Statistical Mechanics of the Anisotropic Linear Heisenberg Model*

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The anisotropic Hamiltonian,

$$H=-\tfrac{1}{2}\sum(J_x\sigma_l^x\sigma_{l+1}^x+J_y\sigma_l^y\sigma_{l+1}^y+J_z\sigma_l^z\sigma_{l+1}^z)-m\mathcal{H}\sum\sigma_l^z,$$

of the linear spin array in the Heisenberg model of magnetism is examined. The eigenstate and the partition function for the case $J_z=0$ are obtained exactly for a finite system and for an infinite system with the aid of annihilation and creation operators, and the free energy F of the latter is given by

$$-F/NkT=(1/\pi)\int_0^\pi \ln\{2\cosh[K_x^2+K_y^2+2K_xK_y\cos 2\omega-2C(K_x+K_y)\cos\omega+C^2]^{\frac{1}{2}}\}d\omega,$$

where $K_x=J_x/2kT$, $K_y=J_y/2kT$, $C=m\mathcal{H}/kT$. The case $J_x=J_y=J_z=J$ is discussed with the aid of a high-temperature expansion and of analysis of small systems. Specific heats and susceptibilities in special cases: (i) $J_x=J_y=J$, $J_z=0$, (ii) $J_x=J$, $J_y=J_z=0$, (iii$_f$) $J_x=J_y=0$, $J_z=J>0$, (iii$_a$) $J_x=J_y=0$, $J_z=J<0$, (iv$_f$) $J_x=J_y=J_z=J>0$, (iv$_a$) $J_x=J_y=J_z=J<0$ are compared and it is shown that (i), (iii$_a$), and (iv$_a$) have the characteristic features of the observed parallel susceptibility of an antiferromagnetic substance, (ii) those of perpendicular susceptibility, and (iii$_f$) and (iv$_f$) those of paramagnetic susceptibility, even though they have no singularities. The distribution of the zeros of the partition function is also discussed.

1. INTRODUCTION

BLOCH[1] presented a spin-wave theory in the Heisenberg model of ferromagnetism. He predicted for the temperature dependence of the spontaneous magnetization at low temperatures a $T^{3/2}$ law in cubic crystals. The spin-wave theory was applied also to the antiferromagnetic case by several authors.[2]

For a one-dimensional lattice Bethe[3] developed a detailed theory of spin waves, and Hulthén[4] obtained the exact ground-state energy of a linear antiferromagnet. The exact partition function and wavefunction, however, are not yet known. Kasteleijn[5] introduced an anisotropy parameter and obtained the discontinuity of long-range order vs anisotropy. Objections to his results were raised by several authors.[6–8] The one-dimensional Heisenberg model remains an interesting problem.

In this paper Kasteleijn's anisotropy is generalized by introducing three Cartesian components of the exchange integral J_x, J_y, J_z, and special cases are examined. The case $J_z=0$, the opposite limiting case to the Ising interaction, is treated exactly. The ground state and the partition function are obtained for a finite system taking the end effect into consideration exactly, and the limit $N\to\infty$ is taken. This is a generalization and extension of Nambu's work.[9] The partition function of the finite system is given by (2.30), and that for the infinite system by (2.32). The latter is similar to the Onsager integral[10,11] in the two-dimensional Ising model. The isotropic case is discussed with the aid of a high-temperature expansion and of a small system, $N=6$.

Thermodynamic properties for special cases of (i) $J_x=J_y=J$, $J_z=0$, (ii) $J_x=J$, $J_y=J_z=0$, (iii$_f$) $J_z=J>0$, $J_x=J_y=0$, (iii$_a$) $J_z=J<0$, $J_x=J_y=0$, (iv$_f$) $J_x=J_y=J_z=J>0$, (iv$_a$) $J_x=J_y=J_z=J<0$ are calculated and compared. It is shown that (i), (iii$_a$), and (iv$_a$) have the characteristic features of antiferromagnetic parallel susceptibility, (ii) those of antiferromagnetic perpendicular susceptibility, and (iii$_f$) and (iv$_f$) those of paramagnetic susceptibility, even though they have no singularities.

It is further shown that the ground-state wavefunction of (i) is rather similar to that of (iv$_a$) than to that of (iii$_a$), and that zeros of the partition function in cases (i), (iii$_a$), and (iv$_a$) lie on the negative real axis, while those in cases (iii$_f$) and (iv$_f$) lie on the unit circle in the complex e^{2C} plane for a system $N=6$ ($C=m\mathcal{H}/kT$). These facts show that J_x and J_y play as important roles as negative J_z in antiferromagnetism.

Finally, the spontaneous magnetization obtained by Frank[12] and Mannari[13] for the ferromagnetic case is discussed.

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2. PARTITION FUNCTION

We consider the linear Heisenberg spin lattice in which $S=\frac{1}{2}$. A Born-von Kármán cyclic condition (not the Bethe-Hulthén cyclic condition) is assumed and the lattice points are labeled $l=1,2,\cdots N$. $N+l\equiv l$. We also assume that N is even. The interaction is restricted to nearest-neighbor spins but anisotropy is introduced in the following sense. That is, denoting the Cartesian component of the Pauli spin operator of the lth spin by σ_l^x, σ_l^y, σ_l^z, we introduce the generalized Heitler-London type Hamiltonian,

$$H=-\tfrac{1}{2}\sum_{l=1}^{N}(J_x\sigma_l^x\sigma_{l+1}^x+J_y\sigma_l^y\sigma_{l+1}^y+J_z\sigma_l^z\sigma_{l+1}^z)-m\mathcal{H}\sum_{l=1}^{N}\sigma_l^z, \quad (2.1)$$

where J_x, J_y, J_z are the Cartesian components of the exchange integral, $m=g\mu_B$, g is the g factor, and μ_B is the Bohr magneton. $\mathcal{H}$ is the external magnetic field in the z direction. The direction of our spin array may be in either direction.

The Pauli operator σ_l with respect to the lth spin is expressed as a direct product of σ and 1.

$$\sigma_l^x=\alpha_l^\dagger+\alpha_l,\quad \sigma_l^y=i(\alpha_l^\dagger-\alpha_l),\quad \sigma_l^z=1-2\alpha_l^\dagger\alpha_l, \quad (2.2)$$

$$\begin{aligned}\alpha_l^\dagger&=1\times1\times\cdots\times\alpha^\dagger\times\cdots\times1,\\ \alpha_l&=1\times1\times\cdots\times\alpha\times\cdots\times1,\end{aligned} \quad (2.3)$$

$$\alpha^\dagger=\begin{bmatrix} & 0\\ 1 & \end{bmatrix},\quad \alpha=\begin{bmatrix} & 1\\ 0 & \end{bmatrix}.$$

Here $\alpha^\dagger$ and α are located at the lth position. 1 is the two-dimensional unit matrix and $\times$ denotes the direct product of matrices.

It is well known[9,14] that the introduction of the sign function enables us to express the Heisenberg Hamiltonian in terms of sets of anticommuting operators. However, since the expression where there is anisotropy and where the end effect is taken into consideration does not appear elsewhere, we briefly describe the derivation.

We introduce sets of anticommuting operators $a_l^\dagger$ and a_l with the aid of the sign function ν_l.

$$\nu_l=\prod_{m=1}^{l-1}(1-2n_m)=(-1)^{\Sigma}$$

where

$$\Sigma=\sum_{m=1}^{l-1}n_m$$

and $n_m=\alpha_m^\dagger\alpha_m$.

Let

$$\begin{aligned}\nu_l\alpha_l^\dagger&=a_l^\dagger,\\ \alpha_l\nu_l&=a_l,\end{aligned} \quad (2.4)$$

then

$$\begin{aligned}&[\alpha_l^\dagger,a_m]_+=\delta_{lm}, \qquad n_m=a_m^\dagger a_m,\\ &[a_l^\dagger,a_m^\dagger]_+=0, \qquad [a_l,a_m]_+=0.\end{aligned} \quad (2.5)$$

Hence, (2.1) is transformed to

$$H=-\tfrac{1}{2}\{(J_x+J_y)[\sum_{l=1}^{N-1}(a_l^\dagger a_{l+1}+a_{l+1}^\dagger a_l)-\nu_N a_N^\dagger a_1-\nu_N a_1^\dagger a_N]+(J_x-J_y)[\sum_{l=1}^{N-1}(a_l^\dagger a_{l+1}^\dagger-a_l a_{l+1})-\nu_N a_1^\dagger a_N^\dagger+\nu_N a_1 a_N]$$
$$+J_z[\sum_{l=1}^{N}(1-4a_l^\dagger a_l)+4\sum_{l=1}^{N-1}a_l^\dagger a_l a_{l+1}^\dagger a_{l+1}+4a_N^\dagger a_N a_1^\dagger a_1]\}-m\sum_{l=1}^{N}\mathcal{H}(1-2a_l^\dagger a_l). \quad (2.6)$$

$a_l^\dagger$ and a_l are the spin deviation operators and the reference state $|0\rangle$ is the state where all spins point in the negative z direction. In order to eliminate ν_N in the last end term, we note that[11]

$$\begin{aligned}(1+\nu_N)\nu_N&=(1+\nu_N),\\ (1-\nu_N)\nu_N&=-(1-\nu_N).\end{aligned} \quad (2.7)$$

$\frac{1}{2}(1+\nu_N)$ is a projection on one of the halves of our total space, and $\frac{1}{2}(1-\nu_N)$ is the complementary projection, that is,

$$\begin{aligned}\tfrac{1}{2}(1+\nu_N)+\tfrac{1}{2}(1-\nu_N)&=1,\\ \tfrac{1}{2}(1+\nu_N)\tfrac{1}{2}(1-\nu_N)&=0,\\ [\tfrac{1}{2}(1\pm\nu_N)]^2&=\tfrac{1}{2}(1\pm\nu_N).\end{aligned} \quad (2.8)$$

We can resolve H into two parts by using these projection operators:

$$\begin{aligned}H&=\tfrac{1}{2}(1+\nu_N)H+\tfrac{1}{2}(1-\nu_N)H\\ &=\tfrac{1}{2}(1+\nu_N)H^+ +\tfrac{1}{2}(1-\nu_N)H^-,\end{aligned} \quad (2.9)$$

where

$$H^+=-\tfrac{1}{2}\{(J_x+J_y)[\sum_{l=1}^{N-1}(a_l^\dagger a_{l+1}+a_{l+1}^\dagger a_l)-a_N^\dagger a_1-a_1^\dagger a_N]+(J_x-J_y)[\sum_{l=1}^{N-1}(a_l^\dagger a_{l+1}^\dagger-a_l a_{l+1})-a_N^\dagger a_1^\dagger+a_N a_1]$$
$$+J_z\sum_{l=1}^{N}(1-4a_l^\dagger a_l+4a_l^\dagger a_l a_{l+1}^\dagger a_{l+1})\}-m\mathcal{H}\sum_{l=1}^{N}(1-2a_l^\dagger a_l) \quad (2.10)$$

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and

$$H^{-}=-\tfrac{1}{2}[(J_x+J_y)\sum_{l=1}^{N}(a_l^\dagger a_{l+1}+a_{l+1}^\dagger a_l)+(J_x-J_y)\sum_{l=1}^{N}(a_l^\dagger a_{l+1}^\dagger-a_l a_{l+1})$$

$$+J_z\sum_{l=1}^{N}(1-4a_l^\dagger a_l+4a_l^\dagger a_l a_{l+1}^\dagger a_{l+1})]-m\mathcal{H}\sum_{l=1}^{N}(1-2a_l^\dagger a_l), \quad (2.11)$$

$$a_{N+l}^\dagger\equiv a_l^\dagger,\quad a_{N+l}\equiv a_l.$$

We will find the eigenvalues of each of H^+ and H^- separately, and will take into account the effect of the factors $\frac{1}{2}(1+\nu_N)$ and $\frac{1}{2}(1-\nu_N)$ by selecting half of the eigenvalues of H^+ and half of those of H^-. The two half sets will then constitute the full set of eigenvalues of H.

Let

$$A_k^\dagger=\frac{1}{N^{1/2}}\sum_{l=1}^{N}a_l^\dagger\exp\left[i\pi\left(\frac{kl}{N}-\frac{1}{4}\right)\right],$$
$$A_k=\frac{1}{N^{1/2}}\sum_{l=1}^{N}a_l\exp\left[-i\pi\left(\frac{kl}{N}-\frac{1}{4}\right)\right], \quad (2.12)$$

where

$$A_{2N+k}^\dagger\equiv A_k^\dagger,\quad A_{2N+k}\equiv A_k. \quad (2.13)$$

It is to be noted that the exponent is not $2\pi ik/N$ but $\pi ik/N$. $A_k^\dagger$, A_k make a set of anticommuting operators. Then we have for H^+ space

$$\sum_{l=1}^{N-1}(a_l^\dagger a_{l+1}+a_{l+1}^\dagger a_l)-a_N^\dagger a_1-a_1^\dagger a_N=\sum_{k=1}^{N}(\epsilon^{2k-1}+\epsilon^{-2k+1})A_{2k-1}^\dagger A_{2k-1},$$

$$\sum_{l=1}^{N-1}a_l^\dagger a_{l+1}^\dagger-a_N^\dagger a_1^\dagger=i\sum_{k=1}^{N}\epsilon^{2k-1}A_{2k-1}^\dagger A_{-2k+1}^\dagger,$$

$$\sum_{l=1}^{N-1}a_l a_{l+1}-a_N a_1=-i\sum_{k=1}^{N}\epsilon^{-2k+1}A_{2k-1}A_{-2k+1}, \quad (2.14)$$

$$\sum_{l=1}^{N}a_l^\dagger a_l a_{l+1}^\dagger a_{l+1}=\frac{1}{N}\sum_{k_1=1}^{N}\sum_{k_2=1}^{N}\sum_{k_3=1}^{N}\sum_{k_4=1}^{N}\delta(k_1-k_2+k_3-k_4)\epsilon^{2k_1-2k_2}A_{2k_1-1}^\dagger A_{2k_2-1}A_{2k_3-1}^\dagger A_{2k_4-1},$$

where $\delta(k)$ is the Kronecker δ function and $\epsilon=\exp(i\pi/N)$. Hence,

$$H^+=H_0^++H_1^+, \quad (2.15)$$

$$H_0^+=\sum_{k=1}^{N/2}\{[-(J_x+J_y)\cos\omega_{2k-1}+2m\mathcal{H}](A_{2k-1}^\dagger A_{2k-1}+A_{-2k+1}^\dagger A_{-2k+1})$$
$$+(J_x-J_y)\sin\omega_{2k-1}(A_{2k-1}^\dagger A_{-2k+1}^\dagger+A_{-2k+1}A_{2k-1})-2m\mathcal{H}\}, \quad (2.16)$$

$$H_1^+=-\frac{J_z}{2}\sum_{k=1}^{N}\left[1-4A_{2k-1}^\dagger A_{2k-1}+4\frac{\epsilon^{-2k}}{N}\sum_{k'=1}^{N}\sum_{k''=1}^{N}A_{2k'-1}^\dagger A_{-2k'+1+2k}A_{2k''-1}^\dagger A_{-2k''+1-2k}\right],$$

where $\omega_k=2\pi k/N$.

In a similar way we have

$$H^-=H_0^-+H_1^-,$$

$$H_0^-=[-(J_x+J_y)\cos\omega_0+2m\mathcal{H}]A_0^\dagger A_0+\sum_{k=1}^{N/2-1}\{[-(J_x+J_y)\cos\omega_{2k}+2m\mathcal{H}](A_{2k}^\dagger A_{2k}+A_{-2k}^\dagger A_{-2k})$$
$$+(J_x-J_y)\sin\omega_{2k}(A_{2k}^\dagger A_{-2k}^\dagger+A_{-2k}A_{2k})-2m\mathcal{H}\}+[-(J_x+J_y)\cos\omega_N+2m\mathcal{H}]A_N^\dagger A_N, \quad (2.17)$$

$$H_1^-=-\frac{J_z}{2}\sum_{k=1}^{N}\left[1-4A_{2k}^\dagger A_{2k}+4\frac{\epsilon^{-2k}}{N}\sum_{k'=1}^{N}\sum_{k''=1}^{N}A_{2k'}^\dagger A_{-2k'+2k}A_{2k''}^\dagger A_{-2k''+2k}\right].$$

Let $N_k = A_k^\dagger A_k$, then

$$\sum_{l=1}^{N} n_l = \sum_{k=1}^{N} N_{2k-1} = \sum_{k=1}^{N} N_{2k},$$

$$\sum_{l=1}^{N}\sum_{l'=1}^{N} n_l n_{l'} = \sum_{k=1}^{N}\sum_{k'=1}^{N} N_{2k-1}N_{2k'-1} = \sum_{k=1}^{N}\sum_{k'=1}^{N} N_{2k}N_{2k'}.$$

Hence

$$\prod_{l=1}^{N}(1-2n_l) = \prod_{k=1}^{N}(1-2N_{2k-1}) = \prod_{k=1}^{N}(1-2N_{2k}). \tag{2.18}$$

Thus, the projection operator is invariant in the transformation from l space to k space.

In the following we treat the case $J_z=0$. When we determine the canonical transformation

$$A_k = u_k\beta_k + v_k\beta_{-k}^\dagger,\quad A_k^\dagger = u_k\beta_k^\dagger + v_k\beta_{-k},\quad u_{-k}=u_k,\quad v_{-k}=-v_k,\quad u_k^2+v_k^2=1, \tag{2.19}$$

in such a way that the coefficient of $\beta_k^\dagger\beta_{-k}^\dagger + \beta_{-k}\beta_k$ vanish, u_k, v_k and the Hamiltonian in k subspace are derived to be

$$\begin{aligned} u_k^2 &= \frac{1}{2}\left(1+\frac{(J_x+J_y)\cos\omega_k}{[J_x^2+J_y^2+2J_xJ_y\cos 2\omega_k - 4m\mathcal{H}(J_x+J_y)\cos\omega_k + 4m^2\mathcal{H}^2]^{1/2}}\right),\\ v_k^2 &= \frac{1}{2}\left(1-\frac{(J_x+J_y)\cos\omega_k}{[J_x^2+J_y^2+2J_xJ_y\cos 2\omega_k - 4m\mathcal{H}(J_x+J_y)\cos\omega_k + 4m^2\mathcal{H}^2]^{1/2}}\right),\\ H_k &= [J_x^2+J_y^2+2J_xJ_y\cos 2\omega_k - 4m\mathcal{H}(J_x+J_y)\cos\omega_k + 4m^2\mathcal{H}^2]^{1/2}(\beta_k^\dagger\beta_k + \beta_{-k}^\dagger\beta_{-k} - 1),\quad (k=1,2\cdots N-1). \end{aligned} \tag{2.20}$$

Then

$$H_0^+ = \sum_{k=1}^{N/2}[-(J_x+J_y)\cos\omega_{2k-1} + H_{2k-1}]. \tag{2.21}$$

H_0^- is given in a similar way except for the end effect. Since the expression in the parenthesis in (2.20) is $\begin{pmatrix}0&\\&1\end{pmatrix}\times\begin{pmatrix}1&\\&1\end{pmatrix}+\begin{pmatrix}1&\\&1\end{pmatrix}\times\begin{pmatrix}0&\\&1\end{pmatrix}-\begin{pmatrix}1&\\&1\end{pmatrix}\times\begin{pmatrix}1&\\&1\end{pmatrix}$, the eigenvalues and the eigenfunctions of (2.20) are given by

$$\left.\begin{matrix}\lambda_k^{(1)}\\ \lambda_k^{(2)}\end{matrix}\right\} = \pm[J_x^2+J_y^2+2J_xJ_y\cos 2\omega_k - 4m\mathcal{H}(J_x+J_y)\cos\omega_k + 4m^2\mathcal{H}^2]^{1/2}, \tag{2.22}$$

$$\psi_k^{(1)} = \beta_k^\dagger\beta_{-k}^\dagger|0\rangle,\quad \psi_k^{(2)} = |0\rangle, \tag{2.23}$$

$$\lambda_k^{(3)} = \lambda_k^{(4)} = 0, \tag{2.24}$$

$$\psi_k^{(3)} = \beta_k^\dagger|0\rangle,\quad \psi_k^{(4)} = \beta_{-k}^\dagger|0\rangle, \tag{2.25}$$

where $|0\rangle$ is the reference state in (β_k,β_{-k}) representation.

H_0 and H_N, end terms in H_0^-, are two-dimensional matrices. Since the terms $-(J_x+J_y)\cos\omega_k$ for $\frac{1}{2}N\pm k$ cancel in the sum, the eigenvalues of H^+ are given by

$$E^+ = \sum_{k=1}^{N/2}\left\{\begin{matrix} +[J_x^2+J_y^2+2J_xJ_y\cos 2\omega_{2k-1} - 4m\mathcal{H}(J_x+J_y)\cos\omega_{2k-1} + 4m^2\mathcal{H}^2]^{\frac{1}{2}}\\ -[J_x^2+J_y^2+2J_xJ_y\cos 2\omega_{2k-1} - 4m\mathcal{H}(J_x+J_y)\cos\omega_{2k-1} + 4m^2\mathcal{H}^2]^{\frac{1}{2}}\\ 0\\ 0 \end{matrix}\right\}, \tag{2.26}$$

where $\sum\{\ \}$ means the sum of all $(4^{N/2})$ possible combinations. The projection operator $\frac{1}{2}(1+\nu_N)$ makes us select as the eigenvalues of $\frac{1}{2}(1+\nu_N)H^+$ the sign combinations where the difference between the number of + signs and − signs has the same parity as $N/2$. We write this selection rule as $N(+)-N(-)\equiv N/2 \pmod 2$.

Similarly

$$E^{-}=\pm[\tfrac{1}{2}(J_x+J_y)\cos\omega_0-m\mathcal{H}]+\sum_{k=1}^{N/2-1}\left\{\begin{matrix}+[J_x^2+J_y^2+2J_xJ_y\cos2\omega_{2k}-4m\mathcal{H}(J_x+J_y)\cos\omega_{2k}+4m^2\mathcal{H}^2]^{\frac{1}{2}}\\ -[J_x^2+J_y^2+2J_xJ_y\cos2\omega_{2k}-4m\mathcal{H}(J_x+J_y)\cos\omega_{2k}+4m^2\mathcal{H}^2]^{\frac{1}{2}}\\ 0\\ 0\end{matrix}\right\}$$

$$\pm[\tfrac{1}{2}(J_x+J_y)\cos\omega_N-m\mathcal{H}]. \quad (2.27)$$

The projection operator $\frac{1}{2}(1-\nu_N)$ makes us select as the eigenvalues of $\frac{1}{2}(1-\nu_N)H^-$ the sign combinations in which the sum of the difference between the number of + signs and − signs in $\sum_{k=1}^{\frac{1}{2}N-1}$ and half of the difference of + signs and of − signs in the 0th term and the Nth term has the opposite parity to that of $N/2$. We write this selection rule schematically as $N(+)-N(-)\equiv\frac{1}{2}N+1$ (mod 2).

Let

$$J_x/2kT=K_x,\quad J_y/2kT=K_y,\quad m\mathcal{H}/kT=C. \quad (2.28)$$

The partition function Z_{2k-1}^+ in $(2k-1)$th subspace is obtained by direct summation of $\sum_{i=1}^4\exp(-E_i/kT)$:

$$Z_{2k-1}^+=2^2\cosh^2[K_x^2+K_y^2+2K_xK_y\cos2\omega_{2k-1}-2C(K_x+K_y)\cos\omega_{2k-1}+C^2]^{\frac{1}{2}}. \quad (2.29)$$

$Z_{2k}^-(k=1,2,\cdots N-1)$ is given by a similar expression.

Taking the allowable sign combinations due to the projection operator $\frac{1}{2}(1+\nu_N)$ or $\frac{1}{2}(1-\nu_N)$, and the end effect into consideration, we obtain the partition function Z of the anisotropic Hamiltonian of the Heisenberg model $J_z=0$ in the following form.

$$Z/\tfrac{1}{2}2^N=\sum_{k=1}^{N/2}\cosh^2[K_x^2+K_y^2+2K_xK_y\cos2\omega_{2k-1}-2C(K_x+K_y)\cos\omega_{2k-1}+C^2]^{1/2}$$

$$+\prod_{k=1}^{N/2}\sinh^2[K_x^2+K_y^2+2K_xK_y\cos2\omega_{2k-1}-2C(K_x+K_y)\cos\omega_{2k-1}+C^2]^{1/2}$$

$$+\{\prod_{k=1}^{N/2-1}\cosh^2[K_x^2+K_y^2+2K_xK_y\cos2\omega_{2k}-2C(K_x+K_y)\cos\omega_{2k}+C^2]^{1/2}\}\cosh(K_x+K_y-C)\cosh(K_x+K_y+C)$$

$$-\{\prod_{k=1}^{N/2-1}\sinh^2[K_x^2+K_y^2+2K_xK_y\cos2\omega_{2k}-2C(K_x+K_y)\cos\omega_{2k}+C^2]^{1/2}\}$$

$$\times\sinh(C-K_x-K_y)\sinh(C+K_x+K_y). \quad (2.30)$$

In the case of $J_x=J_y$ $(K_x=K_y=K)$, (2.30) is simplified to

$$Z=\tfrac{1}{2}2^N\{\sum_{k=1}^{N/2}\cosh^2(C-2K\cos\omega_{2k-1})+\prod_{k=1}^{N/2}\sinh^2(C-2K\cos\omega_{2k-1})$$

$$+[\prod_{k=1}^{N/2-1}\cosh^2(C-2K\cos\omega_{2k})]\cosh(C-2K)\cosh(C+2K)$$

$$-[\prod_{k=1}^{N/2-1}\sinh^2(C-2K\cos\omega_{2k})]\sinh(C-2K)\sinh(C+2K)\}. \quad (2.31)$$

When we take the limit $N\to\infty$, we have $\omega_{2k}\simeq\omega_{2k-1}$, the second and the fourth term of (2.30) cancel, and the first term and the third term become equal, and hence we have

$$\ln(\lambda/2)\equiv\lim_{N\to\infty}(1/N)\ln(Z/2^N)=\frac{1}{\pi}\int_0^\pi\ln\cosh[K_x^2+K_y^2+2K_xK_y\cos2\omega-2C(K_x+K_y)\cos\omega+C^2]^{1/2}d\omega. \quad (2.32)$$

Free energy F is given by $-NkT\ln\lambda$.

This expression is similar to the Onsager integral for the two-dimensional Ising model.[10,11]

The free energy F in the case of no magnetic field is

$$-\frac{F}{NkT}=\ln\lambda=\frac{1}{\pi}\int_0^\pi \ln\{2\cosh[K_x^2+K_y^2+2K_xK_y\cos2\omega]^{1/2}\}d\omega. \quad (2.33)$$

The magnetization M is given by

$$\frac{M}{Nm}=\frac{1}{\pi}\int_0^\pi \frac{C-(K_x+K_y)\cos\omega}{[K_x^2+K_y^2+2K_xK_y\cos2\omega-2C(K_x+K_y)\cos\omega+C^2]^{1/2}} \times\tanh[K_x^2+K_y^2+2K_xK_y\cos2\omega-2C(K_x+K_y)\cos\omega+C^2]^{1/2}d\omega. \quad (2.34)$$

The susceptibility χ in zero magnetic field is

$$\frac{kT\chi}{Nm^2}=\frac{1}{\pi}\int_0^\pi\Big[\frac{(K_x+K_y)^2\cos^2\omega}{(K_x^2+K_y^2+2K_xK_y\cos2\omega)\cosh^2(K_x^2+K_y^2+2K_xK_y\cos2\omega)} +\frac{(K_x-K_y)^2\sin^2\omega\tanh(K_x^2+K_y^2+2K_xK_y\cos2\omega)^{1/2}}{(K_x^2+K_y^2+2K_xK_y\cos2\omega)^{3/2}}\Big]d\omega. \quad (2.35)$$

The internal energy E is given by

$$\frac{E}{N}=-\frac{kT}{\pi}\int_0^\pi [K_x^2+K_y^2+2K_xK_y\cos2\omega-2C(K_x+K_y)\cos\omega+C^2]^{1/2} \times\tanh[K_x^2+K_y^2+2K_xK_y\cos2\omega-2C(K_x+K_y)\cos\omega+C^2]^{1/2}d\omega. \quad (2.36)$$

3. SPECIAL CASES

In this section we list the thermodynamic quantities in two special cases of the results in the preceding section. $k=J/2kT$ for all cases.

(i) $J_x=J_y=J$, $J_z=0$

Free energy:

$$-\frac{F}{NkT}=\ln\lambda=\frac{1}{\pi}\int_0^\pi \ln[2\cosh(C-2K\cos\omega)]d\omega. \quad (3.1)$$

Internal energy in zero field (Fig. 1):

$$\frac{E}{NJ}=-\frac{2}{\pi}\int_0^{\pi/2}\tanh(2K\cos\omega)\cos\omega d\omega. \quad (3.2)$$

Specific heat in zero field (Fig. 2):

$$\frac{C}{Nk}=\frac{4K^2}{\pi}\int_0^\pi \frac{\cos^2\omega}{\cosh^2(2K\cos\omega)}d\omega. \quad (3.3)$$

Magnetization [Fig. 4(a)]:

$$\frac{M}{Nm}=\frac{1}{\pi}\int_0^\pi \tanh(C-2K\cos\omega)d\omega. \quad (3.4)$$

When the temperature tends to zero, the magnetization tends to ($\tanh x\sim x/|x|$ for large $|x|$)

$$\frac{M}{Nm}=1, \qquad (m\mathcal{H}\geqslant J)$$
$$=\frac{2}{\pi}\sin^{-1}\left(\frac{C}{2K}\right)=\frac{2}{\pi}\sin^{-1}\left(\frac{m\mathcal{H}}{J}\right), \qquad (-J\leqslant m\mathcal{H}\leqslant J) \quad (3.5)$$
$$=-1, \qquad (m\mathcal{H}\leqslant\mathcal{H}).$$

Zero-field susceptibility (Fig. 3):

$$\frac{kT\chi}{Nm^2}=\frac{1}{\pi}\int_0^\pi\frac{d\omega}{\cosh^2(2K\cos\omega)}. \quad (3.6)$$

(ii) $J_x=J$, $J_y=J_z=0$

It is evident that the free energy in zero field, and hence the zero-field internal energy and the specific heat are the same as those of the Ising model.[15] The magnetization and the susceptibility, however, are not the same as the Ising model, since the external magnetic field is perpendicular to the easy axis.

Free energy:

$$-\frac{F}{NkT}=\ln\lambda =\frac{1}{\pi}\int_0^\pi \ln\{2\cosh[K^2+C^2-2KC\cos\omega]^{1/2}\}d\omega. \quad (3.7)$$

[15] H. A. Kramers and G. H. Wannier, Phys. Rev. 60, 252, 263 (1941).

Magnetization [Fig. 4(b)]:

$$\frac{M}{Nm}=\frac{1}{\pi}\int_0^\pi \frac{(C-K\cos\omega)\tanh[K^2+C^2-2KC\cos\omega]^{1/2}}{[K^2+C^2-2KC\cos\omega]^{1/2}}d\omega. \quad (3.8)$$

When the temperature tends to zero, the magnetization is expressed by the complete elliptic integrals of the first kind $\mathbf{K}(k)$ and of the second kind $\mathbf{E}(k)$.

$$\frac{M}{Nm}=\frac{2}{\pi}\left\{\frac{C-K}{2C}\mathbf{K}\left[\frac{2(KC)^{1/2}}{K+C}\right]+\frac{K+C}{2C}\mathbf{E}\left[\frac{2(KC)^{1/2}}{K+C}\right]\right\}. \quad (3.9)$$

When $C<K$, this simplifies to

$$\frac{M}{Nm}=\frac{2}{\pi}\left[\frac{K}{C}\mathbf{E}\left(\frac{C}{K}\right)-\left(\frac{K}{C}-\frac{C}{K}\right)\mathbf{K}\left(\frac{C}{K}\right)\right]. \quad (3.10)$$

Zero-field susceptibility (Fig. 3):

$$\frac{kT\chi}{Nm^2}=\frac{1}{2}\left[\frac{1}{\cosh^2 K}+\frac{\tanh K}{K}\right]. \quad (3.11)$$

4. GROUND STATE

Now we consider the ground state in the case of no magnetic field.

In case (i) we have from (2.26) and (2.27)

$$E^+=\sum_{k=1}^{N/2}\left\{\begin{matrix}+2J\cos\omega_{2k-1}\\-2J\cos\omega_{2k-1}\\0\\0\end{matrix}\right\}, \quad (4.1)$$

and

$$E^-=\pm J\cos\omega_0+\sum_{k=1}^{N/2-1}\left\{\begin{matrix}+2J\cos\omega_{2k}\\-2J\cos\omega_{2k}\\0\\0\end{matrix}\right\}\pm J\cos\omega_N. \quad (4.2)$$

The lowest energy state in either E^+ space or in E^- space is realized by taking the $-$ sign in $0\leqslant k<N/4$ and $+$ sign in $N/4<k\leqslant N/2$ for the case $J>0$. Sign of the term with $k=N/4$ is optional. Since $N(+)-N(-)=0$ in E^- for odd $N/2$ and in E^+ for even $N/2$, and $N(+)-N(-)=1$ in E^- for even $N/2$ and in E^+ for odd $N/2$, this selection of signs is allowable, and the lower energy is given by E^+ or by E^- according as $N/2$ is even or odd. The corresponding eigenfunction is either

$$\Psi_0=[\prod_{k>N/4}^{N/2} A_{2k-1}{}^\dagger A_{-2k+1}{}^\dagger]|0\rangle \quad (4.3)$$

for even $N/2$, or

$$\Psi_0=[\prod_{k>N/4}^{N/2-1} A_{2k}{}^\dagger A_{-2k}{}^\dagger]A_N{}^\dagger|0\rangle \quad (4.3')$$

for odd $N/2$. The case $J<0$ can be treated in a similar way. The ground state is nondegenerate irrespective of sign of J. In both cases ($J>0$ and $J<0$), when N is sufficiently large, summation is replaced by integration and we have

$$E_0/N|J|=-2/\pi=-0.6366. \quad (4.4)$$

In case (ii) the lowest energy states (with no magnetic field) of E^+ and of E^- are the same and the selection rule of the sign combination shows that the both states are allowable irrespective of the sign of J and irrespective of the parity of $N/2$. We, thus, have the doubly degenerate ground states which are the same as the Ising model ($E/N|J|=-\frac{1}{2}$).

The ground-state wave function in the case (iv$_f$) is $N+1$ fold degenerate and the energy is the same as in the case (iii), while that in the case (iv$_a$) is nondegenerate. These values of the ground states should be compared with that in case (iv$_a$) obtained by Hulthén,

$$E_0/N|J|=-2\ln 2+\tfrac{1}{2}=-0.8863. \quad (4.5)$$

The ground-state energy in the general $J_z=0$ case is obtained from (2.38) by taking the limit $T\to 0$.

$$\frac{E_0}{N}=-\frac{1}{2\pi}\int_0^\pi (J_x^2+J_y^2+2J_xJ_y\cos 2\omega)^{1/2}d\omega$$
$$=-(1/\pi)(J_x+J_y)\mathbf{E}(2(J_xJ_y)^{1/2}/(J_x+J_y)). \quad (4.6)$$

Now we consider the ordering property in the ground state. We define the ferromagnetic and antiferromagnetic long-range order operator by

$$\xi_F=\frac{1}{N}(\sum_{l=1}^{N/2}\sigma_{2l}{}^z+\sum_{l=1}^{N/2}\sigma_{2l+1}{}^z)$$
$$=\frac{1}{N}\sum_{k=1}^{N/2}A_{2k}{}^\dagger A_{2k}, \quad (4.7)$$

and

$$\xi_A=\frac{1}{N}(\sum_{l=1}^{N/2}\sigma_{2l}{}^z-\sum_{l=1}^{N/2}\sigma_{2l+1}{}^z)$$
$$=\frac{1}{N}\sum_{k=1}A_{2k}{}^\dagger A_{2k+N}, \quad (4.8)$$

respectively. The expectation value of ξ_F in the ground state is 1 and -1 (doubly degenerate) in case (iii$_f$), and $(N-2i)/N$ $(i=0.1, \cdots N)$ in case (iv_f) [$(N+1)$-fold degenerate]. The expectation value of ξ_A in the ground state is 1 and -1 in the case (iii_a) (doubly degenerate), and zero in cases (i) and (iv_a) (nondegenerate), since up and down orientations are equivalent.

As a short-range order we define

$$\rho=\frac{1}{N}\sum_{l=1}^{N}\sigma_l^z\sigma_{l+1}^z. \tag{4.9}$$

ρ is the z component of the Hamiltonian multiplied by $-2/J_zN$. The expectation value of ρ in the ground state in case (i) is

$$\bar{\rho}=-\frac{2}{\pi^2}\int_{\pi/2}^{3\pi/2}\int_{\pi/2}^{3\pi/2}\cos(\omega_1-\omega_2)d\omega_1 d\omega_2$$
$$=-4/\pi^2=-0.4053 \tag{4.10}$$

for $N\rightarrow\infty$. The corresponding value for the case (iv_a) is -0.59 (read from his Fig. 3 in our unit) by Orbach[6] and -0.40 by Davis[8] (read from his Fig. 2).

5. DISCUSSIONS

The thermodynamic quantities derived in the preceding sections [case (i) and (ii)], together with the case of Ising model[15] (iii_f), (iii_a), and the isotropic case (iv_f), (iv_a) (by high-temperature series expansions[16]) have been calculated numerically and are shown in Figs. 1 to 4.

The specific heat in cases (i), (ii), and (iii) has a maximum though it is not a singularity. The specific heat in (iii_f) and (iii_a) is the same, while that in (iv_f) and that in (iv_a) differ slightly and may resemble (iii) in the low-temperature region. The susceptibility in cases (iii_f) and (iv_f) starts from infinity and decreases monotonically as the temperature increases. This is a characteristic feature of observed paramagnetic susceptibility. The susceptibility in (i), (iii_a), and (iv_a) starts from zero and has a maximum. This is a char-

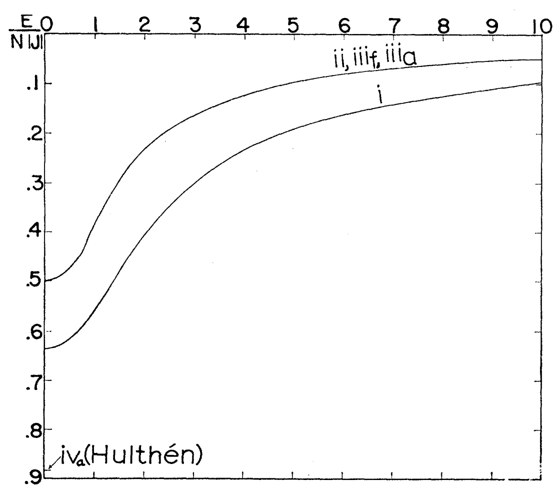

FIG. 1. Internal energy vs temperature. The ordinate and abscissa denote $E/N|J|$ and $2kT/|J|$, respectively. (i) is Eq. (3.2); (ii), (iii_f), and (iii_a) are $-\frac{1}{2}\tanh|K|$.

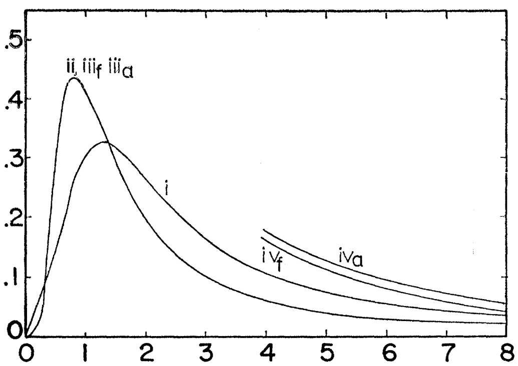

FIG. 2. Specific heat vs temperature. The ordinate and abscissa denote C/Nk and $2kT/|J|$, respectively. (i) is Eq. (3.3); (ii), (iii_f), and (iii_a) are $K^2/\cosh^2K$; (iv) $3K^2-6K^3-15K^4+60K^5\cdots$.

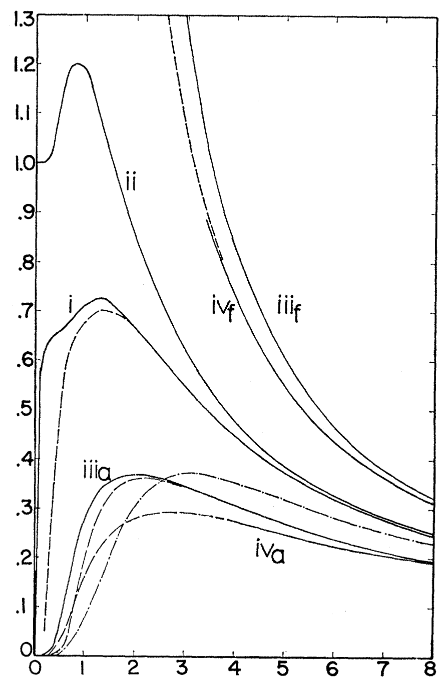

FIG. 3. Susceptibility vs temperature. The ordinate and abscissa denote $|J|\chi/Nm^2$ and $2kT/|J|$, respectively. Solid line shows the exact curves. (i) is Eq. (3.6), (ii) (3.13), (iii)$\pm2Ke^{2K}$, (iv)$\pm2K[1+2K-(8/3)K^3+(10/3)K^4+(28/5)K^5+(266/15)K^6\cdots]$. + and − correspond to f and a cases, respectively. Dashed line uniting to each solid line shows that of the system $N=6$ corresponding to respective cases. Dash-dotted line shows that calculated by Syozi's result.

[16] G. S. Rushbrooke and P. J. Wood, Proc. Phys. Soc. (London) **68**, 1161 (1955); see C. Domb, *Advances in Physics*, edited by N. F. Mott (Taylor and Francis, Ltd., London, 1960), Vol. 9, p. 329.

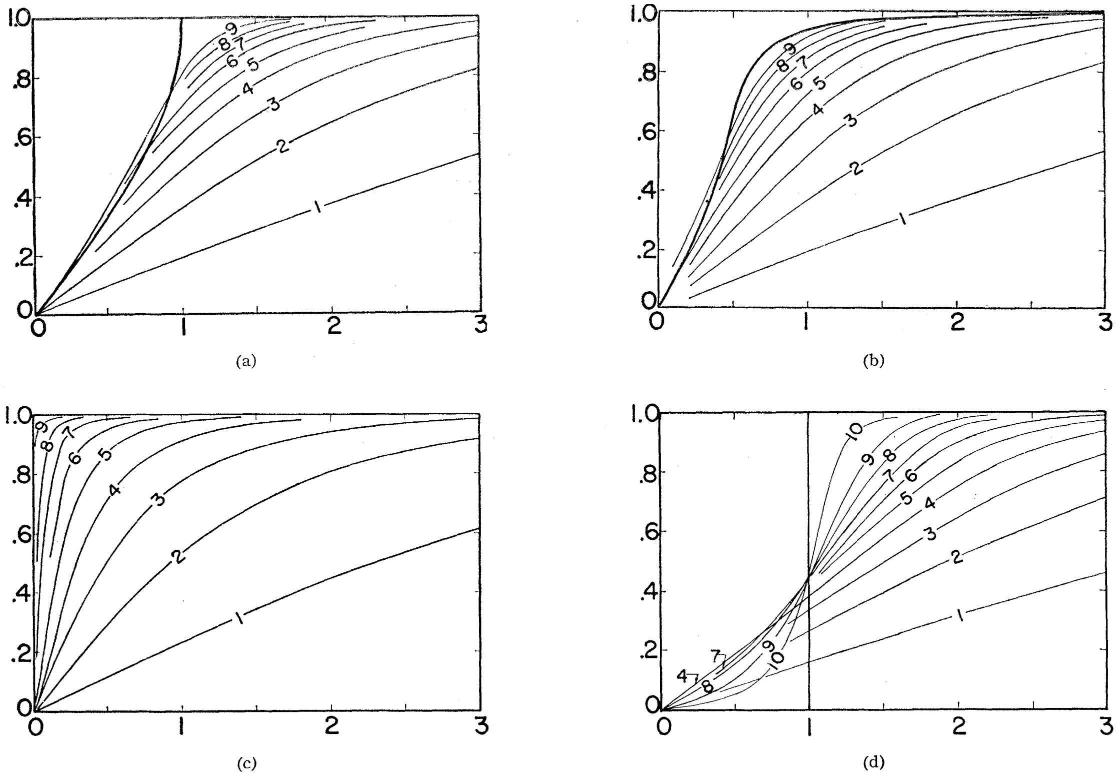

FIG. 4. Magnetization vs magnetic field. The ordinate and abscissa denote M/Nm and $m\mathcal{H}/|J|$. (a) case (i), Eq. (3.4); (b) case (ii), Eq. (3.10); (c) and (d) cases (iii_f) and (iii_a), $\sinh C/[\sinh^2 C+\exp(-4K)]^{1/2}$. The number associated to each curve shows the following temperature. Bold line indicates the limit curve at $T=0$.

No.	$\tanh K$	$2kT/J=1/K$	No.	$\tanh K$	$2kT/J$
1	0.1	9.96655	6	0.6	1.44270
2	0.2	4.93261	7	0.7	1.15300
3	0.3	3.23081	8	0.8	0.91024
4	0.4	2.36045	9	0.9	0.67925
5	0.5	1.82048	10	0.9866	0.40000 [only (d)]

acteristic feature of the observed parallel susceptibility of an antiferromagnetic substance. On the other hand, the susceptibility in case (ii), perpendicular susceptibility of the anisotropic Heisenberg model with Ising interaction, starts from finite value and has a maximum. This is a characteristic feature of the observed perpendicular susceptibility of an antiferromagnetic substance. The susceptibility for the isotropic case obtained by Syozi,[17] which can be rewritten as

$$\frac{kT\chi}{Nm^2}=\frac{1}{\pi}\int_0^{\pi}\frac{d\omega}{\cosh^2[2K(1+\cos^2\omega)^{1/2}]},$$

has been also calculated numerically and shown in Fig. 3.

It is interesting to note that the susceptibility in case (i) looks like a parallel susceptibility, since in both cases (i) and (ii) the spins lie in the xy plane in the classical picture.

Since the exact solution of the isotropic case is not yet known, the susceptibilities of the finite system $N=6$ in cases (i), (iii_f), (iii_a), (iv_f), and (iv_a) have been calculated (dashed line in Fig. 3) and compared.[18] Susceptibilities of the finite system $N=6$ in cases (i), (iii_f), and (iii_a) are surprisingly close to those of infinite system. It is, hence, expected that susceptibilities of the system $N=6$ in cases of (iv_f) and (iv_a) in Fig. 3 are good approximations for $N\rightarrow\infty$.

The magnetization vs magnetic field in several cases are also compared. It is well known that the magnetization of the Ising model with ferromagnetic interaction, case (iii_f), tends to a step function when the temperature tends to zero [Fig. 4(d)]. On the other hand, the magnetization of the Ising model with antiferromagnetic interaction (iii_a) tends to another kind of step function which has a critical field when the temperature is zero. That is, all spins orient to the direction of the field, $M/Nm=\pm1$, when $|m\mathcal{H}|>2|J|$, while antiferromag-

[17] I. Syozi, Busseiron Kenkyu No. 39, 55 (1951).

[18] The partition function for the system $N=6$ can be calculated from (2.31) in case (i), and from the eigenvalues obtained by R. Serber [J. Chem. Phys. 2, 697 (1934)] in case (iv).

netic short-range order exists, and $M/Nm=0$ when $|m\mathcal{H}|<2|J|$ (magnetization is zero). The case (i) is somewhat similar to the above case (iii_a). Below the critical field, however, magnetization decreases gradually (3.5). The magnetization in case (ii) is also similar, but is a smooth function (3.9) of the magnetic field even when the temperature is zero. It is expected that such cooperative properties, which can be seen only at $T=0$ in one-dimensional lattice, will be seen up to the critical temperature and the maximum of specific heat and the susceptibility will become the singularity in two- or three-dimensional lattices.

In the above discussion, we have seen that J_x and J_y play important roles in antiferromagnetism, as well as negative J_z. Indeed, in the system $N=6$, the ground-state wave function of case (iv_a) resembles more closely that of (i) than that of (iii_a) (see Appendix). Moreover, the zeros of the partition function of the system $N=6$ in the complex e^{2C} plane are found to lie on the unit circle in the cases (iii_f) and (iv_f), while they lie on the negative real axis in the cases (i), (iii_a), and (iv_a). It is highly probable that this is valid for any N. This is a generalization of Yang-Lee's theorem[19] to the Heisenberg model.

In the spin-wave theory of Bloch, the fact that the spontaneous magnetization does not exist in a one-dimensional system is indicated by the fact that the integral expressing the magnetization diverges as the magnetic field tends to zero. A similar divergence appears in the one-dimensional case also in Dyson's theory.[20] The nonexistence of the magnetization, however, should be accompanied by the vanishing of the integral expressing the magnetization as shown in our cases (i) and (ii). The divergence results from use of Bose statistics.

On the other hand, Frank[12] and Mannari[13] obtained the spontaneous magnetization of a one-dimensional Heisenberg model of a ferromagnet by using Fermi statistics. The reason for this will now be considered. We write the Hamiltonian (2.1) or (2.6) as

$$H=H_x+H_y+H_z^{(1)}+H_z^{(2)}+H_{\mathcal{H}},$$

where H_x and H_y are the σ_x- and σ_y-dependent part, $H_{\mathcal{H}}$ is the $\mathcal{H}$-dependent part, $H_z^{(1)}$ is the constant part and quadratic part of the annihilation and the creation operators, and $H_z^{(2)}$ is the quartic part of them. In the preceding section $H_x+H_y+H_{\mathcal{H}}$ was diagonalized. Frank and Mannari's unperturbed Hamiltonian is $H_x+H_y+H_z^{(1)}$ and the unperturbed partition function can be derived from the results of the preceding section at once, and their magnetization $M_{\text{Frank-Mannari}}$ is related to (3.5) by

$$M_{\text{FM}}(C,K)=M_{K_x=K_y=K,K_z=0}(C+2K,\,K).$$

[19] C. N. Yang and T. D. Lee, Phys. Rev. **87**, 404, 410 (1952). See also S. Katsura, Progr. Theoret. Phys. (Kyoto) **13**, 571 (1955); **16**, 589 (1956).

[20] F. J. Dyson, Phys. Rev. **102**, 1217, 1230 (1956).

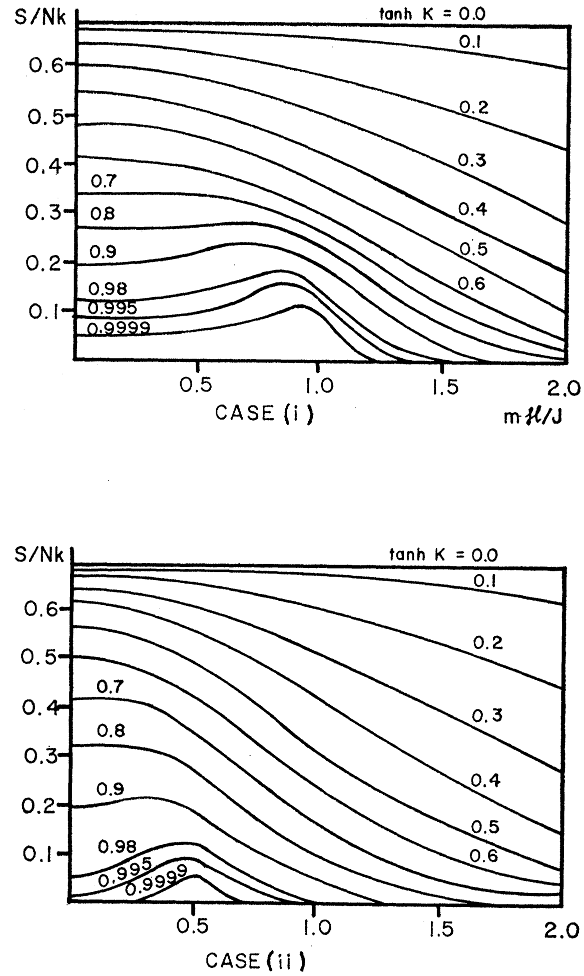

FIG. 5. The entropy as functions of the magnetic field and the temperature.

Their spontaneous magnetization $M_{\text{FM}}(0,K)$ is nothing but $M_{K_x=K_y=K,K_z=0}(2K,K)$ in (3.4). $M_{\text{FM}}(C,K)$ has no symmetric property: $M_{\text{FM}}(C,K)\neq -M_{\text{FM}}(-C,K)$ while (3.4) has. Even when $H_z^{(2)}$ is treated by the perturbation method, this asymmetry cannot be removed. In the perturbation method, $H_z^{(1)}$ and $H_z^{(2)}$ should be regarded as a perturbation as a whole in order to discuss the spontaneous magnetization.

Note added in proof. In the course of publication the author found that the free energy of infinite system without magnetic field agrees with the results of E. Lieb, T. Schultz, and D. Mattis [Ann. Phys. (New York) **16**, 407 (1961)] and that the perpendicular susceptibility agrees with the results of M. E. Fisher [Physica **26**, 618 (1960)]. The author acknowledges helpful correspondences with Dr. D. Mattis and with Dr. M. E. Fisher.

Note added in proof. The author also proved that in the cases (i) and (ii) [see Fig. 5] at the temperature absolute zero there is neither such an anomalous entropy as shown in the Ising antiferromagnetic case (iii_a)

[J. E. Brooks and C. Domb, Proc. Roy. Soc. (London) **A207**, 343 (1951), J. C. Bonner and M. E. Fisher (private communication)] nor that as shown in the super exchange antiferromagnet [M. E. Fisher, Proc. Roy. Soc. (London) **A256**, 502 (1960)]. That is, $S=0$ at $T=0$ irrespective of below, at, and above the critical magnetic field, though S has a maximum nearly at $m\mathcal{H}=J$ in (i) or at $m\mathcal{H}=J/2$ in (ii), respectively, at sufficiently low temperature.

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APPENDIX

The ground state for the system $N=6$ in case (i) is obtained from (4.3′), and that in case ($\mathrm{iv_a}$) is obtained by solving (2.6). Here the ground-state wavefunctions are listed to show the similarity between (i) and ($\mathrm{iv_a}$).

$$\Psi_0(J,J,0)=\mathrm{const}A_4{}^\dagger A_6{}^\dagger A_8{}^\dagger|0\rangle$$

$$=\frac{1}{\sqrt{2}}[\tfrac{1}{2}(a_1{}^\dagger a_3{}^\dagger a_5{}^\dagger-a_2{}^\dagger a_4{}^\dagger a_6{}^\dagger)+\tfrac{1}{3}(a_1{}^\dagger a_4{}^\dagger a_6{}^\dagger-a_2{}^\dagger a_5{}^\dagger a_1{}^\dagger+a_3{}^\dagger a_6{}^\dagger a_2{}^\dagger-a_4{}^\dagger a_1{}^\dagger a_3{}^\dagger+a_5{}^\dagger a_2{}^\dagger a_4{}^\dagger-a_6{}^\dagger a_3{}^\dagger a_5{}^\dagger$$

$$-a_2{}^\dagger a_3{}^\dagger a_5{}^\dagger+a_3{}^\dagger a_4{}^\dagger a_6{}^\dagger-a_4{}^\dagger a_5{}^\dagger a_1{}^\dagger+a_5{}^\dagger a_6{}^\dagger a_2{}^\dagger-a_6{}^\dagger a_1{}^\dagger a_3{}^\dagger+a_1{}^\dagger a_2{}^\dagger a_4{}^\dagger)$$

$$+\tfrac{1}{6}(-a_1{}^\dagger a_2{}^\dagger a_3{}^\dagger+a_2{}^\dagger a_3{}^\dagger a_4{}^\dagger-a_3{}^\dagger a_4{}^\dagger a_5{}^\dagger+a_4{}^\dagger a_5{}^\dagger a_6{}^\dagger-a_5{}^\dagger a_6{}^\dagger a_1{}^\dagger+a_6{}^\dagger a_1{}^\dagger a_2{}^\dagger)]|0\rangle. \quad \text{(A1)}$$

$$\Psi_0(J,J,J)=\mathrm{const}\times\left[A_4{}^\dagger A_6{}^\dagger A_8{}^\dagger+\frac{7-2\sqrt{13}}{2}A_2{}^\dagger A_6{}^\dagger A_{10}{}^\dagger+\frac{11-3\sqrt{13}}{4}(A_8{}^\dagger A_{10}{}^\dagger A_0{}^\dagger+A_0{}^\dagger A_2{}^\dagger A_4{}^\dagger)\right]|0\rangle$$

$$=\frac{1}{\sqrt{2}}[0.676766(a_1{}^\dagger a_3{}^\dagger a_5{}^\dagger-a_2{}^\dagger a_4{}^\dagger a_6{}^\dagger)$$

$$+0.293892(a_1{}^\dagger a_4{}^\dagger a_6{}^\dagger-a_2{}^\dagger a_5{}^\dagger a_1{}^\dagger+a_3{}^\dagger a_6{}^\dagger a_2{}^\dagger-a_4{}^\dagger a_1{}^\dagger a_3{}^\dagger+a_5{}^\dagger a_2{}^\dagger a_4{}^\dagger-a_6{}^\dagger a_3{}^\dagger a_5{}^\dagger$$

$$-a_2{}^\dagger a_3{}^\dagger a_5{}^\dagger+a_3{}^\dagger a_4{}^\dagger a_6{}^\dagger-a_4{}^\dagger a_5{}^\dagger a_1{}^\dagger+a_5{}^\dagger a_6{}^\dagger a_2{}^\dagger-a_6{}^\dagger a_1{}^\dagger a_3{}^\dagger+a_1{}^\dagger a_2{}^\dagger a_4{}^\dagger)$$

$$+0.088983(-a_1{}^\dagger a_2{}^\dagger a_3{}^\dagger+a_2{}^\dagger a_3{}^\dagger a_4{}^\dagger-a_3{}^\dagger a_4{}^\dagger a_5{}^\dagger+a_4{}^\dagger a_5{}^\dagger a_6{}^\dagger-a_5{}^\dagger a_6{}^\dagger a_1{}^\dagger+a_6{}^\dagger a_1{}^\dagger a_2{}^\dagger)]|0\rangle, \quad (J<0). \quad \text{(A2)}$$

The ground-state energies in cases (i) and ($\mathrm{iv_a}$) of the system $N=6$ are $-2/3=-0.6667$ and $-(2+\sqrt{13})/6=-0.9343$, which agree with (4.4) and (4.5), respectively, fairly well. The short-range order in cases (i) and ($\mathrm{iv_a}$) of the system $N=6$ are -0.4444 and -0.6228, which agree with (4.10) and with the value of Orbach,[6] respectively, fairly well.