# Existence of Néel order at T=0 in the spin- $\frac{1}{2}$ antiferromagnetic Heisenberg model on a square lattice

### Shoudan Liang\*

Department of Physics and Material Research Laboratory, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801

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It is known that if the ground state of the spin- $\frac{1}{2}$  antiferromagnetic Heisenberg model is not Néel ordered, the two-point function must satisfy an upper bound. In this paper, the spin-spin correlation function for the ground state is computed on a  $32 \times 32$  square lattice using a projection Monte Carlo method. The correlation function at short distance (about four lattice spacing) violates this bound, which implies that the ground state must have long-ranged Néel order. I have also estimated the staggered magnetization to be  $m^+=0.304\pm0.004$  in the thermodynamic limit.

# I. INTRODUCTION

The most distinct feature of the high- $T_c$  superconductors is their nearly decoupled copper-oxygen planes. Neutron-scattering experiments show<sup>1</sup> that in undoped compounds the coupling between electrons in the planes are described by a spin- $\frac{1}{2}$  antiferromagnetic Heisenberg model. At low temperatures, weak interplane coupling allows ordering, and long-ranged Néel order has been observed. The temperature dependence of the correlation function as well as the dynamical correlations measured in the neutron-scattering experiments is well accounted for<sup>2</sup> by a nonlinear  $\sigma$  model with quantum fluctuations in the parameter regime having a Néel-ordered ground state.<sup>2,3</sup> From the spin-wave theory,<sup>4</sup> however, we expect to have large corrections from quantum fluctuations at low dimensions and for small spins.<sup>5</sup> For the spin- $\frac{1}{2}$  case in two dimensions, the problem at hand, it is natural to suspect that Néel order may be destroyed by either strong quantum fluctuations<sup>6</sup> or by topological defects.<sup>7</sup> It has been found that the topological term does not exist in the continuum limit<sup>8</sup> and both numerical calculations<sup>9-12</sup> and series expansion<sup>13</sup> suggest a Néel-ordered ground state. On the other hand, variational calculations show that there is a disordered state with energy very close to an ordered one<sup>14</sup> and a rigorous statement about the long-ranged order should be useful.

A rigorous proof of the existence of Néel order for the Heisenberg model has recently been extended to lower spins.<sup>15,16</sup> We now know that Néel order exists in three dimensions for all spins, and in two dimensions for spins greater than or equal to one. Furthermore, a bound on the two-point correlation function has been established<sup>15</sup> which if violated would imply a Néel order in the ground state. The correlation function obtained in the Monte Carlo simulation by Gross *et al.*<sup>10</sup> violates the bound starting at r=5 but that calculation is not done at zero temperature and the finite-size effects are not known.

In this paper, I report calculations of the two-point correlation function in the ground state using a new Monte Carlo method that preserves the SU(2) symmetry

for lattices with up to  $32 \times 32$  spins. Finite-size effects are carefully analyzed. Comparing the data on  $L \times L$  lattices with L=16 and 32, I find that correlation functions for  $|\mathbf{r}| \leq L/4$  do not depend strongly on the lattice size L and are good approximations to the infinite-sized system with accuracy of half of a percent. I have also obtained off axes two-point functions. This allows me to construct a slightly better bound. Data for  $32 \times 32$  lattice violate this bound starting at  $|\mathbf{r}| = \sqrt{17}$ . This implies that the ground state is Néel ordered. I have also estimated the groundstate energy per site  $e_0 = -0.6696 \pm 0.0008$  and the staggered magnetization moment  $m^+=0.304\pm0.004$  (in this unit  $m^+=0.5$  for the Néel state) in excellent agreement with the spin-wave theory and the recent series expansion result.<sup>13</sup> Our two-point function is about 10% below the result of Ref. 10 for a distance that is not too short.

Our method starts from a good trial wave function having an energy within 0.2% of the ground state. Then a projector [similar to  $\exp(-\beta H)$  where H is the Hamiltonian] is applied to the trial state to extrapolate to the ground state. I use a discrete projector so my method is exact in the sense that there is no number that has to be set small. A similar approach has been applied to quantum-spin chains.<sup>17</sup> In the next section, I introduce the trial wave function. Sec. III describes the projection method and Sec. IV presents the results of the calculation. The violation of the infrared bound is discussed in Sec. V.

## **II. TRIAL WAVE FUNCTION**

A  $L \times L$  square lattice with L even can be equally divided into A and B sublattices. Let  $(ij) = \uparrow_i \downarrow_j - \downarrow_i \uparrow_j$  denote a singlet bond between i and j. Connecting every site on the A and B sublattices with bonds defines a singlet state for  $N = L^2$  spins,

$$|c\rangle = \prod_{\substack{i\alpha \in A \\ j\alpha \in B}} (i_{\alpha}, j_{\alpha}) .$$
<sup>(1)</sup>

Because of the identity (m,n)(k,l)+(m,k)(l,n)

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Since the ground state of Heisenberg Hamiltonian  $H = J \sum_{\langle ij \rangle} S_i \cdot S_j$  is a singlet, we write a trial wave function in the valence bond basis as<sup>14</sup>

$$|\varphi_{\mathrm{tr}}\rangle = \sum_{\substack{i\alpha \in A \\ j\alpha \in B}} h(i_1 - j_1) \dots h(i_n - j_n)(i_1, j_1) \dots (i_n, j_n) \quad (2)$$

Here I have factorized the weight for a singlet state into a product of weights for its individual bonds. Because of this, (2) is an approximation to the ground state. The weight function h(i-j) is positive because of the Marshall sign rule<sup>18</sup> which essentially says that the ground-state wave function is nodeless in the hard-core boson representation.<sup>11(a)</sup>.

The wave function (2) includes state of different types.<sup>14</sup> When h(i-j) is a constant, independent of the distance, (2) is long-range ordered. In fact it is the Néel state projected into the singlet subspace. On the other extreme, when h(i-j) is short ranged

$$h(x,y) = \delta_{x,1}\delta_{y,0} + \delta_{x,0}\delta_{y,1}$$

[here we have redefined h(x,y) = h(i-j) with  $x = |i_x - j_x|$  and  $y = |i_y - j_y|$ ], (2) is the disordered dimer state. The best weight h(x,y) for the Heisenberg Hamiltonian is between these two limits.

To simplify the parametrization, notice that the symmetries of the square lattice allow us to restrict to the region where  $x \ge y$ . Also under the periodic boundary condition, h(L-x,y)=h(x,y) for  $0 \le x < L/2$ , and similarly for y. Notice further that h(x,y)=0 when x + y is even because no bond connects sites in the same sublattice. Since energy is more sensitive to h(x,y) at short distances, we therefore choose h(1,0)=1 (this sets the normalization), and let h(3,0), h(2,1) be free variational parameters. At larger distances the weight is controlled by  $h(x,y)=\alpha \exp[-\beta(x+y)]$  with  $\alpha, \beta$  being variational parameters.

A Monte Carlo algorithm<sup>14</sup> is readily constructed to compute the multidimensional sum in

$$\frac{\langle \varphi_{\rm tr} | \mathbf{S}_i \cdot \mathbf{S}_j | \varphi_{\rm tr} \rangle}{\langle \varphi_{\rm tr} | \varphi_{\rm tr} \rangle} = \frac{1}{\langle \varphi_{\rm tr} | \varphi_{\rm tr} \rangle} \sum_{c_1, c_2} \left[ \prod_{c_1} h \prod_{c_2} h \langle c_1 | c_2 \rangle \right] \times \frac{\langle c_1 | \mathbf{S}_i \cdot \mathbf{S}_j | c_2 \rangle}{\langle c_1 | c_2 \rangle} , \quad (3)$$

where the combination in the large parentheses is defined as  $P(c_1,c_2)$ —the probability for having the pair of  $(c_1,c_2)$  states. This is possible because h(x,y) is always positive and because the following formulas convert computing of the matrix elements for two valence bond states  $|c_1\rangle, |c_2\rangle$  to counting loops.<sup>14</sup> (i)  $\langle c_1|c_2\rangle = 2^{N(c_1,c_2)}$ , where  $N(c_1,c_2)$  is the number of loops in the bond covering obtained by putting bonds from  $|c_1\rangle$  and  $|c_2\rangle$  on the same lattice. (ii)  $\langle c_1 | \mathbf{S}_i \cdot \mathbf{S}_j | c_2 \rangle = 0$  when *i* and *j* belong to two different loops and

$$\langle c_1 | \mathbf{S}_i \cdot \mathbf{S}_j | c_2 \rangle = \pm \frac{3}{4} \langle c_1 | c_2 \rangle$$

when i and j belong to the same loop. We have the plus sign when i and j are on the same sublattice, and minus sign otherwise.

The Monte Carlo process samples the pair of state  $(c_1, c_2)$  according to the probability distribution  $P(c_1, c_2)$ . The elementary step in generating a new pair  $(c'_1, c_2)$  [or  $(c_1, c'_2)$ ] is to change two bonds in  $c_1$  (or  $c_2$ ) as follows: select at random two sites on the same sublattice across a diagonal of a plaquette; exchange bonds connected with the sites, then go to the new state  $c'_1$  according to probability  $P(c'_1, c_2)/P(c_1, c_2)$ .

Using this method we can compute the energy for a given weight h(x,y). The search for the best weight is made easier by the fact that the derivatives of the energy with respect to h(x,y) can all be obtained directly from the Monte Carlo time series.  $\partial E / \partial \ln h(x,y)$  is proportional to

$$\langle n(x,y)H \rangle - \langle n(x,y) \rangle \langle H \rangle$$
,

where  $\langle \rangle$  is the average over the Monte Carlo time and n(x,y) is the number of bonds that span distance x, y in the two directions.

The best variational parameters for L=8,16,32 are listed in Table I. The energies of the best trial states is almost indistinguishable from the energies of the ground states within statistical error of  $\pm 0.0008$  J. These trial states all have long-ranged Néel order. But in comparison with the ground state, they underestimate the staggered moment by a few percent. This is due to the truncation made for the weight at large distance.

TABLE I. The best variational parameters for the state defined in Eq. (2) on  $L \times L$  lattices. The parametrization is discussed in the text. Also listed are the variational energies and the ground-state energies computed by our projection method. The numbers in brackets are the estimated errors. Thus 0.6730(4) means  $-0.6730\pm0.0004$ . Energies are per site in the unit of J.

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L	8	16	32
h(3,0)	0.0885	0.0874	0.0860
h(2,1)	0.131	0.125	0.121
α	0.150	0.138	0.136
β	-0.245	-0.326	-0.351
Variational			
Energy	-0.6730(4)	-0.6694(4)	-0.6690(4)
Ground-state			
Energy	-0.6738(4)	-0.6704(6)	-0.6696(8)

#### **III. PROJECTION METHOD**

Although the energy of our variational wave function can be made very close to the ground-state value, the two-point function at a large distance is not necessarily so. To obtain the true ground state, we use a projection method.

The trial wave function can always be expanded in terms of eigenstates of the Hamiltonian

$$|\varphi_{\rm tr}\rangle = a_0 |E_0\rangle + a_1 |E_1\rangle + \dots$$

where  $|E_0\rangle$  is the ground state and  $|E_1\rangle$  is the first singlet excited state having the same symmetry as the trial wave function. We define a projected state  $|n\rangle$  using projector

$$H - W = J \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4}) ,$$
  
$$|n\rangle = (H - W)^n |\varphi_{\mathrm{tr}}\rangle .$$
(4)

It is easy to see that

$$|n\rangle = (E_0 - W)^n a_0 \{ |E_0\rangle + (a_1/a_0) [(E_1 - W)/(E_0 - W)]^n \times |E_1\rangle + \dots \}.$$

Thus,  $|n\rangle$  approaches the ground state for large *n* if  $|(E-W)/E_0-W|| < 1$  for all the energy *E* of the singlet states in the energy spectrum. This latter condition is satisfied for the Heisenberg model since the energy spectrum is bounded from both above and below:  $E_F > E \ge E_0$ , where  $-E_F = -JN/2$  is the ground-state energy of the ferromagnetic Heisenberg model (with *J* changed to -J in the Hamiltonian).

The reason for choosing

$$J\sum_{\langle ij\rangle}Q_{ij}\!=\!J\sum_{\langle ij\rangle}{(\mathbf{S}_i\!\cdot\!\mathbf{S}_j\!-\!\frac{1}{4})}$$

as projector in Eq. (3) is because  $Q_{ij}$  preserves the valence bond structure:  $Q_{ij}(i,j) = -(i,j)$ ;

$$Q_{ii}(i,l)(k,j) = -(i,j)(k,l)/2$$

So that the projection of a valence bond state  $|c\rangle$  is a sum over valence bond states

$$\left(\sum_{\langle ij \rangle} Q_{ij}\right)^{n} | c \rangle = \sum_{\{Q_{ij}\}} \prod_{\alpha} Q_{i_{\alpha}j_{\alpha}} | c \rangle , \qquad (5)$$

each term in the sum on the right-hand side of Eq. (5) is a valence bond state. In the Monte Carlo evaluation of matrix elements  $\langle n | \mathbf{S}_i \cdot \mathbf{S}_j | n \rangle$  for the projected state in Eq. (4), one needs to sum over products of operators like the ones in Eq. (5). Because  $Q_{ij}$  preserves the valence bond structure, the summation can be done simultaneously with the sampling over the trial state. The multiplications in Eq. (4) are done directly. They are the most time consuming part of the calculation. For example, for a  $32 \times 32$  lattice, *n* has to be as large as 6000. Therefore sampling over the operator products is performed less frequently. In the actual calculation, relative ratio of  $\frac{1}{16}$  is used. The final answer does not depend on this ratio al-

though the statistical error does.

The expectation value of

$$C_n(\mathbf{r}) = \langle n | \mathbf{S}_{\mathbf{O}} \cdot \mathbf{S}_{\mathbf{r}} | n \rangle / \langle n | n \rangle$$

for the projected state defined in Eq. (4) approaches the ground-state value  $C(\mathbf{r})$  exponentially fast,

$$C_n(\mathbf{r}) = (-1)^{x+y} C(\mathbf{r}) + \delta(\mathbf{r}) \exp(-\Delta n) , \qquad (6)$$

where  $\mathbf{r} = (x, y)$  and  $\Delta$  is determined by

$$\exp(-\Delta) = |(E_1 - W)/(E_0 - W)|$$
,

and  $E_1$  is the first excitation energy.

# **IV. RESULTS**

As a test for the algorithm we have computed energy on a  $4 \times 4$  lattice for several  $|n\rangle$ . The variational parameter h(x,y) is deliberately set away from the optimal one, and the exponential decay is evident (see Fig. 1).

We next measure the two-point function on larger lattices. To do this we first compute the two-point function on the projected state  $|n\rangle$  for several different values of *n* for a given lattice size. Then we extrapolate according to Eq. (6) to the ground-state value  $C(\mathbf{r})$ . We have data for  $L \times L$  lattices with L=8,16,22,32. For each fixed L and *n*, we made 16 independent runs from which the average and the statistical uncertainties of the two-point function were obtained.

To determine the ground-state two-point function  $C(\mathbf{r})$ as well as  $\delta(\mathbf{r})$  and  $\Delta$  in Eq. (5), we need to know  $C_n(\mathbf{r})$  for at least three different values of *n*. The standard  $\chi^2$  fitting is then applied using the statistical errors measured from 16 sets of data. Notice that if  $\Delta$  is fixed, getting  $C(\mathbf{r})$  and  $\delta(\mathbf{r})$  from  $C_n(\mathbf{r})$  for any  $|\mathbf{r}| > 1$  requires a linear leastsquares fitting  $[C(\mathbf{r}=0)$  is 0.75, a constant;  $C(|\mathbf{r}|=1)$  follows different extrapolation with a  $2\Delta$  gap]. The best  $\Delta$  is obtained then by minimizing the sum over all  $\mathbf{r}$  of deviation squares weighted by statistical error.

Uncertainty in  $\Delta$  is large for the large lattices because of the statistical fluctuation. But since the energy-gap scales as  $(E_1 - E_0)/J = A/L$ , we can determine the con-



FIG. 1. A test of the algorithm on a  $4 \times 4$  lattice. Plotted are the energy per site e(n) (shown as squares) of states  $|n\rangle$  defined in Eq. (3) vs *n*. The energies is subtracted by the known ground-state energy  $E_0 = -0.70178$ . All the energies are in the unit of *J*. The solid line is a fit to the exponential form  $E(n)=E_0+a\exp(-2\Delta n), \Delta=0.21$ .

stant A from data on a small system. This is done on a  $8 \times 8$  lattice. To get  $\Delta$  we use  $C_n(\mathbf{r})$  at six different values of n (at  $n\Delta = 1.4$ , 1.9, 2.8, 3.7, 5.6, 7.4). From this we obtain  $\Delta = 0.029$ . This translates to a gap  $(E_1 - E_0)/J = 17.1/L$  which is substantially larger than the gap to the lowest triplet excitation.

For other lattice sizes, the gap parameter  $\Delta$  used in the fitting is computed from  $\Delta = 0.029(8/L)^3$  ( $\Delta$  goes as  $1/L^3$  because  $E_0$  is proportional to  $L^2$ ). Figure 2 compares the gaps  $\Delta$  computed from this formula with ones that best fit the data. The difference is always less than 50%. Shifting  $\Delta$  by 50% changes  $C(\mathbf{r})$  by 0.3% at the largest distance and by about 0.1% at the distance a quarter of the system size.

For lattices with L=16, 22, and 32, the ground-state correlations  $C(\mathbf{r})$  are extrapolated from three values of nwith  $n\Delta$  ranging from 0.9 to 2.8. The correlation function is shown in Fig. 3. To a good approximation, the two-point function depends only on  $|\mathbf{r}|$ . At a large distance,  $C(\mathbf{r})$  goes to a constant indicating a long-rangeordered ground state. The approach to the constant can be fitted to both exponential form and power-law form. The statistical error coming from the Monte Carlo simulation is  $\pm 0.0004$ . The estimated error of the fitting procedure [taken to be 5% of  $\delta(\mathbf{r})$  in Eq. (5)] is largest at the longest distance and is also about  $\pm 0.0004$ .

There are several ways to measure the staggered magnetization. One way is to look at the correlation function at largest distance C(L/2, L/2) or C(L/2, 0) as a function of system size L and extrapolate as a function of 1/L.<sup>10,19</sup> The other is to compute the total amount

$$M = \left[\frac{1}{L^2} \sum_{\mathbf{x}} \epsilon(\mathbf{x}) \mathbf{S}(\mathbf{x})\right]^2, \qquad (7)$$

where  $\epsilon(\mathbf{x})$  is +1 on the *A* sublattice and -1 on the *B* sublattice. There is a large finite-size correction to this moment. In Fig. 4 we plot the extrapolation of these three quantities to the thermodynamic limit. From this we estimate

 $m^+=0.304\pm0.004.$ 

Three quantities give three different extrapolated values of  $m^+$ . This is the major source of error (see the caption for Fig. 4).



FIG. 2. The parameter  $\Delta$  in Eq. (6) that best fits the data (shown as circles) compared with the one used in the actual fitting (solid line).



FIG. 3. The spin-spin correlation function in the ground state as a function of Euclidean distance at short (a) and long (b) distances. The largest error is estimated at 0.5% which is about the size of the dots in (b) and a fraction of a dot in (a). The correlation function falls on a common curve. The deviations at  $|\mathbf{r}| = L/2$  are dual to finite-size effects.



FIG. 4. The staggered magnetization is extrapolated to the thermodynamic limit from the data on finite-sized lattices. The moment defined by Eq. (7) is extrapolated as a linear function of 1/L to get  $m^{+2}=0.0904$  using data for L=8, 16, 22, and 32. But  $m^{+2}$  changes to 0.0922 if only the data for L=16, 22, and 32 is used. From the correlation function for the largest distance on axes, C(L/2,0), we get  $m^{+2}=0.0938$ . Finally from C(L/2,L/2),  $m^{+2}=0.0912$  is obtained. For the two latter fits, values for  $m^{+2}$  are independent of whether the L=8 point is included or not in the fits.

## **V. THE INFRARED BOUND**

There is a connection between the existence of longranged Néel order in the ground state and the values of the correlation function at finite distances.<sup>20,15,16</sup> Bounds can be established for the two-point function. In the following, we construct a slightly better bound following Kennedy *et al.*<sup>15</sup> before comparing them with our data.

For a finite square lattice with periodic boundary conditions, let us define

$$g_{\mathbf{q}} = \frac{1}{3} \sum_{\mathbf{x}} e^{-\iota \mathbf{q} \cdot \mathbf{x}} \langle \mathbf{S}_{\mathbf{0}} \cdot \mathbf{S}_{\mathbf{x}} \rangle ,$$

where  $\langle \rangle$  denotes the normalized ground-state expectation value and  $g_q$  is real and positive. Then we have following infrared bound,<sup>15</sup>

$$g_{\mathbf{q}} \leq f_{\mathbf{q}}, \quad q \neq (\pi, \pi)$$

where

$$f_{q} = (|e_{0}|E_{q}/12E_{q+Q})^{1/2},$$
  
$$E_{q} = 2 - \cos(q_{x}) - \cos(q_{y}).$$

 $\mathbf{q} = (q_x, q_y)$  and  $e_0$  is the ground-state energy per site.

A nonzero Néel moment corresponds to a  $\delta$  function in  $g_q$  at  $q = (\pi, \pi)$  for the infinite volume limit. Following



FIG. 5. This graph compares the left- (data) and right-hand (bounds) sides of Eq. (8). The infrared bound is violated starting at  $|\mathbf{r}|=4$ . This implies the ground state is Néel ordered. The data is taken from L=32 lattice. The total error is 0.4% which is invisible in this graph.

Kennedy et al.<sup>15</sup> we define

$$\widetilde{g}(\mathbf{r}) = \frac{1}{M} \sum_{|\mathbf{x}| \leq r} (-1)^{m+n} \langle \mathbf{S}_0 \cdot \mathbf{S}_{\mathbf{x}} \rangle ,$$

where  $M = \sum_{|\mathbf{x}| \le r} 1$  is the total number of terms in the sum, and the sum is over all sites  $\mathbf{x} = (m, n)$  having  $(m^2 + n^2)^{1/2} \le r$ . We have added all the terms with  $|\mathbf{x}| \le r$  because from Fig. 3 we know that the two-point function depend only on  $|\mathbf{x}|$  and because this gives us a slightly better upper bounds.

If the Néel moment is zero, we must have

$$\tilde{g}(\mathbf{r}) \leq 3 \int_{0}^{2\pi} \frac{dq_x}{2\pi} \int_{0}^{2\pi} \frac{dq_y}{2\pi} \frac{1}{M} \left[ \sum_{|\mathbf{x}| \leq r} (-1)^{m+n} \cos(mq_x + nq_y) \right]_{+} f_q , \qquad (8)$$

where  $[w]_+$  is equal to w if  $w \ge 0$  and is zero otherwise. The integral is evaluated numerically. The integrable singularity at  $(\pi, \pi)$  must be treated with care.

Figure 5 shows that both sides of Eq. (8) as a function of r using data for L=32 lattice. The ground-state energy per site is taken to be  $e_0 = -0.6696$ . Since the finitesize correction to the energy per bond is proportional to  $1/L^3$ , we expect the finite-size correction for the correlation function at short distances to follow the same form. Judging from the two-point function at short distances plotted in Fig. 3(a), we conclude that the finite-size correction for  $|\mathbf{r}| \le 4.5$  is about 0.2%. The estimated error in this region is also 0.2%.

# VI. CONCLUSION

I have computed the spin-spin correlation function in the ground state for the spin- $\frac{1}{2}$  antiferromagnetic Heisenberg model on  $L \times L$  square lattices for L=8, 16, 22, and 32. I have used a new method which starts from a resonating valence bond wave function before projecting to the ground state. The energy of the variational state is within 0.2% of the ground-state energy which is estimated to be  $e_0/J = -0.6696 \pm 0.0008$  per site. I have found a Néel ordered ground state with the staggered magnetization in the infinite volume limit  $m^+=0.304\pm004$  (in this unit  $m^+=0.5$  for the Néel state).

After analyzing the finite-size corrections and statistical errors, I have shown that the two-point function on  $32 \times 32$  lattice at distance less than 8 approximates the infinite large lattice very well with error of less than a percent. The two-point function at short distance (starting at  $\sqrt{17}$ ) exceeds the upper bound constructed following Kennedy *et al.*<sup>15</sup> This means that the ground state is Néel ordered.

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- \*Present address: Department of Physics, Pennsylvania State University, University Park, PA 16802.
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