

# Spin-wave analysis to the spatially anisotropic Heisenberg antiferromagnet on a triangular lattice

Adolfo E. Trumper\*

The Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, P.O. Box 586, 34100 Trieste, Italy

(Received 12 October 1998; revised manuscript received 22 March 1999)

We study the phase diagram at  $T=0$  of the antiferromagnetic Heisenberg model on the triangular lattice with spatially anisotropic interactions. For values of the anisotropy very close to  $J_\alpha/J_\beta=0.5$ , conventional spin-wave theory predicts that quantum fluctuations melt the classical structures, for  $S=1/2$ . For the regime  $J_\beta < J_\alpha$ , it is shown that the incommensurate spiral phases survive until  $J_\beta/J_\alpha=0.27$ , leaving a wide region where the ground state is disordered. The existence of such nonmagnetic states suggests the possibility of spin-liquid behavior for intermediate values of the anisotropy. [S0163-1829(99)03529-8]

For a long time frustrated quantum antiferromagnets have been intensively studied. In this context, the antiferromagnetic Heisenberg model on a triangular lattice is a prototype for such systems. From the proposition of Anderson and Fazekas that this model is a candidate to exhibit spin-liquid behavior,<sup>1</sup> a lot of work was done to understand the nature of its ground state. Although there is a general conviction that the ground state is ordered with a magnetic vector  $\mathbf{Q}=(4\pi/3,0)$ ,<sup>2,3</sup> some authors found a situation very close to a critical one or no magnetic order at all, leaving the answer still controversial.<sup>4,5</sup> A systematic way to study the role of frustration is to vary the strength of the exchange interaction along the bonds. Recently Bhaumik *et al.*<sup>6</sup> explored the existence of collinear phases on triangular and pentagonal lattices and proposed that the critical value of the anisotropy, below which the ground state has collinear order, can be taken as a measure of frustration.

From the experimental point of view, the unconventional properties of the organic superconductors  $\kappa$ -(BEDT-TTF)<sub>2</sub>X and their similarities with the cuprates<sup>8</sup> renewed the interest in the triangular topology. In particular, it was argued<sup>7,9</sup> that the Hubbard model on a triangular lattice with anisotropic interactions at half filling could be a good candidate to explain such properties. In the limit of strong coupling this model can be mapped to the Heisenberg model with anisotropic interactions  $J_\alpha=t_\alpha^2/U$ ,  $J_\beta=t_\beta^2/U$ , where  $t_\alpha$  and  $t_\beta$  are the anisotropic hoppings. Furthermore, experiments suggest that the relevant values of  $J_\alpha/J_\beta$  are about 0.3–1 (see for details Ref. 9), so the combined effect of anisotropy and frustration will take an important role in these materials.

In this paper we address the phase diagram of the Heisenberg model on the triangular lattice with spatially anisotropic interactions by mean of conventional spin-wave theory. Our approach provides the values of anisotropy where nonmagnetic states appear signaling the possible existence of spin-liquid behavior.

The Hamiltonian is

$$H = J_\alpha \sum_{\mathbf{r}, \delta_\alpha} \mathbf{S}_\mathbf{r} \cdot \mathbf{S}_{\mathbf{r}+\delta_\alpha} + J_\beta \sum_{\mathbf{r}, \delta_\beta} \mathbf{S}_\mathbf{r} \cdot \mathbf{S}_{\mathbf{r}+\delta_\beta}, \quad (1)$$

where  $J_\alpha$  and  $J_\beta$  are positive and correspond to interactions along directions  $\delta_\alpha$  and  $\delta_\beta$ , respectively (see Fig. 1). In order to develop a linear spin-wave theory, we need to know

previously the classical phase diagram. Basically, we replace the spin operators by classical vectors on the  $x$ - $y$  plane and minimize the energy which is equivalent to find the magnetic vector  $\mathbf{Q}$  satisfying

$$J_{\mathbf{Q}} \leq J_{\mathbf{k}}, \forall \mathbf{k},$$

where

$$J_{\mathbf{k}} = J_\alpha \cos(k_x) + J_\beta 2 \cos\left(\frac{k_x}{2}\right) \cos\left(\frac{k_y \sqrt{3}}{2}\right). \quad (2)$$

The minimization of Eq. (2) can be carried on easily for each value of  $\mu = J_\alpha/J_\beta$  and it can be shown that there are two kinds of phases.

(i) Collinear: this state is characterized by  $\mathbf{Q}_{\text{col}} = (0, 2\pi/\sqrt{3})$ , and it is stable in the region  $0 \leq \mu \leq 0.5$ . The case  $\mu=0$  is topologically equivalent to a square lattice and  $\mathbf{Q}_{\text{col}}$  on a triangular lattice produces the same magnetic structure than  $(\pi, \pi)$  on a square one.

(ii) Incommensurate spiral: in this state  $\mathbf{Q}_{\text{spi}} = (2Q, 0)$ , where  $Q = \cos^{-1}(-1/2\mu)$ , and it is stable in the region  $0.5 < \mu < \infty$ . For  $\mu=1$  we have the pure frustrated case which corresponds to the 120° commensurate spiral order and for  $\mu=\infty$  we have infinite decoupled classical chains each one Néel ordered.

In Fig. 2 we represent the possible values of  $\pm \mathbf{Q}$  in the Brillouin zone for different values of  $\mu$ . Using the invariance in  $\mathbf{k}$  space under translations  $\mathbf{G} = (\pm 2\pi, \mp 2\pi/\sqrt{3})$  we can

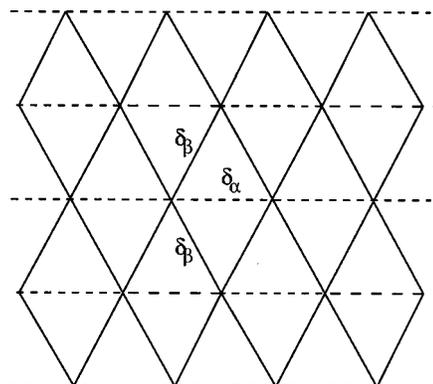


FIG. 1. Structure of the anisotropic bonds in a triangular lattice.

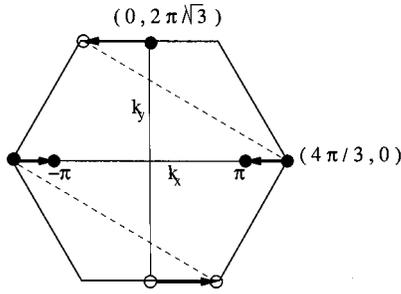


FIG. 2. Magnetic vectors  $\pm \mathbf{Q}$  for different values of  $\mu$  starting from  $\mu=0$  with  $(0, 2\pi/\sqrt{3})$  and ending at  $\mu=\infty$  with  $(\pi, 0)$ , in the Brillouin zone. The equivalence between empty and filled circles, represented by dashed lines, shows the continuity of the classical transitions.

see that the transition between all the possible states is continuous. We are interested in how the transition between these classical states is affected by quantum fluctuations. The strategy to perform the spin-wave calculation is the one-sublattice description. We apply a uniform twist of the coordinate frame in such a way that  $x$ -axis direction coincides, in each site, with the direction of the classical structure. This allows us to incorporate quantum fluctuations in a unique way for collinear and spiral phases. The next steps are well known<sup>10</sup> and we only describe the procedure. (i) The angular momentum operators are expressed by mean of the Holstein-Primakov transformation, (ii) the Hamiltonian is expanded to order  $1/S$  (quadratic order in bosons), (iii) after Fourier transforming, the Hamiltonian can be diagonalized by a Bogoliubov transformation resulting in

$$H = E_c + \frac{1}{2} \sum_{\mathbf{k}} [E(\mathbf{k}) - \gamma_A(\mathbf{k})] + \frac{1}{2} \sum_{\mathbf{k}} E(\mathbf{k}) (\alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + \alpha_{-\mathbf{k}}^\dagger \alpha_{-\mathbf{k}}),$$

where

$$E_c = NS^2 [J_\beta \cos(\mathbf{Q} \cdot \boldsymbol{\delta}_\beta) + J_\alpha \cos(\mathbf{Q} \cdot \boldsymbol{\delta}_\alpha) + J_\beta \cos(\mathbf{Q} \cdot \boldsymbol{\delta}_\beta)]$$

and

$$E(\mathbf{k}) = [\gamma_A^2(\mathbf{k}) - \gamma_B^2(\mathbf{k})]^{-1/2} \quad (3)$$

with

$$\gamma_A(\mathbf{k}) = \frac{S}{2} \sum_{\delta=\delta_\alpha, \delta_\beta} J_\delta \cos(\mathbf{k} \cdot \boldsymbol{\delta}) [1 + \cos(\mathbf{Q} \cdot \boldsymbol{\delta})] - 2 \cos(\mathbf{Q} \cdot \boldsymbol{\delta}),$$

$$\gamma_B(\mathbf{k}) = S \sum_{\delta=\delta_\alpha, \delta_\beta} J_\delta \cos(\mathbf{k} \cdot \boldsymbol{\delta}) [\cos(\mathbf{Q} \cdot \boldsymbol{\delta}) - 1].$$

The compact equation (3) gives the dispersion relation for all the different phases labeled by  $\mathbf{Q}$ . In particular, for  $\mu=0$  we recover the spin wave spectrum of the square lattice while for  $\mu=1$  we obtain the triangular one (spatially isotropic). Independently of the value of  $\mathbf{Q}$  it can be checked that  $E(\mathbf{k})=0$  for  $\mathbf{k}=\mathbf{0}, \pm \mathbf{Q}$ , and these zero modes are the three Goldstone modes related to the complete symmetry-breaking

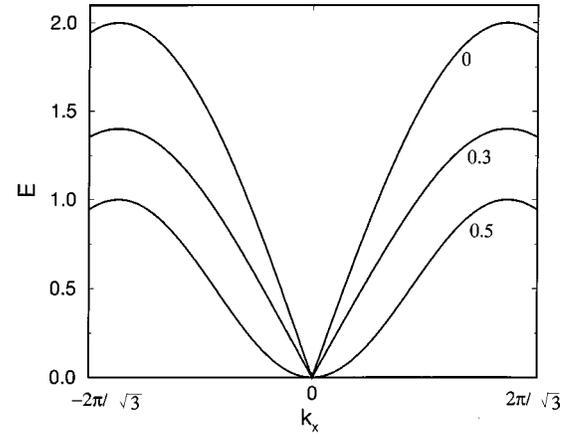


FIG. 3. Relation dispersion  $E(\mathbf{k})$  along  $k_x$  direction for different values of  $\mu = J_\alpha/J_\beta$  and  $S=1/2$ .

of the  $SU(2)$  invariance. However, for collinear phase  $\mathbf{Q}$  is equivalent to  $-\mathbf{Q}$  and two zero modes are recovered. Maybe the most interesting result is that if we expand  $E(\mathbf{k})$  near these zeros the behavior of  $E(\mathbf{k})$  is linear for all  $\mu \neq 1/2$ , while for  $\mu = 1/2$ , around  $\mathbf{k}=(0,0)$  and along the direction of  $k_x$  it becomes quadratic showing the softening of the spin-wave modes for all  $S$  (see Fig. 3). This is manifested in the magnetization

$$m_0 = \left( S + \frac{1}{2} \right) - \frac{\sqrt{3}}{2} \int_{\text{BZ}} \frac{dk_x dk_y}{(2\pi)^2} \frac{\gamma_A(\mathbf{k})}{2E(\mathbf{k})}, \quad (4)$$

where the integration is over the Brillouin zone of the triangular lattice. In the second term of Eq. (4) the integrand diverge for  $\mathbf{k}=\mathbf{0}, \pm \mathbf{Q}$  but the integral remains finite in two dimensional (2D) for all  $\mu \neq 1/2$ , while for  $\mu = 1/2$  quantum fluctuations are amplified, because of the quadratic behavior of  $E(\mathbf{k})$  near  $\mathbf{k}=(0,0)$ , and it can be proved<sup>19</sup> that the integral contribute with a finite but large enhancement of quantum correction to the magnetization. In order to estimate the region where the system is disordered for  $S=1/2$ , we calculated the quantum corrected magnetization for each classical structure. In what follows we rescale  $\mu \rightarrow \eta = \mu/(1+\mu)$ . This allows us to capture all the possible values of  $\mu$  in a finite range  $0 \leq \eta \leq 1$ . Figure 4 shows that spin-wave theory predicts a collinear phase at  $\eta=0$  with  $m_0=0.303$  and as we increase the frustration it is weakened continuously getting disordered just before the classical value  $\eta=1/3$ . Immediately after this value, an incommensurate order is stabilized starting from  $m_0=0$  and it becomes more robust as we approach the spatially isotropic case  $\eta=0.5$  where the structure is commensurate,  $\mathbf{Q}=(4\pi/3, 0)$ , and  $m_0=0.239$ . If we continue increasing  $\eta$  incommensurate structures appear again with decreasing  $m_0$  until the critical value  $\eta=0.79$  where magnetization vanishes. Beyond this value, the ground state is disordered. We note that the singular behavior obtained near  $\eta=1/3$  does not appear in previous studies of this model. In fact, Gazza *et al.*<sup>11</sup> performed a Schwinger boson mean field theory and found a continuous transition from collinear to spiral phases at  $\eta=0.375$  but with a nonvanishing magnetization  $m_0 \sim 0.175$ . However, inclusion of Gaussian fluctuations in this theory would tend to decrease the order, as it is known to occur in highly frustrated cases,<sup>12,3</sup>

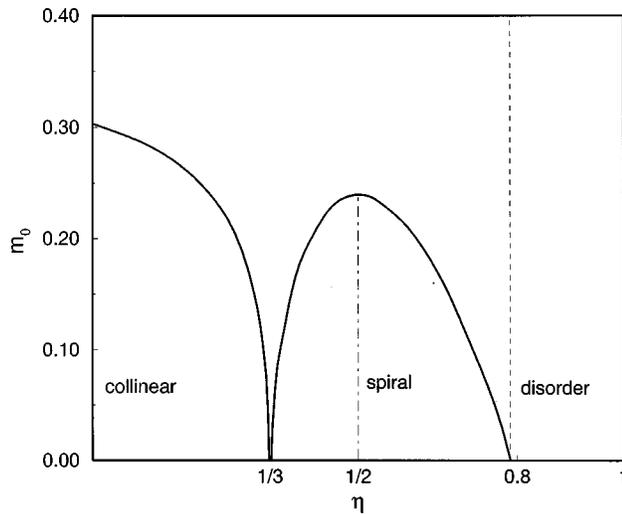


FIG. 4. Quantum corrected magnetization vs  $\eta$  for spin  $S = 1/2$ . The dot-dashed line indicates the location of commensurate spiral Néel order.

reaching probably more accord with our spin wave results. The same happens with both theories in the  $J_1$ - $J_2$  model on a square lattice.<sup>13,14,12</sup> One should take into account that our system can be thought as a Heisenberg model on a square lattice with interactions to first and second neighbors, but only along one of the diagonals.<sup>18</sup>

On the other hand, for the regime  $J_\beta < J_\alpha$ , the critical value  $\eta = 0.79$  means that the system disorders at  $J_\beta/J_\alpha = 0.27$ . This should be compared with the spin wave value for the square case,<sup>16</sup>  $J_\perp/J_\parallel \sim 0.03$ , where the difference in one order of magnitude shows that the way in which fluctuations overcome the ordering is different. However, in the regime around  $\eta = 1$  the spin wave calculation is not reliable any more since quantum fluctuations are divergent in the 1D limit. In particular, numerical techniques<sup>15</sup> predict that in the square case an infinitesimal coupling is required to take the chains away from criticality and get ordered. A similar cal-

ulation should be done for our model in the regime of weakly coupled chains and it is left for a future work.

In conclusion, we have studied the Heisenberg model on a triangular lattice with spatially anisotropic interactions by mean of a spin-wave analysis. We calculated the classical and quantum corrected phase diagram at  $T=0$  for the whole range of parameters  $\eta = J_\alpha/(J_\alpha + J_\beta)$  obtaining different regimes: collinear, incommensurate spirals, and disorder phases. The nonmagnetic region found very near the singular value  $\eta = 1/3$  for  $S = 1/2$  suggests the possible existence of a spin-liquid phase. A similar scenario occurs in the  $J_1$ - $J_2$  and  $J_1$ - $J_3$  model on a square lattice.<sup>13,17</sup> It is clear from our approximation that it should be more probable to find a spin-liquid behavior near  $\eta = 1/3$  than in other region of the diagram between collinear and spiral phases. Though this region is small, it is just located in the range where the experimental values of  $J_\alpha/J_\beta$  are relevant for organic superconductors  $\kappa$ -(BEDT-TTF)<sub>2</sub>X. Moreover, in the regime of  $J_\beta < J_\alpha$  we found that quantum fluctuations destroy the order at  $J_\beta/J_\alpha = 0.27$  leaving a wide region where the ground state is disordered.

Finally, we would like to stress that by applying a simple approximation such as spin-wave theory we have obtained a very rich phase diagram. Of course, we have not demonstrated the existence of spin-liquid phases but the appearance of nonmagnetic regions indicates the possible location of them. Another quantities like spin gap or correlation functions are needed to explore more deeply the nature of these phases, and it requires more powerful techniques.

We recently became aware of two works performed on this model. The first one by Zheng *et al.*<sup>18</sup> using series expansion technique where their prediction are, in general, similar to the phase diagram obtained in this work. The second one, Merino *et al.*<sup>19</sup> using the same technique of the present work.

The author acknowledges the useful discussions with A. Ceccatto, S. Sorella, and E. Jagla. This work was supported by Consejo Nacional de Investigaciones Científicas y Técnicas of Argentina.

\*Electronic address: Trumper@ifir.ifir.edu.ar

<sup>1</sup>P. Fazekas and P. W. Anderson, *Philos. Mag.* **30**, 423 (1974).

<sup>2</sup>D. A. Huse and V. Elser, *Phys. Rev. Lett.* **60**, 2531 (1988); R. Deutscher and H. U. Everts, *Z. Phys. B* **93**, 77 (1993); B. Bernu, C. Lhuillier, and L. Pierre, *Phys. Rev. Lett.* **69**, 2590 (1992); B. Bernu, P. Lecheminant, C. Lhuillier, and L. Pierre, *Phys. Rev. B* **50**, 10 048 (1994).

<sup>3</sup>L. O. Manuel, A. E. Trumper, and H. A. Ceccatto, *Phys. Rev. B* **57**, 8348 (1998).

<sup>4</sup>H. Nishimori and H. Nakanishi, *J. Phys. Soc. Jpn.* **57**, 626 (1988); **58**, 2607 (1989); **58**, 3433 (1989); N. Elstner, R. R. P. Singh, and A. P. Young, *Phys. Rev. Lett.* **71**, 1629 (1993); K. Yang, L. K. Warman, and S. M. Girvin, *ibid.* **70**, 2641 (1993).

<sup>5</sup>P. W. Leung and K. J. Runge, *Phys. Rev. B* **47**, 5861 (1993).

<sup>6</sup>U. Bhaumik and I. Bose, *Phys. Rev. B* **58**, 73 (1998).

<sup>7</sup>H. Kino and H. Fukuyama, *J. Phys. Soc. Jpn.* **65**, 2158 (1996).

<sup>8</sup>R. H. McKenzie, *Science* **278**, 820 (1997).

<sup>9</sup>R. H. McKenzie, *Condens. Matter Phys.* **18**, 309 (1998).

<sup>10</sup>Th. Jolicoeur and J. C. Le Guillou, *Phys. Rev. B* **40**, 2727 (1989);

S. J. Miyake, *J. Phys. Soc. Jpn.* **61**, 983 (1992); A. Chubukov, S. Sachdev, and T. Senthil, *J. Phys.: Condens. Matter* **6**, 8891 (1994).

<sup>11</sup>C. J. Gazza and H. A. Ceccatto, *J. Phys.: Condens. Matter* **5**, L135 (1993).

<sup>12</sup>A. E. Trumper, L. O. Manuel, C. J. Gazza, and H. A. Ceccatto, *Phys. Rev. Lett.* **78**, 2216 (1997).

<sup>13</sup>P. Chandra and B. Doucot, *Phys. Rev. B* **38**, 9335 (1988).

<sup>14</sup>F. Mila, D. Poilblanc, and C. Bruder, *Phys. Rev. B* **43**, 7891 (1991).

<sup>15</sup>T. Sakai and M. Takahashi, *J. Phys. Soc. Jpn.* **58**, 3131 (1989).

<sup>16</sup>A. Parola, S. Sorella, and Q. F. Zhong, *Phys. Rev. Lett.* **71**, 4393 (1993); **71**, 2158 (1996).

<sup>17</sup>P. Locher, *Phys. Rev. B* **41**, 2537 (1990).

<sup>18</sup>Z. Weihong, R. H. McKenzie, and R. R. P. Singh, *Phys. Rev. B* **59**, 14 367 (1999).

<sup>19</sup>J. Merino, R. H. McKenzie, J. B. Marston, and C. H. Chung, *J. Phys.: Condens. Matter* **11**, 2965 (1999).