Two-dimensional Heisenberg antiferromagnet: A numerical study

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We describe a numerical simulation of the isotropic spin-$\frac{1}{2}$ Heisenberg antiferromagnet on square lattices of size 4×4, 6×6, and 8×8. A Hamiltonian Monte Carlo method is used to measure the energies of the lowest-lying singlet and triplet states, and we extrapolate these results to give estimates of the properties of large antiferromagnets. Our result for the ground-state energy per spin is $E_0/N^2=-0.672\pm0.001$ for an infinite system. Within our statistical accuracy, the singlet-triplet gap behaves as $E_1-E_0\approx 2.1/N$, which implies that the infinite system is gapless.

I. INTRODUCTION

It is widely believed that high-temperature superconductivity in the new ceramic materials[1] arises from the properties of holes in two-dimensional spin lattices, for example, in planes of hybridized Cu^{2+} ions in La_2CuO_4.[2] Various proposals have appeared in the literature for the detailed mechanism underlying the superconductivity. These include the existence of a resonating-valence-bond (RVB) ground state and Bose condensates advocated by Anderson and co-workers[2,3] and Kivelson and co-workers,[4] a related RVB spin-liquid droplet model due to Lee, Zhang, and Chang,[5] a spin-bag charge carrier consisting of bound-hole pairs suggested by Schrieffer,[6] electron-electron binding due to hole-electron interactions suggested by Chi and Nagi,[7] and others which have been reviewed in the literature.[8] These proposals are usually substantiated by approximate solutions of the two-dimensional Hubbard model or the closely related Heisenberg model with a hopping term, as these are believed to provide a good description of the physics of electrons and holes in the superconductors. Each of these mechanisms is plausible *a priori* as one need only incorporate antiferromagnetic ordering[9] and the essential presence of holes[10] to insure qualitative agreement with experimental results reported for La_2CuO_4.

In principle one can test these proposals in the context of the Hubbard and Heisenberg models by carrying out numerical simulations. Unfortunately, this approach is limited by the difficulty of accurately simulating large spin systems. High-accuracy studies using direct diagonalization methods (the Lanczos algorithm in particular) have at present attained limits of 24 spins for the one-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet[11] and 27 spins[12] for the two-dimensional system on a triangular lattice. As the superconductivity appears with a fractional hole doping of only a few percent,[10,13] it is probably necessary to study systems having ~100 spins in order to resolve the relevant effects as a function of doping. This is a much larger system than can be studied at present using direct diagonalization of the Hamiltonian, which has storage requirements that increase exponentially with the number of degrees of freedom.

For the numerical study of large spin systems one must presumably employ a stochastic "Monte Carlo" algorithm; Hamiltonian methods of this type have previously been applied to one-dimensional Heisenberg antiferromagnetic chains of up to 48 spins for spin-$\frac{1}{2}$ (Ref. 14) and 32 spins for spin-1.[15] With a sufficiently well chosen importance sampling algorithm, numerical simulations of two-dimensional spin systems of comparable size can be carried out without difficulty. As a preliminary exercise we have applied the "guided random walk" method of Barnes, Daniell, and Story[14,16] to the isotropic spin-$\frac{1}{2}$ Heisenberg antiferromagnet; as this model has been studied in the literature in a number of approximations it serves as a convenient trial application.

For the sake of completeness we note that there also exist Monte Carlo methods for studying the properties of two-dimensional spin systems at finite temperature. These methods have previously been applied to spin systems on large lattices, for example, to the two-dimensional Hubbard model on an 8×8 lattice[17] and the Heisenberg model on a 32×32 one.[18] These techniques are complementary to our approach in that they typically find increasing errors as the temperature is decreased; for example, the method used by Lee *et al.* is a numerical simulation of an expansion of the partition function in powers of $1/k_BT$. For this reason it may prove difficult to obtain accurate results for some properties of the ground state of a quantum-spin system using these methods. These techniques are also inappropriate for studies of long-range order in the isotropic case, as the Mermin-Wagner theorem[19] implies that this can only exist at zero temperature in two dimensions.

At present little is known about the ground state and excited states of the two-dimensional antiferromagnet. Lieb, Schultz, and Mattis[20] have shown that chains having half-integer spin are gapless (assuming translational invariance of the ground state); this however does *not* apply to the two-dimensional square lattice. This was noted by Affleck,[21] who argues that this unproven result is nonetheless probably correct. The possibility of long-range order in the ground state of the spin-$\frac{1}{2}$ system is also unresolved. A spin-wave calculation due to Anderson[22] suggests the existence of long-range order in the isotropic case. Rigorous results include proofs by Fröhlich and Lieb[23] that the two-dimensional anisotropic spin-S

Heisenberg antiferromagnet possesses Néel order for all S at sufficiently small temperature and transverse coupling, and by Neves and Perez,[24] who showed that long-range order exists in the ground state of the isotropic system for $S \geq \frac{3}{2}$.

Numerical studies have been carried out at zero temperature by Oitmaa and Betts[25] on periodic lattices up to 4×4 in extent, and at finite temperature by Lee, Joannopoulos, and Negele[18] on square lattices up to 32×32. Oitmaa and Betts gave results for the ground-state energy per spin and the staggered magnetization of the two-dimensional isotropic system using direct diagonalization. With our normalization they found $E_0/N^2=-0.702$ on the 4×4 lattice, and their estimate for an infinite system was $E_0/N^2=-0.655\pm0.005$. The approximate calculations summarized in Table II have yielded a number of E_0/N^2 estimates within a few percent of this value. Their estimate of a finite staggered magnetization on an infinite lattice is frequently cited as evidence for Néel ordering in the ground state, although ambiguities in the extrapolation procedure noted in more recent studies of the triangular lattice[26] imply a corresponding uncertainty in this result. The finite-temperature study of Lee *et al.* gave numerical results for the internal energy, the specific heat, and the susceptibility of this system, and from this the authors inferred the existence of a gap that scaled as $1/N$ on $N\times N$ square lattices. A numerical simulation on a moderately large lattice at zero temperature might improve our understanding of this system by providing more accurate estimates of the energy levels or by searching for evidence of long-range order.

In this paper we address the first of these problems and determine the ground-state energy per spin and the singlet-triplet energy gap from numerical simulations of 4×4, 6×6, and 8×8 lattices. These finite-N results are then extrapolated to give estimates for an infinite system.

II. THE METHOD

As the random-walk algorithm employed here has been discussed elsewhere in an application to the one-dimensional Heisenberg antiferromagnet,[14] we merely summarize the technique and will describe in detail only those changes which were implemented in generalizing to two dimensions. The algorithm allows one to generate ground-state energies and expectation values from the Euclidean-time wave function $\psi(\mathcal{S},\tau)$ by following the evolution of a sequence of random walks. We assume that a Hamiltonian H and a space of configurations $\{\mathcal{S}\}$ which can be used as a complete set of basis states $\{|\mathcal{S}\rangle\}$ for the quantum system have been specified. In this case we take for $\{\mathcal{S}\}$ the $2^{N^2}\mathcal{S}_z$-diagonal spin states on an $N\times N$ square lattice, and the Hamiltonian is divided into an $\{|\mathcal{S}\rangle\}$ diagonal part H_0 and an interaction part H_I which has no diagonal matrix elements;

$$H=H_0+H_I \ , \tag{1}$$

$$H_0=\sum_{\langle\hat{i}\hat{j}\rangle} S_z^{\hat{i}}S_z^{\hat{j}} \ , \tag{2}$$

$$H_I=-\tfrac{1}{2}\sum_{\langle\hat{i}\hat{j}\rangle}(S_+^{\hat{i}}S_-^{\hat{j}}+S_-^{\hat{i}}S_+^{\hat{j}}) \ . \tag{3}$$

Here, $\sum_{\langle\hat{i}\hat{j}\rangle}$ denoted a sum over nearest-neighbor spins. The minus sign in H_I is induced by the unitary transformation $U=\exp[-i\sum_{\hat{i}}\pi(i_x+i_y)S_z^{\hat{i}}]$, which changes the phase of down-spin basis vectors as $|\downarrow\rangle\rightarrow-|\downarrow\rangle$ on a "checkerboard" of sites. This change in the sign of H_I is convenient because it gives all weight factors the same overall sign.

The algorithm requires that we generate an ensemble of $N_{\rm rw}$ random walks in the configuration space $\{\mathcal{S}\}$ of the system, each of which follows a trajectory $\mathcal{S}_m(\tau)(m=1,\ldots,N_{\rm rw})$ in Euclidean time. These trajectories are determined by the rule that we start at a specified initial configuration $\mathcal{S}(0)$, and with each time step h_τ we attempt a transition from the current configuration $\mathcal{S}(\tau)$ to another configuration $\mathcal{S}'(\tau+h_\tau)$ with a probability of success given by

$$p(\mathcal{S}\rightarrow\mathcal{S}')=N_{\mathcal{S}\mathcal{S}'}r_{\mathcal{S}\mathcal{S}'}h_\tau \ . \tag{4}$$

The configuration $\mathcal{S}'$ is chosen at random from the set of $N_{\mathcal{S}\mathcal{S}'}$ "allowed" configurations for which the matrix element $\langle\mathcal{S}'|H_I|\mathcal{S}\rangle$ is nonzero. The stepping rate $r_{\mathcal{S}\mathcal{S}'}$ is an arbitrary positive number, provided that the resulting $p(\mathcal{S}\rightarrow\mathcal{S}')$ is small compared to unity. The $\{r_{\mathcal{S}\mathcal{S}'}\}$ comprise the algorithm's importance-sampling mechanism; they are chosen to encourage the random walk to move towards configurations expected to have a large overlap with the ground state.

A weight factor $w_m(\tau)$ is associated with the mth random walk, and these weight factors are defined so that their histogram in configuration space $\{\mathcal{S}\}$ gives the Euclidean-time wave function $\psi(\mathcal{S},\tau)$ when averaged over an infinite number of random walks. The weight factor $w_m(\tau)$ is determined from the path followed by the mth walk, the matrix elements of H and the stepping rates $\{r_{\mathcal{S}\mathcal{S}'}\}$ according to

$$w_m(\tau)=\exp\left[-\sum_{\mathcal{S}}c_{\mathcal{S}}T_{\mathcal{S}}[0,\tau]\right]\prod_{\substack{\mathcal{S}\rightarrow\mathcal{S}'\\ \text{transitions}}}\left[-\frac{\langle\mathcal{S}'|H_I|\mathcal{S}\rangle}{r_{\mathcal{S}\mathcal{S}'}}\right] , \tag{5}$$

where

$$c_{\mathcal{S}}=E_0(\mathcal{S})-\sum_{\mathcal{S}'}r_{\mathcal{S}\mathcal{S}'} \ . \tag{6}$$

$T_{\mathcal{S}}[0,\tau]$ is the time the mth walk was at the configuration $\mathcal{S}$ between the start and τ, and $E_0(\mathcal{S})$ is the eigenvalue of H_0 on $|\mathcal{S}\rangle$.

For this application we have chosen an exponential form for $r_{\mathcal{S}\mathcal{S}'}$,

$$r_{\mathcal{S}\mathcal{S}'}=R\exp\left[-\frac{S}{R}\Delta a\right] , \tag{7}$$

where R and S are adjustable guidance parameters and Δa is the change in spin alignment which the transition $\mathcal{S}\rightarrow\mathcal{S}'$ would induce

$$\Delta a\equiv\Delta\left[\sum_{\langle\hat{i}\hat{j}\rangle}S_z^{\hat{i}}S_z^{\hat{j}}\right] . \tag{8}$$

This simple generalization of the $R-S\Delta a$ used in the one-dimensional problem is automatically positive definite for positive R. For $S/R>0$ this $r_{\mathcal{S}\mathcal{S}'}$ guides the random

walks preferentially towards Néel order. We determine approximate optimum values of R and S by minimizing the variance of the log weights $\{\ln(w_{n_i})\}$; this suppresses the statistical errors of energies and matrix elements measured using these weight factors. The estimated optimum values used in our simulations were $R=0.5$ and $S=0.2$.

Although a histogram of the weight factors in (5) could be used to generate the explicit wave function $\psi(\mathcal{S},\tau)$, in practice there are too many basis states to construct such a histogram, and we instead use the weight factors to determine energies and matrix elements directly as described in Ref. 14. To measure ground-state energies we evaluate the mean weight $\langle w(\tau)\rangle$ at two Euclidean times, τ_1 and $\tau_2>\tau_1$. (The angle brackets signify an average over random walks.) If the state $|\mathcal{S}(0)\rangle$ corresponding to the initial configuration $\mathcal{S}(0)$ has a nonzero amplitude in the ground state, at large Euclidean times the normalized weight-factor histogram will approach

$$|\psi_0\rangle\langle\psi_0|\mathcal{S}(0)\rangle e^{-E_0\tau}, \tag{9}$$

so the mean weight satisfies

$$\lim_{\tau\to\infty}\langle w(\tau)\rangle \simeq \kappa e^{-E_0\tau}. \tag{10}$$

This allows an estimate of the ground-state energy which becomes exact as τ_1 approaches infinity,

$$E_0^{\rm est}(\tau_1)=\frac{1}{(\tau_2-\tau_1)}\ln\left[\frac{\langle w(\tau_1)\rangle}{\langle w(\tau_2)\rangle}\right]. \tag{11}$$

Corrections to the asymptotic value of $E_0^{\rm est}(\tau_1)$ due to excited states give this energy estimate an explicit time dependence of the form

$$\lim_{\tau_1\to\infty}E_0^{\rm est}(\tau_1)\simeq E_0+ce^{-(E_0'-E_0)\tau_1}, \tag{12}$$

where E_0' is the energy of the first excited state above E_0 which also couples to the state $|\mathcal{S}(0)\rangle$.

The numerically determined estimate $E_0^{\rm est}(\tau_1)$ is only equal to the true ground-state energy E_0 in the triple limit $h_\tau\to 0$, $N_{\rm rw}\to\infty$, and $\tau_1\to\infty$. As in Ref. 14 we have tested for systematic errors due to h_τ, $N_{\rm rw}$, and τ_1 dependence, and have included appropriate corrections in our reported values for the energies. The h_τ step size was chosen to be $0.2/N^2$; finite h_τ dependence was only visible in our results on the 4×4 lattice. For that case only we corrected for finite h_τ bias by measuring $E_0^{\rm est}(\tau_1)$ and $E_1^{\rm est}(\tau_1)$ at the smaller step size $h_\tau=0.1/N^2$ and extrapolating the two sets of measurements to $h_\tau=0$ as in Sec. III C of Ref. 14. Bias due to a finite random-walk ensemble size was studied by partitioning the weight factors from a set of $N_{\rm rw}$ random walks into two sets of $N_{\rm rw}/2$, four sets of $N_{\rm rw}/4$, and so forth, and recalculating the energies from each partition. The bias estimated in this manner was incorporated in our fitted energies, although it was found to be smaller than the statistical error in all the measurements used in our fits. Bias due to finite τ_1 was studied by carrying our $E_0^{\rm est}(\tau_1)$ measurements at a sequence of τ_1 values, and these results were then fitted to the expected three-parameter asymptotic form (12) after the inclusion of h_τ and $N_{\rm rw}$ corrections.

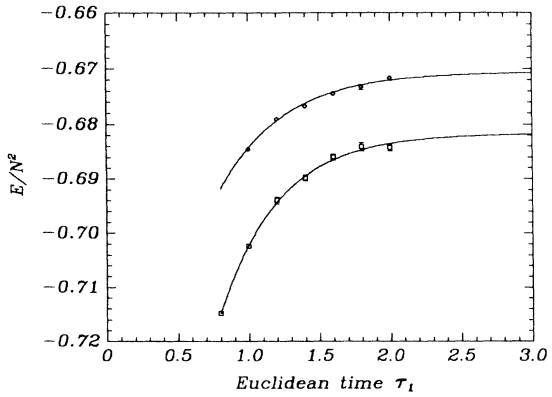

FIG. 1. Energy per spin vs Euclidean time for the 6×6 lattice.

The number of configurations used for each $E_0^{\rm est}(\tau_1)$ [or $E_1^{\rm est}(\tau_1)$] measurement on the 4×4 lattice was 2^{16}, divided into 8 runs of 2^{13} random walks each to generate statistical errors. Measurements were carried out at τ_1 values of 0.8 to 2.0 in steps of 0.2 and at 3.0, and the results were fitted to (12) after inclusion of the other bias corrections. On the 6×6 and 8×8 lattices central processing unit (CPU) time constraints restricted us to 8 runs of 2^{12} walks each. On the 6×6 lattice the above values of τ_1 between 0.8 and 2.0 were used, and on the 8×8 we used these and an additional measurement at $\tau_1=2.5$. The second Euclidean time τ_2 was taken to be $2\tau_1$ except on the 8×8 lattice, where it was decreased to $\tau_1+1.0$ to compensate for the increased weight-factor variance. (The effect of different choices for τ_2 is discussed in more detail in Ref. 14.) This procedure for generating finite-τ_1 energy estimates was not followed strictly in every case; on the 6×6 lattice we did not carry out a $\tau_1=0.8$ measurement of $E_1^{\rm est}$ because E_1 was determined to sufficient accuracy by the higher-τ_1 measurements, and we also used the results of several earlier runs in our fits. These additional measurements were generated during preliminary tests, and incorporating them slightly improved our final statistical accuracy.

TABLE I. Measured energy levels of the two-dimensional Heisenberg antiferromagnet.

N	4	6	8	∞
E_0/N^2	-0.7025 ± 0.0006	-0.6815 ± 0.0007	-0.6766 ± 0.0016	-0.6727 ± 0.0009
E_1/N^2	-0.6660 ± 0.0002	-0.6702 ± 0.0004	-0.6718 ± 0.0016	-0.6720 ± 0.0005
E_1-E_0	0.584 ± 0.010	0.407 ± 0.029	0.31 ± 0.14	0.052 ± 0.085

The fits of the finite τ_1 energy estimates $E_0^{\rm gst}(\tau_1)$ (lower curve) and $E_1^{\rm gst}(\tau_1)$ (upper curve) on the 6×6 lattice to the expected asymptotic form (12) are shown in Fig. 1; our results for the energies per spin on this lattice in Table I are the fitted values of the asymptotes E_0 and E_1. The E_0 and E_1 evaluations were distinguished by the choice of the starting configuration $\mathcal{S}(0)$; this was a pure Néel state for the singlet (E_0) measurements and a Néel state with a single flipped spin for the triplet (E_1) measurements.

The Monte Carlo calculations were performed on micro VAX-II, Sun-4, and CRAY X-MP computers. As an indication of the CPU time used, the measurement of $E_0^{\rm gst}(\tau_1=2.0)$ on the 8×8 lattice using 2^{15} random walks required 1940 CRAY seconds, and this was our longest run. The Sun-4 and micro VAX-II were approximately 10 and 60 times slower in execution of this program. The total CPU time required to accumulate the energy estimates used for our final results corresponds to approximately 15 CRAY hours.

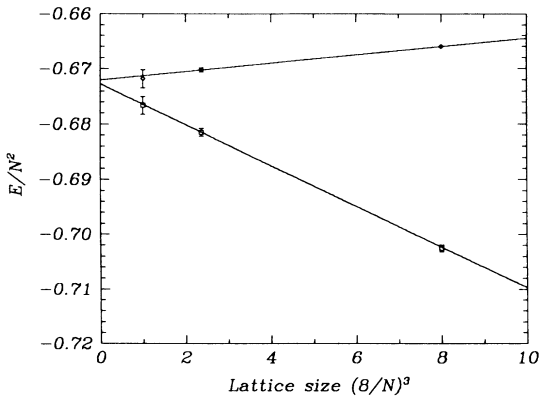

FIG. 2. Extrapolation of E_0/N^2 (lower curve) and E_1/N^2 to infinite square lattices.

III. RESULTS AND DISCUSSION

Our final results for the energy per spin of the lowest-lying singlet and triplet states and the singlet-triplet energy gap E_1-E_0 on the 4×4, 6×6, and 8×8 lattices are given in Table I.

To obtain estimates for infinite-lattice energies we fitted the finite-N numbers to the assumed asymptotic forms

$$\frac{E_i(N)}{N^2}=\frac{E_i(N)}{N^2}\bigg|_{N=\infty}+c_iN^{-3}\ , \tag{13}$$

and independently to

$$(E_1-E_0)\big|_N=(E_1-E_0)\big|_{N=\infty}+\kappa N^{-1}\ . \tag{14}$$

These forms were motivated by the large-N behavior of the one-dimensional system[27] and by inspection of our data. The resulting estimates for an infinite system are also given in Table I, and the data and the corresponding fits to (13) are shown in Fig. 2.

As the ground-state energy per spin on an infinite system is given by both the E_0/N^2 and E_1/N^2 asymptotes, we combined these to obtain our final estimate of

$$\lim_{N\to\infty}\frac{E_0(N)}{N^2}=-0.6724\pm0.0005\ . \tag{15}$$

Of course there remain systematic errors due to the assumption of the asymptotic forms (13) and (14) which we cannot easily determine, but the convergence of E_0/N^2 and E_1/N^2 to within 0.001 suggests that the systematic errors are no larger than this.

Our value for the 4×4 ground-state energy agrees with the result found by Oitmaa and Betts, but our energies on larger lattices are somewhat more negative than expected given their extrapolation. Our estimate of the ground-state energy per spin on an infinite lattice is also more negative than the results found by most of the approximate calculations which have appeared in the literature. For comparison these are summarized in Table II with our normalization convention.

We find that this system is gapless to within the numerical accuracy of our simulation; the singlet-triplet energy gap E_1-E_0 appears to converge to zero as κ/N, where $\kappa\approx2.1$. This is consistent with the results of Lee, Joan-

TABLE II. Summary of E_0/N^2 estimates for an infinite square lattice.

E_0/N^2	Method	Reference
−0.641	Variational	28
−0.641	Variational	29
−0.642	Variational	30
−0.643	Variational	31
−0.655±0.005	Direct diag.	25
−0.656	Variational	32
−0.658	Spin wave $1/S$	22,33
−0.659	Variational	34
−0.664	Perturbative	35
−0.6666	Mean-field theory	25
−0.670	Spin wave $1/S^2$	33,36
−0.6724±0.0005	Random walks	. . .
−0.716	Perturbative	37

nopoulos, and Negele,[18] and is reminiscent of the large-N behavior of the one-dimensional system.[27]

IV. CONCLUSIONS

We have shown that a Monte Carlo simulation of a moderately large two-dimensional Heisenberg antiferromagnet at zero temperature is feasible, and that it is possible to extrapolate to estimates of the properties of infinite systems with relatively small statistical errors. As this system is very similar to models proposed for the high-temperature superconductors, it should also be possible to study these systems numerically using Monte Carlo techniques. In future work we hope to investigate hole-hole interactions and the effect of holes on long-range order; these effects are widely held to be central to the physics of high-temperature superconductivity, but detailed numerical studies in two-dimensional systems such as the Heisenberg and Hubbard models have not been attempted.

Note added in proof. The apparent $E_0^{\downarrow}$ in Fig. 1 represents an average over many excited states and hence is larger than it would be at infinite Euclidean time. We are grateful to D. A. Huse for noting this discrepancy.

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