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Exact diagonalization study of the frustrated Heisenberg model

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The spin-$\frac{1}{2}$ frustrated Heisenberg model is studied on a square lattice using the modified Lanczos technique. Frustration is introduced in the system through an additional coupling along the diagonals of the plaquettes. On a 4×4 lattice the ground state smoothly interpolates between two asymptotic Néel-like limits. However, on a narrow region of parameter space we find that the lowest-lying levels above the ground state are singlets rather than triplets, suggesting the existence of a new phase in the thermodynamic limit.

What are the properties of the ground state of a two-dimensional Heisenberg model with frustration? This question was raised some time ago by Anderson[1] in the context of the spin-$\frac{1}{2}$ triangular lattice. A new spin-liquid state [the resonating-valence-bond (RVB) state] has been proposed as a candidate for the ground state of frustrated systems.[2] The recent discovery of high-T_c superconductors has induced considerable work in this area because it is believed that the introduction of doping in the half-filled Hubbard model is similar to adding frustration to a spin system.[3] That may destabilize the Néel state in favor of a RVB-like state. Other speculations link the ground state of the frustrated Heisenberg model with the fractional quantum Hall state.[4]

However, the existence of a spin-liquid ground state for some physically realistic spin-$\frac{1}{2}$ antiferromagnet in 2D has not been shown. Recently, a step forward in that direction has been given: a 2D Heisenberg model with frustration was studied in Ref. 5 using conventional spin-wave techniques. A small region in parameter space was found where the ordered states are melted by fluctuations. That opens the possibility of the existence of a disordered ground state in that region. Since spin-wave techniques are based on the evaluation of fluctuations around ordered states in the large S limit, other approaches (specially numerical methods) are necessary to analyze the $S=\frac{1}{2}$ model. However, an analysis of the Heisenberg model with frustration using Monte Carlo techniques is very difficult because negative weights are induced in the calculation. So far, the only reliable method for this type of problem is the study of small lattices using the Lanczos approach. In this paper we present an exact diagonalization analysis of the frustrated Heisenberg model using a modification of the Lanczos method[6] that has been recently used in the study of the unfrustrated 2D Heisenberg model[7] and related problems.[8]

We have studied the model described by the Hamiltonian

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

where $\mathbf{S}_\mathbf{i}$ is a spin-$\frac{1}{2}$ operator at site $\mathbf{i}$ of a two dimensional square lattice with periodic boundary conditions. $\hat{\mathbf{e}}(=\hat{\mathbf{e}}_x$ or $\hat{\mathbf{e}}_y)$ denotes unit vectors in the two directions while $\hat{\mathbf{d}}(=\hat{\mathbf{e}}_x\pm\hat{\mathbf{e}}_y)$ denotes vectors along the diagonals of the plaquettes. In this paper we take $J_1=2.0$. For $J_2=0$ convincing evidence has been presented[7,9,10] showing that the ground state is Néel-like. The coupling J_2 introduces frustration in the problem so the Néel state cannot be the ground state for large enough values of J_2. However, in that limit the system decouples into two unfrustrated sublattices each one with Néel order. Classically ($S=\infty$), the change from one regime to another occurs (abruptly) at $J_2/J_1=0.5$. Around this region in parameter space is where we have the possibility of finding a new phase for the $S=\frac{1}{2}$ model once quantum fluctuations are properly taken into account.

What sizes and geometries of lattices are more adequate for our search of an intermediate phase in the frustrated Heisenberg model? It is certainly important to keep the main symmetries of the bulk lattice. For that purpose special square lattices can be constructed.[9] However, from them we should exclude those lattices where $N/2=$odd (N is the number of sites) otherwise for large values of J_2 the system would be divided into two frustrated sublattices. Then, it is convenient to analyze square lattices with special geometries[9] having 4,8,16,... sites.[11,12]

As numerical technique we use the modified Lanczos method.[6] Our main results are the following: The four-site lattice can be solved analytically. There is a crossing of levels at $J_2=1.0$ between the only two possible singlets of this lattice without additional intermediate phases. More interesting are the results for an 8-site lattice (for the geometry of this lattice see Fig. 1 of Ref. 9). In this case we have 14 singlets. In Fig. 1 we show the energies of the lowest-lying levels. We found that these energies are straight lines as a function of J_2. At $J_2=1.0$ there is again a crossing between two singlet states. The staggered magnetizations change abruptly at this point since a crossing is like a first-order phase transition. However, note that at exactly $J_2=1.0$ a third singlet becomes degenerate with the other two Néel-like states (then there is an intermediate phase in this problem at only one point).

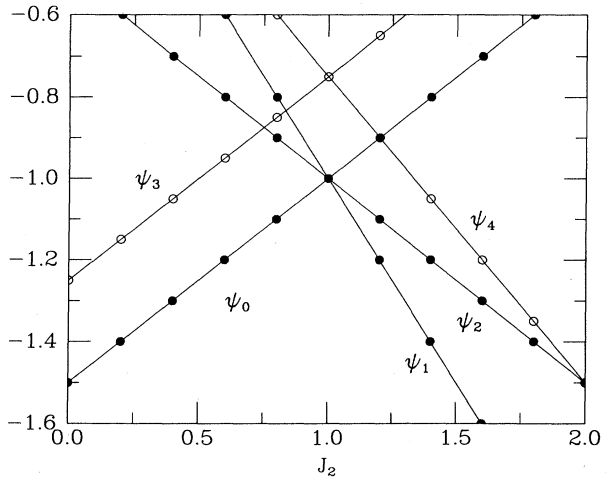

FIG. 1. The energy of the lowest-lying levels of the 8-site lattice. Shown are the singlet ground states ψ_0, ψ_1 and a close third singlet ψ_2. Also shown are the two lowest-energy triplet states ψ_3 and ψ_4.

This interesting detail is important to understand some unexpected results below.

In Fig. 2 we show the ground-state energy (E_0) vs J_2 for a 16-site (4×4) lattice (in many systems this size of the lattice has proven to be large enough to capture the essential physics of the problem). The momentum $\mathbf{k}$ of the ground state is $\mathbf{k}=(0,0)$. Although for J_2 between 1.0 and 1.3 there is a rapid change in the slope of E_0, the crossover between the two asymptotic Néel limits seems to be smooth, quite different from the results on the 4- and 8-site lattices. This suggests that there is no crossing of levels in the ground state of this model for any value of J_2. In Fig. 2 we also show the energies of the lowest-lying excited states with nonzero momentum (these states are very easy to study with our technique simply by changing the quantum numbers of the starting configuration). For small J_2 the first excited state is a triplet and has $\mathbf{k}=(\pi,\pi)$, while at large J_2 it is also a triplet but with $\mathbf{k}=(\pi,0)$ or $(0,\pi)$ (doubly degenerate due to the decoupling of the lattice into two sublattices). These states will become the spin waves of the Néel states in the thermodynamic limit. For large and small J_2 the other states with nonzero momenta are at much higher energies. This is the typical behavior of a Néel ordered system. However, note that in the region where E_0 rapidly changes curvature, the first excited state with nonzero momentum is a singlet with $\mathbf{k}=(0,\pi)$ or $(\pi,0)$ rather than a triplet. This suggests that we may find new results in that intermediate region as shown below.

In Fig. 3 we show the square of the staggered magnetization defined as

$$M_1^2=\left\langle\left[\frac{1}{N}\sum_i(-1)^{|i|}S_i^z\right]^2\right\rangle. \tag{2}$$

We have also measured the staggered magnetization (M_2^2) in one of the two sublattices in which the system decouples at large J_2. The results show that M_1^2 at $J_2=0$ has a large value typical of a Néel state. For $J_2\approx 1.2$ this magnetization has already decreased (smoothly) to a small number. In the same region of parameter space M_2^2 increases also smoothly. From Fig. 2 we observe that there is a narrow region where both magnetizations are small and in that regime we may find a new phase in the thermodynamic limit (the continuity of the magnetizations suggest second-order phase transitions). Bigger lattices are clearly necessary to clarify whether the two magnetizations vanish (in the bulk limit) at different points or not.

Analyzing the number of iterations (τ) required by our numerical method to converge to the ground-state energy with an accuracy of 10^{-9} we find that it has a clear peak at $J_2\approx 1.35$. Relaxation times are usually related with the difference in energy ΔE between the ground state and the first excited state through $\tau\approx 1/\Delta E$. Then this result suggests the existence of another singlet state with zero

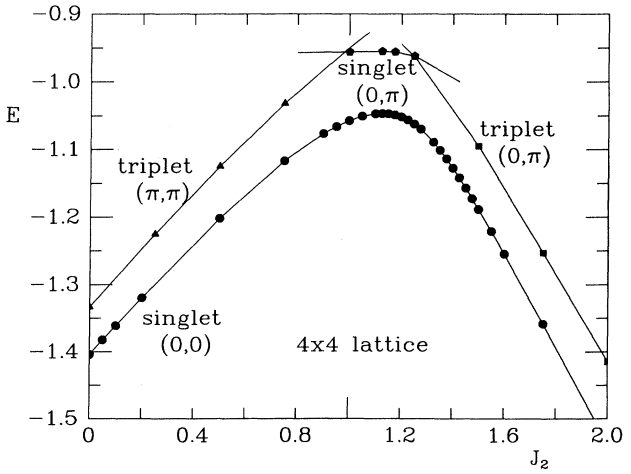

FIG. 2. Energy of the ground state (per site) on a 4×4 lattice vs J_2. Also shown are the first excited states with nonzero momentum and the momentum of each state.

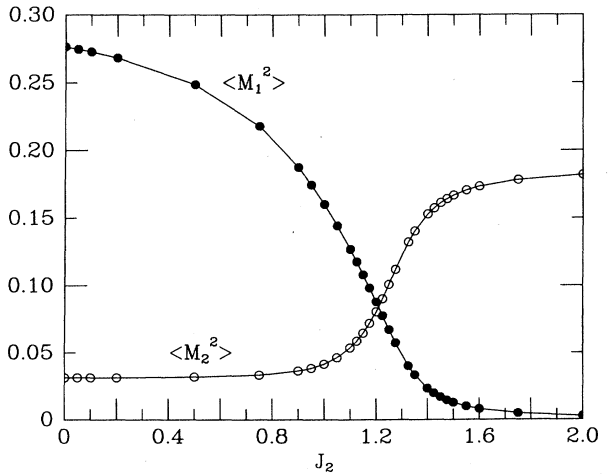

FIG. 3. Staggered magnetizations M_1^2 and M_2^2 vs J_2 on a 4×4 lattice. The error is smaller than the points.

momentum very close to the ground state. They may easily become degenerate or cross in the thermodynamic limit.

To study this excited (singlet zero momentum) state with our numerical method we need to use as a starting configuration a state orthogonal to the ground state. In principle, that can be accomplished by selecting as a trial function the state $|\psi_{\text{trial}}\rangle = |\phi\rangle - \langle\phi|\psi_0\rangle|\psi_0\rangle$, where $|\phi\rangle$ is arbitrary (as long as its projection on the excited state is nonzero) and $|\psi_0\rangle$ is the ground state previously calculated. However, we found that in practice it is simpler to obtain an orthogonal state by inspection of the ground state. For example, if two states $|a_1\rangle, |a_2\rangle$ of the S_z basis appear in the ground state with weights α_1, α_2, respectively, then a state orthogonal to the ground state is $|\psi_{\text{trial}}\rangle = |a_1\rangle - \alpha_1/\alpha_2|a_2\rangle$. This is the method we used and, in general, it produces good results. For example, evaluating the ground-state energy E_0 with error 10^{-9} we get an accuracy of 10^{-5} in the energy of the first excited state. If we continue the iterations after an error of 10^{-5} is reached, the state decays into the ground state because originally it had a projection on the ground state due to small errors in α_1, α_2. We can generalize these ideas for higher excited states, but of course the accuracy of each new excited state is poorer than the previous one.

Applying this technique we found the remarkable result shown in Fig. 4(a) (some special values of the energies are also presented in Table I). In the region $J_2 \approx (1.1,1.5)$ there is another singlet state with zero momentum (E_1), very close to the ground state. Note that the gap between these two states is much smaller than the gap between the triplet (E_T) and the singlet (E_0) states at $J_2=0$ (see also Fig. 2) which we know will become degenerate in the thermodynamic limit. In Fig. 4(a) we also show some points corresponding to a second excited state (E_2). Those values have error bars because of the difficulty in stabilizing the state against a decay into the ground state.[13]

One possibility is that the two almost degenerate states are the equivalent of the Néel states ψ_0 and ψ_1 of Fig. 1 with a small gap opened between them (which is possible since they have the same quantum numbers). However, if an interchange of states effectively has occurred then the excited state should have magnetic properties opposite to those of the ground state, as ψ_0 and ψ_1 have on the 8-site lattice. We have evaluated the magnetizations in the excited state and they are qualitatively very similar to those of the ground state, not the opposite.

Then we have a more interesting situation where on a finite region of parameter space the lowest-lying levels above the ground state are singlets rather than triplets. Consider, for example, the following scenario: Suppose that the states whose energies are denoted by E_0 and E_2 (or some other excited state) in Fig. 4(a) correspond to the states ψ_0 and ψ_1 on the 8-site lattice (Fig. 1) with a gap opened. Then the singlet (E_1) of Fig. 4(a) is in correspondence with ψ_2 of Fig. 1 which was degenerate with the ground state at one-point on the 8-site lattice.[14] Then in the interval $J_2 \approx (1.1,1.5)$ we may have a new disordered ground state[15,16] (the staggered magnetizations are very small in that region). The "one point" new phase of the 8-site lattice corresponds now to a finite region.

It is very difficult to imagine that the fact that the lowest-lying excited states are singlets rather than triplets can be a finite-size effect. Then, we conjecture a phase diagram for this model as shown in Fig. 4(b). Since the magnetizations behave very smoothly we expect second-

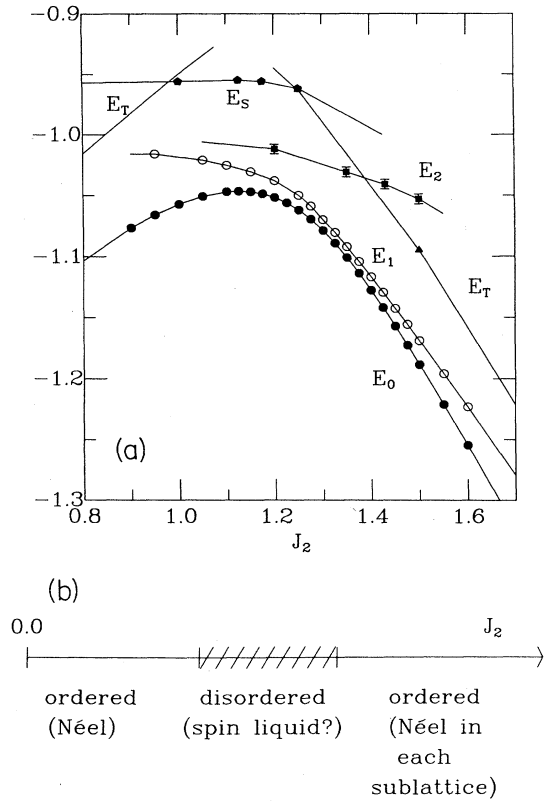

FIG. 4. (a) Ground-state energy (E_0) and first excited-state energy (E_1) (per site) on a 4×4 lattice as a function of J_2 near the degeneracy region. Also shown is the second excited-state energy (E_2). The three states are singlets with $\mathbf{k}=(0,0)$. For comparison, we also show the triplet (E_T) and singlet (E_S) states of Fig. 2. (b) Possible phase diagram of the Heisenberg model with frustration in the thermodynamic limit.

TABLE I. Ground-state energy (E_0) and first excited-state energy (E_1) per site (both singlets with zero momentum) of the 2D Heisenberg model with frustration as a function of J_2 on a 4×4 lattice. The error is in the last digit.

J_2	E_0	E_1
0.950	−1.065978	−1.0160
1.100	−1.047189	−1.0254
1.150	−1.047183	−1.0307
1.200	−1.051792	−1.0380
1.325	−1.089305	−1.0804
1.400	−1.127716	−1.1169
1.500	−1.188546	−1.1691
1.600	−1.254670	−1.2233
1.750	−1.358437	−1.3072

order phase transitions separating the different phases. This represents the first evidence of the existence of a new intermediate phase in the spin-$\frac{1}{2}$ frustrated Heisenberg model.

Our lattice is not big enough to address finer details about the properties of the new disordered phase. Does the very small gap found between the first two singlets vanish in the bulk limit? If this is true then we have a new phase with a degenerate ground state (probably having massless excitations). A second possibility is that the almost-zero singlet-singlet gap is an artifact of our lattice and the bulk limit has a finite gap. In that case, the excitations of the disordered phase may be massive (as suggested in the RVB states with short-range bonds).

Of course considerable work is still needed. That work should be along two main directions. (a) To check the influence of finite size effects in our results it is important to study a square lattice with 20 sites (bigger lattices do not have the correct symmetries or are too big for Lanczos methods). This case will require considerably more computer time not only because the number of states in the Hilbert space is larger than for the 16-site case (factor ≈ 6) but also because the gap between singlets may be even smaller increasing the number of iterations needed for a good convergence. (b) The second area of investigation is the study of the properties of the first excited state. Here we will find that a clear definition of a spin-liquid state is unknown (in other words, the operator whose susceptibility diverges in a RVB phase is unknown to us).[17] Work along these lines is in progress.

Note added. After completion of this work we learned of a calculation by F. Figueirido *et al.*[18] with results similar to ours.

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[11]In practice 24–26 sites are the maximum that can be handled using exact diagonalization techniques due to memory constraints introduced by the huge size of the Hilbert space.

[12]In Ref. 7 we found that the analysis of nonsquare systems such as a 4×6 lattice can suggest misleading results for the thermodynamic limit.

[13]We have not analyzed the singlet zero momentum subspace beyond E_{2_u} but it is possible that other states may appear before E_T is reached in Fig. 4(a).

[14]A possible way to check this scenario is to measure the magnetizations of the second excited state and see if they are opposite to those of the ground state. However, this work is very difficult because that second excited state cannot be stabilized long enough to measure the magnetization with a small error.

[15]This interval is shifted towards higher values of J_2 with respect to the classical "critical" point $J_2=1.0$. However, in Ref. 5 the disordered region for spin-$\frac{1}{2}$ was approximately between $J_2\approx0.8$ and 1.0. This suggests that in spin-wave techniques corrections in $1/S$ are needed to get good quantitative predictions for $S=\frac{1}{2}$.

[16]A spin-Peierls state (valence-bond crystal) has also been recently numerically excluded as a candidate for the ground state of the intermediate phase [S. Kivelson (private communication)].

[17]Perhaps the study of the overlap of the ground state with RVB states may help in this problem. However, since even in the case $J_2=0$ that overlap may be very large, such a study may not be conclusive.

[18]F. Figueirido, A. Karlhede, S. Kivelson, S. Sondy, M. Rocek, and D. Rokhsar (unpublished).