Variational estimation of the ground-state energy of the frustrated Heisenberg model

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By using the variational spin-wave theory introduced by R. Kubo, we rigorously evaluate an upper bound on the ground-state energy of the antiferromagnetic Heisenberg model with the next-nearest-neighbor interactions on the simple-cubic and the square lattices. We employ two types of trial wave functions: One assumes the usual Néel-type ordering and the other assumes so-called strip-type antiferromagnetic ordering with collinear sublattice magnetizations. The obtained upper bound is employed to prove the existence of Néel-type long-range order in the weakly frustrated region.

I. INTRODUCTION

Quantum effects in antiferromagnetic spin systems are recently attracting intense interest. Once frustrations are introduced to a spin system, the properties of the system may change drastically. The interplay of quantum effects and frustrations is also a challenging problem to theorists. We consider in this paper the antiferromagnetic Heisenberg (AFH) model on the square or the simple-cubic lattice with both nearest-neighbor (NN) and next-nearest-neighbor (NNN) interactions, which is a typical example of frustrated quantum spin systems. The ground state of this system changes its character according to the strength λ (≥ 0 throughout this paper) of the NNN interactions. For small λ, the ground state will be the usual Néel state, where the NNN interactions incorporate frustrations. On the other hand, for large λ, another type of antiferromagnetic ordering will be realized as a result of the prevailing NNN interactions, and in this case the NN interactions will be the cause of the frustrations [in three dimensions (3D) the situation is rather complicated because the NNN interactions are frustrated by themselves]. For intermediate λ, there should be a transition (or transitions) between them, whose nature we still do not understand well and which is now under active investigation.[1-8]

In the mean-field approximation, a transition occurs at $\lambda=\lambda_0\equiv 1/[2(\nu-1)]$, where ν (=2 or 3) denotes the dimensionality of the lattice. For $\lambda>\lambda_0$, the mean-field ground state has a continuous degeneracy besides the rotational symmetry of the total spin. On the square lattice, two sublattices order antiferromagnetically in themselves and the mean-field energy is independent of the angle between the staggered magnetizations of the two sublattices. On the simple-cubic lattice, the spin structure is a mixture of the three strip-type orderings with staggered magnetizations perpendicular to each other. The energy does not depend on the ratio of three components of the staggered magnetization each with wave vectors $(0,\pi,\pi)$, $(\pi,0,\pi)$, and $(\pi,\pi,0)$. At $\lambda=\lambda_0$, all the states with vanishing total spins on unit plaquettes are degenerate. In the linear spin-wave theory, the continuous degeneracy at $\lambda>\lambda_0$ is lifted and the state with collinear spin structure is stabilized.[9] Let us call this state a "strip state" since spins are aligned parallel along one of the lattice axes.[3] In the plane (the line for $\nu=2$) perpendicular to this axis, spins are ordered antiferromagnetically. At $\lambda\sim\lambda_0$, the mean-field ground state, assuming finite staggered magnetization, is not justified since the reduction of the staggered magnetization due to spin-wave fluctuations exceeds the assumed value. So Chandra and Doucot[1] argued that the spin liquid state appears even for large S in such a region at $\lambda\sim\lambda_0$ on the square lattice. The ground state with the long-range dimer order was suggested in this region by using a perturbational calculation[2] as well as a finite-size study.[3] On the other hand, Wen, Wilczek, and Zee[4] discussed the possible appearance of a chiral spin state which violates P and T symmetry at $\lambda\gtrsim 0.5$. The system was studied also by exactly diagonalizing finite-size clusters.[3,5,6]

In a previous work,[10] we established in this system an inequality on the Duhamel spin two-point function, extending the method by Dyson, Lieb, and Simon (DLS).[11] That inequality, called "Gaussian domination," holds at $\lambda\leq\lambda_0$. Using the method of infrared bounds,[11,12] which was established for quantum systems by DLS, we proved rigorously that Néel-type long-range order (LRO) exists in the ground state at $0\leq\lambda<\lambda_c(S)$. Estimates for the critical value $\lambda_c(S)$ were given, except for the $S=\frac{1}{2}$ model on the square lattice, where the existence of LRO is still to be proved even for the case without frustration.[13] As will be shown in Sec. V, an upper bound on the ground-state energy is necessary in the proof. It is desirable to have a good upper bound so that a large value of $\lambda_c(S)$ is obtained. This motivation has led us to the present work, in which we calculate the ground-state energy by using a variational spin-wave theory.[14] A preliminary account of this work has been presented in Ref. 15.

Although there are many theories which are called variational, those which give rigorous bounds on the energy in the thermodynamic limit are few. Many theories where the energy is evaluated analytically include some uncontrolled approximations in their calculations.[16,17] Recently, many attempts where the energy is evaluated in numerical ways appeared.[18] Though the energy obtained in these methods seems to be quite accurate, they include finite-size effects and/or statistical errors and cannot be regarded as upper bounds.

The variational spin-wave theory which we employ was introduced by Kubo[14] to evaluate the energy of the AFH model on the square and bcc lattices. In this theory we take the ground-state wave function of a spin-wave Hamiltonian as a trial function. The expectation value of the energy for this trial function is evaluated without approximation to lead to an analytic expression. The expression includes infinite-series expansions and parameters, which are defined as integrations. If we evaluate the infinite series as partial sums, the bounds on the errors can be rigorously evaluated and numerical integrations for the parameters can be done quite precisely. Though the obtained energy may not be called excellent as an approximation in view of the present standard, it shows a considerable improvement from the mean-field value. On the other hand, the spin-wave spectrum which minimizes the energy is revealed to have a finite-energy gap, even though the state has LRO. This contradicts Goldstone's theorem,[19] and we cannot put much physical meaning in either the state itself or the spin-wave spectrum. The method, however, is useful as it gives a rigorous bound and also can be easily applied to any type of ordering and/or to various spin systems such as the *XXZ* model, and so on.

The plan of the paper is as follows. In Sec. II we briefly review the formulation of the variational spin-wave theory based on the usual Néel-type ordering. The results are shown in Sec. III. In Sec. IV we present the theory based on the strip state with its results. In Sec. V we examine the existence of Néel-type LRO using the results obtained in Sec. III. The last section is devoted to a summary and discussion.

II. VARIATIONAL SPIN-WAVE THEORY

The key idea of the variational spin-wave theory is to transform a spin Hamiltonian into an equivalent boson Hamiltonian. This is done by employing a modified Holstein-Primakoff transformation,[14] which is given as

$$S_\alpha^z = S - [n_\alpha] \,,\quad S_\alpha^+ = \sqrt{2S} f_\alpha a_\alpha \,,\quad S_\alpha^- = \sqrt{2S} a_\alpha^\dagger f_\alpha, \text{ on the } A \text{ sublattice} ; \tag{2.1a}$$

and

$$S_\beta^z = -S + [n_\beta] \,,\quad S_\beta^+ = \sqrt{2S} b_\beta^\dagger f_\beta \,,\quad S_\beta^- = \sqrt{2S} f_\beta b_\beta, \text{ on the } B \text{ sublattice} ; \tag{2.1b}$$

where a_α (b_β) is a Bose operator on the A (B) sublattice, $n_\alpha = a_\alpha^\dagger a_\alpha$ ($n_\alpha = b_\alpha^\dagger b_\alpha$), and

$$f_\alpha = f(n_\alpha) \,. \tag{2.2}$$

The function $f(i)$ of an integer i is defined as

$$f(i) \equiv \left[1 - \frac{[i]}{2S}\right]^{1/2} \left[\frac{1+[i]}{1+i}\right]^{1/2} , \tag{2.3}$$

where

$$[i] \equiv i \bmod (2S+1) \,. \tag{2.4}$$

The symbol $[n_\alpha]$ means that the definition (2.4) of [ ] applies to the eigenvalues of the operator n_α. This transformation changes a spin operator of the magnitude S to an operator in a boson space, which may be represented by a direct sum of the infinite number of the original $(2S+1)$-dimensional spin matrices. Then the Hamiltonian expressed with these "spin" operators is represented by an infinite matrix, which is a direct sum of the infinite number of the original Hamiltonian matrices. Therefore, the spectrum of the transformed boson Hamiltonian is the same as the original one, though every state is infinitely degenerate. We are able to bound the ground-state energy of the boson Hamiltonian, i.e., that of the original spin Hamiltonian, from above by using a variational wave function. On the other hand, the relation between the ground-state energy of the boson Hamiltonian and the original spin one is not known if a conventional Holstein-Primakoff or Dyson-Maleev transformation is employed.

The Hamiltonian we consider is

$$H = \sum_{\alpha\in\Lambda} \sum_{m=1}^{\nu} \mathbf{S}_\alpha \cdot \mathbf{S}_{\alpha+\delta_m} + \lambda \sum_{\alpha\in\Lambda} \sum_{(m,n)} \mathbf{S}_\alpha \cdot (\mathbf{S}_{\alpha+\delta_m+\delta_n} + \mathbf{S}_{\alpha+\delta_m-\delta_n}) \,, \tag{2.5}$$

where Λ denotes the square ($\nu=2$) or the simple-cubic ($\nu=3$) lattice with periodic boundary conditions containing $|\Lambda|$ lattice sites and $\mathbf{S}_\alpha$ is a spin operator with the magnitude S at the site α on Λ. The lattice constant is assumed to be unity, and $\boldsymbol{\delta}_m$ denotes a unit vector in the mth direction. $\sum_{(m,n)}$ means a sum over pairs of two different directions. Throughout this paper the parameter λ is assumed positive, and so the NN and NNN interactions compete with each other.

For $\lambda \le \lambda_0$, the ground state of this system has Néel-type LRO according to the mean-field theory. So we construct first a variational wave function based on the Néel state as the starting classical ground state. We examine another wave function in Sec. IV.

Starting from the usual Néel state, the Hamiltonian is transformed to a boson Hamiltonian as

$$H = -\nu[1-(\nu-1)\lambda]|\Lambda|S^2 + 2\nu[1-(\nu-1)\lambda]S \sum_{\alpha\in\Lambda} [n_\alpha] - \sum_{\alpha\in\Lambda} \sum_{m=1}^{\nu} [n_\alpha][n_{\alpha+\delta_m}] + \lambda \sum_{\alpha\in\Lambda} \sum_{(m,n)} [n_\alpha]([n_{\alpha+\delta_m+\delta_n}] + [n_{\alpha+\delta_m-\delta_m}])$$

$$+S\left[\sum_{\alpha\in A}\left[\sum_{m=1}^{\nu} f_\alpha a_\alpha f_{\alpha+\delta_m} b_{\alpha+\delta_m} + \lambda \sum_{(m,n)} f_\alpha a_\alpha a^\dagger_{\alpha+\delta_m+\delta_n} f_{\alpha+\delta_m+\delta_n}\right]\right.$$

$$\left. + \sum_{\beta\in B}\left[\sum_m f_\beta b_\beta f_{\beta+\delta_m} a_{\beta+\delta_m} + \lambda \sum_{(m,n)} f_\beta b_\beta b^\dagger_{\alpha+\delta_m-\delta_n} f_{\alpha+\delta_m-\delta_n}\right] + \text{H.c.}\right] , \tag{2.6}$$

where $\sum_{\alpha\in A}$ and $\sum_{\beta\in B}$ denote sums over α on the A sublattice and β on the B sublattice, respectively.

As was shown in Ref. 14, the expectation value of H for the ground-state wave function of a Hamiltonian described by bilinear forms of Bose operators can be calculated exactly, and the result is expressed as follows:

$$\langle H\rangle_0 = -\nu|\Lambda|S^2\left[[1-(\nu-1)\lambda]\left[1-\frac{1}{S}[AG(A)+BG(B)]\right] + \sum_{m=1}^{\nu}\left[\frac{1}{S^2}F_{0m} - \frac{2}{S}F_{1m}\right]\right.$$

$$\left. -\lambda\sum_\Delta\left[\frac{1}{S^2}(G^A_{0\Delta}+G^B_{0\Delta}) + \frac{2}{S}(G^A_{1\Delta}+G^B_{1\Delta})\right]\right] , \tag{2.7}$$

where

$$G(x) = 1 - \frac{(2S+1)x^{2S}}{(1+x)^{2S+1} - x^{2S+1}} , \tag{2.8}$$

$$F_{0m} = AG(A)BG(B) + C_m C_m^*\left[1-[1-G(A)]^2(1+A^{-1})^{2S} - [1-G(B)]^2(1+B^{-1})^{2S}\right.$$

$$\left. + \sum_{\omega,\omega'}\frac{\omega}{1+A-\omega A}\,\frac{\omega'}{1+B-\omega' B}\,\frac{1}{(1+A-\omega A)(1+B-\omega' B) - (\omega-1)(\omega'-1)C_m C_m^*}\right] , \tag{2.9}$$

$$F_{1m} = C_m \sum_{i,j,k=0}^{\infty} f(i+j)f(i+k)\frac{(i+j+k+1)!}{i!j!k!}[A(1+B) - C_m C_m^*]^k [B(1+A) - C_m C_m^*]^j$$

$$\times (C_m C_m^* - AB)^i [(1+A)(1+B) - C_m C_m^*]^{-2-i-j-k} , \tag{2.10}$$

$$G^A_{0\Delta} = F_{0m}(B \Longrightarrow A,\ C_m \Longrightarrow A_\Delta) , \tag{2.11a}$$

$$G^B_{0\Delta} = F_{0m}(A \Longrightarrow B,\ C_m \Longrightarrow B_\Delta) , \tag{2.11b}$$

$$G^A_{1\Delta} = F_{1m}(B \Longrightarrow A,\ C_m \Longrightarrow A_\Delta) , \tag{2.12a}$$

and

$$G^B_{1\Delta} = F_{1m}(A \Longrightarrow B,\ C_m \Longrightarrow B_\Delta) . \tag{2.12b}$$

The vectors pointing to NNN sites are denoted by Δ ($\equiv \delta_m \pm \delta_n$), and $\sum_\Delta$ means a sum over them. The symbol ω or ω' denotes one of the $(2S+1)$th roots of unity, and $\sum_\omega$ denotes the sum over the roots. The expression above is dependent on the variational parameters through A, B, C_m, A_Δ, and B_Δ, which are defined using the Fourier transforms of the Bose operators

$$a_{\mathbf{q}} = \left[\frac{2}{|\Lambda|}\right]^{1/2} \sum_{\alpha\in A} e^{-i\mathbf{q}\cdot\alpha} a_\alpha , \tag{2.13a}$$

and

$$b_{\mathbf{q}} = \left[\frac{2}{|\Lambda|}\right]^{1/2} \sum_{\alpha\in B} e^{i\mathbf{q}\cdot\alpha} b_\alpha , \tag{2.13b}$$

as

$$A = \frac{2}{|\Lambda|}\sum_{\mathbf{q}}\langle a^\dagger_{\mathbf{q}} a_{\mathbf{q}}\rangle_0 ,$$

$$C_m = \frac{2}{|\Lambda|}\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\delta_m}\langle a_{\mathbf{q}} b_{\mathbf{q}}\rangle_0 , \tag{2.14}$$

$$A_\Delta = \frac{2}{|\Lambda|}\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\Delta}\langle a^\dagger_{\mathbf{q}} a_{\mathbf{q}}\rangle_0 ,$$

and B (B_Δ) is given by replacing $a_{\mathbf{q}}$ by $b_{\mathbf{q}}$ in A (A_Δ). We assumed the translational and the inversion symmetry. The symbol $\sum_{\mathbf{q}}$ means a sum over wave vectors in the reduced Brillouin zone. For derivation of these formulas, readers should refer to Ref. 14. We note, however, that our expression does not completely agree with that obtained in Ref. 14, which leads to a different value of the energy from Ref. 14 at $\lambda=0$.[20]

III. RESULTS OF THE THEORY BASED ON THE NÉEL STATE

As a trial wave function, we employ the ground-state wave function $\Psi_0(\alpha,\delta)$ of the variational Hamiltonian

$H_{\rm var}$, which is written as

$$H_{\rm var}=2\nu S\sum_{\mathbf{q}}[1-(\nu-1)\delta(1-\eta_{\mathbf{q}})](a_{\mathbf{q}}^{\dagger}a_{\mathbf{q}}+b_{\mathbf{q}}^{\dagger}b_{\mathbf{q}})$$
$$+2\nu\alpha S\sum_{\mathbf{q}}\gamma_{\mathbf{q}}(a_{\mathbf{q}}b_{\mathbf{q}}+a_{\mathbf{q}}^{\dagger}b_{\mathbf{q}}^{\dagger})\ , \qquad (3.1)$$

where

$$\gamma_{\mathbf{q}}=\frac{1}{2\nu}\sum_{m=1}^{\nu}(e^{i\mathbf{q}\cdot\boldsymbol{\delta}_m}+e^{-i\mathbf{q}\cdot\boldsymbol{\delta}_m}) \qquad (3.2a)$$

and

$$\eta_{\mathbf{q}}=\frac{1}{2\nu(\nu-1)}\sum_{\Delta}e^{i\mathbf{q}\cdot\Delta}\ . \qquad (3.2b)$$

$H_{\rm var}$ is chosen to have the same wave-vector dependence with the conventional spin-wave Hamiltonian which is obtained from Eq. (2.6) except for the variational parameters α and δ. We restrict ourselves to $0\le\alpha\le1$ and $0\le\delta\le1/2(\nu-1)$. When $\alpha=1$ and $\delta=\lambda$, $H_{\rm var}$ coincides with the usual spin-wave Hamiltonian. From the assumed symmetries, $\langle a^{\dagger}a\rangle=\langle b^{\dagger}b\rangle$, and $C_m(A_\Delta)$ does not depend on m (Δ); we obtain

TABLE I. Variational parameters α and δ, which minimize the energy for the (a) two- and (b) three-dimensional frustrated AFH model with $S=\frac{1}{2}$ together with the minimized energy which is normalized by the mean-field energy at $\lambda=0$. The energy of $S=1$ model is also tabulated. These values are obtained by the variational spin-wave theory based on the Néel state.

(a)

λ	0.0	0.02	0.04	0.06	0.08	0.10	0.12	
α	0.890	0.890	0.889	0.888	0.887	0.887	0.886	
δ	0.6×10^{-3}	0.014	0.028	0.041	0.056	0.069	0.083	
$E(S=\frac{1}{2})$	−1.279	−1.261	−1.243	−1.226	−1.208	−1.191	−1.117	
$E(S=1)$	−1.153	−1.135	−1.116	−1.098	−1.080	−1.062	−1.044	
λ	0.14	0.16	0.18	0.20	0.22	0.24	0.26	0.28
α	0.885	0.885	0.883	0.883	0.882	0.881	0.880	0.879
δ	0.096	0.109	0.123	0.136	0.149	0.162	0.175	0.188
$E(S=\frac{1}{2})$	−1.156	−1.138	−1.121	−1.104	−1.087	−1.070	−1.053	−1.035
$E(S=1)$	−1.026	−1.008	−0.990	−0.972	−0.954	−0.936	−0.919	−0.901
λ	0.30	0.32	0.34	0.36	0.38	0.40	0.42	0.44
α	0.878	0.877	0.875	0.874	0.873	0.871	0.870	0.869
δ	0.201	0.213	0.238	0.251	0.263	0.275	0.287	0.299
$E(S=\frac{1}{2})$	−1.019	−1.002	−0.985	−0.968	−0.952	−0.933	−0.919	−0.902
$E(S=1)$	−0.884	−0.866	−0.849	−0.832	−0.915	−0.798	−0.781	−0.764
λ	0.46	0.48	0.50	0.52	0.54	0.56	0.58	0.60
α	0.868	0.866	0.876	0.865	0.863	0.862	0.860	0.859
δ	0.311	0.323	0.226	0.334	0.345	0.357	0.368	0.379
$E(S=\frac{1}{2})$	−0.886	−0.870	−0.854	−0.838	−0.822	−0.806	−0.791	−0.775
$E(S=1)$	−0.748	−0.731	−0.715	−0.699	−0.683	−0.667	−0.652	−0.637

(b)

λ	0.0	0.02	0.04	0.06	0.08	0.10	0.12		
α	0.922	0.920	0.918	0.916	0.914	0.912	0.910		
δ	0.1×10^{-3}	0.015	0.031	0.046	0.061	0.076	0.090		
$E(S=\frac{1}{2})$	−1.181	−1.114	−1.110	−1.075	−1.040	−1.005	−0.971		
$E(S=1)$	−1.096	−1.059	−1.022	−0.985	−0.949	−0.913	−0.877		
λ	0.14	0.16	0.18	0.20	0.22	0.24	0.25	0.26	0.28
α	0.907	0.905	0.902	0.899	0.896	0.892	0.891	0.889	0.885
δ	0.105	0.119	0.133	0.146	0.159	0.172	0.179	0.185	0.197
$E(S=\frac{1}{2})$	−0.937	−0.903	−0.870	−0.837	−0.805	−0.773	−0.785	−0.742	−0.711
$E(S=1)$	−0.841	−0.806	−0.772	−0.737	−0.704	−0.671	−0.655	−0.639	−0.608

$$\langle H\rangle_0=-\nu|\Lambda|S^2\left[[1-(\nu-1)\lambda]\left[1-\frac{2}{S}AG(A)\right]+\left[\frac{1}{S^2}F_0-\frac{2}{S}F_1\right]-\lambda(\nu-1)\left[\frac{1}{S^2}G_0+\frac{2}{S}G_1\right]\right], \quad (3.3)$$

where F_0, F_1, G_0, and G_1 are given by putting $A=B$, $C\equiv C_m=C_m^*$, and $A'\equiv A_\Delta=A_\Delta^*$ in Eqs. (2.9)–(2.12). The parameters A, C, and A' are expressed in terms of integrations as

$$A=-\frac{1}{2}+\frac{1}{2(2\pi)^\nu}\int_{-\pi}^{\pi}\frac{\Lambda_{\mathbf{k}}}{(\Lambda_{\mathbf{k}}^2-\alpha^2\gamma_{\mathbf{k}}^2)^{1/2}}d^\nu k, \quad (3.4a)$$

$$C=-\frac{1}{2(2\pi)^\nu}\int_{-\pi}^{\pi}\frac{\alpha\gamma_{\mathbf{k}}^2}{(\Lambda_{\mathbf{k}}^2-\alpha^2\gamma_{\mathbf{k}}^2)^{1/2}}d^\nu k, \quad (3.4b)$$

and

$$A'=\frac{1}{2(2\pi)^\nu}\int_{-\pi}^{\pi}\frac{\eta_{\mathbf{k}}\Lambda_{\mathbf{k}}}{(\Lambda_{\mathbf{k}}^2-\alpha^2\gamma_{\mathbf{k}}^2)^{1/2}}d^\nu k, \quad (3.4c)$$

where

$$\Lambda_{\mathbf{k}}\equiv 1-(\nu-1)\delta(1-\eta_{\mathbf{k}}). \quad (3.5)$$

Now we examine the infinite series F_1 and G_1. From Eq. (3.4), the following inequalities for A, C, and A' hold:

$$A>|A'|\geq 0, \quad A+1>-C>A, \quad A(A+1)>C^2. \quad (3.6)$$

Numerical estimation reveals that $A'>0$ for parameters considered. Taking into account of these inequalities, we easily see that F_1 is a convergent negative term series (see the Appendix). The situation for G_1 is more complicated since it is revealed to be an alternating-term series. However, it is also absolutely convergent. If we sum only a finite number of first terms of G_1, an upper bound on the contribution from the rest of the series is easily estimated, as shown in the Appendix. So an upper bound on $\langle H\rangle_0$ is obtained by substituting upper bounds on F_1 and G_1 in Eq. (3.3).

The minimum of $\langle H\rangle_0$ in the (α,δ) plane has been found by using a computer search. The results are tabulated in Table I for $S=\frac{1}{2}$ and 1. Figure 1 displays the energy as a function of λ for $S=\frac{1}{2}$ and $\nu=2$. The energy obtained by the mean-field and linear spin-wave theories is also shown for reference. The result for $S=\frac{1}{2}$ and $\nu=3$ is displayed in Fig. 2. The present results are close to the energy $E_{\rm SW}$ by the spin-wave theory when λ is small for both $\nu=2$ and 3, but as λ increases our results continue to increase almost linearly with λ and the difference from $E_{\rm SW}$ increases. We note here that the value 1.279 at $\lambda=0$ for $\nu=2$ is slightly different from 1.294 obtained in Ref. 14. The "staggered magnetization," i.e., $S-\langle[n_\alpha]\rangle_0$, for $S=\frac{1}{2}$ ($S=1$) and $\nu=2$ is 0.428 (0.889) at $\lambda=0$ and decreases gradually to 0.390 (0.781) at $\lambda=0.6$. The magnetization is less reduced than that estimated by the spin-wave theory and persists at even $\lambda\geq\lambda_0$, where Néel-type LRO is unstable in the mean-field theory. This is due to the fact that the energy is minimized at $\alpha<1$ and $\delta<\lambda$, as shown in Table I. The spin-wave spectrum has, therefore, a finite gap for the parameters minimizing the energy.

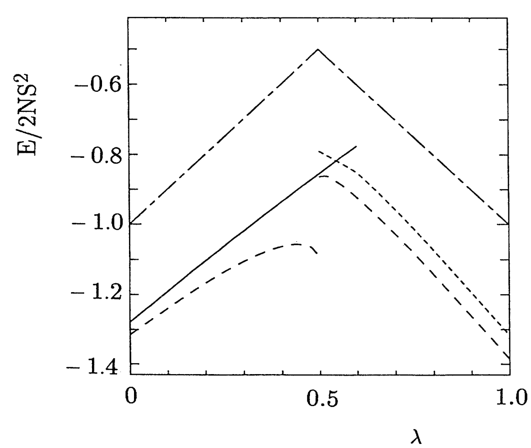

FIG. 1. Ground-state energy in two dimensions for $S=\frac{1}{2}$. The solid and dotted lines show the upper bound obtained by the variational spin-wave theory based on the Néel and strip states, respectively. The dashed line is the ground-state energy by conventional spin-wave theory. The mean-field energy is drawn as a dot-dashed line.

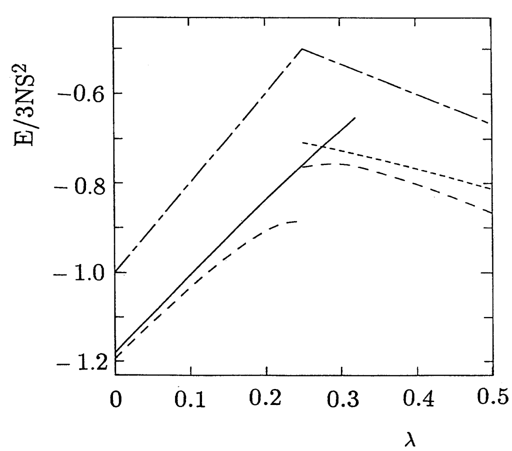

FIG. 2. Ground-state energy in three dimensions for $S=\frac{1}{2}$. The solid and dotted lines show the upper bound obtained by the variational spin-wave theory based on the Néel and strip states, respectively. The dashed line is the ground-state energy by conventional spin-wave theory. The mean-field energy is drawn as a dot-dashed line.

IV. VARIATIONAL SPIN-WAVE THEORY BASED ON THE STRIP STATE

For $\lambda > \lambda_0$, the ground state is the strip state[21] according to the conventional spin-wave theory.[9] We construct therefore the variational spin-wave theory starting from the classical ground state with strip-type ordering. This state contains two sublattices composed of strips extending in one direction (let us assume the direction as $m=1$) where spins are ordered parallel to each other. A spin has two parallel NN spins and $2(\nu-1)$ antiparallel NN spins. Among $2\nu(\nu-1)$ NNN spins, $4(\nu-1)$ NNN spins are parallel to a spin and $2(\nu-1)(\nu-2)$ NNN spins antiparallel.

Following the procedure described in Sec. II, we transform the Hamiltonian (2.4). Then the expectation value is written by assuming the symmetry between the A and the B sublattices as

$$\langle H\rangle_0 = -|\Lambda| S^2 \left[[(\nu-1)(4-\nu)\lambda+\nu-2]\left[1-\frac{2}{S}AG(A)\right]+\frac{1}{S^2}[(\nu-1)F_{02}-F_{01}]-\frac{2}{S}[(\nu-1)F_{12}+G_{11}] + \frac{(\nu-1)\lambda}{S^2}[2G_{0\Delta_{12}}-(\nu-2)G_{0\Delta_{23}}]-\frac{2(\nu-1)\lambda}{S}[2G_{1\Delta_{12}}+(\nu-2)G_{1\Delta_{23}}]\right], \tag{4.1}$$

where F_{0m}, F_{1m}, $G_{0\Delta_{nm}}$, G_{1m}, and $G_{1\Delta_{nm}}$ are defined by using Eqs. (2.9) and (2.10) as

$$F_{0m}=F_{0m}(B\Longrightarrow A)\ , \tag{4.2a}$$

$$F_{1m}=F_{0m}(B\Longrightarrow A)\ , \tag{4.2b}$$

$$G_{0\Delta_{nm}}=F_{0m}(B\Longrightarrow A,\ C_m\Longrightarrow A_{\Delta_{nm}})\ , \tag{4.2c}$$

$$G_{1m}=F_{1m}(B\Longrightarrow A,\ C_m\Longrightarrow A_{\delta_m})\ , \tag{4.2d}$$

and

$$G_{1\Delta_{nm}}=F_{1m}(B\Longrightarrow A,\ C_m\Longrightarrow A_{\Delta_{nm}})\ . \tag{4.2e}$$

The variational Hamiltonian is written as

$$H_{\rm var}=2S\sum_{\mathbf q}M_{\mathbf q}(a_{\mathbf q}^\dagger a_{\mathbf q}+b_{\mathbf q}^\dagger b_{\mathbf q}) +2\alpha S\sum_{\mathbf q}N_{\mathbf q}(a_{\mathbf q}b_{\mathbf q}+a_{\mathbf q}^\dagger b_{\mathbf q}^\dagger)\ , \tag{4.3}$$

where

$$M_{\mathbf q}\equiv[(\nu-1)(4-\nu)\delta+\nu-2]+\cos q_1+2\delta\eta'_{\mathbf q}\ , \tag{4.4}$$

$$N_{\mathbf q}\equiv\gamma'_{\mathbf q}(1+2\delta\cos q_1)\ , \tag{4.5}$$

$$\gamma'_{\mathbf q}\equiv\sum_{m>1}\cos q_m\ ,\qquad \eta'_{\mathbf q}\equiv{\sum_{(m,n)}}'\cos q_m\cos q_n\ , \tag{4.6}$$

where $\sum'_{(m,n)}$ denotes a sum over pairs of m and n, neither of which equals 1. Of course, $\eta'_{\mathbf q}=0$ in two dimensions. The variational parameters α and δ are restricted to the region $0\le\alpha\le1$ and $[2(\nu-1)]^{-1}\le\delta$. By putting $\alpha=1$ and $\delta=\lambda$, $H_{\rm var}$ reduces to the conventional spin-wave Hamiltonian. We have

$$A=-\frac{1}{2}+\frac{1}{2(2\pi)^\nu}\int_{-\pi}^{\pi}\frac{M_{\mathbf q}}{(M_{\mathbf q}^2-\alpha^2N_{\mathbf q}^2)^{1/2}}d^\nu q\ , \tag{4.7a}$$

$$C_m=-\frac{\alpha}{2(2\pi)^\nu}\int_{-\pi}^{\pi}\frac{\cos q_m N_{\mathbf q}}{(M_{\mathbf q}^2-\alpha^2N_{\mathbf q}^2)^{1/2}}d^\nu q\ , \tag{4.7b}$$

and

$$A_\Delta=\frac{1}{2(2\pi)^\nu}\int_{-\pi}^{\pi}\frac{e^{i\mathbf q\cdot\Delta}M_{\mathbf q}}{(M_{\mathbf q}^2-\alpha^2N_{\mathbf q}^2)^{1/2}}d^\nu q\ . \tag{4.7c}$$

We have evaluated the infinite series appearing in F_{0m}, F_{1m}, G_{1m}, $G_{0\Delta_{nm}}$, and $G_{1\Delta_{nm}}$ as in Sec. III. The expectation values of the energy are tabulated in Table II and are shown in Fig. 1 and 2. The energy obtained is slightly higher than $E_{\rm SW}$, as seen in figures. The spin-wave spectrum has a finite gap in this case also, as in the theory based on the Néel state. We observe that for $\lambda\gtrsim\lambda_0$ the energy of the strip state is higher than that of the Néel state. So, in such a region, we adopt the latter as an upper bound of the ground-state energy.

V. EXISTENCE OF NÉEL-TYPE LRO

We have shown in the previous paper[10] that the Néel-type LRO exists at $\lambda\le\lambda_0$ if the following inequality is satisfied:

$$\lim_{|\Lambda|\to\infty}\left[-\frac{1}{3\nu}e(\lambda)\right] >\frac{1}{\nu}\int^{(+)}\frac{d^\nu q}{(2\pi)^\nu}\tilde g_{\mathbf q}^{(i)}\left[-\sum_{m=1}^{\nu}\cos q_m -2\lambda\sum_{(m,n)}\cos q_m\cos q_n\right]\ , \tag{5.1}$$

where $e(\lambda)$ denotes the ground-state energy per spin and the right-hand side is integrated only in the region where the integrand is positive. The function $\tilde g_{\mathbf q}^{(i)}$ is an upper bound on $g_{\mathbf q}^{(i)}=\langle S_{\mathbf q}^iS_{-\mathbf q}^i\rangle$, the correlation function of the Fourier transform of a spin operator

$$\mathbf S_{\mathbf q}=\frac{1}{\sqrt{|\Lambda|}}\sum_{\alpha\in\Lambda}e^{-i\mathbf q\cdot\alpha}\mathbf S_\alpha\ . \tag{5.2}$$

In the present case, $\tilde g_{\mathbf q}^{(i)}$ is independent of i and, by using "Gaussian domination," is expressed as[11,22,25]

$$\tilde g_{\mathbf q}^{(i)}=\tfrac{1}{2}(B_{\mathbf q}^{(i)}C_{\mathbf q}^{(i)})^{1/2}\ , \tag{5.3}$$

where

TABLE II. Minimized energy obtained by the variational spin-wave theory based on the strip state with $S=\frac{1}{2}$ and 1. It is normalized by the mean-field energy at $\lambda=0$. (a) is for the two-dimensional model, and (b) is for three-dimensional model.

(a)

λ	0.50	0.52	0.54	0.56	0.58	0.60	0.62	
$E(S=\frac{1}{2})$	−0.789	−0.801	−0.813	−0.825	−0.837	−0.851	−0.870	
$E(S=1)$	−0.663	−0.675	−0.689	−0.706	−0.725	−0.744	−0.764	
λ	0.64	0.66	0.68	0.70	0.72	0.74	0.76	0.78
$E(S=\frac{1}{2})$	−0.891	−0.912	−0.934	−0.957	−0.980	−1.003	−1.026	−1.050
$E(S=1)$	−0.785	−0.805	−0.826	−0.848	−0.869	−0.891	−0.912	−0.934
λ	0.80	0.82	0.84	0.86	0.88	0.90	0.92	0.94
$E(S=\frac{1}{2})$	−1.073	−1.097	−1.121	−1.145	−1.169	−1.194	−1.218	−1.242
$E(S=1)$	−0.956	−0.978	−1.000	−1.022	−1.044	−1.066	−1.089	−1.111
λ	0.96	0.98	1.00					
$E(S=\frac{1}{2})$	−1.267	−1.291	−1.316					
$E(S=1)$	−1.133	−1.156	−1.178					

(b)

λ	0.25	0.26	0.28	0.30	0.32	0.34	0.36
$E(S=\frac{1}{2})$	−0.708	−0.711	−0.718	−0.726	−0.733	−0.741	−0.749
$E(S=1)$	−0.622	−0.626	−0.633	−0.641	−0.650	−0.660	−0.669
λ	0.38	0.40	0.42	0.44	0.46	0.48	0.50
$E(S=\frac{1}{2})$	−0.758	−0.766	−0.775	−0.783	−0.794	−0.803	−0.812
$E(S=1)$	−0.679	−0.689	−0.699	−0.710	−0.720	−0.731	−0.742

$$B_{\mathbf{q}}^{(i)}=\frac{1}{2}[E_\nu(\mathbf{q}-\mathbf{Q})-2\lambda H_\nu(\mathbf{q})]^{-1}, \tag{5.4}$$

$$C_{\mathbf{q}}^{(i)}=\frac{4}{3}S\left[S+\frac{1}{2\nu}\right]E_\nu(\mathbf{q}) +\frac{8}{3}\lambda S\left[S+\frac{1}{2\nu(\nu-1)}\right]H_\nu(\mathbf{q}), \tag{5.5}$$

$$E_\nu(\mathbf{q})=\sum_{m=1}^{\nu}(1-\cos q_m), \tag{5.6}$$

and

$$H_\nu(\mathbf{q})=\sum_{(m,n)}(1-\cos q_m\cos q_n). \tag{5.7}$$

A sufficient condition for the existence of LRO is obtained by replacing $e(\lambda)$ in inequality (5.1) with an upper bound on the ground-state energy. In our previous paper, we employed the mean-field energy as an upper bound. In Table III we show $\lambda_c(S)$ obtained by using the energy shown in Table I. The region where LRO exists is considerably extended by the improvement of the upper bound on the energy. This suggests that the Néel state is fairly stable against frustrations generated by NNN interactions.

VI. SUMMARY AND DISCUSSION

We have estimated the ground-state energy of the AFH model with the NN and NNN interactions on the square and simple-cubic lattices by using a variational spin-wave theory. The obtained energy is slightly higher than E_{SW} for both $\lambda\gtrsim 0$ (2.8% higher at $\lambda=0$ for $S=\frac{1}{2}$, $\nu=2$) and $\lambda\gtrsim 1$ (4.9% at $\lambda=1$ for $S=\frac{1}{2}$, $\nu=2$). The difference is slightly larger in two dimensions than in three dimensions for $S=\frac{1}{2}$ at $\lambda=0$. When λ is close to λ_0, the discrepancy between our estimation and E_{SW} is rather large. The ratio amounts to 1.19 at $\lambda=\frac{1}{2}$ for $S=\frac{1}{2}$ and $\nu=2$. This, we consider, is because the present results are too high, and in addition, E_{SW} is too low. As shown in Fig. 1, the energy obtained by the variational

TABLE III. Critical values $\lambda_c(S)$ estimated by using the upper bounds on the ground-state energy in Table I. The values in parentheses show the critical values obtained by using the mean-field energy (Ref. 10).

	$\lambda_c(S)$	
S	3D	2D
$\frac{1}{2}$	0.05 (0.002)	
1	0.18 (0.158)	0.16 (0.072)

spin-wave theory shows almost linear dependence on λ both for Néel and strip states. This means our variational state is rather rigid against the variation of λ and so may not simulate well the real ground state, which might change its character drastically around $\lambda=\lambda_0$. On the other hand, in two dimensions the conventional spin-wave theory will break down near $\lambda=\lambda_0$ where the reduction of the sublattice magnetization exceeds the assumed value of the classical ground state. When λ approaches λ_0 from both sides, E_{SW} decreases with divergent derivatives at $\lambda=\lambda_0$. This strongly suggests that E_{SW} is underestimated in this region. Really, a higher-order correction was shown to give a positive contribution.[7]

As seen in Figs. 1 and 2, the energy obtained by the theory based on the Néel state is lower than that based on the strip state at $\lambda \gtrsim \lambda_0$. Therefore, the upper bound on the ground-state energy has a maximum at λ_m which is larger than λ_0. The value λ_m for $S=\frac{1}{2}$ is 0.55 and 0.27 for $\nu=2$ and 3, respectively. The exact diagonalization study[3] of finite-size clusters for $\nu=2$ also gave $\lambda=0.58$ for $S=\frac{1}{2}$.

It might be possible that in the quantum system the Néel-type ground state exists stably even at λ larger than λ_0. Quite recently, using the modified spin-wave theory,[23] Nishimori and Saika[8] concluded that at $\lambda \sim 0.6$ there exists a first-order phase transition between the Néel and strip states. But it would be too bold to extract any conclusion on the character of the ground state around $\lambda \gtrsim \lambda_0$ from our result. First, as has been mentioned above, the obtained energy seems to be not very good in this region, and second, if it were good, one could not say much about the character of the true ground state of a many-body system from a variational calculation. It would be an interesting problem to find a better variational wave function in this region for which the energy can be estimated rigorously. One of the candidates is the variational wave function by Suzuki and Miyashita,[17] for which the energy was recently estimated exactly at $\lambda=0$.[24]

We have used the upper bound obtained by the variational spin-wave theory to prove the existence of Néel-type LRO. As a result, we have extended the region where LRO is affirmed to exist. It is, however, impossible to extend the region to $\lambda=\lambda_0$ in two dimensions for any S by the method of the infrared bounds since the integration in inequality (5.1) diverges at $\lambda=\lambda_0$. On the contrary, it is in principle possible to extend the region to $\lambda=\lambda_0$ in three dimensions and was actually done for $S \geq 4$.[10] It should be noted also that no LRO of spins with a wave vector $\mathbf{q}$ other than $(\pi,\ldots,\pi)$ exists at $\lambda \leq \lambda_0$, since $g_{\mathbf{q}}^{(i)}$ is bounded above for such a wave vector.

APPENDIX

Here we examine the series

$$F_1=C\sum_{i,j,k=0}^{\infty} f(i+j)f(i+k)\frac{(i+j+k+1)!}{i!j!k!}[A(1+A)-C^2]^{j+k}(C^2-A^2)^i[(1+A)^2-C^2]^{-2-i-j-k}$$

$$=C\sum_{i=0}^{\infty}\sum_{J=0}^{\infty}\left[\sum_{j=0}^{J} f(i+j)f(i+J-j)\frac{(i+J+1)!}{i!(J-k)!k!}\right][A(1+A)-C^2]^J(C^2-A^2)^i[(1+A)^2-C^2]^{-2-i-J} \quad \text{(A1)}$$

and

$$G_1=A'\sum_{i,j,k=0}^{\infty} f(i+j)f(i+k)\frac{(i+j+k+1)!}{i!j!k!}[A(1+A)-A'^2]^{j+k}(A'^2-A^2)^i[(1+A)^2-A'^2]^{-2-i-j-k} . \quad \text{(A2)}$$

From inequalities (3.6), it is seen that $C<0$, $X\equiv(1+A)^2-C^2>0$, $Y\equiv A(1+A)-C^2>0$, and $Z\equiv C^2-A^2>0$, and therefore F_1 is a negative-term series. We show that F_1 has a lower bound. For the simplicity, we assume that the spin magnitude is a half. In this case we have

$$f(j)=\begin{cases}0, & j=\text{odd}\\ (j+1)^{-1/2}, & j=\text{even}\end{cases} , \quad \text{(A3)}$$

and $f(i+j)f(i+J-j)$ is not zero only for $(i,J,j)=$(even,even,even) or (odd,even,odd). We have

$$F_1=\frac{1}{X^2}\sum_{J=0}^{\infty}{}'\sum_{i=0}^{\infty}(i+1)S_{i,J}\left[\frac{Y}{X}\right]^J\left[\frac{Z}{X}\right]^i , \quad \text{(A4)}$$

where

$$S_{i,J}\equiv\sum_{j=0}^{J}{}''\frac{(i+J+1)!}{(i+1)!j!(J-j)!\sqrt{(i+j+1)(i+J-j+1)}} , \quad \text{(A5)}$$

and $\sum_{J=0}^{\infty\prime}$ denotes a sum over even J and $\sum_{j=0}^{J\prime\prime}$ denotes a sum over even (odd) j if i is even (odd). Since

$$S_{i,J} \le \frac{(i+J+1)!2^{J-1}}{(i+1)!J!\sqrt{(i+j+1)(i+J-j+1)}} \tag{A6}$$

holds, we obtain the inequality

$$\begin{aligned} F_1 &\ge \frac{C}{2X^2} \sum_{J=0}^{\infty}{}' \sum_{i=0}^{\infty} \frac{(i+J+1)!}{(i+1)!J!} \left[\frac{2Y}{X}\right]^J \left[\frac{Z}{X}\right]^i + X^{-2}\left[1-\frac{Z}{X}\right]^{-1} \\ &\ge \frac{1}{2} C X^{-2} \left[\left[1-\frac{2Y}{X}\right]\left[1-\frac{2Y}{X}-\frac{Z}{X}\right]\right]^{-1} . \end{aligned} \tag{A7}$$

As $(2Y+Z)/X<1$ is confirmed numerically for parameters studied, F_1 is bounded below and so convergent.

In the same way,we can show that the series obtained by replacing all the terms in G_1 with their absolute values is bounded by

$$\frac{A'}{X'^2}\left\{\left[1-\frac{Z'}{X'}\right]^{-1}+\frac{1}{2}\left[\left[1-\frac{2Y'}{X'}\right]\left[1-\frac{2Y'}{X'}-\frac{Z'}{X'}\right]\right]^{-1}\right\}, \tag{A8}$$

where $X' \equiv (1+A)^2 - A'^2 (>0)$, $Y' \equiv (1+A)A - A'^2 (>0)$, and $Z' \equiv |A'^2 - A^2|$. As $(2Y'+Z')/X'<1$ also holds for parameters studied, G_1 is absolutely convergent. To obtain an upper bound of $\langle H \rangle_0$, we replace G_1 by a sum of finite terms plus an error bound. If we take terms up to $i=i_0$ and $J=2j_0$ into account, then the error R is bounded as

$$\begin{aligned} |R| \le \frac{A'}{2X'Z} \Bigg[&\left[1-\frac{2Y'}{X'}-\frac{Z'}{X'}\right]^{-1} - \left[1-\frac{2Y'}{X'}\right] - 1 + \left[1-\frac{Z'}{X'}\right]^{-1}\left[\frac{Z'}{X'}\right]^{i_0+2} \\ &- \sum_{\substack{1 \le i \le i_0+1 \\ 0 \le j \le 2j_0+1}} \frac{(i+j)!}{i!j!}\left[\frac{Z'}{X'}\right]^i \left[\frac{2Y'}{X'}\right]^j \Bigg] . \end{aligned} \tag{A9}$$

We have employed $i_0=15$ and $j_0=15$ in the actual calculation and have found that the error according to the truncation of the series has practically no significance for parameters minimizing the energy.

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