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One-Dimensional Heisenberg Model at Finite Temperature

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A set of integral equations which describes the thermodynamic properties of one-dimensional Heisenberg model is obtained. From these equations one can calculate the energy, entropy and magnetization of the system at given temperature and magnetic field. We have succeeded in reproducing the known exact results in the limiting cases of zero temperature, infinite temperature and infinite magnetic field.

§ 1. Introduction

The exact solution of the one-dimensional Heisenberg model was treated by many authors.[1)~6)] Hulthén[2)] calculated the ground state energy of the antiferromagnet. The spin wave spectrum from the antiferromagnetic ground state was obtained by des Cloiseaux and Pearson.[3)] Griffiths[4)] calculated the magnetization curve at zero temperature. These authors treated the case where all quasi-momenta are real. But in the general case the quasi-momenta are complex numbers and form bound state of spin waves. This fact was already pointed out by Bethe.[1)] Katsura[5)] treated the bound state of two spin waves and calculated its contribution to the partition function of the Heisenberg model in the limit of strong magnetic field. Ovchinikov[6)] calculated the spectrum of the bound state of spin waves as an elementary excitation from the ground state.

On the other hand Yang and Yang[7)] were successful in treating the thermodynamics of the one-dimensional Bose gas with repulsive delta-function interaction. They generalized the theory of Lieb and Liniger[8)] for Bose gas at zero temperature. In this problem Bethe's hypothesis is applicable and fortunately all quasi-momenta are real. Yang and Yang[7)] derived the integral equation for distribution function of quasi-momenta and obtained many interesting results.

In this paper we treat the thermodynamics of the one-dimensional Heisenberg model in the same way as Yang and Yang.[7)] The interaction may be ferromagnetic or antiferromagnetic. The difficulty is how to treat the complex quasi-momenta. Our derivation of integral equations in §§ 2 and 3 has some ambiguous points. But these integral equations have been solved in some special cases and give the known exact results as shown in §§ 4∼6.

§ 2. Theory of eigenstates in a finite system

We consider the one-dimensional Heisenberg model with the Hamiltonian

$$\mathcal{H}=J\sum_{i=1}^{N}(S_i^xS_{i+1}^x+S_i^yS_{i+1}^y+S_i^zS_{i+1}^z-\tfrac{1}{4})+2\mu_0H\sum_{i=1}^{N}S_i^z,$$
$$\boldsymbol{S}_{N+1}=\boldsymbol{S}_1\,. \tag{2·1}$$

Suppose that there are M down-spins and $N-M$ up-spins. Following Bethe[1)] we write the eigenfunctions Ψ as follows:

$$\Psi=\sum_{x_1<x_2<\cdots<x_M}\Phi(x_1,x_2,\cdots,x_M)S_{x_1}^-S_{x_2}^-\cdots S_{x_M}^-|0\rangle\,, \tag{2·2a}$$

$$\Phi(x_1,x_2,\cdots,x_M)=\sum_P\exp\{i(\sum_j k_{Pj}x_j+\sum_{\substack{j<l\\Pj>Pl}}\phi_{PjPl})\}\,. \tag{2·2b}$$

Here k_1, k_2, $\cdots$, k_M are quasi-momenta, P are permutations of 1, 2, $\cdots$, M, and ϕ_{jl} is defined by

$$2\cot(\phi_{jl}/2)=\cot(k_j/2)-\cot(k_l/2)\,. \tag{2·3}$$

One can easily see that the wave function (2·2) with the condition (2·3) is an eigenstate of the Hamiltonian (2·1) with the energy eigenvalue

$$E=-J\sum_{j=1}^{M}(1-\cos k_j)+\mu_0H(2M-N)\,. \tag{2·4}$$

The periodic boundary condition

$$\Phi(x_1,x_2,\cdots,x_{M-1},N+1)=\Phi(1,x_1,x_2,\cdots,x_{M-1})$$

is satisfied, if we put

$$e^{ik_jN}=\prod_{\substack{l\neq j\\l=1}}^{M}\exp(i\phi_{jl}),\qquad j=1,2,\cdots,M\,. \tag{2·5}$$

For simplicity we introduce the parameters Λ_1, Λ_2, $\cdots$, Λ_M, which are defined by

$$\Lambda_j\equiv\cot(k_j/2)\,.$$

Using these new parameters Eqs. (2·2), (2·4) and (2·5) are transformed as

$$\Phi(x_1,x_2,\cdots,x_M)=\sum_P\prod_{j=1}^{M}e^{x_j}(\Lambda_{Pj})\prod_{\substack{i<l\\Pi>Pl}}e\left(\frac{\Lambda_{Pl}-\Lambda_{Pi}}{2}\right), \tag{2·6}$$

$$E=\sum_{j=1}^{M}\left(-\frac{2J}{\Lambda_j^2+1}+2\mu_0H\right)-N\mu_0H \tag{2·7}$$

and

$$e^N(\Lambda_j)=\prod_{\substack{i\neq j\\l=1}}^{M}e\left(\frac{\Lambda_j-\Lambda_i}{2}\right),\qquad j=1,2,\cdots,M\,, \tag{2·8}$$

where $e(x)\equiv(x+i)/(x-i)$.

Theorem 1. The wave function (2·6) vanishes if $\Lambda_i=\Lambda_j$ for $i\neq j$. This is directly proved from (2·6). If two Λ's are same, all terms are cancelled.

Conjecture 1. Complex Λ always forms a bound state with several other Λ's. For a bound state of n-Λ's the real parts of Λ's are the same and the imaginary parts are $(n-1)i$, $(n-3)i$, $\cdots$ $-(n-3)i$ and $-(n-1)i$ within the accuracy of $O(\exp(-\delta N))$, $\delta>0$.

This conjecture is the most fundamental assumption of this paper. We are not able to prove this exactly. But the assumptions of this kind have been used by many authors.[1),5),6)] So we develop our theory assuming this conjecture to be valid.

Consider the case where M_n bound states of n-Λ's exist. We designate Λ's as

$$\Lambda_\alpha^{n,j}, \qquad \alpha=1,2,\cdots,M_n\,,$$

where the suffix n means that this belongs to the bound state of n-Λ's, the suffix j specified the imaginary part of Λ. Now we designate the real part of $\Lambda_\alpha^{n,j}$ by Λ_α^n. From the conjecture 1 we have

$$\Lambda_\alpha^{n,j}=\Lambda_\alpha^n+i(n+1-2j)+O(\exp(-\delta N)), \qquad j=1,2,\cdots,n,\ \delta>0.$$

From Eq. (2·8) we have

$$e^N(\Lambda_\alpha^{n,j})=\prod_{(m,\beta)\neq(n,\alpha)} e\left(\frac{\Lambda_\alpha^{n,j}-\Lambda_\beta^m}{m-1}\right)e\left(\frac{\Lambda_\alpha^{n,j}-\Lambda_\beta^m}{m+1}\right)\prod_{j'\neq j} e\left(\frac{\Lambda_\alpha^{n,j}-\Lambda_\alpha^{n,j'}}{2}\right),$$

$$j=1,2,\cdots n\,. \tag{2·9}$$

Taking a product of these n-equations we have

$$e^N(\Lambda_\alpha^n/n)=\prod_{j=1}^n e^N(\Lambda_\alpha^{n,j})=\prod_{(m,\beta)\neq(n,\alpha)} E_{nm}(\Lambda_\alpha^n-\Lambda_\beta^m), \tag{2·10}$$

where

$$E_{nm}(x)=\begin{cases} e\left(\dfrac{x}{|n-m|}\right)e^2\left(\dfrac{x}{|n-m|+2}\right)e^2\left(\dfrac{x}{|n-m|+4}\right)\cdots e^2\left(\dfrac{x}{m+n-2}\right)e\left(\dfrac{x}{m+n}\right) \\ \qquad\qquad\qquad\qquad\qquad\qquad \text{for } n\neq m\,, \\ e^2\left(\dfrac{x}{2}\right)e^2\left(\dfrac{x}{4}\right)\cdots e^2\left(\dfrac{x}{2n-2}\right)e\left(\dfrac{x}{2n}\right) \qquad \text{for } n=m\,. \end{cases}$$

The logarithm of these equations gives

$$N\theta(\Lambda_\alpha^n/n)=2\pi I_\alpha^n+\sum_{(m,\beta)\neq(n,\alpha)}\Theta_{nm}(\Lambda_\alpha^n-\Lambda_\beta^m), \tag{2·11}$$

where

$$\theta(x)=2\tan^{-1}(x)$$

and

$$\Theta_{nm}(x)=\begin{cases} \theta(x/|n-m|)+2\theta(x/(|n-m|+2))+\cdots+2\theta(x/(n+m-2))+\theta(x/(n+m)) \\ \qquad\qquad\qquad\qquad\qquad\qquad \text{for } n\neq m\,, \\ 2\theta(x/2)+2\theta(x/4)+\cdots+2\theta(x/(2n-2))+\theta(x/2n) \qquad \text{for } n=m\,. \end{cases}$$

$I_\alpha{}^n$ is an integer (half odd integer) if $N-M_n$ is odd (even) and should satisfy

$$|I_\alpha{}^n| \leqq \tfrac{1}{2}(N-\sum_{m=1}^{\infty} t_{nm}M_m - 1), \tag{2·12a}$$

where

$$t_{nm} = \begin{cases} 2\,\mathrm{Min}(n, m) & \text{for } n \neq m\,, \\ 2n-1 & \text{for } n=m\,. \end{cases} \tag{2·12b}$$

All of the eigenstates can be specified by a set of half integers $I_\alpha{}^n$. For example the antiferromagnetic ground state is characterized by $M_1=M$, $0=M_2=M_3=\cdots$,

$$I_\alpha{}^1 = \frac{M-1}{2},\ \frac{M-3}{2},\ \cdots,\ -\frac{M-1}{2}.$$

The ferromagnetic ground state is

$$0=M_1=M_2=\cdots.$$

We prove in Appendix A that the number of the sets $\{I_\alpha{}^n\}$ which satisfy (2·12a) is $\binom{N}{M}-\binom{N}{M-1}$. Then one can easily see that Eq. (2·11) has at least one solution for a given set of $I_\alpha{}^n$. So we have at least $\binom{N}{M}-\binom{N}{M-1}$ solutions for fixed $S=S_z=\frac{1}{2}(N-2M)$. Wave functions for $S_z=S-1$, $S-2$, $\cdots$, $-S+1$, $-S$ are obtained by operation of the spin descending operator to the wave function (2·2a). So we have at least $\binom{N}{M}$ eigenstates for fixed S_z $(|S_z|=\frac{1}{2}(N-2M))$. On the other hand we know that Hilbert space for the $S_z=\pm\frac{1}{2}(N-2M)$ is expanded by the set of $\binom{N}{M}$ states

$$S_{x_1}^- S_{x_2}^- \cdots S_{x_M}^- |0\rangle\,,\quad 1 \leqq x_1 < x_2 \cdots < x_M \leqq N \qquad \text{for } S_z \geqq 0$$

or

$$S_{x_1}^- S_{x_2}^- \cdots S_{x_{N-M}}^- |0\rangle\,,\quad 1 \leqq x_1 < x_2 \cdots < x_{N-M} \leqq N \qquad \text{for } S_z < 0\,.$$

Therefore if we assume the conjecture 1 to be valid, the solution of (2·11) should be unique and the set of all eigenfunctions constructed in the above-mentioned way should be a complete set.

§ 3. Integral equations in the limit $N\to\infty$

From theorem 1 one can easily see that $I_\alpha{}^n \neq I_\beta{}^n$ for $\alpha\neq\beta$. This means that M_n half integers satisfiyng (2·12a) are taken as $I_\alpha{}^n$ and the others are omitted. We write these omitted half integers as $J_\beta{}^n$ and define the corresponding Λ^n values by

$$2\pi J_\beta{}^n = N h_n(\Lambda_\beta{}^n)\,,$$

where

$$Nh_n(\Lambda) \equiv \theta\left(\frac{\Lambda}{n}\right) - \sum_{(m,\alpha)} \Theta_{nm}(\Lambda - \Lambda_\alpha{}^m).$$

We call these Λ_n values which correspond to omitted integers as "holes of Λ^n". Let us consider the limit $N \to \infty$. We put the distribution functions of Λ^n as $\rho_n(\Lambda)$ and these of holes of Λ^n as $\rho_n{}^h(\Lambda)$. Equations (2·11) are rewritten as

$$\theta\left(\frac{k}{n}\right) = h_n(k) + \sum_m \int_{-\infty}^{\infty} \Theta_{nm}(k-k')\rho_m(k')dk',$$

$$\frac{dh_n(k)}{dk} = 2\pi(\rho_n(k) + \rho_n{}^h(k)), \qquad n=1, 2, \cdots,$$

where variable Λ^n's are replaced by k, which shonld not be confused with quasi-momenta k_j's. By the differentiation we have

$$\frac{1}{\pi}\frac{n}{k^2+n^2} = \rho_n{}^h(k) + \sum_{m=1}^{\infty} A_{nm}\rho_m(k), \qquad n=1, 2, \cdots, \tag{3·1}$$

where A_{nm} is an operator defined by

$$A_{nm} \equiv [|n-m|] + 2[|n-m|+2] + 2[|n-m|+4] + \cdots + 2[n+m-2] + [n+m], \tag{3·2}$$

and $[n]$ is an operator defined by

$$[n]f(k) \equiv \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{n}{n^2+(k-k')^2} f(k')dk',$$

$$[0]f(k) \equiv f(k),$$

where f is an arbitrary function of k. The energy per site is

$$E/N = \sum_{n=1}^{\infty} \int g_n(k)\rho_n(k)dk - \mu_0 H, \tag{3·3a}$$

where

$$g_n(k) = -\frac{2nJ}{k^2+n^2} + 2n\mu_0 H. \tag{3·3b}$$

For simplicity we put that $\int \cdots dk$ means $\int_{-\infty}^{\infty} \cdots dk$. The magnetization to the z-direction is

$$S_z/N = \frac{1}{2} - \sum_{n=1}^{\infty} n \int \rho_n(k)dk. \tag{3·4}$$

Now we consider the entropy of the state when the distribution function $\rho_n(k)$ and $\rho_n{}^h(k)$ are given. In a small interval from k to $k+dk$ there are $\rho_n(k)Ndk$ particles and $\rho_n{}^h(k)Ndk$ holes. Here we put $dk \gg 1/N$. So the entropy for this small interval is

$$\ln\frac{\{(\rho_n+\rho_n{}^h)Ndk\}!}{(\rho_nNdk)!(\rho_n{}^hNdk)!}=\{(\rho_n+\rho_n{}^h)\ln(\rho_n+\rho_n{}^h)-\rho_n\ln\rho_n-\rho_n{}^h\ln\rho_n{}^h\}Ndk\,.$$

Therefore the total entropy per site of this state is given by

$$S/N=\sum_{n=1}^{\infty}\int\{(\rho_n(k)+\rho_n{}^h(k))\ln(\rho_n(k)+\rho_n{}^h(k))$$
$$-\rho_n(k)\ln\rho_n(k)-\rho_n{}^h(k)\ln\rho_n{}^h(k)\}dk\,. \tag{3·5}$$

The free energy $F=E-TS$ should be minimized in the thermodynamically equilibrium state. So we have

$$0=\frac{\delta F}{N}=\sum_{n=1}^{\infty}\int g_n(k)\,\delta\rho_n(k)\,dk-T\sum_{n=1}^{\infty}\int\delta\rho_n\ln\left(1+\frac{\rho_n{}^h}{\rho_n}\right)+\delta\rho_n{}^h\ln\left(1+\frac{\rho_n}{\rho_n{}^h}\right)dk\,. \tag{3·6}$$

From Eq. (3·1) we have

$$\delta\rho_n{}^h=-\sum_{m=1}^{\infty}A_{nm}\delta\rho_m\,.$$

Substituting these into (3·6) one obtains

$$0=\frac{\delta F}{N}=T\sum_{n=1}^{\infty}\int\left\{\frac{g_n(k)}{T}-\ln(1+\eta_n(k))+\sum_{m=1}^{\infty}A_{nm}\ln(1+\eta_m{}^{-1}(k))\right\}\delta\rho_n(k)\,dk\,,$$

where we put $\eta_n(k)\equiv\rho_n{}^h(k)/\rho_n(k)$. Thus we have

$$\ln(1+\eta_n(k))=\frac{g_n(k)}{T}+\sum_{n=1}^{\infty}A_{nm}\ln(1+\eta_m{}^{-1}(k))\,. \tag{3·7}$$

Equation (3·1) is rewritten as

$$\frac{1}{\pi}\frac{n}{k^2+n^2}=\eta_n(k)\,\rho_n(k)+\sum_{m=1}^{\infty}A_{nm}\rho_m(k)\,,\qquad n=1,2,\cdots\,. \tag{3·8}$$

Equation (3·7) is transformed as

$$\ln(1+\eta_1(k))=\frac{g_1(k)}{T}+\sum_{m=1}^{\infty}A_{1m}\ln(1+\eta_m{}^{-1}(k))\,, \tag{3·9a}$$

$$([0]+[2])\ln\eta_1(k)=-\frac{2J}{T}\cdot\frac{1}{k^2+1}+[1]\ln(1+\eta_2(k))\,, \tag{3·9b}$$

$$([0]+[2])\ln\eta_{n+1}(k)=[1]\{\ln(1+\eta_n(k))+\ln(1+\eta_{n+2}(k))\}\,,\quad n=1,2,\cdots\,. \tag{3·9c}$$

Equation (3·8) is transformed as

$$\frac{1}{\pi}\frac{1}{k^2+1}=\eta_1(k)\,\rho_1(k)+\sum_{m=1}^{\infty}A_{1m}\rho_m(k)\,, \tag{3·10a}$$

$$\frac{1}{\pi}\frac{1}{k^2+1}+[1]\eta_2(k)\,\rho_2(k)=([0]+[2])\,(\eta_1(k)+1)\,\rho_1(k)\,, \tag{3·10b}$$

$$[1]\,(\eta_{n+2}(k)\,\rho_{n+2}(k)+\eta_n(k)\,\rho_n(k))=([0]+[2])\,(\eta_{n+1}(k)+1)\,\rho_{n+1}(k). \quad (3\cdot 10\text{c})$$

Here we have used

$$[1]\,(A_{n-1,m}+A_{n+1,m})-([0]+[2])\,A_{nm}=([0]+[2])\,\delta_{nm}.$$

These are coupled integral equations which have infinite unknown functions, and it is not easy to solve these. In the following sections we will solve these in some special cases and give plausible results.

§ 4. Solution in the limit $J/T\to 0$

We take the limit $J/T\to 0$ with the ratio H/T kept finite. In this case it is evident that the $\eta_n(k)$'s are all constant because the transformation $k\to k+C$ does not change the integral equation (3·7) or (3·9). Then Eq. (3·9) can be rewritten as

$$1+\eta_1=z^{-2}\prod_{m=1}^{\infty}(1+\eta_m^{-1})^2, \quad (4\cdot 1\text{a})$$

$$\eta_1^2=1+\eta_2, \quad (4\cdot 1\text{b})$$

$$\eta_{n+1}^2=(1+\eta_n)\,(1+\eta_{n+2}), \qquad n=1,2,\cdots, \quad (4\cdot 1\text{c})$$

where $z=\exp(-\mu_0 H/T)$. (4·1c) is a difference equation of second rank. The general solution is

$$\eta_n=\left[\frac{ba^n-b^{-1}a^{-n}}{a-a^{-1}}\right]^2-1, \quad (4\cdot 2)$$

where a and b should be determined by the initial conditions (4·1a) and (4·1b). One easily obtain $a=b=z$. Thus we have

$$\eta_n=\left[\frac{z^{n+1}-z^{-n-1}}{z-z^{-1}}\right]^2-1 \qquad \text{for } H/T>0, \quad (4\cdot 3\text{a})$$

$$\eta_n=(n+1)^2-1 \qquad \text{for } H/T=0. \quad (4\cdot 3\text{b})$$

Next we solve Eq. (3·10). The Fourier transformation of (3·10c) is

$$0=f(n)\,\{f(n-2)\,\tilde{\rho}_{n-1}(\omega)+f(n+2)\,\tilde{\rho}_{n+1}(\omega)-(e^{|\omega|}+e^{-|\omega|})f(n)\,\tilde{\rho}_n(\omega)\},$$

where

$$f(n)=\frac{z^{n+1}-z^{-n-1}}{z-z^{-1}}. \quad (4\cdot 4)$$

Here we have used that $\eta_n=f(n-1)f(n+1)$ and $\eta_n+1=f^2(n)$. Thus we obtain a difference equation

$$(e^{|\omega|}+e^{-|\omega|})f(n)\,\tilde{\rho}_n(\omega)=f(n-2)\,\tilde{\rho}_{n-1}(\omega)+f(n+2)\,\tilde{\rho}_{n+1}(\omega). \quad (4\cdot 5)$$

The general solution is

$$\tilde{\rho}_n(\omega)=A(\omega)\left\{\frac{e^{-n|\omega|}}{f(n-1)f(n)}-\frac{e^{-(n+2)|\omega|}}{f(n)f(n+1)}\right\}$$
$$+B(\omega)\left\{\frac{e^{n|\omega|}}{f(n-1)f(n)}-\frac{e^{(n+2)|\omega|}}{f(n)f(n+1)}\right\}. \tag{4·6}$$

The initial conditions (3·10a) and (3·10b) are

$$e^{-|\omega|}=f(0)f(2)\tilde{\rho}_1(\omega)+(1+e^{-2|\omega|})\sum_{n=1}^{\infty}e^{-(n-1)|\omega|}\tilde{\rho}_n(\omega),$$
$$-1=f(1)f(3)\tilde{\rho}_2(\omega)-f^2(1)\tilde{\rho}_1(\omega)(e^{|\omega|}+e^{-|\omega|}).$$

Substituting (4·6) we can determine $A(\omega)$ and $B(\omega)$. The result is $A(\omega)=1/f(1)$, $B(\omega)=0$. Then we have

$$\tilde{\rho}_n(\omega)=\frac{1}{f(1)}\left\{\frac{e^{-n|\omega|}}{f(n-1)f(n)}-\frac{e^{-(n+2)|\omega|}}{f(n)f(n+1)}\right\} \tag{4·7a}$$

or in k-representation

$$\rho_n(k)=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{i\omega k}\tilde{\rho}_n(\omega)\,d\omega=\frac{1}{\pi f(1)}\left\{\frac{1}{f(n-1)f(n)}\frac{n}{n^2+k^2}\right.$$
$$\left.-\frac{1}{f(n)f(n+1)}\frac{n+2}{(n+2)^2+k^2}\right\}. \tag{4·7b}$$

Substituting this into (3·4) we have

$$S_z/N=\frac{1}{2}-\sum_{n=1}^{\infty}\frac{n}{f(1)}\left\{\frac{1}{f(n-1)f(n)}-\frac{1}{f(n)f(n+1)}\right\}$$
$$=\frac{1}{2}-\frac{1}{f(1)}\sum_{n=1}^{\infty}\frac{1}{f(n-1)f(n)}. \tag{4·8}$$

Now we prove the identity

$$\sum_{n=1}^{\infty}\frac{1}{f(n-1)f(n)}=z. \tag{4·9}$$

Using the identities

$$\frac{1}{f(0)f(1)}-z=\frac{1}{z+z^{-1}}-z=-\frac{z^2}{f(1)}$$

and

$$\frac{1}{f(n-1)f(n)}-\frac{z^n}{f(n-1)}=-\frac{z^{n+1}}{f(n)}, \qquad n=2,3,\cdots$$

we have

$$\sum_{n=1}^{\infty}\frac{1}{f(n-1)f(n)}-z=\sum_{n=i}^{\infty}\frac{1}{f(n-1)f(n)}-\frac{z^i}{f(i-1)}.$$

Taking the limit $i\to\infty$ and using $z\leqq 1$ we see that the right-hand side is zero. Thus we have proved (4·9). So we have

$$S_z/N=\frac{1}{2}-\frac{z}{f(1)}=\frac{1}{2}\tanh\frac{\mu_0 H}{T}. \tag{4·10}$$

From (3·5) one has the expression of entropy,

$$\begin{aligned}S/N&=\sum_{n=1}^{\infty}\{(1+\eta_n)\ln(1+\eta_n)-\eta_n\ln\eta_n\}\int\rho_n(k)\,dk\\&=\sum_{n=1}^{\infty}\frac{1}{f(1)}\left\{\frac{f(n-1)-f(n+1)}{f(n)}(\ln f(n-1)+\ln f(n+1))\right.\\&\qquad\left.-2\left(\frac{f(n)}{f(n+1)}-\frac{f(n)}{f(n-1)}\right)\ln f(n)\right\}\\&=\ln(z+z^{-1})+\lim_{n\to\infty}\frac{z^{-1}-z}{z^{-1}+z}\ln\frac{f(n+1)}{f(n+2)}\\&=\frac{1}{1+z^2}\ln(1+z^2)+\frac{1}{1+z^{-2}}\ln(1+z^{-2}).\end{aligned} \tag{4·11}$$

The expressions for magnetization and entropy are the same as the well-known properties of free spin. Moreover from (3·3) we have the energy per site,

$$\begin{aligned}E/N&=-\sum_{n=1}^{\infty}\frac{J}{f(1)}\left\{\frac{1}{f(n-1)f(n)}\cdot\frac{1}{n}-\frac{1}{f(n)f(n+1)}\cdot\frac{1}{n+1}\right\}-2\mu_0 HS_z/N\\&=-\frac{J}{f^2(1)}-\mu_0 H\tanh\frac{\mu_0 H}{T}=\frac{J}{4}\left(\tanh^2\frac{\mu_0 H}{T}-1\right)-\mu_0 H\tanh\frac{\mu_0 H}{T}.\end{aligned} \tag{4·12}$$

Here we have used

$$\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{n}{k^2+n^2}\cdot\frac{2n}{k^2+n^2}dk=\frac{1}{n},\qquad \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{n}{k^2+n^2}\cdot\frac{2(n+2)}{k^2+(n+2)^2}dk=\frac{1}{n+1}.$$

§ 5. Expansion of free energy by $z=\exp(-\mu_0 H/T)$

In this section we expand the free energy with $z=\exp(-\mu_0 H/T)$ to fourth order. Consider the case where $\mu_0 H\gg 2|J|$ and $\mu_0 H\gg T$. From Eq. (3·7) we have

$$\begin{aligned}\eta_1^{-1}&=z^2\exp\left(\frac{2K}{k^2+1}\right)(1-[2]\eta_1^{-1}(k))+O(z^6),\\\eta_2^{-1}&=z^4\exp\left(\frac{4K}{k^2+4}\right)+O(z^6),\\\eta_n^{-1}&=O(z^{2n}),\qquad n=3,4,\cdots,\end{aligned} \tag{5·1}$$

where $K=J/T$. From Eq. (3·8) we have

$$\rho_1(k)=\frac{1}{\pi}\eta_1^{-1}(k)\frac{1}{k^2+1}-\eta_1^{-1}(k)([0]+[2])\rho_1(k)+O(z^6),$$

$$\rho_2(k)=\frac{1}{\pi}\eta_2^{-1}(k)\frac{2}{z^2+4}+O(z^6),$$

$$\rho_n(k)=O(z^{2n}),\qquad n=3,4,\cdots. \tag{5·2}$$

The free energy per site is

$$F/N=-\mu_0H+\int_{-\infty}^{\infty}\left(-\frac{2J}{k^2+1}+2\mu_0H-T(1+\eta_1)\ln(1+\eta_1)+T\eta_1\ln\eta_1\right)\rho_1(k)dk$$
$$+\int_{-\infty}^{\infty}\left(-\frac{4J}{k^2+1}+4\mu_0H-T(1+\eta_2)\ln(1+\eta_2)+T\eta_2\ln\eta_2\right)\rho_2(k)dk+O(z^6).$$

Using (5·1) we have

$$-\frac{1}{T}(F/N+\mu_0H)=\int_{-\infty}^{\infty}\left(1+\frac{z^2}{2}\exp\left(\frac{2K}{k^2+1}\right)\right)\rho_1(k)dk+\int_{-\infty}^{\infty}\rho_2(k)dk+O(z^6),$$

and substitution of (5·2) yields

$$=z^2\int_{-\infty}^{\infty}\frac{1}{\pi}\exp\left(\frac{2K}{k^2+1}\right)\frac{dk}{k^2+1}+z^4\left[\int_{-\infty}^{\infty}\frac{1}{\pi}\left\{\exp\left(\frac{K}{k^2+1}\right)-\frac{1}{2}\exp\left(\frac{4K}{k^2+1}\right)\right\}\frac{dk}{k^2+1}\right.$$
$$\left.-2\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{1}{\pi^2}\exp\left(\frac{2K}{k^2+1}+\frac{2K}{k'^2+1}\right)\frac{2}{4+(k-k')^2}\cdot\frac{1}{k^2+1}dkdk'\right]+O(z^6).$$

Put $k=\tan(\theta/2)$ and $k'=\tan(\theta'/2)$. So we have

$$-\frac{1}{T}\left(\frac{F}{N}+\mu_0H\right)=z^2e^KI_0(K)+z^4\left\{-\frac{1}{2}e^{2K}I_0(2K)+e^{K/2}I_0(K/2)\right.$$
$$\left.-\frac{1}{\pi^2}\int_0^\pi\int_0^\pi e^{2K(1-\cos\omega_1\cos\omega_2)}\frac{1-\cos\omega_1\cdot\cos\omega_2}{1-2\cos\omega_1\cdot\cos\omega_2+\cos^2\omega_1}d\omega_1d\omega_2\right\}+O(z^6),$$

where

$$\omega_1=\pi+(\theta+\theta')/2$$

and

$$\omega_2=(\theta-\theta')/2.$$

This result is the same as that of Katsura.[5]

§ 6. Solution in the limit $T\to0$

We put

$$\varepsilon_n(k)\equiv T\ln\eta_n(k).$$

From Eq. (3·7) one obtains

$$\varepsilon_1(k) = -\frac{2J}{k^2+1} + 2\mu_0 H + [2] T \ln\left(1+\exp\left(-\frac{\varepsilon_1(k)}{T}\right)\right)$$
$$+ ([0]+[2]) \sum_{j=1}^{\infty} [j] T \ln\left(1+\exp\left(-\frac{\varepsilon_{j+1}(k)}{T}\right)\right)$$

and

$$\varepsilon_n(k) = 2\mu_0 H + [2] T \ln\left(1+\exp\left(-\frac{\varepsilon_n(k)}{T}\right)\right) + [1] T \ln\left(1+\exp\frac{\varepsilon_{n-1}(k)}{T}\right)$$
$$+ ([0]+[2]) \sum_{j=1}^{\infty} [j] T \ln\left(1+\exp\left(-\frac{\varepsilon_{j+n}(k)}{T}\right)\right), \quad n=2, 3, \cdots.$$

Therefore ε_2, ε_3, $\cdots$ are always positive. So in the limit $T\to 0$ these equations are

$$\varepsilon_1(k) = -\frac{2J}{k^2+1} + 2\mu_0 H - [2]\varepsilon_1^-(k), \tag{6·1}$$

$$\varepsilon_n(k) = 2\mu_0 H + [1]\varepsilon_{n-1}^+(k), \qquad n=2, 3, \cdots, \tag{6·2}$$

where

$$\varepsilon_n^+(k) = \begin{cases} \varepsilon_n(k) & \text{at } \varepsilon_n(k)>0, \\ 0 & \text{at } \varepsilon_n(k)\leqq 0, \end{cases} \qquad \varepsilon_n^-(k) = \begin{cases} 0 & \text{at } \varepsilon_n(k)\geqq 0, \\ \varepsilon_n(k) & \text{at } \varepsilon_n(k)<0. \end{cases}$$

Using the relation $[n][m]=[n+m]$ we have

$$\varepsilon_n(k) = 2(n-1)\mu_0 H + [n-1]\varepsilon_1^+(k), \qquad n=2, 3, \cdots. \tag{6·3}$$

Let us consider the case where $J<\mu_0 H$. In this case $\varepsilon_1(k)$ is always positive and the solution of (6·1) and (6·2) is

$$\varepsilon_n(k) = 2n\mu_0 H - \frac{2nJ}{k^2+n^2}, \qquad n=1, 2, \cdots.$$

Then we have

$$\eta_n=\infty, \qquad \rho_n=0, \qquad S_z/N=\tfrac{1}{2} \quad \text{and} \quad E/N=-\mu_0 H.$$

This solution means that all the spins are parallel to the z-direction.

Next we consider the case $J>\mu_0 H$. The function $\varepsilon_1(k)$ is negative at an interval $[B, -B]$ because $\varepsilon_1(k)$ is a monotonically increasing function of k^2 as will be shown in Appendix B. The parameter B is determined by $\varepsilon_1(B)=0$. Equations for $\rho_n(k)$ are

$$\frac{1}{\pi}\cdot\frac{1}{k^2+1} = \rho_1(k) + \frac{1}{\pi}\int_{-B}^{B} \frac{2\rho_1(k')}{4+(k-k')^2} dk', \tag{6·4}$$

$$\rho_n(k) = 0; \qquad n=2, 3, \cdots. \tag{6·5}$$

Then we have

$$S_z/N=\frac{1}{2}-\int_{-B}^{B}\rho_1(k)\,dk, \tag{6·6}$$

$$E/N=\int_{-B}^{B}f_1(k)\rho_1(k)\,dk-\mu_0 H. \tag{6·7}$$

The properties of these integral equations are investigated by Griffiths and by Yang and Yang.[4] Griffiths calculated the magnetization curve and magnetic susceptibility of the one-dimensional Heisenberg antiferromagnet at zero-temperature and estimated magnetic susceptibility as $\mu_0^2/4\pi^2 J$. Yang and Yang proved Griffiths' conjecture.

§ 7. Discussion

One can calculate all of the excitation spectra from the thermodynamically equilibrium state as Yang and Yang[7] did in the problem of Bose system. Details will be given in later papers.

The author believes that this theory can be generalized to the problem of anisotropic Heisenberg model. If the integral equations for anisotropic Heisenberg model are obtained, many physically interesting results will be found.

We have obtained integral equations for thermodynamics of one-dimensional electron gas with repulsive and attractive delta-function potential by using the method which was used in this paper. The integral equations of ground state energy was already given by Gaudin[9] and Yang.[10] The thermodynamics of one-dimensional Hubbard model the ground state of which was treated by Lieb and Wu[11] is also reduced to a set of integral equations. Details will be given in subsequent papers.

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Appendix A

Here we prove the number of sets $\{I_\alpha^n\}$ which satisfy (2·12a) is $\binom{N}{M}-\binom{N}{M-1}$. It is clear that the number of sets $\{I_\alpha^n\}$ is

$$\sum_{\substack{\alpha_1+2\alpha_2+\cdots+M\alpha_M=M\\ \alpha_i\geq 0}}\prod_{i=1}^{M}\binom{N-\sum_{j=1}^{M}t_{ij}\alpha_j}{\alpha_j} \tag{A·1}$$

from the condition (2·12a), where $\binom{N}{M}$ is binomial coefficient and defined by

$$\binom{N}{M} \equiv \frac{N(N-1)(N-2)\cdots(N-M+1)}{M!}.$$

The summation (A·1) is rewritten as

$$(\mathrm{A}\cdot 1) = \sum_{\alpha_M=0}^{\infty} \binom{N-2M+\alpha_M}{\alpha_M} \sum_{\alpha_{M-1}=0}^{\infty} \binom{N-2M+2\alpha_M+\alpha_{M-1}}{\alpha_{M-1}} \cdots$$

$$\times \sum_{\alpha_2=0}^{\infty} \binom{N-2M+2(\alpha_3+2\alpha_4+3\alpha_5+\cdots)+\alpha_2}{\alpha_2} \binom{N-M+\alpha_3+2\alpha_4+3\alpha_5+\cdots}{N-2\alpha_2-3\alpha_3-\cdots}. \tag{A·2}$$

We can easily see that

$$\sum_{\alpha_2=0}^{\infty} \binom{N-2M+2(\alpha_3+2\alpha_4+3\alpha_5+\cdots)+\alpha_2}{\alpha_2} \binom{N-M+\alpha_3+2\alpha_4+3\alpha_5+\cdots}{M-2\alpha_2-3\alpha_3-\cdots}$$

$= $the coefficient of $x^{M-3\alpha_3-4\alpha_4-5\alpha_5-\cdots}$ of the Taylor expansion of

$$(1-x^2)^{-(N-2M+2(\alpha_3+2\alpha_4+3\alpha_5+\cdots))-1}(1+x)^{N-M+\alpha_3+2\alpha_4+3\alpha_5+\cdots}$$

$= M$-th order coefficient of $\{(1-x)^2(1+x)\}^{M-1}(1-x)^{-N+1}$

$$\times \prod_{n=3}^{M} \{x^n/(1-x)^{2(n-2)}(1+x)^{(n-2)}\}^{\alpha_n}.$$

Using the relation

$$\sum_{\alpha=0}^{\infty} \binom{B+\alpha}{\alpha} X^\alpha = (1-X)^{-B-1},$$

we have easily

$$(\mathrm{A}\cdot 1) = M\text{-th order coefficient of } (1+x)^{N-M}\{\prod_{j=2}^{M}(1-u_j^{-1}(x))\}^{-N+2M-1}, \tag{A·3}$$

where $u_j(x)$ are functions determined by

$$(u_{j+1}-1)^2 = u_j u_{j+2} \tag{A·4}$$

and

$$u_2 = \frac{1}{x^2}, \qquad u_3 = \frac{(1-x)^2(1+x)}{x^3}. \tag{A·5}$$

The general solution of defference equation (A·4) is

$$u_j = \left(\frac{ba^j - b^{-1}a^{-j}}{a-a^{-1}}\right)^2. \tag{A·6}$$

Parameters a and b are determined from the initial conditions (A·5) and we have

$$a=b=\frac{1}{2}\left(\sqrt{\frac{1-3x}{x}}+\sqrt{\frac{1+x}{x}}\right). \tag{A·7}$$

We can easily prove that $u_j^{-1}(x)=O(x^j)$. So we have

$$\prod_{M+1}^{\infty}(1-u_j^{-1}(x))=1+O(x^{M+1})$$

and therefore

$$(\mathrm{A}\cdot 3)=M\text{-th order coefficient of }(1+x)^{N-M}\{\prod_{j=2}^{\infty}(1-u_j^{-1}(x))\}^{-(N-2M+1)}. \tag{A·8}$$

We can easily see that

$$u_j-1=f_{j-1}f_{j+1}, \qquad u_j=f_j^2,$$

where $f_j=(ba^j-b^{-1}a^{-j})/(a-a^{-1})$. So we have

$$\prod_{j=2}^{\infty}(1-u_j^{-1}(x))=(1-u_2^{-1})\prod_{j=3}^{\infty}\left(\frac{f_{j-1}f_{j+1}}{f_j^2}\right)=(1-x^2)\frac{f_2}{f_3}\lim_{n\to\infty}\frac{f_{n+1}}{f_n}=(1-x^2)\sqrt{\frac{u_2(x)}{u_3(x)}}a,$$

and substituting (A·5) and (A·7)

$$=\frac{1+x+\sqrt{(1+x)(1-3x)}}{2}.$$

Substituting this into (A·8) we have

$$(\mathrm{A}\cdot 8)=N-M+1\text{-th order coefficient of }(1+x)^{N-M}\left(\frac{1-\sqrt{1-(4x/1+x)}}{2}\right)^{N-2M+1}. \tag{A·9}$$

The function of the right-hand side is expanded by binomial theorem as follows:

$$2^{-N+2M-1}\sum_{S=0}^{\infty}\sum_{r=0}^{\infty}(-1)^{S+r}\binom{N-2M+1}{S}\binom{S/2}{r}(4x)^r(1+x)^{N-M-r}.$$

Fortunately in the case $r\neq N-M+1$ the coefficient of x^{N-M+1} is zero for the term $(4x)^r(1+x)^{N-M-r}$. So one has

$$(\mathrm{A}\cdot 9)=2^{N+1}\sum_{S=0}^{\infty}(-1)^{N-M+1+S}\binom{N-2M+1}{S}\binom{S/2}{N-M+1}$$

$$=\frac{1}{2^{N-2M}}\cdot\frac{N!(N-2M+1)!}{(N-M+1)!(N-M)!}\sum_{r=0}^{\infty}(-1)^r\binom{N-M}{r}\binom{2N-2M-2r}{N}. \tag{A·10}$$

We can easily see

$$\sum_{r=0}^{\infty}(-1)^r\binom{N-M}{r}\binom{2N-2M-2r}{N}$$

$$=N-2M\text{-th order coefficient of }(1-x^2)^{N-M}(1-x)^{-N-1}$$

$$=N-2M\text{-th order coefficient of }(1+x)^{N-M}(1-x)^{-M-1}$$

$$=\sum_{r=0}^{N-2M}\frac{(N-M)!}{r!(N-2M-r)!M!}=(1+1)^{N-2M}\frac{(N-M)!}{M!(N-2M)!}.$$

Substituting this into (A·10) we have finally

$$(\mathrm{A}\cdot 1) = (\mathrm{A}\cdot 10) = \frac{N!(N-2M+1)}{(N-M+1)!M!} = \binom{N}{M} - \binom{N}{M-1}.$$

Appendix B

Here we prove the solution of (6·1), namely $\varepsilon_1(k)$, is a monotonically increasing function of k^2. By the Fourier transformation, Eq. (6·1) is transformed as follows:

$$\varepsilon_1(k) = -\frac{\pi J}{2}\operatorname{sech}\frac{\pi k}{2} + \mu_0 H + \int_{\varepsilon_1(k')>0} R(k-k')\,\varepsilon_1(k')\,dk', \tag{B·1}$$

where

$$R(x) = \frac{1}{4\pi}\int_{-\infty}^{\infty}\frac{1}{1+(x-y)^2}\operatorname{sech}\frac{\pi y}{2}dy\,.$$

Now we seek the solution of (B·1) by iteration:

$$\varepsilon_1^{(0)}(k) = -\frac{\pi J}{2}\operatorname{sech}\frac{\pi k}{2} + \mu_0 H, \tag{B·2}$$

$$\varepsilon_1^{(n)}(k) = -\frac{\pi J}{2}\operatorname{sech}\frac{\pi k}{2} + \mu_0 H + \int_{\varepsilon_1^{(n-1)}(k')>0} R(k-k')\,\varepsilon_1^{(n-1)}(k')\,dk', \quad n=1, 2, \cdots. \tag{B·3}$$

We can easily see that

$$\varepsilon_1^{(0)} < \varepsilon_1^{(1)} < \varepsilon_1^{(2)} < \cdots \qquad \text{and} \qquad \varepsilon_1^{(n)} < 2\mu_0 H\,.$$

So the series $\varepsilon_1^{(n)}$ converges. From Eq. (B·3) we see that $\varepsilon_1^{(n)}(k)$ is a monotonically increasing function of k^2 if $\varepsilon_1^{(n-1)}(k)$ is such a function. As $\varepsilon_1^{(0)}$ is a monotonically increasing function of k^2, $\lim_{n\to\infty}\varepsilon_1^{(n)}(k) = \varepsilon_1(k)$ is also such a function.

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Note added in proof: M. Gaudin gave integral equations for the thermodynamics of the Heisenberg-Ising model at $\Delta \geq 1$. In the limit $\Delta \to 1$ his equations are equivalent to those which were given in this paper [see M. Gaudin, Phys. Rev. Letters **26** (1971), 1301]. The author derived integral equations with finite unknowns for the thermodynamics of this model at $|\Delta| < 1$. These will be given in a separate paper.