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Monte Carlo simulations of the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on a square lattice

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Motivated by the possible connection between superconductivity in the newly discovered oxide superconductors and the magnetic behavior of these materials, we have carried out numerical simulations to determine the sublattice magnetization $m^{\dagger}$ in the ground state of the spin-$\frac{1}{2}$ antiferromagnet on the square lattice with nearest-neighbor interactions. Lattices with $N=L\times L$ spins, where $L\leq 12$, were used. Extrapolating our results for rotationally invariant correlation functions to the thermodynamic limit, we obtain a much smaller value than obtained previously by exact diagonalization on lattices with sizes up to $N=16$. For the staggered magnetization, we find $m^{\dagger}=0.30\pm 0.02$ in units where the saturation value is $\frac{1}{2}$. This agrees with the result of spin-wave theory and a recent reanalysis of the perturbation expansion away from the Ising limit.

There has been a lot of interest in two-dimensional spin-$\frac{1}{2}$ magnetic systems following the discovery of the oxide superconductors[1] and the ensuing suggestion[2] that superconductivity in these materials might be related to their magnetic properties. Hence, not only the superconducting compounds, but also the related insulating materials, such as La_2CuO_4, have recently been studied.[3] It is therefore an appropriate time to gain an improved understanding of spin-$\frac{1}{2}$ magnetic insulators in two dimensions. Of particular interest is the ground-state staggered magnetization $m^{\dagger}$ of the Heisenberg antiferromagnet, which is reduced from its Néel, or classical, value because of zero-point fluctuations. Previous calculations of $m^{\dagger}$ have used spin-wave theory,[4] and perturbation theory away from the Ising limit.[5] In addition, Oitmaa and Betts[6] (referred to as OB) have carried out exact diagonalization on small finite lattices of up to 16 spins.

In the note we compute the staggered magnetization in the ground state of the spin-$\frac{1}{2}$ antiferromagnet on a square lattice by quantum Monte Carlo simulations. With this technique, we can study lattices with $N=L\times L$ spins, where $L\leq 12$, much larger than was possible in the earlier finite-size calculations of OB. This is important because the extrapolation to $N=\infty$ in OB was incorrect, but to verify this one needs to study a larger range of sizes. We find $m^{\dagger}=0.30\pm 0.02$, which is consistent with the result of spin-wave calculations and a recent reanalysis of the perturbation expansions by Huse.[7] We comment further on the relation between our results and those of OB at the end of the paper.

The Hamiltonian that we study is

$$H=\sum_{\langle i,j\rangle}\sigma_i\cdot\sigma_j\ , \tag{1}$$

where the σ_i are Pauli spin operators on the sites of a square lattice with $N=L\times L$ spins. Periodic boundary conditions are applied. The interactions run over nearest-neighbor pairs only and we have set the exchange constant to unity. We use the "world-line" Monte Carlo algorithm[8] in which one divides the Hamiltonian into two pieces H_1 and H_2, where H_1 and H_2 each incorporate the Hamiltonian of every fourth square, as shown in Fig. 1, in such a way that each bond on the lattice is included in either H_1 or H_2. It is easy to compute matrix elements of either H_1 or H_2 separately because they each split into the Hamiltonians of noninteracting squares. Unfortunately, H_1 and H_2 do not commute, so, to determine the partition function and expectation values, one uses the Trotter formula:[8]

$$\exp[-\beta(H_1+H_2)] = \lim_{m\to\infty}\left[\exp\left(\frac{-\beta H_1}{m}\right)\exp\left(\frac{-\beta H_2}{m}\right)\right]^m . \tag{2}$$

Inserting complete sets of states between the different factors, one sees that the partition function becomes that of a classical model in one higher dimension, with $2m$ "time slices" in the "time" direction. Periodic boundary conditions must be applied in this direction to represent the fact that a trace is being taken. At each site there is an Ising-

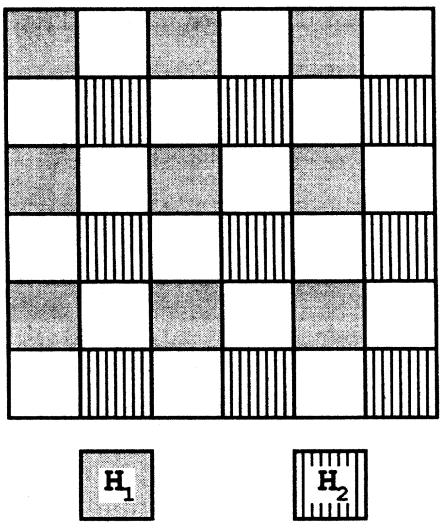

FIG. 1. The checkerboard breakup of the square lattice, showing how the Hamiltonian is divided into two pieces, H_1 and H_2, such that every bond lies in either H_1 or H_2.

like variable which takes values ± 1 and describes whether the spin is up or down. The statistical weight of a given spin configuration is simply the product of matrix elements of $\exp(-\Delta\tau H_{sq})$ for each of the shaded cubes in Fig. 2, where $\Delta\tau=\beta/m$ and H_{sq} is the Hamiltonian of a single square. More precisely, if the two planes perpendicular to the time direction in a shaded cube have their four spins in states described by labels a and b, where $1\leq a,b\leq 2^4$, then the contribution of that shaded cube to the statistical weight is $\langle a|\exp(-\Delta\tau H_{sq})|b\rangle$. Note that the Hamiltonian conserves the total magnetization M^z, which is therefore the same at each time slice.

It is also straightforward to see that the expectation value of any operator A, which conserves the total z component of spin between the two time slices of a single cube, is given by

$$\langle A\rangle=\sum_c A_c P(c) , \tag{3}$$

where c denotes a configuration of the spins at all time slices, A_c is the value of A in this configuration at any one time slice, so for the first time slice this would be

$$A_c=\langle 1|A|1\rangle , \tag{4}$$

$|1\rangle$ denotes the configuration at the first time slice, and P_c is the probability of a particular configuration, namely,

$$P_c=\frac{\langle 1|e^{-\Delta\tau H_1}|2\rangle\langle 2|e^{-\Delta\tau H_2}|3\rangle\cdots\langle 2m-1|e^{-\Delta\tau H_1}|2m\rangle\langle 2m|e^{-\Delta\tau H_2}|1\rangle}{\sum_{1,2,\ldots,2m}\langle 1|e^{-\Delta\tau H_1}|2\rangle\langle 2|e^{-\Delta\tau H_2}|3\rangle\cdots\langle 2m-1|e^{-\Delta\tau H_1}|2m\rangle\langle 2m|e^{-\Delta\tau H_2}|1\rangle} , \tag{5}$$

where $|i\rangle$ denotes the configuration at the ith time slice.

In the Monte Carlo technique, one takes a statistical sample of the spin configurations using standard techniques[9] which generate configurations with probability P_c. Clearly any local move conserves M^z. The ground state, which is our principle interest, has $M^z=0$ so the simulation is restricted to this subspace. As discussed elsewhere,[10] the elementary move is to take a cube in Fig. 2 which is unshaded but has shaded cubes above and below it and which has identical configurations on the top and bottom squares, and to replace these squares with a new configuration (keeping the top and bottom squares the same as each other). The move is accepted with probability $R/(1+R)$ where R is the ratio of the product of matrix elements for the new configuration divided by the product of matrix elements for the old configuration. The matrix elements only differ for those shaded cubes which are neighbors of the unshaded one, so this is fairly straightforward to implement.

With just this move, however, the algorithm does not sample all configurations with $M^z=0$, so two other moves have been included. The first of these causes the "world lines" for two up spins, say, to twist around each other. This is accomplished by searching for a "plaquette," which is in a Néel state, in a "tower" above one of the empty squares in Fig. 1. The spins of this plaquette are then inverted with the same probability as in the elementary move above. Finally, a nonlocal move is included to generate states of different "winding number."[10] This is carried out by looking for a line of spins, in either the x or y space direction at a given time slice, which is in a Néel state, and inverting these spins with the usual probability. For small sizes, inclusion of the nonlocal moves makes a substantial difference to the results. For the larger sizes, the difference appears to be smaller and the acceptance rate becomes very low. Nonetheless, we have preferred to use the same program, including nonlocal moves for *all* sizes, and we perform one sweep of each type of move in turn.

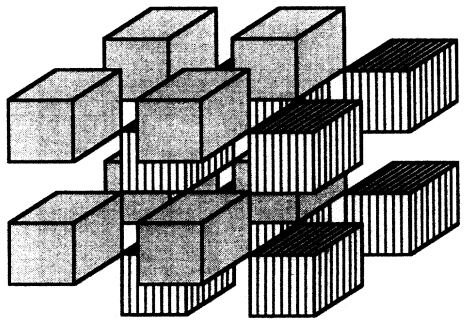

FIG. 2. The three-dimensional lattice on which one simulates an effective classical problem. At each point on the lattice there is a variable taking values ± 1, which indicates whether the spin is up or down. The statistical weight of a given configuration is the product of matrix elements of $\exp(-\Delta\tau H_{sq})$, where H_{sq} is the Hamiltonian of a single square, between the states of the top and bottom squares of the *shaded* cubes.

We wish to compute the staggered magnetization. This can be deduced from the mean-square staggered magnetization, defined by

$$S(\mathbf{q}_c)=\frac{1}{N^2}\left\langle\left[\sum_{x,y}\tilde{S}^z(x,y)\right]^2\right\rangle , \tag{6}$$

where $\mathbf{q}_c$ is the wave vector of the staggered magnetization, x and y are the coordinates of a site on the lattice, and

$$\tilde{S}^z(x,y)=\tfrac{1}{2}\epsilon_{x,y}\sigma^z(x,y) , \tag{7}$$

where $\epsilon_{x,y}$ is $+1$ or -1 depending on which sublattice the site (x,y) lies. The staggered magnetization can also be obtained from the correlation between spins as far apart as possible on the lattice, i.e.,

$$C_{L/2}=\frac{1}{N}\sum_{x,y}\langle\tilde{S}^z(x,y)\tilde{S}^z(x+L/2,y+L/2)\rangle . \tag{8}$$

For $L\rightarrow\infty$, where contributions from short-range order can be neglected, both $S(\mathbf{q}_c)$ and $C_{L/2}$ reduce to $(m^\dagger)^2/3$, the factor of 3 appearing because the ground state of the Heisenberg model is rotationally invariant,[7] whereas values quoted for $m^\dagger$ assume that the symmetry has been

broken in the z direction. Hence, we have

$$m^{\dagger} = \langle \tilde{S}_i^z \rangle = \lim_{L \to \infty} \sqrt{3S(\mathbf{q}_c)} = \lim_{L \to \infty} \sqrt{3C_{L/2}} \ . \tag{9}$$

It is important to check that the simulations are in equilibrium. To verify this we started the simulation both from an ordered (Néel) state and a completely random initial state (the same at each time slice). For each size we did this for a (roughly) logarithmically increasing set of values of the number of sweeps (increasing both the equilibrium sweeps and the subsequent sweeps where measurement takes place). To obtain reasonable statistics, we did each of these runs several, generally five, times. For each size, we verified that the results from the Néel start and the random start were independent of the simulation time for the longer runs and, furthermore, that they agreed with each other within the statistical errors. For $L=12$, which demanded the most computer time, and for $\Delta\tau=0.1$, we did 5 runs with 30000 sweeps (of each of the 3 types of moves) for equilibration followed by 70000 steps for the averaging and 1 run equilibrating for 100000 sweeps and averaging for another 300000. These were carried out both for a random and a Néel start. In addition, many shorter runs were performed. Except for $L=12$, we performed similar sets of runs for several different values of $\Delta\tau$, as discussed below.

Three extrapolations have to be made to compute the value of $m^{\dagger}$ in the ground state. First, one has to let the temperature T tend to zero. This is accomplished by checking that T is sufficiently low that the results are independent of T. For the data presented here we used $\beta = T^{-1} = 10$ except for the largest size $L=12$, where $\beta=15$ was taken. Second, one has to take the limit $\Delta\tau \to 0$, otherwise errors are made in the use of the Trotter formula, Eq. (2). The error in calculating expectation values[11] is proportional to $\Delta\tau^2$ so we plot in Fig. 3 the values obtained for $C_{L/2}$ for $L=4$ and $\beta=10$ against $\Delta\tau^2$. The results seem to be consistent with a linear variation and, furthermore, the intercept at $\Delta\tau=0$ gives a value of 0.0608 ± 0.0010, which agrees with the result $4C_{L/2} = 0.240$ obtained by OB from exact diagonalization. This provides a very useful check on the program. Except for $L=12$, we did a full set of runs, as described above, for at least four values of $\Delta\tau$. However, to reduce computer time, we only did $\Delta\tau=0.1$ for $L=12$. We found that the slope of the plots against $\Delta\tau^2$ did not vary very strongly with L, so we estimated the slope for $L=12$ from that of the smaller sizes.

The final extrapolation is, of course, to infinite system size. OB assumed that the leading finite-size corrections to $S(\mathbf{q}_c)$ and $C_{L/2}$ vary as N^{-1}. However, as also noticed by Huse,[7] spin-wave fluctuations give rise to a spin-spin correlation function which varies as the inverse of the distance, i.e.,

$$\langle \tilde{S}_i^z \tilde{S}_j^z \rangle \simeq \frac{1}{r_{ij}} \ , \tag{10}$$

so the leading finite-size corrections vary as $1/L$ rather than $1/N$. This is clearly apparent in Fig. 4, in which we display our main results, and a quadratic fit to the data. The extrapolated values of $S(\mathbf{q}_c)$ and $C_{L/2}$ which should be equal, are indeed very close, the fit giving 0.0295 and 0.0309, respectively. This should be compared with the saturation value of $\frac{1}{12}$. Our extrapolation is much smaller than the value of 0.059 for $S(\mathbf{q}_c)$ obtained by OB assuming a $1/N$ extrapolation and using only data on small sizes up to $N=16$. Interestingly though, plotting OB's data versus $1/\sqrt{N}$ rather than $1/N$, and performing a linear least-squares fit we find a value for $N=\infty$ quite similar to ours. From Eq. (9) we find

$$m^{\dagger} = 0.30 \pm 0.02 \ , \tag{11}$$

or in other words, 60% of the saturation value. The error was estimated from the range of quadratic fits which gave a reasonable description of the data. A cubic fit gives a very similar value for $m^{\dagger}$. Our value for $m^{\dagger}$ agrees,

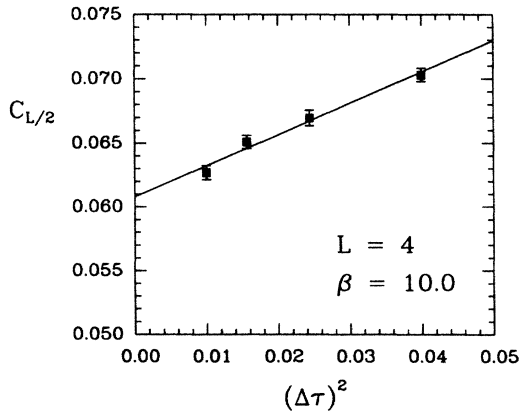

FIG. 3. A plot of the correlation function $C_{L/2}$ against $\Delta\tau^2$ for $L=4$ with $\beta=10$. As discussed in the text, a linear variation is expected theoretically, and the data seem to be consistent with this. The line is least-squares fit. Extrapolation of the fit to $\Delta\tau=0$ gives the value 0.0608 ± 0.0010, which agrees well with the result $4C_{L/2}=0.240$ obtained by Oitmaa and Betts (Ref. 6) from exact diagonalization.

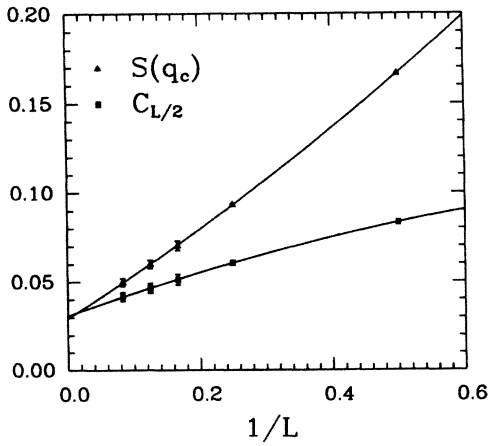

FIG. 4. Data for $S(\mathbf{q}_c)$ and $C_{L/2}$, defined in Eqs. (6) and (8), are plotted against L^{-1}, as discussed in the text. The lines are quadratic least-squares fits. The intercepts on the vertical axis, which should be equal, are indeed very close and we find the values 0.0295 and 0.0309, respectively.

within the error bars, with the spin-wave estimate[4] of 0.303, and the recent analysis of the perturbation expansion away from the Ising limit by Huse,[7] who finds $m^{\dagger}=0.313$. It is surprising that spin-wave theory seems to be so accurate even for spin $\frac{1}{2}$. The leading correction to the spin-wave result is of order $1/(zS)$, where z is the coordination number, and is known to vanish, as discussed by Stinchcombe.[4] However, it appears that the coefficient of the next term in the expansion must either vanish or be very small to account for the accuracy of the spin-wave prediction. It would therefore be interesting to understand corrections to spin-wave theory in greater detail. OB missed the factor of 3 in Eq. (9) which, to a large extent, cancels the error in their extrapolation to $N=\infty$, so their quoted result, $m^{\dagger}=0.24$, differs by only 20% from ours. However, including the factor of 3, OB's value would be increased to $m^{\dagger}=0.42$.

To conclude, we have shown, fairly convincingly, that the staggered magnetization in the spin-$\frac{1}{2}$ antiferromagnet on a square lattice is finite and is, furthermore, very close to the spin-wave value. It would be interesting to use similar techniques to investigate the ground-state properties of this model on other two-dimensional lattices.

Note added in proof: We have recently also computed the ground-state energy. Extrapolating our results to $L=\infty$ by assuming an L^{-3} dependence, as in spin-wave theory, we find $E/E_{\text{Néel}}=1.340\pm0.004$, where $E_{\text{Néel}}$ is the energy of the Néel state.

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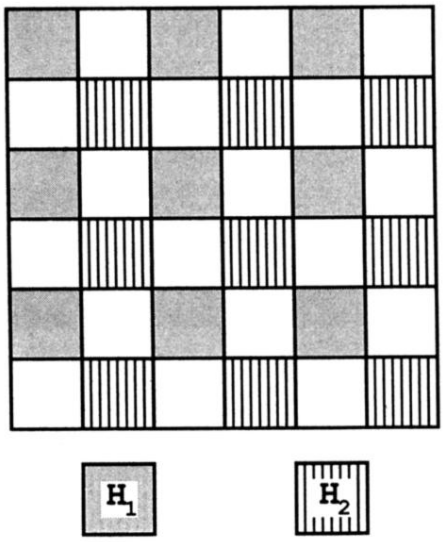
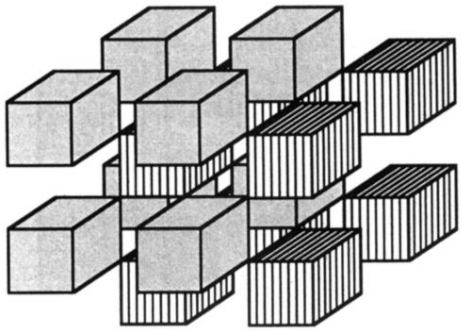


FIG. 1. The checkerboard breakup of the square lattice, showing how the Hamiltonian is divided into two pieces, H_1 and H_2, such that every bond lies in either H_1 or H_2.



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