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Long-Range Order in the *XXZ* Model

Hidetoshi Nishimori,[1] Kenn Kubo,[2] Yukiyasu Ozeki,[1] Yasuhiro Tomita,[1] and Tatsuya Kishi[2]

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The existence of long-range order is proved under certain conditions for the antiferromagnetic quantum spin system with anisotropic interactions (XXZ model) on the simple cubic or the square lattice. In three dimensions (the simple cubic lattice), finite long-range order exists at sufficiently low temperatures for any anisotropy Δ ($\geqslant 0$) if $S \geqslant 1$, and for $0 \leqslant \Delta < 0.29$ (XY-like) or $\Delta > 1.19$ (Ising-like) if $S = 1/2$. In two dimensions (the square lattice), ground-state long-range order exists under the following conditions: for any anisotropy ($\Delta \geqslant 0$) if $S \geqslant 3/2$; $0 \leqslant \Delta < 0.032$ (XY-like) or $0.67 < \Delta < 1.34$ (almost isotropic) or $\Delta > 1.80$ (Ising-like) if $S = 1$; $\Delta > 1.93$ (Ising-like) if $S = 1/2$. We conjecture that the two-dimensional spin-1/2 XY model ($\Delta = 0$) has finite ground-state long-range order. Numerical evidence supporting this conjecture is given.

KEY WORDS: Long-range order; quantum effects; anisotropy.

1. INTRODUCTION

The existence of long-range order in quantum spin systems has been a challenging problem ever since the discovery of exchange interaction by Heisenberg. Recent resurgence of interest in this old problem is partly due to the possible relation of magnetic properties of certain oxide compounds to the basic mechanism of high-temperature superconductivity.[(1)] Let us recall what has been established rigorously on the conditions for the existence of long-range order in quantum spin systems in three and lower dimensions. On the simple cubic lattice, the XY model with $S \geqslant 1/2$ has finite long-range order at low temperatures.[(2,3)] The same is true for the antiferromagnetic Heisenberg model with $S \geqslant 1$ on the simple cubic

[1] Department of Physics, Tokyo Institute of Technology, Oh-okayama, Meguro-ku, Tokyo 152, Japan.

[2] Institute of Physics, University of Tsukuba, Ibaraki 305, Japan.

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lattice.[2] In one and two dimensions, no long-range magnetic order is present at finite temperatures as long as the exchange interaction is isotropic or XY-like.[4] The Ising-like system has finite long-range order at low temperatures even in two dimensions.[5] In the ground state of the antiferromagnetic Heisenberg model on the square lattice, Neves and Perez[6] proved finiteness of long-range order for $S \geqslant 1$.[3] The same technique was applied to the two-dimensional hexagonal lattice to show the existence of antiferromagnetic long-range order for $S \geqslant 3/2$.[7] Kubo[3] analyzed the XY model on the square lattice to show finiteness of ground-state long-range order for $S \geqslant 3/2$.

The purpose of the present paper is to generalize the methods developed in the above papers to include the exchange anisotropy Δ. Let us summarize the results here for convenience. The model system is defined by the Hamiltonian

$$H = \sum_{\boldsymbol{\alpha}} \sum_{\boldsymbol{\delta}} (S^x_{\boldsymbol{\alpha}} S^x_{\boldsymbol{\alpha}+\boldsymbol{\delta}} + S^y_{\boldsymbol{\alpha}} S^y_{\boldsymbol{\alpha}+\boldsymbol{\delta}} + \Delta S^z_{\boldsymbol{\alpha}} S^z_{\boldsymbol{\alpha}+\boldsymbol{\delta}}) \qquad (\Delta \geqslant 0) \tag{1}$$

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

(i) In three dimensions the system at sufficiently low temperatures has finite long-range order in the thermodynamic limit if $S \geqslant 1$ (Δ is arbitrary if nonnegative). The spin-1/2 system has long-range order if $0 \leqslant \Delta < 0.29$ or $\Delta > 1.19$.

(ii) In the ground state of the two-dimensional system, a sufficient condition for finiteness of long-range order is $S \geqslant 3/2$ (arbitrary $\Delta \geqslant 0$). If $S = 1$, Δ should satisfy $0 \leqslant \Delta < 0.032$ or $0.67 < \Delta < 1.34$ or $\Delta > 1.80$ in order that we can prove the existence of long-range order. The spin-1/2 system has long-range order in the ground state if $\Delta > 1.93$.

We further conjecture that the two-dimensional spin-1/2 XY model ($\Delta = 0$) has finite long-range order in its ground state. Although we failed to prove this conjecture, strong numerical evidence is given to support this claim. No conclusive result has been reached on the spin-1/2 isotropic Heisenberg model ($\Delta = 1$) in two dimensions.

[3] As pointed out by Affleck *et al.*,[7] Eq. (9) of ref. 6 contains a trivial error in the factor on the left-hand side. As a consequence, Neves and Perez actually proved the existence of long-range order for $S \geqslant 1$, not only for $S \geqslant 3/2$ as they mentioned.

The main part of the paper is the next section, where the general strategy is described and the $S \geqslant 1$ case is treated explicitly. The spin-1/2 problem has special characteristics and is discussed in Section 3. Final remarks are given in the last section.

2. THE CASE OF $S \geqslant 1$

2.1. Definition and Notation

We first fix the notation. The Fourier transform of the spin operator $\mathbf{S}_\alpha$ is defined by

$$\hat{\mathbf{S}}_\mathbf{p} = \frac{1}{\sqrt{|\Lambda|}} \sum_{\alpha \in \Lambda} e^{-i\mathbf{p}\cdot\boldsymbol{\alpha}} \mathbf{S}_\alpha \tag{2}$$

where Λ is the set of lattice sites, $|\Lambda|$ denotes the total number of sites, and $\mathbf{p}$ is chosen such that periodic boundary conditions are satisfied. Let $\langle \cdots \rangle$ represent the thermal average with respect to the Hamiltonian (1). The symbol (A, B) denotes the Duhamel two-point function

$$(A, B) = Z^{-1} \int_0^1 \mathrm{Tr}(e^{-x\beta H} A e^{-(1-x)\beta H} B)\, dx \tag{3}$$

where Z is the partition function and β is the inverse temperature. The commutator of A and B is written as usual $[A, B]$.

The existence of antiferromagnetic long-range order is defined by

$$(m^{(j)})^2 = \lim_{\Lambda \to \infty} \frac{1}{|\Lambda|} \langle \hat{S}^{(j)}_\mathbf{p} \hat{S}^{(j)}_{-\mathbf{p}} \rangle_{\mathbf{p} = (\pi, \pi, \pi)} > 0 \tag{4}$$

for $j = x$, y, or z at sufficiently low temperatures in three dimensions, or

$$(m^{(j)})^2 = \lim_{\Lambda \to \infty} \lim_{\beta \to \infty} \frac{1}{|\Lambda|} \langle \hat{S}^{(j)}_\mathbf{p} \hat{S}^{(j)}_{-\mathbf{p}} \rangle_{\mathbf{p} = (\pi, \pi)} > 0 \tag{5}$$

in two dimensions. The wave number $\mathbf{p}$ in (4) and (5) is chosen to represent staggered magnetization.

2.2. Basic Theorems

The following are the basic theorems describing sufficient conditions for the existence of finite long-range order in the model (1).

Theorem 1. (Dyson, Lieb, and Simon,[2] referred to as DLS). Suppose that there exist functions $D^{(j)}$, $B_{\mathbf{p}}^{(j)}$, and $C_{\mathbf{p}}^{(j)}$ satisfying

(i) $\langle S_{\alpha}^{(j)} S_{\alpha}^{(j)} \rangle \geqslant D^{(j)}(\beta)$

(ii) $(\hat{S}_{\mathbf{p}}^{(j)}, \hat{S}_{-\mathbf{p}}^{(j)}) \leqslant \beta^{-1} B_{\mathbf{p}}^{(j)}, \qquad p_i \neq \pi$ for some i ($=x$, y, or z)

(iii) $c_{\mathbf{p}}^{(j)} \equiv \langle [\hat{S}_{\mathbf{p}}^{(j)}, [\beta H, \hat{S}_{-\mathbf{p}}^{(j)}]] \rangle \leqslant \beta C_{\mathbf{p}}^{(j)}$

where $j = x$, y, or z. Then the long-range order $(m^{(j)})^2$ is finite at sufficiently low temperatures if

(iv) $2D^{(j)}(\infty) > \frac{1}{(2\pi)^{\nu}} \int d\mathbf{p}\, (B_{\mathbf{p}}^{(j)} C_{\mathbf{p}}^{(j)})^{1/2}$

and

(v) $\int d\mathbf{p}\, B_{\mathbf{p}}^{(j)} < \infty$

where ν represents the lattice dimensionality and the integral is over $-\pi \leqslant p_j \leqslant \pi$ for all j.

Remark 1. Condition (v) is not satisfied in two dimensions, as will be shown later. Thus, this theorem is useful only in three dimensions.

Remark 2. In condition (ii), we can choose $B_{\mathbf{p}}^{(j)}$ as temperature independent, as seen in Theorem 5 below. In contrast, the expectation value of the double commutator $C_{\mathbf{p}}^{(j)}$ in (iii) should have temperature dependence. In actual applications, however, we do not investigate this temperature dependence explicitly because satisfaction of condition (iv), both sides of which are evaluated at $T = 0$, guarantees the existence of long-range order at sufficiently low (but nonvanishing) temperatures. For this reason, the symbol $\langle \cdots \rangle$ should be regarded as the expectation value by the ground-state wave function hereafter. See DLS for details.

The above theorem holds also if one sums various quantities over j.

Theorem 2. (DLS). The long-range order

$$m^2 = \sum_{j=x,\, y,\, z} (m^{(j)})^2 \tag{6}$$

is finite if the following five relations are satisfied.

(i) $\sum_j \langle S_{\alpha}^{(j)} S_{\alpha}^{(j)} \rangle \geqslant \sum_j D^{(j)}(\beta) \equiv D$

(ii) $\sum_j (\hat{S}_{\mathbf{p}}^{(j)}, \hat{S}_{-\mathbf{p}}^{(j)}) \leqslant \beta^{-1} \sum_j B_{\mathbf{p}}^{(j)} \equiv \beta^{-1} B_{\mathbf{p}}, \qquad p_i \neq \pi \quad (i = x,\ y, \text{ or } z)$

(iii) $\sum_j c_{\mathbf{p}}^{(j)} \leqslant \sum_j \beta C_{\mathbf{p}}^{(j)} \equiv \beta C_{\mathbf{p}}$

(iv) $2D > \frac{1}{(2\pi)^\nu} \int d\mathbf{p}\, (B_{\mathbf{p}} C_{\mathbf{p}})^{1/2}$

(v) $\int d\mathbf{p}\, B_{\mathbf{p}} < \infty$ (7)

The ground-state long-range order in two dimensions has been investigated by Neves and Perez.[6]

Theorem 3. (Neves and Perez). Suppose that conditions (i)–(iii) of Theorem 1 are satisfied. Then the ground-state long-range order is finite if condition (iv) is also satisfied.

Remark. Neves and Perez have shown that the condition (v) of Theorem 1, which does not hold in two dimensions, is not required to prove the existence of ground-state long-range order if one takes the low-temperature limit $\beta \to \infty$ first and then the thermodynamic limit $|\Lambda| \to \infty$ [see their Eq. (5) and the argument following it]. If the order of the two limits is reversed, the theorem of Mermin and Wagner[4] applies (as long as $\Delta \leqslant 1$) and no long-range order exists.

Theorem 3 holds also if one sums various quantities over j.

Theorem 4. (Neves and Perez). The long-range order

$$m^2 = \sum_{j=x,\,y,z} (m^{(j)})^2$$

is finite in the ground state if conditions (i)–(iv) of Theorem 2 are satisfied.

Theorem 5. (DLS). The spin system (1) satisfies condition (ii) of Theorem 1 with

$$B_{\mathbf{p}}^{(j)} = 1/(2E'_{\mathbf{p}}) \qquad (j = x \text{ or } y) \tag{8}$$

$$B_{\mathbf{p}}^{(z)} = 1/(2\Delta E'_{\mathbf{p}}) \tag{9}$$

where

$$E'_{\mathbf{p}} = \sum_{\boldsymbol{\delta}} (1 + \cos \mathbf{p} \cdot \boldsymbol{\delta}) \tag{10}$$

Explicitly, in two dimensions,

$$E'_{\mathbf{p}} = 2 + \cos p_1 + \cos p_2$$

and in three dimensions

$$E'_{\mathbf{p}} = 3 + \cos p_1 + \cos p_2 + \cos p_3$$

Remark 1. The above result is DLS's Theorem 6.1 slightly modified to accommodate anisotropy Δ. Lemma 6.1 of DLS remains unchanged if $\Delta \neq 1$, but the derivation of the upper bound on the Duhamel two-point function from Lemma 6.1 needs modification. See their proofs of Theorems 4.1 and 4.2.

Remark 2. Condition (v) of Theorem 1 and condition (v) of Theorem 2 are satisfied in three dimensions with $B_{\mathbf{p}}^{(j)}$ given above. In two dimensions the integral diverges. Consequently, only Theorems 3 and 4 give useful criteria for finiteness of long-range order in two dimensions.

Proposition 1. (DLS). $c_{\mathbf{p}}^{(j)}$ is nonnegative for any $\mathbf{p}$.

Proof. The double commutator is equal to a Duhamel two-point function

$$c_{\mathbf{p}}^{(j)} = ([\hat{S}_{\mathbf{p}}^{(j)}, \beta H], [\beta H, \hat{S}_{-\mathbf{p}}^{(j)}])$$

as is apparent from DLS's Eq. (27). The right-hand side of the above equation is nonnegative according to DLS's Eq. (22). ▮

Proposition 2. The nearest neighbor correlation functions satisfy

$$-\langle zz \rangle \geqslant -\langle xx \rangle \geqslant 0 \qquad \text{if} \quad \Delta \geqslant 1$$

and

$$-\langle xx \rangle \geqslant |\langle zz \rangle| \qquad \text{if} \quad 0 \leqslant \Delta \leqslant 1$$

where

$$\langle xx \rangle \equiv \langle S_{\boldsymbol{\alpha}}^x S_{\boldsymbol{\alpha}+\boldsymbol{\delta}}^x \rangle$$

and

$$\langle zz \rangle \equiv \langle S_{\boldsymbol{\alpha}}^z S_{\boldsymbol{\alpha}+\boldsymbol{\delta}}^z \rangle$$

Proof. It is straightforward to evaluate the double commutator

$$C_{\mathbf{p}}^{(z)} = \beta^{-1} c_{\mathbf{p}}^{(z)} = -4E_{\mathbf{p}} \langle xx \rangle \tag{11}$$

where

$$E_{\mathbf{p}} = \sum_{\boldsymbol{\delta}} (1 - \cos \mathbf{p} \cdot \boldsymbol{\delta})$$

If Proposition 1 is applied to (11) at $p_j = \pi$ (all j), it readily follows that

$$-\langle xx \rangle \geqslant 0 \tag{12}$$

Next we apply the same proposition to

$$C_{\mathbf{p}}^{(x)} = \beta^{-1} c_{\mathbf{p}}^{(x)} = -2 \sum_{\boldsymbol{\delta}} (1 - \Delta \cos \mathbf{p} \cdot \boldsymbol{\delta}) \langle xx \rangle - 2 \sum_{\boldsymbol{\delta}} (\Delta - \cos \mathbf{p} \cdot \boldsymbol{\delta}) \langle zz \rangle \tag{13}$$

at $p_j = 0$ (all j) and $p_j = \pi$ (all j), to derive the following relations:

$$(1 - \Delta)(\langle zz \rangle - \langle xx \rangle) \geqslant 0 \tag{14a}$$

$$-(1 + \Delta)(\langle zz \rangle + \langle xx \rangle) \geqslant 0 \tag{14b}$$

Equations (12) and (14) are sufficient to prove Proposition 2. ∎

2.3. General Criteria for Finiteness of Long-Range Order

First, we apply the above theorems to the Ising-like region.

Proposition 3. The long-range order $(m^{(z)})^2$ is finite (at sufficiently low temperatures in three dimensions and at $T = 0$ in two dimensions) if $\Delta \geqslant 1$ and

$$2^{1/2} \Delta S > \nu K_\nu (\Delta + 2)^{1/2}$$

where

$$\nu K_\nu = (2\pi)^{-\nu} \int d\mathbf{p} \, (E_{\mathbf{p}} / E'_{\mathbf{p}})^{1/2}$$

Proof. As mentioned in Remark 2 of Theorem 5, condition (v) of Theorem 1 is satisfied in three dimensions. Condition (ii) is satisfied according to Theorem 5. Hence we check conditions (i), (iii), and (iv). The double commutator $C_{\mathbf{p}}^{(z)}$ has already been given in (11). Condition (iv) is then written as

$$2D^{(z)}(\infty) > \frac{1}{(2\pi)^\nu} \int d\mathbf{p} \left[\frac{-4E_{\mathbf{p}} \langle xx \rangle}{2\Delta E'_{\mathbf{p}}} \right]^{1/2} \tag{15}$$

To evaluate $D^{(z)}(\infty)$, a lower bound on $\langle (S_{\boldsymbol{\alpha}}^z)^2 \rangle$ in the low-temperature limit, we first note that

$$\langle (S_{\boldsymbol{\alpha}}^z)^2 \rangle^2 = \langle (S_{\boldsymbol{\alpha}}^z)^2 \rangle \langle (S_{\boldsymbol{\alpha}+\boldsymbol{\delta}}^z)^2 \rangle \geqslant \langle S_{\boldsymbol{\alpha}}^z S_{\boldsymbol{\alpha}+\boldsymbol{\delta}}^z \rangle^2 = \langle zz \rangle^2$$

from translational invariance and the Schwartz inequality. By taking account of the fact that $-\langle zz \rangle$ is not negative according to Proposition 2, we write the above relation as

$$\langle (S^z_{\alpha})^2 \rangle \geqslant -\langle zz \rangle \tag{16}$$

The low-temperature limit of the right-hand side of (16) is chosen as $D^{(z)}(\infty)$. Thus, (15) is satisfied if

$$-\langle zz \rangle > \frac{(-\langle xx \rangle)^{1/2}}{(2\Delta)^{1/2}} \nu K_\nu \tag{17}$$

Using Proposition 2, we replace $-\langle xx \rangle$ on the right-hand side by $-\langle zz \rangle$ to derive the following sufficient condition:

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

The left-hand side of (18) is further bounded as

$$-\langle zz \rangle \geqslant \frac{\Delta S^2}{\Delta + 2} \tag{19}$$

To prove (19), we apply the variational principle to the Hamiltonian (1) with the variational wave function ϕ satisfying $S^z_{\alpha}\phi = S\phi$ if α is on one of the sublattices and $S^z_{\alpha}\phi = -S\phi$ if α is on the other sublattice:

$$\langle \phi | H | \phi \rangle = -\nu |\Lambda| \Delta S^2 \geqslant \nu |\Lambda| (2\langle xx \rangle + \Delta \langle zz \rangle) \tag{20}$$

where the expectation values on right-hand side are evaluated by the true ground-state wave function. Equation (20) and Proposition 2 lead to the following inequality:

$$-(2+\Delta)\langle zz \rangle \geqslant -(2\langle xx \rangle + \Delta\langle zz \rangle) \geqslant \Delta S^2$$

which is (19). Equations (18) and (19) are sufficient to prove Proposition 3. ∎

Explicitly, $2K_2 = 1.39$ and $3K_3 = 1.157$ have been obtained from numerical integration. Proposition 3 then states that long-range order exists under the following conditions.

(i) $\nu = 3$: $S \geqslant 3/2$ and $\Delta \geqslant 1$, or $S = 1$ and $\Delta > 1.54$
or $S = 1/2$ and $\Delta > 4.01$

(ii) $\nu = 2$: $S \geqslant 2$ and $\Delta \geqslant 1$, or $S = 3/2$ and $\Delta > 1.17$
or $S = 1$ and $\Delta > 1.95$, or $S = 1/2$ and $\Delta > 5.32$

Much better bounds for the spin-1/2 case will be given in Section 3.

The next problem is the XY-like region.

Proposition 4. The long-range order $(m^{(x)})^2$ is finite (at sufficiently low temperatures in three dimensions and at $T=0$ in two dimensions) if $0 \leqslant \Delta \leqslant 1$ and

$$2S > \nu K_\nu[(2+\Delta)(1+\Delta)]^{1/2}$$

Proof. Condition (iv) of Theorem 1 is written explicitly as, using $C_{\mathbf{p}}^{(x)}$ given in (13),

$$2D^{(x)}(\infty) > [-\langle xx\rangle - \Delta\langle zz\rangle]^{1/2} f_\nu(r_1) \tag{21}$$

where

$$\begin{aligned} f_\nu(x) &= \frac{1}{(2\pi)^\nu}\int d\mathbf{p}\left[\left(\nu - x\sum_{\boldsymbol{\delta}}\cos\mathbf{p}\cdot\boldsymbol{\delta}\right)\Big/E'_{\mathbf{p}}\right]^{1/2} \\ r_1 &= \frac{\langle zz\rangle + \Delta\langle xx\rangle}{\langle xx\rangle + \Delta\langle zz\rangle} \end{aligned} \tag{22}$$

To evaluate $f_\nu(r_1)$, we first point out that r_1 lies in the interval $-1 \leqslant r_1 \leqslant 1$, which is a direct consequence of Proposition 2. Since $f_\nu(x)$ is a monotone increasing function of x if $x \leqslant 1$, as shown in Appendix A, one may replace $f_\nu(r_1)$ by $f_\nu(1) = \nu K_\nu$ in (21). To estimate $D^{(x)}(\infty)$, a lower bound on $\langle (S_\alpha^x)^2\rangle$ in the low-temperature limit, we replace $\langle (S_\alpha^x)^2\rangle$ by $-\langle xx\rangle$ for the same reason as in the derivation of (16). The correlation $-\langle zz\rangle$ on the right-hand side of (21) may be replaced by $-\langle xx\rangle$ according to Proposition 2. In this way we obtain a sufficient condition for the existence of finite long-range order as

$$2(-\langle xx\rangle)^{1/2} > (1+\Delta)^{1/2}\,\nu K_\nu \tag{23}$$

The variational principle as used in the proof of Proposition 3 (choosing the Néel state in the x direction as ϕ) leads to

$$-\langle xx\rangle \geqslant \frac{S^2}{2+\Delta} \tag{24}$$

Equations (23) and (24) lead to Proposition 4. ∎

From Proposition 4, we have the following result. Sufficient conditions for finiteness of long-range order are

(i) $\nu = 3$: $S \geqslant 3/2$ and $0 \leqslant \Delta \leqslant 1$, or $S = 1$ and $0 \leqslant \Delta < 0.299$

(ii) $\nu = 2$: $S \geqslant 2$ and $0 \leqslant \Delta \leqslant 1$, or $S = 3/2$ and $0 \leqslant \Delta < 0.72$, or $S = 1$ and $0 \leqslant \Delta < 0.023$

If $S = 1/2$, there is no region of Δ satisfying the condition of Proposition 4 in three dimensions as well as in two dimensions.

It is advantageous to use Theorems 2 and 4 to treat the almost isotropic region $\Delta \sim 1$.

Proposition 5. The long-range order m^2 is finite (at sufficiently low temperatures in three dimensions and at $T = 0$ in two dimensions) if

$$S(S+1) > \rho^{1/2} \left(1 + \frac{1}{2\Delta}\right)^{1/2} \nu K_\nu \tag{25}$$

where $\rho = -2\langle xx \rangle - \Delta \langle zz \rangle$.

Proof. It is straightforward to verify that condition (iv) of Theorem 2 is written as

$$2S(S+1) > 2\rho^{1/2} \left(1 + \frac{1}{2\Delta}\right)^{1/2} f_\nu(r_2) \tag{26}$$

where $r_2 = -[\langle zz \rangle + (1 + \Delta)\langle xx \rangle]/\rho$. Note here that r_2 satisfies $-1 \leqslant r_2 \leqslant 1$ (as shown by applying Proposition 1 to $c_{\mathbf{p}}^{(x)} + c_{\mathbf{p}}^{(y)} + c_{\mathbf{p}}^{(z)}$ in the same way as in the proof of Proposition 4) and that $f_\nu(x)$ is an increasing function of $x (\leqslant 1)$. Therefore $f_\nu(r_2)$ in (26) may be replaced by $f_\nu(1) = \nu K_\nu$. This completes the proof. ▮

Remark. The quantity $\rho(1 + 1/2\Delta)$ in (25) is a monotone decreasing function of Δ if $0 \leqslant \Delta < 1$ and is monotone increasing if $\Delta > 1$ (see Appendix B). Therefore if (25) for a fixed S is satisfied in some interval $\Delta_{c1} < \Delta < \Delta_{c2}$, this interval should include the isotropic case $\Delta = 1$.

Explicit upper bounds for ρ can be evaluated by diagonalizing finite-size clusters following Anderson[25] (see also Appendix C of DLS): Numerical diagonalization of the operator

$$H_{\text{c}} = \sum_{\langle ij \rangle} J_{ij}(S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z)$$

on finite-size clusters yields a bound on the lowest eigenvalue of the total Hamiltonian (1) which is proportional to ρ. The result is as follows. If $\nu = 2$ and $S = 1$, the inequality (25) is satisfied when $0.67 < \Delta < 1.34$, as displayed in Fig. 1a, from numerical diagonalization of the finite-size system in Fig. 1b (a 9-spin cluster). [Note that we have chosen $J_{ij} = 1/2$ on the boundary bonds in Fig. 1b and $J_{ij} = 1$ in interior. With this choice, the total Hamiltonian (1) of the original system is written as a sum of the cluster Hamiltonian H_{c} with the center site 0 (Fig. 1b) placed on every four sites (so that the boundary bond of a cluster is shared with the neighboring

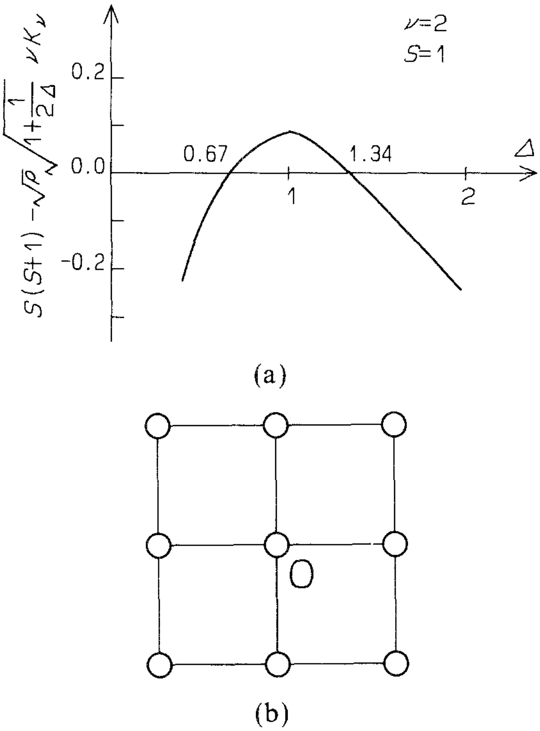


Fig. 1. (a) Difference of the left-hand side and the right-hand side of (25) (with ρ replaced by an upper bound as described in the text) in the case of $\nu = 2$ and $S = 1$. The inequality (25) is satisfied in the range $0.67 < \Delta < 1.34$. (b) The lowest eigenvalue of this 9-spin cluster has yielded a bound on ρ, from which Fig. 1a has been drawn.

cluster). Thus, from the variational principle, the lowest eigenvalue E_0 of H is bounded from below by the lowest eigenvalue of H_c multiplied by $|\Delta|/4$. This fact, together with the relation $-\nu\,|\Delta|\,\rho = E_0$, has been used to derive the above result.] If $\nu = 2$ and $S = 3/2$, our sufficient condition for the existence of long-range order is $0.26 < \Delta < 2.66$ (Fig. 2a), which was derived by diagonalizing the 5-spin cluster of Fig. 2b. In three dimensions, we have found the condition for $S = 1$ as $0.294 < \Delta < 2.40$ (Fig. 3a) by numerical diagonalization of the 7-spin cluster in Fig. 3b.

It is convenient to summarize the results here from three different regions ($0 \lesssim \Delta \lesssim 1$, $\Delta \sim 1$, and $\Delta \gtrsim 1$). In three dimensions, the long-range order is finite at low temperatures if $S \geqslant 1$ for any $\Delta \geqslant 0$. In two dimensions, the ground state has finite long-range order if $S \geqslant 3/2$ for any $\Delta \geqslant 0$; if $S = 1$ in two dimensions, the condition is $0 \leqslant \Delta < 0.023$ or $0.67 < \Delta < 1.34$ or $\Delta > 1.95$.

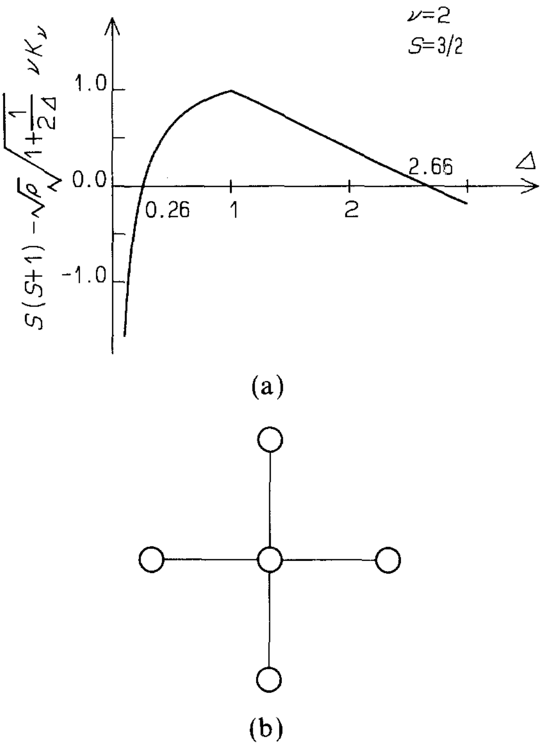


Fig. 2. (a) The same diagram as Fig. 1a in the case of $\nu = 2$, $S = 3/2$. (b) The 5-spin cluster to calculate a bound on ρ for $\nu = 2$, $S = 3/2$.

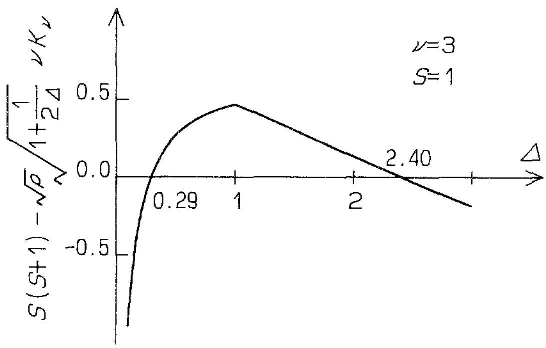
2.4. Improvements of the Estimates for $\nu = 2$, $S = 1$

It is possible slightly to improve the bounds $0 \leqslant \Delta < 0.023$ and $\Delta > 1.95$ derived in the case of $\nu = 2$ and $S = 1$. We first discuss the Ising-like region ($\Delta \geqslant 1$). In the sufficient condition (17) for finiteness of long-range order, we replace $-\langle xx \rangle$ by the following maximum possible value:

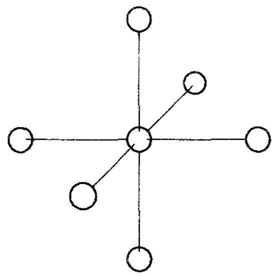
$$-\langle xx \rangle \leqslant -\tfrac{1}{3}\langle \mathbf{S}_\alpha \cdot \mathbf{S}_{\alpha+\delta} \rangle \geqslant \tfrac{5}{12} \tag{27}$$

where the first inequality is a consequence of Proposition 2, while the second comes from the bound $-\langle \mathbf{S}_\alpha \cdot \mathbf{S}_{\alpha+\delta} \rangle \leqslant S(S + 1/2\nu)$.[25] The left-hand side of (17) may be replaced by $\Delta/(\Delta + 2)$ from (19). Thus the condition reduces to

$$\frac{\Delta}{\Delta + 2} > \left(\frac{5}{12}\right)^{1/2} \frac{1.39}{(2\Delta)^{1/2}} \tag{28}$$



(a)



(b)

Fig. 3. (a) The same diagram as Fig. 1a in the case of $\nu = 3$, $S = 1$. (b) The 7-spin cluster to derive a bound on ρ for $\nu = 3$, $S = 1$.

where we have used $\nu K_\nu = 1.39$ for $\nu = 2$. Equation (28) is satisfied in the range $\Delta > 1.80$. This is a small improvement over the previous result, $\Delta > 1.95$.

Next we treat the XY-like region $0 \leqslant \Delta \leqslant 1$. In condition (21) we replace r_1 by its maximum possible value

$$r_{\max} = \frac{17\Delta + 10}{5\Delta^2 + 10\Delta + 12}$$

which is derived by noting that $-\langle xx \rangle \geqslant 1/(2 + \Delta)$ [condition (24)] and $-\langle zz \rangle \leqslant 5/12$ [as shown in a similar way as in the derivation of (27)]. We further replace $-\langle zz \rangle$ in the square root of (21) by its maximum value 5/12. Then (21) is reduced to

$$\frac{-2\langle xx \rangle}{(-\langle xx \rangle + 5/12\Delta)^{1/2}} > f_\nu(r_{\max}) \tag{29}$$

using $\langle (S_\alpha^x)^2 \rangle \geqslant -\langle xx \rangle$. As the left-hand side of the above inequality is monotone increasing in $-\langle xx \rangle$, it is possible to replace $-\langle xx \rangle$ by the minimum value $1/(2+\Delta)$. In this way, both sides of (29) are written as explicit functions of Δ. Numerical evaluation of the integral function f_ν shows that (29) is satisfied if $\Delta \leqslant 0.032$.

We summarize the results of this and the preceding subsections as a theorem.

Theorem 7. On the simple cubic lattice, the system (1) has finite long-range order at low temperatures if $S \geqslant 1$ and $\Delta \geqslant 0$. On the square lattice, the ground-state long-range order is finite if $S \geqslant 3/2$ and $\Delta \geqslant 0$; when $S = 1$ in two dimensions, Δ should satisfy $0 \leqslant \Delta < 0.032$ or $0.67 < \Delta < 1.34$ or $\Delta > 1.80$.

3. THE SPIN-1/2 PROBLEM

3.1. Rigorous Results

A special advantage of the spin-1/2 systems is that $\langle (S_\alpha^x)^2 \rangle$ and $\langle (S_\alpha^z)^2 \rangle$ can be calculated explicitly as 1/4. In the Ising-like region, the condition (15) is thus written as

$$\frac{1}{4} > \frac{(-\langle xx \rangle)^{1/2}}{(2\Delta)^{1/2}} \nu K_\nu \tag{30}$$

The correlation function $-\langle xx \rangle$ may be replaced by its maximum possible value $S(S+1/2\nu)/3$ for the same reason as in Section 2.4. Therefore, (30) is satisfied for $\Delta > 1.19$ if $\nu = 3$ and $\Delta > 1.93$ if $\nu = 2$.

In the XY-like region, the criterion (21) is rewritten as

$$\frac{1}{4} > \frac{(1+\Delta)^{1/2}}{2} (-\langle xx \rangle)^{1/2} \nu K_\nu \tag{31}$$

for the same reasons as in the proof of Proposition 4. We now replace $-\langle xx \rangle$ in (31) by its maximum possible value $1/4\sqrt{3}$, which was derived by DLS in their Appendix C. [Note that the bound $-\langle xx \rangle \leqslant S(S+1/2\nu)/3$ (which is smaller than $1/4\sqrt{3}$ if $S = 1/2$ and $\nu = 2$), valid in the Ising-like region, is not applicable if $\Delta \geqslant 1$.] Then (31) is satisfied for $0 \leqslant \Delta < 0.29$ if $\nu = 3$, and no positive Δ satisfies (31) if $\nu = 2$. These results are summarized as follows.

Theorem 8. The system (1) with $S = 1/2$ has long-range order at sufficiently low temperatures in three dimensions if $0 \leqslant \Delta < 0.29$ or $\Delta > 1.19$. In the ground state of the two-dimensional model, long-range order exists if $\Delta > 1.93$.

3.2. Conjecture

In consideration of recent activities in the investigation of the ground-state properties of the two-dimensional systems,[7–24] it should be of great interest to discuss the case $\nu = 2$ and $S = 1/2$ with $0 \leqslant \Delta \leqslant 1$ in more detail.

As for the antiferromagnetic Heisenberg model ($\Delta = 1$), the present approach is totally inconclusive: The sufficient condition (26) is hardly satisfied even if the best numerical estimates of the correlation functions of the infinite-size system[10] are used in (26).

In contrast, condition (21) applied to the XY model ($\Delta = 0$) is satisfied if one uses the estimates of Oitmaa and Betts[10]:

$$\langle xx \rangle = -1.08/8, \qquad \langle zz \rangle = -0.038 \tag{32}$$

If $S = 1/2$, condition (21) for $\Delta = 0$ reduces to

$$\tfrac{1}{2} > (-\langle xx \rangle)^{1/2} f_2(\langle zz \rangle / \langle xx \rangle) \tag{33}$$

If one insertes (32) into (33), numerical evaluation of the integral function f_2 yields 0.487 as the right-hand side of (33). Therefore, the inequality is satisfied, implying finiteness of long-range order. The only problem is that the values (32) are not exact!

To check more precisely if the condition (33) is possibly satisfied, we calculated numerically the ground-state nearest-neighbor correlation functions on the finite-size square lattices with periodic boundary conditions of Oitmaa–Betts[10] type. The lattice size ranges from $|\Lambda| = 8$ to $|\Lambda| = 20$. The results are listed in Table I. We rewrite (33) as

$$\tfrac{1}{2} > g(-2\langle xx \rangle, -\langle zz \rangle) \tag{34}$$

where

$$g(u, v) = \frac{1}{(2\pi)^2} \int d\mathbf{p} \left(\frac{u - v \cos p_1 - v \cos p_2}{2 + \cos p_1 + \cos p_2} \right)^{1/2} \tag{35}$$

Table I. Nearest Neighbor Correlation Functions of the Spin-1/2 *XY* Model on the Finite-Size Square Lattices of Oitmaa–Betts Type[10]

$\lvert\Lambda\rvert$	$-4\langle S^x_\alpha S^x_{\alpha+\delta} \rangle$	$-4\langle S^z_\alpha S^z_{\alpha+\delta} \rangle$
8	0.586302	0.215909
10	0.576083	0.201172
16	0.562486	0.182339
18	0.559552	0.177784
20	0.558057	0.175975

The expectation values in (34) should be taken by the ground-state wave function in the infinite-size limit $|\Lambda| \to \infty$. If one nevertheless replaces those correlation functions by the finite-size data in Table I, (34) is satisfied for $|\Lambda| \geqslant 16$ ($g = 0.512$, 0.506, 0.499, 0.497, 0.497 for $|\Lambda| = 8$, 10, 16, 18, 20, respectively). Now we notice in Table I that the correlations $-\langle xx \rangle$ and $-\langle zz \rangle$ monotonically decrease as $|\Lambda|$ increases. Since the function $g(u, v)$ is monotone increasing both in u (as is verified from differentiation by u) and in v (as is checked by the same calculations as in Appendix A) in the parameter region of interest ($u \geqslant 2v$), the infinite-size correlation would satisfy (34). Therefore we arrive at the following conjecture.

Conjecture 1. The spin-1/2 XY model has finite ground-state long-range order on the square lattice.

Remark 1. As is clear from the above argument, this conjecture would be proved if one could show

$$-\langle xx \rangle_\infty \leqslant -\langle xx \rangle_{|\Lambda|}$$
$$-\langle zz \rangle_\infty \leqslant -\langle zz \rangle_{|\Lambda|}$$

where ∞ and $|\Lambda|$ denote the system size at which the expectation value is taken. Note that the finite-size systems on the right-hand side of the above equations should have periodic boundary conditions. Otherwise the inequality may be reversed.

Remark 2. Oitmaa and Betts[10] also predict finite long-range order from their finite-size data. The main advantage of the present approach over that of Oitmaa and Betts is that the existence of long-range order can be discussed only in terms of short-range correlations. Since short-range correlation functions are much less affected by finite-size effects than are long-range correlations, the reliability of the present method would exceed that of a simple extrapolation of finite-size long-range correlation data to $|\Lambda| \to \infty$, as employed by Oitmaa and Betts[10] and followers.[11–15]

4. FINAL REMARKS

If the spin is larger than 1/2 ($S = 1$, 3/2,...), the existence of long-range order has been established for almost all values of positive Δ in two and three dimensions. The most interesting case of $S = 1/2$ and $0 \leqslant \Delta \leqslant 1$ in two dimensions remains unsettled. While we conjecture the existence of finite long-range order in the spin-1/2 XY model on the square lattice in agreement with several authors,[8–10,16,17,19–23] finite-lattice calculations on the ferromagnetic XY model on the triangular lattice indicate vanishing long-range order in the infinite-size limit.[11,15] Since the triangular lattice has more interacting bonds per site than the square lattice, the ordering is naively expected to be stronger on the triangular lattice than on the square lattice as long as the interactions are ferromagnetic (i.e., no frustration is present). Thus, we are in an apparently conflicting situation; finiteness of long-range order is concluded from the present (and other) methods whereas vanishing of the same quantity is suggested from direct extrapolation of finite-size data of long-range correlations. In consideration of Remark 2 of Conjecture 1, the present approach seems to be more reliable than the direct extrapolation method of finite-size data. Rigorous proof of the property of the correlation functions mentioned in Remark 1 of Conjecture 1 is a waited.

We have discussed the existence of long-range order defined in (4) and (5). The existence of a phase transition is not immediately proved even if (4) or (5) is established. Fortunately, as discussed by DLS, the following nonclustering property of the infinite-volume state can be proved under the same conditions of the theorems in the text:

$$\lim_{\Lambda' \to \infty} \left[\lim_{\Lambda \to \infty} \left\langle \left(|\Lambda'|^{-1} \sum_{\alpha \in \Lambda'} S_\alpha^{(j)} \right)^2 \right\rangle_\Lambda \right] \neq 0$$

This relation implies the existence of multiple phases and therefore of a phase transition. See DLS for details.

NOTE ADDED

After submission of this paper, new developments have been observed on the present and related problems. Kennedy, Lieb, and Shastry (KLS)[28] generalized the method of DLS to prove the existence of long-range order in the three-dimensional spin-1/2 Heisenberg antiferromagnet with couplings anisotropic in lattice space. They also presented new sufficient conditions for the existence of long-range order. KLS proceeded to prove the existence of long-range order in the *XY* model in two and larger dimensions.[29] Kubo and Kishi[30] proved, independently of the second paper of KLS, the existence of long-range order for all $S \geqslant 1/2$ and $\Delta \geqslant 0$ in three dimensions and for $S \geqslant 1/2$ and $\Delta \geqslant 0$ excluding $0.13 < \Delta < 1.78$ when $S = 1/2$ in two dimensions. Ozeki, Nishimori, and Tomita (ONT)[31] refined the techniques to prove the existence of long-range order in two dimensions excluding the range $0.20 < \Delta < 1.72$ when $S = 1/2$. The two-dimensional hexagonal lattice has also been treated by ONT to improve the result of Affleck *et al.*[7] The range of exclusion cited above in the case of $S = 1/2$ has been replaced by $0.20 < \Delta < 1.67$ in the paper of Nishimori and Ozeki.[32] They also conjectured that the range would become as small as $0.59 < \Delta < 1.10$ if one assumes monotonicity of nearest neighbor correlations as functions of the system size.

APPENDIX A. MONOTONICITY OF $f_\nu(x)$

We prove that $f'_\nu(x) \geqslant 0$ if $x \leqslant 1$. Differentiation of the definition (22) yields

$$f'_\nu(x) = -\frac{1}{2(2\pi)^\nu} \int d\mathbf{p} \frac{h(\mathbf{p})}{\{[\nu + h(\mathbf{p})][\nu - xh(\mathbf{p})]\}^{1/2}}$$

where

$$h(\mathbf{p}) = \sum_{\boldsymbol{\delta}} \cos \mathbf{p} \cdot \boldsymbol{\delta}$$

Since the range of integration is $-\pi \leqslant p_j \leqslant \pi$ and the integrand is periodic with period 2π, one may change the variables from p_j to $\pi - p_j$. Then h changes the sign, and therefore the sign of $f'_\nu(x)$ is equal to that of

$$-h\left(\frac{1}{[(\nu + h)(\nu - xh)]^{1/2}} - \frac{1}{[(\nu - h)(\nu + xh)]^{1/2}}\right) \tag{A.1}$$

The sign of the quantity in the outer brackets of (A.1) is equal to that of $-h$ if $x \leqslant 1$, since

$$(\nu - h)(\nu + xh) - (\nu + h)(\nu - xh) = 2\nu h(x - 1)$$

Hence (A.1) is not negative. This completes the proof.

APPENDIX B. DERIVATIVE OF $\rho(1 + 1/2\Delta)$

To investigate monotonicity of $F(\Delta) \equiv \rho(1 + 1/2\Delta)$, we first note that ρ is the ground-state energy of the model (1) divided by $-\nu\,|\Delta|$. Therefore, using the first-order perturbation theory,

$$\frac{\partial \rho}{\partial \Delta} = -\frac{1}{\nu\,|\Delta|}\left\langle \frac{\partial H}{\partial \Delta}\right\rangle = -\langle zz \rangle \tag{B.1}$$

where the expectation value is taken by the ground-state wave function. It is thus straightforward to show that

$$\frac{\partial F}{\partial \Delta} = \frac{\langle xx \rangle}{\Delta^2} - \langle zz \rangle \tag{B.2}$$

Proposition 2 and (B.2) are sufficient to prove $\partial F/\partial \Delta < 0$ when $0 \leqslant \Delta < 1$ and $\partial F/\partial \Delta > 0$ for $\Delta > 1$.

If the system size is finite, the derivative $\partial \rho/\partial \Delta$ is not necessarily continuous at $\Delta = 1$, as seen in Figs. 1a, 2a, and 3a. This fact comes from the degeneracy of the ground state at $\Delta = 1$ for a system with the number of sites on one of the sublattices unequal to that on the other.[26,27] Continuity of $\partial \rho/\partial \Delta = -\langle zz \rangle$ is expected to be recovered in the thermodynamic limit.

REFERENCES

1. P. W. Anderson, *Science* **235**:1196 (1987).
2. F. J. Dyson, E. H. Lieb, and B. Simon, *J. Stat. Phys.* **18**:335 (1978).
3. K. Kubo, *Phys. Rev. Lett.* **61**:110 (1988).
4. N. D. Mermin and H. Wagner, *Phys. Rev. Lett.* **17**:1133 (1966).
5. J. Frörich and E. H. Lieb, *Commun. Math. Phys.* **60**:233 (1978).
6. E. J. Neves and J. F. Perez, *Phys. Lett.* **114A**:331 (1986).
7. I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, *Commun. Math. Phys.* **115**:477 (1988).
8. P. W. Anderson, *Phys. Rev.* **86**:694 (1952).
9. R. Kubo, *Phys. Rev.* **87**:568 (1952).
10. J. Oitmaa and D. D. Betts, *Can. J. Phys.* **56**:897 (1978).
11. S. Fujiki and D. D. Betts, *Can. J. Phys.* **64**:876 (1986).
12. S. Fujiki and D. D. Betts, *Can. J. Phys.* **65**:76 (1987).
13. S. Fujiki, *Can. J. Phys.* **65**:489 (1987).
14. S. Fujiki and D. D. Betts, *Prog. Theor. Phys.* **1986** (Suppl. 87):268.
15. H. Nishimori and H. Nakanishi, *J. Phys. Soc. Jpn.* **57**:626 (1988).
16. T. Oguchi, H. Nishimori, and Y. Taguchi, *J. Phys. Soc. Jpn.* **55**:323 (1986).
17. J. D. Reger and A. P. Young, *Phys. Rev. B* **37**:5978 (1988).
18. S. Miyashita, *J. Phys. Soc. Jpn.* **57**:1934 (1988).
19. M. Suzuki and S. Miyashita, *Can. J. Phys.* **56**:902 (1978).
20. S. Miyashita, *J. Phys. Soc. Jpn.* **53**:44 (1984).
21. M. Kohmoto, *Phys. Rev. B* **37**:3812 (1988).
22. D. A. Huse and V. Elser, *Phys. Rev. Lett.* **60**:2531 (1988).
23. D. A. Huse, *Phys. Rev. B* **37**:2380 (1988).
24. R. R. P. Singh, M. P. Gelfand, and D. A. Huse, *Phys. Rev. Lett.* **61**:2484 (1988).
25. P. W. Anderson, *Phys. Rev.* **83**:1260 (1951).
26. E. H. Lieb and D. C. Mattis, *J. Math. Phys.* **3**:749 (1962).
27. H. Nishimori, *J. Stat. Phys.* **26**:839 (1981).
28. T. Kennedy, E. H. Lieb, and B. S. Shastry, *J. Stat. Phys.* **53**:1019 (1988).
29. T. Kennedy, E. H. Lieb, and B. S. Shastry, *Phys. Rev. Lett.* **61**:2582 (1988).
30. K. Kubo and T. Kishi, *Phys. Rev. Lett.* **61**:2585 (1988).
31. Y. Ozeki, H. Nishimori, and Y. Tomita, *J. Phys. Soc. Jpn.* **58**:82 (1989).
32. H. Nishimori and Y. Ozeki, *J. Phys. Soc. Jpn.* **58**:1027 (1989).