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The Ground-State Energy of the Heisenberg Antiferromagnet with Anisotropic Exchange Interaction

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The ground-state energy of the Heisenberg antiferromagnet with the XY-like anisotropy is examined with the use of a revised form of the Holstein-Primakoff transformation. The energy is calculated perturbationally with $1/S$ as an expansion parameter, S being the magnitude of spin. The contribution from the kinematical interaction of spin waves is shown to be of the order of $\exp(-aS)$ $(a>0)$ except for the linear chain, and accordingly negligible in the asymptotic expansion in $1/S$. The obtained ground-state energy agrees up to $1/S^2$ with that obtained earlier for bipartite lattices. For non-bipartite lattices, there is an extra term of $O(1/S^2)$ which has not been considered hitherto. The coefficient of the order $1/S^2$ for the triangular lattice is calculated numerically.

§ 1. Introduction

In a recent paper,[1] Nishimori and the present author obtained the ground-state energy of the anisotropic Heisenberg antiferromagnetic model in an expansion with respect to the inverse of magnitude of spin, S, using an enhanced form of Villain's spin wave theory.[2] Up to the order of $1/S^2$, the result agrees with that obtained from the Holstein-Primakoff spin wave theory.[3),4)]

The agreement of these results obtained from two different theories, suggests that the result would be exact to the order of $1/S^2$. In these calculations, the kinematical interactions are neglected. They are of different form in these two theories. It seems plausible that the contribution from the kinematical interaction can be neglected for the calculation of the ground-state energy in the asymptotic expansion in $1/S$.

In the Holstein-Primakoff theory,[5] spin operators are represented by bosons whose number is limited less than $2S+1$. Usual treatment neglects the restriction on boson numbers in the expectation that its effect is small in the limit $S\to\infty$. As far as the present author knows, there is few estimate to what order the kinematical interaction is negligible in the calculation of the ground-state energy.

Dyson[6] gave an estimate of the effect of the kinematical interaction on the temperature dependence of thermodynamic quantities of ferromagnets near 0K as $\exp[-JSz/4kT]$, where J is the exchange energy and z is the coordination number of the lattice. This estimate might seem to justify the expectation mentioned above. However the Bogoliubov transformations utilized for the study of the ground state and the thermal excitation are different in their connection with the kinematical condition on boson numbers.

In the present paper, the ground-state energy is calculated with the use of an extended form of the Holstein-Primakoff transformation. The ground-state energy is calculated perturbationally with $1/S$ as a small parameter.

The contribution from kinematical interaction is explicitly calculated and shown to be of the order of $\exp(-aS)$ $(a>0)$ except for the linear chain. Accordingly, it can be neglected in the asymptotic expansion in $1/S$. The coefficient of the expansion is shown to be exact which is obtained upon neglecting the kinematical interaction.

When the lattice is a non-bipartite one, there is an extra contribution which has not been considered so far. Hence the coefficient of the order $1/S^2$ for this type of lattices is different from that previously obtained. Calculation of the coefficient is done numerically for the triangular lattice.

§ 2. Kinematical interaction

The anisotropic Heisenberg model considered in this paper is represented by the Hamiltonian

$$H=\sum_{<ij>}[J_\perp(S_i^xS_j^x+S_i^yS_j^y)+J_{/\!/}S_i^zS_j^z], \qquad (J_\perp \geq J_{/\!/} \geq 0) \tag{2·1}$$

where we take the sum over all nearest neighbor pairs $\langle ij\rangle$.

In the present and the next sections, the lattice is assumed to consist of two sub-lattices. For such lattices, spins in two sublattices are oriented antiparallel in the easy plane in the classical limit. If we choose the new z-axis for each spin in the direction of its classical orientation, while the new y-axis is chosen for all spins parallel to the direction of the original z-axis, we have

$$H=-J_\perp\sum_{<ij>}\left[S_i^zS_j^z+\frac{1+\Delta}{4}(S_i^+S_j^++S_i^-S_j^-)+\frac{1-\Delta}{4}(S_i^+S_j^-+S_i^-S_j^+)\right]. \tag{2·2}$$

In the above we have put $\Delta=J_{/\!/}/J_\perp$ and $S^\pm=S^x\pm iS^y$.

In order to express the kinematical interaction explicitly, a revised form is used of the Holstein-Primakoff transformation of spin operators. This form was first introduced by Kubo,[7] and utilized later in various connections by Goldhirsch, Levich and Yakhot,[8] and by Agranovich and Toshich.[9]

In the Holstein-Primakoff method,[5] the spin is represented by bosons whose number is limited smaller than $2S+1$. This limitation constitutes the kinematical interaction of spin waves. In the revised form of the transformation, the states which include bosons more than or equal to $2S+1$ are associated to spin states according to the following rule:

$$S^z=S-\mathrm{Mod}(N,2S+1)\,. \tag{2·3}$$

Here, N is the number of bosons and $\mathrm{Mod}(N,2S+1)$ represents the remainder of N divided by $2S+1$. In the following it will be denoted simply as $[N]$ after Kubo.[7] If we use the number representation for bosons, spin operators are expressed as

$$S^z=S\sum_{N=0}^{\infty}(1-[N]/S)|N\rangle\langle N|\,, \tag{2·4a}$$

$$S^+=\sqrt{2S}\sum_{N=0}^{\infty}\sqrt{1-[N]/2S}\sqrt{[N]+1}\,|N\rangle\langle N+1|\,, \tag{2·4b}$$

and S^- is given as the Hermitian conjugate of S^+.

There is no matrix element between states of different sector. The sector is distinguished according to the integer $(N-[N])/(2S+1)$. Since the matrix element within each sector is the same as that of the original spin operator, the use of (2·4a) and (2·4b) instead of original spin operators in the Hamiltonian apparently gives the same energy eigenvalues.

Substitution of (2·4a) and (2·4b) into (2·2) leads to

$$H=-\sum_{<ij>}\sum_{N_i}\sum_{N_j}\left(1-\frac{[N_i]+[N_j]}{S}+\frac{[N_i][N_j]}{S^2}\right)|N_i, N_j\rangle\langle N_i, N_j|$$

$$-\frac{1}{S}\sum_{<ij>}\sum_{N_i}\sum_{N_j}\left(1-\frac{[N_i]}{2S}\right)^{1/2}\left(1-\frac{[N_j]}{2S}\right)^{1/2}\sqrt{[N_i]+1}\sqrt{[N_j]+1}$$

$$\times\left[\frac{1+\varDelta}{2}|N_i, N_j\rangle\langle N_i+1, N_j+1|+\frac{1-\varDelta}{2}|N_i, N_j+1\rangle\langle N_i+1, N_j|+\text{h.c.}\right]. \quad (2\cdot5)$$

In the above and hereafter, the energy is expressed in units of $J_\perp S^2$.

If we expand (2·5) in $1/S$, retain terms of order up to $1/S$ and replace $[N]$'s by N's, we obtain the harmonic Hamiltonian H_1. Separating H into H_1 and the remaining terms, we have

$$H=-N_Lz/2+H_1+H_1'+H_2+H_2'+O(1/S^3)\,, \quad (2\cdot6\text{a})$$

$$H_1=S^{-1}\sum_{<ij>}\left[b_i^\dagger b_i+b_j^\dagger b_j-\frac{1+\varDelta}{2}(b_i^\dagger b_j^\dagger+b_ib_j)-\frac{1-\varDelta}{2}(b_i^\dagger b_j+b_ib_j^\dagger)\right], \quad (2\cdot6\text{b})$$

$$H_1'=(z/S)\sum_i\sum_{N_i}([N_i]-N_i)|N_i\rangle\langle N_i|$$

$$-S^{-1}\sum_{<ij>}\sum_{N_i}\sum_{N_j}(\sqrt{[N_i]+1}\sqrt{[N_j]+1}-\sqrt{N_i+1}\sqrt{N_j+1})$$

$$\times\left(\frac{1+\varDelta}{2}|N_i, N_j\rangle\langle N_i+1, N_j+1|+\frac{1-\varDelta}{2}|N_i, N_j+1\rangle\langle N_i+1, N_j|+\text{h.c.}\right), \quad (2\cdot6\text{c})$$

$$H_2=-S^{-2}\sum_{<ij>}\left\{n_in_j-\frac{1+\varDelta}{8}(n_ib_ib_j+b_in_jb_j+b_i^\dagger n_ib_j^\dagger+b_i^\dagger b_j^\dagger n_j)\right.$$

$$\left.-\frac{1-\varDelta}{8}(n_ib_ib_j^\dagger+b_ib_j^\dagger n_j+b_i^\dagger n_ib_j+b_i^\dagger n_jb_j)\right\}, \quad (2\cdot6\text{d})$$

where n_i and n_j are number operators, z is the coordination number of the lattice, and N_L is the total number of lattice sites. The expression for H_2' is omitted; it is the difference between the $1/S^2$ order term and H_2, the latter being obtained from the former by replacing $[N]$'s by N's. Terms containing boson operators more than six are of higher order in $1/S$, because the boson operator appears in the form $(b/\sqrt{S})$.

The kinematical interaction is expressed explicitly as H_1' and H_2'. Looking H_1 as the unperturbed Hamiltonian and treating other terms as small perturbation, we apply the perturbational calculation of the ground-state energy formulated by Goldstone.[10)]

Diagonalization of H_1 is done by Fourier-transforming b_i's into $b_{\boldsymbol{k}}$'s, and then by applying the Bogoliubov transformation upon $b_{\boldsymbol{k}}$ and $b^\dagger_{-\boldsymbol{k}}$:

$$b_i=N_L^{-1/2}\sum_{\boldsymbol{k}}b_{\boldsymbol{k}}\exp(i\boldsymbol{kr}_i)\,, \quad (2\cdot7\text{a})$$

$$b_{\boldsymbol{k}}=\alpha_{\boldsymbol{k}}\cosh\theta_{\boldsymbol{k}}+\alpha^\dagger_{-\boldsymbol{k}}\sinh\theta_{\boldsymbol{k}}\,, \quad (2\cdot7\text{b})$$

$$\tanh(2\theta_{\boldsymbol{k}})=\tanh(2\theta_{-\boldsymbol{k}})=(1+\varDelta)\gamma_{\boldsymbol{k}}/[2-(1-\varDelta)\gamma_{\boldsymbol{k}}]\,, \quad (2\cdot7\text{c})$$

$$\gamma_k = z^{-1}\sum_l \exp(i\boldsymbol{k}\boldsymbol{d}_l)\,, \tag{2·7d}$$

where $\boldsymbol{d}_l$'s represent the relative position of the nearest neighbors. Thus we have

$$H_1 = -(z/2S)\sum_k [1-\sqrt{1-\gamma_k}\sqrt{1+\Delta\gamma_k}] + (z/S)\sum_k \sqrt{1-\gamma_k}\sqrt{1+\Delta\gamma_k}\,\alpha_k^\dagger \alpha_k\,. \tag{2·8}$$

Now we are in a position to investigate the effect of kinematical interaction H_1' and H_2'. First we note the relation

$$|M\rangle\langle N| = \iint C^{\pm}_{MN}(x,y)^* \exp\{\pm i(x+iy)b^\dagger \pm i(x-iy)b\}\,dxdy/\pi\,, \tag{2·9a}$$

$$C^{\pm}_{MN}(x,y) \equiv \langle M|\exp\{\pm i(x+iy)b^\dagger \pm i(x-iy)b\}|N\rangle\,. \tag{2·9b}$$

The derivation of the relation as well as the expression of $C^{\pm}_{MN}(x,y)$ is described in the Appendix.

Especially we have

$$C^{\pm}_{NN}(x,y) = \exp\left[-\frac{1}{2}(x^2+y^2)\right] L_N(x^2+y^2)\,, \tag{2·10a}$$

$$C^{\pm}_{NN+1}(x,y) = \mp i(x+iy)\exp\left[-\frac{1}{2}(x^2+y^2)\right] L_N^1(x^2+y^2)\,. \tag{2·10b}$$

In the above, $L_n^r(z)$ is the associated Laguerre polynomial and $L_n(z)=L_n^0(z)$.[11]

Using these relations, the expectation value in the ground state, $\mathrm{Ex}(O)$, of an operator O in H_1', can be calculated as follows. For example,

$$\mathrm{Ex}(|N_i\rangle\langle N_i|) = \frac{2}{\sqrt{A_1+1}\sqrt{A_2+1}}\sum_{m=0}^{\infty}(-)^{N_i}\binom{-\frac{1}{2}}{m}\binom{-\frac{1}{2}}{N_i-m}\left(\frac{A_1-1}{A_1+1}\right)^m\left(\frac{A_2-1}{A_2+1}\right)^{N_i-m}, \tag{2·11a}$$

$$A_1 \equiv N_L^{-1}\sum_k \sqrt{1+\Delta\gamma_k}/\sqrt{1-\gamma_k}\,,\quad A_2 \equiv N_L^{-1}\sum_k \sqrt{1-\gamma_k}/\sqrt{1+\Delta\gamma_k}\,. \tag{2·11b}$$

Similar but more complicated expressions are obtained for the expectation values of other operators in H_1'. Details of these calculations are presented in the Appendix.

If the larger of A_1 and A_2 is denoted as $A(>1)$, the following inequality can be obtained:

$$\mathrm{Ex}(|N_i\rangle\langle N_i|) < \mathrm{const}\times p^{N_i}, \quad p \equiv (A-1)/(A+1)\,. \tag{2·12}$$

It is to be noted that N_i contributing to (2·11a) is larger than or equal to $2S+1$.

For lattices other than the linear chain we have an estimate as

$$\mathrm{Ex}(H_1') = O(S^n p^{2S+1}), \qquad p<1 \text{ and } n<\infty\,. \tag{2·13}$$

For the linear chain, A is logarithmically divergent; p is equal to unity.

The effect of the kinematical interaction cannot be shown to be small even in the limit of large S. As signaled by the divergence of A, the spin wave treatment of the linear chain antiferromagnet seems to involve some problems to be solved.

Estimate of $\mathrm{Ex}(H_2')$ as well as the off-diagonal matrix element of H_1' is similar; they are exponentially small as S tends to infinity except for the linear chain.

We are, therefore, led to the conclusion that the kinematical interaction in the Holstein-Primakoff method is exponentially small in the limit $S\to\infty$ except for the linear chain. Also these considerations establish that H_2 is of the order of $1/S^2$. It looks proportional to $1/S^2$ as it stands in (2·6d), but the summation with respect to N_i that extends to infinity might give rise to some dependence on S. It is the exponential dependence on N_i which guarantees that H_2 is really of the order of $1/S^2$.

§ 3. Expansion in $1/S$

The only contribution of order of $1/S^2$ comes from the expectation value of H_2. It can be evaluated with the help of Wick's theorem and with the use of the average values

$$\langle b_i^\dagger b_i\rangle = N_L^{-1}\sum_k \sinh^2\theta_k = \frac{1}{4}(A_1+A_2-2)\,, \tag{3·1a}$$

$$\langle b_i^\dagger b_j\rangle = \langle b_i b_j^\dagger\rangle = N_L^{-1}\sum_k \gamma_k \sinh^2\theta_k = \frac{1}{4}(B_1+B_2)\,, \tag{3·1b}$$

$$\langle b_i b_i\rangle = \langle b_i^\dagger b_i^\dagger\rangle = N_L^{-1}\sum_k \sinh\theta_k\cosh\theta_k = \frac{1}{4}(A_1-A_2)\,, \tag{3·1c}$$

$$\langle b_i b_j\rangle = \langle b_i^\dagger b_j^\dagger\rangle = N_L^{-1}\sum_k \gamma_k \sinh\theta_k\cosh\theta_k = \frac{1}{4}(B_1-B_2)\,, \tag{3·1d}$$

where we have put

$$A_1 \equiv N_L^{-1}\sum_k \exp(2\theta_k) = N_L^{-1}\sum_k \sqrt{1+\Delta\gamma_k}/\sqrt{1-\gamma_k}\,, \tag{3·2a}$$

$$A_2 \equiv N_L^{-1}\sum_k \exp(-2\theta_k)\,, \tag{3·2b}$$

$$B_1 \equiv N_L^{-1}\sum_k \gamma_k \exp(2\theta_k)\,, \tag{3·2c}$$

$$B_2 \equiv N_L^{-1}\sum_k \gamma_k \exp(-2\theta_k)\,. \tag{3·2d}$$

The expectation value of H_2 is given as

$$\mathrm{Ex}(H_2) = -(z/8S^2)[(1-J_1)^2+(1-\Delta^2)B_2^2/2]\,, \tag{3·3a}$$

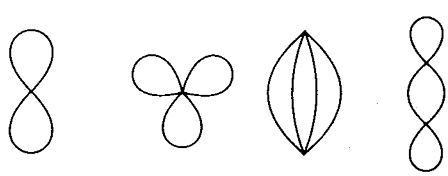

Fig. 1. Diagrams of $O(1/S^2)$ and $O(1/S^3)$ for bipartite lattices. (a): $O(1/S^2)$, (b)～(d): $O(1/S^3)$.

$$J_1 \equiv A_1 - B_1 = N_L^{-1} \sum_{\boldsymbol{k}} \sqrt{1+\Delta\gamma_{\boldsymbol{k}}}\sqrt{1-\gamma_{\boldsymbol{k}}}\,. \tag{3·3b}$$

The result is the same with that obtained previously from an enhanced form of Villain's spin wave theory.[1)]

In passing, we note that the correction of the ground-state energy to a given order can be estimated with the aid of Goldstone's perturbational calculation as depicted in Fig. 1. In (2·6a), omitted higher order terms contain more than four and even number of $(b/\sqrt{S})$ and $(b^\dagger/\sqrt{S})$. To each vertex in Fig. 1, $2n$ $(n\geq 2)$ lines (respresenting $\alpha_{\boldsymbol{k}}$ or $\alpha_{\boldsymbol{k}}^\dagger$) are attached; the factor associated with each line is proportional to $1/S$. The diagram with m lines and q vertices is of the order of S^{-m+q-1}, since the number of energy denominators in the perturbational calculation is equal to $q-1$, each contributing a factor proportional to S.

§ 4. Triangular lattice

For non-bipartite lattices, there is another contribution of order $1/S^2$. In these lattices, neighboring spins are not antiparallel but mutually oriented with a certain angle in the Néel state. In the triangular lattice, for example, three spins on the corners of the triangle are mutually oriented with 120 degrees each other.

As a result, when the Hamiltonian is expressed in terms of spin operators each quantized in the direction of the classical orientation, there are terms which are present because the quantization axes in neighboring sites are neither parallel nor antiparallel. For simplicity, we will restrict our study in the following to such lattices for which the classical spins are all oriented in the easy plane.

With an appropriate choice of the S^x-axis for each sublattice in the easy plane, the Hamiltonian is rewritten as

$$H = \sum_{<ij>} \{\cos(\phi_i-\phi_j)(S_i^z S_j^z + S_i^x S_j^x) + \sin(\phi_i-\phi_j)(S_i^x S_j^z - S_i^z S_j^x) + \Delta S_i^y S_j^y\}\,, \tag{4·1}$$

where ϕ_i indicates the classical direction of the spin at site i referred to a certain fixed direction in the easy plane. Expanded in $1/S$, the new term contains an odd number of b and $b^\dagger$; the part containing one b or $b^\dagger$ operator cancels out. The remaining lowest order term has three $b^\dagger$ or b's and is of the order of $S^{-3/2}$; the expectation value is zero and the second-order perturbational calculation gives a contribution of order $1/S^2$.

The three-boson operator part is given as

$$H_{3/2} = 2^{-1/2} S^{-3/2} \sum_i (b_i + b_i^\dagger) \sum_j \sin(\phi_i - \phi_j)\, n_j\,, \tag{4·2}$$

where the j-sum extends to all the nearest neighbors of i. Expressing b_i and $b_i^\dagger$ in $\alpha_{\boldsymbol{k}}$ and $\alpha_{\boldsymbol{k}}^\dagger$, and retaining the terms that contribute to the second-order perturbational calculation, we have

$$H_{3/2}^0 = 2if(2S)^{-3/2} z N_L^{-1/2} \sum_{\boldsymbol{q}} \beta(\boldsymbol{q}) \exp(2\theta_{\boldsymbol{q}})\, \alpha_{\boldsymbol{q}}^\dagger$$

$$\times \sum_{k} \alpha_k^\dagger \alpha^\dagger_{-(k+q)} \cosh\theta_q \sinh\theta_{k+q} + \text{h.c.}, \tag{4·3a}$$

$$\beta(\boldsymbol{q}) \equiv z^{-1} \sum_i \text{sgn}[\sin(\phi_i - \phi_j)] \sin[\boldsymbol{q}(\boldsymbol{r}_i - \boldsymbol{r}_j)], \tag{4·3b}$$

$$f \equiv |\sin(\phi_i - \phi_j)|. \tag{4·3c}$$

We have assumed that the angle between spins is the same for all nearest-neighbor pairs.

The $1/S^2$ contribution from $H_{3/2}^0$ is

$$\Delta E = -N_L \frac{4(fz)^2}{(2S)^3 3! N_L^2} \sum_k \sum_q \frac{F(\boldsymbol{k}, \boldsymbol{q})^2}{\omega(\boldsymbol{k}) + \omega(\boldsymbol{q}) + \omega(\boldsymbol{k}+\boldsymbol{q})}$$

$$= -N_L z \frac{f^2}{3c(2S)^2} \frac{1}{N_L^2} \sum_k \sum_q \frac{F(\boldsymbol{k}, \boldsymbol{q})^2}{\nu(\boldsymbol{k}) + \nu(\boldsymbol{q}) + \nu(\boldsymbol{k}+\boldsymbol{q})}, \tag{4·4a}$$

$$F(\boldsymbol{k}, \boldsymbol{q}) \equiv \beta(\boldsymbol{k}) \exp(2\theta_k) \sinh(\theta_k + \theta_{k+q}) + \beta(\boldsymbol{q}) \exp(2\theta_q) \sinh(\theta_k + \theta_{k+q})$$

$$- \beta(\boldsymbol{k}+\boldsymbol{q}) \exp(2\theta_{k+q}) \sinh(\theta_k + \theta_q), \tag{4·4b}$$

$$\omega(\boldsymbol{k}) = czS^{-1}\nu(\boldsymbol{k}), \qquad \nu(\boldsymbol{k}) \equiv \sqrt{1-\gamma_k}\sqrt{1+\Delta\gamma_k/c}, \tag{4·4c}$$

$$c \equiv |\cos(\phi_i - \phi_j)|. \tag{4·4d}$$

In the first line of (4·4a) $\boldsymbol{k}$ and $\boldsymbol{q}$ are taken independently in the first Brillouin zone. The result should be divided by 3! because the same set of three magnons $(\boldsymbol{k}, \boldsymbol{q}, -(\boldsymbol{k}+\boldsymbol{q}))$ appears 3! times in the sum.

Besides the contribution calculated above which is represented by Fig. 2(a), there is also a term represented by Fig. 2(b). The value of the term is indefinite when the interaction is strictly isotropic in the easy plane. The value becomes definite and equals to zero, if we interpret the Hamiltonian (2·1) as a limit that a certain crystal anisotropy tends to zero which stabilizes a particular Nẽel configuration.

Adding (4·4a) to (3·3a), we obtain the ground-state energy, E_0, up to $1/S^2$

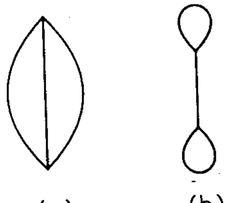

Fig. 2. Extra diagrams of $O(1/S^2)$ for non-bipartite lattices.

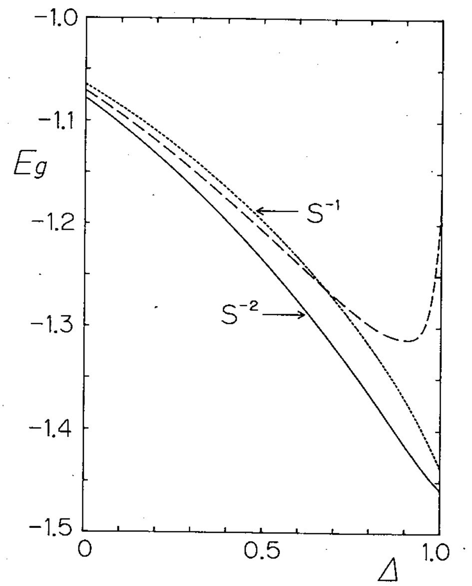

Fig. 3. Ground-state energy of the spin-1/2 antiferromagnet on the triangular lattice, $E_g = E_0 / (1.5 N_L J_\perp S^2)$ given by (4·5a), as a function of the exchange anisotropy $\Delta = J_{/\!/}/J_\perp$. The solid line represents the energy including all terms up to $O(1/S^2)$. The energy up to $O(1/S)$ is plotted with a dotted line, and a broken line represents the energy excluding I_2, the $O(1/S^2)$ contribution from the 3-boson term.

Table I. Coefficient of $1/(2S)^2$ for the triangular lattice.

Δ	0.0	0.2	0.4	0.6	0.8	1.0
I_1	.00616	.00965	.01105	.00585	−.01994	−.25430
I_2	.00716	.01283	.02161	.03665	.06776	.27566
C_2	.01332	.02248	.03266	.04250	.04782	.02136

$$E_0/(N_L z J_\perp c S^2/2) = -[1+(1-J_1)/S + C_2/(2S)^2], \quad C_2 = I_1 + I_2, \tag{4·5a}$$

$$I_1 = (1-J_1)^2 + [1-(\Delta/c)^2] B_2{}^2/2, \tag{4·5b}$$

$$I_2 = \frac{2f^2}{3c^2} N_L{}^{-2} \sum_{\boldsymbol{k}} \sum_{\boldsymbol{q}} \frac{F(\boldsymbol{k}, \boldsymbol{q})^2}{\nu(\boldsymbol{k}) + \nu(\boldsymbol{q}) + \nu(\boldsymbol{k}+\boldsymbol{q})}. \tag{4·5c}$$

In the above, B_2 and J_1 are given by (3·2d) and (3·3b) where Δ is replaced by Δ/c.

Some numerical results for I_1, I_2 and C_2 for the triangular lattice are listed in Table I. The dependence of the ground-state energy upon Δ is depicted for $S=1/2$ in Fig. 3.

§ 5. Summary and discussion

The ground-state energy of the anisotropic Heisenberg antiferromagnet was examined in the form of asymptotic expansion in $1/S$. The effect of the kinematical interaction of spin waves was estimated by expressing the interaction in an explicit form of the Hamiltonian and by calculating its expectation value in the unperturbed ground state.

Calculation shows that contribution from the kinematical interaction to the energy is of the order of $\exp(-aS)$, a being a positive constant; it can be neglected for the asymptotic expansion in $1/S$ except for the linear chain. Also the exponential smallness of contributions from the states with many bosons makes definite the order of each of remaining terms in the Hamiltonian. Thus we can select the contribution of a given order in $1/S$ on the basis of Goldstone's perturbational calculation.

The exponential dependence on S reminds us of Dyson's result mentioned in § 1. According to Dyson, some thermodynamic quantities of ferromagnets have the temperature dependence $\exp[-JSz/4kT]$. It is due to the suppression of the thermal fluctuation by the kinematical interaction. In the present calculation, a similar effect is considered concerning the fluctuation of the quantum origin because the ground state of antiferromagnets is under investigation. In spite of the difference in the origin of fluctuations, the interplay of the fluctuation and the kinematical interaction gives rise to an effect which has similar dependence on S.

For the linear chain, the effect of the kinematical interaction cannot be shown to be small because of the divergence of A_1 defined by (2·11a). The expectation value of the boson number N_i is also divergent because it is equal to $(A_1+A_2-2)/4$. Apparently the contribution is by no means negligible which comes from the states with $N_i \geq 2S+1$. It seems that some problems remain in the spin-wave treatment of one-dimensional antiferromagnets.

For bipartite lattices, the only term of $O(1/S^2)$ is the expectation value of the 4-boson term of the Hamiltonian. The result agrees with the previous ones.

For non-bipartite lattices, however, the second-order perturbational energy from the 3-boson term is of $O(1/S^2)$ and is to be included. Calculation of the $O(1/S^2)$ term was done numerically for the triangular lattice. As shown in Fig. 3, the expectation value of the 4-boson term alone gives an anomalous increase of energy near $\Delta \sim 1$. When the contribution from the 3-boson term is added, the anomaly is canceled; the dependence on Δ is similar to that for bipartite lattices.

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Appendix

The expression for the matrix element (2·9b) in the text is readily obtained as

$$C^{\pm}_{MN}(x,y) \equiv \langle M|\exp\{\pm i(x\pm iy)b^\dagger \pm i(x-iy)b\}|N\rangle$$

$$=\begin{cases} \sqrt{M!/N!}\exp\left[-\frac{1}{2}(x^2+y^2)\right]L_M{}^{N-M}(x^2+y^2)[\pm i(x-iy)]^{N-M}, & (M\le N) \\ \sqrt{N!/M!}\exp\left[-\frac{1}{2}(x^2+y^2)\right]L_N{}^{M-N}(x^2+y^2)[\pm i(x+iy)]^{M-N}. & (M\ge N) \end{cases} \quad (A\cdot 1)$$

In the above, $L_n{}^r(z)$ is the associated Laguerre polynomial. It is easily seen that $C^{\pm}_{MN}(x,y)$'s constitute a set of orthogonal functions in the xy-plane

$$\iint C^{\pm}_{IJ}(x,y)^* C^{\pm}_{MN}(x,y)\,dxdy/\pi = \delta_{I-J,M-N}\delta_{J,N} = \delta_{I,M}\delta_{J,N}\,. \quad (A\cdot 2)$$

By virtue of (A·2), the relation (2·9a) in the text is derived from the representation

$$\exp[\pm i(x+iy)b^\dagger \pm i(x-iy)b] = \sum_M\sum_N C^{\pm}_{MN}(x,y)|M\rangle\langle N|\,. \quad (A\cdot 3)$$

In order to calculate the expectation value Ex$(|N\rangle\langle N|)$, it is convenient to introduce the generating function

$$F(s) \equiv \sum_{N=0}^{\infty} s^N \mathrm{Ex}(|N\rangle\langle N|) = \mathrm{Ex}(\sum s^N|N\rangle\langle N|)\,. \quad (A\cdot 4)$$

Using the expression (2·9a) for $|N\rangle\langle N|$ and the generating function for the Laguerre polynomials, we have

$$F(s) = \iint \frac{dxdy}{\pi}\frac{1}{1-s}\exp\left[-\frac{1}{2}\frac{1+s}{1-s}(x^2+y^2)\right]\mathrm{Ex}(\exp[\pm i(x+iy)b_i{}^\dagger \pm i(x-iy)b_1])\,. \quad (A\cdot 5)$$

Transforming b_i and $b_i{}^\dagger$ into α_k and $\alpha_k{}^\dagger$, and remembering that the ground state is the vacuum for α_k's, the expectation value in (A·5) is calculated as

$$\mathrm{Ex}(\exp[\pm i(x+iy)b_i{}^\dagger \pm i(x-iy)b_i]) = \exp\left(-\frac{1}{2}A_1x^2 - \frac{1}{2}A_2y^2\right), \quad (A\cdot 6a)$$

$$A_1 \equiv N_L^{-1}\sum_k \exp(2\theta_k), \quad A_2 \equiv N_L^{-1}\sum_k \exp(-2\theta_k)\,. \tag{A·6b}$$

Substituting Eq. (A·6a) into Eq. (A·5), we obtain

$$F(s) = \frac{2}{\sqrt{A_1+1}\sqrt{A_2+1}}\left(1-\frac{A_1-1}{A_1+1}s\right)^{-1/2}\left(1-\frac{A_2-1}{A_2+1}s\right)^{-1/2}. \tag{A·7}$$

From (A·7), (2·11a) in the text is easily obtained.

Similarly, the expectation values of $|N_i, N_j\rangle\langle N_i, N_j|$, $|N_i, N_j\rangle\langle N_i+1, N_j+1|$ and $|N_i, N_j+1\rangle\langle N_i+1, N_j|$, where the sites i and j are any of nearest neighbor pairs, are calculated with the help of the following generating functions:

$$U(s, t) \equiv \sum_{N_i}\sum_{N_j} s^{N_i} t^{N_j} \mathrm{Ex}(|N_i, N_j\rangle\langle N_i, N_j|)\,, \tag{A·8a}$$

$$V(s, t) \equiv \sum\sum s^{N_i} t^{N_j} \mathrm{Ex}(|N_i, N_j\rangle\langle N_i+1, N_j+1|)\sqrt{N_i+1}\sqrt{N_j+1}\,, \tag{A·8b}$$

$$W(s, t) \equiv \sum\sum s^{N_i} t^{N_j} \mathrm{Ex}(|N_i, N_j+1\rangle\langle N_i+1, N_j|)\sqrt{N_i+1}\sqrt{N_j+1}\,. \tag{A·8c}$$

These functions are expressed in the form of 4-fold integrals over x, y, x' and y'. The integrands contain a common factor

$$\mathrm{Ex}(\exp[\pm i(x+iy)b_i^\dagger \pm i(x-iy)b_i \pm i(x'+iy')b_j^\dagger \pm i(x'-iy')b_j])$$
$$= \exp\left[-\frac{1}{2}A_1(x^2+x'^2) + B_1 xx' - \frac{1}{2}A_2(y^2+y'^2) + B_2 yy'\right], \tag{A·9a}$$

$$B_1 \equiv N_L^{-1}\sum_k \gamma_k \exp(2\theta_k), \qquad B_2 \equiv N_L^{-1}\sum_k \gamma_k \exp(-2\theta_k)\,. \tag{A·9b}$$

Integration gives the generating functions as

$$U(s, t) = 4[(A_1+1)^2 - B_1^2]^{-1/2}[(A_2+1)^2 - B_2^2]^{-1/2}$$
$$\times [1 - R_1(s+t) + Q_1 st]^{-1/2}[1 - R_2(s+t) + Q_2 st]^{-1/2}\,, \tag{A·10a}$$

$$\frac{1}{2}[V(s, t) + W(s, t)] = \frac{4B_1}{(A_1+1)^2 - B_1^2}[1 - R_1(s+t) + Q_1 st]^{-1} U(s, t)\,, \tag{A·10b}$$

$$\frac{1}{2}[V(s, t) - W(s, t)] = \frac{-4B_2}{(A_2+1)^2 - B_2^2}[1 - R_2(s+t) + Q_2 st]^{-1} U(s, t)\,, \tag{A·10c}$$

$$R_n \equiv [(A_n^2 - 1) - B_n^2]/[(A_n+1)^2 - B_n^2]\,, \quad (n=1, 2) \tag{A·10d}$$

$$Q_n \equiv [(A_n - 1)^2 - B_n^2]/[(A_n+1)^2 B_n^2]\,. \quad (n=1, 2) \tag{A·10e}$$

If we would expand the generating functions in powers of s and t, we could calculate the expectation values of operators which appear in H_1'. For the purpose of estimating the magnitude of $\mathrm{Ex}(H_1')$, it suffices to evaluate such quantities as

$$\sum_{N_i}([N_i] - N_i)\sum_{N_j}\mathrm{Ex}(|N_i, N_j\rangle\langle N_i, N_j|) \equiv \sum_N([N] - N) f_N\,. \tag{A·11}$$

Summation with respect to N_j is effected by simply setting $t=1$ in $U(s, t)$. Expanding $U(s, 1)$ in powers of s, we can have an estimate of the summand of the N-summation in

(A·11).

$$f_N = U(0,1)\sum_{r=0}^{N}(-)^N\binom{-\frac{1}{2}}{r}\binom{-\frac{1}{2}}{N-r}\left(\frac{R_1-Q_1}{1-R_1}\right)^r\left(\frac{R_2-Q_2}{1-R_2}\right)^{N-r}. \tag{A·12}$$

Noting the relation

$$(R_n-Q_n)/(1-R_n)=(A_n-1)/(A_n+1)\,, \qquad (n=1,2) \tag{A·13}$$

we obtain

$$f_N/U(0,1)\le\sum_{r=0}^{N}(-)^N\binom{-\frac{1}{2}}{r}\binom{-\frac{1}{2}}{N-r}\left(\frac{A-1}{A+1}\right)^N=\left(\frac{A-1}{A+1}\right)^N\equiv p^N\,, \tag{A·14}$$

where A is the larger of A_1 and A_2. Since the summation in (A·11) is restricted to $N\ge 2S+1$, the sum is of the order of Sp^{2S+1}. Similar estimates can be obtained for other terms in H_1'.

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