j(x) & \text{for } \varepsilon_j(x)\ge 0,\\ 0 & \text{for } \varepsilon_j(x)<0,\end{cases}\qquad \varepsilon_j^-\equiv\varepsilon_j-\varepsilon_j^+ .$$

For $J>0$ and $H\ge 0$, $\varepsilon_j(j\ge 2)$ are always positive. From Eqs. (3·5), ε_1 is given as the solution of the integral equation

$$\varepsilon_1=-Aa_1(x)+2\mu_0 H-\int_{-\infty}^{\infty}T_{1,1}(x-x')\varepsilon_1^-(x')dx'.$$

The function $\varepsilon_1(x)$ is a monotonously increasing function of x^2 and is negative in a certain region $[-B,B]$. Therefore $\eta_1(x)$ is zero in this region and infinite outside this region. Linear integral equations (3·1) are written as

$$a_1(x)=\rho_1(x)+\int_{-B}^{B}T_{1,1}(x-x')\rho_1(x')dx' \quad \text{for } |x|<B. \tag{I·2}$$

For $J<0$ and $H\ge 0$, $\varepsilon_j(j\ne\nu_1)$ are always positive, and ε_{ν_1} is given by

$$\varepsilon_{\nu_1}=-Aa_{\nu_1}+2\mu_0 H+\int_{-\infty}^{\infty}T_{\nu_1,\nu_1}(x-x')\varepsilon_{\nu_1}^-(x')dx' .$$

In the same way as in the above paragraph we obtain

$$a_{\nu_1}(x)=-\rho_{\nu_1}(x)+\int_{-B}^{B}T_{\nu_1,\nu_1}(x-x')\rho_{\nu_1}(x')dx' . \tag{I·3}$$

The integral equations (I·2) and (I·3) are equivalent to those obtained by Orbach.[7)]

Next we discuss the X-Y-Z model. In the limit $T\to 0$, Eqs. (4·10) and (4·16) are written as

$$\varepsilon_j(x)=(1-2\delta_{m_{i-1},j})s_i*\varepsilon_{j-1}^{+}+s_i*\varepsilon_{j+1}^{+}\quad \text{for } m_{i-1}\leq j\leq m_i-2\,,$$

$$\varepsilon_j(x)=(1-2\delta_{m_{i-1},j})s_i*\varepsilon_{j-1}^{+}+d_i*\varepsilon_j{}^{+}+s_{i+1}*\varepsilon_{j+1}^{+}\quad \text{for } j=m_i-1\,,$$

$$\varepsilon_0{}^{+}=-A\delta(x),\quad \lim_{j\to\infty}\frac{\varepsilon_j}{n_j}=0,\quad A=\pi J_z\zeta^{-1}\,\mathrm{sn}(2\zeta)\,. \tag{I·4}$$

For $J_z>0$, we have

$$\varepsilon_1(x)=-As_1(x)\qquad \text{and}\qquad \varepsilon_j=0\quad \text{for } j\geq 2\,. \tag{I·5}$$

For $J_z<0$, we have $\varepsilon_j=0$ for $j>\nu_1$ and

$$\varepsilon_0=|A|\delta(x),$$

$$\varepsilon_j=s_1*(\varepsilon_{j-1}+\varepsilon_{j+1}),\quad j=1,2,\cdots,\nu_1-2\,,$$

$$\varepsilon_{\nu_1-1}=s_1*\varepsilon_{\nu_1-2}+d_i*\varepsilon_{\nu_1-1}$$

and

$$\varepsilon_{\nu_1}=-s_2*\varepsilon_{\nu_1-1}\,. \tag{I·6}$$

This set of equations is solved analytically by the Fourier transformation and the result is given by

$$\varepsilon_j(x)=\frac{|A|}{2Q}\sum_{n=-\infty}^{\infty}\exp\left(\frac{n\pi ix}{Q}\right)\frac{\mathrm{ch}((p_0+1-j)n\pi/Q)}{\mathrm{ch}((p_0+1)n\pi/Q)},\quad j=1,2,\cdots,\nu_1-1\,,$$

$$\varepsilon_{\nu_1}=-\frac{|A|}{2Q}\sum_{n=-\infty}^{\infty}\exp\left(\frac{n\pi ix}{Q}\right)\frac{1}{2\,\mathrm{ch}((p_0-1)n\pi/Q)}\,. \tag{I·7}$$

Substituting (1·5) and (I·7) into (4·13), we obtain the exact ground-state energy of the X-Y-Z model by Baxter.[8)]

References

1) M. Takahashi, Prog. Theor. Phys. **46** (1971), 401.
2) M. Gaudin, Phys. Rev. Letters **26** (1971), 1301.
3) M. Takahashi, Phys. Letters **36A** (1971), 325.
4) J.D. Johnson, B.M. McCoy and C.K. Lai, Phys. Letters **38A** (1972), 143.
5) M. Takahashi and M. Suzuki, Phys. Letters A (in press).
6) H. Bethe, Z. Phys. **71** (1931), 205.
7) R. Orbach, Phys. Rev. **112** (1955), 309.
L.R. Walker, Phys. Rev. **116** (1959), 1089.
J. des Cloizeaux and M. Gaudin, J. Math. Phys. **7** (1966), 1384.
C.N. Yang and C.P. Yang, Phys. Rev. **147** (1966), 303; **150** (1966), 321, 327; **151** (1966), 258.

8) R.J. Baxter, Phys. Rev. Letters **26** (1971), 832, 834; Ann. of Phys. **70** (1972), 193, 323.
9) C.N. Yang and C.P. Yang, J. Math. Phys. **10** (1969), 1115.
10) S. Katsura and S. Inawashiro, J. Math. Phys. **5** (1964), 1091.
11) S. Katsura, Phys. Rev. **127** (1962), 1508.
E.H. Lieb, T.D. Schultz and D.C. Mattis, Ann. of Phys. **16** (1961), 941.