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Ground-State Long-Range Order in the Two-Dimensional *XXZ* Model

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We prove the existence of Néel-type long-range order in the ground state of the spin-1/2 *XXZ* model with Δ(exchange anisotropy)>1.67 on the square lattice. We further show the existence of long-range order for $\Delta>1.10$ and $0\leqq\Delta<0.59$ by assuming monotonicity of nearest neighbor correlations as functions of the system size. The assumption of monotonicity is supported by numerical calculations.

The two-dimensional quantum spin system has been attracting attention recently for its possible relation to the mechanism of high-temperature superconductivity.[1)] We discuss here one of the important aspects of this problem, i.e., the existence of Néel-type long-range order in the ground state of the spin-1/2 *XXZ* model. The Hamiltonian is

$$H=\sum_{\langle ij\rangle}(S_i^xS_j^x+S_i^yS_j^y+\Delta S_i^zS_j^z), \qquad (1)$$

where the summation runs over the nearest neighbor pairs on the square lattice. In a previous paper[2)] we proved the existence of long-range order for $\Delta>1.72$ and $0\leqq\Delta<0.20$ using the method originally developed by Dyson, Lieb and Simon.[3)] More precisely, in the *XY*-like region ($0\leqq\Delta\leqq1$), we showed that

$$\lim_{\Lambda\to\infty}\frac{1}{|\Lambda|}g^{(x)}_{p=(\pi,\pi)}>0, \qquad (2)$$

for $0\leqq\Delta<0.20$, where $|\Lambda|$ is the lattice size and

$$g_p^{(x)}=\frac{1}{|\Lambda|}\sum_{\alpha,\beta}\mathrm{e}^{-\mathrm{i}p\cdot\alpha+\mathrm{i}p\cdot\beta}\langle S_\alpha^xS_\beta^x\rangle. \qquad (3)$$

The summation in (3) extends over all lattice sites and the brackets $\langle\ \ \rangle$ denote the average by the ground-state wave function. Similarly, we proved in the Ising-like region ($\Delta\geqq1$) that

$$\lim_{\Lambda\to\infty}\frac{1}{|\Lambda|}g^{(z)}_{p=(\pi,\pi)}>0, \qquad (4)$$

for $\Delta>1.72$. In the present paper, the inequality (4) is proved for an extended range $\Delta>1.67$. It is further shown that (2) holds when $0\leqq\Delta<0.59$ if one assumes monotonicity of the nearest neighbor correlations as functions of the system size (which is verified numerically). Under similar assumptions, we show that (4) holds for $\Delta>1.10$.

Let us start the argument with the case of the Ising-like anisotropy $\Delta\geqq1$. A sufficient condition for the existence of long-range order has been derived[4)] as

$$-\langle zz\rangle>\sqrt{\frac{-\langle xx\rangle}{2\Delta}}\,\Gamma_2, \qquad (5)$$

where $\langle zz\rangle$ (or $\langle xx\rangle$) denotes the nearest neighbor correlation function $\langle S_0^zS_1^z\rangle$ (or $\langle S_0^xS_1^x\rangle$) of the infinite-size system. The quantity Γ_2 is an integral:

$$\Gamma_2=\int\frac{^{(+)}\mathrm{d}^2p}{2(2\pi)^2}\sqrt{\frac{2-\cos p_1-\cos p_2}{2+\cos p_1+\cos p_2}}\times(-\cos p_1-\cos p_2)=0.646. \qquad (6)$$

Here, the symbol (+) means that the integral is limited to the region in the first Brillouin zone where the integrand is positive. To see if (5) is satisfied for a given Δ, we proceed to derive a lower bound on the lhs and an upper bound on the rhs of (5). For this purpose, we point out that the correlation $-\langle xx\rangle$ is bounded from above by the value of the same quantity at $\Delta=1$ (which will be denoted as $-\langle xx\rangle_{\mathrm{H}}$). The reason is as follows.

The ground-state energy per bond,

$$e\equiv 2\langle xx\rangle+\Delta\langle zz\rangle, \tag{7}$$

has a derivative,[5)]

$$\frac{\partial e}{\partial\Delta}=\langle zz\rangle, \tag{8}$$

which leads to

$$\frac{\partial^2 e}{\partial\Delta^2}=\frac{\partial\langle zz\rangle}{\partial\Delta}\leqq 0, \tag{9}$$

according to the concavity of the free energy (or the energy at $T=0$).[6)] The quantity in the middle expression of (9) is equal to $-(2/\Delta)\,\partial\langle xx\rangle/\partial\Delta$, as verified by explicitly differentiating (7) and comparing the result with (8). Hence $-\langle xx\rangle$ is a monotone decreasing function of Δ. This implies that $-\langle xx\rangle$ at a certain Δ ($\geqq 1$) is bounded from above by $-\langle xx\rangle_{\rm H}$. In this way, we are allowed to replace $-\langle xx\rangle$ on the rhs of (5) with $-\langle xx\rangle_{\rm H}$.

The correlation $-\langle zz\rangle$ on the lhs of (5) is bounded from below as

$$-\langle zz\rangle=\frac{2\langle xx\rangle-e}{\Delta}\geqq\frac{2\langle xx\rangle_{\rm H}-e_{\rm v}}{\Delta}, \tag{10}$$

where $e_{\rm v}$ is a variational energy. From these estimations, the sufficient condition (5) is reduced to

$$\frac{2\langle xx\rangle_{\rm H}-e_{\rm v}}{\Delta}>\sqrt{\frac{-\langle xx\rangle_{\rm H}}{2\Delta}}\,\Gamma_2. \tag{11}$$

We use the variational energy given in the Appendix of ref. 2 in the lhs of (11). A lower bound on the lhs and an upper bound on the rhs of (11) are obtained by substituting an upper bound on $-\langle xx\rangle_{\rm H}$ (which gives a lower bound on $\langle xx\rangle_{\rm H}$). Our best upper bound $-\langle xx\rangle_{\rm H}\leqq 0.11895$ has been derived as follows.

Let us consider a finite-size system described by the Hamiltonian

$$H_{\rm f}=\sum_{\langle ij\rangle}J_{ij}\boldsymbol{S}_i\cdot\boldsymbol{S}_j, \tag{12}$$

with free boundary conditions. The positive exchange interaction J_{ij} depends on $\langle ij\rangle$ in general. We denote the lowest eigenvalue of $H_{\rm f}$ as $E_0(\{J_{ij}\})$. Then, the expectation value of $H_{\rm f}$ with respect to the ground-state wave function of the uniform infinite-size system (all $J_{ij}=1$) satisfies

$$\langle H_{\rm f}\rangle\geqq E_0(\{J_{ij}\}). \tag{13}$$

Since the infinite-size system is translationally invariant, (12) and (13) lead to

$$\langle\boldsymbol{S}_i\cdot\boldsymbol{S}_j\rangle\sum_{\langle ij\rangle}J_{ij}\geqq E_0(\{J_{ij}\}),$$

or, by making use of the equivalence of three axes,

$$3\langle xx\rangle_{\rm H}\geqq E_0(\{J_{ij}\})/\sum_{\langle ij\rangle}J_{ij},$$

which is equivalent to

$$-\langle xx\rangle_{\rm H}\leqq -E_0(\{J_{ij}\})/3\sum_{\langle ij\rangle}J_{ij}. \tag{14}$$

This inequality (14) holds for any $\{J_{ij}\}$. Therefore, the problem of finding a good upper bound on $-\langle xx\rangle_{\rm H}$ is reduced to that of searching for a $\{J_{ij}\}$ which gives the lowest value of rhs of (14). Our best result $-\langle xx\rangle_{\rm H}\leqq 0.11895$ was obtained for the lattice of Fig. 1. Thus, everything in (11) has been given explicitly, and we have found that (11) is satisfied when $\Delta>1.67$.

A further improvement is achieved by assuming monotonicity of $-\langle xx\rangle$ and $-\langle zz\rangle$ as functions of the system size. From the numerical data in Fig. 2 (which were calculated for finite-size systems with periodic boundaries of the Oitmaa-Betts type[7)]), we think it plausible that $-\langle zz\rangle$ for a fixed Δ (>1) increases monotonically with $|\Delta|$ in the asymptotic region $|\Delta|\gg 1$. The reason is as follows. In Fig. 2, the system size dependence of $-\langle zz\rangle$ changes in the range $1<\Delta<1.08$;

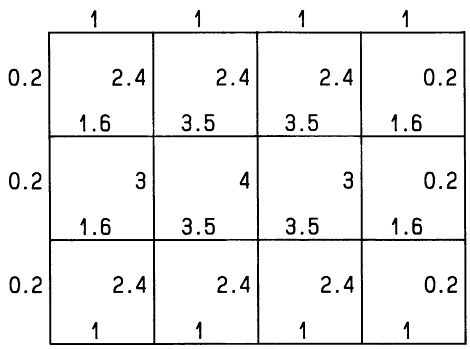

Fig. 1. The ground-state energy of this finite-size lattice with free boundaries gives an upper bound 0.11895 to $-\langle xx\rangle_{\rm H}$ of the infinite-size system. The numbers indicate the relative magnitude of the antiferromagnetic exchange interactions $\{J_{ij}\}$.

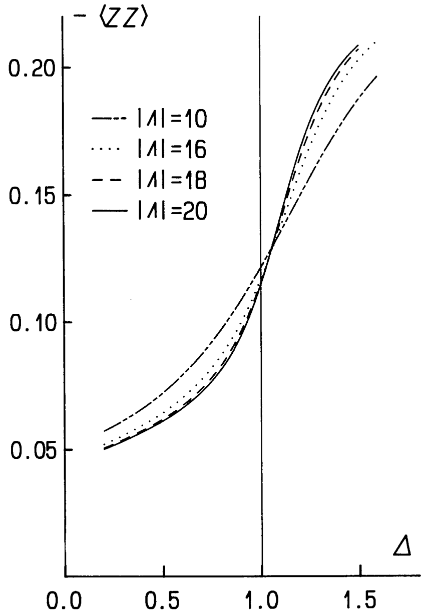

Fig. 2. The nearest neighbor correlation $-\langle zz\rangle$ calculated for various finite-size systems of the Oitmaa-Betts type.[7]

the crossing point $\Delta_c(|\Lambda_1|, |\Lambda_2|)$ (at which $-\langle zz\rangle$ for $|\Lambda_1|$ is equal to $-\langle zz\rangle$ for $|\Lambda_2|$) satisfies $1<\Delta_c(20,18)<\Delta_c(18,16)<\Delta_c(16,10)<1.08$ (see Fig. 3). This observation suggests that, for any $\Delta>1$, $-\langle zz\rangle$ will eventually increase with $|\Lambda|$. In particular, the range $\Delta>1.08$ seems to be already in the asymptotic region, even for $|\Lambda|$ as small as 10. As for the other correlation function $-\langle xx\rangle$, this quantity is monotone decreasing with the system size $|\Lambda|$ ($\leqq 20$) for all positive Δ, as shown in Fig. 4. Therefore, it is reasonable to assume that, if $\Delta\geqq 1.08$, $-\langle zz\rangle$ of the infinite-size system is bounded from below by its value at $|\Lambda|=20$, and $-\langle xx\rangle$ is bounded from above by the value at $|\Lambda|=20$. When $\Delta=1.10$, $-\langle zz\rangle$ for $|\Lambda|=20$ is 0.14175 and $-\langle xx\rangle$ is 0.10114. The sufficient condition (5) is satisfied by these values. We note that (5) is not satisfied at $\Delta=1.09$ even if monotonicity of the nearest neighbor correlations is assumed.

The same argument applies to the XY-like region $0\leqq\Delta\leqq 1$. The nearest neighbor correlations $-\langle xx\rangle$ and $-\langle zz\rangle$ are seen to be monotone decreasing as $|\Lambda|$ increases when $0\leqq\Delta\leqq 1$ (Figs. 2 and 4). We use this fact in the following sufficient condition for (2) to hold:[4]

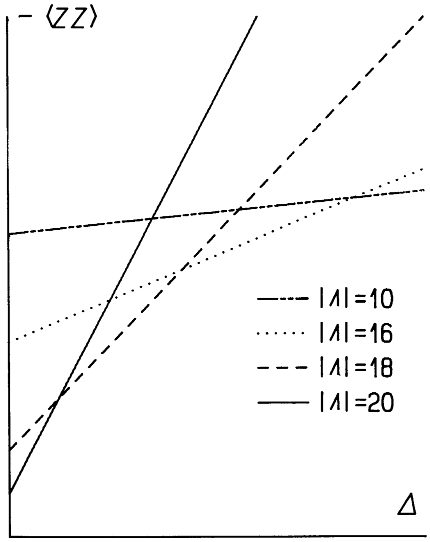

Fig. 3. Schematic diagram of the dependence of $-\langle zz\rangle$ on $|\Lambda|$ and Δ in the region $1<\Delta<1.08$. From this figure, we expect that $-\langle zz\rangle$ for any fixed $\Delta>1$ will increase with $|\Lambda|$ if $|\Lambda|$ is larger than some critical value $|\Lambda_c(\Delta)|$. This figure represents only the relative position of the four curves; these curves are too close to each other to be distinguished clearly in the real scale.

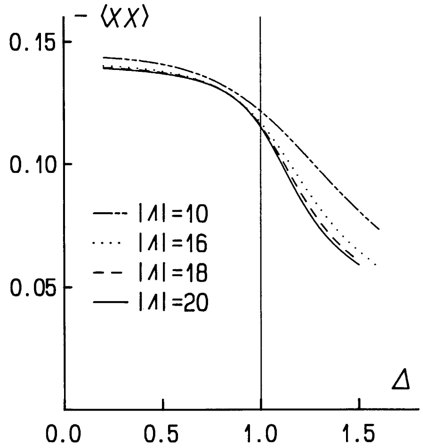

Fig. 4. The correlation $-\langle xx\rangle$ of the same lattices as in Fig. 2.

$$-2\langle xx\rangle>\sqrt{-\langle xx\rangle-\Delta\langle zz\rangle}\,h_2(r), \qquad (15)$$

where

$$h_2(r)=\int\frac{{}^{(+)}d^2p}{2(2\pi)^2}\sqrt{\frac{2-r\cos p_1-r\cos p_2}{2+\cos p_1+\cos p_2}}\times(-\cos p_1-\cos p_2), \qquad (16)$$

with

$$r=\frac{\langle zz\rangle/\langle xx\rangle+\Delta}{1+\Delta\langle zz\rangle/\langle xx\rangle}. \quad (17)$$

The above-mentioned assumption on monotonicity implies

$$-2\langle xx\rangle=-e+\Delta\langle zz\rangle\geqq-e_{\rm v}+\Delta\langle zz\rangle_{|\Delta|=20}, \quad (18)$$

and therefore,

$$R\equiv\frac{-\langle zz\rangle}{-\langle xx\rangle}\leqq\frac{-\langle zz\rangle_{|\Delta|=20}}{(-e_{\rm v}+\Delta\langle zz\rangle_{|\Delta|=20})/2}\equiv R_{\rm max}. \quad (19)$$

Since $-\langle xx\rangle$ is non-negative,[5] (19) leads to

$$-\langle zz\rangle\leqq-R_{\rm max}\langle xx\rangle. \quad (20)$$

If we replace $-\langle zz\rangle$ in the square root of (15) by the upper bound (20), we have

$$2\sqrt{-\langle xx\rangle}>\sqrt{1+R_{\rm max}}\,h_2(r). \quad (21)$$

A lower bound on the lhs of (21) is given by (18). An upper bound on the rhs of (21) is derived if we note that $h_2(r)$ is a monotone increasing function of r.[5] This monotonicity means that r of (17) should be replaced by its largest possible value, which is achieved when R is equal to $R_{\rm max}$. Thus, everything in (21) has been given explicitly. By use of the variational energy of Suzuki and Miyashita[8] as $e_{\rm v}$ in (18) and (19), we have found that (21) is satisfied when $0\leqq\Delta\leqq0.59$. This completes our argument in the XY-like region.

As has been pointed out by Kennedy *et al.*,[9] the present criterion (5) or (15) for the existence of long-range order is unlikely to be satisfied by the isotropic Heisenberg antiferromagnet ($\Delta=1$) even if the best numerical estimate of the correlation function is used. A new approach should be developed to resolve the case of the isotropic model.

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