New 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 $(J_2/J_1)_{c2} = 0.38$, and the first order transition from the spin liquid state to the collinear state at $(J_2/J_1)_{c1} = 0.60$. We have found evidence for two new 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 $(J_2/J_1)_{c4} = 0.34 \pm 0.04$. We also present an independent calculation of $(J_2/J_1)_{c2} = 0.38$ using a new 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 non-perturbative methods are needed to analyze the latter regime.

An important insight into the disordered regime was achieved by field-theory methods [4] and dimer series expansions [5]. 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 new 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. [10] 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 new 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) $\sigma$-model.

The Hamiltonian of the $J_1 - J_2$ model reads:

$$H = J_1 \sum_{nn} S_i \cdot S_j + J_2 \sum_{nnn} S_i \cdot S_j,$$

(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 [4-6] and therefore we start our consideration from 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

$$\chi_q \propto G_q(\omega = 0) \sim Z_q/\omega_q^2,$$

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

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

$$F_P = \sum_{i,j} (-1)^{i} S_{i,j} \cdot S_{i,j+1},$$

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. Results for $1/\chi_P$ are shown in Fig. 2. The value of $1/\chi_P$ vanishes at $g_{c3} = 0.50 \pm 0.02$ and this is the critical point for the second order quantum phase transition from a simple columnar dimerized state to the 8-fold 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) $\sigma$-model. The critical indexes for this model are $[4]: \nu \approx 0.630$, $\eta \approx 0.034$. Therefore one shall expect $\gamma = 2(\nu - \eta) \approx 1.19$. On the other hand the Dlog Padé approximants to the series $\chi_P$ give $\gamma = 0.9 \pm 0.1$. 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.

$$|s\rangle = a_2 |tt\rangle + a_3 |ttt\rangle + a_4 |tttt\rangle + \ldots$$

We would like to stress that there is very strong mixing between two-triplet and multi-triplet bound states. This mixing was the reason why vanishing of the singlet gap at $g = g_{c3}$ was missed in Reference [8]. In Ref. [9] analysis of the singlet excitation was based on a two-particle Bethe-Salpeter equation with further account of multi-particle 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 multi-particle bound state with relatively small two particle component. The mixing between two-particle and multi-particle components of the singlet excitation varies with $g$ and this effect cannot be taken into account in the non-linear $\sigma$-model 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 $\sigma$-model 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 $Sp(N)$, $N \rightarrow \infty$ field theory suggests that the dimer order appears 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) $\sigma$-model in spite of an additional dimer order parameter. The additional gapless excitation is irrelevant to the critical dynamics because this excitation has extremely large size [3]: $r \sim 1/(g - g_c)^M$, $M \gg 1$. Another possibility is that $g_{c1} < g_{c2}$ and hence there are two separated quantum phase transitions [13]. The transition at $g_{c2} = 0.38$ is still described by the nonlinear O(3) $\sigma$-model, while the transition at $g_{c1}$ is of the O(1)$\times$O(1)-type. So in the vicinity of the point $g_{c1}$ there is an additional effective singlet field which can condense either at momentum $k = (\pi, 0)$ or $(0, \pi)$. The sign degeneracy of the scalar field together with the momentum degeneracy gives a four-fold degenerate ground state which exactly corresponds to the degeneracy of the spin-dimerized state. 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 $\Delta_s$ vanishes. An external field which is coupled to the singlet excitation, $\langle s | F | 0 \rangle \neq 0$, 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 $\Delta_s^2$.

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.

$$F_D = \sum_{i,j} (-1)^i S_{i,j} \cdot S_{i+1,j}.$$  

In this calculation we use the usual Ising series expansion up to seventh order. Note that in spite of the similarity between (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 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 the case of an irrelevant singlet [9] the quasiparticle residue is extremely small, $Z \propto (g - g_c)^M$, $M \gg 1$ and hence the susceptibility has no divergence at the critical point. Thus we conclude from Fig. 3 that $g_{c1} = 0.34 \pm 0.04,$
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. There is no doubt that the irrelevant gapless singlet excitation at $g \approx g_{c2}$ also exists, but it has an exponentially small residue and hence its contribution to the susceptibility is negligible.

The final result we report here is a new way of estimating $g_{c2} \approx 0.38$. The previous best calculation [15] was based on vanishing of the triplet gap in the spin liquid phase. A previous attempt [15] 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 new estimate is based on Ising expansions for the staggered magnetization in the Néel state. The transitions at $c_1$, $c_2$, $c_3$ correspondingly. Energies of the $\sigma$-model. The energy of the triplet excitation vanishes at $g \leq g_{c2}$; 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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FIG. 5. Schematic phase diagram and the excitation spectra of the $J_1 - J_2$ model. Solid lines show the triplet gap, the dashed lines show the gaps of the relevant singlets, and the dotted line shows the gap of the irrelevant singlet.
Fig. 1
Fig. 5

- Simple Neel state
- Neel state with columnar dimerization
- Columnar dimerized spin liquid
- Columnar dimerized spin liquid with plaquette type modulation
- Collinear state

Critical points:
- O(1)xO(1) critical point
- O(3) critical point
- O(1) critical point

1st order transition