

## Ising phase in the $J_1$ - $J_2$ Heisenberg model

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The two-dimensional Heisenberg antiferromagnet on the square lattice with nearest ( $J_1$ ) and next-nearest ( $J_2$ ) neighbor couplings is investigated in the strong frustration regime ( $J_2/J_1 > 1/2$ ). A new effective field theory describing the long wavelength physics of the model is derived from the quantum Hamiltonian. The structure of the resulting nonlinear sigma model allows us to recover the known spin wave results in the collinear regime, supports the presence of an Ising phase transition at finite temperature, and suggests the possible occurrence of a nonmagnetic ground state breaking rotational symmetry. By means of Lanczos diagonalizations we investigate the spin system at  $T=0$ , focusing our attention on the region where the collinear order parameter is strongly suppressed by quantum fluctuations and a transition to a nonmagnetic state occurs. Correlation functions display a remarkable size independence and allow us to identify the transition between the magnetic and nonmagnetic region of the phase diagram. The numerical results support the presence of a nonmagnetic phase with orientational ordering.

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### I. INTRODUCTION

Frustrated low-dimensional spin systems are still extensively investigated since they show rich phase diagrams and exhibit unusual quantum phases. A typical example is the square-lattice  $J_1$ - $J_2$  model; a Heisenberg antiferromagnet with competing couplings ( $J_1, J_2 > 0$ ) between nearest neighbor ( $\langle \rangle$ ) and next-nearest neighbor ( $\langle \langle \rangle \rangle$ ) spins,

$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + J_2 \sum_{\langle \langle i,k \rangle \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_k, \quad (1)$$

where  $\hat{\mathbf{S}}_i$  are spin operators. By varying the frustration ratio  $\alpha = J_2/J_1$ , quantum phase transitions between magnetically ordered and disordered phases can take place at  $T=0$ . The interest in the 2D frustrated antiferromagnets has deep theoretical motivations in the characterization of disordered spin liquids (or Bose liquids). Moreover, several magnetic materials have been synthesized nowadays where frustration plays a dominant role.<sup>1</sup> In particular, the specific interest on the frustrated Heisenberg model on a square lattice raised with the discovery of vanadate compounds, whose magnetic behavior is likely to be described by the  $J_1$ - $J_2$  Hamiltonian.<sup>2</sup>

In the classical limit ( $S \rightarrow \infty$ ) at weak frustration, the ground state (GS) has conventional Néel order with magnetic wave vector  $\mathbf{Q} = (\pi, \pi)$  for  $\alpha < 0.5$ . Above this threshold, the two sublattices are antiferromagnetically ordered but remain free to rotate with respect to each other and the GS manifold has an  $O(3) \times O(3)$  degeneracy, larger than expected on the basis of the  $O(3)$  symmetry of the Hamiltonian. Weak quantum fluctuations, via the *order by disorder* mechanism, can be included by use of spin wave theory, and are shown to select a collinear ordered state with magnetic wave vector  $\mathbf{Q} = (\pi, 0)$  or  $(0, \pi)$ , reducing the GS degeneracy to  $O(3) \times Z_2$ . In fact, the collinear state breaks both the  $O(3)$  spin rotational invariance of the Heisenberg Hamiltonian and the  $\pi/2$  rotational symmetry of the square lattice ( $Z_2$ ). In the  $S \rightarrow \infty$  limit, according to spin wave theory,<sup>3</sup> the critical coupling  $\alpha_c = 1/2$  marks the first order transition between the

collinear and the Néel phase. However, when quantum fluctuations are taken into account beyond perturbation theory (at least) one intermediate phase is expected to separate the two magnetically ordered phases.<sup>1</sup>

Nevertheless, on the basis of a very recent perturbative numerical renormalization group analysis no evidence for an intermediate phase has been found and it has been proposed that a direct and unexpected second order phase transition may occur at the classical critical point.<sup>4</sup>

The aim of this work is to investigate the quantum phase transition occurring at  $T=0$  as the frustration ratio  $\alpha$  is decreased, i.e., when the collinear order is suppressed by quantum fluctuations. To this purpose, the effective long-wavelength action of the two-dimensional quantum model in the regime of strong frustration is mapped into a nonlinear sigma model (NLSM) in 2+1 dimension. This is the first time that the mapping, originally proposed by Haldane for a Heisenberg chain,<sup>5</sup> is properly generalized to the strongly frustrated  $J_1$ - $J_2$  model. On the basis of the symmetries of the NLSM action, an Ising phase, breaking the  $\pi/2$  rotational symmetry of the square lattice and preserving the  $O(3)$  spin rotational invariance, may exist both at low and zero temperature. While the stability of this phase at finite temperature has been previously investigated,<sup>6-9</sup> it has never been explicitly examined if such an Ising state is stable at zero temperature for some values of the frustration ratio lower than the one corresponding to the onset of the collinear order. Lanczos diagonalizations support this scenario via a careful examination of both the excitation spectrum and the correlation functions. A nonmagnetic valence bond nematic phase with orientational ordering is the most favorable candidate as a ground state in a portion of the phase diagram.

### II. NONLINEAR SIGMA MODEL FOR THE COLLINEAR PHASE

Among the various theoretical approaches adopted for the  $J_1$ - $J_2$  model in the regime of weak frustration, the NLSM

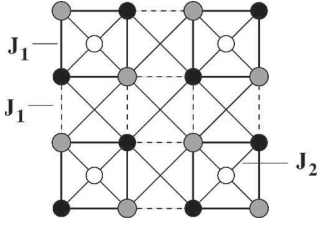


FIG. 1. Lattice of the  $J_1$ - $J_2$  model. The lattice spacing is  $a$ . Grey and black circles denote  $+$  and  $-$  sublattice sites, respectively, while white circles the center of each plaquette, where the fields  $\hat{\mathbf{n}}_+$ ,  $\hat{\mathbf{n}}_-$  and  $\mathbf{L}_+$ ,  $\mathbf{L}_-$  are defined.

method is particularly suitable for the study of the phase transition between a magnetically ordered state and a disordered phase. The 2D frustrated Heisenberg antiferromagnet with  $\alpha < \alpha_c$  is mapped to a  $O(3)$  NLSM in  $D=2+1$  dimension,<sup>10,11</sup> which indeed shows a second order (quantum) phase transition to a nonmagnetic state at  $T=0$ . When frustration is strong and the GS is collinear, the mapping to a 3D classical model is still possible, but the effective long-wavelength action is no longer a conventional  $O(3)$  NLSM.

Here we generalize the original mapping proposed by Haldane for the microscopic derivation of the long-wavelength, low-energy effective theory of one-dimensional quantum antiferromagnets in the Néel phase,<sup>5</sup> to the  $J_1$ - $J_2$  model in the strong frustration regime, where collinear order is expected. By using the Trotter formula and a coherent state basis in the spin Hilbert space, the partition function of the system is written in a path integral representation as

$$\mathcal{Z} = \int \mathcal{D}\hat{\Omega} \exp(-S[\hat{\Omega}]), \quad (2)$$

where  $\hat{\Omega}_i(t)$  is a classical  $O(3)$  vector field defined on each lattice site, normalized to  $\hat{\Omega}_i^2(t)=1$  and  $S$  is the action at a temperature  $\beta^{-1}$ ,

$$S[\hat{\Omega}(\tau)] = -iS \sum_i \omega[\hat{\Omega}_i(\tau)] + \int_0^\beta d\tau \mathbf{H}[\hat{\Omega}(\tau)]. \quad (3)$$

The first (purely imaginary) term is the Berry phase<sup>5</sup> and  $\mathbf{H}[\hat{\Omega}]$  is the expectation value of the Hamiltonian operator on the coherent states basis,

$$\mathbf{H}[\hat{\Omega}] = S^2 J_1 \sum_{\langle i,j \rangle} \hat{\Omega}_i \cdot \hat{\Omega}_j + S^2 J_2 \sum_{\langle\langle i,k \rangle\rangle} \hat{\Omega}_i \cdot \hat{\Omega}_k. \quad (4)$$

In the regime of strong frustration it is convenient to separate the lattice in the two sublattices which will be labeled  $+$  and  $-$ , respectively. Following Haldane,<sup>5</sup> we split the spatially oscillating spin state  $\hat{\Omega}_i$  on the sublattice  $+$  ( $-$ ) as the sum of two orthogonal smooth vector fields, describing the local Néel order  $\hat{\mathbf{n}}_+$  ( $\hat{\mathbf{n}}_-$ ) and the transverse fluctuations  $\mathbf{L}_+$  ( $\mathbf{L}_-$ ), satisfying the constraints  $\hat{\mathbf{n}}_+^2=1$  ( $\hat{\mathbf{n}}_-^2=1$ ) and  $\hat{\mathbf{n}}_+ \cdot \mathbf{L}_+ = 0$  ( $\hat{\mathbf{n}}_- \cdot \mathbf{L}_- = 0$ ). In order to carry out the splitting between the uniform and staggered fluctuations keeping the right number of independent variables, we proceed by partitioning the lattice in plaquettes as shown in Fig. 1. Then we define the Néel

fields ( $\hat{\mathbf{n}}_+$ ,  $\hat{\mathbf{n}}_-$ ) and the associated fluctuations ( $\mathbf{L}_+$ ,  $\mathbf{L}_-$ ) in the center of each plaquette as follows:

$$\hat{\Omega}\left(x + \frac{a}{2}, y + \frac{a}{2}\right) = \eta \hat{\mathbf{n}}_+(\mathbf{r}) \sqrt{1 - \left|\frac{\mathbf{L}_+(\mathbf{r})}{S}\right|^2} + \frac{\mathbf{L}_+(\mathbf{r})}{S}, \quad (5)$$

$$\hat{\Omega}\left(x + \frac{a}{2}, y - \frac{a}{2}\right) = \eta \hat{\mathbf{n}}_-(\mathbf{r}) \sqrt{1 - \left|\frac{\mathbf{L}_-(\mathbf{r})}{S}\right|^2} + \frac{\mathbf{L}_-(\mathbf{r})}{S}, \quad (6)$$

where  $\eta = \pm 1$ ,  $a$  is the spacing of the original lattice and  $\mathbf{r} = (x, y)$  is the coordinate of the plaquette centers which define a square superlattice of spacing  $2a$ . In the continuum limit, to second order in space and time derivatives and keeping the lowest order in  $1/S$ , the partition function is written as

$$\mathcal{Z} = \int \mathcal{D}\hat{\mathbf{n}}_\pm \mathcal{D}\mathbf{L}_\pm \delta(\hat{\mathbf{n}}_+ \cdot \mathbf{L}_+) \delta(\hat{\mathbf{n}}_- \cdot \mathbf{L}_-) e^{-S}, \quad (7)$$

where

$$S = \int d^2\mathbf{x} \int_0^\beta d\tau \mathcal{L}$$

and the Lagrangian is

$$\mathcal{L} = \mathbf{L}^T \mathbf{A} \mathbf{L} - \mathbf{B}^T \mathbf{L} + \mathbf{K}_1 + \mathbf{K}_2. \quad (8)$$

$\mathcal{D}\hat{\mathbf{n}}_\pm$  and  $\mathcal{D}\mathbf{L}_\pm$  mean integration over the Néel fields and the fluctuations in both the sublattices and the six component array  $\mathbf{L}^T = (\mathbf{L}_+, \mathbf{L}_-)$  gathers the (three) components of the two fluctuation fields  $\mathbf{L}_+^\alpha$  and  $\mathbf{L}_-^\alpha$ . The scalars  $\mathbf{K}$  are defined as

$$\begin{aligned} \mathbf{K}_1 &= -S^2 J_1 (\partial_y \hat{\mathbf{n}}_+ \cdot \partial_y \hat{\mathbf{n}}_- - \partial_x \hat{\mathbf{n}}_+ \cdot \partial_x \hat{\mathbf{n}}_-), \\ \mathbf{K}_2 &= S^2 J_2 \sum_{k=\pm} [(\nabla \hat{\mathbf{n}}_k)^2 + k \partial_x \hat{\mathbf{n}}_k \cdot \partial_y \hat{\mathbf{n}}_k], \end{aligned} \quad (9)$$

while the  $6 \times 6$  matrix  $\mathbf{A}$  is written in block form as

$$\mathbf{A} = \frac{1}{a^2} \begin{pmatrix} 2J_2 & J_1 \\ J_1 & 2J_2 \end{pmatrix} \quad (10)$$

and the array  $\mathbf{B}^T = (\mathbf{B}_+, \mathbf{B}_-)$  is given by

$$\begin{aligned} \mathbf{B}_+ &= \frac{-i}{2a^2} (\hat{\mathbf{n}}_+ \times \partial_\tau \hat{\mathbf{n}}_+) + \frac{SJ_1}{a} \vec{\gamma}_- + \frac{2SJ_2}{a} \vec{\gamma}_+, \\ \mathbf{B}_- &= \frac{-i}{2a^2} (\hat{\mathbf{n}}_- \times \partial_\tau \hat{\mathbf{n}}_-) + \frac{SJ_1}{a} \vec{\gamma}_+ + \frac{2SJ_2}{a} \vec{\gamma}_-, \end{aligned}$$

with

$$\vec{\gamma}_+ = \partial_x \hat{\mathbf{n}}_+ + \partial_y \hat{\mathbf{n}}_+, \quad \vec{\gamma}_- = \partial_x \hat{\mathbf{n}}_- - \partial_y \hat{\mathbf{n}}_-.$$

To this order in derivatives the Berry phase contributions  $i\omega[\hat{\mathbf{n}}_+(\tau)]$  and  $i\omega[\hat{\mathbf{n}}_-(\tau)]$  identically vanish.<sup>12</sup> Performing the Gaussian integration of the partition function with respect to fluctuations needs some care due to the constraints  $\hat{\mathbf{n}}_+ \cdot \mathbf{L}_+ = 0$  and  $\hat{\mathbf{n}}_- \cdot \mathbf{L}_- = 0$  which limit the integration to the transverse components of the spin fluctuations  $\mathbf{L}_+^\perp$  and  $\mathbf{L}_-^\perp$ . In

order to release the constraint, we first multiply the partition function by a constant factor  $F$  (which does not affect the physical properties of the model) written as a Gaussian integral over two auxiliary scalar fields  $v_+$  and  $v_-$ ,

$$F = \int \mathcal{D}v_{\pm} e^{-\int d^2x \int_0^{\beta} d\tau (L^{\parallel})^T A L^{\parallel}},$$

where  $\mathbf{L}_{\pm}^{\parallel} = v_{\pm} \hat{\mathbf{n}}_{\pm}$  ( $\mathbf{L}_{\pm}^{\parallel} = v_{\pm} \hat{\mathbf{n}}_{\pm}$ ). By defining the vector  $\mathbf{L}_{\pm} = \mathbf{L}_{\pm}^{\parallel} + \mathbf{L}_{\pm}^{\perp}$  ( $\mathbf{L}_{\pm} = \mathbf{L}_{\pm}^{\parallel} + \mathbf{L}_{\pm}^{\perp}$ ), the integral over fluctuations  $\mathcal{I}$  in Eq. (7) can be written as

$$\mathcal{I} = \int \mathcal{D}\mathbf{L}_{\pm} e^{-\int d^2x \int_0^{\beta} d\tau [(\mathbf{L}^{\perp})^T A \mathbf{L}^{\perp} + (\mathbf{L}^{\parallel})^T A \mathbf{L}^{\parallel} - \mathbf{B}^T \mathbf{L}^{\perp}]},$$

where  $\mathbf{L}_{\pm}^{\perp}$  is explicitly given by  $\mathbf{L}_{\pm}^{\perp} = \mathbf{L}_{\pm} - (\mathbf{L}_{\pm} \cdot \hat{\mathbf{n}}_{\pm}) \hat{\mathbf{n}}_{\pm}$  ( $\mathbf{L}_{\pm}^{\perp} = \mathbf{L}_{\pm} - (\mathbf{L}_{\pm} \cdot \hat{\mathbf{n}}_{\pm}) \hat{\mathbf{n}}_{\pm}$ ). As a result, the partition function is written as an unconstrained integral over the fields  $\mathbf{L}_{\pm}$  and  $\hat{\mathbf{n}}_{\pm}$ . The Lagrangian maintains the same formal structure (8) with a modified matrix  $A$  and array  $B$ ,

$$\begin{aligned} \tilde{A}_{ik}^{\alpha\beta} &= A_{ik}(\delta^{\alpha\beta} - n_i^{\alpha} n_i^{\beta} - n_k^{\alpha} n_k^{\beta} + 2(n_i \cdot n_k) n_i^{\alpha} n_k^{\beta}), \\ \tilde{B}_i^{\alpha} &= B_i^{\alpha} - (\mathbf{B}_i \cdot \hat{\mathbf{n}}_i) \hat{n}_i^{\alpha}, \end{aligned} \quad (11)$$

where Latin indices  $i, k = \pm$  identify the sublattice and Greek superscripts run over the three spin components. In practice, the Gaussian integration has been performed by diagonalizing the matrix  $\tilde{A}$  on its eigenvector basis  $\{u_i^{\alpha}(l)\}_l$  with  $l = 1, \dots, 6$  so that the effective Lagrangian density is expressed in terms of the eigenvalues  $\{\lambda_l\}_l$

$$\mathcal{L} = \mathbf{K}_1 + \mathbf{K}_2 - \frac{1}{4} \sum_l \lambda_l^{-1} b_l^2, \quad b_l = \sum_{i,\alpha} \tilde{B}_i^{\alpha} u_i^{\alpha}(l). \quad (12)$$

After tedious but straightforward calculations, the resulting effective Lagrangian is written as

$$\mathcal{L}[\hat{\mathbf{n}}_+, \hat{\mathbf{n}}_-] = \mathcal{L}_S + \mathcal{L}_A + \mathcal{L}_{\times} \quad (13)$$

with

$$\begin{aligned} \mathcal{L}_S &= \sum_{i=\pm} \left\{ \frac{S^2 J_2}{2} |\nabla \hat{\mathbf{n}}_i|^2 + \frac{J_2}{8a^2 D^*} (\partial_{\tau} \hat{\mathbf{n}}_i)^2 \right\}, \\ \mathcal{L}_A &= -\frac{S^2 J_1}{2} (\partial_y \hat{\mathbf{n}}_+ \cdot \partial_y \hat{\mathbf{n}}_- - \partial_x \hat{\mathbf{n}}_+ \cdot \partial_x \hat{\mathbf{n}}_-), \\ \mathcal{L}_{\times} &= \frac{J_1 J_2^2}{2a^2 D} (\hat{\mathbf{n}}_+ \cdot \partial_{\tau} \hat{\mathbf{n}}_-) (\partial_{\tau} \hat{\mathbf{n}}_+ \cdot \hat{\mathbf{n}}_-) + \frac{J_1^2 J_2}{8a^2 D} [(\hat{\mathbf{n}}_+ \cdot \partial_{\tau} \hat{\mathbf{n}}_-)^2 \\ &\quad + (\partial_{\tau} \hat{\mathbf{n}}_+ \cdot \hat{\mathbf{n}}_-)^2] - \frac{J_1}{8a^2 D^*} \sigma (\partial_{\tau} \hat{\mathbf{n}}_+ \cdot \partial_{\tau} \hat{\mathbf{n}}_-), \end{aligned}$$

where  $D^* = 4J_2^2 - \sigma^2 J_1^2$ ,  $D = D^* (4J_2^2 - J_1^2)$ , and  $\sigma = \hat{\mathbf{n}}_+ \cdot \hat{\mathbf{n}}_-$  is the ‘‘Ising order parameter.’’ The Lagrangian density  $\mathcal{L}$  preserves the  $O(3)$  symmetry of the microscopic Hamiltonian (1) but breaks the invariance of the model under  $\pi/2$  lattice rotation due to the adopted coarse graining procedure.<sup>6</sup> However, the original rotational invariance reflects in the additional  $Z_2$  symmetry of our Lagrangian under the simulta-

neous action of  $\pi/2$  rotation and inversion of one field:  $(x, y) \rightarrow (-y, x)$  and  $\hat{\mathbf{n}}_{\pm} \rightarrow -\hat{\mathbf{n}}_{\pm}$ . The global symmetry group of the resulting field theory is therefore  $O(3) \times Z_2$ .

In order to check the correctness of the effective Lagrangian density  $\mathcal{L}$ , we compare the dispersion relation arising from a saddle point evaluation of the partition function to the known spin wave results. The saddle point configuration corresponds to the minimum of the action, i.e., to a homogeneous and static configuration characterized by two independent unit vectors  $\hat{\mathbf{n}}_+^0$  and  $\hat{\mathbf{n}}_-^0$  which describe one of the degenerate classical ground states. By expanding up to second order in fluctuations  $\hat{\mathbf{n}}_+ = \hat{\mathbf{n}}_+^0 + \delta \hat{\mathbf{n}}_+$  ( $\hat{\mathbf{n}}_- = \hat{\mathbf{n}}_-^0 + \delta \hat{\mathbf{n}}_-$ ) and performing the Gaussian integration we get precisely the same result of spin wave theory in the long wavelength limit.<sup>6,14</sup> The low energy excitations are described by four branches labeled by  $\lambda = \pm 1$  and  $\eta = \pm 1$  whose dispersions are given by

$$\begin{aligned} \omega^2(\mathbf{k}) &= 4S^2 \{ k_x^2 (2J_2 + \eta J_1) (2J_2 + \eta J_1 \cos \theta) + k_y^2 (2J_2 + \lambda J_1) \\ &\quad \times (2J_2 - \lambda J_1 \cos \theta) \}, \end{aligned} \quad (14)$$

where  $\theta$  is the angle between the two Néel fields:  $\cos \theta = \hat{\mathbf{n}}_+^0 \cdot \hat{\mathbf{n}}_-^0$ . Accordingly, perturbation theory on the effective action shows that the lowest free energy is attained when the staggered magnetizations of the two sublattices  $\hat{\mathbf{n}}_+^0$  and  $\hat{\mathbf{n}}_-^0$  are either parallel or antiparallel. The collinear order is stabilized by quantum fluctuations. This picture is believed to be correct in the limit of large frustration ratio  $\alpha$ . By lowering  $\alpha$ , fluctuations are enhanced and a quantum phase transition is expected to occur at zero temperature before reaching the (classical) limiting value  $\alpha = 0.5$ . On the basis of the symmetries of the effective model, an intermediate regime characterized by vanishing staggered magnetization  $\langle \hat{\mathbf{n}}_+ \rangle = \langle \hat{\mathbf{n}}_- \rangle = 0$  and possibly a finite Ising order parameter  $\langle \sigma \rangle = \hat{\mathbf{n}}_+ \cdot \hat{\mathbf{n}}_- \neq 0$  may be present. This hypothetical state would break the rotational symmetry of the lattice preserving the  $SU(2)$  spin symmetry. Due to the coarse graining carried out in the microscopic Hamiltonian, such a state may correspond either to a translationally invariant ‘‘valence bond nematic’’ phase where valence bonds display orientational ordering or to a valence bond crystal (VBC) which breaks the translational symmetry.

A low energy, long wavelength effective field theory for collinear antiferromagnets was put forward in a seminal paper by Chandra, Coleman, and Larkin.<sup>6</sup> At variance with our approach, in that work, quantum fluctuations were integrated out by use of a perturbative spin-wave approximation and the analysis was limited to the finite temperature domain. In this way, CCL predicted a finite temperature Ising transition in two dimensions: Even if at  $T=0$  both sublattices display finite staggered magnetization in zero field, long-range Néel order disappears at any finite temperature, since thermal fluctuations are known to restore the continuous symmetries in two spatial dimensions.<sup>15</sup> CCL suggested that the previously defined Ising order parameter  $\sigma$  may preserve long-range order up to a nonzero critical temperature. Recently the presence of such a finite temperature transition has been the subject of several investigations.<sup>7-9</sup>

The CCL approach, however, cannot be directly applied to the study of the zero temperature limit because the effects

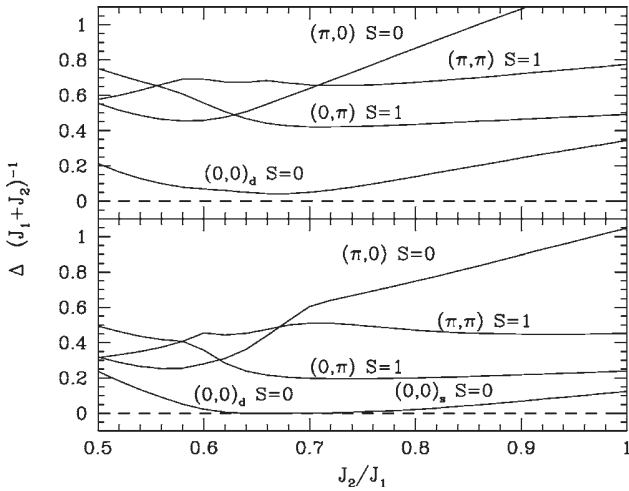


FIG. 2. Low energy states referenced to the GS as a function of the frustration ratio  $\alpha=J_2/J_1$  in the  $4\times 4$  (upper panel) and  $6\times 6$  (lower panel) cluster.

of quantum fluctuations are considered only within perturbation theory. In order to clarify the relationship between our effective field theory and the CCL approach, it is convenient to specialize the Lagrangian  $\mathcal{L}[\hat{\mathbf{n}}_+, \hat{\mathbf{n}}_-]$  to a class of field configurations of the form  $\hat{\mathbf{n}}(\mathbf{r}, t)_+ = \hat{\mathbf{n}}(\mathbf{r})_+^0 + \delta\hat{\mathbf{n}}(\mathbf{r}, t)_+$  ( $\hat{\mathbf{n}}(\mathbf{r}, t)_- = \hat{\mathbf{n}}(\mathbf{r})_-^0 + \delta\hat{\mathbf{n}}(\mathbf{r}, t)_-$ ) characterized by weak fluctuations ( $\delta\hat{\mathbf{n}}(\mathbf{r}, t)$ ) on top of a slowly varying *time independent* (i.e., classical) configuration ( $\hat{\mathbf{n}}(\mathbf{r})$ ). Expanding  $\mathcal{L}$  to second order in the fluctuations and performing the gaussian integration, by use of the result (14), we recover the CCL result. This approach can be justified at large frustration ratios  $\alpha$  (i.e., deep in the collinear regime) where quantum fluctuations are not able to severely affect the classical ground state. However, in order to analyze the quantum transition between collinear order and a disordered phase at  $T=0$ , it is necessary to take into account the effects of quantum fluctuations beyond the spin wave approximation, i.e., we have to study the full effective Lagrangian (13).

### III. LANCZOS DIAGONALIZATIONS

By means of Lanczos diagonalizations (LD) we try to clarify if an Ising state can be stabilized when the long range collinear order fades away, as suggested by the field theoretical approach.

Lanczos diagonalizations have been performed on the  $4\times 4$  and  $6\times 6$  square clusters for spin  $S=1/2$ . By means of LD we obtain the energy spectrum, providing indications of possible changes in the nature of the GS which occur by increasing the frustration ratio.<sup>16,17</sup> In the collinear phase, due to the spatial symmetry breaking, four classes (*towers*) of states with different spatial symmetries are expected to become degenerate: the lowest representative of these classes are an *s*-wave and a *d*-wave singlet at momentum  $(0,0)$  and two triplets at momenta  $(0,\pi)$  and  $(\pi,0)$ . The low energy spectrum as a function of the frustration ratio is shown in Fig. 2. While the behavior of the model for  $\alpha\sim 0.5$  has been

the subject of several investigations<sup>1</sup> and is still a debated problem, here we will concentrate on the GS properties in the regime of larger frustration  $\alpha\gtrsim 0.6$ . A clear tendency to break the rotational symmetry is suggested by the quasidegeneracy of the *s*-wave and *d*-wave singlets which actually cross each other in the  $6\times 6$  cluster. However, this does not rule out the possible occurrence of the collinear phase down to  $\alpha=0.6$ , since the energy gap of the triplet at  $(0,\pi)$  is shown to decrease with the lattice size. The  $(\pi,0)$  singlet gap also decreases with size although it remains considerably larger than the lowest singlet gap and in fact comparable to the  $(\pi,\pi)$  triplet gap which is believed to be finite in the thermodynamic limit for  $\alpha>0.5$ . The  $(\pi,\pi)$  singlet (not shown in figure) is much higher in energy. Therefore, from the ordering of the low energy states we may conclude that: (i) rotational symmetry is broken for  $\alpha\gtrsim 0.6$ ; (ii) triplet states are gapped for  $\alpha\leq 0.62$ ; (iii) the columnar VBC phase is unlikely to occur, at least for  $\alpha\gtrsim 0.62$ ; and (iv) other VBC phases, like a plaquette state,<sup>11,18,19</sup> are not compatible with the observed ordering of levels in the energy spectrum.<sup>20</sup>

The quasidegeneracy between the *s*-wave ( $|s\rangle$ ) and *d*-wave ( $|d\rangle$ ) singlets in the extended range  $0.6<\alpha<0.7$  allows us to consider the two real linear combinations of these states as good representations of the symmetry broken phases which are physically realized in the thermodynamic limit. This is particularly convenient since in a non rotationally invariant state, like  $(|s\rangle\pm|d\rangle)/\sqrt{2}$ , the rotational order parameter  $\hat{O}_r = \hat{S}_r \cdot \hat{S}_{r+\hat{x}} - \hat{S}_r \cdot \hat{S}_{r+\hat{y}}$  (where  $\hat{x}$  and  $\hat{y}$  are the two primitive vectors of the lattice) may acquire a nonzero value. If the two singlets are degenerate and  $\langle\hat{O}_r\rangle$  remains finite in the thermodynamic limit, rotational symmetry breaking occurs in the model.<sup>21</sup> In the thermodynamic limit, this procedure would be fully equivalent to the usual way to evaluate order parameters in terms of the asymptotic behavior of correlation functions  $\langle\hat{O}_r\hat{O}_0\rangle$ . However, in small clusters, we believe that our approach is less affected by finite size effects. The two (quasi) degenerate states have vanishing momentum and then the order parameter  $\langle\hat{O}_r\rangle$  is translationally invariant i.e. independent of  $\mathbf{r}$ . The numerical results are displayed in Fig. 3 together with the probability of finding next neighbor singlets both on horizontal  $P_x$  and vertical  $P_y$  bonds.

A strong anisotropy is present: The order parameter is large and the singlet probability strongly differs in the two spatial directions. Remarkably, around  $\alpha\sim 0.60$ ,  $P_y\sim 0.25$  is compatible with a disordered configuration, while  $P_x$  gets close to the limit characterizing the Heisenberg chain. In essence, the whole system seems to behave as a collection of spin chains weakly coupled in the transverse direction. As  $\alpha$  grows,  $P_x$  stays almost constant, while  $P_y$  decreases, leaving room to the formation of vertical triplets; the system is moving toward the collinear phase.

In order to better characterize the phase diagram we also investigated the behavior of spin correlations. The Fourier transform  $S(\mathbf{k})$  of  $\langle S_0^z S_n^z \rangle$  along a closed path in the Brillouin zone has been calculated both for the *s*-wave and *d*-wave singlet and the results are shown in Fig. 4. The close similarity between the spin correlations in the two states indeed

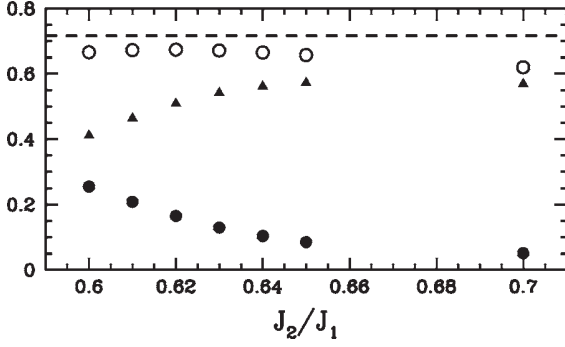


FIG. 3. Properties of the symmetry broken state: Ising order parameter  $\hat{O}$  (triangles); Probability to find next neighbors singlets in a given direction;  $P_\mu = \langle 1 - \frac{1}{2}(\hat{S}_r + \hat{S}_{r+\hat{\mu}})^2 \rangle$ . Empty dots:  $P_x$ , Full dots:  $P_y$ . Dashed line:  $P_x$  for independent Heisenberg chains.

confirms that they both contain the same physics. At  $J_2 = 0.55J_1$   $S(\mathbf{k})$  exhibits a peak at momentum  $(\pi, \pi)$  suggesting that the dominant (short range) correlations are still antiferromagnetic.<sup>22</sup> In the range  $0.60 \lesssim \alpha \lesssim 0.62$   $S(\mathbf{k})$  is remarkably flat and does not show significant size dependence. Instead it seems that for larger frustration  $\alpha$  the system is going to sustain a transition to a collinear phase. Finally, at  $\alpha = 0.7$  the  $(\pi, 0)$  peak in fact grows quite substantially with the size, signaling the onset of the collinear order parameter. A remarkable common feature of the LD results is the collapse of the  $4 \times 4$  and  $6 \times 6$  data on the same smooth curve *except* (possibly) at a single wave vector, which identifies the dominant periodicity in the spin correlations. The LD data then allow for an accurate evaluation of the full momentum

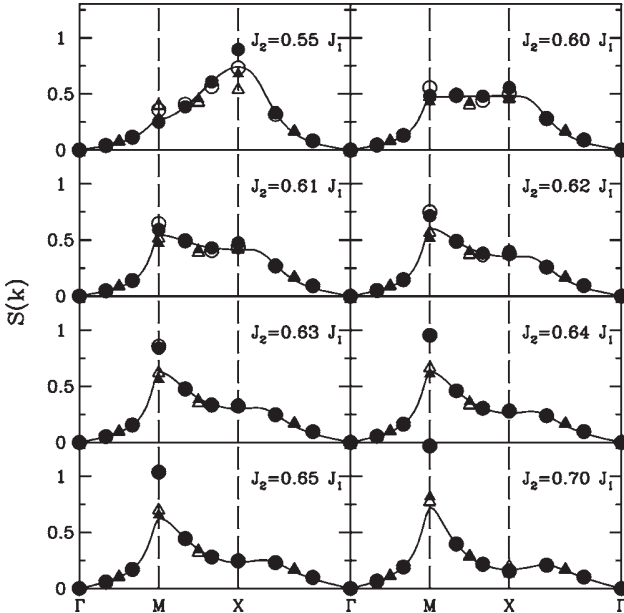


FIG. 4. Magnetic structure factor along a closed path in the Brillouin zone from  $\Gamma = (0, 0)$  to  $M = (0, \pi)$ , to  $X = (\pi, \pi)$  and back to  $\Gamma$ . Full (empty) triangles:  $S(\mathbf{k})$  evaluated on the lowest  $s$ -wave ( $d$ -wave) singlet for a  $4 \times 4$  cluster; Full (empty) dots:  $S(\mathbf{k})$  evaluated on the lowest  $s$ -wave ( $d$ -wave) singlet for a  $6 \times 6$  cluster.

dependence of the magnetic structure factor; we performed a fit of the numerical data (also shown in Fig. 4) with a parameterized form inspired by the spin wave theory results.<sup>23</sup> The chosen function represents quite accurately the numerical data except at the single wave vector where the order parameter sets in and a singular contribution develops in the thermodynamic limit.

#### IV. CONCLUSIONS

In this paper we derived, for the first time, the long wavelength, low energy effective field theory describing quantum and thermal fluctuations in the collinear phase of frustrated 2D antiferromagnets. The resulting NLSM is written in terms of two fields describing the local Néel order parameter of the two sublattices and is invariant under the  $O(3) \times Z_2$  symmetry group. On the basis of this formalism we are led to predict the possible occurrence of a nonmagnetic ground state breaking rotational symmetry for suitable values of the frustration ratio. In order to investigate this possibility, we also performed Lanczos diagonalizations. By a careful inspection of the numerical results we found evidence for the occurrence of the predicted valence bond nematic ground state in a region around  $\alpha \sim 0.6$ . The evaluation of the magnetic structure factor in small clusters also showed that the short range spin correlations of the  $J_1$ - $J_2$  model are remarkably size independent. This observation may be very useful in the interpretation of accurate neutron scattering data on frustrated 2D antiferromagnets.

According to spin wave theory the  $J_1$ - $J_2$  model displays a first order phase transition at  $\alpha_c = 0.5$  between a Néel and a collinearly ordered region in the classical limit ( $S \rightarrow \infty$ ). When quantum fluctuations are taken into account an intermediate  $SU(2)$  invariant phase is stabilized. Many different candidates have been proposed as possible ground states in this region: gapped or gapless spin liquids,<sup>22,24</sup> VBC's with columnar<sup>16,19,20,25</sup> or plaquette patterns.<sup>11,18,19</sup>

At any finite temperature, the continuous spin rotational symmetry, broken in the collinear phase, is restored and only the breaking of the symmetry corresponding to the order parameter  $\sigma = \hat{\mathbf{n}}_+ \cdot \hat{\mathbf{n}}_-$  can in principle survive up to a finite critical temperature defining a phase transition which lies in the 2D Ising universality class.<sup>6</sup> The hypothesis that as  $T \rightarrow 0$  the transition line ends in a point different from the one corresponding to the onset of the collinear order can not be excluded *a priori*. In such a case, the ground state in a portion of the intermediate  $SU(2)$  invariant region may be a valence bond nematic phase with some orientational ordering. This possible scenario is consistent with the suggestions of the analytical results based on the NLSM action and has been confirmed by a LD analysis.

Because of the quasidegeneracy in the energy spectrum in a region around  $\alpha \sim 0.60$ , a state characterized by an orientational symmetry breaking is very likely to occur, ruling out the fully symmetric spin liquid. Similarly, the ordering of excited states is not compatible with the plaquette VBC.

A careful analysis of the low energy spectrum and of the correlation functions suggests that a zero temperature transition takes place at  $\alpha_c \sim 0.62$ . The transition separates the large  $\alpha$  collinear phase and an intermediate gapped regime breaking the  $\pi/2$  rotational symmetry of the lattice. Thus on the basis of our investigations we argue that such a phase may be conveniently thought of as “nematic” ordering of valence bonds and anticipates an isotropic spin liquid (or a VBC) which is likely to occur at lower  $\alpha$ .

A direct transition between the collinear phase and a VBC should be of the first order, the two phases having different order parameters. Instead the transition to the Ising phase may be of second order being related just to the vanishing of the sublattice staggered magnetization. Our analysis is not able to discriminate between second order and weakly first order transition; Monte Carlo simulations of the NLSM action derived here will be helpful to supplement LD data in order to clarify this issue.

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<sup>12</sup>This is true within the  $O(3)$  NLSM approach where it is assumed that the Néel field is well defined at all points in  $(2+1)$  dimensional space-time. However if this assumption is relaxed to allow “hedgehog” (spatial) singularities of the Néel field then a dependence on the quantized value of the spin  $S$  appears and the

Berry term may contribute to the Boltzmann weight of the configuration (Ref. 13).

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