Long-range order without broken symmetry: Two-dimensional Heisenberg antiferromagnet at zero temperature

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We have calculated the probability distribution for staggered magnetization at $T=0$ for the two-dimensional (2D) antiferromagnetic Heisenberg model (2D AFH) on a series of finite lattices up to 26 sites. We find that the singlet ground state of the 2D AFH possesses long-range magnetic order without broken symmetry. We also study the lowest triplet state and find that it becomes degenerate with the ground state in the thermodynamic limit. This state does exhibit broken symmetry on a finite lattice. The value of the staggered magnetization in the thermodynamic limit is also obtained by extrapolation. We compare our results with the results obtained by other methods and discuss the relevance to the high-T_c superconductive oxide compounds.

As a venerable quantum spin model, the Heisenberg model has played an important role in our understanding of magnetism since it was proposed in the early times of quantum mechanics. Last year's vigorous research on the newly found high-T_c superconductive oxide compounds has fueled renewed interest on the two-dimensional antiferromagnetic Heisenberg model (2D AFH). It has been proposed as a basic frame for various theories about possible new superconductivity mechanisms.[1-4] Many authors start from expanding the Hubbard model in the strong coupling limit. This procedure yields an effective Hamiltonian, which usually has an antiferromagnetic Heisenberg term, plus a hopping term combined with Gutzwiller-type projection operators to eliminate doubly-occupied-site states. Thus, a solid knowledge of this model, especially the knowledge of its ground state, is now of great urgency; we need to explore new facts and resolve old controversies.

One longstanding controversy is whether long-range order (LRO) exists at zero temperature in the 2D AFH. As early as 1952, Anderson used a semiclassical spin-wave approach to attack this model, calculating the ground-state energy and the staggered magnetization.[5] This approach was then elaborated by Kubo,[6] and later Oguchi proved that the next order correction to their results is negligibly small.[7] Of course, the basic assumption of spin-wave theory is that LRO does exist, and quantum fluctuations only cause spins to undergo small fluctuations around a common direction. Before this assumption is confirmed by other techniques, its validity can only be judged by the consistency between this assumption and the results predicted by it. Under this assumption, a staggered magnetization of 0.303, defined such that the saturation value is $\frac{1}{2}$, has been obtained. Then came Mermin and Wagner's rigorous proof[8] that a 2D Heisenberg model cannot sustain LRO at any finite temperature. It makes the situation at $T=0$ more intriguing, and many results were published in the years that followed. Perturbation methods give results of magnetic order close to preceding value.[9] Variational results do not seem to appear frequently in the reference lists, possibly because the staggered magnetization value obtained, 0.402, is too high to be believable.[10] Nevertheless, we include variational results in Table I together with other results obtained by various methods. Ten years ago, Oitmaa and Betts (OB) published their finite lattice study on 2D AFH and XY model,[11] in which they claimed LRO exists in both models. However, for AFH on a square lattice, only three lattice sizes, i.e., 8-site, 10-site, and 16-site were used. Later, Monte Carlo simulations on the 2D half-filled Hubbard model showed evidence of LRO for nonzero Coulomb interaction.[12] The half-filled Hubbard model reduces to an effective AFH for large Coulomb interaction. So it seems fair to say that the prevailing perception among physicists is that LRO exists at $T=0$ for 2D AFH. This perception, however, was recently challenged by Fujiki and Betts himself.[13] Based on work on the triangular lattice, they reanalyzed the XY data on square lattices up to size 20 sites. Their work highlighted the difficulty in the extrapolation process. Whether one finds LRO or not can depend on what kind of fitting formula one uses. Last year Anderson suggested that the ground state of the 2D AFH on a square lattice is probably a case of the resonating-valence-bond (RVB) state.[1] His hypothesis further raises doubts about the existence of LRO.[14] Recently, Reger and Young (RY) performed a world-line Monte Carlo simulation for the 2D AFH up to lattice size 12×12.[15] They found that the staggered magnetization m has a finite value of 0.30 ± 0.02 in the infinite-size and zero-temperature limit. Meanwhile, Huse[16] reanalyzed Parrinello and Arai's[9] cumulant series, obtaining a value of 0.313 for the staggered magnetization. So, the spin-wave approximation, perturbation method, and Monte Carlo simulation all give a finite staggered magnetization around 0.3; Oitmaa and Bett's original result (derived from their $\langle N_\alpha^2\rangle/N^2$ value) was 0.42; and Tang and Lin's recent result is 0.245 (Ref. 17); in the latter work seven square lattices up to 26 sites were used.

To extrapolate the properties of an infinite system from

TABLE I. The various results for the staggered magnetization of the 2D Heisenberg antiferromagnet. The numerical results (last three entries in the table) are for the staggered magnetization $m=(\langle m^2\rangle)^{1/2}$ as defined in Eq. (4). In Ref. 11, results for m_z^2 were quoted, as pointed out by Huse (Ref. 16). In the last row, for the present work, only the result for the singlet ground state is quoted.

Method	Author	Ref.	Staggered magnetization
Spin wave	P. W. Anderson	5	0.303
Perturbation	H. L. Davis	9	0.382
Perturbation	M. Parrinello and T. Arai	9	0.362
Perturbation	D. A. Huse	10	0.313
Variational	R. R. Bartkowski	10	0.402
Monte Carlo	J. D. Reger and A. P. Young	15	0.30±0.02
Finite lattice	J. Oitmaa and D. D. Betts	11	0.42
Finite lattice	S. Tang and H. Q. Lin	17	0.245
Finite lattice	S. Tang and J. E. Hirsch	Present work	0.25±0.03

the information collected on a series of finite systems is now a well-established procedure in statistical mechanics. This procedure usually gives reliable results. Exact calculations on small lattices are an important complement and check on computer simulations on larger lattice systems. Possible sources of errors in simulation studies, such as Reger and Young's, are the Trotter approximation, the necessity to extrapolate from finite temperature, and possible metastability in the Monte Carlo simulation; exact diagonalization does not encounter these problems, but of course can only reach substantially smaller lattice sizes. Here we reexamine the exact 2D AFH ground states and low-lying excited states of seven square lattices, of size $N=4$, 8, 10, 16, 18, 20, and 26. Those N can be written as $N=l^2+m^2$, where l,m is zero or integer, and $l+m$ is even. The accuracy of the ground states was checked by acting the total magnetic moment matrix $\mathbf{S}^2$ and the Hamiltonian matrix H on them, until a genuine singlet state and an energy accurate to ten digits were obtained.

The Heisenberg Hamiltonian is defined as

$$H=2J\sum_{\langle i,j\rangle}\mathbf{S}_i\mathbf{S}_j \ , \tag{1}$$

where $J>0$ for antiferromagnetism, and $\langle i,j\rangle$ runs on all nearest neighbors. This Hamiltonian is a special case of the more general anisotropic Heisenberg model, defined in this work as

$$H=4J\sum_{\langle i,j\rangle}[\gamma S_i^zS_j^z+(1-\gamma)(S_i^xS_j^x+S_i^yS_j^y)] \ . \tag{2}$$

When $\gamma=\frac{1}{2}$, (2) reduces to (1), $\gamma=1$ is the Ising model, and $\gamma=0$ is the quantum XY model. We define the z-direction staggered magnetization as

$$m_z=\frac{1}{N}\sum_i \epsilon_i S_i^z \ , \tag{3}$$

where $\epsilon_i=\pm 1$, depending which sublattice site i belongs to. We also define the mean-square root of the staggered magnetization as

$$m=\frac{1}{N}\left[\left\langle\left[\sum_i \epsilon_i\mathbf{S}_i\right]^2\right\rangle\right]^{1/2} \ , \tag{4}$$

which is what actually calculated by OB (Ref. 11) and RY (Ref. 15) and supposedly, should be equal to the z-direction staggered magnetization calculated by the spin-wave approximations and the perturbation methods. We will call m the staggered magnetization throughout this work.

The ground state on a finite lattice can be written as

$$\Psi_0=\sum_i \alpha_i|i\rangle \ , \tag{5}$$

where i runs on all possible spin configurations. We use eigenvectors of the Ising Hamiltonian as our basis. Every spin configuration has a z-direction staggered magnetization m_z, whose allowed value is from -0.5 to 0.5. Following what Suzuki and Miyashita did for the total magnetic moment $\mathbf{S}^2$ of the XY the model,[18] we calculate the distribution of the probability amplitude α^2 versus m_z. We sum up all α_i^2, where $|i\rangle$ has a particular value of m_z, then plot these sums in Fig. 1(a). The results on the four largest lattices we used are presented. Due to the symmetry, only the non-negative portion of the distribution is actually plotted. The data for the 20-site lattice are their true values, the data for other lattices are scaled so they will give the same area if a histogram is made.

A glimpse at Fig. 1(a) confirms the existence of LRO. There is clearly no tendency for the probability amplitude to peak around 0 as the lattice size increases. It looks very unlikely that a distribution of δ-function type centered at $m_z=0$ will emerge in the thermodynamic limit.

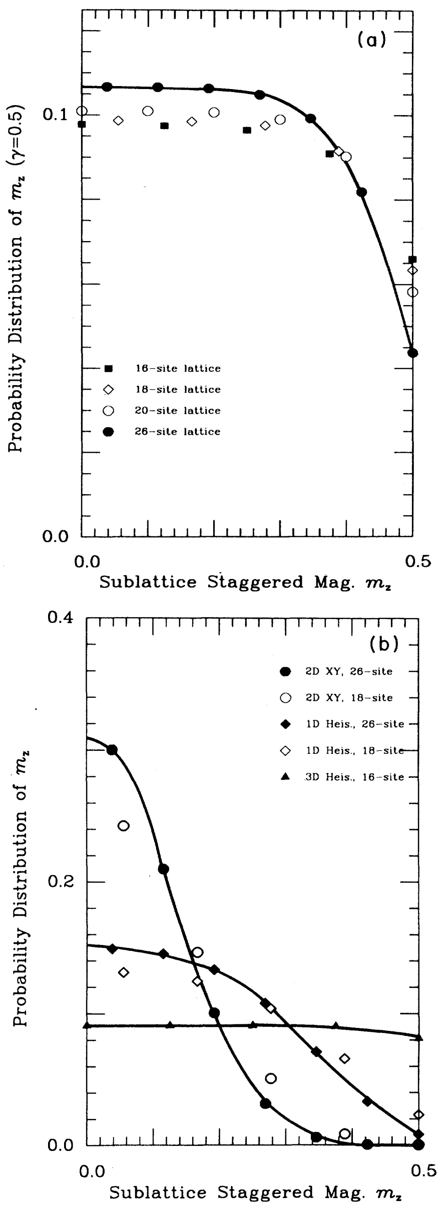

FIG. 1. (a) The probability distribution for the sublattice staggered magnetization m_z. The results on four lattices are presented. The lattice sizes are 16-, 18-, 20-, and 26-site. A line is drawn to guide the eye. For the 20-site lattice, true values are given. For all other lattices, the data are scaled so that a histogram will occupy an area of equal size if it is made. There is no indication of a peak around $m_z=0$. Instead, the curve is almost flat from 0 to 0.25, and only raises very slightly around 0. The curve begins decreasing at 0.25, possibly going to 0 at $m_0=0.5$ in the thermodynamic limit. This feature guarantees a finite staggered magnetization but also gives rise to nonvanishing fluctuations in the thermodynamic limit for m_z. (b) Probability distributions for the 2D XY model on a 18- and 26-site lattice, for the 1D AF Heisenberg chain of 18- and 26-site, and for the 3D AFH on a 16-site trigonal lattice. For the 2D XY model and the 1D AFH, small m_z values have dominant probability. These two models are believed to possess no finite magnetization along z direction at $T=0$. For the 3D AFH, the distribution is almost uniform.

The distribution is essentially flat from 0 to 0.25, then it begins to decrease. For example, for the 26-site lattice, the distribution has a value of 0.08213 at $m_z=\frac{1}{26}$, while this value at $m_z=\frac{5}{26}$ is 0.08186. The Hamiltonian and the ground state of 2D AFH have rotational invariance in spin space. If a finite staggered magnetization m_0 exists, all points (m_x,m_y,m_z) located on the spherical surface $m_0^2=m_x^2+m_y^2+m_z^2$ should have equal probability amplitude. This spherical distribution will lead to a uniform distribution for m_z from $m_z=-m_0$ to $m_z=m_0$, and 0 outside the interval $[-m_0,m_0]$. The distribution showed in Fig. 1(a) is consistent with the preceding observation. This flatness of the probability distribution is absent in the systems whose lack of LRO at $T=0$ is exactly known. For comparison, the same distribution data of the 2D XY model on 18- and 26-site lattice, and of the one-dimensional (1D) AF Heisenberg on 18- and 26-site chain, are plotted in Fig. 1(b). We set the interaction to be antiferromagnetic in our calculation for the XY model. It is believed that the XY model has no z-component magnetization in the thermodynamic limit.[11] In Fig. 1(b), more than half of the probability amplitude concentrates between the interval $m_z=\pm\frac{1}{26}$ for the 2D XY model. A similar feature is showed by the 1D AFH. We see that the cusp centered at $m_z=0$ becomes higher and narrower as the lattice size increases. The distribution for the three-dimensional (3-D) AF Heisenberg model on a 16-site trigonal lattice is also plotted in Fig. 1(b).[19] It shows the same flat feature. Because the lattice is relatively small and the staggered magnetization in this lattice is larger than the saturation value 0.5, we see an almost uniform distribution from $m_z=0$ to $m_z=\pm0.5$.

In order to calculate the value of the staggered magnetization, we construct a squared staggered magnetization matrix,

$$\mathbf{M}^2=\left[\sum_i \epsilon_i \mathbf{S}_i\right]^2 , \tag{6}$$

and this matrix is applied to the 2D AFH ground state to obtain m^2. The results on our seven lattices, together with the ground-state energy, are listed in Table II. Our data fitting procedure is the following: first we try to fit the data linearly with a dependence $N^{-1/2}$, N^{-1}, and N^{-2}, then we pick up the one which gives the best fit, and add one or two more terms of higher power to the fitting formula, if the addition will not overdo the fitting. For those small lattices, the correction terms may be as large as, or even larger than, the asymptotic value, and to fit the data too well is equally dangerous as to fit the data too poorly. In order to make the fitting biased to larger lattices, we assign a weight proportional to the lattice size to the data points. The mean squared staggered magnetization m^2 on the seven lattices are fitted with a form

$$m^2(N)=m^2(\infty)+a_1N^{-1/2}+a_2N^{-1} . \tag{7}$$

The second term in the right-hand side of (7) is predicted by spin-wave theory.[16] We searched for a best exponent from 0 to 2 by using a least-squares method, and found the best value is 0.495 for our m^2 data, so this term truly makes sense. The diagonal element of the matrix $\mathbf{M}^2$ is

TABLE II. The calculated values of the energy and mean-square staggered magnetization, the z component of the mean-square staggered magnetization for the 2D AFH ground state (singlet $S=0$) and the lowest excitation state (triplet, $S=1$ and $S^z=0$).

Lattice	Ground state Energy E_0	Ground state Staggered magnetization	Ground state z compt.	Lowest excited state Energy E_1	Lowest excited state Staggered magnetization	Lowest excited state z compt.
4	−2.000 000	0.500 000	0.166 667	−1.000 000	0.375 000	0.250 000
8	−1.500 000	0.375 000	0.125 000	−1.250 000	0.343 750	0.212 500
10	−1.460 014	0.338 041	0.112 660	−1.292 820	0.324 232	0.195 347
16	−1.403 560	0.276 527	0.092 176	−1.331 236	0.271 956	0.164 607
18	−1.387 972	0.268 603	0.089 534	−1.331 482	0.263 698	0.159 249
20	−1.381 616	0.257 731	0.085 910	−1.334 919	0.254 130	0.153 242
26	−1.368 904	0.233 899	0.077 966	−1.339 931	0.232 594	0.139 677
∞	−1.344±0.002	0.064±0.014	0.021±0.005	−1.344±0.002		0.042±0.008

$$\sum_i (S_i^x S_i^x + S_i^y S_i^y) + \left[\sum_i \epsilon_i S_i^z\right]^2 . \tag{8}$$

This form gives rise to the third term in (7). In our previous calculations[17] m^2 was only fitted to $N^{-1/2}$. In Fig. 2 we plotted the fitting curves for m^2. The limiting value is

$$m^2 = 0.064 \pm 0.014 , \tag{9}$$

which gives a staggered magnetization value as

$$m_0 = 0.25 \pm 0.03 . \tag{10}$$

This value is smaller than all previous results except the ones obtained by finite lattice studies,[17] but it seems consistent with the tendency of the probability distribution for the staggered magnetization.

Thus, our analysis confirms that the 2D Heisenberg antiferromagnetic possesses long-range order at zero temperature. But as a singlet, the ground state itself cannot break the rotational symmetry of the staggered magnetization. For the classical Heisenberg model at $T=0$, although the Hamiltonian has rotational invariance in spin space as does its quantum counterpart, the ground state is infinitely degenerate, and the spins are "frozen" along a special direction, i.e., the system settles in one of the degenerate ground states, so the rotational symmetry is broken when long-range order sets in at $T=0$. For a quantum Heisenberg ferromagnet, the z component of the magnetic moment is a constant of motion, a special direction is chosen after we choose our basis. In the case of a quantum antiferromagnet, the situation is totally different. The staggered magnetization is not a constant of motion, and its direction changes constantly. In the isotropic $S=0$ state, any direction has equal probability at any time. The two Néel states in our basis do not have any special meaning for the ground state. As shown by Kaplan using an exactly solvable model, a singlet without broken symmetry can possess LRO.[20] The same situation is clearly shown in Fig. 1(a); there is no peak at the two Néel states ($m_z = \pm 0.5$); there is also no peak around the extrapolated m_0 values, and no tendency to develop a peak around these values as the lattice size grows. The same situation also occurs in three dimensions, as indicated by the results on the 3D 16-site lattice in Fig. 1(b).

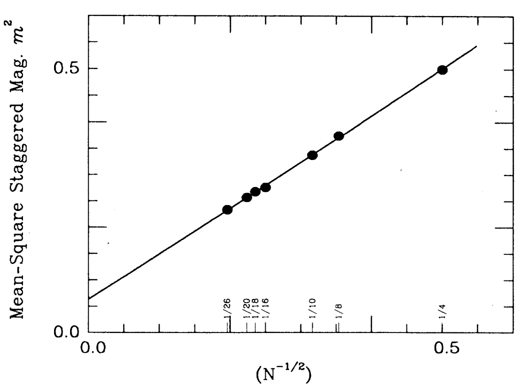

FIG. 2. The extrapolation of the mean-square staggered magnetization m^2 for the ground state. Though the line looks straight vs $N^{-1/2}$, the correction term proportional to N^{-1} is taken into account. The limiting value is 0.064 ± 0.014, which yields a staggered magnetization of 0.25 ± 0.03.

The preceding observation indicates that one should be careful in doing a direct comparison of the results obtained by different methods. On one hand, exact finite lattice studies[11,17] and Monte Carlo simulation[15] treat the ground state of 2D AFH as a singlet invariant under spin rotation. On the other hand, perturbation and spin-wave approximation start from a broken-symmetry state. The perturbation method takes an Ising-like interaction in Eq. (2) as the unperturbed Hamiltonian. In the spin-wave approach, it is implicitly assumed that the probability distribution peaks at the Néel states, and that these two Néel states will be decoupled in the thermodynamic limit, i.e., the distribution peaks should grow higher and narrower at the expense of those spin configurations which have m_z around 0, so the tunneling rate between these two peaks vanishes as $N \to \infty$. This is very different from the flat probability distribution found in Fig. 1.

The spin-wave picture implicitly assumes that an infinitesimal staggered field has picked out the z direction as the direction of the staggered magnetization. To understand the connection with our results, we have to take into account the effect of the low-lying excited states. When $\gamma = 1$ in Eq. (2), i.e., in the Ising limit, the ground state is a doublet. On a finite lattice, the two Néel states can form two independent linear combinations; one is the sum of the Néel states, the other is the difference between them. When γ decreases from 1 and the exchange interaction is turned on, the sum (difference) will become the ground state by mixing with other spin configurations, if the lattice has $4n(4n+2)$ sites. Meanwhile, the difference (sum) will also become the lowest excited state by mixing with other spin configurations. At the Heisenberg point where $\gamma=0.5$, the ground state becomes a singlet, while the lowest excited state is a triplet. This scenario is similar to what happens in the 1D case,[21] and has been checked by us through direct calculations on finite lattices. It is believed that there is no energy gap for the 2D AFH.[22] Recently, Barnes and Swanson calculated the ground state and the lowest excitation energies by a projector Monte Carlo method on lattices up to 8×8 sites.[23] Their results shows that there is probably no energy gap in the thermodynamic limit. Though their extrapolation formula is different from ours, their energy estimate is very close to ours. Our results for energies are listed in Table II, and plotted in Fig. 3. The results indicate the excitation spectrum is gapless as predicted by spin-wave theory. For this triplet state in the $S_z=0$ sector, the probability distribution of the sublattice staggered magnetization m_z does have a peaked structure, as one would expect from the following symmetry argument. The total magnetic moment $\mathbf{S}$ is the sum of the two z-direction magnetic moments $\mathbf{S}_A$ and $\mathbf{S}_B$, while the staggered magnetic moment $\mathbf{M}$ is equal to $\mathbf{S}_A-\mathbf{S}_B$. Noting $\mathbf{S}_A$ commutes with $\mathbf{S}_B$, we have

$$\mathbf{S}\cdot\mathbf{M}=\mathbf{S}_A^2-\mathbf{S}_B^2=0\ , \tag{11}$$

due to the symmetry between the two sublattices. Thus, the staggered magnetic moment is perpendicular to the total magnetic moment. For the triplet states with $S^z=\pm1$, $\mathbf{M}$ is on the xy plane, for the triplet state with $S^z=0$, $\mathbf{M}$ lies on a plane parallel to the z axis, probably with a dominant z component. In Fig. 4, we plot the probability distribution of m_z for this triplet state on the four largest lattices we used. The mean squared staggered magnetization $\mathbf{M}^2$ values for this triplet state on the seven lattices we used, are also given in Table II. A simple linear fit of the difference of $\mathbf{M}^2$ values between the singlet and the triplet shows that this difference $\Delta\mathbf{M}^2$ can be expressed as

$$\Delta\mathbf{M}^2\simeq c_0+c_2N^{-2}\ , \tag{12}$$

where $c_0=-0.0015\pm0.0013$. Because the difference decays faster than $N^{-1/2}$, we conclude that the triplet and the singlet have the same total mean squared staggered magnetization, besides having the same energy, as one would expect. It is likely that there are also higher S states that become degenerate with the singlet ground state in the thermodynamic limit and have the same total staggered magnetization. But the z components of the total mean squared staggered magnetization can be different in these states. For the triplet, the z component of the mean squared staggered magnetization can be fitted very well by using formula (7). The fitting is plotted in Fig. 5. The limiting value is

$$m_z^2=0.042\pm0.008\ . \tag{13}$$

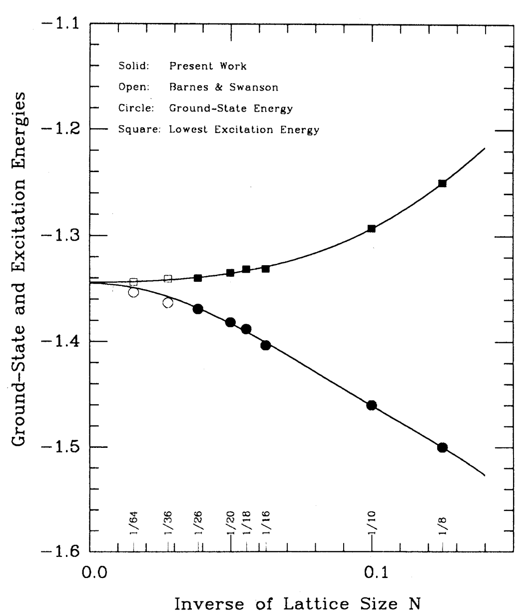

FIG. 3. The extrapolation of the ground-state energy and the lowest excitation energy. We also plotted the results of Barnes and Swanson (Ref. 23). The limiting value is -1.344 ± 0.002. We assume that the data have a form of $E(\infty)+\alpha_2N^{-2}+\alpha_4N^{-4}+\alpha_6N^{-6}$.

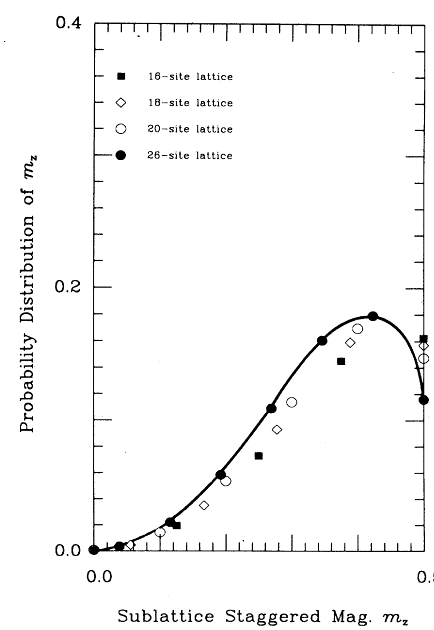

FIG. 4. The probability distribution for the sublattice staggered magnetization m_z for the lowest excited state. The results on four lattices are presented in the same fashion as in Fig. 1. The lattice sizes are 16-, 18-, 20-, and 26-site. A line is drawn to guide the eye. The probability distribution peaks at a value close to the Néel values $m_z=\pm0.5$.

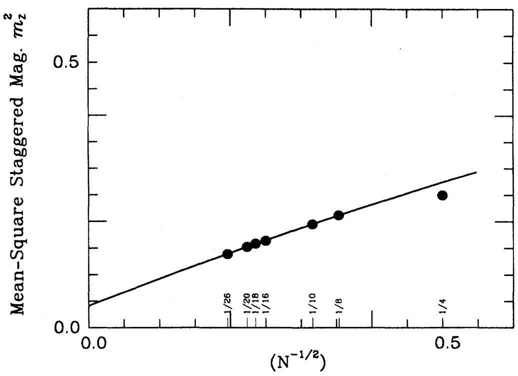

FIG. 5. The extrapolations of the z component of mean-square staggered magnetization m^2 for the lowest excited state. The limiting value is 0.042 ± 0.008.

It is interesting that our extrapolated value for the z component of the mean squared staggered magnetization for the $S^z=0$ triplet is about twice the corresponding value for the singlet.

If a small staggered field h ($h \ll J$) along the z direction is applied to the system, the energy degeneracy in the thermodynamic limit of the singlet ground state and the lowest excited triplet state, and possibly other higher S states will be removed. The singlet ground state will mix predominantly with this lowest triplet state. On the other hand, the triplet state, in turn, will mix with higher S states. Thus, a broken-symmetry state with a staggered magnetization polarized along the direction of the field can be constructed. To calculate the staggered magnetization of this broken-symmetry state under a small field is an interesting problem for further investigation.

The quantum fluctuations in the 2D AFH model can be reduced by a weak third-dimensional coupling. In a real material like La_2CuO_4, such a weak third-dimensional coupling is always present. Below a critical temperature, the Cu-O planes will be strongly coupled. This mechanism could stabilize those low-energy states of the 2D AFH model. If magnetic order does exist on the Cu-O plane in La_2CuO_4 below the Néel temperature, as indicated by the experiment,[4] one would expect the spins on the 2D plane to be described by a broken-symmetry state, a linear combination of the singlet and higher S states. If this is the case, the description given by the resonating-valence-bond theory seems to miss certain essential ingredients, at least before doping, because now the lowest state is not even a singlet.

In summary, we have calculated the staggered magnetization and its probability distribution for the 2D AFH model at $T=0$ on a series of finite lattices. From our calculations, it can be concluded that long-range order exists in this model at $T=0$. For the singlet ground state, only the length of the staggered magnetization is meaningful due to the spin rotational invariance. Our result of the mean-square root of the staggered magnetization, 0.25 ± 0.03, is slightly below the experimentally observed $0.6\mu_B$ (Ref. 25) staggered magnetization in La_2CuO_4, which corresponds to 0.27 in our unit (full moment of Cu^{2+} is $1.1\mu_B$). There are, however, two additional effects: charge fluctuation will reduce the long-range order, and a weak third-dimensional coupling reduces the quantum fluctuations in the plane and thus increases the order.

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