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Long-Range Order in Antiferromagnetic Quantum Spin Systems

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The existence of long-range order is proved under certain conditions for the antiferromagnetic XYZ model on the simple cubic or the square lattice. In particular, the spin-1/2 XXZ model on the square lattice is shown to have ground-state long-range order if the exchange anisotropy Δ satisfies $0\leqq\Delta<0.20$ or $\Delta>1.72$, which improves the result of Kubo and Kishi. The existence of long-range order of the z-component of the spin operator is proved for the XXZ model with XY-like anisotropy ($0\leqq\Delta\leqq 1$) under certain conditions. A similar result is shown to hold for the long-range order in the x-direction for the Ising-like model ($\Delta\geqq 1$). The XXZ model on the two-dimensional hexagonal lattice is proved to have finite ground-state long-range order for any value of $\Delta(\geqq 0)$ if $S\geqq 1$ and for $\Delta>2.55$ when $S=1/2$.

§1. Introduction

Possible relevance of magnetism to the mechanism of high-temperature superconductivity[1] has aroused active debates on the ground-state properties of the two-dimensional quantum spin systems.[2] One of the important outstanding problems is whether long-range order exists or not in the ground state of the two-dimensional antiferromagnetic XXZ model. The answer should depend on the spin quantum number S and the exchange anisotropy Δ. The best rigorous result obtained so far is due to Kubo and Kishi[3] who showed the existence of long-range order for arbitrary Δ (as long as it represents antiferromagnetic interactions) if the spin quantum number satisfies $S\geqq 1$ on the square lattice. They have also proved that the two-dimensional spin-1/2 model has finite long-range order if Δ is close to the limit of the XY model ($0\leqq\Delta<0.13$) or Δ is larger than 1.78 (Ising-like). Although this settles the controversy on the existence of ground-state long-range order in the spin-1/2 XY model ($\Delta=0$) in two dimensions,[4] the isotropic Heisenberg antiferromagnet ($\Delta=1$) still escapes rigorous analysis.

The method of Kubo and Kishi has its basic origin in the theory of Dyson, Lieb and Simon (DLS).[5] These latter authors derived a sufficient condition for the existence of long-range order at low temperatures in three- (and higher-) dimensional systems. The DLS theory has since been applied by Neves and Perez[6] to the ground-state problem of the two-dimensional Heisenberg model. Further refinement of the theory has been achieved by Nishimori *et al.*[7] and Kennedy *et al.*[8] by generalizing the method to the XXZ model or by providing improved sufficient conditions for the existence of long-range order. Kubo and Kishi made full use of these existing techniques to prove the above-mentioned results.

It is the purpose of the present paper to generalize the idea of Kubo and Kishi to show the following results. First, we treat the XYZ model instead of the XXZ model and derive the parameter region in which long-range order certainly exists at low temperatures on the simple cubic lattice or at $T=0$ on the square lattice. In the special case of the spin-1/2 XXZ model on the square lattice, we prove the existence of long-range order in the range of $0\leqq\Delta<0.20$ and $\Delta<1.72$, which is an improvement over Kubo and Kishi's $0\leqq\Delta<0.13$ and $\Delta<1.78$. Second, we prove that long-range order along the nonprincipal axis (e.g., z-axis in the XY-like region) exists in the XXZ model on the square or the simple cubic lattice if the nearest-neighbor correlations are continuous functions of Δ in the neighborhood of $\Delta=1$. Third, we apply the present method to the two-dimensional hexagonal lattice to prove the existence of ground-state long-range order for any $\Delta\geqq 0$ if $S\geqq 1$ and for $\Delta>2.55$ if $S=1/2$.

These three problems are discussed in the succeeding three sections, followed by a brief summary in the last section.

§2. *XYZ* model

The model Hamiltonian is defined by

$$H=\sum_{\alpha}\sum_{\delta}(J_x S_\alpha^x S_{\alpha+\delta}^x+J_y S_\alpha^y S_{\alpha+\delta}^y+J_z S_\alpha^z S_{\alpha+\delta}^z), \tag{2.1}$$

where α denotes a lattice site on the square or the simple cubic lattice with periodic boundary conditions, δ is the unit vector to one of the nearest neighbor sites. The number of δ is equal to the lattice dimensionality, ν. The exchange parameters J_x, J_y and J_z should not be negative. In the following, we use the symbol $g_p^{(i)}$ to denote the spin correlation of the ith component ($i=x, y, z$) with the wave number p:

$$g_p^{(i)}=\langle S_p^i S_{-p}^i\rangle, \tag{2.2}$$

where the Fourier transformation is defined by

$$S_p^i=\frac{1}{\sqrt{|\Lambda|}}\sum_{\alpha}e^{-ip\cdot\alpha}S_\alpha^i. \tag{2.3}$$

Here the total number of sites is represented by $|\Lambda|$. The expectation value is understood as being taken by the ground-state wave function throughout this paper. In this connection, we note that the existence of long-range order is established in the following at sufficiently low temperatures in three dimensions, or at $T=0$ in two dimensions. See DLS and ref. 6 for details on this point.

It is straightforward to derive the sum rule[8]

$$\langle S_\alpha^i S_{\alpha+\delta}^i\rangle=\frac{1}{\nu|\Lambda|}\sum_p g_p^{(i)}\sum_{m=1}^{\nu}\cos p_m, \tag{2.4}$$

where use has been made of translational invariance as well as equivalence of δ in any direction in evaluating the expectation value on the left-hand side of (2.4). Finiteness of Néel-type long-range order in the direction i is equivalent to

$$\lim_{\Lambda\to\infty}\frac{1}{|\Lambda|}g_p^{(i)}>0,$$

with $p=(\pi, \pi)$ in two dimensions or $p=(\pi, \pi, \pi)$ in three dimensions.[5] This fact, together with the sum rule (2.4), yields the following necessary and sufficient condition for finiteness of long-range order in the thermodynamic limit:

$$-\langle S_\alpha^i S_{\alpha+\delta}^i\rangle>\int\frac{d^\nu p}{(2\pi)^\nu}g_p^{(i)}\left(-\frac{1}{\nu}\sum_m\cos p_m\right). \tag{2.5}$$

By replacing the integrand in (2.5) with an upper bound, we obtain a sufficient condition as[8]

$$-\langle S_\alpha^i S_{\alpha+\delta}^i\rangle>\int^{(+)}\frac{d^\nu p}{(2\pi)^\nu}\tilde{g}_p^{(i)}\left(-\frac{1}{\nu}\sum_m\cos p_m\right), \tag{2.6}$$

where $(+)$ means that the integral is restricted to the region where the integrand is positive. The function $\tilde{g}_p^{(i)}$ is given by[5]

$$\tilde{g}_p^{(i)}=\frac{1}{2}(B_p^{(i)}C_p^{(i)})^{1/2}, \tag{2.7}$$

where

$$B_p^{(i)}=\frac{1}{2J_i E_p'}, \tag{2.8}$$

with

$$E_p'=\sum_m(1+\cos p_m) \tag{2.9}$$

and

$$C_p^{(i)}=\langle[S_p^{(i)}, [H, S_{-p}^{(i)}]]\rangle. \tag{2.10}$$

Let us first discuss the parameter region $J_x\geqq J_y\geqq J_z$. Since the appropriate long-range order is that of the spin component $i=x$, we have calculated the double commutator (2.10) with $i=x$ to find

$$C_p^x=-2\nu J_y\langle yy\rangle-2\nu J_z\langle zz\rangle+2(J_z\langle yy\rangle+J_y\langle zz\rangle)\sum_m\cos p_m,$$

where $\langle jj\rangle$ ($j=x, y, z$) is an abbreviation of $\langle S_\alpha^j S_{\alpha+\delta}^j\rangle$. Hence, the sufficient condition (2.6) is written as, using (2.7) to (2.10),

$$-2\langle xx\rangle\sqrt{J_x}>\sqrt{-J_y\langle yy\rangle-J_z\langle zz\rangle}\int^{(+)}\frac{d^\nu p}{(2\pi)^\nu}\sqrt{\frac{\nu-r\sum\cos p_m}{\nu+\sum\cos p_m}}\left(-\frac{1}{\nu}\sum_m\cos p_m\right), \tag{2.11}$$

where

$$r=\frac{J_z\langle yy\rangle+J_y\langle zz\rangle}{J_y\langle yy\rangle+J_z\langle zz\rangle}. \tag{2.12}$$

Since the integrand of (2.11) is a monotone increasing function of r,[7] one may replace r by its maximum value. This maximum value is 1, because

$$r-1=\frac{(\langle yy\rangle-\langle zz\rangle)(J_z-J_y)}{J_y\langle yy\rangle+J_z\langle zz\rangle}\leqq 0, \tag{2.13}$$

which follows from

$$-\langle yy\rangle\geqq-\langle zz\rangle\geqq 0, \tag{2.14}$$

in the present parameter region. Equation (2.14) can be proved by the same technique as in the proof of Proposition 2 of Nishimori *et al.*[7] The condition (2.11) is thus replaced by

$$-2\langle xx\rangle\sqrt{J_x}>\sqrt{-J_y\langle yy\rangle-J_z\langle zz\rangle}\,\Gamma_\nu, \tag{2.15}$$

where Γ_ν denotes the integral appearing in (2.11) with $r=1$. Further simplification comes from the inequality

$$-\langle xx\rangle\geqq-\langle yy\rangle\geqq-\langle zz\rangle\geqq 0, \tag{2.16}$$

the first relation of which can be proved in a similar manner as the proof of (2.14). Using (2.16) in (2.15), a new sufficient condition is found:

$$2\sqrt{-J_x\langle xx\rangle}>\sqrt{J_y+J_z}\,\Gamma_\nu. \tag{2.17}$$

We next estimate a lower bound of $-\langle xx\rangle$ by applying the variational principle to the Hamiltonian (2.1) with the Néel-state wave function in the x-direction:[7]

$$J_x\langle xx\rangle+J_y\langle yy\rangle+J_z\langle zz\rangle\leqq -S^2J_x. \tag{2.18}$$

According to (2.16), the inequality (2.18) implies

$$-\langle xx\rangle\geqq\frac{S^2J_x}{J_x+J_y+J_z}. \tag{2.19}$$

From (2.17) and (2.19), we derive the final condition for the existence of long-range order as

$$2SJ_x>\Gamma_\nu\sqrt{(J_x+J_y+J_z)(J_y+J_z)}. \tag{2.20}$$

This is a generalization of Kubo and Kishi's condition (2.13). It does not lose generality to set $J_x=1$ in the Hamiltonian. We use this unit of energy in the following.

In three dimensions, the integral Γ_3 is evaluated as 0.350. Then it is straightforward to verify that (2.20) is satisfied for any allowed value of the parameters ($S\geqq 1/2$, $0\leqq J_z\leqq J_y\leqq 1$). In two dimensions, Γ_2 is 0.646, which leads to the existence of long-range order if $S\geqq 1$ for any value of J_y and J_z in the present parameter region. In the case of $S=1/2$ in two dimensions, the inequality (2.20) is satisfied only if $0\leqq J_y+J_z\leqq 1.13$. This parameter range is depicted in Fig. 1.

The sufficient condition in the other parameter regions (such as $J_y\geqq 1\geqq J_z$) can be obtained simply by permuting x, y and z in (2.20). The three-dimensional model with arbitrary S or the two-dimensional model with $S\geqq 1$ is found to have long-range order for any value of the exchange interactions. A restriction exists in the case of $S=1/2$, $\nu=2$, as shown in Fig. 1. In this figure, long-range order has been found to exist in the unshaded region. The line $J_y=1$ corresponds to the *XXZ* model (J_z is usually denoted as Δ in this model). The result of Kubo and Kishi (who proved the existence of long-range order for

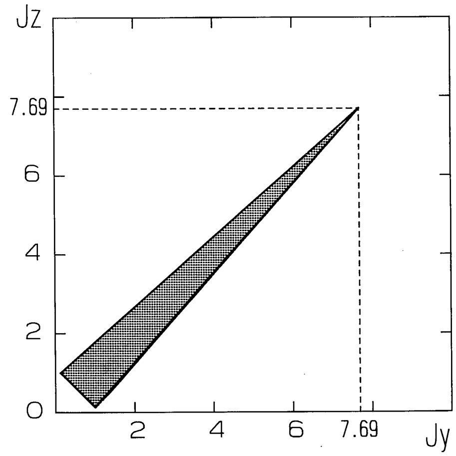

Fig. 1(a). The unshaded region represents the range where we can prove the existence of ground-state long-range order for the spin-1/2 *XYZ* model on the square lattice.

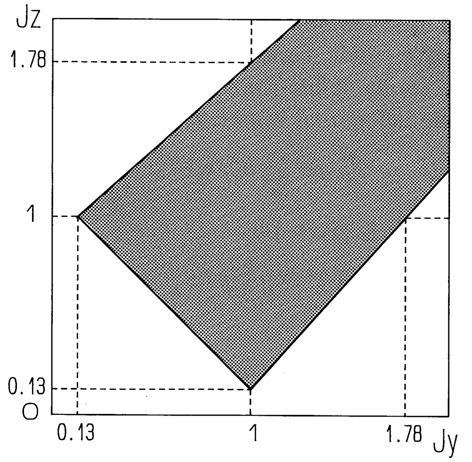

Fig. 1(b). An enlargement of Fig. 1(a) in the neighborhood of the origin.

$\Delta<0.13$ and $\Delta>1.78$) is reproduced. The line $J_z=0$ represents the "anisotropic XY model" which is seen to have long-range order for any $J_y \geqq 0$.

It is possible to improve the bound $\Delta<0.13$, $\Delta>1.78$ for the spin-1/2 XXZ model by using better variational wave functions to estimate the ground-state energy better than in (2.18). In the XY-like region ($\Delta \leqq 1$), by denoting the variational energy per bond as e, the sufficient condition derived from (2.17) is

$$-e>\Gamma_\nu^2 \frac{(2+\Delta)(1+\Delta)}{4}, \tag{2.21}$$

which should be compared with (2.20). We have found that the trial function of Suzuki and Miyashita[9] satisfies (2.21) when $\Delta<0.20$ by numerically minimizing their expression (4.2) of the ground-state energy (see Fig. A.3). In the Ising-like region ($\Delta \geqq 1$), the condition corresponding to (2.21) is

$$-e>\Gamma_\nu^2 \frac{2+\Delta}{2\Delta}. \tag{2.22}$$

We have found that the Néel state with short-range spin fluctuations, as described in the Appendix, satisfies (2.22) in the range $\Delta>1.72$. The spin-1/2 isotropic model $\Delta=1$ in two dimensions escapes the best estimate of the ground-state energy as suggested by Kennedy *et al.*[8] A different approach is required to settle this case.

§3. Long-Range Order in the Nonprincipal Axis

The long-range order discussed in the previous section is that of the spin component i which has the property that J_i has the largest value in the Hamiltonian (2.1). A natural question arises on what happens to long-range order of other components of spin operators. We investigate this problem in the present section, restricting ourselves to the XXZ model ($J_x=J_y=1$, $J_z=\Delta$) for simplicity.

If the system is XY-like ($0 \leqq \Delta \leqq 1$), the long-range order of our interest is related to $\langle S_p^z S_{-p}^z \rangle$. The condition (2.6) with (2.7) to (2.10) thus reads

$$-\langle zz \rangle > \sqrt{\frac{-\langle xx \rangle}{2\Delta}} \int^{(+)} \frac{d^\nu p}{(2\pi)^\nu} \sqrt{\frac{E_p}{E_p'}} \left(-\frac{1}{\nu} \sum_m \cos p_m \right) = \sqrt{\frac{-\langle xx \rangle}{2\Delta}} \Gamma_\nu, \tag{3.1}$$

where $E_p=\nu-\sum \cos p_m$, and the commutator

$$C_p^{(z)}=-4E_p\langle xx \rangle,$$

has been used. The zz-correlation on the left-hand side of (3.1) is bounded from below as

$$-\langle zz \rangle \geqq \frac{S^2+2\langle xx \rangle}{\Delta}, \tag{3.2}$$

according to the variational principle with the trial wave function of the Néel state in the x-direction.[7] By replacing $-\langle zz \rangle$ in (3.1) with the right-hand side of (3.2) and solving the inequality for $-\langle xx \rangle$, we find that long-range order in the z-direction exists if

$$-16\langle xx \rangle < \Delta \Gamma_\nu^2+8S^2-\Gamma_\nu \sqrt{\Delta(\Delta\Gamma_\nu^2+16S^2)}. \tag{3.3}$$

To see whether (3.3) is satisfied when $\Delta \leqq 1$, we evaluate this inequality in the isotropic case $\Delta=1$. Since the left-hand side is bounded from above by $16S(S+1/2\nu)/3$ if $\Delta=1$,[5] (3.3) is satisfied if

$$\frac{16}{3} S \left(S+\frac{1}{2\nu} \right) < \Gamma_\nu^2+8S^2-\Gamma_\nu \sqrt{\Gamma_\nu^2+16S^2}. \tag{3.4}$$

One easily finds that (3.4) is satisfied if $S \geqq 3/2$

when $\nu=2$ ($\Gamma_2=0.646$) or if $S\geqq 1$ when $\nu=3$ ($\Gamma_3=0.350$). Now we notice that the right-hand side of (3.3) is a continuous function of Δ. Therefore, if the left-hand side is also continuous in the neighborhood of $\Delta=1$ in the thermodynamic limit, (3.3) is satisfied by sufficiently large S in a range $\Delta_c(S)<\Delta$ with $\Delta_c(S)<1$.

A similar argument can be given on the long-range order in the x-direction in the Ising-like region ($\Delta\geqq 1$). Using the method of §2, we can derive the following condition for the existence of this long-range order:

$$-2\langle xx\rangle>\sqrt{-\langle xx\rangle-\Delta\langle zz\rangle}\Gamma_\nu. \qquad (3.5)$$

The correlation $-\langle xx\rangle$ on the right-hand side of (3.5) can be replaced by $-\langle zz\rangle$ since $-\langle zz\rangle\geqq-\langle xx\rangle$ in the Ising-like region.[7] The correlation function on the left-hand side should be replaced by a lower bound in order to obtain a sufficient condition for the existence of long-range order. The variational wave function of the Nêel state in the z-direction gives

$$-2\langle xx\rangle\geqq\Delta S^2+\Delta\langle zz\rangle. \qquad (3.6)$$

In this way, the inequality (3.5) has been written only in terms of the correlation $-\langle zz\rangle$. After some rearrangement, the inequality reads

$$\begin{aligned}-4\Delta^2\langle zz\rangle<2(1+\Delta)\Gamma_\nu^2+4\Delta^2S^2\\ -2\Gamma_\nu\sqrt{1+\Delta}\sqrt{(1+\Delta)\Gamma_\nu^2+4\Delta^2S^2}.\end{aligned} \qquad (3.7)$$

In the case of $\Delta=1$, we may replace the left-hand side by the upper bound $4S(S+1/2\nu)/3$. Then the inequality (3.7) ($\Delta=1$) is seen to be satisfied if $S\geqq 3/2$ when $\nu=2$ or if $S\geqq 1$ when $\nu=3$. Therefore, assuming continuity of the correlation $-\langle zz\rangle$ in the neighborhood of $\Delta=1$, we conclude that the Ising-like model ($\Delta\geqq 1$) with sufficiently large S has long-range order in the x-direction if Δ is not far from 1.

§4. Long-Range Order on the Hexagonal Lattice

As has been pointed out by DLS, the present method is applicable to the two-dimensional hexagonal lattice. Affleck *et al.*[10] actually carried out this program to prove the existence of long-range order of the isotropic model ($\Delta=1$) with $S\geqq 3/2$. We apply the technique described in the previous sections to improve their result. Following Affleck *et al.*,[10] let us define the Fourier transformation on the hexagonal lattice as

$$S^i_{p,\pm}=\sum_\alpha h^\pm_p(\alpha)S^i_\alpha, \qquad (4.1)$$

where $h^\pm_p$ is given by

$$\begin{aligned}h^\pm_p(\alpha)=(\mp)^\alpha\exp\{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{\alpha}+\mathrm{i}(-)^\alpha\phi(\boldsymbol{p})/2\}\\ /\sqrt{|\Lambda|}.\end{aligned} \qquad (4.2)$$

The factor $(\mp)^\alpha$ on the right-hand side is $+$ if α is on one of the sublattices (even site) and $\mp$ if it is on the other one (odd site). The factor $\phi(\boldsymbol{p})$ represents the phase of

$$\varepsilon(\boldsymbol{p})=\sum_{m=1}^{3}\exp(\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{\delta}_m), \qquad (4.3)$$

where $\boldsymbol{\delta}_m$ denotes the unit vector to the nearest neighbor site. The wave number $\boldsymbol{p}$ ranges over the first Brillouin zone of one of the sublattices. The phase $\phi(\boldsymbol{p})$ cannot be defined when $\boldsymbol{p}$ satisfies $\varepsilon(\boldsymbol{p})=0$. However, this indefiniteness of the phase is irrelevant to the following arguments because such points do not have finite measure in the first Brillouin zone. The inverse transformation is

$$S^i_\alpha=\sum_{t=\pm}\sum_p h^t_p(\alpha)^*S^i_{p,t}, \qquad (4.4)$$

where the asterisk signifies conjugation. By making use of this Fourier transformation and translational and rotational invariance, it is rather straightforward to derive the sum rule

$$\begin{aligned}\langle S^i_\alpha S^i_{\alpha+\delta}\rangle=-\frac{1}{3|\Lambda|}\sum_t\sum_p t\langle S^i_{p,t}S^i_{-p,t}\rangle\\ \times|\varepsilon(\boldsymbol{p})|.\end{aligned} \qquad (4.5)$$

Since the existence of Nêel-type long-range order is represented by positivity of $\langle S^i_{0,+}S^{i*}_{0,+}\rangle/|\Lambda|$ (as can be checked by using (4.1) and noticing that $\langle S^i_{0,-}S^{i*}_{0,-}\rangle/|\Lambda|$ is either vanishing, or of much smaller order than $\langle S^i_{0,+}S^{i*}_{0,+}\rangle/|\Lambda|$), the necessary and sufficient condition for the existence of long-range order in the i-direction is

$$-\langle S^i_\alpha S^i_{\alpha+\delta}\rangle>\frac{1}{3|\Lambda|}\sum_t\sum_{p\neq 0}t|\varepsilon(\boldsymbol{p})|\langle S^i_{p,t}S^{i*}_{p,t}\rangle,$$

or, in the thermodynamic limit,

$$-\langle S^i_\alpha S^i_{\alpha+\delta}\rangle > \frac{1}{6|B|}\int_B d^2p\,|\varepsilon(p)|(\langle S^i_{p,+}S^{i*}_{p,+}\rangle - \langle S^i_{p,-}S^{i*}_{p,-}\rangle), \tag{4.6}$$

where B denotes the Brillouin zone. Since both expectation values in the integrand of (4.6) are positive semi-definite, we obtain a sufficient condition by dropping the second term on the right-hand side of (4.6):

$$-\langle S^i_\alpha S^i_{\alpha+\delta}\rangle > \frac{1}{6|B|}\int_B d^2p\,|\varepsilon(p)|\langle S^i_{p,+}S^{i*}_{p,+}\rangle. \tag{4.7}$$

Let us apply the condition (4.7) to the XY-like region ($0\leqq\varDelta\leqq 1$) of the XXZ model. Following Affleck *et al.*,[10] we replace the expectation value of the product of spin operators on the right-hand side of (4.7) ($i=x$) by its upper bound $(B^{(x)}_p C^{(x)}_p)^{1/2}/2$, where

$$B^{(x)}_p = \frac{1}{3-|\varepsilon(p)|}, \tag{4.8}$$

$$\begin{aligned} C^{(x)}_p &= \langle [S^x_{p,+}, [H, S^{x*}_{p,+}]]\rangle \\ &= -3\varDelta\langle zz\rangle - 3\langle xx\rangle \\ &\quad -(\varDelta\langle xx\rangle + \langle zz\rangle)|\varepsilon(p)|. \end{aligned} \tag{4.9}$$

The resulting inequality is

$$-\langle xx\rangle > \frac{\sqrt{-\langle xx\rangle - \varDelta\langle zz\rangle}}{12}\frac{1}{|B|}\int_B d^2p\,|\varepsilon(p)| \times\sqrt{\frac{3+r|\varepsilon(p)|}{3-|\varepsilon(p)|}}, \tag{4.10}$$

where

$$r = \frac{\varDelta\langle xx\rangle + \langle zz\rangle}{\langle xx\rangle + \varDelta\langle zz\rangle}.$$

Since $r\leqq 1$ (as derived from $-\langle xx\rangle \geqq -\langle zz\rangle$[7]) and the right-hand side of (4.10) is monotone increasing in r,[7] we are allowed to set $r=1$ in (4.10) to obtain a new sufficient condition for the existence of long-range order. The inequality reduces to a more tractable form by replacing $-\langle zz\rangle$ with $-\langle xx\rangle$ on the right-hand side, which is valid when $\varDelta\leqq 1$, and $-\langle xx\rangle$ on the left-hand side with its lower bound $S^2/(2+\varDelta)$ (see (2.19)). The final condition is

$$12S > \sqrt{(2+\varDelta)(1+\varDelta)}\,I, \tag{4.11}$$

where

$$I = \frac{1}{|B|}\int_B d^2p\,|\varepsilon|\sqrt{\frac{3+|\varepsilon|}{3-|\varepsilon|}} = 5.07. \tag{4.12}$$

The inequality is satisfied by all $\varDelta\leqq 1$ if $S\geqq 3/2$ and by $\varDelta<0.92$ if $S=1$.

The Ising-like region $\varDelta\geqq 1$ is treated in a similar manner. The inequality (4.7) is applied with $i=z$. The relevant quantities corresponding to (4.8) and (4.9) are[10]

$$\begin{aligned} B^{(z)}_p &= \frac{1}{\varDelta(3-|\varepsilon(p)|)}, \\ C^{(z)}_p &= \langle [S^z_{p,+}, [H, S^{z*}_{p,+}]]\rangle \\ &= -2(3+|\varepsilon(p)|)\langle xx\rangle. \end{aligned}$$

The sufficient condition then reads

$$-\langle zz\rangle > \frac{\sqrt{-\langle xx\rangle}}{6\sqrt{2\varDelta}}I, \tag{4.13}$$

with the same I as in (4.12). In the Ising-like region, $-\langle xx\rangle$ is bounded from above by $-\langle zz\rangle$, and $-\langle zz\rangle$ is bounded from below by $\varDelta S^2/(\varDelta+2)$. Therefore, we obtain the condition as

$$6\sqrt{2}\varDelta S > I\sqrt{\varDelta+2}. \tag{4.14}$$

This relation is satisfied by any $\varDelta\geqq 1$ if $S\geqq 3/2$ and by $\varDelta>1.04$ if $S=1$. As for the spin-1/2 case, the range of $\varDelta$ satisfying (4.14) is $\varDelta>2.55$.

We have proved that the XXZ model on the two-dimensional hexagonal lattice has ground-state long-range order for any $\varDelta\geqq 0$ if $S\geqq 3/2$, for $\varDelta>1.04$ or $0\leqq\varDelta<0.92$ if $S=1$, and for $\varDelta>2.55$ if $S=1/2$. An improvement on the spin-1 case is possible by employing a better variational wave function to estimate a lower bound on the left-hand side of (4.7). (Remember that a simple Néel state was used in the above argument.) This idea is carried out in the Appendix by introducing short-range spin fluctuations into the Néel state. The sufficient condition derived from (4.10) or (4.13) is

$$-e > \frac{(2+\varDelta)(1+\varDelta)}{12^2}I^2 \quad (0\leqq\varDelta\leqq 1), \tag{4.15}$$

or

$$-e > \frac{2+\varDelta}{72\varDelta}I^2 \quad (\varDelta\geqq 1), \tag{4.16}$$

where e is the variational energy. These inequalities are satisfied by any $\Delta \geqq 1$ when $S=1$, as shown in the Appendix.

§5. Summary

We have proved that the antiferromagnetic XYZ model on the three-dimensional simple cubic lattice has long-range order at sufficiently low temperatures for any value of the exchange parameters J_x, J_y and J_z in the Hamiltonian (2.1), irrespective of the spin quantum number S. In the ground state of the same model on the square lattice, the existence of long-range order has been proved for any J_x, J_y and J_z in the case of $S \geqq 1$. As for the spin-1/2 model, the region we can prove the existence of long-range order is limited to the unshaded part of Fig. 1. By specializing to the XXZ model ($J_x=J_y=1$, $J_z=\Delta$), we could improve the result on the spin-1/2 model on the square lattice to show the existence of long-range order in the range $\Delta>1.72$ and $0 \leqq \Delta < 0.20$.

The existence of long-range order in the z-direction in the XY-like case ($\Delta \leqq 1$) of the XXZ model has been proved for sufficiently large S assuming continuity of the nearest-neighbor correlation as a function of Δ. The same has been shown on the long-range order in the x-direction in the Ising-like region ($\Delta \geqq 1$).

The existence of ground-state long-range order has been proved for the XXZ model on the two-dimensional hexagonal lattice with arbitrary $\Delta \geqq 0$ and $S \geqq 1$ or with $\Delta > 2.55$ and $S=1/2$.

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Appendix: Upper Bound of the Ground-State Energy

First, we derive an upper bound of the ground-state energy of the spin-1 XXZ model on the hexagonal lattice using a simple variational method. The case of the spin-1/2 model on the square lattice will be discussed later.

Let us start with the Néel state in the z-direction, $|N\rangle$, in which all S_α^z on one of the sublattices (even sites) are $+1$, and those on odd sites are -1. The energy per bond of this state, which is greater than the true ground-state energy, is given by

$$e_0 = -\Delta. \tag{A·1}$$

To obtain a better upper bound, it is useful to operate $(1+\lambda S_\alpha^- S_\beta^+/2S)$ to the Néel state for the nearest neighboring sites (α, β). The first site α is an even site while β is odd. In actual calculations of matrix elements, it is essential to factorize the wave function into local parts. For this purpose, we apply the above operator only to the bonds drawn in solid lines in Fig. A·1. These solid lines (which we call a-bonds) form isolated hexagonal plaquettes and the remaining bonds (b-bonds) connect these plaquettes. Then the trial function with a real parameter λ is

$$|\Phi_\lambda\rangle = \prod_p \prod_{(\alpha,\beta)\in p} \left(1+\frac{\lambda}{2S} S_\alpha^- S_\beta^+\right) |N\rangle, \tag{A·2}$$

where the first product is taken over all isolated plaquettes, and the second one is over all nearest-neighboring pairs in a plaquette p. Note that Bartkowski[11] used a similar trial function with the same local operator $(1+\cdots)$ applied to all bonds. Our function (A·2) is much simpler in evaluating various quantities. The energy per bond of this state is given by

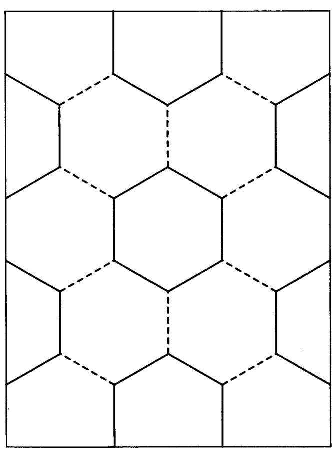

Fig. A·1. Spin-fluctuations introduced to the bonds on hexagons drawn in solid lines.

$$e(\lambda)=\frac{2}{3}e_a(\lambda)+\frac{1}{3}e_b(\lambda), \quad (\text{A}\cdot 3)$$

$$e_a(\lambda)=\langle\Phi_\lambda|\frac{1}{2}(S_0^+S_{\delta_a}^-+S_0^-S_{\delta_a}^+)+\Delta S_0^zS_{\delta_a}^z|\Phi_\lambda\rangle/\langle\Phi_\lambda|\Phi_\lambda\rangle, \quad (\text{A}\cdot 4\text{a})$$

$$e_b(\lambda)=\langle\Phi_\lambda|\Delta S_0^zS_{\delta_b}^z|\Phi_\lambda\rangle/\langle\Phi_\lambda|\Phi_\lambda\rangle, \quad (\text{A}\cdot 4\text{b})$$

where the pair $(0, \delta_a)$ is on an a-bond and $(0, \delta_b)$ is on a b-bond. Note that the operator $(1+\lambda S_\alpha^-S_\beta^+/2S)$ commutes with the other ones belonging to different plaquettes. If F is an operator consisting of spins of only one particular plaquette p_0, such as $S_0^zS_{\delta_a}^z$, the matrix element $\langle\Phi_\lambda|F|\Phi_\lambda\rangle$ is written as a product of single-plaquette-related quantities as

$$\begin{aligned}\langle\Phi_\lambda|F|\Phi_\lambda\rangle&=\langle N|\prod_{(\alpha,\beta)\in p_0}\left(1+\frac{\lambda}{2S}S_\alpha^+S_\beta^-\right)(F)\prod_{(\alpha',\beta')\in p_0}\left(1+\frac{\lambda}{2S}S_{\alpha'}^-S_{\beta'}^+\right)\\&\quad\times\prod_{p\neq p_0}\left\{\prod_{(\alpha,\beta)\in p}\left(1+\frac{\lambda}{2S}S_\alpha^+S_\beta^-\right)\prod_{(\alpha',\beta')\in p}\left(1+\frac{\lambda}{2S}S_{\alpha'}^-S_{\beta'}^+\right)\right\}|N\rangle\\&=\langle n|\prod_{(\alpha,\beta)}\left(1+\frac{\lambda}{2S}S_\alpha^+S_\beta^-\right)(F)\prod_{(\alpha',\beta')}\left(1+\frac{\lambda}{2S}S_{\alpha'}^-S_{\beta'}^+\right)|n\rangle\\&\quad\times\left\{\langle n|\prod_{(\alpha,\beta)}\left(1+\frac{\lambda}{2S}S_\alpha^+S_\beta^-\right)\prod_{(\alpha',\beta')}\left(1+\frac{\lambda}{2S}S_{\alpha'}^-S_{\beta'}^+\right)|n\rangle\right\}^{N_p-1},\end{aligned} \quad (\text{A}\cdot 5)$$

where N_p is the number of isolated plaquettes $(=|\Lambda|/6)$. The ket $|n\rangle$ denotes the Néel state in the six-spin space of a single plaquette. Consequently, matrix elements in (A·4a) can be expressed as

$$\langle\Phi_\lambda|\Phi_\lambda\rangle=I_0(\lambda)^{N_p}, \quad (\text{A}\cdot 6\text{a})$$

$$\langle\Phi_\lambda|S_0^zS_{\delta_a}^z|\Phi_\lambda\rangle=I_0(\lambda)^{N_p-1}I_{zz}(\lambda), \quad (\text{A}\cdot 6\text{b})$$

$$\langle\Phi_\lambda|S_0^+S_{\delta_a}^-|\Phi_\lambda\rangle=\langle\Phi_\lambda|S_0^-S_{\delta_a}^+|\Phi_\lambda\rangle=I_0(\lambda)^{N_p-1}I_{+-}(\lambda), \quad (\text{A}\cdot 6\text{c})$$

where

$$I_0(\lambda)=\langle n|\prod_{(\alpha,\beta)}\left(1+\frac{\lambda}{2S}S_\alpha^+S_\beta^-\right)\prod_{(\alpha',\beta')}\left(1+\frac{\lambda}{2S}S_{\alpha'}^-S_{\beta'}^+\right)|n\rangle, \quad (\text{A}\cdot 7\text{a})$$

$$I_{zz}(\lambda)=\langle n|\prod_{(\alpha,\beta)}\left(1+\frac{\lambda}{2S}S_\alpha^+S_\beta^-\right)(S_0^zS_{\delta_a}^z)\prod_{(\alpha',\beta')}\left(1+\frac{\lambda}{2S}S_{\alpha'}^-S_{\beta'}^+\right)|n\rangle, \quad (\text{A}\cdot 7\text{b})$$

$$I_{+-}(\lambda)=\langle n|\prod_{(\alpha,\beta)}\left(1+\frac{\lambda}{2S}S_\alpha^+S_\beta^-\right)(S_0^+S_{\delta_a}^-)\prod_{(\alpha',\beta')}\left(1+\frac{\lambda}{2S}S_{\alpha'}^-S_{\beta'}^+\right)|n\rangle. \quad (\text{A}\cdot 7\text{c})$$

The matrix element of $S_0^zS_{\delta_b}^z$, which contains the spins of two plaquettes, can be expressed similarly as

$$\langle\Phi_\lambda|S_0^zS_{\delta_b}^z|\Phi_\lambda\rangle=-I_0(\lambda)^{N_p-2}I_z(\lambda)^2, \quad (\text{A}\cdot 8)$$

where

$$I_z(\lambda)=\langle n|\prod_{(\alpha,\beta)}\left(1+\frac{\lambda}{2S}S_\alpha^+S_\beta^-\right)(S_0^z)\prod_{(\alpha',\beta')}\times\left(1+\frac{\lambda}{2S}S_{\alpha'}^-S_{\beta'}^+\right)|n\rangle. \quad (\text{A}\cdot 9)$$

Using (A·3) to (A·4), (A·6) to (A·9), we obtain

$$e(\lambda)=\frac{2}{3}(I_{+-}+\Delta I_{zz})/I_0-\frac{\Delta}{3}(I_z/I_0)^2. \quad (\text{A}\cdot 10)$$

Noting that $(S_\alpha^+)^3=(S_\alpha^-)^3=0$ for $S=1$, the I's are found as

$$I_0=1+6\lambda^2+15\lambda^4+22\lambda^6+15\lambda^8+6\lambda^{10}+\lambda^{12}, \quad (\text{A}\cdot 11\text{a})$$

$$I_{zz}=-1-3\lambda^2-3\lambda^4-2\lambda^6-3\lambda^8-3\lambda^{10}-\lambda^{12}, \quad (\text{A}\cdot 11\text{b})$$

$$I_{+-}=2\lambda+10\lambda^3+22\lambda^5+22\lambda^7+10\lambda^9+2\lambda^{11}, \quad (\text{A}\cdot 11\text{c})$$

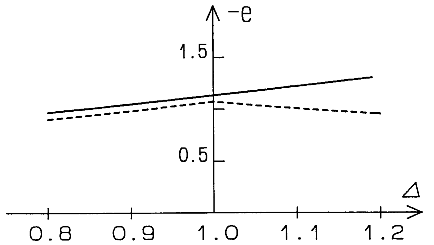

Fig. A·2. The variational energy (A·10) of the spin-1 model on the hexagonal lattice is drawn in a solid line. The right-hand sides of (4.15) and (4.16) shown by a dashed line are always smaller than the corresponding left-hand sides.

$$I_z=1+4\lambda^2+5\lambda^4-5\lambda^8-4\lambda^{10}-\lambda^{12}. \qquad (\mathrm{A\cdot 11d})$$

Substituting these into (A·10), and estimating the minimum value numerically, we can obtain the upper bound of the ground-state energy as a function of Δ. The results are shown in Fig. A·2.

An upper bound of the ground-state energy of the spin-1/2 XXZ model on the square lattice can be estimated quite similarly. In this case, a four-spin cell is chosen as the isolated plaquette, and (A·3) and (A·10) are replaced by

$$e(\lambda)=\frac{1}{2}e_a(\lambda)+\frac{1}{2}e_b(\lambda)$$

$$=\frac{1}{2}(I_{+-}+\Delta I_{zz})/I_0-\frac{\Delta}{2}(I_z/I_0)^2. \qquad (\mathrm{A\cdot 12})$$

From $(S_\alpha^+)^2=(S_\alpha^-)^2=0$ for $S=1/2$, the I's in (A·7) and (A·9) are calculated as

$$I_0=1+4\lambda^2+4\lambda^4, \qquad (\mathrm{A\cdot 13a})$$

$$I_{zz}=-\frac{1}{4}(1+4\lambda^4), \qquad (\mathrm{A\cdot 13b})$$

$$I_{+-}=\lambda(1+2\lambda^2), \qquad (\mathrm{A\cdot 13c})$$

$$I_z=\frac{1}{2}(1-4\lambda^4). \qquad (\mathrm{A\cdot 13d})$$

The results are shown in Fig. A·3. The variational energy thus obtained is better than that of Suzuki and Miyashita[9] in the region ($\Delta \gtrsim 1.5$), but is worse in the XY-like region ($0 \leqq \Delta \leqq 1$).

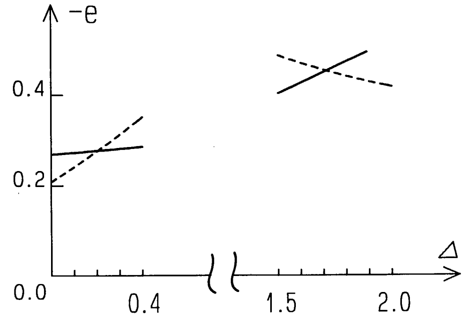

Fig. A·3. In the XY-like region ($\Delta<1$) of the spin-1/2 model on the square lattice, the variational energy of Suzuki and Miyashita[9] (solid line) satisfies (2.21) in the range $\Delta<0.20$. The dashed line corresponds to the right-hand side of (2.21). In the Ising-like region ($\Delta>1$), the energy (A·12) (solid line) satisfies (2.22) when $\Delta>1.72$.

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