Ground-state properties of the two-dimensional antiferromagnetic Heisenberg model

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The ground-state energy, staggered magnetization, and correlation function are computed for the two-dimensional spin-$\frac{1}{2}$ quantum antiferromagnetic Heisenberg model (believed to be relevant to the high-temperature superconducting materials without doping) on lattices up to 24×24 by Monte Carlo methods extrapolated to zero temperature. A more accurate value for the ground-state energy is determined by the method of Neumann and Ulam by extrapolating from lattices up to 12×12.

I. INTRODUCTION

In the past year, a wealth of experimental data has demonstrated the existence of strong antiferromagnetic (AF) correlations in the small doping limit of high-T_c superconducting materials.[1] The most detailed studies exist for La_2CuO_4 single crystals. The copper atoms form planes, and the chemical and magnetic properties are all suggestive of there being a localized spin $\frac{1}{2}$ on each copper. The zero-temperature resistance is infinite unless the material is "doped" (say, by adding strontium) which adds mobile holes to the Cu-O planes and eventually leads to superconductivity.

Neutron scattering measurements are all consistent with a two-dimensional simple square Heisenberg antiferromagnet provided the doping is zero. No order is expected at nonzero temperatures, and the observed three-dimensional ordering is consistent with a weak interlayer exchange which in addition is frustrated.[2] The anisotropy in spin space is very small ($\lesssim 6\times10^{-3}$), and the in-plane correlation length[3] can grow to ~50 lattice constants before three-dimensional (3D) ordering ensues. The zero-temperature moment and the in-plane correlation length are in accord with one's expectations for a 2D Heisenberg model, though the experimental error bars are quite large.

On the purely theoretical side some doubts have been expressed that conventional AF order exists for spin $\frac{1}{2}$ at zero temperature.[4] A rigorous proof of order exists for spin 1 and larger,[5] but similar estimates fail for spin $\frac{1}{2}$ since the zero-point motion is more pronounced. More generally one would like to know whether the spin-$\frac{1}{2}$ Heisenberg model obeys what appears to be the long-wavelength theory for higher spins, namely the nonlinear sigma (NLσ) model.[6] This description is particularly useful in a numerical context since it facilitates the calculation of corrections due to finite size and nonzero temperature. But again spin $\frac{1}{2}$ is furthest from the large-spin limit for which one has an analytically tractable expansion.

Clearly, to settle either question some nontrivial spin-$\frac{1}{2}$ calculation has to be done. The NLσ model cannot be used until it is demonstrated that sufficient local order exists to define the AF order parameter. The most convincing evidence of that would be a Monte Carlo renormalization-group calculation. Almost as good is an evaluation of the magnitude of the staggered magnetization, which for the 12×12 lattice we find to be about 80% of the Néel value. Hence it is reasonable to evaluate finite-size effects using the NLσ model which we do below.

The first numerical evaluation of the staggered order magnetization was done by Oitmaa and Betts[7] for 16 and fewer spins. (In order to go from the z component of staggered magnetization [ω_z in Eq. (18) of this work] to the full staggered magnetization [ω, Eq. (5)], a factor of $\sqrt{3}$ is necessary. With this factor of $\sqrt{3}$ the result of Oitmaa and Betts becomes $\omega=0.84$ in our units, which is significantly higher than the other values collected in Table III.) Recently, Reger and Young[8] have performed a Monte Carlo calculation for the staggered magnetization, essentially the same as the one presented here. Since a number of extrapolations are necessary, we feel it is useful to have two completely independent sets of measurements available so readers can assess for themselves the systematic errors. We also note that Huse[9] has arrived at a similar estimate for the long-range order from series.

We also find the ground-state energy by the method of Neumann and Ulam and find some disagreement with a very recent calculation of Barnes and Swanson.[10] Finally, we examine the correlation function at zero temperature which has not been reported on previously.

II. FINITE-SIZE CORRECTIONS

As noted above, finite-size corrections are most easily evaluated from the NLσ model action, which in imaginary time form reads

$$S=\frac{\rho_0}{2}\int_0^\beta d\tau\int d^2x\left[(\partial_x\mathbf{\Omega})^2+\frac{1}{c_0^2}(\partial_\tau\mathbf{\Omega})^2\right], \tag{1}$$

where ρ_0 and c_0 are, respectively, a bare stiffness constant and spin-wave velocity, and the AF order parameter $\mathbf{\Omega}$ obeys the constraint $\mathbf{\Omega}^2=1$. The Hamiltonian version is

$$\mathcal{H}=\tfrac{1}{2}\int[\rho_0(\partial_x\mathbf{\Omega})^2+\chi_0^{-1}m^2]d^2x\ , \tag{2}$$

where m is a magnetization density and χ_0 the bare susceptibility. The commutators are

$$\begin{aligned}&[\Omega_i(\mathbf{x}),m_j(\mathbf{y})]=i\epsilon^{ijk}\Omega_k(\mathbf{x})\delta^2(\mathbf{x}-\mathbf{y})\ ,\\ &[\Omega_i(\mathbf{x}),\Omega_j(\mathbf{y})]=0\ ,\\ &[m_i(\mathbf{x}),m_j(\mathbf{y})]=i\epsilon^{ijk}m_k(\mathbf{y})\delta^2(\mathbf{x}-\mathbf{y})\ .\end{aligned} \tag{3}$$

$\mathbf{\Omega}(\mathbf{x})$ and $\mathbf{m}(\mathbf{x})$ behave like coordinates and angular momentum on a sphere for each site $\mathbf{x}$. The Lagrangian is recovered by setting $\partial_\tau\mathbf{\Omega}=\mathbf{m}\times\mathbf{\Omega}$ and $c_0^2=\rho_0/\chi_0$, noting that $\mathbf{\Omega}(\mathbf{x})\cdot\mathbf{m}(\mathbf{x})=0$.

The connection between the variables in equation (2) and a lattice spin model[6] is given by summing over some "block" of spins B and setting

$$\mathbf{\Omega}=\frac{1}{\mu_1}\sum_{\mathbf{x}\in B}\epsilon(\mathbf{x})S(\mathbf{x}),\quad \mathbf{m}=\sum_{\mathbf{x}\in B}\mathbf{S}(\mathbf{x})\ , \tag{4}$$

where μ_1 is chosen to correctly normalize $\mathbf{\Omega}$ and scales with N_B, the number of spins in B, $\epsilon(\mathbf{x})=1(-1)$ on the even (odd) sites of the lattice and $\mathbf{S}(\mathbf{x})\cdot\mathbf{S}(\mathbf{x})=s(s+1)$. In appropriate variables,[6] it has been shown that $\rho_0=O(s)$, $c_0^2=O(1)$ for $s\to\infty$ and hence for sufficiently large s the ensemble e^{-S} has long-range order in $\mathbf{\Omega}$, i.e., $\langle\mathbf{\Omega}\rangle\neq0$.

There is, however, a subtle difference between the ground state of a quantum Heisenberg antiferromagnet on a square lattice and the ground state of the Hamiltonian (2) that should be noted. Namely, on any finite lattice, Lieb, Schultz, and Mattis[11] have shown that the Heisenberg ground state is a singlet and hence the expectation value of any vector operator, in particular $\mathbf{\Omega}$, is zero. More generally in any eigenstate $|M\rangle$ of $\int m_i$, the commutators (3) imply $\langle M|\mathbf{\Omega}|M\rangle=0$. The Lagrangian form of the NLσ model, however, is equivalent to a classical model for which there is conventional long-range order. These contrasting statements about $\langle\mathbf{\Omega}\rangle$ can be reconciled by imagining that the lattice ground state involves an average over the direction of $\mathbf{\Omega}$, whose square, all agree is nonzero. We elaborate on this idea below, but for the moment we wish to emphasize an analogy with superfluidity or BCS superconductivity.

There the order parameter is a complex number, whose expectation value in any state with a fixed number of particles is zero by virtue of commutation relations similar to (3).[12] Hence to prepare an ensemble with a nonzero order parameter it is necessary to superimpose states with different numbers of particles. The greater the spread in number, the more accurately can one define the phase of the order parameter.

We now repeat these uncertainty principal arguments for the quantum antiferromagnet. In so doing we will have to include in our ensemble, states above the ground state, and it is of interest to estimate their energy.

To simplify the notation, we make the associations $(1/\mu_2 N)\int\mathbf{\Omega}_i\Longleftrightarrow\mathbf{r}$ and $\int m_i\Longleftrightarrow L_i$, since the commutation relations are the same. We fix μ_2 by imposing $\langle\mathbf{r}^2\rangle=1$. An ensemble with the staggered order along $\hat{\mathbf{z}}$ has the properties

$$\langle x\rangle=\langle y\rangle=0,\quad \langle z\rangle=1-O(1/\Lambda)\ ,$$

and

$$\langle(z-\langle z\rangle)^2\rangle\leq O(1/\Lambda)\ ,$$

where Λ is defined by these equations; it may be as large as N, but can be smaller. Hence by the constraint, $\langle x^2+y^2\rangle\leq O(1/\Lambda)$. The uncertainty relations, e.g., $\langle x^2\rangle\langle L_y^2\rangle\geq\langle z\rangle^2$, imply $\langle L_x^2+L_y^2\rangle\geq O(\Lambda)$. Therefore the components of the magnetization perpendicular to the staggered order must have a spread of $O(\Lambda^{1/2})$, which necessitates superimposing values of the total spin $S=0,1,2,\ldots,O(\Lambda^{1/2})$ in the ensemble in order to achieve the desired order in $\mathbf{\Omega}$. From (2) the energy difference scales as $\sim S^2/(\chi_0 N)$ since the excess magnetization (m) will be $\sim S/N$ and uniformly distributed to minimize the energy.

To proceed further with finite-size effects, we rely on the heuristic idea that a renormalization-group calculation can be done without modification for a finite system until the block size approaches the system size. Hence all the complicated nonlinear interactions in (1) and (2) should do no more than renormalize the coefficients in the linearized long-wavelength theory. These arguments are not wholly trivial and are considered more carefully in Ref. 13. One useful consequence is that the part of the ground-state energy dependent on the total spin is precisely $S(S+1)/(2\chi N)$, where χ is the physical, long-wavelength susceptibility.

On this basis, the finite-size corrections to the total energy can be estimated from spin-wave theory and scale as $N^{-1/2}$, i.e., just the energy of the lowest spin-wave mode in the finite system. The corrections to the total staggered magnetization are somewhat different.

In any spin-singlet state, the staggered long-range order may be calculated from

$$\omega^2=\lim_{N\to\infty}\frac{1}{N^2}\left\langle 0\left|\left[\sum_{\mathbf{x}}\epsilon(\mathbf{x})\mathbf{S}(\mathbf{x})\right]^2\right|0\right\rangle\ . \tag{5}$$

Finite-size corrections to ω^2 follow from the NLσ model correlation function:

$$\delta(\omega^2)\sim\frac{1}{N}\int\langle L(\mathbf{x})L(0)\rangle\ , \tag{6}$$

where $L=\langle\mathbf{\Omega}\rangle\cdot(\mathbf{\Omega}-\langle\mathbf{\Omega}\rangle)$. From (1), $\langle L(\mathbf{x})L(0)\rangle$ is found to go as q^{-2} in momentum space, where q is a $2+1$ dimensional wave number. Fourier transforming back we find at zero temperature $\langle L(\mathbf{x})L(0)\rangle\sim1/x$ for x large, or $\delta(\omega^2)\sim N^{-1/2}$.

A nonzero temperature, of course, is nothing but a finite size in the imaginary time direction. To make the temperature cutoff comparable to the spatial one, the spin-wave scaling $T\sim N^{-1/2}$ should be used since the Lagrangian is isotropic in $\mathbf{x}$ and τ if appropriate units are chosen.

There is one remaining subtlety related to the singlet

character of the antiferromagnetic ground state and the low-lying excited states with higher total spin that were noted above. Although these states are too few to be thermodynamically important, the associated energy gap for large N is less than that for spin waves (N^{-1} rather than $N^{-1/2}$), and they are included in the Monte Carlo calculation since we extrapolate the temperatures to zero as $T \sim N^{-1/2}$.

In any large but finite ordered system, there is a single degree of freedom associated with the order parameter integrated over the entire sample. Typically this may be treated classically and is assigned some fixed direction by breaking the symmetry. The quantum antiferromagnet is more interesting since the order parameter does not commute with a conserved quantity, $\int m$, which one is allowed to control in doing thermodynamics. Let $\mathbf{r}$ be $\int \boldsymbol{\Omega}$ normalized to $\langle \mathbf{r}^2 \rangle = 1$ as before and assume the system is in an eigenstate of total spin S and z component M. Then we conjecture that there is a piece of the density matrix diagonal in $\hat{\mathbf{r}}$ described by a wave function equal to the spherical harmonic $Y_{SM}(\hat{r})$. Therefore, in a correlation function such as $\langle S_z(0) S_z(\mathbf{x}) \rangle$ there is an additive piece proportional to $\int d\hat{\mathbf{r}} |Y_{SM}|^2 z^2$. Changing a single quantum of spin will change the correlation function by a nonzero amount. [Similar conclusions follow from a model in which the spins on each sublattice are combined ferromagnetically into two $O(N)$ spins which are then added to yield the total spin $S \ll N$.] Of course, in any physical system there are small anisotropies which orient $\boldsymbol{\Omega}$ and smear the magnitude of the total spin in the perpendicular directions.

In the present paper we will mostly be concerned with ensembles with $M=0$. Thus the S dependence of $\langle S_z(0) S_z(x) \rangle$ is proportional to

$$\int d\hat{\mathbf{r}}\, z^2 |Y_{SO}|^2 = \frac{2S^2+2S-1}{4S^2+4S-3} ,$$

which is $\frac{1}{3}$ for $S=0$ but larger for $S>0$. Mixing in higher-S states increases the magnitude of z-z correlations. For an unconstrained ensemble with $T \sim N^{-1/2}$ (but $M=0$) thermal fluctuations populate all $S \leq O(N^{1/4})$. Therefore decreasing the temperature increases (makes less negative), $\langle S_z(\mathbf{x}) S_z(\mathbf{x}+\hat{\mathbf{e}}) \rangle$, where $\hat{\mathbf{e}}$ is a unit vector in either the $\hat{\mathbf{x}}$ or $\hat{\mathbf{y}}$ direction. If one incorrectly assumed the total energy was $6\langle S_z(\mathbf{x}) S_z(\mathbf{x}+\hat{\mathbf{e}}) \rangle$, then it would appear that the specific heat was negative. While the extrapolation to $N \to \infty$ can in principle be improved by these ideas, the magnitude of the effect is of order the sampling errors for our data.

Further analysis shows that the renormalized stiffness constant and spin-wave velocity appear in various finite-size correction terms. In a Monte Carlo calculation, however, the statistical error bars preclude their determination this way. Obviously χ can be determined directly from the energy as a function of (magnetic field) H or $\int m^z$, and ρ would follow from the excess energy in a lattice with an odd number of rows or columns.

III. NUMERICAL METHODS AND ALGORITHMIC DETAILS

We want to evaluate expectation values for the 2D spin-$\frac{1}{2}$, quantum, isotropic, antiferromagnetic Heisenberg model:

$$\langle O \rangle = \frac{1}{Z} \mathrm{tr} O e^{-\beta H}, \quad Z = \mathrm{tr} e^{-\beta H} ,$$
$$H = \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j , \tag{7}$$

where β is the inverse temperature, $\mathbf{S}$ is a vector of Pauli matrices, and the summation is over all nearest-neighbor pairs. Note that in our notation the Hamiltonian is dimensionless.

One of the two numerical techniques used in this work is the *quantum Monte Carlo method*.[14,15] The basic idea is to write

$$H = \sum_{i=1}^{r} H_i \tag{8}$$

for the 2D system, where the terms in each of the H_i are chosen to commute among themselves. Since

$$e^{-\beta H} = \lim_{m \to \infty} \left[\prod_{i=1}^{r} e^{-\beta H_i / m} \right]^m , \tag{9}$$

intermediate states can be inserted to obtain

$$Z = \lim_{m \to \infty} \sum_{\alpha} \langle \alpha_1 | e^{-\beta H_1 / m} | \alpha_2 \rangle \times \langle \alpha_2 | e^{-\beta H_2 / m} | \alpha_3 \rangle \cdots \langle \alpha_{rm} | e^{-\beta H_r / m} | \alpha_1 \rangle . \tag{10}$$

There is considerable freedom in the partitioning of H into the H_i. Our choice is to take $r=4$ and partition the pair interactions of H as shown in Fig. 1 for a 4×4 lattice.

The intermediate states α_j can be chosen to correspond to spins up or down on each site and may be considered to be states with differing fictitious times j. In this way the quantum 2D system has been transformed to a classical 3D system. Using the commutivity of the terms in each of the H_i, matrix elements in (10) can each be factorized into a product of four-spin matrix elements which can be easily calculated exactly for each of the 16 possible four-spin configurations (see, for example, Ref. 16). Ten of the 16 four-spin matrix elements turn out to be 0. Thus the great majority of spin configurations have zero weight and must be avoided in any stochastic sampling method. This prevents updating a single spin at a time by Monte Carlo methods, but one can sample the "allowed" configurations by updating several spins simultaneously. To be able to perform all local changes we simultaneously update four cubes of spins stacked in the time direction, involving 16 spins; at least 6 of these 16 spins are unaltered in the updating, however.

This updating is efficiently carried out by storing a look-up table of all of the allowed subconfigurations of 16 spins (of which there are 8192). Along with each

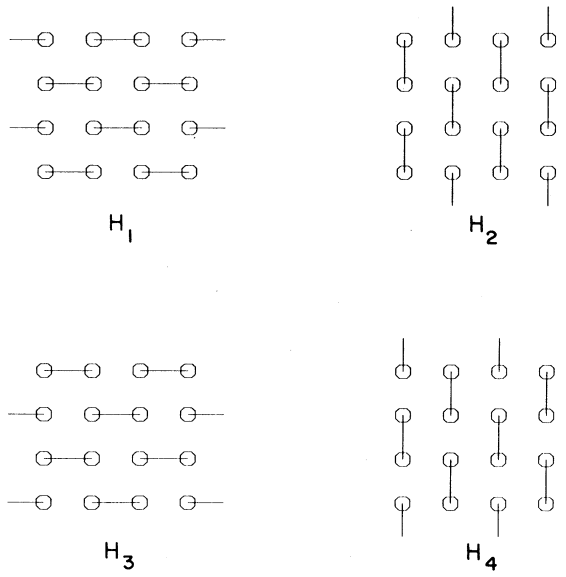

FIG. 1. The pair interactions of the Hamiltonian are partitioned into H_1, H_2, H_3, and H_4 as indicated here for a 4×4 lattice with periodic boundary conditions.

subconfiguration we store all possible subconfiguration updates which are compatible with the spin environment (this number turns out to be 1 or 2) and the Monte Carlo probability for each to be chosen (which depends on β/m). Each 16-spin subconfiguration in the lattice is updated during one "sweep." Typically hundreds of thousands of sweeps are carried out for each value of temperature and lattice size.

This local updating procedure does not sample all the states in (10). First one cannot reach configurations consisting of closed strings of up (or down) spins which wind around one or more times in the spatial directions (we used periodic boundary conditions in both the spatial and temporal directions). In constructing these strings one removes ambiguities by the convention that spins are connected vertically (i.e., in the time direction) rather than diagonally when such a choice exists and never horizontally. Then it is clear that choosing boundary conditions so that the spatial boundary consists only of up spins removes the winding number configurations. Thus they are but a finite-size effect and must disappear as the size of the system goes to ∞. Numerically we find that restricting the winding number to be zero (by starting with it zero and doing only local updating) we obtain results for the energy, staggered magnetization, and correlation function on a 4×4 lattice which agree with the exact results within our $\leq 1\%$ errors (see below), so the effect of winding number configurations can be safely neglected even for small lattices.

The other quantity these local rules preserve is $S_z^{\text{total}} \equiv \sum_{\mathbf{x}} S_z(\mathbf{x})$. While it would be possible to nonlocally flip an entire string of up (or down) spins in the time direction to change S_z^{total}, the Monte Carlo acceptance rate of such a nonlocal update becomes very small as the size in the time direction m goes to ∞. We avoid these updates altogether by recognizing that the ground state of the Heisenberg model is a singlet $S_z^{\text{total}}=0$.[11] Since we are interested in the ground-state behavior of the system we restrict our simulation to that subspace of states and take the temperature, $T\rightarrow 0$. Quite generally, even at finite temperature one expects a canonical and microcanonical ensemble to give identical correlation functions in the thermodynamic limit.

We checked for ergodicity on a $4\times4\times8$ lattice by starting with random-allowed spin configurations with $S_z^{\text{total}}=0$ and performing simulated annealing to try to reach the classical Néel configuration consisting of alternating spins on each time slice. After tens of thousands of such runs it was found that the only configurations which could not be locally updated into the classical Néel state were those with strings of spins winding around the spatial lattice. As discussed above, such configurations are irrelevant in the thermodynamic limit.

The extrapolation to infinite temporal extent m has been examined by several authors.[17] For the quantities measured here, the expectation values have been shown to be even in m and so corrections to the $m\rightarrow\infty$ limit begin at $O(1/m^2)$ (see for example, Fig. 3). Also, for sufficiently large $\beta=1/T$, it has been shown that the expectation values considered here become functions of $(\beta/m)^2$ only, for fixed $L(=N^{1/2})$. So for each size lattice, we fix β to be sufficiently large as to approximate zero temperature, and then take measurements for a variety of small $(\beta/m)^2$ in order to extrapolate $(\beta/m)^2\rightarrow 0$. The extrapolations are carried out by fitting the small $(\beta/m)^2$ data to a quadratic in $(\beta/m)^2$. [For sufficiently large lattices the variation with respect to $(\beta/m)^2$ has been shown to be independent of size.[17] We used this fact to reduce the computational cost for the 24×24 lattice by evaluating expectation values for only one value of $(\beta/m)^2$ and using the $(\beta/m)^2$ extrapolation obtained for the 12×12 lattice to take the $m\rightarrow\infty$ limit.] This then gives the ground-state properties of the finite-size system. Making these measurements on systems of size 4×4 up to 24×24 we then attempt the thermodynamic extrapolation $L\rightarrow\infty$.

For a more accurate estimation of the ground-state energy we used a numerical algorithm, first suggested by Neumann and Ulam,[18] that stochastically implements the direct iteration method to find the dominant eigenvalue of a large matrix T (in our case the negative of the Hamiltonian). It can be considered a simplified version of the Green's function Monte Carlo method,[19] and it has been used in the evaluation of eigenvalues of the transfer matrix of classical spin systems[20] and in the study of the one-dimensional spin-1 Heisenberg antiferromagnet.[21] One starts with a set $S_0=\{|i\rangle\}$ of M_0 elements of a basis and transforms each $|i\rangle$ into m_j copies of the basis element $|j\rangle$ chosen with a probability $P_{i,j}$ in such a way that the following equation

$$m_j P_{i,j} = \langle j|T|i\rangle \tag{11}$$

is true on average. Otherwise the choice of $P_{i,j}$ is largely arbitrary. After this operation, we end up with a set S_1

containing $M_1=\Sigma_j m_j$ basis elements. The process is repeated k times ending up with a set S_k of M_k "*random walkers.*" By appropriately scaling T one can maintain the value of all the M_k close to a target value M. For k and M large, the vector $\sum |i\rangle$, where the sum is over the set S_k, stochastically approximates the highest eigenvector of the system, and the dominant eigenvalue of T, λ, can be obtained by

$$\lambda=\lambda(M)+O\left[\frac{1}{M}\right], \tag{12}$$

where

$$\lambda(M)=\left\langle\frac{M_{k+1}}{M_k}\right\rangle, \tag{13}$$

with the average taken over different values of k.

For the Heisenberg antiferromagnet in the square lattice we used for the basis elements $\{|i\rangle\}$ the standard eigenvectors of the z component of the spin at each point with a trivial phase rotation in one of the sublattices to guarantee that the off-diagonal elements of T in this basis are non-negative. By adding a convenient constant to T, its diagonal elements were also made non-negative. We used values of k up to 10^4–10^5, neglecting the first few hundred values. The bias due to the finite number of random walkers was corrected by calculating $\lambda(M)$ for several values of M and extrapolating it to the limit $M\to\infty$. Typical values of M used in our calculations range from 10^3 to 5×10^4. The form of the transition probability $P_{i,j}$ from the state $|i\rangle$ to the state $|j\rangle$ was taken to be

$$P_{i,j}=\frac{\langle j|T|i\rangle}{\sum_j\langle j|T|i\rangle}. \tag{14}$$

IV. RESULTS

A. The energy

We describe next the results for the energy obtained with the stochastic random-walk method described in Sec. III (Neumann-Ulam method). We used lattices of sizes 4×4, 6×6, 8×8, and 12×12. When this work was almost completed we received a report by Barnes and Swanson[10] that also uses a random-walk approach, although different than the one used in our study, to compute the ground-state energy of the 2D Heisenberg antiferromagnet with lattices up to 8×8 spins. Our results are summarized in Fig. 2 and compared to their reported values with our conventions for the energy in Table I. Both results are very close, but significantly different, and give extrapolated values for the ground-state energy per site in the thermodynamic limit that differ by 1% (seven standard deviations). This is a small difference but it can be of importance in variational studies of the ground state, in which a precise value of the energy is a good indicator as to the accuracy of the variational approximation. To double check our program we computed the exact value of the energy in the 4×4 case to a high degree of accuracy in the sectors with total spin $S=0$ and $S=1$ using the direct iterative power method (see also Ref. 7, where the $S=0$ value is calculated). These results are also quoted in Table I. Our results obtained using the stochastic method for these cases agree within error bars with the exact values. The $S=0$ value quoted by Barnes and Swanson is one of their standard deviations smaller

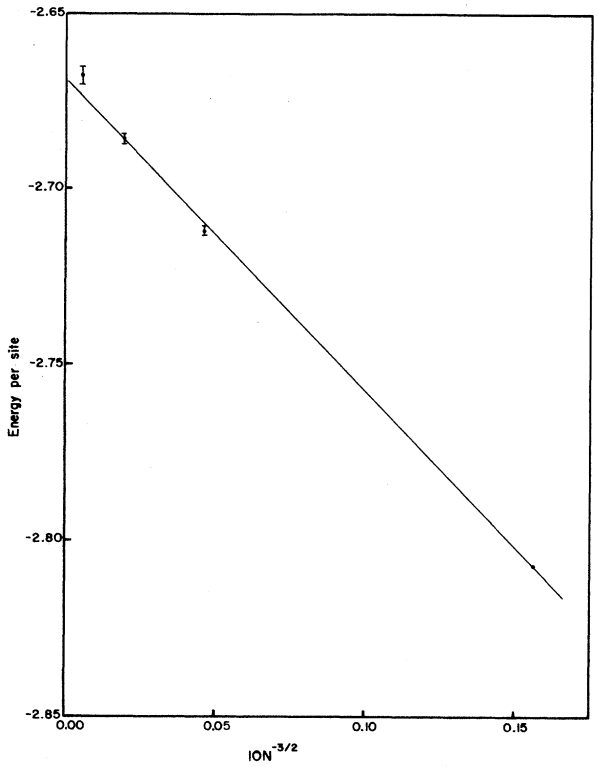

FIG. 2. Neumann-Ulam method measurements of the energy per site as a function of lattice size and a fit to $AN^{-3/2}+B$.

TABLE I. The energy per site as a function of lattice size and total spin S.

Size and sector		Measured values	Ref. 7 values	Exact values
4×4	$S=0$	$-2.807\,10\pm0.000\,34$	-2.810 ± 0.0024	$-2.807\,120\,8$
4×4	$S=1$	$-2.662\,32\pm0.000\,20$	-2.664 ± 0.0008	$-2.662\,471\,2$
6×6	$S=0$	-2.7120 ± 0.0013	-2.726 ± 0.0028	
8×8	$S=0$	-2.6860 ± 0.0015	-2.706 ± 0.0064	
12×12	$S=0$	-2.6680 ± 0.0026		
∞	$S=0$	-2.6689 ± 0.0030	-2.6908 ± 0.0036	

than the exact value, and their $S=1$ value is two standard deviations smaller (see Table I). These discrepancies could be attributed to statistical fluctuations but could also signal a small systematic error in their results. A further study of the energy of the system for states with total spin greater than zero is underway, and it will be reported elsewhere.[22] The corrections to the total energy of the ground state scale extremely well with the size of the system as $1/L$, as explained in Sec. II, even for the 4×4 lattice. Fitting our data to a function of this form we obtain an extrapolated value for the ground-state energy per site in the thermodynamic limit of

$$E_0=-2.669\pm0.003\ , \tag{15}$$

where the error is only due to the statistical errors of the fit, and no attempt has been made to include higher-order corrections to the scaling law. This is to be compared with a recent variational calculation by Huse and Elser[23] of -2.6552, which is only 0.5% higher. The coefficient of the $N^{-3/2}$ term in Fig. 2 was -8.85.

The energy was also measured by the quantum Monte Carlo method described in Sec. III. The results are much less accurate than are obtained using Neumann-Ulam, but serve as a crude check on both methods. We measured $\langle S_z(\mathbf{x})S_z(\mathbf{x}+\hat{\mathbf{e}})\rangle$, where $\hat{\mathbf{e}}$ is a unit vector in either the $\hat{\mathbf{x}}$ or $\hat{\mathbf{y}}$ direction, and used the fact that the ground state is rotationally invariant (Sec. II) which implies

$$E_0=6\lim_{\beta\to\infty}\langle S_z(\mathbf{x})S_z(\mathbf{x}+\hat{\mathbf{e}})\rangle\ . \tag{16}$$

First the $L=4$ (4×4 lattice) measurements were carried out for various β and $(\beta/m)^2$ as shown in Fig. 3. Note the saturation to a universal function of $(\beta/m)^2$ as $\beta\to\infty$ (Sec. III). The $(\beta/m)^2\to0$ extrapolation was then carried out as discussed in Sec. III, resulting in Fig. 4 for the dependence of $\langle S_z(\mathbf{x})S_z(\mathbf{x}+\hat{\mathbf{e}})\rangle$ on β. The errors shown are statistical only. It is clear that within those errors this method agrees with the exact result for $\beta\to\infty$ (see Table I) with no evidence of any contribution from the "winding number configurations" discussed in Sec. III. The estimator for E_0 plotted in Fig. 4 increases with decreasing temperature and continues to do so for larger L. This may be attributed to the lack of explicit rotational symmetry in our numerical scheme and the admixture of higher total-S states discussed at the end of Sec. II.

On larger lattices we worked at fixed $\beta=2L$ (see Sec. II) and obtained the results shown in Fig. 5 with E_0 approximated by $6\langle S_z(\mathbf{x})S_z(\mathbf{x}+\hat{\mathbf{e}})\rangle$ at $\beta=2L$. The error bars exhibited here are also statistical only. There are also systematic errors, e.g., in ignoring terms higher order in $(\beta/m)^2$ in taking the $m\to\infty$ limit, which appear to be of the same order as the statistical errors. But the largest error here is seen to be due to working at $\beta=2L$ rather than infinity (recall Fig. 4). This appears to give an ~2–3 % error which looms large in Fig. 5 because of the meager size dependence of the energy and the much greater accuracy of the Neumann-Ulam data.

B. The staggered magnetization

The ground-state staggered magnetization ω may be defined by

$$\omega^2=\lim_{N\to\infty}\frac{1}{N^2}\left\langle 0\left|\left[\sum_{\mathbf{x}}\epsilon(\mathbf{x})\mathbf{S}(\mathbf{x})\right]^2\right|0\right\rangle\ , \tag{17}$$

where ϵ was defined in Sec. II. By rotational invariance of the ground state we may also obtain ω by the thermo-

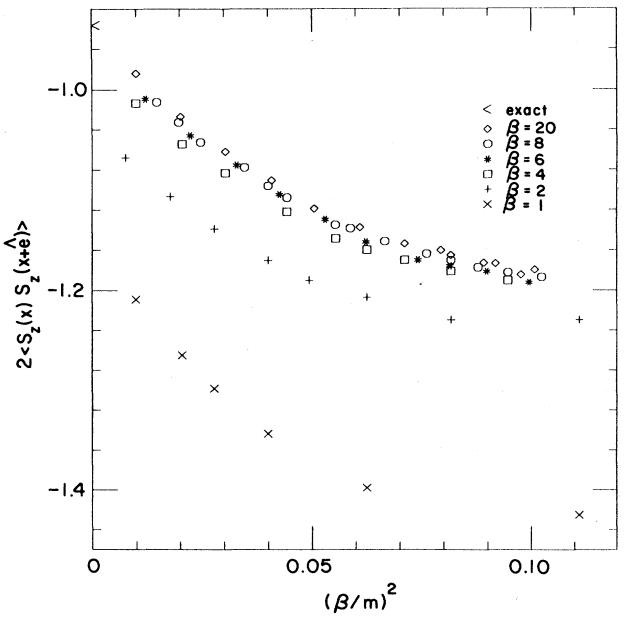

FIG. 3. Measurements of $2\langle S_z(\mathbf{x})S_z(\mathbf{x}+\hat{\mathbf{e}})\rangle$ for a 4×4 lattice with various values of temperature and temporal lattice size (m). Statistical errors are of order the size of the symbols.

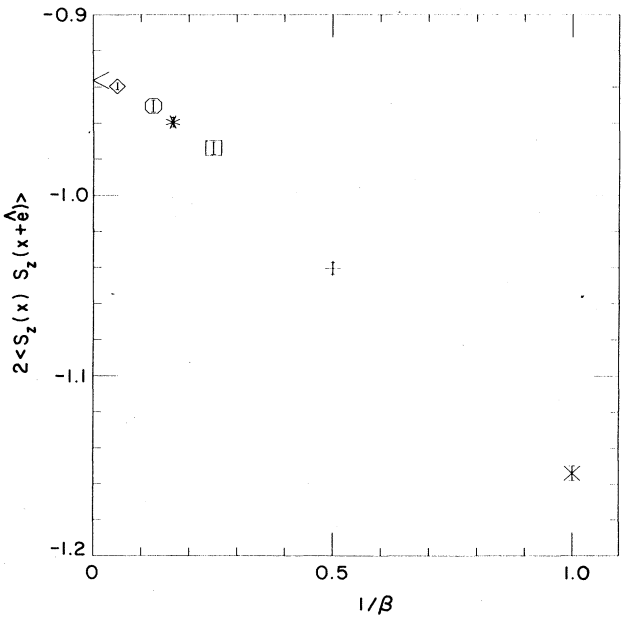

FIG. 4. The temperature dependence of $2\langle S_z(\mathbf{x})S_z(\mathbf{x}+\hat{\mathbf{e}})\rangle$ for a 4×4 lattice obtained by extrapolation of Fig. 3 to infinite m.

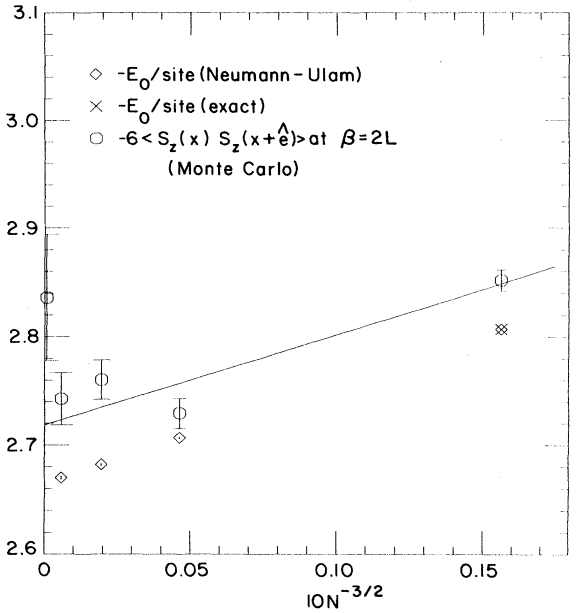

FIG. 5. Lattice size dependence of an approximation to the energy per site, $6\langle S_z(\mathbf{x})S_z(\mathbf{x}+\hat{\mathbf{e}})\rangle$ at $\beta=2L$, compared to the Neumann-Ulam measurements of the energy per site shown in Fig. 2. The line is a fit which does not include the $L=24$ data point (see text) and disagrees with the Neumann-Ulam measurements because of finite temperature effects.

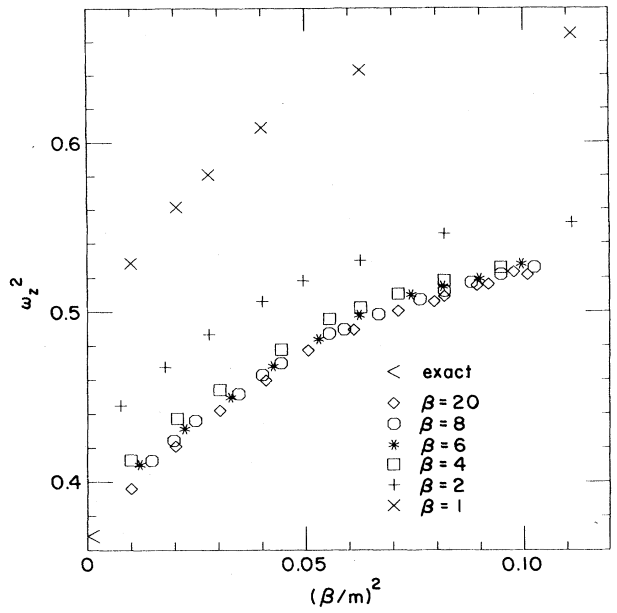

FIG. 6. Measurements of ω_z^2 for a 4×4 lattice with various values of temperature and m. Statistical errors are of order the size of the symbols.

dynamic limit of

$$\omega_z^2 \equiv \frac{1}{N^2}\left\langle 0 \left| \left[\sum_{\mathbf{x}} \epsilon(\mathbf{x}) S_z(\mathbf{x}) \right]^2 \right| 0 \right\rangle \rightarrow \frac{\omega^2}{3} \quad \text{as } L\rightarrow\infty \ . \tag{18}$$

If $\omega\neq0$, then only the long-distance part of the correlation function contributes to (18), so in either case we can also obtain ω via the correlation function half way across and half way diagonally across the lattice:

$$C_{L/2} = \frac{1}{L^2}\sum_{x,y} |\langle 0|S_z(x,y)S_z(x,y+L/2)|0\rangle| \rightarrow \frac{\omega^2}{3} \quad \text{as } L\rightarrow\infty \tag{19}$$

(where L is assumed even) and

$$C_{L/2,L/2} = \frac{1}{L^2}\sum_{x,y} \langle 0|S_z(x,y)S_z(x+L/2,y+L/2)|0\rangle \rightarrow \frac{\omega^2}{3} \quad \text{as } L\rightarrow\infty \ . \tag{20}$$

We measured ω by all of Eqs. (18), (19), and (20).

In Fig. 6 we show ω_z^2 for a 4×4 lattice for various β and $(\beta/m)^2$. After extrapolating to $(\beta/m)^2=0$, Fig. 7 is obtained. Within (statistical) errors we obtain the exact value of (18) for $L=4$, $\beta\rightarrow\infty$ (Ref. 7) (we have calculated this by use of direct iterative power method to be 0.368 702 848 151 0). On larger lattices we again worked at fixed $\beta=2L$. A sample plot is shown in Fig. 8 for $L=8$. For this size lattice, the values for $\beta=16$ should be within $O(0.01)$ of the infinite-β limit.

The same analysis was carried out in evaluating $C_{L/2}$ and $C_{L/2,L/2}$. The final results are summarized in Fig. 9. All the errors are statistical only, except for the 24×24 data in which the errors shown are 1.5 times statistical (see Sec. III). We extrapolated each data set linearly in

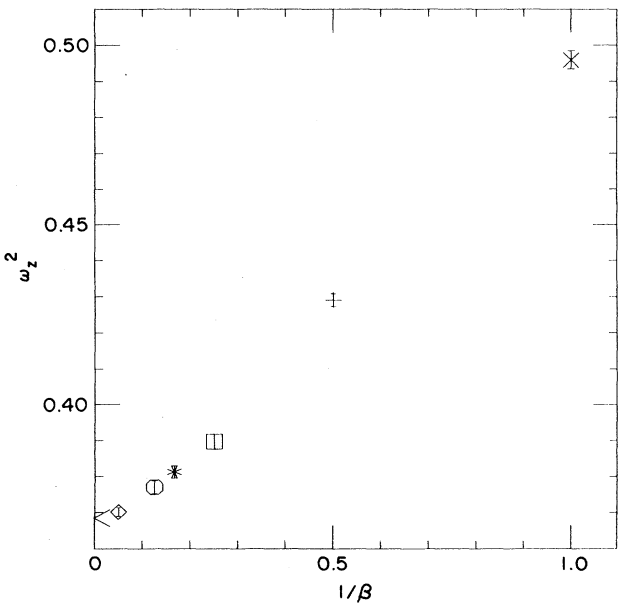

FIG. 7. The temperature dependence of ω_z^2 for a 4×4 lattice obtained by extrapolation of Fig. 6 to infinite m.

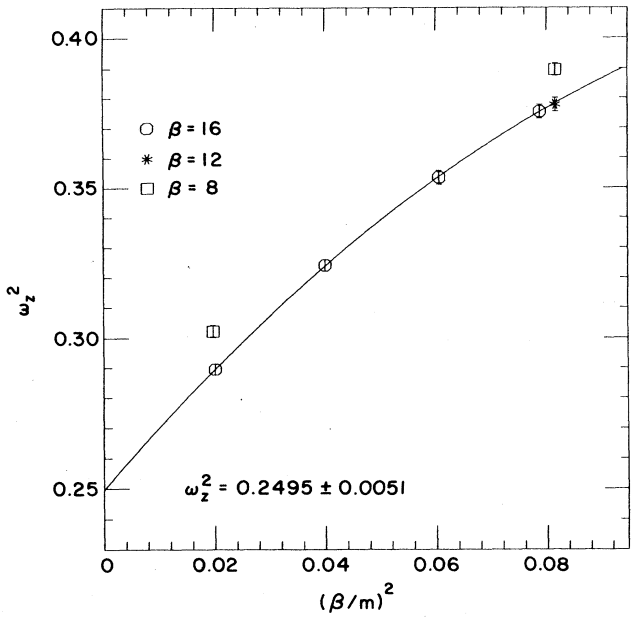

FIG. 8. ω_z^2 on a 8×8 lattice. The fit of the $\beta=16$ data is of the form $A+B(\beta/m)^2+C(\beta/m)^4$.

$1/L$ to estimate the thermodynamic limits, but did not include the $L=24$ data in the fit because of the problem of the thermally excited higher-total-spin states discussed at the end of Sec. II. Since we have the singlet-triplet spacings explicitly for a number of different N from the stochastic iteration method, we find

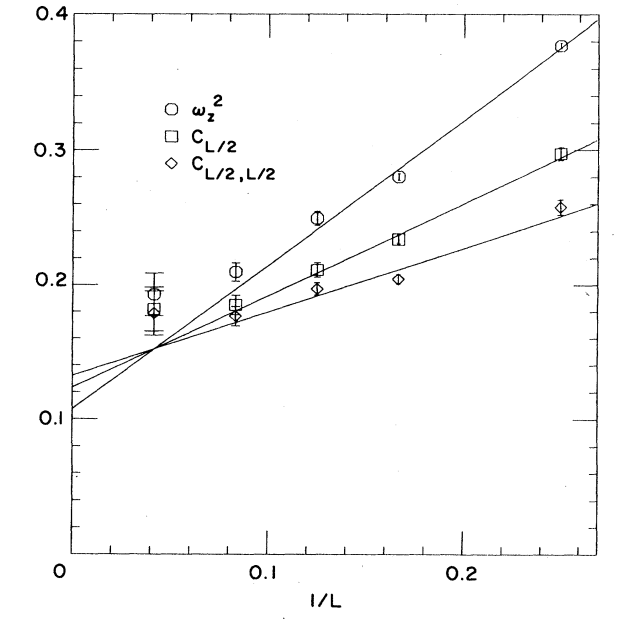

FIG. 9. Lattice size dependence of ω_z^2, $C_{L/2}$, and $C_{L/2,L/2}$ linearly extrapolated in $1/L$ to the thermodynamic limit. The $L=24$ data was not used in the extrapolation because of the contribution of the thermally excited higher-spin states discussed in Sec. II.

TABLE II. Our Monte Carlo values of ω_z^2, $C_{L/2}$, and $C_{L/2,L/2}$ compared to those of Reger and Young (Ref. 8). Finite-temperature corrections were subtracted from the values obtained in Fig. 9 as described in the text. Combined statistical and systematic errors are around the 20% level for each quantity.

Quantity ($L\to\infty$)	This work	Ref. 8
ω_z^2	0.099	0.118
$C_{L/2}$	0.111	
$C_{L/2,L/2}$	0.114	0.124

$$\exp\{\beta[E_0(S=1)-E_0(S=0)]\}\lesssim O(1)$$

for $L\leq 8$ and $\beta=2L$. Hence we expect a flattening of the curve around $L=12$ as is observed. A crude attempt was made to eliminate the finite-temperature effects by using the $\beta=\infty$ numbers for 4×4 to shift all the points, i.e., by adding to the $L\to\infty$ limit of each measured quantity $Q=\omega_z^2$, $C_{L/2}$, and $C_{L/2,L/2}$, the amount

$$[Q(L=4,\beta=\infty)-Q(L=4,\beta=2L)]\ .$$

This shift is comparable to what one would have inferred from Fig. 8 for 8×8. The larger values of N are systematically high due to the inclusion of $S\geq1$ states. The results are given in Table II (in our convention) and compared to other Monte Carlo results of Reger and Young.[8] Our combined statistical and systematic errors for each of the three quantities are estimated to be about the 20% level, similar to the errors quoted in Ref. 8.

It should be pointed out that the agreement between the two sets of Monte Carlo results occurred despite several significant differences between our calculation and

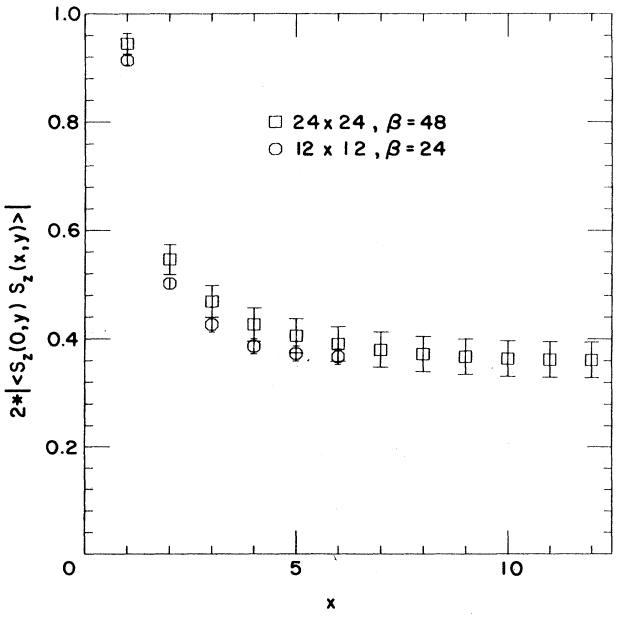

FIG. 10. Correlation function along a lattice axis on 12×12 and 24×24 lattices.

TABLE III. Our value for the ground-state staggered magnetization ω compared to previous estimates.

Quantity	This work	Ref. 8	Ref. 24	Ref. 9	Ref. 23
ω	0.57±0.05	0.60±0.04	0.606	0.626	0.71

that of Reger and Young. In particular, they went to smaller $(\beta/m)^2$ and extrapolated linearly (two parameters) in that quantity rather than quadratically (three parameters) as we did. They partitioned the Hamiltonian into $r=2$ pieces [see Eq. (8)] rather than our $r=4$. We worked at a lower temperature for the largest systems. They ran with only one value of m for their largest system: $L=12$; we used four values. Their thermodynamic extrapolations of ω_z^2 and $C_{L/2,L/2}$ versus $1/L$ included quadratic terms; ours were only linear.

Averaging our measurements for the quantities ω_z^2, $C_{L/2}$, $C_{L/2,L/2}$, each of which approximates $\omega^2/3$, we obtain an estimate for ω: $\omega=0.57\pm0.05$. This is compared in Table III to the Monte Carlo result of Reger and Young, spin-wave results,[24] a reanalyzed perturbative expansion away from the Ising limit,[9] and the variational calculation of Huse and Elser.[23]

C. The correlation function

Although the correlation function at finite temperature has been previously measured,[25] there have been no reports of it at zero temperature. We measured the correlation function along the x axis for the various size lattices. For $L=12$ and $L=24$ the situation is as shown in Fig. 10. The error bars for the $L=12$ lattice are statistical only; those for the $L=24$ lattice are 1.5 times statistical. The $m\to\infty$ limit of the $L=24$ data was obtained by using $L=12$ finite-m correction (see Sec. III) for the corresponding x. For $x>6$ and $L=24$ we simply used the $x=6$, $L=12$ shift since the correction is nearly constant beyond $x=3$. It is seen that the correlation function quickly approaches the asymptotic limit given by the staggered magnetization.

V. SUMMARY

In this paper we have presented results for the ground-state values of the energy, staggered magnetization, and correlation function for the quantum antiferromagnetic Heisenberg model. The energy value is determined to 0.1% accuracy and disagrees with a previous measurement.[10] The staggered magnetization is about 11 standard deviations above zero and is in agreement with previous measurements (see Table III). The correlation function is seen to approach its asymptotic value within a few lattice spacings.

The finite-size corrections deduced from the NLσ model are consistent with observations, particularly for the energy in Fig. 2. The energy of the higher total-spin states is also in accord with our expectations and will be discussed in Ref. 22. Some indication of the bias incurred by mixing in states with total $M>0$, noted at the end of Sec. II, was apparent in Fig. 9. Subtle topological corrections to (2) have been proposed in Ref. 26 which could be missed in a numerical simulation.

Noted added in proof. A very recent Monte Carlo calculation by Reger, Riera, and Young[27] obtained $E_0=-2.680\pm0.002$ in marginal agreement with our value. We thank Peter Young for communicating that value to us in advance of publication.

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