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Ground-state and low-lying excitations of the Heisenberg antiferromagnet

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Monte Carlo methods are used to determine the exact ground-state energy of the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on two-dimensional square periodic lattices up to size 32×32. The extrapolated ground-state energy for infinite lattice size is -0.33459 ± 0.00005. In addition, splittings between the ground state and the lowest spin-1 and -2 excitations are determined as a function of lattice size. The scaling of both the ground-state energy and the gap are in agreement with that predicted by spin-wave theory over a wide range of lattice sizes. In particular, numerical results demonstrate convincingly the lack of a gap for infinite systems, and that the gap for finite systems scales with the inverse volume of the lattice. Finally, we present results for the ground-state spin-correlation function. Our approximate results for larger lattices indicate that the staggered magnetization is 0.34 ± 0.01 in units where the saturated value is $\frac{1}{2}$.

I. INTRODUCTION

The two-dimensional Heisenberg antiferromagnet is the subject of much current theoretical interest, and many analytical and numerical studies have examined its low-temperature properties. We have employed a method closely related to Green's-function Monte Carlo[1] (GFMC) to determine the low-energy states of this Hamiltonian. GFMC and related methods have proven to be very successful in determining ground-state properties of a wide variety of quantum many-body systems, including solid and liquid helium,[2,3] one-dimensional Hubbard models,[4] and atomic and molecular[5] systems.

We have used GFMC to study the ground state on relatively large lattices, obtaining the exact ground-state energy of lattices from size 4×4 to 32×32. In addition to this $S=0$ ground state, the lowest-energy spin-1 and -2 excitations can be determined by calculating the ground states in the $S_z=1$ and 2 sectors. These energies are obtained as a function of lattice size in order to compare with scaling predictions of spin wave and other analytic theories.

Finally, we present results for the spin-correlation function for a variety of lattice sizes. Results for the spin-correlation function are not exact, as they are based upon a linear extrapolation from variational results. The necessity and accuracy of this extrapolation are discussed below. Our results, however, do indicate the possibility that larger lattices are necessary for an accurate extrapolation to infinite volume, and that the staggered magnetization is somewhat larger than previously believed.

II. METHOD

Green's-function Monte Carlo methods solve for the ground state by iterating the equation

$$\{\Psi_T\Psi^{n+1}\}=[\Psi_T F(H)\Psi_T^{-1}]\{\Psi_T\Psi^n\}\,. \tag{1}$$

$F(H)$ can be any function of the Hamiltonian which projects out the ground state, Ψ_T is a trial or importance function which is used to guide the random walk, and Ψ is the true ground-state wave function. For the Heisenberg antiferromagnet, $H=\sum_{\langle i,j\rangle}\mathbf{s}_i\cdot\mathbf{s}_j$, with the sum running over all nearest-neighbor pairs.

The wave function for the Heisenberg antiferromagnet may be written in the basis of definite third components of spin on each lattice site: $\Psi=\sum A[\sigma_i^z]\otimes\chi[\sigma_i^z]$, where A represents the amplitude for a particular spin configuration χ, and the sum runs over all possible spin configurations. For the ground state, only terms with an equal number of up and down spins contribute, and Marshall[6] has shown that the amplitude A has a positive or negative sign, respectively, if there are an even or odd number of up spins on one of the sublattices.

It is trivial to show that if we absorb this sign into the definition of the basis χ, the operator $-(\sigma_i^x\sigma_j^x+\sigma_i^y\sigma_j^y)$ has purely positive off-diagonal matrix elements between different states on the lattice. It is possible to absorb the signs in this way only for a bipartite lattice, and here we limit ourselves to square lattices. A variety of evolution operators $F(H)$ project out the ground state, including $F(H)=1-tH$ for a small time step t. This choice of F avoids any time step error, since the Hamiltonian enters only linearly. We have chosen to use an approximate evolution operator which has a finite, but small, time-step error

$$F(H)=\mathcal{S}\prod_{\langle i,j\rangle}\exp(-\Delta\tau\mathbf{s}_i\cdot\mathbf{s}_j)\,, \tag{2}$$

where $\mathcal{S}$ indicates a symmetrization over all orderings of noncommuting spin pairs. This propagator allows one to perform an explicit sum over all nearest-neighbor pairs, which may limit the statistical errors associated with the branching of the population. In addition, it may be useful for "forward walking" or "shadow" wave functions, which can, in principle, be used to obtain exact results for all expectation values. This evolution operator differs from the true $\exp(-H\Delta\tau)$ by terms of third order in $\Delta\tau$, which produce very small finite time-step errors, as is demonstrated in Sec. III.

We begin with a set of spin configurations drawn from the square of a trial wave function. We then iterate Eq.

(1), diagonalizing the operator $\mathbf{s}_i \cdot \mathbf{s}_j$ and sampling the new spin configuration s' from the original configuration s and the importance transformed kernel $\Psi_T(s') \times \exp(-\Delta\tau \mathbf{s}_i \cdot \mathbf{s}_j)\Psi_T^{-1}(s)$. Weights are introduced as required, and branching techniques employed to retain a finite variance for large total propagation times τ. The procedure is repeated as necessary to ensure convergence to the ground state. The energy can be obtained from a mixed estimate E_{mix},

$$E_{\text{mix}} = \langle \Psi | H | \Psi_T \rangle / \langle \Psi | \Psi_T \rangle , \tag{3}$$

or a growth estimate E_{gr},

$$\exp(-\Delta\tau E_{\text{gr}}) = \langle \Psi^{n+1} | \Psi_T \rangle / \langle \Psi^n | \Psi_T \rangle . \tag{4}$$

In order to obtain accurate results, it is important to choose a good trial function Ψ_T. In addition to its direct value in minimizing the variance of the mixed estimate, an accurate trial function will greatly reduce the population fluctuations. We use the wave function given by Huse and Elser in Ref. 7:

$$A[\sigma_i^z] = \prod_{i<j} \exp[-u(r_{ij}) s_i^z s_j^z] , \tag{5}$$

where $u(r_{ij}) = u_1$ for i,j nearest neighbors, and k/r_{ij}^l otherwise. The variational parameters are u_1, k, and l. This wave function has the advantage of simplicity and accuracy, yielding a variational ground-state energy of $-0.3319(1)$. A disadvantage of this trial function, however, is that it is not an eigenstate of the total spin S. In particular, the expectation value of $\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y$ shows long-range order, but $\sigma_i^z \sigma_j^z$ does not. This property may limit the accuracy of results for quantities other than the energy, especially for the spin-correlation function.

Ground-state expectation values other than the energy are extrapolated from the variational and mixed estimates $\langle \Psi | O | \Psi \rangle \approx 2\langle \Psi_T | O | \Psi \rangle - \langle \Psi_T | O | \Psi_T \rangle$. This extrapolation is accurate to first order in the difference between the trial and exact wave functions. Other techniques, such as forward walking, are available to estimate these quantities, but are subject to a comparatively large statistical error.

III. RESULTS

Figure 1 plots the results obtained for the ground-state energy per bond for lattices from size 4×4 to 32×32. It is possible to determine the 4×4 ground-state energy without resorting to stochastic algorithms, and we have used the eigenvalue (-0.35089) (Refs. 8 and 9) to check our method. In Fig. 1, the energies are plotted versus $(10/L)^3$, where L is the length of one side of the lattice. Spin-wave theories (and related arguments[10]) predict a finite-size scaling of this type.

Our results for the ground-state energy confirm this scaling, with no statistically significant deviations from 32×32 down to 4×4 lattices, an extremely small system. The straight line in Fig. 1 is a fit to all of the energies of the form $E(L) = E(\infty) + c/L^3$, with the infinite volume limit $E(\infty)$ being -0.33459, and the linear term

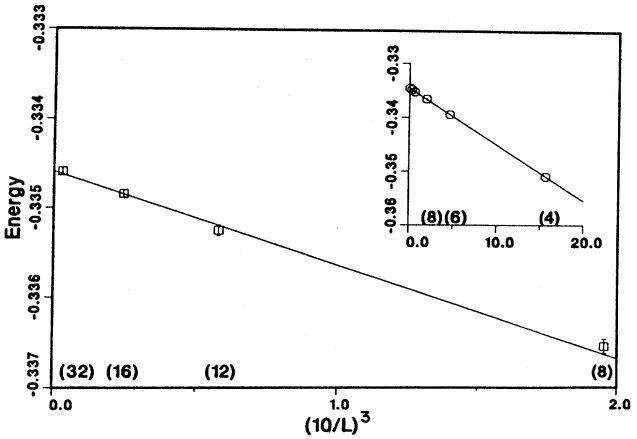

FIG. 1. Ground-state energy vs $(10/L)^3$ for $L\times L$ lattices. The line is a linear fit to the results of the numerical simulations, which are indicated by points with error bars. The inset shows results on small lattices, larger lattices are also indicated in the main figure.

$c = -1.043$. This value of c corresponds to a spin-wave velocity of 1.45 according to the analysis of Neuberger and Ziman,[10] with an uncertainty of approximately 7%.

In order to determine the errors associated with these results, we must examine the finite time-step error as well as the statistical error. The latter alone is indicated in Fig. 1, but the time-step error may be examined by using larger time steps $\Delta\tau$. For the 32×32 lattice, the resulting ground-state energies are shown in Table I. The leading error in the kernel is of order $\Delta\tau^3$, corresponding to an error of order $\Delta\tau^2$ in the ground-state energy. Equating our propagator to the exponential of an approximate Hamiltonian and evaluating the anticommutators in the propagator to third order in $\Delta\tau$, one obtains

$$\tilde{H} = H + (\Delta\tau^2/48)(12\langle \mathbf{s}_i \cdot \mathbf{s}_j \rangle_{\text{NN}} - 8\langle \mathbf{s}_i \cdot \mathbf{s}_j \rangle_D - 4\langle \mathbf{s}_i \cdot \mathbf{s}_j \rangle_L) . \tag{6}$$

The first term in angular brackets is the nearest-neighbor correlation, and D and L stand for diagonal and linear sites connected by two links, respectively.

Table I presents the growth and mixed estimates for the ground-state energy on a 32×32 lattice as a function of the time step $\Delta\tau$. The finite time-step error may be examined by looking at the difference between the mixed estimate and the sum of the growth energy plus a perturbative estimate of $\langle H - \tilde{H} \rangle$. Measuring the spin-correlation function, we have calculated a perturbative contribution of 0.00033(1) for $\Delta\tau = 0.05$. Adding this result to the growth estimate produces the best growth approximation

TABLE I. Time-step dependence.

$\Delta\tau$	E_{mix}	E_{gr}	$E_{\text{gr}} + \langle H - \tilde{H} \rangle$
0.05	−0.33459(2)	−0.33490(2)	−0.33457(3)
0.10	−0.33458(3)	−0.33580(3)	−0.33448(5)
0.20	−0.33434(8)	−0.33869(11)	−0.33341(20)

to the energy, given in the last column of Table I.

A more accurate extrapolation can be obtained from the mixed estimate alone. It is apparent from the first column of Table I that the statistical errors are larger than the finite time-step errors in this simulation. Combining the uncertainty of the extrapolation with the statistical errors, we obtain $E(\infty) = -0.33459 \pm 0.00005$. Recent resonating-valence-bond (RVB) variational calculations[11] give an upper bound of -0.3344 for trial functions which incorporate long-range bonds.

The results for the energy gap as a function of lattice size are shown in Fig. 2. The total energy difference between the lowest spin-1 or spin-2 state and the ground state is expected to scale inversely with the lattice size L^2. Our results support this conclusion; in particular, the fact that there is no gap for infinite lattices. The scaling does not seem to extend to very small lattice sizes, however, as the spin-1 4×4 state shows significant deviations from scaling. The gaps obtained in these simulations range from 0 to 0.6 while the total energies range from -11 to approximately -170.

Finally, we present results for the spin-correlation function in Figs. 3 and 4. Figure 3 shows the variational and GFMC results for the 16×16 and 32×32 lattices, demonstrating the reduction in correlation obtained with GFMC. The diagonal and on-axis correlations at $L/2$ are nearly identical on the 32×32 lattice. Figure 4 recasts these results as a function of $1/L$; the correlation functions at $L/2$ for a variety of lattice sizes are indicated by open symbols and the results on the 32×32 lattice by closed symbols. The results on the 32×32 lattice are in good agreement with the predicted[10,12] linear extrapolation in $1/L$. The results for the correlation at $L/2$ as a function of lattice size seem to imply that the scaling region is not reached until $L \sim 16$, however. This is consistent with a conjecture by Huse[12] that lattices with more than 100 sites are necessary for accurate extrapolations.

Our results for the diagonal $(L/2, L/2)$ correlation on smaller (8×8 and 12×12) lattices appear to be statistically consistent with those of Reger and Young.[13] However,

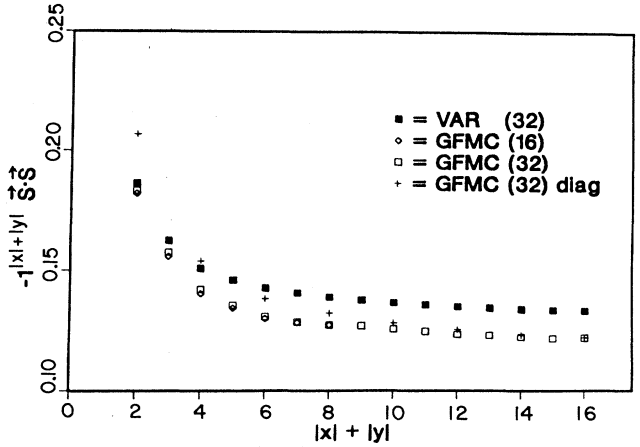

FIG. 3. The staggered spin-correlation function $-1^{|x|+|y|}\mathbf{s}_i \cdot \mathbf{s}_j$. Both variational and extrapolated GFMC results (see text) are shown for two lattice sizes. Unless otherwise indicated, the displacement direction is along the x or y axis.

our results for larger lattices imply an infinite volume limit of 0.117(5) for the spin-correlation function at large distance, while their extrapolation yields approximately 0.09. The difference may result from the fact that we have disregarded any results on small lattices ($L \leq 8$) in our extrapolation.

This value of the long-range correlation implies a staggered magnetization of 0.34(1), somewhat larger than previous numerical work[13] and results of spin-wave theory and other analytical estimates,[12] which predict a value in the range of 0.30 to 0.31. Some of this discrepancy could be due to our extrapolation method, but the best RBV variational results[11] also predict a higher magnetization, ~ 0.33. One could hope to obtain more reliable results for the correlation function by employing forward-walking techniques, which attempt to evaluate an expectation value through

$$\langle \Psi | O | \Psi \rangle = \langle \Psi_T | \exp(-H\tau) O | \Psi \rangle / \langle \Psi_T | \exp(-H\tau) | \Psi \rangle .$$

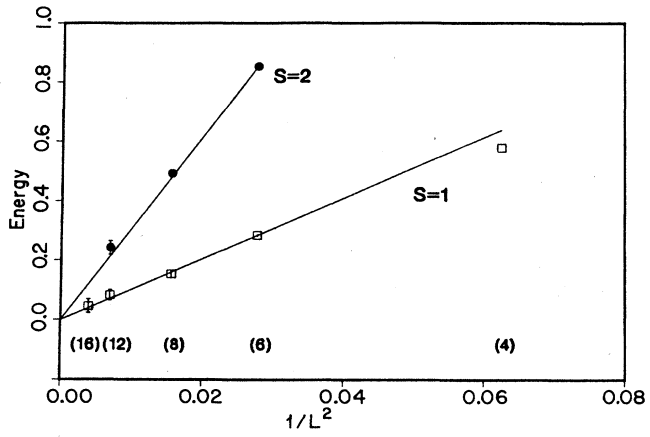

FIG. 2. The energy gap as a function of $1/L^2$ for spin-1 and spin-2 states. The open squares and solid circles give the simulation results for the spin-1 and spin-2 excitation energies, respectively. The solid lines are linear fits to the $L = 6$ points.

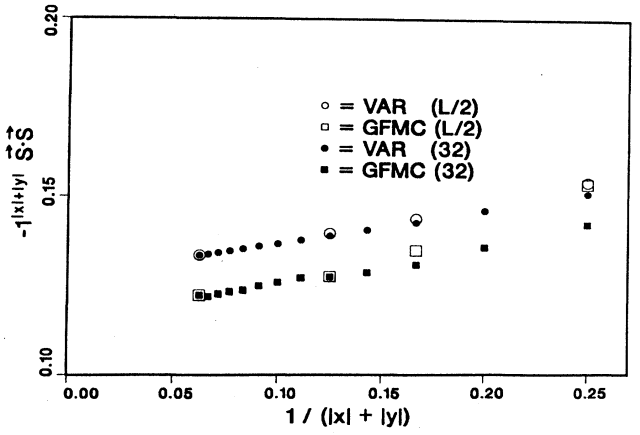

FIG. 4. The staggered spin-correlation function vs the inverse of the displacement along one axis. Open symbols indicate the results at a displacement of $L/2$ for various L, while solid symbols present results for the 32×32 lattice.

Experiments with small lattices indicate that the statistical errors are quite large, however.

In summary, we have been able to obtain very accurate energy expectation values for the low-lying states of the Heisenberg antiferromagnet on large lattices. These results offer dramatic evidence of the accuracy of the scaling predictions of spin-wave theories and other analytic theories. Our results also suggest the necessity of looking at large lattice sizes in order to accurately determine the infinite volume limit of the spin-correlation function.

Note added in proof. Manousakis (private communication) has recently obtained a variational wave function with more accurate long-range correlations, which should allow more reliable determinations of the staggered magnetization.

ACKNOWLEDGMENTS

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