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Ground-State Properties and Phase Diagram of the Quantum *XXZ* Antiferromagnet on a Triangular Lattice

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Long-range order, especially chiral order, in the two-dimensional spin $\frac{1}{2}$ XXZ antiferromagnet $H=J\Sigma(S_i^xS_j^x+S_i^yS_j^y+\Delta S_i^zS_j^z)$ on a triangular lattice is studied, partially by showing exact ground states and partially using the spin-wave theory. Exact ground states in the region $\Delta\leq-0.5$ are found. These states are not disordered by quantum fluctuation. Most of the ground states at $\Delta=-0.5$ have a so-called 120° structure. Ground-state properties in the region $-0.5\leq\Delta\leq1$ are studied using the spin-wave theory. It is shown that quantum fluctuations are enhanced in the ground states as Δ is increased. The phase diagram of the relevant system at low temperatures is also discussed using the spin-wave theory.

§1. Introduction

As Villain[1)] pointed out, the ground-state degeneracy of chirality in the frustrated classical XY model on two-dimensional lattices causes an Ising-type phase transition at finite temperatures.[2-4)] The classical antiferromagnetic XXZ model on a triangular lattice (the classical AFT XXZ model) described by the Hamiltonian $H=J\Sigma(S_i^xS_j^x+S_i^yS_j^y+\Delta S_i^zS_j^z)$ with $-0.5<\Delta<1$ has the same properties in the low-temperature phase as those of the XY model, since the ground states have a so-called 120° structure and are discretely degenerate with chirality. Miyashita[5)] studied this system using Monte Carlo simulation and showed that a chiral-order phase-transition appears at finite temperatures. He found that a reentrant phase transition occurs for the model $\Delta>-0.5$, which is caused by the non-trivial degeneracy of the ground states at $\Delta=-0.5$.

In the quantum case, systems are fluctuating with frustration and quantum effects.[6,7)] Existence of chiral order has been studied by many authors in the two-dimensional $S=\frac{1}{2}$ AFT XY model. Results of studies using the exact diagonalization[8)] in finite clusters with different size are not consistent with each other.[9,10)] Thus the size of calculated clusters is not enough large to predict properties of infinite systems. A critical point appeared in a study using the Monte Carlo method.[11)] In a study using high-temperature series-expansions, no critical point was found.[12)] In the previous paper,[13)] we studied this $S=\frac{1}{2}$ AFT XXZ model using the super-effective-field theory[14)] and we concluded, from the size-dependence of critical temperatures, that a chiral order exists at finite temperatures at least in the region $-0.5\leq\Delta\leq0.5$. For the case near the symmetry of the Heisenberg model, say $\Delta>0.5$, the size of the clusters is not large enough to conclude the existence of the chiral order.

In the present paper we show exact ground states of a special model, which is the two-dimensional AFT XXZ model with $\Delta=-0.5$. These ground states have the degeneracy of chirality and the sublattice magnetization is fully ordered in these states. We study the properties of ground states in the model with Δ larger than -0.5 using the spin-wave theory and we show how the quantum effects change the sublattice magnetization and chirality as Δ is increased. Our approach to the study of frustrated quantum spin systems is contrary to that by Fazekas and Anderson.[6)] They continued the disordered ground states changing Δ from infinity to 1. We study the ground states by changing Δ from an ordered region, say -0.5, to 1. At the end of the present paper, we study thermal properties in this model using the spin-wave theory[15,16] and discuss a phase diagram on chiral order considering all the above results together with our previous ones.[13]

In the next section we show exact ground states of the quantum XXZ model with $\Delta=-0.5$ and $\Delta<-0.5$. In §3 we study the properties of ground states in the quantum XXZ model with various values of Δ using the spin-wave theory. In §4 thermal properties of the model $\Delta\sim-0.5$ are studied and the phase diagram of chiral order is discussed. Section 5 contains summary and discussion.

§2. Exact Ground States of the Quantum AFT XXZ Model with $\Delta\leq-0.5$

The ground states of the $S=\frac{1}{2}$ XXZ antiferromagnet on the triangular lattice are exactly found here in the region with $\Delta\leq-0.5$. We briefly derive them and discuss the properties of them.

2.1 Case of $\Delta=-0.5$

First we consider the ground states in the $S=1/2$ AFT XXZ model with $\Delta=-0.5$. It is convenient to change the spin-space and define the Hamiltonian as

$$H=J\sum_{\langle i,j\rangle}\left(\sigma_i^z\sigma_j^z+\sigma_i^x\sigma_j^x-\frac{1}{2}\sigma_i^y\sigma_j^y\right), \quad (2.1)$$

where the summation is taken over all nearest-neighbour pairs of sites and σ^a $(a=x, y, z)$ are the Pauli matrices. In this way we choose the quantized axis on the plane to which all the spin-vectors belong in the ground states of the classical model. Here we consider the following two states,

$$|\mathrm{GS}.1\rangle=U\,|\text{all spins}\uparrow\rangle,$$
$$|\mathrm{GS}.2\rangle=U^\dagger\,|\text{all spins}\uparrow\rangle, \quad (2.2)$$

where $\sigma^z|\uparrow\rangle=|\uparrow\rangle$ and $\sigma^z|\downarrow\rangle=-|\downarrow\rangle$ and U is a rotation operator defined by

$$U\equiv\exp\left(i\frac{\pi}{3}\sum_{i\in\mathrm{B\,sub}}\sigma_i^y-i\frac{\pi}{3}\sum_{i\in\mathrm{C\,sub}}\sigma_i^y\right). \quad (2.3)$$

This operator rotates all the spins on the sublattice B through the angle $2\pi/3$ and on the sublattice C through the angle $-2\pi/3$ about the y axis. With this operator, quantum spins have the 120° structure. These states have a form similar to the trial wavefunction which was proposed by Miyashita[17] and by Betts and Miyashita[18] as the ground state of the $s=\frac{1}{2}$ AFT XY model.

From now we show that the states $|\mathrm{GS}.1\rangle$ and $|\mathrm{GS}.2\rangle$ belong to the ground states. First we indicate that the state $|\text{all spins}\uparrow\rangle$ is one of the ground states of the transformed Hamiltonian, $U^\dagger HU$, which is given by

$$U^\dagger HU=-\frac{J}{2}\sum_{\langle i,j\rangle}(\sigma_i^z\sigma_j^z+\sigma_i^x\sigma_j^x+\sigma_i^y\sigma_j^y)+\frac{\sqrt{3}\,J}{2}\sum_{(i\to j)}(\sigma_i^z\sigma_j^x-\sigma_i^x\sigma_j^z). \quad (2.4)$$

This Hamiltonian (2.4) is divided into cell-Hamiltonians which are defined on each triangular cell as shown in Fig. 1, namely

$$U^\dagger HU=\sum_{\triangle(i,j,k)}U^\dagger H_{\triangle(i,j,k)}U, \quad (2.5)$$

where $\triangle(i,j,k)$ indicates the upward triangular cell labeled with the sites i, j and k. The cell-Hamiltonian is given by

$$U^\dagger H_{\triangle(1,2,3)}U=-\frac{J}{2}\sum_{\substack{\langle i,j\rangle=\\ \langle 1,2\rangle,\langle 2,3\rangle,\langle 3,1\rangle}}(\sigma_i^z\sigma_j^z+\sigma_i^x\sigma_j^x+\sigma_i^y\sigma_j^y)$$
$$+\frac{\sqrt{3}\,J}{2}\sum_{\substack{(i\to j)=\\ (1\to 2),(2\to 3),(3\to 1)}}(\sigma_i^z\sigma_j^x-\sigma_i^x\sigma_j^z). \quad (2.6)$$

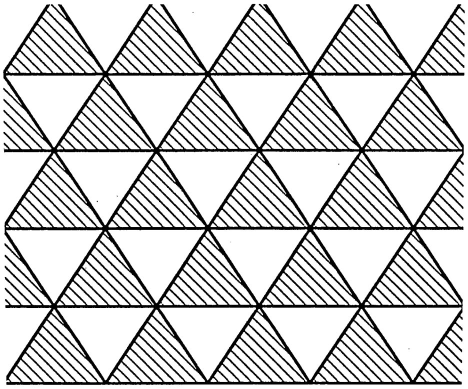

Fig. 1. A triangular lattice is divided into shaded triangular cells. The cell-Hamiltonians are defined on each shaded cell.

The state $|\text{all spins}\uparrow\rangle$ is one of the eigenstates of this cell-Hamiltonian and the eigenvalue of this state is $-1.5J$. Then we show that the state $|\text{all spins}\uparrow\rangle$ has a minimum energy. The cell-Hamiltonian (2.6) can be easily diagonalized in a triangular cell and all the eigenstates and all the eigenvalues can be evaluated. From a straightforward calculation, we have found that the state $|\uparrow\uparrow\uparrow\rangle$ is one of the ground states of the transformed cell-Hamiltonian (2.6) and that the ground-state energy is $-1.5J$. We show that the operator $H_{\triangle(1,2,3)}+1.5J$ is positive semidefinite in the space of spin states on the total space. We construct orthonormal bases of spin states on the total lattice with the spin-configurations $|\uparrow\rangle$ or $|\downarrow\rangle$ on each site. For example, one of the bases is $|\psi_m\rangle=|\uparrow\downarrow\uparrow\uparrow\uparrow\cdots\rangle$. This state is the product of a three-spin state on the sites 1, 2 and 3 and a spin-state on other sites as

$$|\psi_m\rangle=|\uparrow\downarrow\uparrow\rangle_\triangle\otimes|\uparrow\uparrow\cdots\rangle', \tag{2.7}$$

where $|\uparrow\uparrow\cdots\rangle'$ denotes a state $|\psi_m\rangle$ except the three sites 1, 2 and 3. Each three-spin state on the sites 1, 2 and 3 in these bases can be represented with the eigenstates of the cell-Hamiltonian $U^\dagger H_{\triangle(1,2,3)}U$ as

$$|\uparrow\downarrow\uparrow\rangle_\triangle=\sum_{n=1}^{8}a_m(n)\,|\phi_n\rangle_\triangle, \tag{2.8}$$

where $|\phi_n\rangle_\triangle$ $(n=1,\cdots,8)$ denote the eigenstates of the cell-Hamiltonian $U^\dagger H_{\triangle(1,2,3)}U$ in the triangular cell $\triangle(1,2,3)$ as

$$U^\dagger H_{\triangle(1,2,3)}U\,|\phi_n\rangle_\triangle=\varepsilon_n\,|\phi_n\rangle_\triangle. \tag{2.9}$$

Thus any spin-configuration $|\psi_m\rangle$ can be written as

$$|\psi_m\rangle=\sum_{n=1}^{8}a_m(n)\,|\phi_n\rangle_\triangle\otimes|\psi_m\rangle', \tag{2.10}$$

where $|\psi_m\rangle'$ denotes a state $|\psi_m\rangle$ except the three sites 1, 2 and 3. Using this representation, any state $|\Psi\rangle$ which is constructed with a linear combination of $|\psi_m\rangle$ can be represented as

$$|\Psi\rangle=\sum_m\alpha_m\,|\psi_m\rangle$$
$$=\sum_m\alpha_m\sum_{n=1}^{8}a_n(m)\,|\phi_n\rangle_\triangle\otimes|\psi_m\rangle'. \tag{2.11}$$

The expectation value of the operator $H_{\triangle(1,2,3)}+1.5J$ with respect to this state is

$$\langle\Psi|\,H_\triangle+1.5J\,|\Psi\rangle=\sum_l\sum_m\alpha_l^*\alpha_m\sum_{n=1}^{8}a_n^*(l)a_n(m)'\,\langle\psi_l|\psi_m\rangle'(\varepsilon_n+1.5J)$$
$$=\sum_{n=1}^{8}\Big(\sum_l\alpha_l a_n(l)|\psi_l\rangle'\Big)^\dagger\Big(\sum_m\alpha_m a_n(m)|\psi_m\rangle'\Big)(\varepsilon_n+1.5J). \tag{2.12}$$

As mentioned above, the minimum value of ε_n is $-1.5\,J$. Then we summarize the above discussions as follows. For any state $|\Psi\rangle$ on the total lattice, the expectation value of the operator $U^\dagger H_{\triangle(1,2,3)}U+1.5J$ is always positive or zero as

$$\langle\Psi|\,U^\dagger H_{\triangle(1,2,3)}U+1.5J\,|\Psi\rangle\geq 0. \tag{2.13}$$

Thus the operator $U^\dagger H_{\triangle(1,2,3)}U+1.5J$ is positive semidefinite. Then the total operator $U^\dagger HU+1.5NJ$, which is given by the summation of the cell-operator $U^\dagger H_\triangle U+1.5J$, is also positive semidefinite. From the results that the state $|\text{GS.1}\rangle$ belongs to the eigenstates, that the eigenvalues of these states are all equal to $-1.5JN$ and that the minimum energy of the operator $U^\dagger HU$ is $-1.5NJ$, we conclude that the state $|\text{GS.1}\rangle$

belongs to the ground states of the total Hamiltonian (2.1).

In the same way, the state $|\text{spin all}\uparrow\rangle$ is also shown to be one of the eigenstates of the transformed Hamiltonian $UHU^\dagger$ and it takes a minimum energy. Then the state $|\text{GS}.2\rangle$ is also shown to be one of the ground states of the Hamiltonian (2.1).

These ground states are not fluctuating with quantum effect and have fully-ordered sublattice-magnetization and chirality. The signs of the chirality are opposite to each other as follows:

$$\langle \text{GS}.1|Q|\text{GS}.1\rangle=-\frac{3}{4}$$

$$\langle \text{GS}.2|Q|\text{GS}.2\rangle=\frac{3}{4}, \qquad (2.14)$$

where Q is the order parameter of the chiral order defined by

$$Q=\frac{1}{3N}\frac{1}{2\sqrt{3}}\sum_{\langle i\to j\rangle}(\sigma_i^z\sigma_j^x-\sigma_i^x\sigma_j^z), \qquad (2.15)$$

where N is the number of sites. Here we briefly discuss some interesting properties of these ground-states. The ground states are degenerate with rotated states, namely with $R|\text{GS}.1\rangle$ and $R|\text{GS}.2\rangle$, where

$$R=\exp\left(i\frac{\theta}{2}\sum_i\sigma_i^y\right), \qquad (2.16)$$

since the Hamiltonian (2.1) has the O(2) symmetry. However, there is another type of degeneracy. The rotated states

$$|\text{GS}.1'\rangle=UR_3|\text{all spins}\uparrow\rangle=R_3'|\text{GS}.1\rangle, \qquad (2.17)$$

also belong to the ground states, where

$$R_3=\exp\left(i\frac{\theta}{2}\sum_i\sigma_i^y\right)\exp\left(i\frac{\phi}{2}\sum_i\sigma_i^x\right), \qquad (2.18)$$

and

$$\begin{aligned}R_3'&=UR_3U^\dagger\\&=\exp\left(i\frac{\theta}{2}\sum_i\sigma_i^y\right)\\&\quad\times\exp\left\{i\frac{\phi}{2}\left(\sum_A\sigma_i^x+\sum_B\left(-\frac{1}{2}\sigma_i^x+\frac{\sqrt{3}}{2}\sigma_i^z\right)+\sum_C\left(-\frac{1}{2}\sigma_i^x-\frac{\sqrt{3}}{2}\sigma_i^z\right)\right)\right\}. \qquad (2.19)\end{aligned}$$

Because the state $|\uparrow\uparrow\uparrow\rangle$ is also one of the ground states of the transformed Hamiltonian $R_3^\dagger U^\dagger H_\triangle UR_3$ which is given by

$$\begin{aligned}R_3^\dagger U^\dagger H_{\triangle(1,2,3)}UR_3=&-\frac{J}{2}\sum_{\substack{\langle i,j\rangle=\\\langle 1,2\rangle,\langle 2,3\rangle,\langle 3,1\rangle}}(\sigma_i^z\sigma_j^z+\sigma_i^x\sigma_j^x+\sigma_i^y\sigma_j^y)\\&+\frac{\sqrt{3}J}{2}\sum_{\substack{(i\to j)=\\(1\to 2),(2\to 3),(3\to 1)}}\{\cos\phi(\sigma_i^z\sigma_j^x-\sigma_i^x\sigma_j^z)-\sin\phi(\sigma_i^x\sigma_j^y-\sigma_i^y\sigma_j^x)\}. \qquad (2.20)\end{aligned}$$

Similarly the states $|\text{GS}.2'\rangle=U^\dagger R_3|\text{all spins}\uparrow\rangle$ belong to the ground states.

The Hamiltonian (2.1) is not invariant with respect to $R_3^\dagger$, namely

$$R_3'^\dagger HR_3'\neq H. \qquad (2.21)$$

Only the ground-state energy is invariant under the irregular O(3) transformation, R_3'. This degeneracy of the ground states is the same as that of the corresponding classical model.[5] The states $|\text{GS}.1'\rangle$ have negative values of the chirality as

$$\langle \text{GS}.1'|Q|\text{GS}.1'\rangle=-\frac{3}{4}\cos^2\phi, \qquad (2.22)$$

and $|\text{GS}.2'\rangle$ have positive one. The transformation R_3' corresponds to closing the umbrella of spins which has the 120° structure and changes the absolute value of the chirality between 3/4 and 0, but never changes the sign. Thus the ground states have degeneracy of the chirality and the irregular O(3) symmetry.

Most of the ground states, $|\text{GS.1}'\rangle$ (and $|\text{GS.2}'\rangle$), have a scalar chiral order[19] defined by the operator

$$E=E_{123}=S_1\cdot(S_2\times S_3), \tag{2.23}$$

because we have

$$\begin{aligned}\langle \text{GS.1}'|E|\text{GS.1}'\rangle&=\langle \text{all spins}\uparrow|R_3^{\dagger}U^{\dagger}EUR_3|\text{ all spins}\uparrow\rangle\\ &=-\frac{3\sqrt{3}}{2}\sin\phi\cos^2\phi\neq 0.\end{aligned} \tag{2.24}$$

2.2 Ferromagnetic Ising-like model ($\Delta<-0.5$)

Next we consider the region $\Delta<-0.5$ in which the interactions of spin-z-components namely ferromagnetic Ising interactions are dominant. Here we use the following Hamiltonian

$$H=J\sum_{\langle i,j\rangle}(\sigma_i^x\sigma_j^x+\sigma_i^y\sigma_j^y+\Delta\sigma_i^z\sigma_j^z). \tag{2.25}$$

The ground-states are given by

$$\begin{aligned}|\text{GS.3}\rangle&=|\text{all spins}\uparrow\rangle,\\ |\text{GS.4}\rangle&=|\text{all spins}\downarrow\rangle,\end{aligned} \tag{2.26}$$

where the states $|\uparrow\rangle$ and $|\downarrow\rangle$ are the eigenstates of the Pauli operator σ^z. These states have a ferromagnetic order and no chiral order.

We show the proof that these two states belong to the ground states. Clearly these states, $|\text{GS.3}\rangle$ and $|\text{GS.4}\rangle$ are the eigenstates of the Hamiltonian (2.25) and the eigenvalues of both states are $3\Delta NJ$. Then we indicate here that the states (2.26) have a minimum energy. We again divide the Hamiltonian (2.25) into the cell-Hamiltonians which are given by

$$H_{\triangle(1,2,3)}=J\sum_{\substack{\langle i,j\rangle=\\ \langle 1,2\rangle,\langle 2,3\rangle,\langle 3,1\rangle}}(\sigma_i^x\sigma_j^x+\sigma_i^y\sigma_j^y+\Delta\sigma_i^z\sigma_j^z). \tag{2.27}$$

Clearly the states (2.26) are also the eigenstates of this cell-Hamiltonian. From direct diagonalization of the cell-Hamiltonian, we have found that states $|\uparrow\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\downarrow\rangle$ are the ground states of the cell-Hamiltonian (2.27) in $\Delta\leq-0.5$ and the eigenvalue is $3\Delta J$. From this result we conclude, in the same way as shown in the previous subsection, that the operator $H_{\triangle(1,2,3)}-3\Delta J$ is positive semidefinite in the spin-space on the total lattice. In this way it has been proved that all the eigenvalues of the Hamiltonian H are larger than $3\Delta JN$ or just equal to it.

Thus $|\text{GS.3}\rangle$ and $|\text{GS.4}\rangle$ belong to the eigenstates and the eigenvalue of these states, $3\Delta JN$, is the minimum energy of the operator H. Consequently we conclude that the states $|\text{GS.3}\rangle$ and $|\text{GS.4}\rangle$ belong to the ground states of the total Hamiltonian (2.25). As shown in the above proof, the states (2.26) belong also to the ground states of the XXZ model with $\Delta=-0.5$.

§3. Spin-Wave Expansion

Here we estimate values of the sublattice-magnetization and the chirality in ground states of the quantum spin S AFT XXZ model with $\Delta\geq-0.5$ using the spin-wave theory[15,16,20] and we discuss how the ground states change from those for the model with $\Delta=-0.5$ as Δ is increased. As shown in the previous section, the ground states of the quantum AFT XXZ model with $\Delta=-0.5$ are the same as those of the classical model. By increasing Δ from -0.5, quantum effects are introduced into the ground states and their physical values differ from those of the corresponding classical model. We have used the

Holstein-Primakoff transformation to expand the spin operator and have calculated some physical values up to the first order of $1/S$.

At zero temperature, spins have the 120° structure in the plane in the classical AFT *XXZ* model with $-0.5<\Delta<1$. We expand the quantum Hamiltonian from this classical ground state. The quantized axis on each site is defined, so that the axes have the 120° structure. Oguchi[20] first applied this method to the Heisenberg model on the triangular lattice.

We choose the quantized axes in the *XY* plane as in §2.1. Namely we use the Hamiltonian

$$H=J\sum(S_i^zS_j^z+S_i^xS_j^x+\Delta S_i^yS_j^y), \tag{3.1}$$

where S^α ($\alpha=x, y, z$) denote spin operators. With the operator

$$U=\exp\left(i\frac{2\pi}{3}\sum_{i\in B}S_i^y-i\frac{2\pi}{3}\sum_{i\in C}S_i^y\right), \tag{3.2}$$

the Hamiltonian (3.1) is transformed as

$$U^\dagger HU=-\frac{J}{2}\sum_{\langle i,j\rangle}(S_i^zS_j^z+S_i^xS_j^x-2\Delta S_i^yS_j^y)+\frac{\sqrt{3}\,J}{2}\sum_{(i\to j)}(S_i^zS_j^x-S_i^xS_j^z). \tag{3.3}$$

Spin operators are expanded using the Holstein-Primakoff transformation

$$S_i^+=\sqrt{2S-a_i^\dagger a_i}\,a_i$$
$$S_i^-=a_i^\dagger\sqrt{2S-a_i^\dagger a_i}$$
$$S_i^z=S-a_i^\dagger a_i, \tag{3.4}$$

where $\{a_i\}$ denote boson operators. This transformation corresponds to an expansion from the ground state $|\mathrm{GS}.1\rangle$ for $\Delta=-0.5$. The sublattice-magnetization is given by

$$U^\dagger MU=\sum_i S_i^z, \tag{3.5}$$

and the chiral order parameter is transformed as

$$U^\dagger QU=\frac{1}{4}\sum_{\langle i,j\rangle}(S_i^zS_j^z+S_i^xS_j^x)-\frac{1}{4\sqrt{3}}\sum_{(i\to j)}(S_i^zS_j^x-S_i^xS_j^z). \tag{3.6}$$

Using the boson operators $\{a_k^\dagger, a_k\}$ and by expanding them with respect to $1/S$ up to the first order, the Hamiltonian (3.3) is transformed as

$$U^\dagger HU=-\frac{3NJS(S+1)}{2}+\frac{3JS}{4}\sum_k\{2-(1-2\Delta)\gamma_k\}(a_k^\dagger a_k+a_ka_k^\dagger)-\frac{3J(1+2\Delta)S}{4}\sum_k\gamma_k(a_{-k}a_k+a_k^\dagger a_{-k}^\dagger), \tag{3.7}$$

where $\{\boldsymbol{k}\}$ denote wave vectors in the first Brillouin zone of the triangular lattice and

$$\gamma_k=\frac{1}{3}\{\cos\boldsymbol{e}_1\cdot\boldsymbol{k}+\cos\boldsymbol{e}_2\cdot\boldsymbol{k}+\cos(\boldsymbol{e}_1-\boldsymbol{e}_2)\cdot\boldsymbol{k}\}, \tag{3.8}$$

where $\boldsymbol{e}_i$ ($i=1, 2$) denote unit vectors of the lattice. Using the transformation

$$a_k=b_k\cosh\theta_{-k}-b_{-k}^\dagger\sinh\theta_k$$
$$a_k^\dagger=-b_{-k}\sinh\theta_k+b_k^\dagger\cosh\theta_{-k}, \tag{3.9}$$

we diagonalize the Hamiltonian (3.7) as

$$U^\dagger HU=-\frac{3NJS(S+1)}{2}+\frac{3JS}{4}\sum_k\{(1+2\Delta\gamma_k)\exp(2\theta_k)+(1-\gamma_k)\exp(-2\theta_k)\}(b_k^\dagger b_k+b_kb_k^\dagger), \tag{3.10}$$

where

$$\exp(2\theta_k)=\sqrt{\frac{1-\gamma_k}{1+2\Delta\gamma_k}}. \tag{3.11}$$

In the ground state, the expectation values of the number of bosons with nonvanishing momenta $\{\boldsymbol{k}\}$ are zero, namely $\langle b_k^\dagger b_k\rangle_g=0$ in the region $-0.5\leq\Delta\leq 1$, since the spectrum of a boson, ε_k, is always positive. The ground-state energy is given by

$$\langle U^\dagger HU\rangle_g=-\frac{3NJS(S+1)}{2}+\frac{3JS}{2}\sum_k\sqrt{(1-\gamma_k)(1+2\Delta\gamma_k)}, \tag{3.12}$$

in the region $-0.5\leq\Delta\leq 1$ and it is shown in Fig. 2(a) (and Tables I and II). The sublattice magnetization (3.5) is transformed as

$$U^\dagger MU=N\left(S+\frac{1}{2}\right)-\frac{1}{2}\sum_k\cosh 2\theta_k(b_k^\dagger b_k+b_k b_k^\dagger)+\frac{1}{2}\sum_k\sinh 2\theta_k(b_k^\dagger b_{-k}^\dagger+b_{-k}b_k), \tag{3.13}$$

and the expectation value of it in the ground state is given by

$$\langle U^\dagger MU\rangle_g=N\left(S+\frac{1}{2}\right)-\frac{1}{4}\sum_k\left\{\sqrt{\frac{1-\gamma_k}{1+2\Delta\gamma_k}}+\sqrt{\frac{1+2\Delta\gamma_k}{1-\gamma_k}}\right\}. \tag{3.14}$$

The calculated values in the region $-0.5\leq\Delta\leq 1$ are shown in Fig. 2(b). The chiral-order parameter (3.6) is written by

$$\begin{aligned}U^\dagger QU=&\frac{3NS(S+1)}{4}-\frac{3S}{8}\sum_k\{2\cosh 2\theta_k-\gamma_k\exp(-2\theta_k)\}(b_k^\dagger b_k+b_k b_k^\dagger)\\&+\frac{3S}{8}\sum_k\{2\sinh 2\theta_k+\gamma_k\exp(-2\theta_k)\}(b_{-k}^\dagger b_k^\dagger+b_k b_{-k}).\end{aligned} \tag{3.15}$$

The expectation values of the chiral-order parameter in the ground state are given by

$$\langle U^\dagger QU\rangle_g=\frac{3NS(S+1)}{4}-\frac{3S}{4}\sum_k\frac{(1+\Delta\gamma_k)\sqrt{1-\gamma_k}}{\sqrt{1+2\Delta\gamma_k}}, \tag{3.16}$$

and are shown in Fig. 2(c).

At $\Delta=-0.5$, the calculated ground-state energy and the calculated values of chirality and sublattice magnetization in the ground states are exactly equal to those of the exact ground states (2.2), though we have expanded them only up to the first order of $1/S$. Namely the remaining higher order terms in $1/S$ do not contribute to these physical quantities at $\Delta=-0.5$.

As Δ is increased, the values of the ground-state energy become lower and lower and the deviation of the sublattice-magnetization becomes larger and larger compared with the classical values. Thus the quantum effects appear and become stronger as the antiferromagnetic Ising interactions are introduced into the Hamiltonian. In comparison with the above two results, the values of the chirality change in a little different way. For the case $\Delta=-0.5$ the estimated value is equal to the exact one. As Δ is increased, the calculated values of the chirality become a little larger than the classical one. In the $S=\frac{1}{2}$ XY model ($\Delta=0$), the value of it is given by $\langle Q\rangle_g/S^2N=0.798$, where the corresponding classical value is given by $\langle Q\rangle_{cl}/N=0.75$. In the quantum model, the eigenvalues of the chiral order parameter on a triangle-cell are 1, 0 and -1. Then it is possible that the value of chirality is enhanced in the quantum case. As the system approaches the Heisenberg model, the value of chirality decreases quickly in the same way as the sublattice-magnetization does.

The values of the ground-state energy are shown in Tables I and II together with the results of other papers. In spite of our simple estimate to expand only up to the first order of $1/S$, our results agree well with other results. In the $S=\frac{1}{2}$ AFT XY model the values of the sublattice magnetization is given by $\langle M\rangle/SN=0.8973$ and the chirality is given by $\langle Q\rangle/S^2N=0.7982$. In the Heisenberg model, we have $\langle M\rangle/SN=0.4780$ and $\langle Q\rangle/S^2N=0.4050$. The value of the chirality estimated

Table I. Ground-state energy per bonds, $E_g/3NJ$, of the quantum AFT XY model.

Method	Ground-state energy
Classical limit	-0.5
Variational method[17]	-0.5233
Finite-lattice method[9,10]	-0.5456
Spin-wave theory $O(1/S^2)$[23-25]	$-0.5172\sim-0.5392$
Spin-wave theory $O(1/S)$	-0.532

Table II. Ground-state energy per bonds, $E_g/3NJ$, of the quantum AFT Heisenberg model.

Method	Ground-state energy
Classical limit	-0.5
Variational method (RVB)[6]	-0.613
Variational method (120° structure)[21]	-0.7156
Finite-lattice method[22,10]	-0.729
Spin-wave theory $O(1/S^2)$[23-25]	$-0.728\sim-0.7488$
Spin-wave theory $O(1/S)$[20]	-0.718

by the exact diagonalization method under the assumption that a long-range order exists in the infinite systems is given by $\lim_{N\to\infty}\langle Q^z Q^z\rangle/S^4N^2=0.556$[10] (or 0.526[9]) in the AFT XY model. Our corresponding value is given by $\langle Q\rangle^2/S^4N^2=0.637$. In the Heisenberg model, the Hamiltonian has the O(3) symmetry. Then the chiral long-range order is isotropic as follows:

$$\lim_{N\to\infty}\frac{1}{N^2}\langle Q^x Q^x\rangle=\lim_{N\to\infty}\frac{1}{N^2}\langle Q^y Q^y\rangle=\lim_{N\to\infty}\frac{1}{N^2}\langle Q^z Q^z\rangle. \quad (3.17)$$

The result by exact diagonalization is given by $\lim_{N\to\infty}\langle Q^z Q^z\rangle/S^4N^2=0.08.$[22] Then the chirality of the system in which the O(3) symmetry of the chirality is spontaneously broken is given by $\langle Q\rangle^2/S^4N^2\sim\lim_{N\to\infty}3\langle Q^z Q^z\rangle/S^4N^2=0.24$. Our corresponding result is given by $\langle Q\rangle^2/S^4N^2=0.164$. In the spin-wave theory, we have estimated the value of it under the assumption that the symmetry has been spontaneously broken by an infinitesimal effective field.

§4. Phase Diagram at Low Temperatures

In this section we discuss a phase diagram at finite temperatures in the quantum AFT XXZ

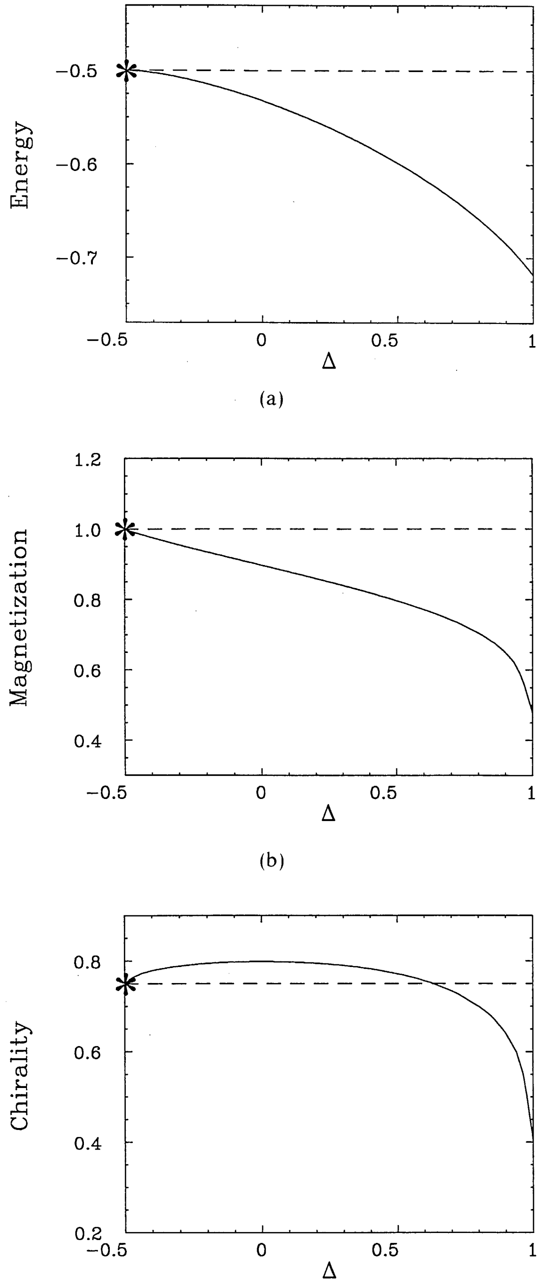

Fig. 2. Evaluated values of (a) energy $E_0/3NJS^2$, (b) sublattice magnetization M/SN, and (c) chirality Q/S^2N in the ground states of the $s=1/2$ AFT XXZ model using the spin-wave expansion up to 1/S order. The parameter Δ means the anisotropy of the z-component interactions. The symbols * denote the exact results of the states $|\mathrm{GS}.1\rangle$ and dashed lines denote values in the classical limit ($S\to\infty$).

model. We consider especially the chiral phase and ferromagnetic one. In the case of the corresponding classical model, the chirality is ordered in the region $-0.5<\Delta<1$ at low temperatures and a ferromagnetic order exists in the region $\Delta<-0.5$.[5] At $\Delta=-0.5$, the ground states are non-trivially degenerate. Miyashita[5] showed that ferromagnetically ordered states are favorite at finite temperatures in the classical model with $\Delta=-0.5$ by calculating the free energy in the harmonic approximation and he showed using Monte Carlo simulation that a reentrant phase transition appears for the model $\Delta>-0.5$. In the AFT plane rotator model, the appearance of the KT transition is also observed near the critical point of the chiral order.[2] There remains a possibility that the KT transition appears also in the quantum case accompanied with or independent of the chiral order phase transition. In this paper we only discuss the order which can be defined as the existence of nonvanishing values of order parameters, namely the chiral order and ferromagnetic order.

In the previous paper[13] we studied the vector chiral order in the $S=\frac{1}{2}$ AFT XXZ model using the super-effective-field theory[14] (SEFT). In the SEFT, all the states of spins in finite clusters are treated exactly and the effect for the relevant system to be infinite is introduced as effective-fields. In this way, the chiral order is studied in a mean-field theoretical approach and physical properties of the infinite system are predicted from the size-dependence of critical temperatures by analyzing with the finite-size scaling. We applied this method to the $S=\frac{1}{2}$ AFT XXZ model and concluded that there exists a chiral long-range order at low temperatures in the region $-0.5\leq\Delta<0.5$.

Here we discuss the phase diagram of the quantum AFT XXZ model using the spin-wave theory. In §3 we have expanded the Hamiltonian in the region $-0.5\leq\Delta\leq1$ as

$$U^{\dagger}HU=\langle U^{\dagger}HU\rangle_g+\sum_k \varepsilon_k b_k^{\dagger} b_k, \qquad (4.1)$$

where $\langle U^{\dagger}HU\rangle_g$ denotes the ground-state energy defined in eq. (3.12) and

$$\varepsilon_k=3JS\sqrt{(1+2\Delta\gamma_k)(1-\gamma_k)}. \qquad (4.2)$$

The expectation value of the chirality at finite temperatures is given by

$$\begin{aligned}\langle U^{\dagger}QU\rangle&=\langle U^{\dagger}QU\rangle_g-\frac{3S}{2}\sum_k\frac{(1+\Delta\gamma_k)\sqrt{1-\gamma_k}}{\sqrt{1+2\Delta\gamma_k}}\langle b_k^{\dagger}b_k\rangle\\&=\langle U^{\dagger}QU\rangle_g-\frac{3S}{2}\sum_k\frac{(1+\Delta\gamma_k)\sqrt{1-\gamma_k}}{\sqrt{1+2\Delta\gamma_k}}\frac{1}{\exp(\beta\varepsilon_k)-1},\end{aligned} \qquad (4.3)$$

where the bracket $\langle\cdots\rangle$ denotes thermal average and $\langle U^{\dagger}QU\rangle_g$ denotes the expectation value of the chirality at ground states, which was given in eq. (3.16). In the region $-0.5<\Delta<1$, a dispersion relation behaves as $\varepsilon_k\sim|k|$ for small k. Then the second term in eq. (4.3), namely deviation of the chirality from ground-state values is finite and small at low temperatures. Then the chirality remains nonvanishing even at finite temperatures. The numerator of the integrand of eq. (4.3) has a zero-point at $\boldsymbol{k}=0$. The existence of this zero-point corresponds to the stableness of the chirality against (long-range) spin-wave excitations.

At $\Delta=-0.5$, we obtain

$$\langle Q\rangle=\frac{3NS^2}{4}-\frac{3S}{4}\sum_k(2-\gamma_k)\frac{1}{\exp(\beta\varepsilon_k)-1}. \qquad (4.4)$$

The dispersion relation is $\varepsilon_k\sim k^2$ for small k. Then the second term becomes divergent as

$$\begin{aligned}\Delta Q&=\frac{3S}{4}\sum_k(2-\gamma_k)\frac{1}{\exp(\beta\varepsilon_k)-1}\\&\sim\beta^{-1}\sum_k\frac{1}{k^2}\to\infty.\end{aligned} \qquad (4.5)$$

This divergence means that the chirality is unstable at $\Delta=-0.5$ against spin-wave excitations. This result suggests that the phase boundary of the chiral order comes to an end at $\Delta=-0.5$ and that the chirality is destroyed at $\Delta=-0.5$ at finite temperatures as shown in Fig. 4.

At $\Delta=1$ energy spectra have other zero-points at the corners of the Brillouin zone. For these modes, the deviation of the chirality ΔQ becomes divergent as

$$\Delta Q \sim \beta^{-1} \sum_{k} \frac{1}{(\boldsymbol{k}-\boldsymbol{k}')^2} \to \infty, \tag{4.6}$$

where $\boldsymbol{k}'$ denotes a momentum at one of the corner points of the Brillouin zone, say $(4\pi/3, 0)$. This result is consistent with the exact proof that there exists no vector chiral order at finite temperatures.[26]

Next we discuss the phase diagram of the ferromagnetic phase. As shown in §2.2, ground states are ferromagnetically ordered in $\Delta \leq -0.5$. We use a transformed Hamiltonian

$$U_z^{\dagger} H U_z = -\frac{J}{2} \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y - 2\Delta S_i^z S_j^z) - \frac{\sqrt{3}\, J}{2} \sum_{(i\to j)} (S_i^x S_j^y - S_i^y S_j^x), \tag{4.7}$$

where

$$H = J \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z), \tag{4.8}$$

and

$$U_z = \exp\left(i\frac{2\pi}{3} \sum_{i\in B} S_i^z - i\frac{2\pi}{3} \sum_{i \in C} S_i^z\right). \tag{4.9}$$

It is shown by the transformation U_z that spin fluctuations become space-translational invariant and that a spin wave with the mode $k\sim 0$ becomes dominant. The Hamiltonian is expanded with the Holstein-Primakoff transformation as

$$U_z^{\dagger} H U_z = 3NS^2 J\Delta + \sum_{k} \varepsilon_k a^{\dagger}(k) a(k), \tag{4.10}$$

where

$$\varepsilon_k = -3SJ(2\Delta + \gamma_k) - \sqrt{3}\, SJ\{\sin \boldsymbol{k}\cdot\boldsymbol{e}_1 - \sin \boldsymbol{k}\cdot\boldsymbol{e}_2 + \sin \boldsymbol{k}\cdot(\boldsymbol{e}_2 - \boldsymbol{e}_1)\}. \tag{4.11}$$

The expectation value of the magnetization is given by

$$M = S - \sum_{k} \langle a^{\dagger}(k) a(k) \rangle = S - \sum_{k} \frac{1}{\exp(\beta\varepsilon_k) - 1}. \tag{4.12}$$

In the region $\Delta < -0.5$, spectra of the boson behave as

$$\varepsilon_k \sim \frac{3SJ}{4}(-8\Delta - 4 + k^2). \tag{4.13}$$

A finite gap exists above the ground states. The appearance of the energy gap comes from the result that the ferromagnetic Ising interaction is dominant in $\Delta < -0.5$. In this region, the ferromagnetic order is stable against the spin-wave fluctuation. The magnetization can be ordered at finite temperatures. As Δ is increased, the energy gap decreases and it vanishes at $\Delta=-0.5$. At $\Delta=-0.5$, the spectra behave as

$$\varepsilon_k \sim \frac{3SJ}{4} k^2. \tag{4.14}$$

Then the deviation of the magnetization becomes divergent as

$$\Delta M \sim \beta^{-1} \sum_{k} \frac{1}{k^2} \to \infty. \tag{4.15}$$

This divergence means that the magnetization is unstable and there is no magnetic order. This result is different from that of the classical model.

At $\Delta=-0.5$, the ground states are non-trivially degenerate. It may be possible that a scalar chiral-order phase appears at finite temperatures by quantum effect in an intermediate phase between the ferromagnetic phase and vector-chiral one, since a scalar chiral order appears in a part of the degenerate ground-states. We calculate the free energy by expanding from various ground states (2.17) to determine which states are favorite at finite temperatures. We use the Hamiltonian (2.1) with $\Delta=-0.5$ and rotate the quantized axes as

$$R^\dagger U^\dagger HUR = -\frac{J}{2}\sum_{\langle i,j\rangle}(S_i^z S_j^z + S_i^x S_j^x + S_i^y S_j^y) - \frac{\sqrt{3}\,J}{2}\sum_{(i\to j)}\{\cos\phi(S_i^z S_j^x - S_i^x S_j^z) - \sin\phi(S_i^y S_j^x - S_i^x S_j^y)\}. \tag{4.16}$$

With $\phi=0$, the quantized axes are in the XY plane and the system has the 120° structure. As ϕ is increased, these axes close as bones of umbrella do. We expand the Hamiltonian (4.16) up to the first order of $1/S$ as

$$R^\dagger U^\dagger HUR = -\frac{3NJS^2}{2} + \sum_k \{3JS(1-\gamma_k) + \sqrt{3}\,JSg_k \sin\phi\}\, a^\dagger(k)a(k), \tag{4.17}$$

where

$$g_k = \sin \boldsymbol{k}\cdot\boldsymbol{e}_1 - \sin \boldsymbol{k}\cdot\boldsymbol{e}_2 + \sin \boldsymbol{k}\cdot(\boldsymbol{e}_2 - \boldsymbol{e}_1). \tag{4.18}$$

This Hamiltonian is already diagonalized. The partition function of this system is given by

$$Z = \mathrm{Tr}\exp(-\beta R^\dagger U^\dagger HUR) = \sum_{n_k=0}^{\infty} \exp(-\beta H_0)\exp(-\beta\sum_k \varepsilon_k n_k), \tag{4.19}$$

where $\beta = 1/k_B T$ and

$$H_0 = -\frac{3NJS^2}{2}, \tag{4.20}$$

and

$$\varepsilon_k = 3JS(1-\gamma_k) + \sqrt{3}\,JSg_k \sin\phi. \tag{4.21}$$

The free energy of this system is given by

$$F = -\beta^{-1}\log Z = H_0 + \beta^{-1}\sum_k \log\{1-\exp(-\beta\varepsilon_k)\}. \tag{4.22}$$

Here we define the following function,

$$f(T) = \sum_k \log\{1-\exp(-\beta\varepsilon_k)\}. \tag{4.23}$$

The values of $f(T)$ at various temperatures are shown in Fig. 3. The free energy of ferromagnetically ordered states which are fluctuating around the ground state (2.17) with $\phi=\pi/2$ is minimum at each temperature. Thus scalar chiral order can not appear at finite temperatures. Even a ferromagnetic order can not appear as mentioned above.

As a conclusion we obtain the phase diagram shown in Fig. 4 by taking into account all the above results and our previous

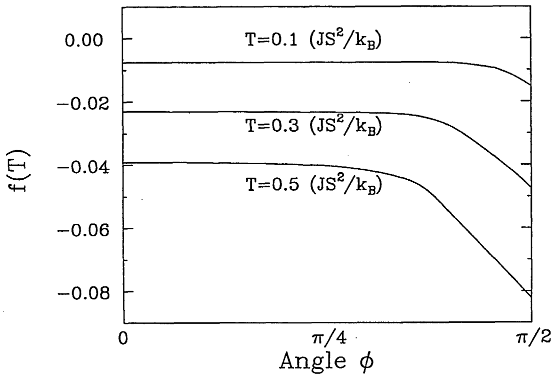

Fig. 3. Values of $f(T)$ at various temperatures. These values are calculated by expanding them from many ground states (2.17) which have different values of parameter ϕ. A ground state with $\phi=0$ has the 120° structure and a state with $\phi=\pi/2$ corresponds to the ferromagnetically ordered state.

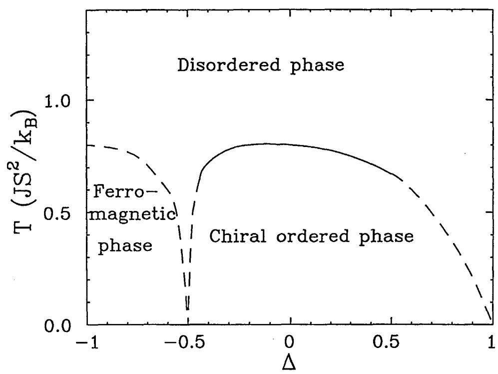

Fig. 4. Phase diagram of the chiral order which we have predicted from the results of the SEFT, SW and exact ground states. The solid-line comes from the results of the SEFT. The dashed-line was predicted from the results of the spin-wave expansion by extending the solid-line.

results[13] of the SEFT. We have extended the phase boundary which was obtained previously from the results of the SEFT and have drawn a line without quantitative accuracy, since we have only discussed whether orders are stable against spin-wave excitations or not and we have not estimated the critical temperatures.

§5. Summary and Discussion

In the present paper we have studied long-range order in the quantum AFT XXZ model. We showed exact ground states in the region $\Delta \leq -0.5$ and studied the ground-state and thermal properties using the spin-wave theory. Considering all the above results, we give the phase diagram of the chiral order in the AFT XXZ model.

For the case $\Delta = -0.5$, most of the exact ground states have a chiral long-range order. This model corresponds to one of the marginal points of the chiral ordered phase. These ground states are almost the same as those of the corresponding classical model. The sublattice-magnetization and the chirality are fully ordered in these states. Using the spin-wave theory, we studied ground-state properties in the region $-0.5 \leq \Delta \leq 1$. As Δ is increased, quantum effects are enhanced in the ground states. Deviations of the sublattice-magnetization become large, but the chirality does not change depending on Δ near $\Delta = 0$. In the antiferromagnetic XY model, systems are not so fluctuating with quantum effect. The sublattice magnetization seems to be ordered at ground states and the chirality seems to be ordered even at finite temperatures. Near the antiferromagnetic Heisenberg model, quantum effects become strong. The values of the magnetization and the chirality are reduced rapidly by quantum fluctuation. Though the estimated magnetization and chirality have non-zero values in the Heisenberg model, the Δ dependence of the magnetization and of the chirality suggests that the Heisenberg model is near the critical point.

Using the spin-wave theory, we have studied the phase diagram at low temperatures and have shown that the chiral order is stable against spin-wave excitations in the region $-0.5 < \Delta < 1$. In the case $\Delta = -0.5$ the chirality is destroyed by long-range spin-wave excitations. It is because the linear dispersion relation $\varepsilon_k \sim |k|$ in the region $-0.5 < \Delta < 1$ becomes of the form $\varepsilon_k \sim k^2$ at $\Delta = -0.5$. In the case of $\Delta \leq -0.5$, the ferromagnetic Ising interaction is dominant. The dispersion relation has a mass gap as $\varepsilon_k \sim m^2 + k^2$. However, this gap vanishes at $\Delta = -0.5$. Then the ferromagnetic order exists at low temperatures in the model with $\Delta < -0.5$ and a long-range spin-wave breaks this order at $\Delta = -0.5$.

As mentioned above, quantum fluctuation is strong in the model near the symmetry of the Heisenberg model, say $\Delta \sim 1$. Then it is possible that the system is not ordered and that the estimated values in the spin-wave approximation remain only apparently to be non-vanishing in this region. There remains a possibility for some differences between classical systems and quantum ones in these regions to appear.

We give a remark that there remains a possibility that any order at finite temperatures exists in the real system of the XXZ model with $\Delta = -0.5$. Indeed, as shown in §2, the Hamiltonian itself is not invariant with any infinitesimal transformation which changes the sign of the magnetization or the chirality. As we showed in our previous paper, the correlation of the chirality in finite clusters is still strong at $\Delta = -0.5$. If an order exists at finite temperatures, a ferromagnetic order may exist and a reentrant transition may occur in the same way as in a classical system, since the free energy of the ferromagnetic phase is lower than that of the chiral phase. To test these possibilities, a more delicate study is needed.

We did not argue the KT transition in this paper. To study the relation between the KT transition and the chiral order phase transition is an interesting problem. To reveal the relation, any study from other approaches is needed.

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