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Spin-wave theory of two-dimensional Heisenberg antiferromagnets: ground states

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Abstract. The ground-state energies and sublattice magnetizations of Heisenberg antiferromagnets with XY-like anisotropy of nearest-neighbour exchange interactions on a two-dimensional triangular lattice, as well as on a two-dimensional square lattice, are studied in the framework of spin-wave theory in the first-order perturbation approximation. To take account of the kinematic interactions the Dyson–Maleev transformation is incorporated with the method proposed by Kubo. When we neglect the kinematic interactions, we obtain the ground-state energies for the $S = 1/2$ models on the triangular lattice, namely -0.1872 for the isotropic exchange interactions and -0.1344 for the XY interactions. The kinematic interactions, however, increase the ground-state energies, and that for the XY interactions becomes -0.1293.

1. Introduction

As the simplest spin model that frustrates quantum-mechanically, the $S = 1/2$ Heisenberg antiferromagnet on a two-dimensional triangular lattice (which we abbreviate as $S = 1/2$ TRHA) has attracted much interest. The study of this model was started with the proposal of its ground state by Anderson [1] and Fazekas and Anderson [2], who pointed out that the ground state is described by a resonating-valence-bond (RVB) state, a kind of spin-liquid state. Since then, the model has been investigated by many authors. In recent research on high-T_c superconductors, the $S = 1/2$ Heisenberg antiferromagnet on a two-dimensional square lattice ($S = 1/2$ SQHA) has also gained much renewed attention in relation to the theory of a possible RVB mechanism of the new superconductivity, being claimed first by Anderson [3]. In particular, the idea of an RVB mechanism was recently developed from the viewpoint of a fractional quantum Hall state by Laughlin [4]. Kalmeyer and Laughlin [5] and Laughlin [6] also stated that the ground state of the former model is equivalent to a fractional quantum Hall state.

In spite of these studies, no one could succeed in proving whether the ground state of $S = 1/2$ TRHA has no Néel order and is a spin-liquid state. Rather, a serious question was presented by Huse and Elser [7]. Making use of a trial wavefunction, they found a ground state that has Néel order and a lower energy than the RVB state given by Anderson [1] and Laughlin's fractional quantum Hall state [4]. The ground state of the TRHA still seems to remain controversial.

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The ground-state energy of the TRHA was first calculated by Oguchi [8] in the approximation of free spin waves by making use of the Holstein–Primakoff (HP) representation. Following this, Miyake [9] developed the study of the ground state of the model with XY-like anisotropy of the exchange interaction in an expansion of $1/S$ up to order $1/S^2$, and obtained fairly good values for the ground-state energy in comparison with the result given by Nishimori and Nakanishi [10], who diagonalized numerically the Hamiltonian matrices of small-spin systems. In the numerical calculation by Miyake, the restriction of the boson number of each spin to be less than $2S + 1$, which is called the kinematic interaction, was not taken into account. Dyson [11] discussed the role of kinematic interactions in ferromagnets and clarified that the contribution of kinematic interactions to the free energy becomes exponentially small at temperatures well below the Curie point. In contrast to ferromagnets, however, the kinematic interaction plays important roles for antiferromagnets with small spins even at $T = 0$, so that including its contribution to the ground-state energy will be important.

In addition to the conventional HP representation of spin operators, there exists a transformation to represent the spin systems in terms of boson operators, which was invented by Dyson [11] and then given in a simplified form by Maleev [12]. Recently by using the Dyson–Maleev (DM) transformation, Takahashi [13] showed in his modified spin-wave theory of the SQHA that the ground-state energy in the first-order approximation of the spin-wave interaction coincides quite well with the value of small-spin systems obtained by means of numerical diagonalization. Encouraged by his success, we use the DM transformation in our present study.

The treatment of the kinematic interaction is generally very difficult. Fortunately, by combining it with the DM transformation we can appropriately adopt the method earlier proposed by Kubo [14]. He extended the boson Hilbert space of the HP representation of spin operators restricted within boson numbers less than $2S + 1$ to infinity with repeated correspondence between the spin states and the boson states.

Recently, we studied the static spin correlation function and the sublattice magnetizations of the ground states of the TRHA and SQHA with XY-like anisotropy of nearest-neighbour exchange interaction in the framework of spin-wave theory by using the DM transformation, and found that up to the second-order approximation of the spin-wave interactions the sublattice magnetizations exhibit an anomalous divergent behaviour only in the case of the isotropic TRHA [15]. We think it is possible that this fact is an indication of the disappearance of the Néel order in the ground state of the $S = 1/2$ isotropic TRHA. In the above study, however, we neglected the contribution of the kinematic interaction. The above fact shows the importance of the kinematic interaction. It can be thought that if the perturbation expansion taking account of the kinematic interaction breaks down at some higher order, the true ground state will be a spin-liquid state.

In this paper we study the ground-state energy of the TRHA on the basis of the same spin-wave theory by using the DM transformation and by taking account of the kinematic interaction in the first-order approximation, as mentioned above to clarify the role of the kinematic interaction. For the purpose of comparison the SQHA is also studied in parallel. This paper is organized as follows. In section 2 we present the DM transformation in connection with Kubo's method and give the expression of the ground-state energy investigated in the successive sections. In section 3 we estimate the ground-state energy of the TRHA by ignoring the kinematic interaction. In spite of the rather crude approximation we obtain fairly good values. The ground-state energies are calculated by taking account of the kinematic interactions in section 4. They are described by series expan-

sions as in Kubo [14]. We find that, in comparison with the values of the previous section, the kinematic interactions raise the ground-state energy significantly for small S. The sublattice magnetization is also discussed in this section. The last section is devoted to concluding remarks.

2. Spin Hamiltonian and boson transformation of spin operators

The spin Hamiltonian that we study is described by

$$H_S = J \sum_{(i,j)} [(S_i^y S_j^y + S_i^z S_j^z) + \Delta S_i^x S_j^x] \tag{2.1}$$

where S_i^α ($\alpha = x, y, z$) is the spin operator at the ith site on a two-dimensional triangular lattice or a square lattice, and (i,j) in the summation is taken over all the pairs of nearest-neighbouring lattice sites. The parameter Δ controls the XY-like anisotropy of the exchange interaction with values within $0 \leqslant \Delta \leqslant 1$; and $J > 0$.

To start our spin-wave theory, we postulate for the TRHA that the ground state of equation (2.1) has a Néel order with three sublattice (namely A, B and C) magnetizations having mutual angles of $2\pi/3$ with each other. We choose the sublattice magnetizations in the yz plane and rotate the spin quantization axis of each lattice site to the direction parallel to the corresponding sublattice magnetization. Then rotation around the x axis for B and C sublattices by angles of $2\pi/3$ and $-2\pi/3$, respectively, yields

$$H_S \to H_S = J \sum_{(i,j)} \{[-\tfrac{1}{2}(S_i^y S_j^y + S_i^z S_j^z) \pm \tfrac{1}{2}\sqrt{3}(S_i^y S_j^z - S_i^z S_j^y)] + \Delta S_i^x S_j^x\} \tag{2.2}$$

where the $\pm$ sign means that if the direction of the sublattice magnetization is rotated by an angle of $-2\pi/3$ ($2\pi/3$) from ith site to jth site then $+$ ($-$) sign is chosen. We also assume the SQHA has a Néel order with two sublattice (A and B) magnetizations.

For later use let us review the DM transformation [11]. We consider the spin operator of magnitude S and introduce the boson annihilation and creation operators, a and $a^\dagger$, which obey the commutation relation

$$aa^\dagger - a^\dagger a = 1. \tag{2.3}$$

If we take the m-boson state $|m) = [1/\sqrt{(m!)}](a^\dagger)^m|0)$, the operator F that satisfies

$$F|m) = F(m)|m)$$
$$F(m) = \begin{cases} 1 & \text{for } m = 0 \text{ or } 1 \\ 1[1 - 1/(2S)] \ldots [1 - (m-1)/(2S)] & \text{for } 2 \leqslant m \leqslant 2S \end{cases} \tag{2.4}$$

can be defined. Then one can easily verify the following relations for the matrix elements of the boson operators and the spin operators:

$$\begin{aligned} &(m|T(S - a^\dagger a)T^{-1}|n) = (S-m)\delta_{mn} = M\delta_{MN} = \langle M|S^z|N\rangle \\ &(m|T\sqrt{(2S)}[1 - a^\dagger a/(2S)]aT^{-1}|n) = [(2S-m)(m+1)]^{1/2}\delta_{m+1\,n} = \langle M|S^+|N\rangle \\ &(m|T\sqrt{(2S)}a^\dagger T^{-1}|n) = [(2S-m+1)m]^{1/2}\delta_{m-1\,n} = \langle M|S^-|N\rangle \end{aligned} \tag{2.5}$$

for $0 \leq m, n \leq 2S$, where $M = S - m$ and $N = S - n$, and $T = F^{1/2}$. Thus we obtain the transformation first introduced by Dyson [11]:

$$\begin{aligned} S^z &= T\Xi^z T^{-1} & \Xi^z &= S - a^\dagger a \\ S^+ &= T\Xi^+ T^{-1} & \Xi^+ &= \sqrt{(2S)}[1 - a^\dagger a/(2S)]a \\ S^- &= T\Xi^- T^{-1} & \Xi^- &= \sqrt{(2S)}a^\dagger. \end{aligned} \tag{2.6}$$

It should be noticed that Ξ^+ is not Hermitian conjugate to Ξ^-, in contrast with the relation between S^+ and S^-, since T is not unitary.

It is in general quite difficult to study spin systems by using equations (2.6) taking account of the kinematic interaction. To avoid this difficulty and to remove the restriction on the boson number, we here adopt Kubo's method [14]. He applied it to the study of the ground state of antiferromagnetic two-sublattice spin systems by using the HP representation and the variational method [14]. Kubo's idea is that we map the m-boson state $|m\rangle$ into the spin state $|M\rangle$ with $M = S - \xi(m)$, where $\xi(m) = m \bmod 2S + 1$. By using this mapping the matrices in the original spin Hilbert space with dimension $(2S + 1)$ are replaced with infinite-dimensional matrices in the boson Hilbert space composed of the infinite number of $(2S + 1)$-dimensional matrices. The new Hamiltonian thus obtained has the same ground-state energy as that of the original spin Hamiltonian. We use this method by combining it with the DM transformation, and obtain instead of equations (2.6) the following alternative transformation:

$$\begin{aligned} S^z &\to T\Xi^z T^{-1} & \Xi^z &= S - \xi(a^\dagger a) \\ S^+ &\to T\Xi^+ T^{-1} & \Xi^+ &= \sqrt{(2S)}[1 - \xi(a^\dagger a)/(2S)]a\eta(a^\dagger a) \\ S^- &\to T\Xi^+ T^{-1} & \Xi^- &= \sqrt{(2S)}\eta(a^\dagger a)a^\dagger \end{aligned} \tag{2.7}$$

where $\eta(a^\dagger a) = [\xi(a^\dagger a)/a^\dagger a]^{1/2}$ and $T = F^{-1/2}$. The new operators $\Xi^\pm$ and Ξ^z in equations (2.7) satisfy the same commutation relations as those of the original spin operators as well as of the operators in equations (2.6), and they also have the same matrix elements as those of the spin operators in each $(2S + 1)$-dimensional subspace.

In the case of the SQHA, use of the antiferromagnetic DM transformation is more appropriate than the use of equations (2.6) or (2.7) [13], which transforms spin operators on sublattice B by

$$\begin{aligned} S^z &\to T\Xi^z T^{-1} & \Xi^z &= -S + \xi(a^\dagger a) \\ S^+ &\to T\Xi^+ T^{-1} & \Xi^+ &= \sqrt{(2S)}\eta(a^\dagger a)a^\dagger[1 - \xi(a^\dagger a)/(2S)] \\ S^- &\to T\Xi^+ T^{-1} & \Xi^- &= \sqrt{(2S)}a\eta(a^\dagger a) \end{aligned} \tag{2.8}$$

instead of equations (2.7).

The above new boson transformation makes equation (2.2) into the new Hamiltonian

$$H_S \to \mathcal{T} H_D \mathcal{T}^{-1} \tag{2.9}$$

$$H_D = J \sum_{(i,j)} (P_{ij} + Q_{ij}) \tag{2.10}$$

where $\mathcal{T} = \Pi_i T_i$. We divided the terms of equation (2.10) into two parts, P_{ij} and Q_{ij}, where P_{ij} (Q_{ij}) consists of the products of the terms of even (odd) number boson

operators, and P_{ij} is given by

$$P_{ij} = (\tfrac{1}{2} + \Delta)S\{[1 - \xi(a_i^\dagger a_i)/(2S)]a_i\eta(a_i^\dagger a_i)[1 - \xi(a_j^\dagger a_j)/(2S)]a_j \times \eta(a_j^\dagger a_j) + \eta(a_i^\dagger a_i)a_i^\dagger\eta(a_j^\dagger a_j)a_j^\dagger\} - (\tfrac{1}{2} - \Delta)S\{[1 - \xi(a_i^\dagger a_i)/(2S)] \times a_i\eta(a_i^\dagger a_i)\eta(a_j^\dagger a_j) + \eta(a_i^\dagger a_i)a_i^\dagger[1 - \xi(a_j^\dagger a_j)/(2S)]a_j\eta(a_j^\dagger a_j)\} - \tfrac{1}{2}[S - \xi(a_i^\dagger a_i)][S - \xi(a_j^\dagger a_j)] \tag{2.11}$$

for the TRHA and by

$$P_{ij} = \tfrac{1}{2}(1 + \Delta)S\{[1 - \xi(a_i^\dagger a_i)/(2S)]a_i\eta(a_i^\dagger a_i)a_j\eta(a_j^\dagger a_j) + \eta(a_i^\dagger a_i)a_i^\dagger\eta(a_j^\dagger a_j)a_j^\dagger \times [1 - \xi(a_j^\dagger a_j)/(2S)]\} - \tfrac{1}{2}(1 - \Delta)S\{[1 - \xi(a_i^\dagger a_i)/(2S)]a_i\eta(a_i^\dagger a_i)\eta(a_j^\dagger a_j)a_j^\dagger \times [1 - \xi(a_j^\dagger a_j)/(2S)] + \eta(a_i^\dagger a_i)a_i^\dagger a_j\eta(a_j^\dagger a_j)\} + [S - \xi(a_i^\dagger a_i)][S - \xi(a_j^\dagger a_j)] \tag{2.12}$$

for the SQHA. The odd term Q_{ij} is not written down explicitly here because in the following approximation its contribution to the ground-state energy becomes zero.

It should be noticed that although H_S is a self-adjoint operator, H_D is not, because of the non-unitarity of $\mathcal{T}$. One should be careful in evaluating the expectation values of such operators.

Let us separate the constant and the quadratic terms of a_i and $a_i^\dagger$ of H_D from the remaining terms, which describe spin-wave interactions. Here we only do this for the TRHA:

$$H_D = H_0 + H_{int} \tag{2.13}$$

$$H_0 = -\tfrac{3}{2}JS^2N + \tfrac{1}{2}JS\sum_{(i,j)}[(\tfrac{1}{2} + \Delta)(a_ia_j + a_j^\dagger a_i^\dagger) - (\tfrac{1}{2} - \Delta)(a_i^\dagger a_j + a_j^\dagger a_i) + (a_i^\dagger a_i + a_j^\dagger a_j)] \tag{2.14}$$

where H_0 describes the free spin-wave Hamiltonian of the present system, which has the same form as the free spin-wave Hamiltonian obtained by the HP representation and is evidently Hermitian. Although H_D is non-Hermitian, as stated above, to evaluate the ground-state energy we can expand it in powers of H_{int} in perturbation theory as in the case of ordinary Hamiltonians. Then the ground-state energy is given by

$$E_G = E_0 + \langle H_{int}U(0, -\infty)\rangle_{conn} \tag{2.15}$$

$$U(0, -\infty) = P\exp\left(-i\int_{-\infty}^{0} d\tau H_{int}^I(\tau)\right) \tag{2.16}$$

$$H_{int}^I(\tau) = \exp(iH_0\tau)H_{int}\exp(-iH_0\tau) \tag{2.17}$$

in which $\langle op\rangle$ denotes the expectation value of op with respect to the ground state of H_0, which we express by $|\Psi_G^0\rangle$ in the following, the suffix 'conn' means that only the connected diagrams must be picked up in the calculation of $\langle op\rangle$, and E_0 is the ground-state energy of H_0 [16]. If we retain up to the first order of H_{int} in equation (2.15) we immediately obtain

$$E_G = \langle\Psi_G^0|H_D|\Psi_G^0\rangle = \langle H_D\rangle. \tag{2.18}$$

In the following sections we evaluate equation (2.18).

3. Ground-state energy without kinematic interaction

In this section we discuss the ground-state energy of the TRHA by using equation (2.18) ignoring the kinematic interaction. The value of the ground-state energy of the SQHA is presented only to compare the results.

The diagonalization of H_0 of the TRHA with $\Delta = 1$ has already been presented by Oguchi [8]. Here we give only the results to use below. We distinguish the boson operators on the three sublattices by writing them as a, b or c, each of which belongs to A, B or C sublattice, respectively. Turning to k-space representation by

$$a_n = (3/N)^{1/2} \sum_k a_k \exp(ikr_n^a) \tag{3.1}$$

etc, where N is the total number of lattice sites of the system and r_n^a denotes the site vector of nth lattice site on the A sublattice, we have

$$\begin{aligned} H_0 = -\tfrac{3}{2}JS^2N + \tfrac{3}{2}JS \sum_k \{&2(a_k^\dagger a_k + b_k^\dagger b_k + c_k^\dagger c_k) \\ &- (\tfrac{1}{2} - \Delta)[\gamma_k(a_k^\dagger b_k + b_k^\dagger c_k + c_k^\dagger a_k) + \text{HC}] \\ &+ (\tfrac{1}{2} + \Delta)[\gamma_k(a_{-k} b_k + b_{-k} c_k + c_{-k} a_k) + \text{HC}]\} \end{aligned} \tag{3.2}$$

where $\gamma_k = [\exp(ik_x) + 2\exp(-ik_x/2)\cos(\sqrt{3}\,k_y/2)]/3$. The wavevector k in the summation is taken over the first Brillouin zone of a sublattice. With the definitions of the quantities $\mu_k^{(j)}$ and $\pi_k^{(j)}$ as

$$\begin{aligned} &\mu_k^{(1)} = 2\,\mathrm{Re}(\kappa_k) \qquad \mu_k^{(2)} = -[\mathrm{Re}(\kappa_k) + i\sqrt{3}\,\mathrm{Im}(\kappa_k)] \qquad \mu_k^{(3)} = \mu_{-k}^{(2)} \\ &\pi_k^{(1)} = 2\,\mathrm{Re}(\lambda_k) \qquad \pi_k^{(2)} = -[\mathrm{Re}(\lambda_k) + i\sqrt{3}\,\mathrm{Im}(\lambda_k)] \qquad \pi_k^{(3)} = \pi_{-k}^{(2)} \end{aligned} \tag{3.3}$$

where $\kappa_k = -(\frac{1}{4} - \frac{1}{2}\Delta)\gamma_k$ and $\lambda_k = (\frac{1}{4} + \frac{1}{2}\Delta)\gamma_k$, H_0 is diagonalized to become

$$H_0 = -\tfrac{3}{2}JS(S+1)N + \sum_{j=1}^{3} \sum_k \varepsilon_k^{(j)}(\alpha_k^{(j)\dagger}\alpha_k^{(j)} + \tfrac{1}{2}) \tag{3.4}$$

where

$$\varepsilon_k^{(j)} = 3JS[(1 + \mu_k^{(j)})^2 - (\pi_k^{(j)})^2]^{1/2} \tag{3.5}$$

($j = 1, 2, 3$) are the three spin-wave modes of the system. Introducing the vector notations of the boson operators,

$$(\Psi_k)^t = (a_k, b_k, c_k, a_{-k}^\dagger, b_{-k}^\dagger, c_{-k}^\dagger) \tag{3.6}$$

$$(\Phi_k)^t = (\alpha_k^{(1)}, \alpha_k^{(2)}, \alpha_k^{(3)}, \alpha_{-k}^{(1)\dagger}, \alpha_{-k}^{(2)\dagger}, \alpha_{-k}^{(3)\dagger}) \tag{3.7}$$

the Bogoliubov transformation matrix that combines equation (3.2) with equation (3.4) is given by

$$\Psi_k = W_k \Phi_k \tag{3.8}$$

$$W_k = \frac{1}{\sqrt{3}} \begin{pmatrix} Z_k & V_{-k}^* \\ V_k & Z_{-k}^* \end{pmatrix} \tag{3.9}$$

where

$$Z_k = \begin{pmatrix} \cosh\theta_k & \cosh\phi_k & \cosh\phi_{-k} \\ \cosh\theta_k & \omega^*\cosh\phi_k & \omega\cosh\phi_{-k} \\ \cosh\theta_k & \omega\cosh\phi_k & \omega^*\cosh\phi_{-k} \end{pmatrix}$$
$$V_k = -\begin{pmatrix} \sinh\theta_k & \sinh\phi_k & \sinh\phi_{-k} \\ \sinh\theta_k & \omega^*\sinh\phi_k & \omega\sinh\phi_{-k} \\ \sinh\theta_k & \omega\sinh\phi_k & \omega^*\sinh\phi_{-k} \end{pmatrix} \tag{3.10}$$

with $\omega = -(1 - i\sqrt{3})/2$. The parameters in equation (3.8) are determined by

$$\tanh(2\theta_k) = \frac{\pi_k^{(1)}}{1+\mu_k^{(1)}} \qquad \tanh(2\phi_k) = \frac{\pi_k^{(2)}}{1+\mu_k^{(2)}} = \frac{\pi_{-k}^{(3)}}{1+\mu_{-k}^{(3)}}. \tag{3.11}$$

From equations (3.3) and (3.5) we find that the $\varepsilon_k^{(j)}$ obey the following symmetry relations:

$$\varepsilon_{-k}^{(1)} = \varepsilon_k^{(1)} \qquad \varepsilon_{-k}^{(2)} = \varepsilon_k^{(3)}. \tag{3.12}$$

One can also easily see that among the three spin-wave modes of equation (3.5) only the first mode ($\varepsilon_k^{(1)}$), in the yz plane, is gapless for any values of the anisotropy parameter and that the other two modes, being out of the yz plane, are gapless only for $\Delta = 1$. The energy gaps of the modes $\varepsilon_k^{(2)}$ and $\varepsilon_k^{(3)}$ grow from zero to a finite value as Δ decreases from $\Delta = 1$ to $\Delta = 0$. Note also that inversion symmetry holds only for θ_k, so that $\theta_k = \theta_{-k}$, but $\phi_k \neq \phi_{-k}$.

Now let us evaluate the ground-state energy, equation (2.18). Ignoring the kinematic interaction in H_{int} and taking advantage of Wick's decomposition theorem to evaluate the expectation value of H_D with respect to $|\Psi_G^0\rangle$, we arrive at the result

$$\begin{aligned} E_G = 3JN\{&-\tfrac{1}{2}S + S[u_0 - (\tfrac{1}{2}-\Delta)u_1 + (\tfrac{1}{2}+\Delta)v_1] + \tfrac{1}{2}(\tfrac{1}{2}-\Delta)(2u_0u_1 + v_0v_1) \\ &- \tfrac{1}{2}(\tfrac{1}{2}+\Delta)(2u_0v_1 + u_1v_0) - \tfrac{1}{2}(u_0^2 + u_1^2 + v_1^2) + \tfrac{1}{8}S(\tfrac{1}{2}+\Delta) \\ &\times [4(u_0^2v_1 + u_0u_1v_0 + u_1^2v_1) + (v_0^2 + 2v_1^2)v_1]\} \end{aligned} \tag{3.13}$$

where

$$\begin{aligned} u_0 &= \langle a_n^\dagger a_n\rangle = \frac{1}{2N}\sum_k [\cosh(2\theta_k) + 2\cosh(2\phi_k)] - \tfrac{1}{2} \\ u_1 &= \langle a_n^\dagger b_m\rangle = \frac{1}{2N}\sum_k \{\sigma_k[\cosh(2\theta_k) - \cosh(2\phi_k)] + \sqrt{3}\,\chi_k\cosh(2\phi_k)\} \\ v_0 &= \langle (a_n^\dagger)^2\rangle = \langle (a_n)^2\rangle = -\frac{1}{2N}\sum_k [\sinh(2\theta_k) + 2\sinh(2\phi_k)] \\ v_1 &= \langle a_n b_m\rangle = \langle a_n^\dagger b_m^\dagger\rangle = -\frac{1}{2N}\sum_k \{\sigma_k[\sinh(2\theta_k) - \sinh(2\phi_k)] + \sqrt{3}\,\chi_k\sinh(2\phi_k)\}. \end{aligned} \tag{3.14}$$

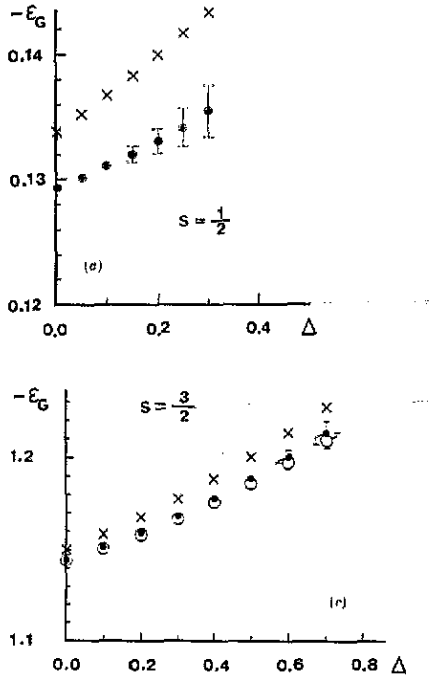
Table 1. The $S = 1/2$ Heisenberg antiferromagnet on a triangular lattice: comparison of the various estimates of the ground-state energy per bond, $-\varepsilon_G = -E_G/3JN$, of (*a*) $\Delta = 1$ (isotropic model) and (*b*) $\Delta = 0$ (XY model). Present theory (i) is the value calculated in section 3 by ignoring the kinematic interaction, and present theory (ii) is that obtained in section 4 by taking it into account. Here only the representative works are listed. In the third column of the table methods are indicated, where (A) means spin-wave theory, (B) numerical diagonalization of Hamiltonian, (C) railroad trestle extrapolation, (D) variational wavefunction and (E) fractional quantum Hall wavefunction.

(*a*) Isotropic model.

$-\varepsilon_G$	Authors	Method	Ref.
0.1872	Present theory (i)	(A)	
0.1823	Nishimori and Nakanishi	(B)	[10]
0.163	Anderson	(C)	[1]
0.1789	Huse and Elser	(D)	[7]
0.1567	Kalmayer and Laughlin	(E)	[5]
0.182	Miyake	(A)	[9]

(*b*) XY model.

$-\varepsilon_G$	Authors	Method	Ref.
0.1344	Present theory (i)	(A)	
0.1293	Present theory (ii)	(A)	
0.1364	Nishimori and Nakanishi	(B)	[10]
0.1348	Miyake	(A)	[9]



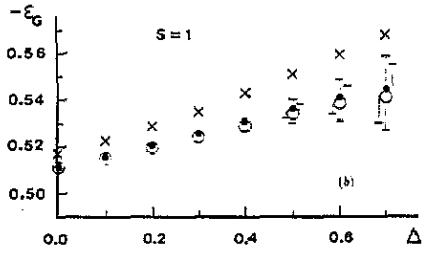


Figure 1. Ground-state energy of Heisenberg antiferromagnet on a triangular lattice: $-\varepsilon_G$ versus Δ for (*a*) $S = 1/2$, (*b*) $S = 1$ and (*c*) $S = 3/2$. The crosses indicate the values without kinematic interaction, and the full circles indicate the values by the Dyson–Maleev transformation taking account of the kinematic interaction. The values by the Holstein–Primakoff representation taking account of the kinematic interaction, which are indicated by the open circles, are also shown for the purpose of comparison. For the error bars attached to the full circles, see text.

Here in equation (3.14) the mth site on the B sublattice is the nearest neighbour of the nth site on the A sublattice, and σ_k and χ_k are the real and imaginary parts of γ_k, respectively.

In table 1 the numerical values of the energy per bond for the $S = 1/2$ TRHA in units of J, $\varepsilon_G = E_G/3JN$, are listed in comparison with the values of the other representative theories, and in figure 1 $-\varepsilon_G$ versus Δ is plotted for $S = 1/2$, 1 and 3/2. Although the approximation in this section is rather crude, the values obtained have relatively good coincidence even for $S = 1/2$ with the values of small-spin systems of $S = 1/2$ obtained by using the numerical diagonalization of the Hamiltonian matrix by Nishimori and Nakanishi [10]. In particular, our value -0.1344 in the case of the $S = 1/2$ XY model ($\Delta = 0$) compares well with their value -0.1364. However, for the isotropic model ($\Delta = 1$) of $S = 1/2$ our value -0.1872 is a little lower than their value -0.1823. In this case our value is also lower than the value of Huse and Elser [7], -0.1789, who calculated it by using the variational calculation of the trial wavefunction described by spin operators (therefore the kinematic interaction is automatically included). This situation will be partly explained by the following consideration. We have ignored the kinematic interaction in the above calculation, which suppresses the zero-point quantum spin fluctuations in the ground state. The effect of the zero-point spin fluctuations becomes large as S becomes small, and since as already stated the energy gaps of two of the three spin-wave modes increase from zero to a finite value as Δ decreases, then the contribution from the zero-point spin fluctuations of these two modes to the ground-state energy decreases as Δ decreases. Hence the effect of the kinematic interaction decreases as S increases and/or Δ decreases. With this consideration we can expect that if the kinematic interaction is taken into account our value of the ground-state energy of $\Delta = 1$ will increase more for smaller S.

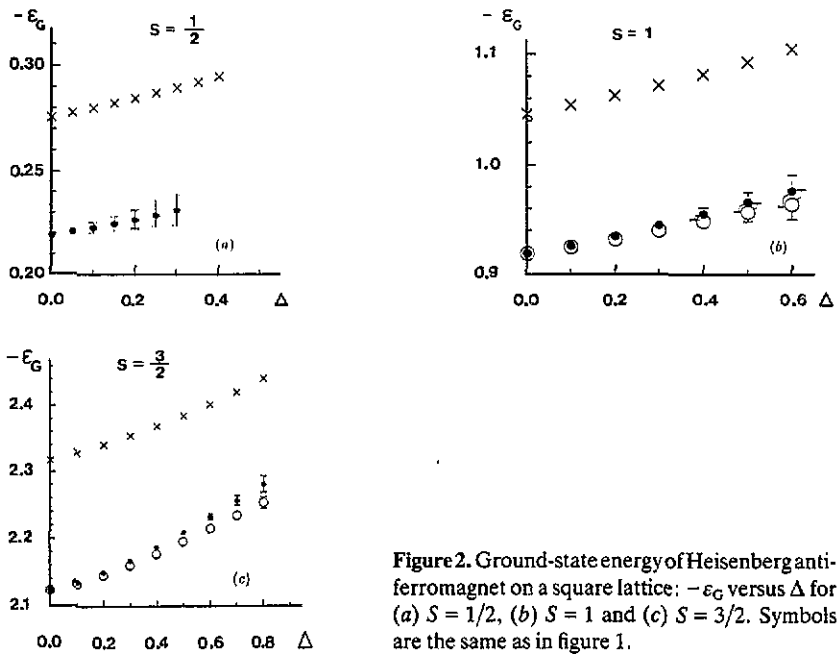


Figure 2. Ground-state energy of Heisenberg antiferromagnet on a square lattice: $-\varepsilon_G$ versus Δ for (*a*) $S = 1/2$, (*b*) $S = 1$ and (*c*) $S = 3/2$. Symbols are the same as in figure 1.

Calculating similarly we also obtain the value of the ground-state energy of the SQHA, -0.3352, which is quite near to the value of the Monte Carlo calculation by Reger, Riera and Young [17], -0.335, as already found by Takahashi [13]. We show $\varepsilon_G = E_G/4JN$ versus Δ for $S = 1/2$, 1 and $3/2$ in figure 2.

These facts tell us that insofar as we calculate the ground-state energy in the first-order approximation of the spin-wave interactions and neglect the kinematic interactions, we get better values by using the DM transformation than by using the HP representation. In the next section the contribution of the kinematic interaction to the ground-state energy is studied.

4. Contribution of kinematic interaction to ground-state energy

Let us evaluate the ground-state energy, equation (2.18), by taking account of the kinematic interaction. In the expectation value of equation (2.10) with respect to the state $|\Psi_G^0\rangle$ there exist terms of the form (i) $D_1 = \langle f(a_i^\dagger a_i)\rangle$, (ii) $D_{20} = \langle f(a_i^\dagger a_i) f(a_j^\dagger a_j)\rangle$, (iii) $D_{21} = \langle f_1(a_i^\dagger a_i) a_i f_2(a_j^\dagger a_j) a_j\rangle$ and $D_{22} = \langle a_i^\dagger f_1(a_i^\dagger a_i) a_j^\dagger f_2(a_j^\dagger a_j)\rangle$ and (iv) $D_{23} = \langle a_i^\dagger f_1(a_i^\dagger a_i) f_2(a_j^\dagger a_j) a_j\rangle$ and $D_{24} = \langle f_1(a_i^\dagger a_i) a_i a_j^\dagger f_2(a_j^\dagger a_j)\rangle$, where $f(n)$, $f_1(n)$ and $f_2(n)$ are some functions and site j is a nearest neighbour to site i. To evaluate these quantities it is convenient to utilize the relations

$$f(a^\dagger a) = \frac{1}{2\pi i}\oint_C \frac{dx}{x} \sum_{n=0}^{\infty} f(n) x^{-n} x^{a^\dagger a} \tag{4.1}$$

and

$$x^{a^\dagger a} = \sum_{p=0}^{\infty} \frac{(x-1)^p}{p!} (a^\dagger)^p (a)^p \tag{4.2}$$

in accordance with Kubo [14], where the integration contour C encircles the origin of the complex x plane. Then, because of equations (4.1) and (4.2), D_1 and the D_{2i} are written as

$$\begin{aligned} D_1 &= \frac{1}{2\pi i}\oint_C \frac{dx}{x} \sum_{n=0}^{\infty} f(n) x^{-n} F_1(x) \\ D_{2i} &= \frac{1}{(2\pi i)^2}\oint_C dx \oint_C dy \frac{1}{xy} \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} f_1(m) f_2(n) \\ &\quad \times \frac{1}{x^m y^n} F_{2i}(x, y) \qquad \text{for } i = 0, 1, 2, 3, 4 \end{aligned} \tag{4.3}$$

where

$$\begin{aligned} F_1(x) &= \sum_{p=0}^{\infty} \frac{(x-1)^p}{p!} W_1(p) \\ F_{2i}(x, y) &= \sum_{p=0}^{\infty}\sum_{q=0}^{\infty} \frac{(x-1)^p (y-1)^q}{p!q!} W_{2i}(p, q) \qquad \text{for } i = 0, 1, 2, 3, 4. \end{aligned} \tag{4.4}$$

In equation (4.4) W_1 and the W_{2i} are defined by

$$\begin{aligned} W_1(p) &= \langle (a_i^\dagger)^p (a_i)^p \rangle \\ W_{20}(p,q) &= \langle (a_i^\dagger)^p (a_i)^p (a_j^\dagger)^q (a_j)^q \rangle \\ W_{21}(p,q) &= \langle (a_i^\dagger)^p (a_i)^{p+1} (a_j^\dagger)^q (a_j)^{q+1} \rangle \\ W_{22}(p,q) &= \langle (a_i^\dagger)^{p+1} (a_i)^p (a_j^\dagger)^{q+1} (a_j)^q \rangle \\ W_{23}(p,q) &= \langle (a_i^\dagger)^p (a_i)^{p+1} (a_j^\dagger)^{q+1} (a_j)^q \rangle \\ W_{24}(p,q) &= \langle (a_i^\dagger)^{p+1} (a_i)^p (a_j^\dagger)^q (a_j)^{q+1} \rangle. \end{aligned} \tag{4.5}$$

We use a slightly different method from that of Kubo [14] to evaluate the quantities $F_1(x)$ and $F_{2i}(x, y)$. The details are shown in the appendix. We eventually get the results

$$\begin{aligned} F_1(x) &= 1/\{[1-(x-1)u_0]^2 - (x-1)^2 v_0^2\}^{1/2} \\ F_{2i}(x,y) &= G_i(x,y) F_2(x,y) \qquad \text{for } i = 1,2,3,4 \end{aligned} \tag{4.6}$$

where

$$\begin{aligned} F_2(x,y) &= 1/[\det(1-R)]^{1/2} \\ R &= \begin{pmatrix} (x-1)u_0 & (x-1)v_0 & (x-1)u_1 & (x-1)v_1 \\ (x-1)v_0 & (x-1)u_0 & (x-1)v_1 & (x-1)u_1 \\ (y-1)u_1 & (y-1)v_1 & (y-1)u_0 & (y-1)v_0 \\ (y-1)v_1 & (y-1)u_1 & (y-1)v_0 & (y-1)u_0 \end{pmatrix} \end{aligned} \tag{4.7}$$

and

$$\begin{aligned} G_0(x,y) &= 1 \\ G_i(x,y) &= \tfrac{1}{2}\mathrm{tr}[B_i(1-R)^{-1}] \qquad \text{for } i = 1,2,3,4. \end{aligned} \tag{4.8}$$

Here the matrices B_i are defined by

$$\begin{aligned} B_1 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ u_1 & v_1 & u_0 & v_0 \\ 0 & 0 & 0 & 0 \\ u_0 & v_0 & u_1 & v_1 \end{pmatrix} \qquad B_2 = \begin{pmatrix} v_1 & u_1 & v_0 & u_0 \\ 0 & 0 & 0 & 0 \\ v_0 & u_0 & v_1 & u_1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\ B_3 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ v_1 & u_1 & v_0 & u_0 \\ u_0 & v_0 & u_1 & v_1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad B_4 = \begin{pmatrix} u_1 & v_1 & u_0 & v_0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ v_0 & u_0 & v_1 & u_1 \end{pmatrix}. \end{aligned} \tag{4.9}$$

Let us write the ground-state energy, equation (2.18), in the case of the TRHA as follows:

$$\begin{aligned} \varepsilon_G = \frac{E_G}{3JN} = \langle P_{ij} \rangle &= -\tfrac{1}{2}S^2 + ST_1 - \tfrac{1}{2}T_{20} + \tfrac{1}{2}(\tfrac{1}{2}+\Delta)(T_{21}+T_{22}) \\ &\quad - \tfrac{1}{2}(\tfrac{1}{2}-\Delta)(T_{23}+T_{24}) \end{aligned} \tag{4.10}$$

where the terms T_1 and T_{2i} are given by

$$\begin{aligned}
T_1 &= \langle \xi(a_i^\dagger a_i) \rangle \\
T_{20} &= \langle \xi(a_i^\dagger a_i)\xi(a_j^\dagger a_j) \rangle \\
T_{21} &= 2S\langle [1 - \xi(a_i^\dagger a_i)/(2S)]a_i \eta(a_i^\dagger a_i)[1 - \xi(a_j^\dagger a_j)/(2S)]a_j \eta(a_j^\dagger a_j) \rangle \\
T_{22} &= 2S\langle \eta(a_i^\dagger a_i)a_i^\dagger \eta(a_j^\dagger a_j)a_j^\dagger \rangle \\
T_{23} &= 2S\langle [1 - \xi(a_i^\dagger a_i)/(2S)]a_i \eta(a_i^\dagger a_i)\eta(a_j^\dagger a_j)a_j^\dagger \rangle \\
T_{24} &= T_{23}.
\end{aligned} \tag{4.11}$$

By using equations (4.6)–(4.9) and putting

$$\begin{aligned}
f(n) &= \xi(n) \\
f_1(n) &= \sqrt{(2S)}[1 - \xi(n)/(2S)]^{1/2}[\xi(n+1)/(n+1)]^{1/2} \\
f_2(n) &= \sqrt{(2S)}[\xi(n+1)/(n+1)]^{1/2}
\end{aligned} \tag{4.12}$$

T_1 and the T_{2i} can be calculated. Expanding $F_1(x)$, $G_i(x, y)$ $(i = 1, 2, 3, 4)$ and $F_2(x, y)$ into Taylor series,

$$\begin{aligned}
F_1(x) &= \sum_{k=0}^{\infty} \frac{F_1^{(k)}}{k!}(x-1)^k \\
G_i(x, y) &= \sum_{k=0}^{\infty}\sum_{l=0}^{\infty} \frac{G_i^{(k,l)}}{k!l!}(x-1)^k(y-1)^l \\
F_2(x, y) &= \sum_{k=0}^{\infty}\sum_{l=0}^{\infty} \frac{F_2^{(k,l)}}{k!l!}(x-1)^k(y-1)^l
\end{aligned} \tag{4.13}$$

we get the following expressions:

$$\begin{aligned}
T_1 &= \sum_{k=0}^{\infty} F_1^{(k)}\delta_S(k) \\
T_{20} &= \sum_{k=0}^{\infty}\sum_{l=0}^{\infty} F_2^{(k,l)}\delta_S(k)\delta_S(l) \\
T_{21} &= \sum_{k=0}^{\infty}\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{G_1^{(k,l)}F_2^{(m,n)}}{k!l!m!n!}\Delta^{k+m}f_1(0)\Delta^{l+n}f_1(0) \\
T_{22} &= \sum_{k=0}^{\infty}\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{G_2^{(k,l)}F_2^{(m,n)}}{k!l!m!n!}\Delta^{k+m}f_2(0)\Delta^{l+n}f_2(0) \\
T_{23} = T_{24} &= \sum_{k=0}^{\infty}\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{G_3^{(k,l)}F_2^{(m,n)}}{k!l!m!n!}\Delta^{k+m}f_1(0)\Delta^{1+n}f_2(0)
\end{aligned} \tag{4.14}$$

where $\Delta^k f(n)$ stands for the kth-order difference of $f(n)$,

$$\Delta^k f(n) = \sum_{m=0}^{k} {}_kC_m(-1)^{k-m}f(n+m) \tag{4.15}$$

and

$$\delta_S(k) = \sum_{m=0}^{k} {}_kC_m(-1)^{k-m}\xi(m). \tag{4.16}$$

We can evaluate ε_G by using equations (4.12)–(4.16) and equation (4.10). The similar calculation for the SQHA can also be performed. We give only its numerical results below the discussion of the results of the TRHA. Notice that T_1 can also be expressed in the form of the integral

$$T_1 = \frac{1}{\pi}\int_0^{\pi} d\theta(u_0 + v_0\cos\theta) \times \left(1 - (2S+1)\frac{(u_0 + v_0\cos\theta)^{2S}}{(1 + u_0 + v_0\cos\theta)^{2S+1} - (u_0 + v_0\cos\theta)^{2S+1}}\right). \tag{4.17}$$

Since the T_{2i} in equation (4.14) are expressed by series expansions, we must sum the first few terms in these series to make a numerical calculation until the values converge within an appropriate accuracy. The convergence is, however, quite poor for $\Delta \sim 1$ and small S. The numerical values of $-\varepsilon_G$ versus Δ are shown in figures 1 and 2, and the values of the TRHA for $\Delta = 0$ are also listed in tables 1 and 2. The numerical summations

Table 2. The values of the ground-state energy per bond $-\varepsilon_G$ of the antiferromagnetic XY model on a triangular lattice for small S estimated by taking account of (lower line) and ignoring (upper line) the kinematic interactions.

S	$-\varepsilon_G$	S	$-\varepsilon_G$	S	$-\varepsilon_G$
1/2	0.13437	1	0.51717	3/2	1.11501
	0.1293		0.5115		1.11445

in T_1 and T_{2i} were performed up to terms of tenth differential order, namely $F_1^{(k)}$ with $k \leqslant 10$, $F_2^{(k,l)}$ with $k + l \leqslant 10$ and $G_i^{(k,l)}F_2^{(m,n)}$ with $k + l + m + n \leqslant 10$. The numerical value of $-\varepsilon_G$ is oscillatory with increasing number of summed terms. When the summations were not converged sufficiently, we gave them by the average of the summed values up to the ninth- and tenth-order terms, and in figures 1 and 2 showed them with error bars. It is unfortunate not to be able to get the values in the isotropic cases. One can see in figures 1 and 2 that as considered in the previous section the kinematic interaction raises the ground-state energy, and the amount of the raise decreases more for larger S and smaller Δ. Comparing the obtained value of $S = 1/2$ TRHA for $\Delta = 0$, $-\varepsilon_G = 0.1293$, with our value in the previous section, 0.1344, and the value of Nishimori and Nakanishi, 0.1364 [10], we find that in the present approximation the kinematic interactions increase the ground-state energy too much to get coincidence with their value. It can be seen that in the case of the SQHA the kinematic interaction also raises the ground-state energy, and the resulting value departs rather from the numerical value given by Reger, Riera and Young [17]. These facts suggest that we must extend the calculation of the perturbation expansion to higher-order terms to include the dynamic effect of the spin-wave interactions and the kinematic interactions.

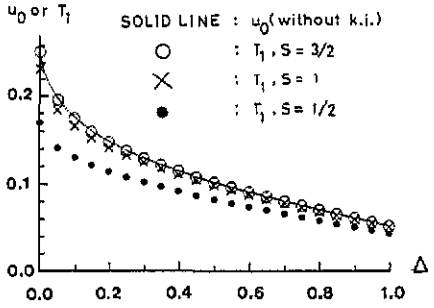


Figure 3. Reduction of sublattice magnetization from the value S for Heisenberg antiferromagnet on a triangular lattice: $u_0 \equiv \langle n \rangle$ and $T_1 \equiv \langle \xi(n) \rangle$ versus Δ, where $n = a_i^\dagger a_i$. In the present approximation the value u_0 does not depend on S.

We can readily apply the above calculation to the HP representation of both models, not by expanding the factor $[1 - a^\dagger a/(2S)]^{1/2}$ in terms of $a^\dagger a/(2S)$. In the case of the TRHA for instance, the T_{2i} in equations (4.11) are replaced by

$$\begin{aligned} T_{21} = T_{22} &= \langle \tilde{f}(a_i^\dagger a_i) a_i \tilde{f}(a_j^\dagger a_j) a_j \rangle \\ T_{23} = T_{24} &= \langle \tilde{f}(a_i^\dagger a_i) a_i a_j^\dagger \tilde{f}(a_j^\dagger a_j) \rangle \end{aligned} \tag{4.18}$$

where

$$\tilde{f}(n) = \sqrt{(2S)}[1 - \xi(n)/(2S)]^{1/2}[\xi(n+1)/(n+1)]^{1/2}. \tag{4.19}$$

The results are also shown in figures 1 and 2. They show the values of the ε_G to be a little larger than those of the DM transformation, and the differences between the values of the HP representation and the DM transformation become negligibly small when the model approaches the XY limit.

Finally let us consider the sublattice magnetization S_{subl}. Instead of the original spin operator S^z we here use equations (2.7). By using the DM transformation the sublattice magnetization is calculated as

$$\langle \Phi_G | S^z | \Phi_G \rangle = S - \langle \Psi_G | \mathcal{T}^2 a_i^\dagger a_i | \Psi_G \rangle / \langle \Psi_G | \mathcal{T}^2 | \Psi_G \rangle \tag{4.20}$$

where $|\Phi_G\rangle$ and $|\Psi_G\rangle = \mathcal{T}|\Phi_G\rangle$ are the ground-state vectors of H_S and H_D, respectively. Therefore retaining only the lowest-order terms in the $1/S$ expansion (free spin-wave approximation) we get

$$S_{subl} = S - u_0. \tag{4.21}$$

When the kinematic interaction is taken into account and equations (2.7) are used instead of the original spin operator S^z, equation (4.21) must be replaced with

$$S_{subl} = S - T_1. \tag{4.22}$$

For the TRHA the plots of u_0 and T_1 versus Δ for $S = 1/2$, 1 and 3/2 are shown in figure 3. We can see that the zero-point spin-wave motions reduce S_{subl} more remarkably for smaller Δ, while the kinematic interactions diminish the reduction of S_{subl} more for smaller Δ and smaller S.

5. Concluding remarks

In the previous sections we have studied the ground-state energies of the Heisenberg antiferromagnets with XY-like anisotropy of nearest-neighbour exchange interactions

on two-dimensional triangular and square lattices, by using the DM transformation within the first-order approximation of spin-wave interaction. The ground-state energies were calculated, first by ignoring the kinematic interaction, and then by taking account of it. We found that the numerical values of the ground-state energy of the TRHA without the kinematic interactions coincide relatively well with the values obtained by the numerical diagonalization method for small-spin systems for $S = 1/2$ and $\Delta = 1$, and that the coincidence is quite good for $S = 1/2$ and $\Delta \simeq 0$. Furthermore, for the SQHA the numerical coincidence is excellent. We also found that the kinematic interactions raise the ground-state energy more for smaller S and larger Δ. However, since the obtained ground-state energy is described in a series and the series converges very poorly for small S and large Δ, we can successfully obtain numerical values only for large S and/or small Δ. The values for $S \simeq 1/2$ and $\Delta = 0$ are seen to be a little larger than the numerical values obtained by the numerical diagonalization method.

We have neglected the dynamic effect of the spin-wave interaction. To take it into account we must calculate the perturbation expansion of H_{int} up to higher order. Miyake [9] studied the contribution of the dynamic effect to the ground-state energy of the TRHA up to $O(S^{-1})$ by using the HP representation and obtained a fairly good value in comparison with that of Nishimori and Nakanishi [10]. The Hamiltonian H_D of the TRHA includes the six-boson terms in addition to the four-boson terms (while the isotropic SQHA has only four-boson interacting terms). Even though these terms in H_D are of $O(S^{-2})$, they give an important numerical contribution to the ground-state energy in the present approximation. This fact suggests that the dynamic effect should be studied, at least up to $O(S^{-2})$. The contribution of the kinematic interaction, which Miyake did not estimate numerically [9], cannot be neglected for small S as shown in this work.

Acknowledgments

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Appendix

We derive equations (4.6)–(4.9) in section 4. Let us consider the following generating function

$$I(x_1, x_2, x_3, x_4) = \langle e^{x_1 a_i^\dagger} e^{x_2 a_i} e^{x_3 a_j^\dagger} e^{x_4 a_j} \rangle \tag{A1}$$

where site j is a nearest neighbour of site i. Then $W_1(p)$ and $W_{2i}(p, q)$ are written as

$$\begin{aligned} W_1(p) &= [(\partial/\partial x_1)^p (\partial/\partial x_2)^p I(x_1, x_2, x_3, x_4)]_{x_1=x_2=x_3=x_4=0} \\ W_{20}(p,q) &= [(\partial/\partial x_1)^p (\partial/\partial x_2)^p (\partial/\partial x_3)^q (\partial/\partial x_4)^q I(x_1,x_2,x_3,x_4)]_{x_1=x_2=x_3=x_4=0} \\ W_{21}(p, q) &= [(\partial/\partial x_1)^p (\partial/\partial x_2)^{p+1} (\partial/\partial x_3)^q (\partial/\partial x_4)^{q+1} I(x_1, x_2, x_3, x_4)]_{x_1=x_2=x_3=x_4=0} \end{aligned} \tag{A2}$$

etc. Using Wick's theorem on the right-hand side of equation (A1) yields

$$I(x_1, x_2, x_3, x_4) = \exp[U(x_1, x_2, x_3, x_4)] \tag{A3}$$

where

$$U(x_1, x_2, x_3, x_4) = (x_1x_2 + x_3x_4)u_0 + (x_1x_4 + x_2x_3)u_1 + \tfrac{1}{2}(x_1^2 + x_2^2 + x_3^2 + x_4^2)v_0 + (x_1x_3 + x_2x_4)v_1. \tag{A4}$$

Then from equations (A2), (A3), (4.5) and (4.6) we obtain the following expressions:

$$\begin{aligned} F_1(x) &= [e^{\Gamma_1} e^{U(x_1,x_2,x_3,x_4)}]_{x_1=x_2=x_3=x_4=0} \\ F_{20}(x, y) &= [e^{\Gamma_2} e^{U(x_1,x_2,x_3,x_4)}]_{x_1=x_2=x_3=x_4=0} \\ F_{2i}(x, y) &= [\Lambda_i e^{\Gamma_2} e^{U(x_1,x_2,x_3,x_4)}]_{x_1=x_2=x_3=x_4=0} \qquad \text{for } i = 1, 2, 3, 4 \end{aligned} \tag{A5}$$

where

$$\begin{aligned} \Gamma_1 &= (x-1)\partial^2/\partial x_1 \partial x_2 \\ \Gamma_2 &= (x-1)\partial^2/\partial x_1 \partial x_2 + (y-1)\partial^2/\partial x_3 \partial x_4 \end{aligned} \tag{A6}$$

and

$$\begin{aligned} \Lambda_1 &= \partial^2/\partial x_2 \partial x_4 \qquad & \Lambda_2 &= \partial^2/\partial x_1 \partial x_3 \\ \Lambda_3 &= \partial^2/\partial x_2 \partial x_3 \qquad & \Lambda_4 &= \partial^2/\partial x_1 \partial x_4. \end{aligned} \tag{A7}$$

Evaluation of $F_1(x)$ and $F_{20}(x, y)$

Let us first evaluate $F_{20}(x, y)$. Since Γ_2 is a second-order differential operator and U is of bilinear form, $F_{20}(x, y)$ becomes

$$F_{20}(x, y) = \sum_{n=0}^{\infty} \frac{\Gamma_2^n U^n}{(n!)^2}. \tag{A8}$$

It is convenient to write Γ_2 and U in a general form, $\Gamma_2 = \Sigma_{\lambda,\mu=1}^4 \Gamma_{\lambda\mu}\partial_\lambda\partial_\mu$ and $U = \Sigma_{\lambda,\mu=1}^4 U_{\lambda\mu}x_\lambda x_\mu$, where $\Gamma_{\lambda\mu} = \Gamma_{\mu\lambda}$ and $U_{\lambda\mu} = U_{\mu\lambda}$ are assumed. Then we have

$$\begin{aligned} \Gamma_2^n U^n &= \sum_P \sum_{\lambda_1} \cdots \sum_{\lambda_{2n}} \Gamma_{\lambda_1\lambda_2} \cdots \Gamma_{\lambda_{2n-1}\lambda_{2n}} U_{\lambda_{P(1)}\lambda_{P(2)}} \cdots U_{\lambda_{P(2n-1)}\lambda_{P(2n)}} \\ &= \sum_P \Pi_P. \end{aligned} \tag{A9}$$

In equation (A9) P stands for a permutation of $2n$ suffices of λ and it runs over all these permutations. Here Π_P consists of the product of connected parts,

$$\Upsilon_m = \sum_{\lambda_1} \cdots \sum_{\lambda_{2m}} \Gamma_{\lambda_1\lambda_2} U_{\lambda_2\lambda_3} \Gamma_{\lambda_3\lambda_4} \cdots \Gamma_{\lambda_{2m-1}\lambda_{2m}} U_{\lambda_{2m-1}\lambda_1} \tag{A10}$$

so that we can write

$$\Pi_P = \Upsilon_{m_1} \Upsilon_{m_2} \cdots \tag{A11}$$

where the condition $m_1 + m_2 + \ldots = n$ must be satisfied.

We classify each Π_P in the summation over P into topologically equivalent terms and count the number of terms that belong to each class. Let us consider the class under the condition, $\Sigma_{k=1} k s_k = n$, which consists of $s_1 \Upsilon_1$, $s_2 \Upsilon_2$ and so on. The number of these topologically equivalent terms is counted through the following considerations:

(i) The number of the ways that n $\Gamma_{\lambda\mu}$ are connected to n $U_{\lambda\mu}$ is $n!4^n$.

(ii) Let us define $R_{\lambda\mu} = 4\Sigma_\gamma \Gamma_{\lambda\gamma} U_{\gamma\mu}$. The number of ways that the n $R_{\lambda\mu}$ are connected to s_1 Y_1, s_2 Y_2 and so on is $n!/s_1!s_2! \ldots$.

(iii) However, factor k is counted too many times for Y_k in (ii) since there is no end in the closed loop. Then one must multiply by the factor $1/(1^{s_1}2^{s_2} \ldots)$ to correct it.

(iv) We have also counted too many times when we connect the k $R_{\lambda\mu}$ into a closed loop Y_k. The factor of 4^n in (i) must be corrected by multiplying by the factor $1/(2^{s_1}2^{s_2} \ldots)$ because in (i) one can always find the same term by relabelling the suffices of the other terms connected in different ways.

Therefore, by collecting all the factors given in (i)–(iv) the summation over P in equation (A9) can be performed as follows:

$$\Gamma_2^n U^n = \sum_{s_1} \sum_{s_2} \delta(s_1 + 2s_2 + \ldots, n)(n!)^2 \prod_{k=1} \frac{1}{s_k!} (2^{2k-1} Y_k/k)^{s_k} \tag{A12}$$

where $\delta(i, j)$ denotes Kronecker's delta. Then equation (A8) becomes

$$F_{20}(x, y) = \prod_{k=1}^{\infty} \sum_{s_k} \frac{1}{s_k!} (2^{2k-1} Y_k/k)^{s_k} = \exp\left(\tfrac{1}{2} \sum_{k=1}^{\infty} \frac{1}{k} 4^k Y_k\right). \tag{A13}$$

Since $Y_k = \mathrm{tr}[(R/4)^k]$, we arrive at the expression

$$F_{20}(x, y) = \exp\left(\tfrac{1}{2} \sum_{k=1} \frac{1}{k} \mathrm{tr}(R^k)\right) = \exp\{-\tfrac{1}{2}\mathrm{tr}[\ln(1 - R)]\}$$

$$= \frac{1}{[\det(1 - R)]^{1/2}} = F_2(x, y). \tag{A14}$$

The matrix R is obtained by using the explicit forms of the matrices Γ and U, and given by equation (4.8).

In the above calculation of $F_{20}(x, y)$, if we use the differential operator Γ_1 instead of Γ_2 we can get $F_1(x)$ straightforwardly by replacing the matrix R with

$$R_1 = (x - 1) \begin{pmatrix} u_0 & v_0 \\ v_0 & u_0 \end{pmatrix} \tag{A15}$$

so that $F_1(x)$ in equation (4.7) is obtained.

Evaluation of $F_{2i}(x, y)$ ($i = 1, 2, 3, 4$)

We can proceed to evaluate $F_{2i}(x, y)$ for $i = 1, 2, 3, 4$ in a similar way to the above calculation, and obtain

$$F_{2i}(x, y) = \sum_{n=1}^{\infty} \frac{1}{(n-1)!n!} \Lambda_i \Gamma_2^{n-1} U^n \tag{A16}$$

as in equation (A8). Writing Λ_i in a general form, $\Lambda_i = \Sigma_{\lambda\mu} \Lambda^i_{\lambda\mu} \partial_\lambda \partial_\mu$, where $\Lambda^i_{\lambda\mu} = \Lambda^i_{\mu\lambda}$, then after the operations of Λ_i and Γ_2 on U in equation (A16) we obtain

$$\Lambda_i \Gamma_2^{n-1} U^n = \sum_P \sum_{\lambda_1} \ldots \sum_{\lambda_{2n}} \Lambda^i_{\lambda_1\lambda_2} \Gamma_{\lambda_3\lambda_4} \ldots \Gamma_{\lambda_{2n-1}\lambda_{2n}} U_{\lambda_{P(1)}\lambda_{P(2)}} \ldots U_{\lambda_{P(2n-1)}\lambda_{P(2n)}}$$

$$= \sum_P \Pi^i_P. \tag{A17}$$

By introducing the disconnected part of order m

$$\Omega^i_m = \sum_{\lambda_1} \dots \sum_{\lambda_{2m}} \Lambda^i_{\lambda_1\lambda_2} U_{\lambda_2\lambda_3} \Gamma_{\lambda_3\lambda_4} U_{\lambda_4\lambda_5} \dots \Gamma_{\lambda_{2m-1}\lambda_{2m}} U_{\lambda_{2m}\lambda_1} \tag{A18}$$

which includes a factor of Λ^i in addition to Γ and U, we can describe Π^i_P by

$$\Pi^i_P = \Omega^i_m \Upsilon_{m_1} \Upsilon_{m_2} \dots \tag{A19}$$

where the condition $m + m_1 + m_2 + \dots = n$ must be satisfied. Analysing the topologically equivalent terms of equation (A17) in a similar manner to the previous calculation and defining $B_{i,\lambda\mu} = 4 \sum_\nu \Lambda^i_{\lambda\nu} U_{\nu\mu}$, we obtain

$$F_{2i}(x, y) = \sum_{n=1} \sum_{m} \sum_{s_1} \sum_{s_2} \dots \delta(m + s_1 + 2s_2 + \dots, n) 2^{2m-1} \Omega^i_m$$

$$\times \prod_{k=1} \frac{1}{s_k!} (2^{2k-1}/k)^{s_k} \Upsilon_k = \tfrac{1}{2} \sum_{m=1} \mathrm{tr}(B_i R^{m-1}) F(x, y)$$

$$= \tfrac{1}{2} \mathrm{tr}[B_i (1 - R)^{-1}] F(x, y) \tag{A20}$$

where the relation $\Omega^i_m = \mathrm{tr}[\Lambda^i U(\Gamma U)^{m-1}] = 4^{-m} \mathrm{tr}(B_i R^{m-1})$ is used. The matrices B_i are easily calculated by using the definition and R. They are given by equation (4.9).

Thus we have derived equations (4.6)–(4.9).

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