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Ground-State Energy of the Heisenberg Model with XY-Like Anisotropy

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We estimate the ground-state energy of the quantum Heisenberg model with XY-like anisotropy on various lattices by a self-consistent harmonic approximation and by an expansion from the classical limit in powers of $1/S$. A spin wave theory due to Villain gives the first order term in $1/S$ and the second order correction is obtained from the iterative solution of equations in the self-consistent harmonic approximation. Our coefficient of the second order term is not exact but we have reasons to believe that it is quite accurate. The second order expansion yields excellent values when comparison is possible with other exact and approximate estimates while the self-consistent harmonic approximation does not always work well. Our methods have the advantage of wide range of applicability and simplicity of the basic physical picture.

§ 1. Introduction

Ground-state properties of the quantum Heisenberg model have continuously attracted attention. It is generally very difficult to find out the correct ground-state and its energy, and a number of exact and approximate methods have been developed. It is convenient to summarize the problem in terms of frustration.[1] First, if the interaction is ferromagnetic, there is no frustration in the system, and classically the ground-state is trivial. A perfect ferromagnetic order sets in and spins are parallel to the z-axis (for an Ising-like anisotropy) or in the XY-plane (for an XY-like anisotropy). However, when quantum effects come into play, this picture no longer holds for XY-like models, and determination of the ground-state and its energy is a non-trivial problem.[2)~4)] On the other hand, the Ising-like model remains trivial at absolute zero even in the presence of quantum effects. Second, in antiferromagnetic models with two sublattices, frustration is again absent and the classical ground-state is determined uniquely (the Néel state) except for trivial degeneracy. For quantum systems, however, the Néel state is not a true eigenstate even with an Ising-like anisotropy. Quantum fluctuations are not negligible and various techniques have been proposed[5] to estimate quantum effects. The third class constitutes of antiferromagnetic systems on non-bipartite lattices. These models have frustration. For frustrated systems it is not easy in general to find out the correct set of classical ground-states (usually there is non-trivial degeneracy). Recent surge of interest in spin glasses has prompted investigation of those frustrated quantum spin systems and several results have been published.[6)~9)]

In the present paper we propose new methods to evaluate quantum fluctuations around a classical ground-state. All of the above-mentioned three classes will be treated in a unified manner. However for frustrated systems with high degeneracy of classical ground-state our approach may not give excellent results because, in such models, transition between different classical ground-states will be more important than fluctuations around one of them. Our approach has its basis on the spin wave theory of

Villain.[10] He introduced a convenient way to express spin operators making natural use of the classical picture of an XY-like ordering. Thus the Ising-like models are beyond our scope. We first develop a spin wave theory, following Villain, to show the basic idea. The ground-state energy is evaluated to first order in $1/S$ (classical state gives the zeroth term). We next present a variational method (or a self-consistent harmonic approximation). To our disappointment, this variational method does not always improve the results of the simple harmonic approximation, sometimes worse than the latter. A major reason for this failure lies, as discussed in detail later, in the finiteness and discreteness of spin operators to be ignored here in this approach. These effects may be called kinematical interactions of spin waves according to Dyson.[11] Deficiencies of the variational method are improved in the expansion of the ground-state energy to second order of $1/S$ to be developed following the variational approach. Our expansion does not yield exact coefficients of the second order term in $1/S$. Nevertheless, we have good reasons to believe that our values are close enough to the exact ones. At least dynamical interactions[11] between spin waves are perfectly taken into account, and so are kinematical interactions although in part. Resulting ground-state energy agrees excellently with available data from other exact and approximate methods when comparison is possible. Thus the expansion to second order gives a unified way to predict the ground-state energy with high accuracy of the Heisenberg model with XY-like anisotropy.

In the next section a harmonic approximation in Villain's variables is presented. The variational approach is developed in §3, followed by the second order expansion in §4. Discussions are given in §5.

§ 2. Harmonic approximation

In this section we study the leading non-trivial quantum correction to the classical ground-state, closely following Villain.[10] The system of our interest is described by the Hamiltonian

$$H=-J_{\perp}\sum_{<ij>}(S_i^xS_j^x+S_i^yS_j^y)-J_{/\!/}\sum_{<ij>}S_i^zS_j^z+D\sum_j(S_j^z)^2\,. \tag{1}$$

The magnitude of a spin will be denoted by S, and we assume $|J_{\perp}|\geq|J_{/\!/}|$ and $D\geq 0$ to represent an XY-like anisotropy. The range of interactions may be arbitrary, but in practice we will often restrict ourselves to nearest neighbor interactions to give definite values of the ground-state energy to be compared with already-known results. According to Villain[10] the spin operators have the following expressions:

$$\begin{aligned} S_j^+&=e^{i\phi_j}\sqrt{\left(S+\frac{1}{2}\right)^2-\left(S_j^z+\frac{1}{2}\right)^2}\,,\\ S_j^-&=\sqrt{\left(S+\frac{1}{2}\right)^2-\left(S_j^z+\frac{1}{2}\right)^2}\,e^{-i\phi_j}\,, \end{aligned} \tag{2}$$

where the new operator ϕ_j satisfies

$$[S_i^z,\ e^{i\phi_j}]=\delta_{ij}e^{i\phi_j}\,. \tag{3}$$

This relation (3) can be derived from the commutation relation

$$[\phi_i, S_j^z]=i\delta_{ij}\,. \tag{4}$$

With a periodic (or an antiperiodic) boundary condition imposed on ϕ_j with periodicity 2π, we may use ϕ_j and S_j^z instead of the original spin operators S_j^x, S_j^y, S_j^z. From (4) one may be inclined to regard ϕ_j and S_j^z as the position and momentum operators, respectively, of a particle on a closed chain of length 2π. However, S_j^z has a finite spectrum $|S_j^z|/S\leq 1$ and it should be distinguished from the momentum operator of a particle. Nevertheless, if S is very large and the anisotropy is XY-like, spins are almost certainly in the XY-plane in the ground-state and S_j^z/S is small. Accordingly in this limit finiteness of S_j^z gives only a small correction and we may safely neglect this property of the operator S_j^z. Discreteness of S_j^z/S (and correspondingly periodicity of ϕ_j) is also a small correction of $O(1/S)$ and thus we ignore it in the first approximation. Then the relation (4) allows us to treat the variables S_j^z and ϕ_j as continuous momentum and position in an infinite space $-\infty<\phi_j<\infty$, which is a part of what we call the harmonic approximation. As it turns out, this approximation yields a quantum correction of $O(1/S)$ to the classical ground-state energy. Taking into account the finiteness and discreteness corresponds apparently to an $O(1/S)$ correction to the harmonic approximation, thus giving an $O(1/S^2)$ correction to the ground-state energy.

In the limit of S infinity, S_j^z/S is vanishing and ϕ_j has a definite classical value $\overline{\phi_j}$ (which is the angle of the classical spin relative to the x-axis). Then $S_j^{\pm}=S\exp(\pm i\overline{\phi_j})$ by (2) and the Hamiltonian is reduced to

$$H=-\frac{1}{2}zNJ_{\perp}\cos(\overline{\phi_i}-\overline{\phi_j})S^2\equiv-\frac{1}{2}zNJ_{\perp}S^2c\,, \tag{5}$$

where z is the number of nearest neighbors and N denotes the system size. To evaluate quantum effects we next expand the exponentials and square roots in (2). Smallness of quantum fluctuations for large S suggests the expansion

$$\exp(i\phi_j)=\exp(i\overline{\phi_j})\left(1+i\theta_j-\frac{1}{2}\theta_j^2+\cdots\right), \tag{6}$$

$$\sqrt{\left(S+\frac{1}{2}\right)^2-\left(S_j^z+\frac{1}{2}\right)^2}=\left(S+\frac{1}{2}\right)\left\{1-\frac{1}{2}\left(S_j^z+\frac{1}{2}\right)^2\Big/\left(S+\frac{1}{2}\right)^2+\cdots\right\}, \tag{7}$$

where $\theta_j=\phi_j-\overline{\phi_j}$. In the harmonic approximation only the second order terms in (6) and (7) are retained. As discussed later, neglected terms in the expansion (which represent dynamical interactions of spin waves as described by Dyson[11]) do not contribute in the first order expansion in $1/S$ of the ground-state energy. The Hamiltonian (1) is now

$$\begin{aligned}H=&-\frac{1}{2}zNJ_{\perp}\left(S+\frac{1}{2}\right)^2c+\frac{1}{2}J_{\perp}cz\sum_j(S_j^z)^2-J_{/\!/}\sum_{<ij>}S_i^zS_j^z\\&+\frac{1}{2}J_{\perp}c\left(S+\frac{1}{2}\right)^2\sum_{<ij>}(\theta_i-\theta_j)^2+D\sum_j(S_j^z)^2\,,\end{aligned} \tag{8}$$

where higher order interactions between S_j^z and ϕ_j have also been ignored. The quadratic form (8) of the continuous canonical operators ϕ_j and S_j^z can be diagonalized by a standard technique. We first Fourier-transform (8) to take advantage of translational symmetry, and then define creation and annihilation operators of a harmonic

oscillator for each value of the wave number k. The result is

$$H=-\frac{1}{2}zNJ_{\perp}\left(S+\frac{1}{2}\right)^2c+\sum_k\omega_k\left(a_k^{\dagger}a_k+\frac{1}{2}\right), \tag{9}$$

where

$$\omega_k=zJ_{\perp}Sc\sqrt{(1-\gamma_k)(1-\Delta\gamma_k/c+2D/czJ_{\perp})} \tag{10}$$

with $\Delta=J_{/\!/}/J_{\perp}$ and

$$\gamma_k=\frac{1}{z}\sum_{\rho}e^{-ik\rho}. \tag{11}$$

The sum in (11) extends over nearest neighbor vectors ρ. Since c represents cosine of the classical angle between neighboring spins, $J_{\perp}c$ is always positive (so that the classical energy (5) is negative) and therefore $\omega_k\geq 0$ as it should. An immediate conclusion from (10) is a linear dispersion relation $\omega_k\sim|k|$ for small k except when $\Delta=c=1$ and $D=0$. The ground-state energy is thus

Table I. Ground-state energy $E_g=|E_0/NJ_{\perp}S^2|$ of the antiferromagnetic spin-1/2 XY-model on various lattices. Our results are listed as $O(1/S)$ (spin wave), $O(1/S^2)$ (expansion to second order) and SCHA (self-consistent harmonic approximation—variational method).

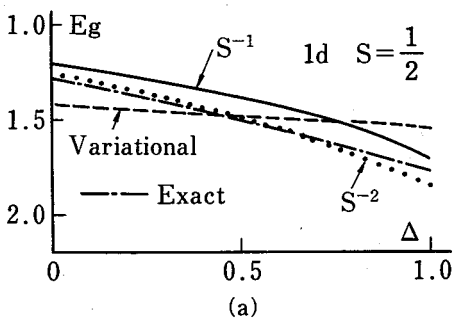
	Classical	$O(1/S)$	$O(1/S^2)$	SCHA	Variational[2),9)]	Exact/ Numerical
linear chain	1	1.199	1.254	1.408	1.185	1.272[14),15)]
square	2	2.167	2.191	2.596	2.149	2.156[3),4)] 2.174[16)]
triangular	1.5	1.596	1.609	1.922	1.57	1.8[7)] 1.76[17),18)]
simple cubic	3	3.152	3.166	3.813	3.140	—
bcc	4	4.152	4.163	5.044	4.136	—

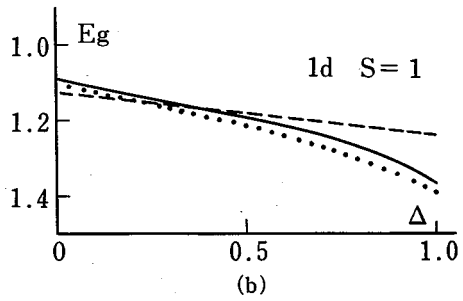
Table II. Ground-state energy E_g of the antiferromagnetic spin-1/2 isotropic Heisenberg model. Our spin wave estimates, $O(1/S)$, agree precisely with the results of conventional (Holstein-Primakoff or semi-classical) methods.[8),12),13)] The $O(1/S^2)$ estimates for bipartite lattices coincide with those of Kubo.[13)]

	Classical	$O(1/S)$	$O(1/S^2)$	SCHA	Variational/ Perturbational	Exact/ Numerical
linear chain	1	1.727	1.859	1.544	1.632 ~1.736[19)~24)]	1.772[25),26)]
square	2	2.632	2.682	2.706	2.564 ~2.656[2),19)~24)]	2.60[3),4)]
triangular	1.5	2.156	1.822	2.039	2.02[9)] ~2.16[27)]	2.76[7)]
simple cubic	3	3.583	3.611	3.914	3.140 ~3.609[2),19)~24)]	—
bcc	4	4.584	4.606	5.143	4.136 ~4.628[2),19)~24)]	—

$$E_g \equiv |H/NJ_\perp S^2|_{T=0} = \frac{1}{2} z|c| \left(1+\frac{1}{S}\right) - \frac{1}{SN}\sum_k \omega_k . \tag{12}$$

The $O(1/S)$ term of the ground-state energy (12) is composed of contributions from smearing of spin length and from zero-point motion of the harmonic oscillator. It is straightforward to verify that the higher order terms than quadratic in ϕ_j and S_j^z in the expansion of the Hamiltonian yield higher order corrections than $1/S$ to the ground-state energy, if we evaluate them by the ground-state eigenvector of the harmonic Hamiltonian (9). As discussed earlier, the finiteness and discreteness of the operators ϕ_j and S_j^z give an $O(1/S^2)$ correction to E_g. Therefore we are justified to claim that (12) is the correct expansion of E_g to $O(1/S)$. Results of explicit numerical evaluations of the energy (12) are listed in Tables I and II and Figs. 1(a)~5(b) for $D=0$. Agreement with available





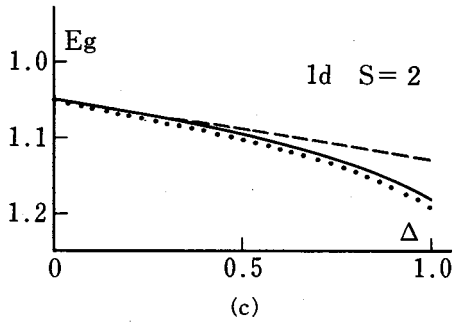
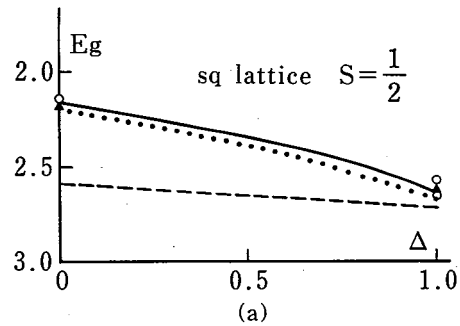


Fig. 1. (a) Ground-state energy $E_g=|E_0/NJ_\perp S^2|$ as a function of the anisotropy $\Delta=J_\parallel/J_\perp$ of the spin-1/2 antiferromagnetic chain. The solid line represents the spin wave results (§2), the dashed line is for the variational method (§3), and the dotted line denotes the second order expansion (§4). The exact solution[28),29)] is exhibited in a dash-dotted line.

(b) Same as in Fig. 1(a) but for $S=1$. Note the difference in energy scales between Figs. 1(a) and (b).

(c) Same as in Fig. 1(a) but for $S=2$.



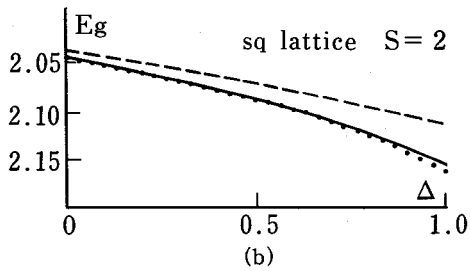


Fig. 2. (a) Ground-state energy E_g of the square lattice antiferromagnet with $S=1/2$. Various methods in this paper are represented by the same symbols as in Fig. 1(a). Representative values found in the literature are denoted by circles (variational/perturbational methods) and triangles (numerical methods). For references see Tables I and II.

(b) Same as in Fig. 2(a) except that $S=2$.

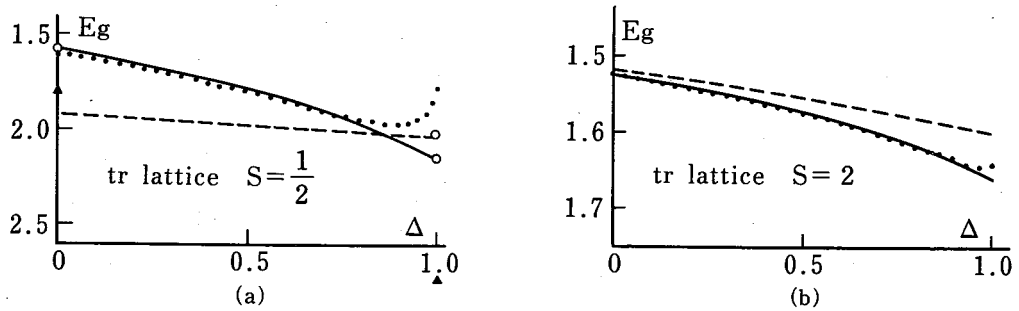


Fig. 3. (a) Ground-state energy E_g for the triangular lattice antiferromagnet with $S=1/2$. Symbols are the same as in Figs. 1(a) and 2(a).
(b) Same as in Fig. 3(a) but $S=2$.

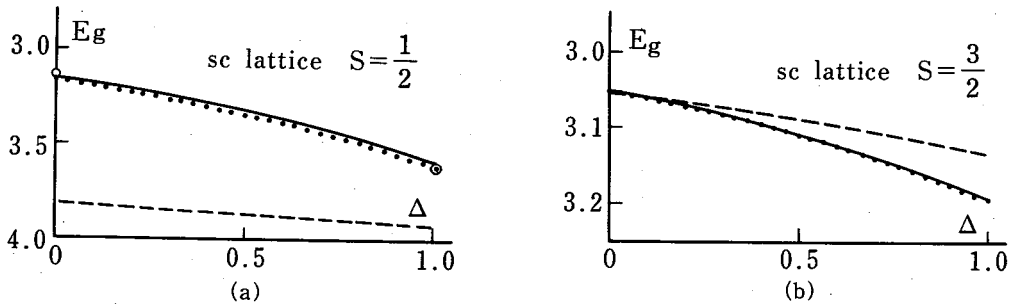


Fig. 4. (a) Ground-state energy E_g of the $S=1/2$ antiferromagnetic Heisenberg model on the simple cubic lattice. We use the same symbols as in Figs. 1(a) and 2(a).
(b) Same as in Fig. 4(a) except that $S=3/2$.

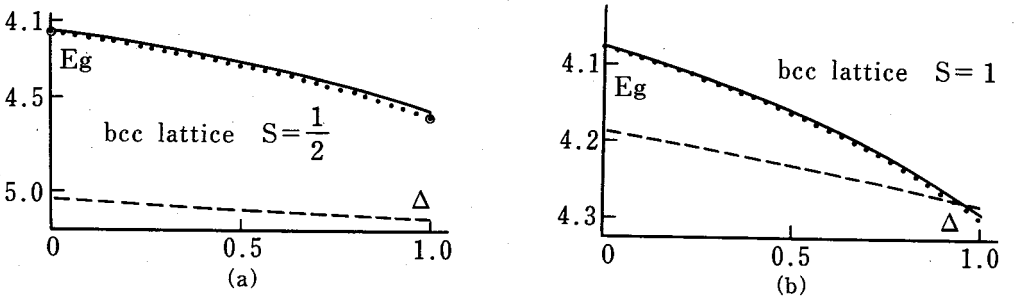


Fig. 5. (a) Ground-state energy E_g of the $S=1/2$ antiferromagnetic Heisenberg model on the body centered cubic lattice. The same symbols are used as before.
(b) Same as in Fig. 5(a) but $S=1$.

data is surprisingly good even for $S=1/2$. In particular, when $\Delta=1$ (isotropic Heisenberg model), our method gives the same value as those from the conventional spin wave theory.[8),12),13)] Advantages of the present method over the conventional Holstein-Primakoff formalism are the simplicity of calculations and the fact that the quantum variables appearing in the theory, ϕ_j and S_j^z, have their natural classical interpretation as an angle and the z-component of a spin.

§ 3. Variational approach

Let us now evaluate the expectation value of the Hamiltonian without expanding the square roots and exponentials in (2). Our variational state is, in essence, the ground-state of the harmonic oscillator (9) with parameters to be varied. The anisotropy D is taken to be vanishing in this and the following sections. As we remarked in §2, finiteness and discreteness of the operator S_j^z are ignored in constructing the ground-state of the harmonic Hamiltonian (9). Hence minimization of the original Hamiltonian (1) using the above-mentioned variational ground-state does not correspond to a genuine variational method. Operators in the Hamiltonian (1) are correct spin operators with finiteness and discreteness while the variational states do not have those properties. Therefore, one should not expect that the ground-state energy thus obtained is an upper bound to the exact value. Nevertheless, our variational method is of significance in that, among other reasons, it enables us to develop a higher order expansion of the ground-state energy as explained in the next section.

For later convenience, we rewrite the relations (2) as

$$S_j^{\pm}=e^{\pm i\phi_j/2}\sqrt{\left(S+\frac{1}{2}\right)^2-(S_j^z)^2}\,e^{\pm i\phi_j/2}. \tag{13}$$

To take into account finiteness of the spin operators at least in part, we multiply the square root in (13) by a step function and use the formula

$$\sqrt{\left(S+\frac{1}{2}\right)^2-(S_j^z)^2}\,\theta\left(\left(S+\frac{1}{2}\right)^2-(S_j^z)^2\right)=\left(S+\frac{1}{2}\right)\int_{-\infty}^{\infty}\frac{d\lambda}{2\lambda}\exp\left\{i\lambda S_j^z\Big/\left(S+\frac{1}{2}\right)\right\}J_1(\lambda), \tag{14}$$

where $J_1(\lambda)$ is the Bessel function of the first order. The operator S_j^z in (14) may be regarded as unbounded because unphysical values of S_j^z (larger than S or smaller than $-S$) are automatically cut off by the step function θ. To distinguish such an unbounded operator from the finite spin variable we denote the former by $\mathscr{S}_j^z$. Then from (13) we have

$$S_j^{\pm}=\left(S+\frac{1}{2}\right)\int_{-\infty}^{\infty}\frac{d\lambda}{2\lambda}J_1(\lambda)\exp\left\{i\lambda\mathscr{S}_j^z\Big/\left(S+\frac{1}{2}\right)\pm i\phi_j\right\} \tag{15}$$

and

$$S_j^z=\frac{1}{2}[S_j^+,\,S_j^-]=i\left(S+\frac{1}{2}\right)\int_{-\infty}^{\infty}d\lambda z(\lambda)\,\exp\left\{i\lambda\mathscr{S}_j^z\Big/\left(S+\frac{1}{2}\right)\right\}, \tag{16}$$

where

$$z(\lambda)=\frac{2S+1}{\pi\lambda}\left(\sin\frac{\lambda}{2S+1}\right)\left(\frac{\sin\lambda}{\lambda}\right)'. \tag{17}$$

The prime in (17) indicates differentiation with respect to λ. With the commutation relation (4) in mind we next define new operators P_j and Q_j and their Fourier transforms:

$$P_j=(\mathscr{S}_j^z-\overline{S_j^z})\Big/\sqrt{S+\frac{1}{2}}=\sum_k P_k e^{ikr_j}/\sqrt{N}\,,$$

$$Q_j=(\phi_j-\overline{\phi_j})\sqrt{S+\frac{1}{2}}=\sum_k Q_k e^{ikr_j}/\sqrt{N}\ , \tag{18}$$

where $\overline{S_j^z}$ and $\overline{\phi_j}$ are classical values of S_j^z and ϕ_j respectively. Since we are interested in the XY-like anisotropy, we actually set $\overline{S_j^z}=0$. From (18) boson-like operators are constructed as

$$\begin{aligned} a_k&=\sqrt{\frac{C_k}{2}}Q_k+i\sqrt{\frac{1}{2C_k}}P_k\ ,\\ a_k^{\dagger}&=\sqrt{\frac{C_k}{2}}Q_{-k}-i\sqrt{\frac{1}{2C_k}}P_{-k}\ , \end{aligned} \tag{19}$$

where C_k is an arbitrary real parameter satisfying $C_k=C_{-k}$. Since ϕ_j and $\mathscr{S}_j^z$ follow the commutation relation (4) (with S_j^z replaced by $\mathscr{S}_j^z$), we find

$$\begin{aligned} &[a_k,\ a_{k'}^{\dagger}]=\delta_{kk'}\ ,\\ &[a_k,\ a_{k'}]=[a_k^{\dagger},\ a_{k'}^{\dagger}]=0\ . \end{aligned} \tag{20}$$

It should be noted here that the present operators a_k and $a_k^{\dagger}$ are different from those in (9) in the preceding section because of the variational parameters $\{C_k\}$ in the definition (19). Strictly speaking, the operators a_k and $a_k^{\dagger}$ obey constraints coming from discreteness of $\mathscr{S}_j^z$ (and hence periodicity of ϕ_j). But the periodicity of ϕ_j is imposed for each j and is therefore reflected to the Fourier-transformed Q_k in a complicated manner. In what follows we ignore this remark and the operators a_k and $a_k^{\dagger}$ in (19) and (20) will be treated as unconstrained bose operators. This is the approximation which prevents us from obtaining correct upper bound estimates of the ground-state energy. This approximation is made in the same spirit as in the preceding section. An improvement here is that the constraint of finiteness of S_j^z appearing in the Hamiltonian has been lifted not as an approximation but by the step function in (14). Another difference from the harmonic approximation is that we calculate the expectation value of the Hamiltonian without expanding the square roots and exponentials in (2). We now express the Hamiltonian in terms of a_k and $a_k^{\dagger}$ with the aid of (15), (16), (18) and (19):

$$\begin{aligned} H=&-\frac{J_{\perp}}{2}\left(S+\frac{1}{2}\right)^2\sum_{<ij>}\Lambda_{\perp}[\exp\{i(\overline{\phi_i}-\overline{\phi_j})\}F_{ij}(\lambda_1,\lambda_2,1)+\text{c.c.}]\\ &-J_{/\!/}\left(S+\frac{1}{2}\right)^2\sum_{<ij>}\Lambda_{/\!/}[F_{ij}(\lambda_1,\lambda_2,0)], \end{aligned} \tag{21}$$

where

$$\Lambda_{\perp}[f(\lambda_1,\lambda_2)]=\int_{-\infty}^{\infty}\frac{d\lambda_1}{2\lambda_1}J_1(\lambda_1)\int_{-\infty}^{\infty}\frac{d\lambda_2}{2\lambda_2}J_1(\lambda_2)f(\lambda_1,\lambda_2),$$

$$\Lambda_{/\!/}[g(\lambda_1,\lambda_2)]=\int_{-\infty}^{\infty}d\lambda_1 z(\lambda_1)\int_{-\infty}^{\infty}d\lambda_2 z(\lambda_2)g(\lambda_1,\lambda_2),$$

$$F_{ij}(\lambda_1,\lambda_2,\mu)=\exp\left[\frac{i}{\sqrt{2S+1}\sqrt{N}}\sum_k a_k e^{ikr_i}\left\{\frac{\mu}{\sqrt{C_k}}(1-e^{-ik\rho})-i\sqrt{C_k}(\lambda_1-\lambda_2 e^{-ik\rho})\right\}\right.$$

$$+\sum_k a_k^\dagger e^{-ikr_i}\left\{\frac{\mu}{\sqrt{C_k}}(1-e^{ik\rho})+i\sqrt{C_k}(\lambda_1-\lambda_2 e^{ik\rho})\right\}\Big]$$

with $\rho=r_i-r_j$. The experience in the preceding section suggests us to take the expectation value of the Hamiltonian by the vacuum of a-bosons. The result is, for a given $\{C_k\}$,

$$E_0(\{C_k\})=-\frac{1}{2}cJ_\perp\left(S+\frac{1}{2}\right)^2 NzA_\perp[\Xi(\lambda_1,\lambda_2,1)]$$
$$-\frac{1}{2}J_{/\!/}\left(S+\frac{1}{2}\right)^2 NzA_{/\!/}[\Xi(\lambda_1,\lambda_2,0)], \tag{22}$$

where

$$\Xi(\lambda_1,\lambda_2,\mu)=\exp\Big[-\frac{1}{2S+1}\frac{1}{N}\sum_k\left\{\frac{\mu}{C_k}(1-\gamma_k)+\frac{C_k}{2}(\lambda_1^2-2\lambda_1\lambda_2\gamma_k+\lambda_2^2)\right\}\Big]. \tag{23}$$

Variating E_0 by each C_k, we finally obtain the extremum value as

$$E_0=-\frac{1}{2}NzcJ_\perp\left(S+\frac{1}{2}\right)^2 A_\perp-\frac{1}{2}NzJ_{/\!/}\left(S+\frac{1}{2}\right)^2 A_{/\!/}, \tag{24}$$

where

$$A_\perp=A_\perp[\Xi(\lambda_1,\lambda_2,1)],$$
$$A_{/\!/}=A_{/\!/}[\Xi(\lambda_1,\lambda_2,0)]. \tag{25}$$

C_k is determined by

$$C_k^2=\frac{J_\perp cA_\perp(1-\gamma_k)}{J_\perp c(B_\perp-C_\perp\gamma_k)+J_{/\!/}(B_{/\!/}-C_{/\!/}\gamma_k)}, \tag{26}$$

where

$$\begin{Bmatrix}B_\perp\\C_\perp\end{Bmatrix}=A_\perp\Big[\begin{Bmatrix}\lambda_1^2\\\lambda_1\lambda_2\end{Bmatrix}\Xi(\lambda_1,\lambda_2,1)\Big] \tag{27}$$

and

$$\begin{Bmatrix}B_{/\!/}\\C_{/\!/}\end{Bmatrix}=A_{/\!/}\Big[\begin{Bmatrix}\lambda_1^2\\\lambda_1\lambda_2\end{Bmatrix}\Xi(\lambda_1,\lambda_2,0)\Big]. \tag{28}$$

These equations have been numerically solved for various lattices and the results are in Tables and Figures. It is observed in these figures that the present variational technique is not necessarily an improvement over the harmonic approximation in §2. A major reason is our ignorance of finiteness and discreteness of S_j^z in the variational state. (Remember that finiteness has been correctly considered only at sites $\langle i, j\rangle$, for which we used (14)~(16), and not at other sites.) Detailed discussions are found in §5.

§ 4. 1/S-expansion to second order

In this section we solve Eq. (26) for C_k iteratively starting from the classical limit

$S\to\infty$. We may alternatively say that (26) will be solved order by order in $1/S$ to derive an expansion of E_0, (24), to second order of $1/S$. Since the method of §3 is basically to evaluate the original Hamiltonian by the harmonic ground-state (which gives exact E_g to $O(1/S)$), we may expect that the ground state energy thus derived by iterative solution of (26) is exact to $O(1/S)$. In fact, the first order term of the expansion in this section agrees with the ground-state energy of the harmonic approximation. Moreover, from a well-known theorem of perturbation theory, our correction term of $O(1/S^2)$ is very accurate because we calculate the next order correction, $O(1/S^2)$, by the eigenstate of the preceding order. However, finiteness and discreteness of S_j^z again prevent us from claiming exactness of our coefficient of $O(1/S^2)$. Let us summarize results, leaving details to the Appendix. The quantities A, B, C appearing in (25), (27), (28) are expanded to first order in $1/S$:

$$\begin{aligned} A_\perp &= 1-(J_1+J_2)/2S\,,\\ A_{/\!/} &= J_3/2S\,,\\ B_\perp &= 1-(J_1-J_2)/2S\,,\\ B_{/\!/} &= 0\,,\\ C_\perp &= J_3/2S\,,\\ C_{/\!/} &= 1\,, \end{aligned} \tag{29}$$

where J_1, J_2, J_3 are defined in (A·5). Inserting the above to (26) we obtain

$$C_k^2=\frac{1-\gamma_k}{1-\Delta\gamma_k/c}\{1-(J_1+J_2)/2S+(J_1-J_2+\gamma_k J_3)/2S(1-\Delta\gamma_k/c)\}. \tag{30}$$

From this expansion of C_k to $O(1/S)$ we can calculate $A_\perp$, $A_{/\!/}$ to $O(1/S^2)$ as

$$A_\perp=1-(J_1+J_2)/2S+(2J_1+2J_2-J_2^2+2J_3^2+3J_1J_2-J_1J_4+J_2J_4-J_3J_5)/8S^2\,, \tag{31}$$

$$A_{/\!/}=J_3/2S-(2J_3+J_1J_3+J_2J_3-J_1J_5+J_2J_5-J_3J_6)/8S^2\,, \tag{32}$$

where J_4, J_5, J_6 are defined in (A·9). It is now straightforward to write down the ground-state energy (24):

$$\begin{aligned} E_g&=|E_0/NJ_\perp S^2|\\ &=\frac{1}{2}|c|z\{1+(1-J_1)/S+(2-4J_1+2J_1^2+(1-\Delta^2/c^2)J_3^2)/8S^2\}, \end{aligned} \tag{33}$$

where we have used (A·11) to eliminate J_2, J_4, J_5, J_6. The integrals J_1 and J_3 are evaluated quite easily numerically and the resulting E_g are in Tables and Figures. In general, the present second order calculation gives very close values to the expected answers, at least much better than the variational estimates in §3 and slightly better than the harmonic approximation in §2. It is somewhat surprising that our result (33) is reduced to that of Kubo,[13] his equation (6·14), when $\Delta=-c=1$. He has calculated the effects of dynamical interactions on the ground-state energy in the Holstein-Primakoff variables starting from the Néel state ordered along the z-axis. Thus (33) is a generalization of Kubo's result to anisotropic interactions ($\Delta<1$) and to non-bipartite

lattices ($c>-1$). Further discussions are found in the next section.

§ 5. Discussion

A major deficiency of the techniques in the present paper lies in our neglect of finiteness and discreteness of spin operators. These properties of S_j^z do not play a role in determining the $O(1/S)$ term of E_g but they do in higher orders increasingly as the order. Nevertheless, since the variational state employed in §3 is basically a harmonic ground-state, we have good control over E_g to $O(1/S^2)$ as remarked in the preceding section from a general theorem of perturbation theory. On the other hand, the variational energy is alternatively regarded as an infinite partial sum of the asymptotic expansion of the true ground-state energy by $1/S$. In the presence of increasingly important kinematical effects we do not have strong reasons to claim reliability of coefficients of higher orders than the second term except for the overall extremization of E_g. Thus we are reasonably allowed to expect that the best value of E_g is obtained if we truncate the expansion at second order. This argument justifies the excellent results in §4. To get the exact coefficient of the $O(1/S^2)$ term, however, we should take into account finiteness and discreteness of S_j^z (kinematical effects) in the harmonic order. (Note that dynamical interactions between spin waves, which arise from higher-than-quadratic terms in the expansion of the square roots and exponentials in the Hamiltonian, are correctly evaluated in §4, since we did not expand square roots and exponentials in (2).) To take into account those kinematical effects is in general difficult; but at least finiteness of neighboring spins is correctly considered in our formulation in §§3 and 4 through the step function in (14). In any event the term of $O(1/S^2)$ is already small even for $S=1/2$ as seen in Figures, and therefore a correction due to finiteness and discreteness is not expected to upset our predicted values by large amount.

Since our method starts from the classical ground-state of the XY-model, the resulting energy should be more reliable in the XY-regime ($|\Delta|\ll 1$) than in the Heisenberg regime ($|\Delta|\lesssim 1$). This general trend is observed in Figures, except for the disturbing discrepancy of the variational energy from other estimates when $S=1/2$ almost in the whole range of Δ. A few reasons have been given above for this discrepancy, but after all we should not expect too much out of the present techniques when $S=1/2$ and $\Delta\lesssim 1$. Another headache comes from the mysterious upturn of the $O(1/S^2)$ energy on the triangular lattice near the isotropic limit ($\Delta\lesssim 1$) as in Figs. 3(a) and (b). This behavior is probably attributed to a breakdown of the XY-like picture, from which we started, in the strongly frustrasted Heisenberg model on the triangular lattice.

As remarked before, our formula (33) of the $1/S$-expansion agrees with the corresponding result of Kubo[13] when $\Delta=-c=1$. This coincidence is accidental because kinematical interactions neglected in both formulas are of different nature from each other (Kubo used the Holstein-Primakoff formalism). On the other hand, in ferromagnets the same method gives the exact temperature dependence of magnetization at low temperatures.[30),31)] Accordingly his formula for the ground-state energy of antiferromagnets on bipartite lattices would be quite accurate (that is, kinematical effects should be small). This argument serves as another support to our claim that the coefficient of $1/S^2$ in our generalization (33) of Kubo's formula is close to the exact value in spite of our negligence of kinematical interactions.

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Appendix

We derive here the expansion (33) of the ground-state energy from relations (24)~(28) in §3. It is convenient to define the following lattice sums:

$$F_1=\frac{1}{2S+1}\frac{1}{N}\sum_k\frac{1-\gamma_k}{C_k},$$

$$F_2=\frac{1}{2S+1}\frac{1}{2N}\sum_k C_k,$$

$$F_3=\frac{1}{2S+1}\frac{1}{N}\sum_k\gamma_k C_k. \tag{A·1}$$

The function Ξ, (23), is then

$$\Xi(\lambda_1,\lambda_2,\mu)=\exp\{-\mu F_1-(\lambda_1^2+\lambda_2^2)F_2+\lambda_1\lambda_2 F_3\}. \tag{A·2}$$

First, let us consider the classical limit $S\to\infty$. It turns out to be consistent to assume $C_k\sim O(1)$. Thus F_1, F_2, F_3 are $O(1/S)$ and may be neglected, yielding $\Xi=1$. For this value of Ξ, it is easy to verify $A_\perp=1$, $A_{/\!/}=0$ from (25). We also notice $B_\perp=1$, $C_\perp=0$, $B_{/\!/}=0$, $C_{/\!/}=1$ in this limit. Now we have from (24)

$$E_g=|E_0/NJ_\perp S^2|=\frac{1}{2}|c|z \tag{A·3}$$

in the classical limit.

To obtain the next order correction to the classical value (A·3), we should expand $A_\perp$ and $A_{/\!/}$ to $O(1/S)$ as seen in (24). $A_\perp$ and $A_{/\!/}$ have their dependence on $1/S$ through F_j ($j=1,2,3$) in Ξ, see (A·2), and the F_j are all of order $1/S$. Hence we first expand $A_\perp$ and $A_{/\!/}$ to first order in F_j:

$$A_\perp=1-F_1-2F_2,$$

$$A_{/\!/}=F_3, \tag{A·4}$$

and then F_j to first order of $1/S$:

$$F_1=\frac{1}{2SN}\sum_k\sqrt{(1-\gamma_k)(1-\Delta\gamma_k/c)}\equiv\frac{J_1}{2S},$$

$$F_2=\frac{1}{4SN}\sum_k\sqrt{(1-\gamma_k)/(1-\Delta\gamma_k/c)}\equiv\frac{J_2}{4S},$$

$$F_3=\frac{1}{2SN}\sum_k\gamma_k\sqrt{(1-\gamma_k)/(1-\Delta\gamma_k/c)}\equiv\frac{J_3}{2S}, \tag{A·5}$$

where we have used the classical value of C_k:

$$C_k=\sqrt{(1-\gamma_k)/(1-\Delta\gamma_k/c)} \tag{A·6}$$

obtained from (26) with $A_\perp=B_\perp=C_{/\!/}=1$ and $A_{/\!/}=B_{/\!/}=C_\perp=0$. We are ready to derive E_g from (A·4) and (A·5) as

$$E_g=\frac{1}{2}|c|z\left(1+\frac{1}{S}-\frac{J_1}{S}\right) \tag{A·7}$$

which agrees with the harmonic approximation (12) in §2.

The next order correction is obtained in a similar manner. We need $A_\perp$ and $A_{/\!/}$ to $O(1/S^2)$ as is apparent from (24). For that, F_j should be expanded to $O(1/S^2)$, see (A·4), which is possible when we have C_k to $O(1/S)$, see (A·1). Thus, with (26) in mind, we first expand $A_\perp$, $A_{/\!/}$, $B_\perp$, $B_{/\!/}$, $C_\perp$, $C_{/\!/}$ to $O(F_j)$ and make use of (A·5). The result is (29) in the text. Next the above expansion (29) is inserted in the right side of (26), yielding the expansion (30) of C_k. We are now able to expand F_j, (A·1), to $O(1/S^2)$:

$$\begin{aligned}
F_1&=J_1/2S+(-2J_1+J_1^2+J_2^2-J_3^2)/8S^2,\\
F_2&=J_2/4S-(2J_2+J_1J_2+J_2^2-J_1J_4+J_2J_4-J_3J_5)/16S^2,\\
F_3&=J_3/2S-(2J_3+J_1J_3+J_2J_3-J_1J_5+J_2J_5-J_3J_6)/8S^2,
\end{aligned} \tag{A·8}$$

where

$$\begin{aligned}
J_4&=\frac{1}{N}\sum_k\sqrt{(1-\gamma_k)/(1-\Delta\gamma_k/c)^3},\\
J_5&=\frac{1}{N}\sum_k\gamma_k\sqrt{(1-\gamma_k)/(1-\Delta\gamma_k/c)^3},\\
J_6&=\frac{1}{N}\sum_k\gamma_k^2\sqrt{(1-\gamma_k)/(1-\Delta\gamma_k/c)}.
\end{aligned} \tag{A·9}$$

It is also necessary to expand $A_\perp$ and $A_{/\!/}$ to $O(F_j^2)$:

$$\begin{aligned}
A_\perp&=1-F_1-2F_2+\frac{1}{2}F_1^2+2F_1F_2-2F_2^2+\frac{1}{2}F_3^2,\\
A_{/\!/}&=F_3+O(F_j^3),
\end{aligned} \tag{A·10}$$

which, together with (A·8), yields (31) and (32). It is straightforward to derive the expansion (33) from (31) and (32) using the relations

$$\begin{aligned}
J_2-\Delta J_3/c&=J_1,\\
J_5-\Delta J_6/c&=J_3,\\
J_4-\Delta J_5/c&=J_2.
\end{aligned} \tag{A·11}$$

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Note added in proof: After submission of the paper we learned that our results are in excellent agreement with numerical estimates by Blöte[32] in one dimension for $S \geqq 1$ as well as for $S=\frac{1}{2}$.