Existence of Long-Range Order in the *XXZ* Model

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The method of Kennedy, Lieb, and Shastry is applied to the antiferromagnetic *XXZ* model to examine the existence of long-range order (LRO). On the 3D simple-cubic lattice LRO is proved to exist for any $S \geqq \frac{1}{2}$ and $\Delta \geqq 0$ at low temperature. On the 2D square lattice LRO exists in the ground state for any $\Delta \geqq 0$ if $S \geqq 1$ and for $0 \leqq \Delta < 0.13$ and $\Delta > 1.78$ if $S = \frac{1}{2}$. The existence of LRO in the ground state of the $S = \frac{1}{2}$ *XY* model ($\Delta = 0$), therefore, has been confirmed, in agreement with the conjecture by Nishimori *et al.* The ground state of the $S = \frac{1}{2}$ antiferromagnetic Heisenberg model in two dimensions still remains to be clarified.

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The rigorous proof for the existence of a phase transition in the Heisenberg ferromagnet or antiferromagnet in three dimensions has stood as a challenging problem for theoretical physicists for many decades. The proof for the antiferromagnet was given for $S \geqq 1$ by Dyson, Lieb, and Simon (DLS)[1] and the proof for $S = \frac{1}{2}$ was given quite recently by Kennedy, Lieb, and Shastry (KLS).[2] The proof for the ferromagnet is still not known. On the other hand, the ground-state properties of the two-dimensional quantum spin systems are attracting intense interest which is inspired by a possible relation to the mechanism of the recently discovered high-T_c superconductors.[3] Although no long-range order (LRO) exists in two dimensions at a finite temperature in the system with a continuous symmetry,[4] the existence of LRO in the ground state is a nontrivial problem. Many numerical works have focused on the spin-$\frac{1}{2}$ antiferromagnetic (AF) Heisenberg model on the square lattice.[5] The question of whether the ground state of that system has LRO or not seems to be not yet clarified. The existence of LRO in the spin model with anisotropic exchange interactions is also an interesting problem.

The fundamental method for the proof of the existence of phase transitions in the quantum spin systems with a continuous symmetry was established by DLS.[1] They proved existence of LRO at a low temperature in the spin-$\frac{1}{2}$ isotropic *XY* model and the AF Heisenberg model with spin $S \geqq 1$ on the 3D simple-cubic lattice. Neves and Perez applied the method of DLS to the ground state of the AF Heisenberg model on the 2D square lattice and proved the existence of LRO for $S \geqq 1$.[6,7] Quite recently, several works appeared and extended the proof. Affleck *et al.* showed the existence of antiferromagnetic LRO in the ground state of the AF Heisenberg model on the 2D hexagonal lattice.[7] Kubo analyzed the *XY* model to show the existence of LRO at a low temperature for $S \geqq 1$ on the simple-cubic lattice and also in the ground state of the square lattice for $S \geqq \frac{3}{2}$.[8] Nishimori *et al.*[9] generalized the analysis to the antiferromagnetic *XXZ* model with the anisotropy parameter Δ ($\geqq 0$) on the simple cubic or the square lattice. They also conjectured the existence of the ground-state LRO in the $S = \frac{1}{2}$ *XY* model on the square lattice, relying on strong numerical evidence. Kennedy, Lieb, and Shastry[2] proved this for the $S = \frac{1}{2}$ AF Heisenberg model on the simple-cubic lattice. They also conjectured the existence of the ground-state LRO in two dimensions, making use of the numerical data of a Monte Carlo calculation by Gross, Sanchez-Velasco, and Siggia.[5] We summarize in Fig. 1 the values of S and Δ for which the existence of LRO has been proved so far. The complete proof is still lacking for $S = \frac{1}{2}$ in three dimensions, and both the $S = 1$ and $\frac{1}{2}$ cases remain to be understood in two dimensions.

In this Letter we apply the method of KLS[2] to the *XXZ* model ($\Delta \geqq 0$). The model we consider is described by the Hamiltonian

$$H = \sum_{\alpha \in \Lambda} \sum_{\delta} (S_\alpha^x S_{\alpha+\delta}^x + S_\alpha^y S_{\alpha+\delta}^y + \Delta S_\alpha^z S_{\alpha+\delta}^z) \quad (\Delta \geqq 0), \tag{1}$$

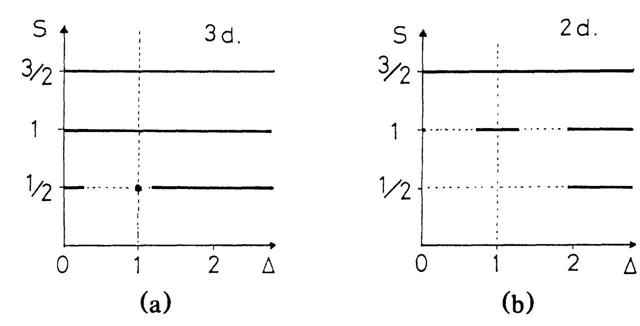

FIG. 1. Bold lines show the values of S and Δ for which the existence of LRO was proved prior to the present work (Refs. 1, 2, and 6–9). (a) 3D simple-cubic lattice: The whole region $\Delta \geqq 0$ for $S \geqq 1$, and two regions $0 \leqq \Delta < 0.29$ and $\Delta > 1.19$ for $S = \frac{1}{2}$ have LRO at a low temperature. For the isotropic point $\Delta = 1$, it was also proved (Ref. 2). (b) 2D square lattice: The whole region $\Delta \geqq 0$ for $S \geqq \frac{3}{2}$, three regions $0 \leqq \Delta < 0.032$, $0.71 < \Delta < 1.30$, and $\Delta > 1.80$ for $S = 1$, and $\Delta > 1.93$ for $S = \frac{1}{2}$ have the ground-state LRO.

where $\boldsymbol{\alpha}$ denotes a lattice site on a finite-size square (or a simple cubic) lattice with periodic boundary conditions. The second summation runs over two (three) vectors to the nearest-neighbor sites along x, y (and z) axes on the square (simple cubic) lattice. Positivity of Δ corresponds to antiferromagnetic interactions.

Let us define

$$g_{\mathbf{p}}^{(i)} = \langle S_{\mathbf{p}}^i S_{-\mathbf{p}}^i \rangle \geqq 0 \quad (i = x,y,z),$$

with

$$S_{\mathbf{p}}^i = |\Lambda|^{-1/2} \sum_{\boldsymbol{\alpha} \in \Lambda} e^{-i\mathbf{p}\cdot\boldsymbol{\alpha}} S_{\boldsymbol{\alpha}}^i,$$

where the angular brackets denote the thermal average, Λ is the set of lattice sites with its total number $|\Lambda|$, and $\mathbf{p}$ belongs to the dual lattice defined by the periodic boundary conditions. We define the antiferromagnetic LRO as

$$[m_{\mathbf{Q}}^{(i)}]^2 = \lim_{\Lambda\to\infty} \frac{1}{|\Lambda|} g_{\mathbf{Q}}^{(i)} = \lim_{\Lambda\to\infty} \left\langle \left[|\Lambda|^{-1} \sum_{\boldsymbol{\alpha}} e^{-i\mathbf{Q}\cdot\boldsymbol{\alpha}} S_{\boldsymbol{\alpha}}^i \right]^2 \right\rangle, \tag{2}$$

where $\mathbf{Q}$ denotes (π,π) or (π,π,π), depending on whether we are considering two or three dimensions. As was shown by the theorem 3.2 of DLS,[1] there exists an upper bound on $g_{\mathbf{p}}^{(i)}$, if there exist $B_{\mathbf{p}}^{(i)}$ and $C_{\mathbf{p}}^{(i)}$ satisfying

$$(S_{\mathbf{p}}^i, S_{-\mathbf{p}}^i) \leqq \beta^{-1} B_{\mathbf{p}}^{(i)}, \tag{3}$$

and

$$\langle [S_{\mathbf{p}}^i, [H, S_{-\mathbf{p}}^i]] \rangle \leqq C_{\mathbf{p}}^{(i)}. \tag{4}$$

The symbol (A,B) denotes the Duhamel two-point function

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

where Z is the partition function and β is the inverse temperature. The upper bound $\tilde{g}_{\mathbf{p}}^{(i)}$ is given by

$$\tilde{g}_{\mathbf{p}}^{(i)} = \tfrac{1}{2} (B_{\mathbf{p}}^{(i)} C_{\mathbf{p}}^{(i)})^{1/2} \coth[\tfrac{1}{2}\beta (C_{\mathbf{p}}^{(i)}/B_{\mathbf{p}}^{(i)})^{1/2}]. \tag{5}$$

KLS[2] used the sum rule for the nearest-neighbor correlation given by

$$\langle S_{\boldsymbol{\alpha}}^i S_{\boldsymbol{\alpha}+\boldsymbol{\delta}}^i \rangle = \frac{1}{\nu |\Lambda|} \sum_{\mathbf{p}} g_{\mathbf{p}}^{(i)} \sum_{m=1}^{\nu} \cos p_m, \tag{6}$$

where ν denotes the lattice dimensionality. Here we have used the fact that the nearest-neighbor correlation does not depend on the direction of the vector δ connecting the neighbors. Using $\tilde{g}_{\mathbf{p}}^{(i)} \geqq g_{\mathbf{p}}^{(i)} \geqq 0$, we can easily see that LRO exists, i.e., $m_{\mathbf{Q}}^{(i)} > 0$, if

$$\lim_{\Lambda\to\infty} [-\langle S_{\boldsymbol{\alpha}}^i S_{\boldsymbol{\alpha}+\boldsymbol{\delta}}^i \rangle] > \int^{(+)} \frac{d^\nu p}{(2\pi)^\nu} \tilde{g}_{\mathbf{p}}^{(i)} \left(-\frac{1}{\nu} \sum_{m=1}^{\nu} \cos p_m \right), \tag{7}$$

where the integration on the right-hand side is done over the region where $0 \leqq p_m \leqq 2\pi$ and the integrand is positive. We take the zero-temperature limit before taking the limit $\Lambda \to \infty$ in the derivation of inequality (7) in order to discuss the ground-state LRO, as was first done by Neves and Perez.[6] Then the hyperbolic cotangent factor of Eq. (5) drops off and all the thermal averages appearing in the following discussions should be replaced by the ground-state expectations. If the ground state is not a singlet, the average over the ground states should be taken. In three dimensions, the existence of the ground-state LRO assures the existence of LRO and a phase transition at sufficiently low temperature.[1]

In the XY region $(0 \leqq \Delta \leqq 1)$, we examine the inequality (7) for $i = x$. As was shown in Ref. 9, we have

$$B_{\mathbf{p}}^{(x)} = (2E'_{\mathbf{p}})^{-1} \text{ for } \mathbf{p} \neq \mathbf{Q}, \tag{8}$$

and

$$C_{\mathbf{p}}^{(x)} = -2 \sum_{m=1}^{\nu} (1 - \Delta \cos p_m) \langle xx \rangle - 2 \sum_{m=1}^{\nu} (\Delta - \cos p_m) \langle zz \rangle, \tag{9}$$

where $E'_{\mathbf{p}} = \sum_{m=1}^{\nu} (1 + \cos p_m)$, and the notation $\langle xx \rangle \equiv \langle S_{\boldsymbol{\alpha}}^x S_{\boldsymbol{\alpha}+\boldsymbol{\delta}}^x \rangle$ and $\langle zz \rangle \equiv \langle S_{\boldsymbol{\alpha}}^z S_{\boldsymbol{\alpha}+\boldsymbol{\delta}}^z \rangle$ is used for nearest-neighbor correlations. The condition (7) is then written as

$$-2\langle xx \rangle > (-\langle xx \rangle - \Delta \langle zz \rangle)^{1/2} h_\nu(r_1), \tag{10}$$

where

$$h_\nu(x) = \int^{(+)} \frac{d^\nu p}{(2\pi)^\nu} \left(-\frac{1}{\nu} \sum_{m=1}^{\nu} \cos p_m \right) \left[\frac{F_{\mathbf{p}}(x)}{E'_{\mathbf{p}}} \right]^{1/2}, \tag{11}$$

$$F_{\mathbf{p}}(x) = \sum_{m=1}^{\nu} (1 - x \cos p_m),$$

and

$$r_1 = \frac{\langle zz \rangle + \Delta \langle xx \rangle}{\langle xx \rangle + \Delta \langle zz \rangle}.$$

One can easily see that $h_\nu(x)$ is a monotone increasing function of x.[9] In the XY region we have the inequality $-\langle xx \rangle \geqq |\langle zz \rangle|$,[8,9] which implies $-1 \leqq r_1 \leqq 1$. We may therefore replace $h_\nu(r_1)$ by $\Gamma_\nu \equiv h_\nu(1)$ in (10). The variational wave function with a Néel order in the x direction gives the lower bound on $-\langle xx \rangle$ as[9]

$$-\langle xx \rangle \geqq S^2/(2+\Delta). \tag{12}$$

As a result we obtain the following proposition:

Proposition 1.—Long-range order $[m_{\mathbf{Q}}^{(x)}]^2$ is finite at a sufficiently low temperature on the 3D simple-cubic lattice and at $T=0$ on the 2D square lattice, if $0 \leqq \Delta \leqq 1$

and

$$2S > \Gamma_\nu[(2+\Delta)(1+\Delta)]^{1/2}, \tag{13}$$

where

$$\Gamma_\nu = \int^{(+)} \frac{d^\nu p}{(2\pi)^\nu} \left[-\frac{1}{\nu} \sum_{m=1}^{\nu} \cos p_m \right] \left[\frac{E_{\mathbf{p}}}{E'_{\mathbf{p}}} \right]^{1/2}, \tag{14}$$

and

$$E_{\mathbf{p}} = \sum_{m=1}^{\nu} (1-\cos p_m). \tag{15}$$

Next we examine the Ising region ($\Delta \geqq 1$) where LRO in z components is considered. Using[9]

$$B_{\mathbf{p}}^{(z)} = (2\Delta E'_{\mathbf{p}})^{-1} \quad (\text{for } \mathbf{p} \neq \mathbf{Q}), \tag{16}$$

and

$$C_{\mathbf{p}}^{(z)} = -4E_{\mathbf{p}}\langle xx \rangle, \tag{17}$$

we rewrite the condition (7) as

$$-\langle zz \rangle > (-\langle zz \rangle / 2\Delta)^{1/2}\Gamma_\nu. \tag{18}$$

The inequality

$$-\langle zz \rangle \geqq -\langle xx \rangle \geqq 0,$$

which holds for $\Delta \geqq 1$, and the variational wave function with a Néel order in the z direction give the lower bound on $-\langle zz \rangle$ as[9]

$$-\langle zz \rangle \geqq \Delta S^2/(\Delta+2). \tag{19}$$

As a result we obtain proposition 2.

Proposition 2.—Long-range order $[m_{\mathbf{Q}}^{(z)}]^2$ is finite at a sufficiently low temperature on the 3D simple-cubic lattice and at $T=0$ on the 2D square lattice, if $\Delta \geqq 1$ and

$$\Delta S > \Gamma_\nu[(2+\Delta)/2]^{1/2}. \tag{20}$$

It should be noted that in the Ising region a phase transition at a finite temperature is expected to occur even in two dimensions since the expected LRO does not have a continuous symmetry. The present method, however, cannot predict a phase transition at finite temperature in two dimensions. The conditions (13) and (20) have the same form as conditions derived in Ref. 9 with Γ_ν replacing νK_ν. The two propositions give the same condition, i.e., $S > (\frac{3}{2})^{1/2}\Gamma_\nu$ for the isotropic model ($\Delta=1$) where the condition of the existence of LRO is most tight. If we use the numerical estimate $\Gamma_3 = 0.350$, we see that the condition is satisfied for $S=\frac{1}{2}$ and $\Delta=1$ as was shown by KLS,[2] and therefore for any $S \geqq \frac{1}{2}$ and $\Delta \geqq 0$ in three dimensions.

In two dimensions Γ_2 is estimated as 0.646, which leads to the existence of the ground-state LRO for $0 \leqq \Delta < 0.13$ and for $\Delta > 1.78$ if $S=\frac{1}{2}$. The region close to the isotropic model remains unresolved. The ground state has LRO for any $\Delta \geqq 0$ if $S \geqq 1$.

In summary, we have shown the existence of LRO at low temperature in the whole region of the antiferromagnetic XXZ model ($\Delta \geqq 0$ for any S) in three dimensions. In two dimensions the ground-state LRO has been shown to exist for $S \geqq 1$ and $\Delta \geqq 0$. For $S=\frac{1}{2}$ the proof has been given except for a region $0.13 < \Delta < 1.78$. The proof includes the XY model ($\Delta=0$) which attracts special interest because of the controversy among numerical works on the triangular lattice.[10]

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Note added.—After submission of this work, we received a preprint from Kennedy, Lieb, and Shastry reporting the existence of LRO in the $S=\frac{1}{2}$ XY model in two dimensions.[11]

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