Phase Diagram of the Frustrated Spin-$\frac{1}{2}$ Heisenberg Antiferromagnet in Two Dimensions

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Using a Lanczos technique we study the frustrated spin-$\frac{1}{2}$ Heisenberg model on square lattices of 16 and 20 sites. Frustration is introduced by an interaction along the diagonals of the plaquettes with coupling $J_2 \gtrsim 0$. For large J_2 we found that the ground state breaks (spontaneously) the lattice rotational symmetry. For intermediate values of J_2, the squares of order parameters associated with spin-Peierls and "twisted" states have a peak while a similar quantity for a chiral state shows no interesting structure.

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The discovery of high-temperature superconductors induced considerable work in the study of two-dimensional (2D) spin systems. This has been mainly motivated by Anderson's claim[1] that the physics of the new materials is closely related to the existence of new non-Néel phases of the 2D spin-$\frac{1}{2}$ Heisenberg model. In fact it has been shown that the Hubbard model with doping can be written, under some approximations, as a Heisenberg model with frustration.[2] While for the unfrustrated case evidence is accumulating that there is Néel order in the ground state, not much is known when frustration is explicitly included in the model. Since fluctuations are very strong in this problem, mean-field studies can only *suggest* a tentative phase diagram and more powerful techniques are needed for a reliable analysis.

In this Letter we study the spin-$\frac{1}{2}$ Heisenberg model with frustration introduced through an additional coupling along the diagonal of the plaquettes of the lattice. This model is defined as

$$H = J_1 \sum_{\mathbf{i},\hat{\mathbf{e}}} \mathbf{S}_\mathbf{i} \cdot \mathbf{S}_{\mathbf{i}+\hat{\mathbf{e}}} + J_2 \sum_{\mathbf{i},\hat{\mathbf{d}}} \mathbf{S}_\mathbf{i} \cdot \mathbf{S}_{\mathbf{i}+\hat{\mathbf{d}}}, \quad (1)$$

and we will refer to it as the J_1-J_2 model. $\mathbf{S}_\mathbf{i}$ are spin-$\frac{1}{2}$ operators located at sites $\mathbf{i}$ of a square lattice with periodic boundary conditions. $\hat{\mathbf{e}}$ $(=\hat{\mathbf{x}},\hat{\mathbf{y}})$ denote unit vectors along the two directions while $\hat{\mathbf{d}}$ $(=\hat{\mathbf{x}} \pm \hat{\mathbf{y}})$ represent vectors along the diagonals of the plaquettes. Classically, the J_1-J_2 model presents two phases: For small J_2 the ground state has Néel order, while for $J_2/J_1 > 0.50$ the system decouples into two Néel sublattices with an energy independent of the angle between the corresponding staggered magnetizations (thus the ground state is highly degenerate). $J_2/J_1 = 0.50$ is the classical transition point where in fact other states (having a uniform but arbitrary spin twist) are also degenerate with the ground state.

Recently the study of the quantum version of this model was initiated with spin-wave techniques (large S) showing that in a small region of parameter space the staggered magnetization may be zero.[3] Also, recently a numerical study of the spin-$\frac{1}{2}$ model was presented[4,5] using a Lanczos method on a 4×4 lattice. In that analysis it was found that for $J_2/J_1 \gtrsim 0.55$ a singlet state with momentum $\mathbf{k}=(0,0)$ was very close to the ground state with a gap much smaller than the spin-wave gap in the Néel phase (for the same finite lattice). In this Letter we continue the analysis of the J_1-J_2 model clarifying the physical meaning of that near degeneracy of the ground state as well as discussing other possible new phases near the classical transition point. Using the modified Lanczos method[6] we have studied square lattices with $N=16$ and 20 (N denotes the number of sites)[7] investigating the spectrum and mean values of special operators in the ground state. Energies have been obtained with a typical accuracy of 10^{-9} that produces errors in the squares of order parameters of 10^{-4}.

Our results are the following: In Fig. 1(a) we show some selected energy levels (including the ground state) for a 4×4 lattice at $J_1 = 2.0$ [actually there are other levels above and in between those shown in Fig. 1(a)]. The energies are per site. The ground state E_+ is a singlet with $\mathbf{k}=(0,0)$. It is even (+) under both a rotation of the lattice in $\pi/2$ and a reflection along a vertical axis. By inspection of the wave function we found that the state E_- [also singlet with $\mathbf{k}=(0,0)$] differs from the ground state under a $\pi/2$ lattice rotation, this excited state having a quantum number -1 (odd) under that operator (and still even under reflections). E_{SW1} and E_{SW2} are spin-wave states (triplets) with $\mathbf{k}=(\pi,\pi)$ and $(0,\pi),(\pi,0)$, respectively, while E_p is the first state of the spectrum odd under reflections with $\mathbf{k}=(0,0)$. E_S have $\mathbf{k}=(0,\pi),(\pi,0)$ and are singlets. The physical meaning of these states will be discussed below. In Fig. 1(b) we present our results for a 20-site lattice. While the behavior of E_{SW1} and E_{SW2} is qualitatively similar to Fig. 1(a), the E_+ and E_- levels cross at $J_2 \approx 1.17 \pm 0.01$ $(J_1 = 2.0)$ where E_- becomes the ground state. The gap between E_- and E_+ is remarkably small near and after the crossing point. This nonuniform behavior of the ground state for large J_2 (i.e., even under rotations for $N=16$ but odd for $N=20$) is likely to be a finite-size effect. Below, we follow the convention that mean values

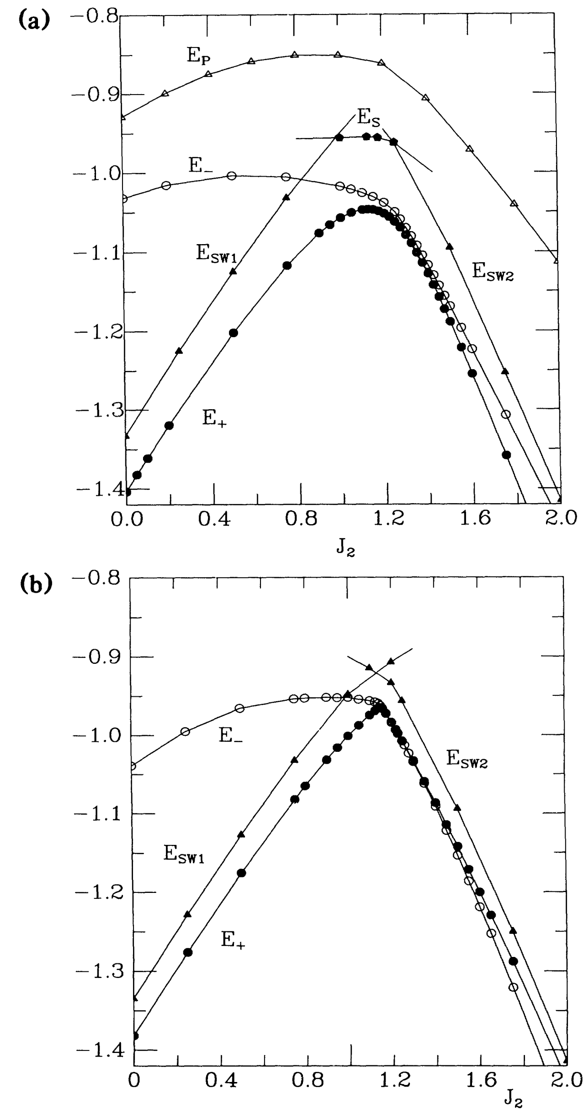

FIG. 1. (a) Some representative energy levels (per site) of the $N=16$ lattice at $J_1=2.0$. E_+ is the ground state, E_- is the first excited state odd under a $\pi/2$ lattice rotation, E_{SW1}, E_{SW2} are spin waves, and E_P, E_S are excited states whose physical meaning is explained in the text. (b) Same as (a) but for $N=20$.

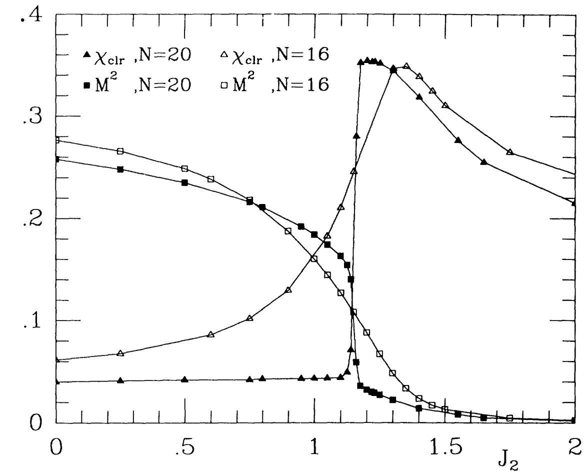

FIG. 2. Squares of order parameter, χ_{clr} and M^2, associated with collinear and Néel states, respectively, vs J_2 ($J_1=2.0$). Solid (open) squares and triangles denote results for $N=20$ ($N=16$) as explained in the figure.

of operators are evaluated in the actual ground state taking into account the crossing levels. We explicitly checked that our qualitative predictions are unchanged if instead of the actual ground state for $N=20$ we consider the state E_+ in calculating expectation values.

Now we analyze the physical meaning of our results. First we concentrate on the near degeneracy between E_+ and E_- for $J_2/J_1 \gtrsim 0.55$ where classically the system decouples into two independent Néel-ordered sublattices. However, for large but finite J_2, thermal and/or quantum fluctuations crucially alter this picture.[8] The J_1 term that couples the two sublattices cannot be neglected. The basic detail is that the coupling between the fluctuations of each sublattice staggered magnetization is maximum when they are parallel or antiparallel. Explicit calculations[9] at large S have shown that the infinite degeneracy of the classical ground state is removed and the system effectively prefers to be locked in a state where the magnetizations have a relative angle of 0 or π. This results in dominant configurations having alternating rows (or columns) of spins up and down (that we will call "strip" or collinear states) that are connected by a lattice rotation of $\pi/2$. However, the tunneling between them is through a high-energy barrier and thus exponentially suppressed. The barrier diverges in the thermodynamic limit and a spontaneous breakdown of the discrete lattice rotational symmetry occurs.

Our results in Fig. 1 clearly support this picture, confirming the validity of the spin-wave calculations[9] even for $S=\frac{1}{2}$. E_+ and E_- correspond to the even and odd combinations of the two collinear states with a splitting caused by tunneling in our finite system. Analyzing the wave functions we found that indeed the classical collinear states have relatively large coefficients. In the collinear states there is a spin-wave mode in the "staggered" direction. They correspond to the states E_{SW2} of Fig. 1. Another way to check the existence of collinear states is by using the order parameter

$$O_i = \mathbf{S}_i \cdot (\mathbf{S}_{i+\hat{x}} + \mathbf{S}_{i-\hat{x}} - \mathbf{S}_{i+\hat{y}} - \mathbf{S}_{i-\hat{y}}) . \quad (2)$$

O_i takes values $+1$ or -1 for the collinear states. It vanishes for a classical Néel state. We have studied the square of this order parameter, defined as $\chi_{clr} = \langle (N^{-1}\sum_i O_i)^2 \rangle$, where the sum is over even sites. If a collinearlike state is the ground state in the bulk limit then χ_{clr} should stay approximately constant with increasing N. In Fig. 2 we show our results for χ_{clr}. For completeness, we also present results for the square of the staggered magnetization, defined as

$$M^2=\left\langle 3\left[\frac{1}{N}\sum_{\mathbf{i}}(-1)^{i_x+i_y}S_{\mathbf{i}}^z\right]^2\right\rangle .$$

$\chi_{\rm clr}$ is small for small J_2 but with increasing J_2 it presents a sharp peak between 1.2 and 1.4 that does not change much with the lattice size. This result gives support to a recent calculation[10] where the Ising-type critical temperature of this model was shown to have a maximum near the classical transition point. The abrupt change in $\chi_{\rm clr}$ and M^2 (and other observables presented below) for $N=20$ is due to the crossing of levels in the ground state, although using the state E_+ instead, the results look very similar. We have not attempted an extrapolation to the bulk limit but from Fig. 2 it is clear that $\chi_{\rm clr}$ is likely to remain finite in that limit for $J_2 \gtrsim 1.2$. Note that the existence of a maximum in $\chi_{\rm clr}$ is correlated with the minimum in the $|E_+ - E_-|$ gap.

Now we analyze the region around $J_2/J_1=0.5$. Here there are many candidates for the ground state. For example, recently Read and Sachdev[11] have shown in a $1/M$ expansion for the SU(M) antiferromagnet that if a non-Néel phase exists in the Heisenberg model then it may exhibit spin-Peierls order. In this state the spins are coupled in short-range singlets forming columns (we will refer to it as the "column" state). Such a configuration breaks the lattice rotational symmetry, it is fourfold degenerate, and its existence can be tested using the complex order parameter,[12]

$$O_{\mathbf{i}}^{\rm col}=\eta(\mathbf{i})\mathbf{S}_{\mathbf{i}}\cdot(\mathbf{S}_{\mathbf{i}+\hat{\mathbf{x}}}+i\mathbf{S}_{\mathbf{i}+\hat{\mathbf{y}}}-\mathbf{S}_{\mathbf{i}-\hat{\mathbf{x}}}-i\mathbf{S}_{\mathbf{i}-\hat{\mathbf{y}}}) ,$$

where $\mathbf{i}$ are even sites and $\eta(\mathbf{i})=+1$ (-1) if both i_x and i_y are even (odd). This operator takes the values 1, i, -1, and $-i$ for the four column states and it vanishes for Néel or collinear states. We studied numerically $\chi_{\rm col}=\langle |N^{-1}\sum_{\mathbf{i}}O_{\mathbf{i}}^{\rm col}|^2\rangle$ (Fig. 3). For the 4×4 lattice it has a peak at $J_2/J_1\approx 0.5$–0.55 indicating that there is an enhancement of the stability of this state in that region. For the 20-site lattice $\chi_{\rm col}$ still has a peak but of lower intensity. Then, we cannot show convincingly the stability of the column state in the bulk limit.[13] Note that the doubly degenerate state E_S [singlets with $\mathbf{k}=(0,\pi)$, $(\pi,0)$] of Fig. 1(a) may be associated with the two additional levels that would become degenerate with E_+ and E_- when $N\to\infty$ if the column state is the ground state.

Another possibility for the ground state in the intermediate region is a "twisted" or helicoidal state which can be obtained from the Néel state by applying a uniform twist Q along some direction (e.g., the x axis). Classically, these states are all degenerate at $J_2/J_1=0.5$ [including $Q=0$ (Néel state) and $Q=\pi$ (collinear states)] and only at that point do they form the ground state. However, if a new term is added to the Hamiltonian that couples spins at a distance of two lattice spacings (along both axis) with coupling constant J_3, then there is a *finite* region around $J_2/J_1=0.5$ where the twisted state is the ground state.[10] Although in our model $J_3=0$, it may be generated dynamically so it is important to analyze the possible existence of such a twisted order. For $S=\frac{1}{2}$ these states can be characterized by the *vector* order parameter,[10] $\mathbf{V}_{\mathbf{i}}=\mathbf{S}_{\mathbf{i}}\times(\mathbf{S}_{\mathbf{i}+\hat{\mathbf{x}}}+\mathbf{S}_{\mathbf{i}+\hat{\mathbf{y}}})$. In Fig. 4 we show $\chi_t=\langle (N^{-1}\sum_{\mathbf{i}}\mathbf{V}_{\mathbf{i}})^2\rangle$. In the intermediate region it has a peak that *increases* its intensity from $N=16$ to 20. An extrapolation to the bulk limit is difficult but it is clear that this state is enhanced near $J_2/J_1\approx 0.5$.

Finally, we present results for chiral order. Recently it has been pointed out[14] that a nonzero expectation value for the operator $O_{\mathbf{i}}^{\rm ch}=\mathbf{S}_{\mathbf{i}}\cdot(\mathbf{S}_{\mathbf{i}+\hat{\mathbf{x}}}\times\mathbf{S}_{\mathbf{i}+\hat{\mathbf{y}}})$ implies chiral-symmetry breaking (and also parity and time-reversal symmetry breaking). We have measured the square of the chiral order parameter, $\chi_{\rm ch}=\langle (N^{-1}\sum_{\mathbf{i}}O_{\mathbf{i}}^{\rm ch})^2\rangle$ (assuming a *uniform* chiral state)

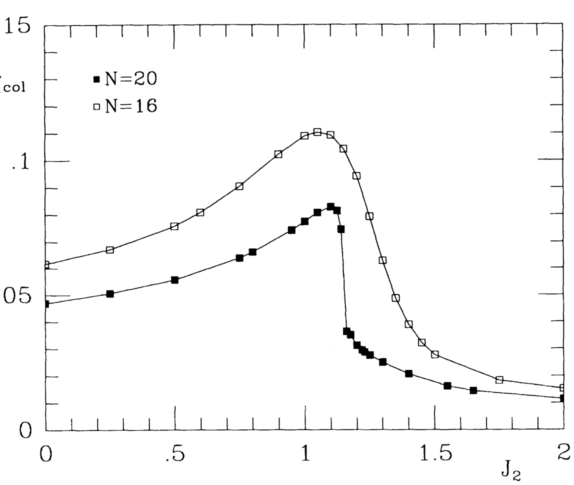

FIG. 3. $\chi_{\rm col}$ (square of the column-state order parameter) vs J_2 ($J_1=2.0$).

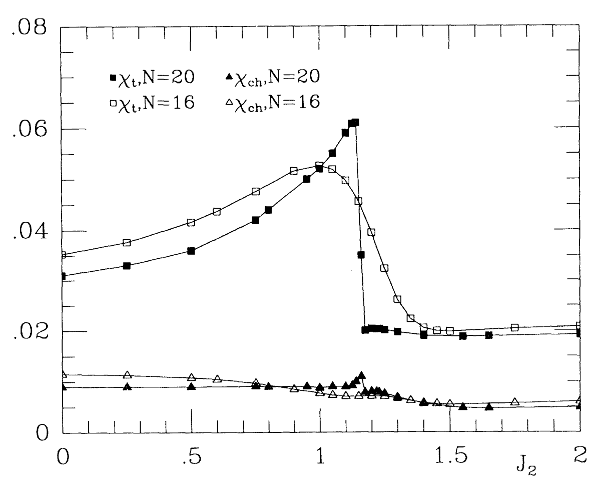

FIG. 4. χ_t and $\chi_{\rm ch}$ (square of the twisted and chiral order parameters, respectively) vs J_2 ($J_1=2.0$).

(Fig. 4). There is no indication of an enhancement of this type of order since χ_{ch} is very flat for both $N=16$ and 20. In Fig. 1(a) we also studied the state E_P which has the lowest energy in the subspace of $\mathbf{k}=(0,0)$ and *odd* under reflection.[15] The gap $|E_P-E_{+,-}|$ is much larger than the spin-wave and the $|E_+-E_-|$ gaps. So in the spectrum there are no indications of a parity-symmetry-breaking ground state either.

Summarizing, our conclusions from a numerical study of small lattices are the following: (i) For large J_2 we found strong evidence that the lattice rotational symmetry is spontaneously broken. This effect appears very clearly when studying both the spectrum and the order parameter and is in good agreement with analytic calculations.[8,9] The symmetry breaking seems to be maximum for $J_2/J_1 \approx 0.6$–0.7 and perhaps a discontinuous transition separates this phase from the others. (ii) In the intermediate region we observed indications of an enhancement of both spin-Peierls and twisted order since both χ_{col} and χ_t have a peak. Bigger lattices are needed to conclusively show the stability of these states. With Lanczos techniques it may be possible in the near future to study $N=32$ which is the next lattice size with all the symmetries of the bulk limit.[7] It is interesting to analyze the possible coexistence of column and twisted order. It is also important to extend these results, including the parameter J_3 that makes the twisted state stable (classically) on a finite region.[16,17] (iii) No evidence of chiral order in this J_1-J_2 model has been found. Of course our lattices may be too small for such a state to be energetically favored (we know very little about typical length scales for this state). Also it would be interesting to know if the chiral order is expected to be uniform (as tested here) or if it presents additional spatial structure. (iv) Finally, note that for all values of J_2/J_1 there seems to be some order parameter corresponding to a symmetry-breaking state that shows some enhancement. Then there is little room in the J_1-J_2 model for resonating-valence-bond (disordered) phases.[18] Again this situation may change when including a J_3 coupling or doping (holes).

After completing this work we received a paper[19] where the column state is claimed to be stable near $J_2/J_1 \approx 0.5$.

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