On the nature of the transition from the spontaneously dimerized to the Néel phase in the two-dimensional $J_1 - J_2$ model

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We analyze the spectrum of the 2D S=1/2 frustrated Heisenberg model near the transition from the spontaneously dimerized spin-liquid phase into the Néel ordered phase. Two excitation branches: the triplet magnon, and the collective singlet mode, both become gapless at the transition point. However we find that the length scales associated with these modes are well separated at the quantum transition. While in the quantum disordered phase the singlet excitation has finite spectral weight and reflects the existence of spontaneous dimer order, near the transition point the size of the singlet bound state grows exponentially with the correlation length, and hence the quasiparticle residue is exponentially small. Therefore the critical dynamics remains in the O(3) universality class in spite of the four gapless modes.

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Quantum phase transitions between magnetically ordered and disordered phases can take place at $T = 0$ by varying the exchange interactions which can drive the spin-spin correlations from long-range behavior, characterized by an infinite correlation length, towards a short-range regime, typical for disordered phases. An example of a quantum model which exhibits such transitions is the two-dimensional (2D), $S = 1/2$ Heisenberg antiferromagnet (HAFM) on a square lattice. While for uniform nearest-neighbor interactions the HAFM has long-range Néel order in the ground state with sub-lattice magnetization $M \approx 0.3$ [1], inclusion of additional interactions, such as dimerization and/or frustration, leads to increased quantum fluctuations and ultimately vanishing of $M$ at a critical coupling. Examples of transitions caused by local alternation of the exchange couplings are the dimerized HAFM [1], the two-layer HAFM [2,3] and the $CaV_4O_9$ lattice (1/5-th depleted square lattice) [4]. In these cases the local dimer or plaquette correlations eventually win over the long-range Néel order, leading to a non-magnetic ground state. Another route towards a magnetically disordered ground state is introduction of frustrating second-neighbor interactions ($J_2$), in addition to the nearest-neighbor ones ($J_1$) (see Fig.1.). The Néel order disappears at $(J_2/J_1)_c \approx 0.4$ in this case [4,5].

An important issue concerning the quantum transitions mentioned above is their universality class. It is generally accepted that the effective low-energy theory for the 2D Heisenberg systems with a collinear (Néel) order parameter is the $O(3)$ non-linear sigma model (NLSM) in 2+1 dimensions [6]. This field theory contains a single effective coupling constant $g$ and, at $T = 0$, describes the ordered Néel phase for $g < g_c$. For $g > g_c$ the NLSM is in a quantum disordered phase with a finite correlation length. However the determination of $g_c$ and the nature of the disordered phase are beyond the field theory formulation and depend on the specific details of the model. In addition, Berry phases associated with instanton tunneling between topologically different configuration are present in the NLSM [7]. In one dimension the Berry phase effects are known to be important, essentially leading to the difference between the excitations in the integer and half odd-integer spin chains [8]. In 2D Berry phases are also present but their role is less clear. If one neglects these purely quantum effects, the universality class of the quantum transitions in the 2D HAFM should be the same as that of the classical $O(3)$ vector model in 3D [9]. Quantum Monte Carlo simulations performed on the two-layer HAFM [10] and the $CaV_4O_9$ lattice HAFM [11] confirm with high accuracy that the quantum transitions in the above two models are in the $O(3)$ universality class. There also has been a report [11] that the 2D dimerized HAFM exhibits a deviation from the $O(3)$ behavior, which is presumably due to the small size lattices studied in the above work. Generally the most accurate Monte Carlo results seem to indicate that the quantum Berry phase effects are not important, at least in the models where the quantum transitions are driven by explicit (exchange driven) dimerization.

On the other hand the $J_1 - J_2$ model, which exhibits a quantum transition due to frustration, has a much better chance for deviation from the $O(3)$ universality class. The reason is that the Berry phases were shown to be relevant and intimately related to the presence of spontaneous dimer (spin-Peierls) order in the quantum disordered phase of this model [12,13]. Within the formalism of the large $N$ expansion for the $Sp(N)$ theory ($N = 1$ being the physical limit), Read and Sachdev [13] found two divergent length scales at the transition from the quantum disordered into the Néel ordered phase. The first one is the usual correlation length $\xi$ which governs the exponential decay of the spin-spin correlations in the disordered phase and is inversely proportional to the (triplet) magnon gap, $\xi \propto 1/\Delta$. The instanton effects however lead to the appearance of spontaneous spin-Peierls correlations and a second gapped singlet mode with a charac-
teristic scale $\xi_{SP}$ (inverse singlet mass). The two scales are related via:

$$\xi_{SP} \sim \xi^{CN}, \ N \gg 1,$$

where $C = C_1 + O(1/N), C_1 \sim 1$. Since $N$ is large one expects $\xi_{SP} \gg \xi$. The presence of two divergent length scales at the transition point would naively suggest a change in the universality class. However, as argued in Ref. [20], the fact that $\xi_{SP}$ is a (large) power of $\xi$, causing the two scales to be well separated near the critical point, is a characteristic feature of a dangerously irrelevant coupling. This means that even though the Berry phases are relevant in the disordered phase, ultimately, near the critical point, their effect disappears. In particular the dimer order parameter $D$ is expected to behave as $D \sim \xi_{SP}^{-1} \sim \Delta^{CN}$ and thus vanishes very fast as the critical point ($\Delta \to 0$) is approached [19]. In this scenario the quantum critical fluctuations of the Néel order parameter are decoupled from the singlet mode and consequently the transition is still of $O(3)$ type. Notice that the above analysis is certainly valid provided the $1/N$ expansion behaves well, since only then the $N \to \infty$ results are relevant to the physical situation $N = 1$. However corrections beyond the $N = \infty$ limit have not been systematically calculated in the literature, due to the complex nature of the problem.

The purpose of the present work is to analyze the structure of the excitation spectrum and the scales that appear near the quantum critical point in order to test the $Sp(N)$ field theory predictions. We work directly with the physical spin problem ($N = 1$) and the approximate scheme that we use is based on a perturbative expansion around the spontaneously dimerized ground state in the quantum disordered phase. First, let us mention that the numerical implementation of this expansion via the dimer series expansion [22] [23], as well as the mean-field [24] and diagrammatic treatments [22], confirm the stability of the spontaneously dimerized phase for intermediate values of frustration. This means that the large $N$ limit captures the essential physics of the problem, even though it cannot be trusted numerically in regards to the exact location of the phase boundaries. However both the series expansions and the diagrammatic method are not accurate enough to calculate reliably the critical exponents near the transition into the Néel phase, since the exponents are not expected to vary considerably. For example the exponent $\nu$ governing the vanishing of the triplet gap: $\Delta \sim (g - g_c)^{\nu}$, is $\nu \approx 0.71$ for the $O(3)$ and $\nu \approx 0.75$ for the $O(4)$ universality class [22]. Such small difference can not be confidenty resolved with the above methods [22]. This is why we will follow a different route, namely we will analyze the possibility of having additional soft modes at the transition (in addition to the triplet mode).

The Hamiltonian of the frustrated Heisenberg antiferromagnet is:

$$H = J_1 \sum_{NN} S_i S_j + J_2 \sum_{NNN} S_i S_j,$$

where $J_1 > 0$ is the nearest-neighbor, and $J_2 > 0$ is the frustrating next-nearest-neighbor exchange coupling on a square lattice (defined as shown in Fig.1). All the spins $S_i = 1/2$. In order to find the excitation spectrum of $H$ we follow closely the treatment of Ref. [22] which is briefly outlined below. The starting point is grouping the spins into dimers (singlets) in the pattern, shown in Fig.1. This configuration (which is degenerate with three others, obtained by translation by one lattice site, rotation by $\pi/2$, and rotation plus translation) was found to be stable in the parameter window $(J_2/J_1)_{c1} < J_2/J_1 < (J_2/J_1)_{c2}$ [22]. Here $(J_2/J_1)_{c1} \approx 0.38$ is the transition point into the Néel phase, the neighborhood of which is the region we want to analyze. The Hamiltonian can be expressed in terms of bosonic operators $t_{\alpha}^\dagger, \alpha = x, y, z$ creating three degenerate triplet excitations from the singlets formed by each pair of spins, as shown in Fig.1. The site index $i$ now numbers the sites on the dimerized lattice. The effective Hamiltonian describing the interactions between the triplets is [22]:

$$H = H_2 + H_3 + H_4,$$

$$H_2 = \sum_{\mathbf{k},\alpha} \left\{ A_\mathbf{k} t_{\mathbf{k}\alpha}^\dagger t_{\mathbf{k}\alpha} + \frac{B_{\mathbf{k}}}{2} \left( t_{\mathbf{k}\alpha}^\dagger t_{-\mathbf{k}\alpha}^\dagger + h.c. \right) \right\}, \quad (4)$$

$$H_3 = \sum_{1+2=3} R(\mathbf{k}_1,\mathbf{k}_2) c_{\alpha\beta\gamma} t_{\mathbf{k}_1\alpha}^\dagger t_{\mathbf{k}_2\beta}^\dagger t_{\mathbf{k}_3\gamma} + h.c., \quad (5)$$

$$H_4 = \sum_{1+2=3+4} \left[ T(\mathbf{k}_1 - \mathbf{k}_3) (\delta_{\alpha\delta} \delta_{\beta\gamma} - \delta_{\alpha\beta} \delta_{\gamma\delta}) + \right.$$

$$+ U \delta_{\alpha\delta} \delta_{\beta\gamma} t_{\mathbf{k}_1\alpha}^\dagger t_{\mathbf{k}_2\beta}^\dagger t_{\mathbf{k}_3\gamma} t_{\mathbf{k}_4\delta} \right], \quad (6)$$

The following definitions are used in Eqs.(4-6): $A_\mathbf{k} = J_1 - (J_1/2) \xi_{k_x} + (J_1 - J_2) \xi_{k_y} - J_2 \xi_{k_z}, \xi_{k_x}, B_{\mathbf{k}} = A_\mathbf{k} - J_1$, and the matrix elements in the quartic and cubic interaction terms: $4T(\mathbf{k}) = J_1 \xi_{k_x} + 2(J_1 + J_2) \xi_{k_y} + 2J_2 \xi_{k_z}, \xi_{k_y}, 4R(\mathbf{p},\mathbf{q}) = -J_1 \gamma_{p\gamma} - 2J_2 \gamma_{p\gamma}, \xi_{p\gamma} - \{p \to q\}$, where we have defined $\xi_k = \cos(k), \gamma_k = \sin(k)$. The $T$ and $R$ terms describe the inter-site interactions arising from the exchange between the dimers. An additional on-site ($U$) term is also introduced and one must set $U \to \infty$. This term reflects the hard-core nature of the bosons which follows from the kinematic constraint on the Hilbert space $t_{\alpha}^\dagger t_{\alpha}^\dagger = 0$. The constraint is necessary in order to ensure that the bosonic Hamiltonian in terms of the triplet operators corresponds uniquely to the original spin Hamiltonian $H$ and no unphysical states appear in the final result. The sums over $\mathbf{k}$ extend over the Brillouin zone of the dimerized lattice, i.e. $-\pi \leq k_x, k_y \leq \pi$. In this notation the Néel ordering wave-vector ($(\pi, \pi)$ of the original lattice) is $Q_{AF} = (0, \pi)$. 

$$H = J_1 \sum_{NN} S_i S_j + J_2 \sum_{NNN} S_i S_j,$$

where $J_1 > 0$ is the nearest-neighbor, and $J_2 > 0$ is the frustrating next-nearest-neighbor exchange coupling on a square lattice (defined as shown in Fig.1). All the spins $S_i = 1/2$. In order to find the excitation spectrum of $H$ we follow closely the treatment of Ref. [22] which is briefly outlined below. The starting point is grouping the spins into dimers (singlets) in the pattern, shown in Fig.1. This configuration (which is degenerate with three others, obtained by translation by one lattice site, rotation by $\pi/2$, and rotation plus translation) was found to be stable in the parameter window $(J_2/J_1)_{c1} < J_2/J_1 < (J_2/J_1)_{c2}$ [22]. Here $(J_2/J_1)_{c1} \approx 0.38$ is the transition point into the Néel phase, the neighborhood of which is the region we want to analyze. The Hamiltonian can be expressed in terms of bosonic operators $t_{\alpha}^\dagger, \alpha = x, y, z$ creating three degenerate triplet excitations from the singlets formed by each pair of spins, as shown in Fig.1. The site index $i$ now numbers the sites on the dimerized lattice. The effective Hamiltonian describing the interactions between the triplets is [22]:

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$$H_2 = \sum_{\mathbf{k},\alpha} \left\{ A_\mathbf{k} t_{\mathbf{k}\alpha}^\dagger t_{\mathbf{k}\alpha} + \frac{B_{\mathbf{k}}}{2} \left( t_{\mathbf{k}\alpha}^\dagger t_{-\mathbf{k}\alpha}^\dagger + h.c. \right) \right\}, \quad (4)$$

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$$H_4 = \sum_{1+2=3+4} \left[ T(\mathbf{k}_1 - \mathbf{k}_3) (\delta_{\alpha\delta} \delta_{\beta\gamma} - \delta_{\alpha\beta} \delta_{\gamma\delta}) + \right.$$
The spectrum of Eq. (3) was studied in Ref. [22] by summing selected infinite series in the perturbative expansion. The dilute Bose gas approximation was used and the diagrams classified in powers of the density of magnons. The diagrammatic treatment was also compared with numerical results obtained by high-order dimer series expansions and the agreement was found to be very good. We will therefore present only diagrammatic results from now on. In the quantum disordered phase \((J_2/J_1)_{c1} < J_2/J_1 < (J_2/J_1)_{c2}\) the triplet excitation spectrum \(\omega(k)\) has a non-zero gap \(\Delta = \omega(Q_{AF})\) which reflects the fact that the dimer configuration is stable. As the critical point \((J_2/J_1)_{c1} = 0.38\) is approached, \(\Delta \to 0\), signaling an instability towards a phase with non-zero Néel order parameter. The variation of \(\Delta\) as a function of frustration is shown in Fig. 2. Let us mention that as we move close to the critical point from the disordered side, the density of triplets increases and is approximately 0.3 at \(J_2/J_1 = 0.38\). This leads, in principle, to a 30\% uncertainty in the results due to the omitted higher order diagrams. However the accuracy in the position of the critical point (0.38) is much better than 30\% because of the steep dependence of the gap on \(J_2/J_1\). Nevertheless, within the accuracy of our calculation the point where \(\Delta \approx 0.05 J_1\) (see Fig. 2) is practically indistinguishable from the critical point.

In Ref. [22] it was pointed out that an additional collective low-energy mode also exists near \((J_2/J_1)_{c1}\). This excitation is a bound state of two triplets with total spin \(S = 0\). We proceed to investigate its properties in more detail. Introducing the total \((Q)\) and the relative \((q)\) momenta of the two triplets forming the bound state, the two-particle singlet is:

\[
|\Psi_Q \rangle = \sum_{q, \alpha} \Psi(q, Q) t^\dagger_{\alpha, 0, Q/2+q} t^\dagger_{\alpha, 0, Q/2-q} |0 \rangle. \tag{7}
\]

The bound state wave-function \(\Psi(q, Q)\) satisfies the integral equation:

\[
\left[ E^S(Q) - \omega_{Q/2+q} - \omega_{Q/2-q} \right] \Psi(q, Q) = \int \frac{dp}{(2\pi)^2} \left\{ -2[T(p-q) + T(p+q)] + U \right\} \Psi(p, Q), \tag{8}
\]

which can be easily derived by noticing that it is equivalent to the two-particle Schrödinger equation: \(H|\Psi_Q \rangle = E^S(Q)|\Psi_Q \rangle\). Here \(E^S(Q)\) is the energy of the collective mode. The function \(T(q)\) is the two-particle scattering amplitude from [3]:

\[
T(k) = \frac{J_1}{4} \cos k_x + \frac{(J_1 + J_2)}{2} \cos k_y + \frac{J_2}{2} \cos k_x \cos k_y. \tag{9}
\]

This interaction leads to attraction between two triplets in the singlet channel. In Eq. (8) the (second-order) contribution of \(H_3\), Eq. (5) into binding has been neglected.

We have checked that the perturbative inclusion of this term indeed leads only to a small change of the results presented below. Since we have to take \(U \to \infty\), the following replacement must be made on the right hand side of Eq. (8): \(U \int dp \Psi(p, Q) \to \lambda\), where \(\lambda\) is a Lagrange multiplier, determined self-consistently from the condition \(\int dq \Psi(q, Q) = 0\). The bound state exists only if a solution of Eq. (8) can be found such that \(E^S(Q) < E_c(Q) = \min_q [\omega(Q/2+q) + \omega(Q/2-q)]\), meaning that it must be below the two-particle scattering continuum \(E_c\). In Fig. 3 we present the numerical solution of Eq. (8) for a fixed value of frustration \((J_2/J_1 = 0.4)\) above the critical value. We have also plotted the one-particle spectrum \(\omega(k)\), and the shaded region is the two-particle scattering region \(E > E_c(k)\). The bound state is stable (non-zero gap) for all \(k\) throughout the disordered phase, with a minimum of the dispersion \(E^S(k)\) at \(k = (0, 0)\). As frustration decreases the singlet gap \(E^S(0,0)\) decreases and appears to vanish at the critical point, as shown in Fig. 2.

We believe that the existence of a singlet bound state at \(k = (0, 0)\) reflects the spontaneous nature of the dimer order. Indeed, we have checked that in models where the dimerization is explicit, i.e. due to stronger exchange on certain bonds, the singlet does not exist in the neighborhood of \(k = (0, 0)\), meaning that its binding energy is zero. The binding energy is defined as \(\epsilon(k) = E_c(k) - E^S(k)\). We have found that \(\epsilon(0,0) = 0\) both in the 2D dimer model (as defined in Ref. [3]) and in the two-layer model (Ref. [4]). Unlike the above two models, the Hamiltonian Eq. (4) does not break any lattice symmetries, but the ground state of Fig. 1 certainly does. It was argued in Ref. [22] that the vanishing of the spontaneous dimer order at the critical point is intrinsically related to the low energy singlet mode. Thus we believe that the singlet bound state reflects the presence of non-zero dimer order parameter in the \(J_1-J_2\) model, i.e. the spontaneous breakdown of the discrete lattice symmetries in the quantum disordered phase.

Even though we have shown that the gaps for both the triplet and singlet modes vanish at the critical point, this does not necessarily mean a departure from the \(O(3)\) universality class which is related to the triplet only. In what follows we will in fact demonstrate that the singlet mode is "irrelevant" at the critical point. Let us start with the observation that the relevancy (or otherwise) of a soft excitation is directly related to its spectral weight. We find, as expected, that the spectral weight of the triplets (the residue of the one-particle Green’s function) stays finite at the transition point. However, the spectral weight of the collective singlet excitation is proportional to the binding energy (which in turn is inversely proportional to the size of the bound-state wave function). Observe that the lower edge of the two-particle continuum at \(k = (0, 0)\), \(E_c(0,0) = 2\omega(Q_{AF}) = 2\Delta\), and since at the transition point \(\Delta \to 0\), the binding energy must...
vanish as well, $\epsilon(0,0) \to 0$. The variation of the binding energy as a function of frustration, obtained by solving Eq. (8) numerically, is shown in Fig. 2. Since we realize that for $\Delta \to 0$ the accuracy of the calculation decreases, let us find the asymptotic behavior of $\epsilon(0,0)$ in this limit analytically. The one-particle dispersion around its minimum has the form: $\omega^2(k) = \Delta^2 c^2 |k - Q_{AF}|^2$, which is valid close to the critical point. The triplet velocity $c$ is known to remain finite at the transition [2, 4], $\Delta c \sim J_1$, where $\Delta \sim 1$ (in units of the inverse lattice spacing) is a characteristic momentum. Denoting the right hand side of Eq. (8) by $\Phi(q, Q)$, the solution of (8) at $Q = (0,0)$ is: $\Psi(q,0) = \Phi(q,0)[E^S - 2\omega(q)]^{-1}$. We define $E^S = E^S(0,0)$ and $\epsilon = \epsilon(0,0)$ from now on. The energy can be found from the condition: $\int dq \Psi(q,0) = 0$. This integral diverges logarithmically at $Q_{AF}$ for small binding:

$$\int \frac{d^2 q}{2\omega(q) - E^S} \sim \frac{\Lambda}{c} + \frac{\Delta}{c^2} \ln \left( \frac{\Delta c}{\epsilon} \right), \quad \epsilon \ll \Delta \ll J_1. \quad (10)$$

We remind that $\epsilon = 2\Delta - E^S$. When estimating the integral, $\Phi(q,0)$ can be replaced by $\Phi(Q_{AF},0)$. This quantity is finite at the critical point which follows from Eq. (8). From (10) we find the binding energy:

$$\epsilon = \epsilon_0 \exp \left( -\frac{\epsilon_1}{\Delta} \right), \quad \Delta \ll J_1, \quad (11)$$

where $\epsilon_0, \epsilon_1 \sim J_1$ are two constants that depend weakly on $J_2$ and are finite at the critical point. The result is similar to the formula for the exponentially small s-wave bound state in a 2D potential [26]. However there are two differences from the usual expression [26]: 1.) the pre-exponential factor in Eq. (11) does not depend on the “mass” $\Delta$ because of the relativistic form of the dispersion near the transition point, and 2.) because of the hard core constraint ($U \to \infty$) the exponent $\epsilon_1$ can not be written as $|\int U dr|^{-1}$, where $U$ is the attractive potential (i.e. the expression in the curly brackets in Eq. (8)),

In Fig. 2 we present a fit of the formula (11) to the numerical solution of (8). The major disagreement occurs only close to the critical point, for $J_2/J_1 < 0.41$. The asymptotically exact solution predicts an exponentially fast vanishing of $\epsilon$ which can not be captured reliably in the numerical solution.

The size $R$ of the bound state (in units of the lattice spacing) is determined by the spatial extent of the wavefunction: $R^2 = \sum_q |\Psi(q)|^2$, where $\Psi$ is assumed normalized. Evaluating this expression for $\Delta \to 0$ leads to

$$R^2 \sim \frac{J_2^2}{\epsilon \Delta} \sim \xi \exp(C_\xi \xi), \quad \xi \gg 1, \quad (12)$$

where $\xi \sim \Delta^{-1}$ is the correlation length, and $C_\xi \sim 1$ is a constant. Thus we find, as expected, that the size increases as the binding energy decreases. At the critical point $R$ diverges exponentially with the correlation length. This in turn implies that the spectral weight of the collective singlet vanishes exponentially fast. Consequently the singlet bound state does not influence the triplet dynamics near the critical point and hence can not change the $O(3)$ universality class.

Unlike the theory of Read and Sachdev [19], our approach does not relate directly the gap in the singlet spectrum and the dimer order parameter. The latter quantity is defined as $D = \langle S_2 S_3 \rangle - \langle S_1 S_2 \rangle$ (see Fig.1.). We have presented arguments [22] that the low-energy singlet affects the dimer order by increasing the quantum fluctuations. This effect becomes stronger and stronger as the critical point is approached and one could ultimately expect that $D$ vanishes. High order dimer series results support this conclusion [22], but can not determine the critical behavior of $D$. Thus we can not verify the prediction of the large-$N$ theory (which follows from Eq. (11)) that $D$ should vanish with a large exponent.

In summary, we have found that in the 2D $J_1 - J_2$ model the critical behavior near the transition between the spontaneously dimerized and the Néel phase is characterized by two soft modes - the usual triplet magnon mode, and a collective singlet excitation. Even though the gap in the singlet spectrum vanishes at the transition, we argue that it does not influence the critical dynamics of triplet excitations. The reason is that the spectral weight of the singlet vanishes exponentially fast at the quantum critical point. We have to note that our picture is different from that of Read and Sachdev [18, 19], based on the large-$N$ expansion. In [18, 19] the singlet gap was found to be much smaller than the triplet one, which in turn leads to the second large length scale. In our picture the singlet gap is approximately equal to two triplet gaps, and the large length scale comes from the size of the singlet bound state. Nevertheless the final conclusion concerning the triplet critical dynamics is the same: the $O(3)$ universality class describes the transition between the Néel ordered and quantum disordered phase.

Finally let us mention that in cases where the ordered phase is characterized by incommensurate correlations (e.g. the triangular lattice Heisenberg model) the critical behavior could be quite different. On semi-classical level the order parameter has $SO(3)$ symmetry and consequently an $O(4)$ universality class is possible [27]. If indeed the $O(4)$ class is realized in this case, the singlet mode should become a truly Goldstone mode at the transition and therefore must have very different properties from the ones found in the present work.

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FIG. 1. The $J_1 - J_2$ model on a square lattice. The circles represent spins paired in singlets in the columnar ladder dimerization pattern.

FIG. 2. Gaps in the one and two-particle excitation spectra. Solid squares, connected by a solid line, represent the triplet gap $\Delta = \omega(Q_{AF})$, and open circles connected with a dashed line represent the gap of the two-particle singlet bound state at $k = (0, 0)$. Open squares are the singlet binding energy, obtained by solving Eq.(8) numerically, while the solid line is the fit, based on the asymptotic formula, Eq.(11), with $\epsilon_0 = 2.85J_1, \epsilon_1 = 1.20J_1$.

FIG. 3. Triplet magnon excitation spectrum (solid line), and the singlet bound state excitation branch (long-dashed line) in the part of the Brillouin zone near $(0, 0)$ and $Q_{AF}$. The shaded area represents the two-magnon scattering continuum. All spectra are calculated diagrammatically for $J_2/J_1 = 0.40$. 

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[27] P. Azaria and B. Delamotte, in Magnetic systems with competing interactions, edited by H.T. Diep, (World Scientific, Singapore, 1994).
Fig. 2.
Fig. 3.