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Modified Spin Wave Theory of the Two-Dimensional Frustrated Heisenberg Model

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The modified spin wave theory of Takahashi is applied to the antiferromagnetic Heisenberg model with next nearest neighbor interactions on the square lattice in the ground state. The result indicates existence of ordered states for any value of the ratio of the nearest and next nearest neighbor interactions in contrast to some of the other theories.

§1. Introduction

The antiferromagnetic Heisenberg model on the square lattice is now believed to have long-range order in the ground state even for $S=1/2$.[1-4] It is an interesting problem whether this long-range order is destroyed by frustration caused, for instance, by next nearest neighbor antiferromagnetic interactions. It has been pointed out that this type of model has close relationship with the Hubbard model with nearly half-filled band.[5] We do not intend, however, to emphasize the electronic aspects of the frustrated system; we will rather investigate how the magnetic long-range order is affected by frustration. For small values of the ratio α of the next nearest neighbor and the nearest neighbor interactions, the conventional two-sublattice Néel ordel survives as proved rigorously by Kishi and Kubo.[6] If α is sufficiently large, the system effectively splits into two interpenetrating square lattices, in each of which the two-sublattice order exists. We call the latter state the four-sublattice Néel state. The most interesting region is that of the intermediate values of α. There the conventional long-range order may be unstable against quantum fluctuations, leading to a new spin state. There have been many papers published on this subject. Chandra and Doucot[7] employed the spin wave theory in the harmonic approximation (to be called the naive spin wave theory in the present paper). They claim that a spin liquid phase exists for some range of α near 0.5 in the sense that the conventional antiferromagnetic long-range order disappears. Hirsch and Tang[8] studied this model by a sublattice-symmetric spin wave theory and exact diagonalization. They predicted a transition to a disordered phase with an energy gap and an exponentially decaying correlation function, rather than to a gapless spin liquid phase. For spin-1/2 systems, numerical diagonalization of small systems was also used by Dagotto and Moreo.[9] They suggested that the order parameter may undergo qualitative change of behavior around $\alpha \simeq 0.58$. Oguchi and Kitatani[10] used the spin wave theory with a spin-boson transformation similar to the Dyson-Maleev transformation to represent the spin variables in terms of bosons. Their equations lead to the same conclusions as those of Chandra and Doucot.[7] Sano *et al.*[11] claim to have confirmed absence of disordered state based upon an extrapolation of numerical data.

In spite of this accumulating amount of investigation, we feel that our understanding of this problem is still at a primitive stage; the naive spin wave theory suffers from undesired infrared divergences at $\alpha=0.5$ which originate in the instability of the classical ground state against quantum fluctuations. Numerical studies give only preliminary suggestions on the magnetic ordering because of smallness of system size. These are the reasons which prompted us to the calculations employing the method of Takahashi.[12]

One of the important features of his method

is the use of the Dyson-Maleev transformation to avoid uncontrolled cutoff of the expansion of irrational functions appearing in the Holstein-Primakoff transformation. Another trick is in the introduction of a chemical potential (or a Lagrange multiplier) to impose the condition of vanishing sublattice magnetization. The latter technique leads to rather satisfactory results if applied to the unfrustated system ($\alpha=0$) at low temperatures: The naive spin wave theory fails to predict the behavior of physical quantities at finite temperatures in two dimensions because of infrared divergences originating in the absence of long-range order. Takahashi[12] succeeded in deriving finite and reasonable values of various quantities by imposing the condition of vanishing magnetization at finite temperatures in two dimensions. Thus, we considered, if this method is applied to the frustrated antiferromagnetic Heisenberg model in the ground state, dievergences of technical (not physical) origin at $\alpha=0.5$ may be removed, revealing the true behavior of the system in the region with strongest effects of frustration. Actually, we have found that for any $\alpha(\geq 0)$ and $S(\geq 1/2)$ there exists finite Néel order of either the two-sublattice or the four-sublattice type. Therefore, the present method predicts no magnetically disordered (or liquid-like) phase. Details of the calculations are presented in the next section, followed by the numerical solutions of the self-consistent equations in §3. The conclusion is given in the last section.

§2. Modified Spin Wave Theory

To develop a spin wave theory, we have to start from the explanation of the classical spin configuration in the ground state of the Hamiltonian

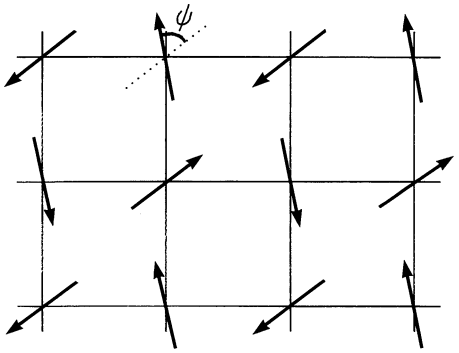

Fig. 1. The four-sublattice Néel state of the classical system. This state is seen to be composed of two interpenetrating square lattices. The relative orientation ψ between the two sublattices is arbitrary. In each of the two sublattices, a rigid two-sublattice Néel state is realized.

$$H=\sum_{\text{n.n.}} \boldsymbol{S}_i\cdot\boldsymbol{S}_j+\alpha \sum_{\text{n.n.n.}} \boldsymbol{S}_i\cdot\boldsymbol{S}_j. \tag{2.1}$$

For $0\leq\alpha<0.5$, the conventional two-sublattice Néel state is the ground state. If α exceeds 0.5, the ground state is replaced by the four sublattice Néel state. The four-sublattice state has infinite degeneracy corresponding to the arbitrary relative orientation of two interpenetrating square lattices (Fig. 1). When $\alpha=0.5$, both of the Néel states are ground states, and in addition, an extra degree of continuous degeneracy emerges. This high degeneracy causes divergences in the naive spin wave calculations.[7,10] We investigate whether or not this classical long-range order is destroyed by quantum fluctuations using the modified spin wave theory.[12]

2.1 *Two-sublattice Néel state*

Let us introduce the antiferromagnetic Dyson-Maleev transformation to rewrite the spin operators in terms of bosons:

$$\begin{aligned} &S_l^-=a_l^\dagger,\quad S_l^+=(2S-a_l^\dagger a_l)a_l,\quad S_l^z=S-a_l^\dagger a_l \quad (l\in \text{A sublattice})\\ &S_p^-=-b_p,\quad S_l^+=-b_p^\dagger(2S-b_p^\dagger b_p),\quad S_p^z=-S+b_p^\dagger b_p \quad (p\in \text{B sublattice}), \end{aligned} \tag{2.2}$$

where a_l and b_p are bose operators satisfying

$$[a_l, a_m^\dagger]=\delta_{lm}$$
$$[b_p, b_q^\dagger]=\delta_{pq},$$

and zero otherwise. By the antiferromagnetic Dyson-Maleev transformation (2.2), the Hamilto-

nian (2.1) is rewritten as

$$H=\frac{1}{2}(\alpha-1)zNS^2+\sum_{\langle lp\rangle}^{\text{n.n.}}\left[S(a_l^\dagger a_l+b_p^\dagger b_p-a_l^\dagger b_p^\dagger-a_l b_p)+\frac{1}{2}a_l^\dagger(b_p^\dagger-a_l)^2 b_p\right]$$
$$+\alpha\sum_{\langle lm\rangle}^{\text{n.n.n.}}\left[S(a_l^\dagger-a_m^\dagger)(a_l-a_m)+\frac{1}{2}a_l^\dagger a_m^\dagger(a_l^\dagger-a_m^\dagger)^2\right]$$
$$+\alpha\sum_{\langle pq\rangle}^{\text{n.n.n.}}\left[S(b_p^\dagger-b_q^\dagger)(b_p-b_q)+\frac{1}{2}(b_p^\dagger-b_q^\dagger)^2 b_p b_q\right]. \tag{2.3}$$

This transformed Hamiltonian does not have terms higher than the fourth order of boson operators in contrast to the representation by the Holstein-Primakoff transformation. One should note here that the eigenvalue spectrum of eq. (2.3) contains unphysical values not included in the original Hamiltonian (2.1) as expected from the fact that the transformed Hamiltonian (2.3) is not Hermitian. This problem comes from the non-unitarity of the Dyson-Maleev transformation (2.2) . Nevertheless, one generally believes that the unphysical states do not affect the ground state properties.[12] We define the Fourier transformation as

$$a_k=\sqrt{\frac{2}{N}}\sum_l \exp(-ik\cdot l)a_l,$$
$$b_k=\sqrt{\frac{2}{N}}\sum_p \exp(-ik\cdot p)b_p^\dagger.$$

We have used non-bold symbols to represent vectors such as $\boldsymbol{k}$, $\boldsymbol{l}$ and $\boldsymbol{p}$ for simplicity of notation. Following Takahashi,[12] we perform a Bogoliubov transformation

$$\alpha_k=a_k\cosh\theta_k-b_k^\dagger\sinh\theta_k$$
$$\beta_{-k}=-a_k\sinh\theta_k+b_{-k}^\dagger\cosh\theta_k,$$

and assume that the density matrix is diagonal in α_k and β_k. We then minimize the free energy by varying θ_k and the energy spectrum ε_k of the diagonal bosons α_k and β_k under the condition $\langle S_z\rangle=0$. To calculate physical quantities, it is necessary to evaluate the expectation values such as $\langle a_i^\dagger b_j\rangle$, $\langle a_i a_j\rangle$ and so on. Using the assumption of diagonal density matrix, we obtain

$$\langle a_l^\dagger b_j\rangle=\langle a_l b_j^\dagger\rangle=0,\ \langle a_l a_l\rangle=\langle a_l^\dagger a_l^\dagger\rangle=0,$$
$$\langle b_j b_m\rangle=\langle b_j^\dagger b_m^\dagger\rangle=0,$$
$$\langle a_l^\dagger a_l\rangle=f(r_l-r_l)-\frac{1}{2}\delta_{ll},$$
$$\langle b_j^\dagger b_m\rangle=f(r_j-r_m)-\frac{1}{2}\delta_{jm},$$
$$\langle a_l b_j\rangle=\langle a_l^\dagger b_j^\dagger\rangle=g(r_l-r_j),$$

where

$$f(r)=\frac{2}{N}\sum_k\cosh 2\theta_k\exp(-ik\cdot r)\left(n_k+\frac{1}{2}\right),$$
$$g(r)=\frac{2}{N}\sum_k\sinh 2\theta_k\exp(-ik\cdot r)\left(n_k+\frac{1}{2}\right).$$

The summation runs over the first Brillouin zone of the sublattice.

Let us restrict our argument hereafter to the ground state defined by $n_k=0$. (Thus the variational parameter ε_k mentioned above does not play a role in the following). From the above expressions, the expectation value of the energy (2.3) is given as

$$E/N=\frac{1}{2}zS^2-\frac{1}{2}\sum_{\text{n.n.}}\left[S+\frac{1}{2}-f(0)+g(\rho)\right]^2$$
$$+\frac{\alpha}{2}\sum_{\text{n.n.n.}}\left[S+\frac{1}{2}-f(0)+f(\delta)\right]^2, \tag{2.4}$$

where ρ is the vector to a nearest neighbor site and δ is to a next nearest neighbor site. The condition $\langle S_z\rangle=0$ is expressed as

$$0=\langle S_z\rangle=S+\frac{1}{2}-f(0). \tag{2.5}$$

Since we are considering the ground state, minimization is carried out only for θ_k,

$$\frac{\partial}{\partial\theta_k}\left[\frac{\langle E\rangle}{4N}-\mu\langle S_l^z\rangle\right]=0, \tag{2.6}$$

where μ is the chemical potential (or the Lagrange multiplier) to be determined by the condition (2.5). From eq. (2.6), θ_k is determined as follows,

$$\tanh\theta_k=\frac{g(\rho)\gamma_k}{g(\rho)-\alpha f(\delta)(1-\gamma_k')-\mu}\equiv\eta_k\gamma_k, \tag{2.7}$$

where

$$\gamma_k=(\cos k_x+\cos k_y)/2,$$
$$\gamma_k'=\cos k_x\cos k_y.$$

Equations (2.5), (2.6) and (2.7) are summarized as a set of self-consistent equations as

$$S+\frac{1}{2}=f(0)=\frac{1}{N}\sum_k\frac{1}{\sqrt{1-\eta_k^2\gamma_k^2}},$$
$$g(\rho)=\frac{1}{N}\sum_k\exp(\mathrm{i}k\cdot\rho)\eta_k\gamma_k\frac{1}{\sqrt{1-\eta_k^2\gamma_k^2}}, \tag{2.8}$$
$$f(\delta)=\frac{1}{N}\sum_k\exp(\mathrm{i}k\cdot\delta)\frac{1}{\sqrt{1-\eta_k^2\gamma_k^2}}.$$

For given values of S and α, eq. (2.8) determines μ, $g(\rho)$ and $f(\delta)$, which make it possible to evaluate various physical quantities.

We proceed to estimate the ground-state energy expanded in the inverse power of S. Another possible path to follow is to adopt the minimum value of the energy (2.4) without expansion by $1/S$. However, it sometimes happens that the asymptotic expansion by $1/S$ yields more reliable results than the raw value of the variational energy.[13] Therefore we accept the expansion method.

First we have to estimate the S-dependence of various quantities. Similarly to the unfrustrated case,[12] the $\boldsymbol{k}=0$ mode in the summations (2.8) determines whether the system has long-range order or not. By explicitly extracting the $\boldsymbol{k}=0$ mode and taking the thermodynamic limit, eq. (2.8) is rewritten as

$$m_0=S+\frac{1}{2}-\frac{1}{2\pi^2}\int_0^\pi\frac{1}{\sqrt{1-\eta_k^2\gamma_k^2}}\,\mathrm{d}^2k, \tag{2.9a}$$
$$g(\rho)=m_0+\frac{1}{2\pi^2}\int_0^\pi\frac{\eta_k\gamma_k^2}{\sqrt{1-\eta_k^2\gamma_k^2}}\,\mathrm{d}^2k, \tag{2.9b}$$
$$f(\delta)=m_0+\frac{1}{2\pi^2}\int_0^\pi\frac{\cos k_x\cos k_y}{\sqrt{1-\eta_k^2\gamma_k^2}}\,\mathrm{d}^2k, \tag{2.9c}$$

where we assumed that η_0 is close to unity for large N

$$\eta_0=1-\frac{C}{N^2}. \tag{2.10}$$

For later convenience, we define here m_0 as

$$m_0=\sqrt{\frac{2}{C}}. \tag{2.11}$$

The present assumption of finite C amounts to the postulation of finite long-range order $m_0>0$. The possibility of vanishing long-range order will be pursued later. Equation (2.9a) determines the S-dependence of m_0, which in turn specifies the S-dependence of $g(\rho)$ and $f(\delta)$. The energy

$$E/N=-2g_1^2+2\alpha f_1^2,$$

is then able to be explicitly expanded in powers of $1/S$ as

$$E/N=-2(1-\alpha)S^2-2S(1-\alpha)-4S(I_1-\alpha I_2), \tag{2.12}$$

where I_1 and I_2 represent integrals appearing in eqs. (2.9b) and (2.9c), respectively.

The relation (2.10) is equivalent to the very small value of μ, of order N^{-2}, as verified from the definition (2.7). If μ takes a finite value in the thermodynamic limit, η_0 deviates from one, and correspondingly m_0 in eq. (2.11) vanishes. This type of behavior emerges as the solution of the set of self-consistent equations

$$g(\rho)=\frac{1}{2\pi^2}\int_0^\pi\frac{\eta_k\gamma_k^2}{\sqrt{1-\eta_k^2\gamma_k^2}}\,\mathrm{d}^2k$$
$$f(\delta)=\frac{1}{2\pi^2}\int_0^\pi\frac{\gamma_k}{\sqrt{1-\eta_k^2\gamma_k^2}}\,\mathrm{d}^2k \tag{2.13}$$

with

$$\eta_k^{-1}=1-\alpha u+\alpha u\cos k_x\cos k_y-\tilde{\mu}, \tag{2.14}$$

where

$$u=f(\delta)/g(\rho), \tag{2.15}$$

and

$$\tilde{\mu}=\mu/g(\rho).$$

Equations (2.13), (2.14) and (2.15) determine $\tilde{\mu}$ and u for given values of α and S, the latter of which controls the problem through the relation

$$S+\frac{1}{2}=\frac{1}{2\pi^2}\int_0^\pi\frac{\mathrm{d}^2k}{\sqrt{1-\eta_k^2\gamma_k^2}}. \tag{2.16}$$

If these equations have appropriate solutions, the energy calculated from $g(\rho)$ and $f(\delta)$ in

eq. (2.13) should be compared with that from eq. (2.9). The solution with lower energy gives the true ground state. Results of numerical evaluation will be given in the next section.

2.2 *Four-sublattice Néel state*

Quite similar procedures as in the two-sublattice case can be taken also in the four-sublattice problem except that four types of bosons should be introduced instead of two. As the starting classical spin configuration, we accept the collinear state ($\psi=\pi$ in Fig. 1). Although the classical system has infinite and continuous degeneracy as mentioned before, we use only the collinear state since quantum fluctuations generally remove continuous classical degeneracy, favoring collinear states.[14] The Dyson-Maleev transformation now reads

$$
\begin{aligned}
&S_l^-=a_l^\dagger,\ S_l^+=(2S-a_l^\dagger a_l)a_l,\ S_l^z=S-a_l^\dagger a_l\ (l\in \text{A sublattice})\\
&S_p^-=-b_p,\ S_p^+=-b_p^\dagger(2S-b_p^\dagger b_p),\ S_p^z=-S+b_p^\dagger b_p\ (p\in \text{B sublattice})\\
&S_{l'}^-=-c_{l'},\ S_{l'}^+=-c_{l'}^\dagger(2S-c_{l'}^\dagger c_{l'}),\ S_{l'}^z=-S+c_{l'}^\dagger c_{l'}\ (l'\in \text{C sublattice})\\
&S_{m'}^-=d_{m'}^\dagger,\ S_{m'}^+=(2S-d_{m'}^\dagger d_{m'})d_{m'},\ S_{m'}^z=S-d_{m'}^\dagger d_{m'}\ (m'\in \text{D sublattice}).
\end{aligned}
$$

The Hamiltonian (2.1) is expressed in terms of bosons, and then a Bogoliubov transformation is applied:

$$
\begin{aligned}
&\sqrt{2}\,a_k=\alpha_k\cosh\theta_k+\beta_k^\dagger\sinh\theta_k+\gamma_k\cosh\phi_k+\delta_k^\dagger\sinh\phi_k,\\
&\sqrt{2}\,b_k=\alpha_k^\dagger\sinh\theta_k+\beta_k\cosh\theta_k+\gamma_k^\dagger\sinh\phi_k+\delta_k\cosh\phi_k,\\
&\sqrt{2}\,c_k=\alpha_k^\dagger\sinh\theta_k+\beta_k\cosh\theta_k-\gamma_k^\dagger\sinh\phi_k-\delta_k\cosh\phi_k,\\
&\sqrt{2}\,d_k=\alpha_k\cosh\theta_k+\beta_k^\dagger\sinh\theta_k-\gamma_k\cosh\phi_k-\delta_k^\dagger\sinh\phi_k.
\end{aligned}
$$

The ground state is assumed to be the vacuum of the transformed bosons α_k, β_k, γ_k and δ_k. The energy is minimized with respect to the angles θ_k and ϕ_k under the restriction of vanishing sublattice magnetization. For vanishingly small values of the chemical potential μ, the results are summarized in the following set of self-consistent equations:

$$
\eta_{1k}=\frac{2\alpha\gamma_k'+\gamma_{ky}u}{2\alpha+u-v(1-\gamma_{kx})},\quad \eta_{2k}=\frac{-2\alpha\gamma_k'+\gamma_{ky}u}{2\alpha+u-v(1+\gamma_{kx})},\tag{2.17}
$$

where

$$
u=\frac{B(\rho)}{A(\delta)},\quad v=\frac{C(\rho)}{A(\delta)},\tag{2.18}
$$

with

$$
\begin{aligned}
A(\delta)&=\frac{1}{N}\sum_k\exp(-\mathrm{i}k\cdot\delta)\left(\frac{\eta_{1k}}{\sqrt{1-\eta_{1k}^2}}-\frac{\eta_{2k}}{\sqrt{1-\eta_{2k}^2}}\right),\\
B(\rho)&=\frac{1}{N}\sum_k\exp(-\mathrm{i}k\cdot\rho)\left(\frac{\eta_{1k}}{\sqrt{1-\eta_{1k}^2}}+\frac{\eta_{2k}}{\sqrt{1-\eta_{2k}^2}}\right),\\
C(\rho)&=\frac{1}{N}\sum_k\exp(-\mathrm{i}k\cdot\rho)\left(\frac{1}{\sqrt{1-\eta_{1k}^2}}-\frac{1}{\sqrt{1-\eta_{2k}^2}}\right),
\end{aligned}\tag{2.19}
$$

and

$$
\gamma_{kx}=\cos k_x,\quad \gamma_{ky}=\cos k_y.
$$

The summation runs over the first Brillouin zone of one of the four sublattices. The condition of vanishing sublattice magnetization is written as

$$
m_0=S+\frac{1}{2}-\frac{1}{N}\sum_{k\neq 0}\left(\frac{1}{\sqrt{1-\eta_{1k}^2}}+\frac{1}{\sqrt{1-\eta_{2k}^2}}\right).\tag{2.20}
$$

The energy is expressed as

$$E/N=-2\alpha A(\delta)^2-B(\rho)^2+C(\rho)^2. \quad (2.21)$$

The expansion by $1/S$ is possible using eq. (2.20), similarly to the two-sublattice case. The expanded form of the energy reads

$$E/N=-2\alpha S^2+2S\{J_4-J_3-\alpha(1-2J_1+2J_2)\}, \quad (2.22)$$

where

$$J_1=\frac{1}{\pi^2}\int_0^{\pi/2}\left(\frac{1}{\sqrt{1-\eta_{1k}^2}}+\frac{1}{\sqrt{1-\eta_{2k}^2}}\right)\mathrm{d}^2k,$$

$$J_2=\frac{1}{\pi^2}\int_0^{\pi/2}\left(\frac{\eta_{1k}}{\sqrt{1-\eta_{1k}^2}}-\frac{\eta_{2k}}{\sqrt{1-\eta_{2k}^2}}\right)\times\cos k_x\cos k_y\,\mathrm{d}^2k,$$

$$J_3=\frac{1}{\pi^2}\int_0^{\pi/2}\left(\frac{\eta_{1k}}{\sqrt{1-\eta_{1k}^2}}+\frac{\eta_{2k}}{\sqrt{1-\eta_{2k}^2}}\right)\cos k_y\,\mathrm{d}^2k,$$

$$J_4=\frac{1}{\pi^2}\int_0^{\pi/2}\left(\frac{1}{\sqrt{1-\eta_{1k}^2}}-\frac{1}{\sqrt{1-\eta_{2k}^2}}\right)\cos k_x\,\mathrm{d}^2k.$$

Equations (2.17) and (2.18) determine u and v for a given α. The order parameter m_0 and the energy are then evaluated for a given S by eqs. (2.20) and (2.22).

The solution with nonvanishing μ is derived similarly. We simply write down the set of self-consistent equations:

$$\eta_{1k}=\frac{2\alpha\gamma_k+\gamma_{ky}u}{2\alpha+u-v(1-\gamma_{kx})+\mu}, \quad (2.23a)$$

$$\eta_{2k}=\frac{-2\alpha\gamma_k+\gamma_{ky}u}{2\alpha+u-v(1+\gamma_{kx})+\mu}, \quad (2.23b)$$

$$S=\frac{1}{\pi^2}\int_0^{\pi/2}\left(\frac{1}{\sqrt{1-\eta_{1k}^2}}+\frac{1}{\sqrt{1-\eta_{2k}^2}}\right)\mathrm{d}^2k-\frac{1}{2}, \quad (2.24)$$

where u, v, A, B and C satisfy the same relations as before, eqs. (2.17), (2.18) and (2.19). These equations (2.23) and (2.24) determine μ, u and v for given α and S. The energy (2.21) thus obtained should be compared with the corresponding energy of nonvanishing m_0 to find out the true ground state.

§3. Solution of the Self-Consistent Equations

We have numerically solved the self-consistent equations derived in the previous section for various values of α and S. We have found that the unphysical divergences at $\alpha=0.5$ appearing in the naive spin wave theory is removed for any finite S. Actually, for finite S, the two-sublattice relations (2.9) have solutions even for α a little larger than 0.5. Solution of eq. (2.9) yields the region of finite long-range order ($m_0>0$) beyond which m_0 becomes negative. Line A of Fig. 2 represents the boundary ($m_0\to 0$) of this region. Equation (2.11) requires that we should restrict ourselves to the region below line A. We have also found that eqs. (2.13) to (2.16) (corresponding to $m_0=0$) do not have solutions below line A. This implies that the two-sublattice Néel order exists at least as a quasi-stable state below A.

As for the four-sublattice case, eqs. (2.17) to (2.20) with nonvanisheing long-range order have solutions for α larger than some $\alpha_0(S)>1/2$. For example, α_0 is 0.56 when $S=1/2$. The vanishing-order equations (2.23) and (2.24) have solutions for $S\gtrsim 1/2$ in a region ($\alpha\geq\alpha_1(S)>1/2$) larger than the above-mentioned case $\alpha\geq\alpha_0$ (i.e., $\alpha_0>\alpha_1$). An example is $\alpha_1=0.55$ for $S=1/2$. However, in the region

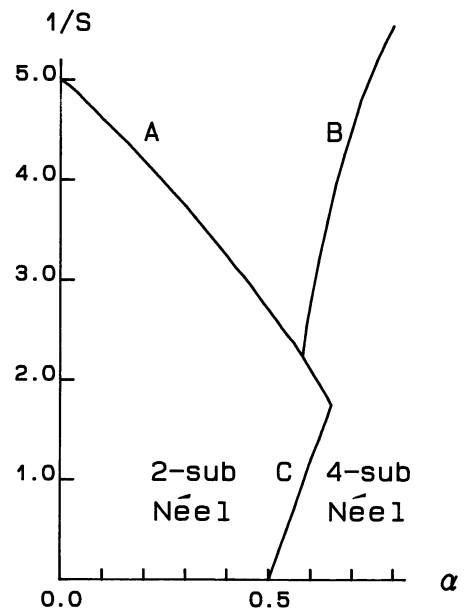

Fig. 2. Phase diagram of the present system at $T=0$ derived from the modified spin wave theory. The two-sublattice Néel state exists below line A and the four-sublattice counterpart does below B. The two types of Néel states coexist at the boundary C.

in which either only the vanishing-order equations have solutions or they have lower enrgy than the nonvanishing-order equation, the ground state enegy of the four-sublattice equation exceeds that of the two-sublattice. Therefore, in any event, the four-sublattice Néel state is not superseded by the non-ordered state, rather by the two-sublattice Néel state. Similarly to the two-sublattice case, the limit of existence of long-range order has been determined by the condition $m_0 \to 0$ in the finite-order equations (2.17) to (2.20). The result is depicted in Fig. 2 as line B.

The energy of the two-sublattice Néel state is equal to that of the four-sublattice state on line C. Therefore, in the region below A and above, C, the system has two-sublattice Néel order while the order is of the four-sublattice type in the region on the right-hand side. No long-range order of the Néel type exists above A and B.

For $S \geq 1$, the system undergoes a simple first order phase transition at $\alpha \gtrsim 1/2$. The situation is a little more complicated if $S=1/2$. As α is increased beyond 0.5, the solution of the two-sublattice equation (2.9) ceases to exist before the energy of the two-sublattice state exceeds that of the four-sublattice state. Therefore the energy jumps to a larger value as one crosses line A to enter the four-sublattice region.

§4. Conclusion

As shown in Fig. 2, we have found that the Néel-type long-range order is not destroyed at any value of α as long as $S \geq 1/2$. Either the two-sublattice or the four-sublattice order exists in spite of strong frustration around $\alpha=0.5$. Of course, the present approximate calculations are not expected to yield quantitatively reliable results; for instance, the limit of the exstence of long-range order (lines A and B in Fig. 2) may actually be located below $S=1/2$ around $\alpha=0.5$. If this is the case, the long-range order is destroyed in the corresponding region of α for $S=1/2$. Nevertheless, one should notice that the qualitative feature of the phase diagram is quite different from that of the naive spin wave theory. In the latter case, the non-ordered phase exists for any large but finite S if α is close to 0.5. The present modified spin wave theory predicts existence of long-range order for sufficiently large S at any α. This difference originates in the successuful removal of unphysical divergences at $\alpha=0.5$ in the present treatment. Although only the spin-1/2 system is predicted to undergo a phase transition of peculiar type with a jump in energy as explained in the previous section, we do not intend to emphasize this difference according to S in the small-S region because of the above-mentioned reasons. Our point is in the qualitative difference of the present phase diagram from the naive spin wave theory in the region close to $\alpha=0.5$ and large S.

Another noteworthy aspect of the phase diagram is the persistence of the two-sublattice Néel state beyond $\alpha=0.5$. Although the classical energy of the two-sublattice state is higher than the four-sublattice counterpart for $\alpha>0.5$, quantum fluctuations work as a larger stabililizing perturbation of the former state than in the latter.

Our conclusion apparently conflicts with some of other theories based on different approaches. One of the most reliable of such would be the perturbation expansion from the pure dimer state by Gelfand *et al.*[15] They predict that a dimerized phase exists in a finite range of α near 0.5 for $S=1/2$. Since, after all, both of our theory and theirs are approximate on different grounds, it seems hardly possible to judge decisively which is more reliable than the other. Further investigation should be continued.

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