Quantum phase transitions in the two-dimensional J_1-J_2 model

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We analyze the phase diagram of the frustrated Heisenberg antiferromagnet, the J_1-J_2 model, in two dimensions. Two quantum phase transitions in the model are already known: the second-order transition from the Néel state to the spin liquid state at $(J_2/J_1)_{c2}\approx 0.38$, and the first-order transition from the spin liquid state to the collinear state at $(J_2/J_1)_{c4}\approx 0.60$. We have found evidence for two second-order phase transitions: the transition from the spin columnar dimerized state to the state with plaquette-type modulation at $(J_2/J_1)_{c3}=0.50\pm 0.02$, and the transition from the simple Néel state to the Néel state with spin columnar dimerization at $(J_2/J_1)_{c1}=0.34\pm 0.04$. We also present an independent calculation of $(J_2/J_1)_{c2}\approx 0.38$ using another approach.

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The nature of the quantum disordered phases of low-dimensional quantum antiferromagnets is a topic of fundamental importance for the physics of quantum magnetism.[1] Such phases can result from mobile holes in an antiferromagnetic background as in the t-J or Hubbard model at finite doping. Alternatively, competition of purely magnetic interactions can also lead to destruction of long-range order. A typical example of the second kind is the J_1-J_2 model which exhibits a quantum disordered (spin-liquid) phase due to second-neighbor frustrating interactions. Even though it has been intensively studied during the last ten years, the J_1-J_2 model apparently still holds many secrets. This model is also an ideal testing ground for the theory of quantum phase transitions because it has very complex dynamics and contains a variety of transitions. Exact diagonalization studies[2] have shown that the excitation spectrum of the model is quite complex and that finite-size effects are large.[3] Spin-wave-like expansions around the simple Néel state (which occurs for small frustration) naturally cannot give any information about the ground state at stronger frustration, and consequently nonperturbative methods are needed to analyze the latter regime.

An important insight into the disordered regime was achieved by field-theory methods[4,5] and dimer series expansions. [6,5,7] The above works have established the range of the disordered regime, $0.38<g<0.60$ ($g=J_2/J_1$), and have also shown that the ground state in this regime is dominated by short-range singlet (dimer) formation in a given pattern (see Fig. 1). The stability of such a configuration implies that the lattice symmetry is spontaneously broken and the ground state is fourfold degenerate. This picture is somewhat similar to the one dimensional situation, where the Lieb-Schultz-Mattis theorem guarantees that a gapped phase always breaks the translational symmetry and is doubly degenerate, whereas gapless excitations correspond to a unique ground state.[8]

Two very recent calculations[9,10] performed by Green function Monte Carlo methods have raised questions on the structure of the intermediate phase. The authors of Ref. 9 claim stability of the ''plaquette RVB'' state at $g\approx 0.5$. Reference 10 comes to a different conclusion: there is a columnar spin dimerized state with plaquette-type modulation along the columns. An additional very interesting observation[10] is that the columnar spin dimerization penetrates into the Néel phase to $g\approx 0.3$. To conclude the list of observations which do not agree with a simple spin liquid with columnar dimerization we mention the divergence in the plaquette susceptibility found in Ref. 7 at $g\sim 0.5$.

In the present paper we elucidate all the above questions and come to the conclusion that two additional quantum critical points exist in the phase diagram of the system. These critical points correspond to a generic type of second-order quantum phase transition considered in Ref. 11. At each of the critical points there is condensation of some singlet excitation and the critical dynamics is described by the nonlinear O(1) field theory.

The Hamiltonian of the J_1-J_2 model reads:

$$H=J_1\sum_{nn}\mathbf{S}_i\cdot\mathbf{S}_j+J_2\sum_{nnn}\mathbf{S}_i\cdot\mathbf{S}_j, \tag{1}$$

where J_1 is the nearest-neighbor, and J_2 is the frustrating next-nearest-neighbor Heisenberg exchange on a square lattice (see Fig. 1). Both couplings are antiferromagnetic, i.e., $J_{1,2}>0$ and the spins $S_i=1/2$. We also use the notation $g=J_2/J_1$. The spin columnar dimerization at $g>g_{c2}$ is well established[4–7] and therefore we start our consideration from

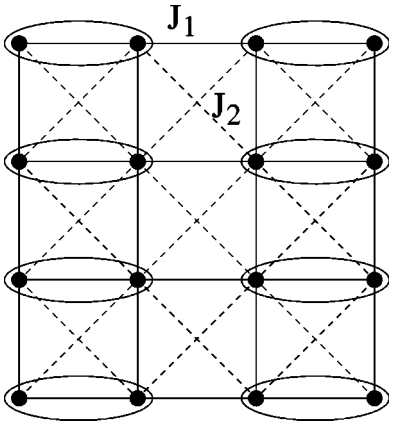

FIG. 1. Schematic picture of the simple columnar dimerized state. The ovals represent two spins coupled into a singlet.

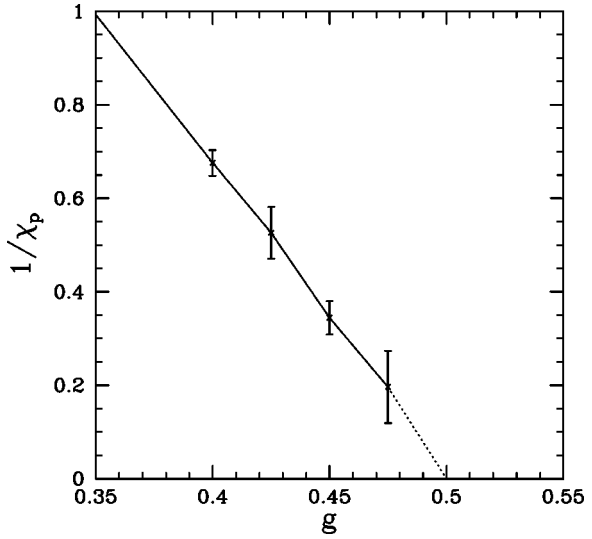

FIG. 2. The plot of $1/\chi_P$, where χ_P is the plaquette susceptibility calculated in the simple columnar dimerized state using dimer series expansion. The value of $1/\chi_P$ vanishes at $g_{c3}=0.50\pm0.02$ indicating a transition to the columnar dimerized state with plaquette-type modulation.

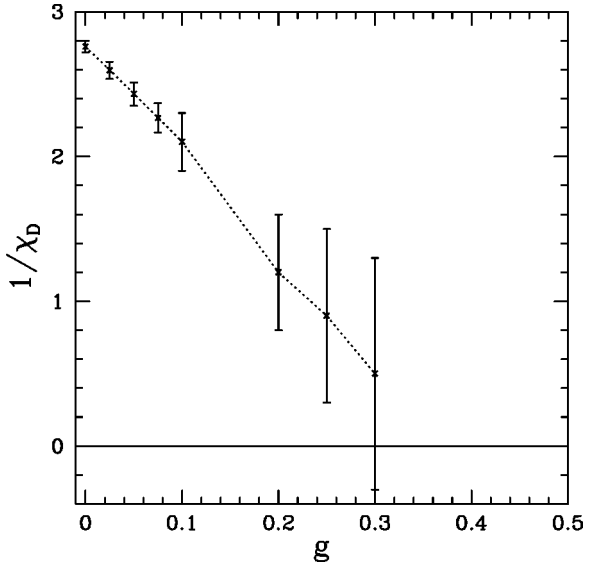

FIG. 3. The plot of $1/\chi_D$, where χ_D is the dimer susceptibility calculated in the simple Néel state using Ising series expansion. The value of $1/\chi_D$ vanishes at $g_{c1}=0.34\pm0.04$ indicating transition to the Néel state with spontaneous spin columnar dimerization.

this state shown schematically in Fig. 1. If there is an instability with respect to some kind of additional ordering then the gap in the spectrum of some singlet excitation must vanish at the corresponding critical point.[11] We do not have a reliable technique for direct calculation of the singlet gap, but we do have a well developed series expansion technique for calculation of static susceptibilities. A static susceptibility is proportional to the corresponding Green's function at zero frequency

$$\chi_{\mathbf{q}} \propto G_{\mathbf{q}}(\omega=0) \sim Z_{\mathbf{q}}/\omega_{\mathbf{q}}^2, \tag{2}$$

where $\omega_{\mathbf{q}}$ is the quasiparticle energy, and $Z_{\mathbf{q}}$ is the quasiparticle residue. So at the critical point $1/\chi$ must vanish approximately as $(g-g_c)^{\gamma}$, with $\gamma=\nu(2-\eta)$, where ν is the critical index for the spectral gap, $\Delta \propto (g-g_c)^{\nu}$, and $\nu\eta$ is the critical index for the quasiparticle residue, $Z \propto (g-g_c)^{\nu\eta}$.

To analyze possible plaquette type modulation we calculate the susceptibility of the spin columnar dimerized state with respect to the field[7]

$$F_P = \sum_{i,j} (-1)^j \mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1}, \tag{3}$$

which breaks the translational symmetry in the direction perpendicular to the dimers. The series has been computed up to the seventh order in the dimerization parameter, and these series are extrapolated by using the standard Padé approximant and the integrated differential approximants.[12] Results for $1/\chi_P$ are shown in Fig. 2, where the errorbar reflect the spread in the Padé approximants. The value of $1/\chi_P$ vanishes at $g_{c3}=0.50\pm0.02$ and this is the critical point for the second-order quantum phase transition from a simple columnar dimerized state to the eightfold degenerate columnar dimerized state with plaquette-type bond modulation in the direction perpendicular to the dimers suggested in Ref. 10. This phase transition is of the generic type considered in Ref. 11 and therefore it is described by 2D nonlinear O(1) field theory.[13] The critical indexes for this model are:[14] $\nu \approx 0.630$, $\eta \approx 0.034$. Therefore one shall expect $\gamma=\nu(2-\eta) \approx 1.2$. On the other hand the Dlog Padé approximants to the series χ_P give $\gamma=0.9\pm0.1$. This is fair agreement, and we offer an explanation for the small discrepancy. The phase transition is related to the condensation of some singlet excitation which can be considered as a bound state of triplet excitations.

$$|s\rangle = a_2|tt\rangle + a_3|ttt\rangle + a_4|tttt\rangle + \ldots . \tag{4}$$

We would like to stress that there is very strong mixing between two-triplet and multitriplet bound states. This mixing was the reason why vanishing of the singlet gap at $g=g_{c3}$ was missed in Ref. 5. In Ref. 5 analysis of the singlet excitation was based on a two-particle Bethe-Salpeter equation with further account of multiparticle contributions as a small perturbation. This assumption was wrong because of the strong mixing. So at $g=g_{c3}$ we have condensation of effectively a multiparticle bound state with relatively small two particle component. The mixing between two-particle and multiparticle components of the singlet excitation varies with g and this effect cannot be taken into account in the nonlinear O(1) field theory which assumes condensation of an ''elementary'' (=structureless) field. Ultimately very close to the critical point the variation of the mixing can be neglected and one shall expect restoration of the pure O(1) field theory behavior. However, it happens in so narrow vicinity of the critical point that the present numerical data cannot assess it.

Let us consider now the appearance of spin dimer order at $g=g_{c1}$ as g is increased from small values. A scenario put forward some time ago[4] and based on the analysis of the $Sp(N)$, $N \to \infty$ field theory suggests that the dimer order ap-

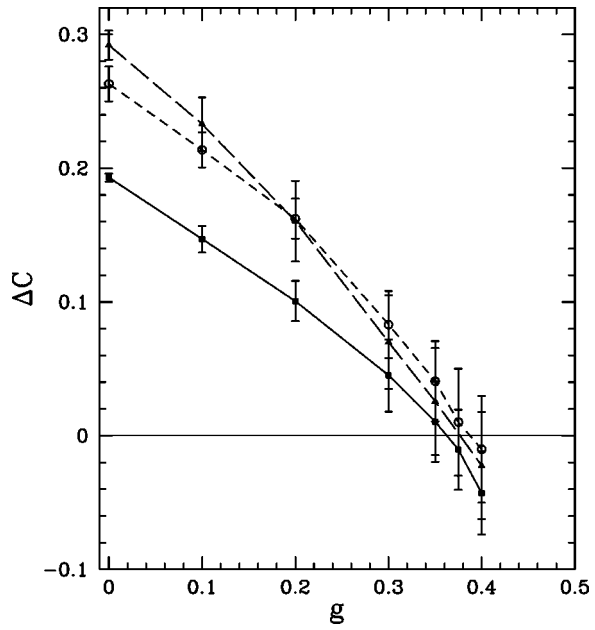

FIG. 4. Plot of the difference $\Delta C=2|\langle \mathbf{S}_i\cdot\mathbf{S}_j\rangle-3\langle S_i^zS_j^z\rangle|$ for 1st neighbors (full line), 2nd neighbors (short dashed line), and 3rd neighbors (long-dashed line) versus $g=J_2/J_1$. The full rotation symmetry of the ground state is restored when $\Delta C=0$.

pears simultaneously with disappearance of the Néel order, $g_{c1}=g_{c2}$. The dynamics in the vicinity of the critical point is described by the nonlinear O(3) field theory in spite of an additional dimer order parameter. The additional gapless excitation is irrelevant to the critical dynamics because this excitation is of extremely large size:[4] $r\sim(g-g_c)^{-M}$, $M\gg1$. Another possibility is that $g_{c1}<g_{c2}$ and hence there are two separated quantum phase transitions.[15] The transition at $g_{c2}=0.38$ is still described by the nonlinear O(3) σ model, while the transition at g_{c1} is of the O(1)×O(1) type.[11] A recent work based on the Green function Monte Carlo method[10] gives a hint in favor of this picture.

Let us give the precise meaning to the terms relevant and irrelevant singlet excitation. We consider a quantum critical point at which the singlet gap Δ_s vanishes. An external field which is coupled to the singlet excitation, $\langle s|F|0\rangle\neq0$, is applied to the system. If the corresponding susceptibility given by Eq. (2) is diverging at the critical point we call this singlet excitation ''relevant.'' If the susceptibility is not diverging we call the singlet excitation ''irrelevant.'' It is clear that for an irrelevant excitation the quasiparticle residue Z vanishes faster than Δ_s^2.

To analyze the problem of spin dimer order we calculate the susceptibility of the Néel state with respect to the external field which probes spin columnar dimerization.

$$F_D=\sum_{i,j}(-1)^i\mathbf{S}_{i,j}\cdot\mathbf{S}_{i+1,j}. \tag{5}$$

In this calculation we use the usual Ising series expansion up to seventh order, the Ising expansion for this model has been discussed in Ref. 16, and will not be repeated here. Note that in spite of the similarity between Eqs. (3) and (5) these are two quite different situations. The field (3) assumes that the dimers aligned along the *i* direction already exist and it probes a possible modulation in the *j* direction. The field (5) is applied to the Néel state and therefore it does not assume any dimer order. The series has been extrapolated in the same way as that for $1/\chi_P$, and the values of $1/\chi_D$ versus g are plotted in Fig. 3. It is clear that $1/\chi_D$ vanishes somewhere in the interval $g\in[0.3,0.4]$, but the data is not precise enough to distinguish g_{c1} from g_{c2}. To distinguish between the two scenarios discussed above we have to realize that Fig. 3 clearly indicates the *relevant* singlet excitation. In a picture with an *irrelevant* singlet[4] the quasiparticle residue is extremely small, $Z\propto(g-g_c)^M$, $M\gg1$, and hence the susceptibility has no divergence at the critical point. Thus we conclude from Fig. 3 that $g_{c1}=0.34\pm0.04$, and that $g_{c1}<g_{c2}$, so there is a region $g_{c1}<g<g_{c2}$, where the spin columnar dimer order and the Néel order coexist. The critical dynamics at g_{c1} is described by the *relevant* gapless singlet excitation.[11] There is no doubt that the *irrelevant* gapless singlet excitation at $g\approx g_{c2}$ also exists, but it has an exponentially small residue[17] and hence its contribution to the susceptibility is negligible.

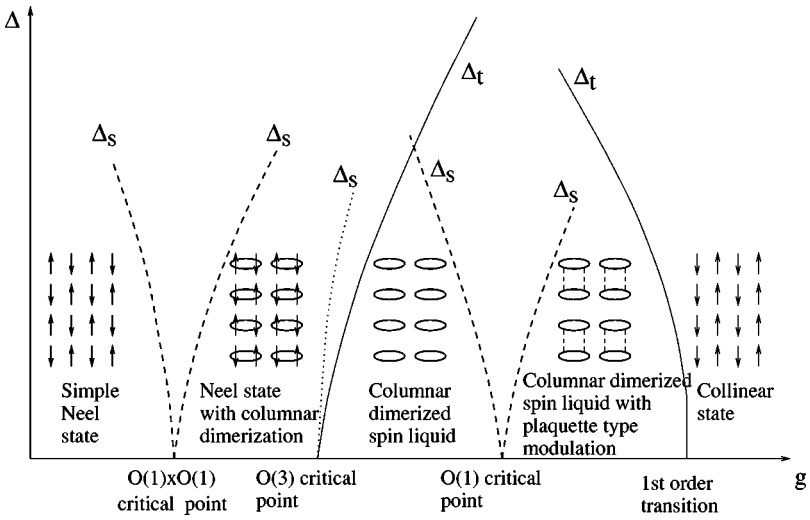

FIG. 5. Schematic phase diagram and the excitation spectra of the J_1-J_2 model. Solid lines show the triplet gap, dashed lines show the gaps of the *relevant* singlets, the dotted line shows the gap of the *irrelevant* singlet.

The final result we report here is another way of estimating $g_{c2} \simeq 0.38$. The previous best calculation[5] was based on vanishing of the triplet gap in the spin liquid phase. A previous attempt[16] to estimate g_{c2} by Ising expansions for the staggered magnetization in the Néel phase showed the magnetization vanishing around 0.4, but the series were erratic in this region and the precision low. The estimate is based on Ising expansions[16] in the Néel phase for the 1st, 2nd, and 3rd neighbor correlators $\langle S_i^x S_j^x \rangle$ and $\langle S_i^z S_j^z \rangle$, where z is the direction of staggered magnetization. The series has been computed up to order 9 for 1st and 2nd neighbor correlators and to order 7 for 3rd neighbor correlator. Again these series are analyzed by using the standard Padé approximant and the integrated differential approximants,[12] and the results for the differences of these correlators are shown in Fig. 4, where the errorbar reflect the spread in the different order of approximants. The transition point is identified by the condition $\langle S_i^x S_j^x \rangle = \langle S_i^z S_j^z \rangle$, corresponding to restoration of spin rotational symmetry to the ground state. This gives $g_{c2} \simeq 0.38(3)$, in excellent agreement with previous results.

In conclusion, the zero-temperature phase diagram and the excitation spectra of the J_1-J_2 model are shown schematically in Fig. 5. There are four critical points: $g_{c1} = 0.34 \pm 0.04$, $g_{c2} \approx 0.38$, $g_{c3} = 0.5 \pm 0.02$, $g_{c4} \approx 0.60$. The states are: $g < g_{c1}$—the simple Néel state, $g_{c1} < g < g_{c2}$—the columnar dimerized Néel state, $g_{c2} < g < g_{c3}$—the simple columnar dimerized spin liquid, $g_{c3} < g < g_{c4}$—the columnar dimerized spin liquid with plaquette type modulation, and $g > g_{c4}$—the collinear state. The transitions at g_{c1} and g_{c3} are second-order phase transitions of the O(1)×O(1) and O(1) symmetry classes correspondingly. Energies of the corresponding *relevant* singlet excitations vanish at the critical points. The transition at g_{c2} is a second-order phase transition described by the nonlinear O(3) field theory. The energy of the triplet excitation vanishes at $g \leqslant g_{c2}$; at the critical point there is also a singlet excitation with zero gap, but this singlet is *irrelevant*. The transition at g_{c4} is probably of first order, but is very close to second order.

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