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Long-Range Order in the Frustrated *XXZ* Model

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We examine the existence of long-range order in the two-dimensional frustrated *XXZ* model with next nearest neighbor interactions using the spin wave theory and the method of infrared bounds. The results show that the *XY*-like system may have essentially the same properties as the isotropic Heisenberg case, while the Ising-like system is very unlikely to show non-classical behavior. We also prove the absence of twisted order.

§1. Introduction

The two-dimensional quantum spin system continues to attract attention. Especially the interplay of frustration and quantum fluctuation is of special interest since it may lead to a non-classical spin state. Chandra and Doucot[1] studied the two-dimensional frustrated Heisenberg model using the naïve spin wave theory. They interpreted their results that the classical states are destroyed in the region of strong frustration to be replaced by a spin liquid state. Oguchi and Kitatani[2] showed that the same results can be derived by the variational spin wave theory.

Various states have been proposed as the candidates of the spin liquid state in this system. Wen *et al.*[3] discussed the possibility of the chiral spin state characterized by a *P* and *T* symmetry breaking. Gelfand *et al.*[4] studied the dimer states using a perturbation theory from the independent pure-dimer Hamiltonian. We pointed out[5] that the modified spin wave theory[6] leads to the classical picture even in the strongly frustrated region. Similar results have been obtained by Xu and Ting,[7] and Mila *et al.*[8]

Numerical researches have also been carried out. Dagotto and Moreo[9] investigated the system by the numerical diagonalization of small size with up to 20 spins. They estimated the various order parameters, Nēel order, collinear order, twisted order, chiral order and dimer order parameters. The data indicated a crossover between two types of classical order. However the system size was too small to conclude the existence or absence of a non-classical state in the crossover region. As another approach Kishi and Kubo[10] proved the existence of Nēel long-range order using infrared bounds method. We proved[11] the absence of spontaneous breakdown of twisted symmetry in this system.

In this paper we investigate how these obtained results may be modified if we introduce an anisotropy, the *XXZ* model. We first use the naive spin wave theory to estimate roughly the stability of the classical picture. We next use the method of infrared bounds originally proposed by Dyson, Lieb and Simon[12] for unfrustrated quantum spin systems. In the case of the present two-dimensional frustrated Heisenberg model, Kishi and Kubo[10] extended the method to prove the existence of Nēel long-range order in a restricted region. We further extend the proof to the anisotropic model. We also prove the absence of twisted order on the same model by exploiting our previous idea.[11]

In §2 we apply the naive spin wave theory to the frustrated system. In §3 we apply the method of infrared bounds to prove the existence of long-range order in a restricted region. We prove the absence of twisted order in §4 by the Bogoliubov inequality in a stronger form. Section 5 is devoted to the conclusion.

§2. Naive Spin Wave Theory

The Hamiltonian of the system of our interest is

$$H=\sum_{\langle n.n.\rangle}(S_i^xS_j^x+S_i^yS_j^y+\Delta S_i^zS_j^z)+\lambda\sum_{\langle n.n.n.\rangle}(S_i^xS_j^x+S_i^yS_j^y+\Delta S_i^zS_j^z). \tag{2.1}$$

Here λ is the ratio of the exchange integral of the nearest neighbor interaction to that of the next nearest neighbor interaction. We concentrate on the ground state problem. When we use the spin wave theory, we start from the classical spin state. In the present model, the Néel state is stable for $0\leq\lambda\leq 1/2$ while the collinear state (Fig. 1) is the classical ground state if $\lambda\geq 1/2$. As seen in Fig. 1, the collinear state is a special case of the four-sublattice antiferromagnet. To evaluate the quantum fluctuation around the classical states, we transform the spin operator to bose operator by the Holstein-Primakoff transformation. In the naive spin wave theory, spin wave interactions are neglected and the boson Hamiltonian is harmonic. Evaluation of physical quantities within this approximation is rather straightforward.[1,2,5] We simply write down the results. Sublattice magnetization in the Ising-like anisotropic case ($\Delta\geq 1$) is

$$\langle S^z\rangle_{\text{Néel}}=S+\frac{1}{2}-\frac{1}{2|\Lambda|}\sum_k\frac{\Delta+\alpha(\eta_k-\Delta)}{[\{\Delta+\alpha(\eta_k-\Delta)\}^2-\gamma_k^2]^{1/2}} \tag{2.2}$$

$$\langle S^z\rangle_{\text{col}}=S+\frac{1}{2}-\frac{1}{2|\Lambda|}\sum_k\frac{2\lambda\Delta+\gamma_{k_x}}{[(2\lambda\Delta+\gamma_{k_x})^2-(2\lambda\eta_k+\gamma_{k_y})^2]^{1/2}}, \tag{2.3}$$

where the summation runs over the first Brillouin zone, $|\Lambda|$ denotes the system size, and $\gamma_k=(\cos k_x+\cos k_y)/2$, $\gamma_{k_x}=\cos k_x$, $\gamma_{k_y}=\cos k_y$, $\eta_k=\cos k_x\cos k_y$. Equation (2.2) is for the Néel-like order parameter ($0\leq\lambda\leq 1/2$) and (2.3) represents the collinear order parameter ($\lambda\geq 1/2$). In the XY-like anisotropic case ($0\leq\Delta\leq 1$)

$$\langle S^z\rangle_{\text{Néel}}=S+\frac{1}{2}-\frac{1}{2|\Lambda|}\sum_k\frac{1+\Delta_-\gamma_k+\lambda(\Delta_+\eta_k-1)}{[\{1+\Delta_-\gamma_k+\lambda(\Delta_+\eta_k-1)\}^2-(\Delta_+\gamma_k+\lambda\Delta_-\eta_k)^2]^{1/2}} \tag{2.4}$$

$$\langle S^z\rangle_{\text{col}}=S+\frac{1}{2}-\frac{1}{2|\Lambda|}\sum_k\frac{2\lambda+\Delta_+\gamma_{k_x}+\Delta_-(2\lambda\eta_k-\gamma_{k_y})}{[\{2\lambda+\Delta_+\gamma_{k_x}+\Delta_-(2\lambda\eta_k-\gamma_{k_y})\}^2-\{\Delta_+(2\lambda\eta_k+\gamma_{k_y})-\Delta_-\gamma_{k_x}\}^2]^{1/2}}. \tag{2.5}$$

Here $\Delta_-=(1-\Delta)/2$, and $\Delta_+=(1+\Delta)/2$. If we follow Chandra and Doucot[1] to determine the phase boundary in the rather crude criterion $\langle S^z\rangle=0$, we obtain the phase diagram given in Figs. 2(a), 2(b) and 2(c).

Let us first discuss the XY-like ($0\leq\Delta\leq 1$) model. As indicated Fig. 2(a), the Néel state reaches the stability limit ($\langle S^z\rangle=0$) before λ becomes $1/2$ for any finite S, and the collinear state also has a negative $\langle S^z\rangle$ for λ close to $1/2$. Thus in the narrow region bounded by these stability limit lines $\langle S^z\rangle_{\text{Néel}}=0$ and $\langle S^z\rangle_{\text{col}}=0$, the first order quantum correction overwhelms the classical picture. If we take this fact naively, as Chandra and Doucot did,[1,2] this intermediate region may have a non-classical spin state, which Chandra and Doucot called the spin liquid state. Quite the same behavior of this system is found in the isotropic Heisenberg case ($\Delta=1$). For instance, the divergence of any two-point correlation function at $\lambda\to 1/2$ is observed for $0\leq\Delta<1$ as well as for $\Delta=1$. Thus the properties of the non-classical spin liquid state, if any, should remain essentially the same if we introduce the XY-like anisotropy. In the Ising-

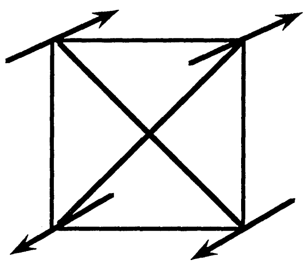

Fig. 1. The collinear state is defined as a special case of the four-sublattice antiferromagnet.

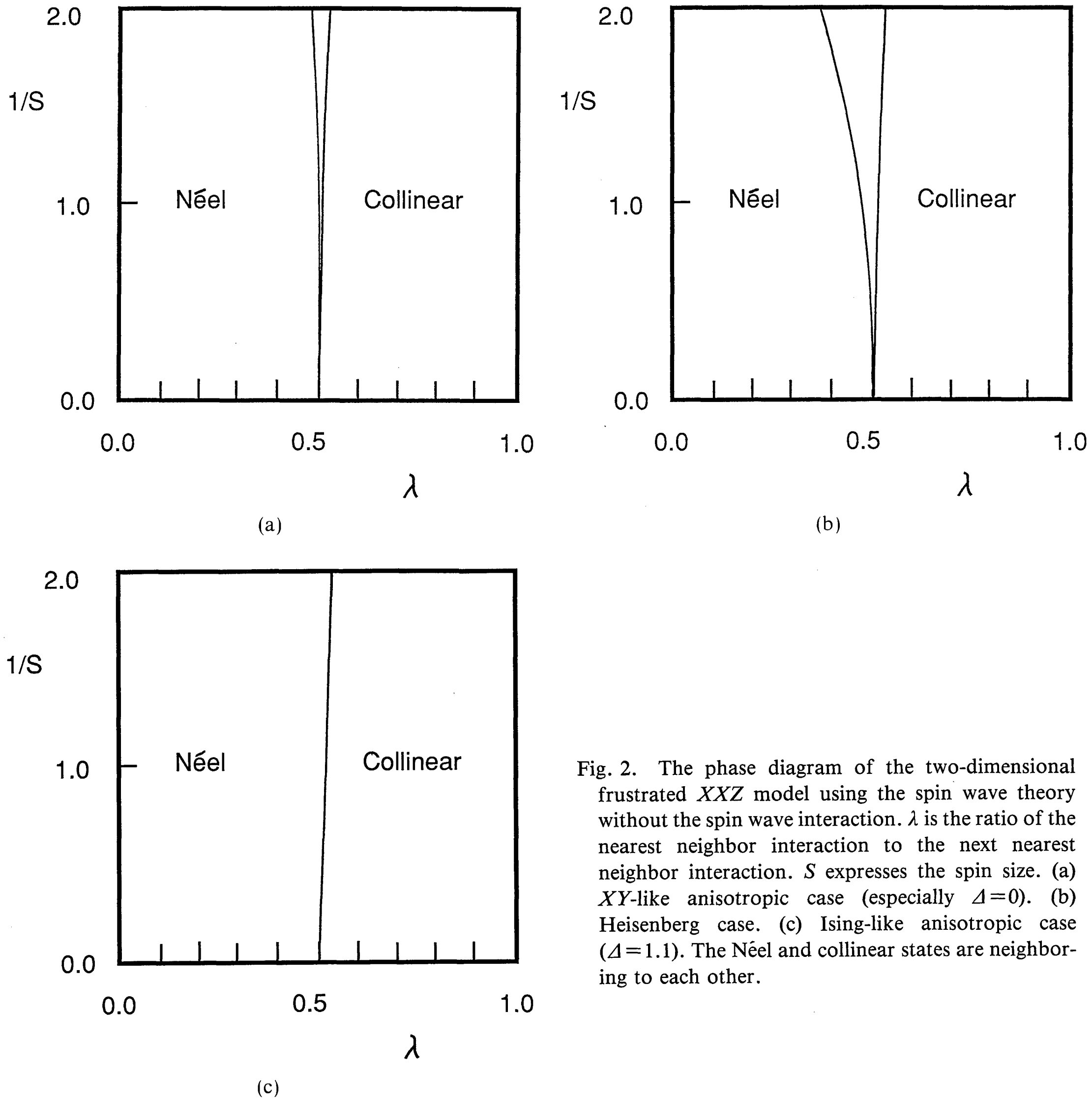

Fig. 2. The phase diagram of the two-dimensional frustrated XXZ model using the spin wave theory without the spin wave interaction. λ is the ratio of the nearest neighbor interaction to the next nearest neighbor interaction. S expresses the spin size. (a) XY-like anisotropic case (especially $\Delta=0$). (b) Heisenberg case. (c) Ising-like anisotropic case ($\Delta=1.1$). The Néel and collinear states are neighboring to each other.

like anisotropic case ($\Delta>1$) the existence of an excitation energy gap leads to the stability of both the Néel state and collinear state near $\lambda=1/2$. Even when the anisotropy parameter is quite close to 1, the spin liquid state phase in the above sense disappears in the large S region. This gives support to the idea that the spin liquid state, if any, has the XY-like nature rather than the Ising-like characteristics. However these arguments are not precise enough to claim the final reliability. The criterion on the stability of the classical limit, $\langle S^z\rangle=0$, may reflect the limit of stability of the naive spin wave theory more strongly than the actual limit of stability of physical state.[5)]

§3. Proof of the Existence of Néel Order

The existence of long-range order in antiferromagnetic quantum spin systems was first proved by Dyson, Lieb and Simon[12)] using the method of infrared bounds. The technique was later applied to the ground-state problem by Neves and Perez.[13)] The reader is referred to these papers as well as those appearing below for technical details. We only outline our argument here. The Néel order parameter to be estimated in this method is defined as

$$\langle [m^i_{(\pi,\pi)}]^2 \rangle \equiv \lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|} g^i_{(\pi,\pi)} = \lim_{|\Lambda|\to\infty} \langle \{ |\Lambda|^{-1} \sum_\alpha (-1)^\alpha S^i_\alpha \}^2 \rangle, \quad (3.1)$$

where

$$g^i_k = \langle S^i_k S^i_{-k} \rangle \quad (3.2)$$

$$S^i_k = \frac{1}{\sqrt{|\Lambda|}} \sum_\alpha e^{ik\cdot\alpha} S^i_\alpha. \quad (3.3)$$

The summation in (3.1) and (3.3) runs over the lattice sites, and i expresses the element of spin operator. To extend the region in which we can prove the existence of Néel order for the isotropic ($\Delta=1$) case, we use the method developed by Wischmann and Müller-Hartmann.[14] In this method to estimate long-range order, we take the linear combination of correlation functions and the spin size, and choose the weighting factor that gives the best result. Now we must estimate the next identity:

$$\mu\langle S^i_0 S^i_0\rangle - \langle S^i_0 S^i_1\rangle - \lambda\langle S^i_0 S^i_2\rangle = (\mu+1+\lambda)\frac{1}{|\Lambda|} g_{(\pi,\pi)} + \frac{1}{2}\int \frac{d^2k}{(2\pi)^2} g^i_k (2\mu - \cos k_1 - \cos k_2 - 2\lambda \cos k_1 \cos k_2), \quad (3.4)$$

where $\langle S^i_0 S^i_1\rangle$ is the nearest neighbor correlation function and $\langle S^i_0 S^i_2\rangle$ is the next nearest neighbor correlation function. We choose the adjustable parameter μ so that the region for which we can prove the existence of long-range order is optimized. This equation allows us to express the Néel-type long-range order (3.1) in terms of short-range order,

$$(\mu+1+\lambda)\langle [m_{(\pi,\pi)}]^2\rangle = \mu\langle S^i_0 S^i_0\rangle - \langle S^i_0 S^i_1\rangle - \lambda\langle S^i_0 S^i_2\rangle - \frac{1}{2}\int \frac{d^2k}{(2\pi)^2} g^i_k (2\mu - \cos k_1 - \cos k_2 - 2\lambda \cos k_1 \cos k_2). \quad (3.5)$$

As it is in general difficult to evaluate g^i_k explicitly, we replace g^i_k by its upper bound $\tilde{g}^i_k$, which leads to the following sufficient condition for the existence of long-range order

$$\mu\langle S^i_0 S^i_0\rangle - \langle S^i_0 S^i_0\rangle - \lambda\langle S^i_0 S^i_2\rangle > \frac{1}{2}\int^{(+)} \frac{d^2k}{(2\pi)^2} \tilde{g}^i_k (2\mu - \cos k_1 - \cos k_2 - 2\lambda \cos k_1 \cos k_2), \quad (3.6)$$

where the range of integration is restricted to the region in which the integrand is positive. For a general anisotropic case ($\Delta \neq 1$), it is difficult to estimate a bound on the first term of the left hand side of (3.6), and therefore we simply put $\mu=0$. Dyson, Lieb and Simon[12] derived an explicit expression of $\tilde{g}^i_k$, which was later applied to the ground-state problem by Neves and Perez.[13] The result is

$$\tilde{g}^i_k = \frac{1}{2}[B^i_k C^i_k]^{1/2}, \quad (3.7)$$

where

$$\beta(S^i_k, S^i_{-k}) \le B^i_k, \quad (3.8)$$

$$\langle [S^i_k, [H, S^i_{-k}]]\rangle \le C^i_k. \quad (3.9)$$

The brackets in (3.8) denote the Duhamel two-point function defined by

$$(A, B) = \frac{1}{Z}\int_0^1 dx \, \mathrm{Tr}\,\{A e^{-\beta x H} B e^{-\beta(1-x)H}\}, \quad (3.10)$$

where β is the inverse temperature and Z is the partition function.

The problem has thus been reduced to the evaluation of the upper bound B^i_k of the Duhamel two-point function and C^i_k of the double commutator. Kishi and Kubo[10] were able to generalize the method of infrared bounds so that it can be applied to the isotropic frustrated quantum spin system ($\Delta=1$). It is not difficult to apply their idea to the case of the general XXZ model (2.1). The result is

$$B_k^i=\frac{1}{2}\{2+\cos k_1+\cos k_2-2\lambda(1-\cos k_1\cos k_2)\}^{-1}, \tag{3.11a}$$

for $i=x$, y and

$$B_k^z=\frac{1}{2\Delta}\{2+\cos k_1+\cos k_2-2\lambda(1-\cos k_1\cos k_2)\}^{-1}. \tag{3.11b}$$

It is straightforward to calculate the double commutator for $i=x$, y:

$$\langle[S_k^i,[H,S_{-k}^i]]\rangle=-2\{(2-\Delta\cos k_1-\Delta\cos k_2)\langle S_0^xS_1^x\rangle+2\lambda(1-\Delta\cos k_1\cos k_2)\langle S_0^xS_2^x\rangle$$
$$+(2\Delta-\cos k_1-\cos k_2)\langle S_0^zS_1^z\rangle+2\lambda(\Delta-\cos k_1\cos k_2)\langle S_0^zS_2^z\rangle\}. \tag{3.12a}$$

In the case of $i=z$ the double commutator is

$$\langle[S_k^z,[H,S_{-k}^z]]\rangle=-4\{(2-\cos k_1-\cos k_2)\langle S_0^xS_1^x\rangle+2\lambda(1-\cos k_1\cos k_2)\langle S_0^xS_2^x\rangle\}. \tag{3.12b}$$

Hence to evaluate an upper bound C_k^i in (3.9), it is necessary to know bounds for the short-range correlation functions. For this purpose we use the following relations for three neighboring spins in Fig. 3:

$$0\le\left\langle\left(\frac{1}{2}S_A+S_B+S_C\right)^2\right\rangle=\frac{1}{4}\langle S_A^2\rangle+\langle S_B^2\rangle+\langle S_C^2\rangle+2\left(\frac{1}{2}\langle S_C\cdot S_A\rangle+\frac{1}{2}\langle S_A\cdot S_B\rangle+\langle S_B\cdot S_C\rangle\right), \tag{3.13a}$$

for the isotropic interaction ($\Delta=1$), and

$$0\le\left\langle\left(\frac{1}{2}S_A^i+S_B^i+S_C^i\right)^2\right\rangle=\frac{1}{4}\langle S_A^{i2}\rangle+\langle S_B^{i2}\rangle+\langle S_C^{i2}\rangle+2\left(\frac{1}{2}\langle S_C^iS_A^i\rangle+\frac{1}{2}\langle S_A^iS_B^i\rangle+\langle S_B^iS_C^i\rangle\right), \tag{3.13b}$$

for general Δ. As seen in Fig. 3, $\langle S_AS_B\rangle$ and $\langle S_CS_A\rangle$ express the nearest neighbor correlation function, and $\langle S_BS_C\rangle$ is for the next nearest neighbor correlation function in (3.13a) and (3.13b). Equation (3.13a) leads to the next relation

$$-\langle S_0\cdot S_2\rangle\le\frac{9}{8}S(S+1)+\langle S_0\cdot S_1\rangle, \tag{3.14}$$

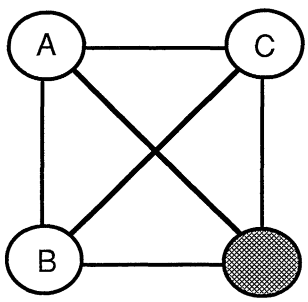

Fig. 3. Three neighboring spins used in the evaluation of short-range order.

for the Heisenberg case. We also use the Anderson bound[12,15] to estimate the lower bound of the nearest neighbor correlation function,

$$-\langle S_i\cdot S_j\rangle\le S\left(S+\frac{1}{4}\right). \tag{3.15}$$

For general Δ, we can get the next inequality from (3.13b):

$$-\langle S_0^iS_2^i\rangle\le\frac{9}{8}S^2+\langle S_0^iS_1^i\rangle. \tag{3.16}$$

We later use the next trivial relation:

$$\langle S_0^iS_0^i\rangle\le S^2. \tag{3.17}$$

We have thus finished the estimation of all short-range correlations appearing in the double commutator. Replacing the next nearest neighbor correlation in (3.12b) by (3.14) and then the nearest neighbor correlation by (3.15), we finally have

$$C_k^z = \frac{4}{3}[(2-\cos k_1 - \cos k_2)S(S+1/4) + 2\lambda(1-\cos k_1 \cos k_2)S(S+7)/8], \tag{3.18a}$$

for the Heisenberg case, and

$$C_k^z = 4[(2-\cos k_1 - \cos k_2)S^2 + 2\lambda(1-\cos k_1 \cos k_2)S^2/8], \tag{3.18b}$$

for the Ising-like case ($\Delta > 1$).

In the XY-like case, we use the next trivial estimations:

$$-S^2 \le \langle S_0^i S_1^i \rangle \le S^2 \tag{3.19a}$$

$$-S^2 \le \langle S_0^i S_2^i \rangle \le S^2. \tag{3.19b}$$

Equations (3.16) and (3.19) allow us to evaluate the upper bound of the double commutator (3.12a) for the XY-like anisotropy:

$$\begin{aligned} C_k^i = 2\,\{&(2-\Delta\cos k_1 - \Delta\cos k_2)S^2 + 2\lambda(1-\Delta\cos k_1\cos k_2)S^2] \\ &+[(2\Delta-\cos k_1-\cos k_2)+2\lambda(\Delta-\cos k_1\cos k_2)]\,S^2 \\ &\times\theta(2\Delta-\cos k_1-\cos k_2)\theta(\Delta-\cos k_1\cos k_2) \\ &-[(2\Delta-\cos k_1-\cos k_2)+2\lambda(\Delta-\cos k_1\cos k_2)]\,S^2 \\ &\times\theta(-2\Delta+\cos k_1+\cos k_2)\theta(-\Delta+\cos k_1\cos k_2) \\ &+[(2\Delta-\cos k_1-\cos k_2)-2\lambda(\Delta-\cos k_1\cos k_2)]\,S^2 \\ &\times\theta(2\Delta-\cos k_1-\cos k_2)\theta(-\Delta+\cos k_1\cos k_2) \\ &+[-(2\Delta-\cos k_1-\cos k_2)+2\lambda(\Delta-\cos k_1\cos k_2)]\,S^2 \\ &\times\theta(-2\Delta+\cos k_1+\cos k_2)\theta(\Delta-\cos k_1\cos k_2)\}, \end{aligned} \tag{3.20}$$

where $\theta(x)$ is the unit step function.

To complete the argument, it is necessary to evaluate bounds on the correlation functions appearing on the left hand side of (3.6). The nearest neighbor correlation function $-\langle S_0^i S_1^i \rangle$ in (3.6) must be replaced by its lower bound if we wish to obtain a sufficient condition for the existence of long-range order. This estimation of a lower bound can be accomplished by a variational inequality with the trivial Néel state wave function applied to the Hamiltonian (2.1):[12)]

$$-\langle S_0^i S_1^i \rangle - \lambda\langle S_0^i S_2^i \rangle \ge \frac{\Delta}{\Delta+2}(1-\lambda)S^2 \quad (\Delta \ge 1) \tag{3.21a}$$

$$-\langle S_0^i S_1^i \rangle - \lambda\langle S_0^i S_2^i \rangle \ge \frac{1}{\Delta+2}(1-\lambda)S^2 \quad (0 \le \Delta < 1). \tag{3.21b}$$

With the bounds (3.8), (3.9) and (3.21) inserted in the inequality (3.6), we finally obtain the explicit form of a sufficient condition for the existence of long-range order in the Heisenberg case as follows:

$$\frac{1}{3}S(S+1)\mu + \frac{1}{3}(1-\lambda)S^2 > \frac{1}{2}\int^{(+)} \frac{d^2k}{(2\pi)^2}\frac{1}{2}[B_k^z C_k^z]^{1/2}(2\mu - \cos k_1 - \cos k_2 - 2\lambda\cos k_1\cos k_2), \tag{3.22}$$

where B_k^z, C_k^z are given in (3.11b) and (3.18a). For the Ising-like case, the inequality is

$$\frac{\Delta}{\Delta+2}(1-\lambda)S^2 > \frac{1}{2}\int^{(+)} \frac{d^2k}{(2\pi)^2}\frac{1}{2}[B_k^z C_k^z]^{1/2}(2\mu - \cos k_1 - \cos k_2 - 2\lambda\cos k_1\cos k_2), \tag{3.23}$$

where B_k^z and C_k^x are given in (3.11b) and (3.18b). For the XY-like anisotropic case, the inequality reads

$$\frac{1}{\Delta+2}(1-\lambda)S^2>\frac{1}{2}\int^{(+)}\frac{d^2k}{(2\pi)^2}\frac{1}{2}[B_k^x C_k^x]^{1/2}(2\mu-\cos k_1-\cos k_2-2\lambda\cos k_1\cos k_2), \quad (3.24)$$

where B_k^x and C_k^x are defined in (3.11a) and (3.20).

Results of numerical evaluation of (3.22), (3.23) and (3.24) are given in Table I and Fig. 4. As seen from comparison of Figs. 2 and 4, the region in which we can prove the existence of Néel-type long-range order is completely included in the region where the naive spin wave theory predicts the same property. The advantage of the present argument is that the existence has been established in a mathematically rigorous way.

§4. Absence of Twisted Order

In this section we prove the absence of twisted order[1,11] in the model using the Bogoliubov inequality. Nishimori and Saika[11] proved this property in the Heisenberg case of this model using the upper bound of the Duhamel two-point function of Kishi and Kubo.[10] For technical reasons, the proof was restricted to the region $0\leq\lambda\leq 1/2$. The same argument is applied here to the general anisotropic problem. In this method we add an external field on a finite system to induce the twisted order,

$$H_e=-h\sum_{\alpha}\varepsilon_\alpha\cos(\boldsymbol{k}\cdot\alpha)S_\alpha^y. \quad (4.1)$$

Here ε_α is 1 on the A sublattice and -1 on the B sublattice. To prove the absence of twisted order, we use the Bogoliubov inequality in a stronger form,[12]

$$|\langle[A,B]\rangle|^2\leq\beta(B^\dagger,B)\langle[A^\dagger,[H,A]]\rangle, \quad (4.2)$$

where $(B^\dagger, B)$ expresses the Duhamel two-point function.

First we prove the absence of twisted order

Table I. λ_c is the phase boundary below which the existence of Néel order is proved by the infrared bounds method.

S	λ_c		
	$\Delta=0.0$	$\Delta=1.0$	$\Delta=3.0$
1/2	—	—	0.076
1	0.233	0.099	0.340
2	0.418	0.365	0.472
3	0.467	0.442	0.486
∞	0.500	0.500	0.500

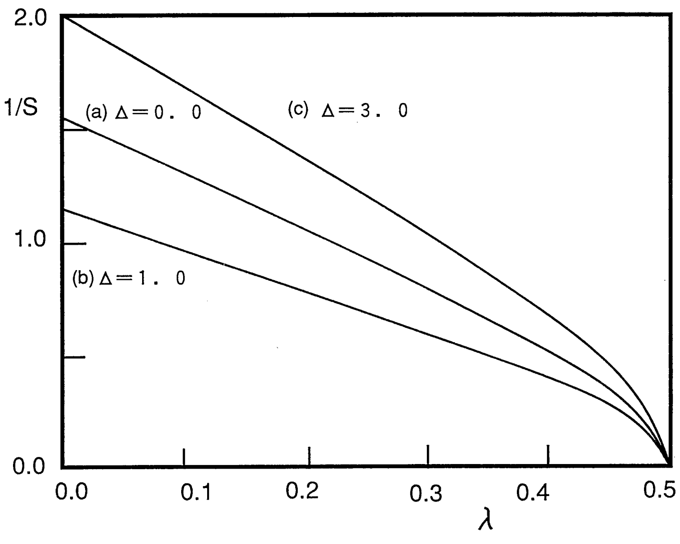

Fig. 4. The boundary of the region in which the existence of Néel-type order can be proved by the method of infrared bounds. (a) XY-like anisotropic case. (b) Heisenberg case. (c) Ising-like anisotropic case.

in the XY-like case. To evaluate the twisted order, we choose A and B as below:

$$A=S^z_{p-k+(\pi,\pi)}=\frac{1}{\sqrt{|\Lambda|}}\sum_\alpha \varepsilon_\alpha e^{-i(p-k)\alpha}S^z_\alpha \quad (4.3)$$

$$B=S^x_{-p}=\frac{1}{\sqrt{|\Lambda|}}\sum_\alpha e^{ip\alpha}S^x_\alpha. \quad (4.4)$$

With (4.3) and (4.4), the left hand side of the Bogoliubov inequality (4.2) gives the twisted order:

$$|\langle[A,B]\rangle|^2=\left\{\frac{1}{|\Lambda|}\sum_\alpha \varepsilon_\alpha \cos(k\cdot\alpha)\langle S^y_\alpha\rangle\right\}^2+\left\{\frac{1}{|\Lambda|}\sum_\alpha \varepsilon_\alpha \sin(k\cdot\alpha)\langle S^y_\alpha\rangle\right\}^2. \quad (4.5)$$

We next use the upper bound of the Duhamel two-point function derived by Kishi and Kubo,[10] (3.11a), (3.11b) as in the previous section. It is straightforward to calculate the double commutator:

$$\begin{aligned}\langle[A^\dagger,[H,A]]\rangle=&-\frac{2}{|\Lambda|}\sum_{\alpha,m}(1-\cos q_m)\{\langle S^x_\alpha S^x_{\alpha+m}\rangle+\langle S^y_\alpha S^y_{\alpha+m}\rangle\}\\&-\frac{2\lambda}{|\Lambda|}\sum_\alpha(1-\cos(q_1+q_2))\,\{\langle S^x_\alpha S^x_{\alpha+1+2}\rangle+\langle S^y_\alpha S^y_{\alpha+1+2}\rangle\}\\&-\frac{2\lambda}{|\Lambda|}\sum_\alpha(1-\cos(q_1-q_2))\,\{\langle S^x_\alpha S^x_{\alpha+1-2}\rangle+\langle S^y_\alpha S^y_{\alpha+1-2}\rangle\}+hm_y, \quad (4.6)\end{aligned}$$

where $q=p-k$, m in the summation expresses the vectors to the nearest neighboring spins and $1+2$ and $1-2$ also express the vectors to the next nearest neighboring spins. We used the definition of the twisted order parameter

$$m_y=\frac{1}{|\Lambda|}\sum_\alpha \varepsilon_\alpha \cos(k\cdot\alpha)\langle S^y_\alpha\rangle. \quad (4.7)$$

The upper bound of the double commutator is given by using the inequality $|\langle S^i_\alpha S^i_{\alpha+\delta}\rangle|\le S^2$, where δ expresses a vector to the nearest neighbor site. We thus have

$$\langle[A^\dagger,[H,A]]\rangle\le 4S^2\,\{2-\cos q_1-\cos q_2+2\lambda(1-\cos q_1\cos q_2)\}+|hm_y|\equiv C_p, \quad (4.8)$$

which should not be confused with C^z_k in (3.18b). We prove the absence of twisted order using following inequality which results from (3.8), (3.11a), (4.2) and (4.8):

$$|\langle[A,B]\rangle|^2\le B^x_p C_p. \quad (4.9)$$

Note that C_p is always finite and B^x_p is finite except when $(p_1,p_2)=(\pi,\pi)$. Since the left hand side of (4.9) does not depend upon p, the minimum value of the right hand side with respect to p yields the optimized upper bound. As seen from (4.8), the right hand side of (4.9) vanishes at $q_1=q_2=0$ unless $(k_1,k_2)=(\pi,\pi)$ when $h\to 0$ after the thermodynamic limit is taken. This implies that (4.5) vanishes, which means the absence of spontaneous symmetry breaking $m_y\to 0$ as inferred from comparison of (4.5) and (4.7).

In the Ising-like anisotropic case, we add an external field parallel to the z axis and choose A and B as below:

$$A=S^x_{p-k+(\pi,\pi)}=\frac{1}{\sqrt{|\Lambda|}}\sum_\alpha \varepsilon_\alpha e^{-i(p-k)\alpha}S^x_j \quad (4.10)$$

$$B=S^y_{-p}=\frac{1}{\sqrt{|\Lambda|}}\sum_\alpha e^{ip\alpha}S^y_k. \quad (4.11)$$

The commutator $[A,B]$ yields the order parameter,

$$|\langle[A, B]\rangle|^2=\left\{\frac{1}{|\Lambda|}\sum_{\alpha}\varepsilon_\alpha\cos(k\cdot\alpha)\langle S^z_\alpha\rangle\right\}^2+\left\{\frac{1}{|\Lambda|}\sum_{\alpha}\varepsilon_\alpha\sin(k\cdot\alpha)\langle S^z_\alpha\rangle\right\}^2. \tag{4.12}$$

The double commutator is evaluated in a similar way as above. The result is

$$\begin{aligned}\langle[A^\dagger, [H, A]]\rangle=&-\frac{1}{|\Lambda|}\sum_{\alpha,m}(\Delta-\cos q_m)\langle S^z_\alpha S^z_{\alpha+m}\rangle-\frac{1}{|\Lambda|}\sum_{\alpha,m}(1-\Delta\cos q_m)\langle S^x_\alpha S^x_{\alpha+m}\rangle\\&-\frac{\lambda}{|\Lambda|}\sum_{\alpha}(\Delta-\cos(q_1+q_2))\langle S^z_\alpha S^z_{\alpha+1+2}\rangle\\&-\frac{\lambda}{|\Lambda|}\sum_{\alpha}(1-\Delta\cos(q_1+q_2))\langle S^x_\alpha S^x_{\alpha+1+2}\rangle\\&-\frac{\lambda}{|\Lambda|}\sum_{\alpha}(\Delta-\cos(q_1-q_2))\langle S^z_\alpha S^z_{\alpha+1-2}\rangle\\&-\frac{\lambda}{|\Lambda|}\sum_{\alpha}(1-\Delta\cos(q_1-q_2))\langle S^x_\alpha S^x_{\alpha+1-2}\rangle+hm_z,\end{aligned} \tag{4.13}$$

where $q=p-k$. The expectation value of the double commutator is finite as in the XY-like case, and the right hand side of the Bogoliubov inequality (4.2) does not diverge unless $(k_1, k_2)=(\pi, \pi)$. Therefore the upper bound of order parameter goes to 0 after taking the thermodynamic and zero-field limits in this order. In this way we have proved the absence of twisted order in the two-dimensional frustrated XXZ model for any anisotropy Δ as long as $\lambda\leq 1/2$. This restriction comes from the limit of applicability of (3.11).[10]

§5. Conclusion

We discussed the existence of long-range order in the two-dimensional quantum frustrated XXZ model at zero temperature. To investigate the characteristics of this system in the strongly frustrated region ($\lambda\simeq 1/2$), we introduced the XXZ anisotropy. Using the naive spin wave theory, the method of infrared bounds and the Bogoliubov inequality, we investigated the validity of the classical picture in this system. First, we used the naive spin wave theory, and obtained the results as seen in Figs. 2(a), 2(b) and 2(c). If we follow Chandra and Doucot[1] in defining the spin liquid state as a region in which the quantum correction is larger than the classical contribution, such a state appears for any XY-like anisotropy ($0\leq\Delta\leq 1$) in the strongly frustrated region $\lambda\simeq 1/2$. With effects of the Ising-like anisotropy, the spin liquid phase disappears even in the strongly frustrated region. These results suggest that the spin liquid phase, if any, is more stable in the XY-like system than in the Ising-like system. However, we should remind the reader that the predictions of the naive spin wave theory may not be taken too seriously in the strongly frustrated region. The idea of asymptotic expansion by $1/S$ may breakdown even when classical states may persist to exist against quantum effects.[11] To confirm the existence of Néel order away from the strongly frustrated region, we used the mathematically rigorous method of infrared bounds. This technique allowed us to estimate a lower bound of long-range order, thus yielding a region in which the existence of long-range order is fully confirmed. The result is in Fig. 4. For technical reasons, it is not possible to discuss the existence of collinear order which may exist beyond $\lambda=1/2$. It is also difficult to discuss the absence of non-classical state by the present method.

In §4 we discussed the absence of twisted order using the Bogoliubov inequality generalizing our previous idea for the Heisenberg case.[11] We proved that for $0\leq\lambda\leq 1/2$ the twisted order cannot be the ground state for any Δ.

The gap between the limits of stability of two classical states, the Néel and collinear, predicted by the naive spin wave theory vanishes as soon as the Ising-like anisotropy is introduced, Fig. 2(c). This fact supports the idea that the non-classical state in the strongly frustrated region, if any, should have XY-like characteristics. Investigation of candidates for non-classical states in the Ising-like region by other methods may clarify appropriateness of the proposed states.

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