Journal of Magnetism and Magnetic Materials 340 (2013) 97–101

Contents lists available at SciVerse ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Bilinear-biquadratic anisotropic Heisenberg model on a triangular lattice

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ARTICLE INFO

Article history:
Received 13 November 2012
Received in revised form
21 January 2013
Available online 8 April 2013

Keywords:
Heisenberg model
Antiferromagnet
Quantum phase transition

ABSTRACT

Motivated by the fact that the study of disordered phases at zero temperature is of great interest, I study the spin-one quantum antiferromagnet with a next-nearest neighbor interaction on a triangular lattice with bilinear and biquadratic exchange interactions and a single ion anisotropy, using a SU(3) Schwinger boson mean-field theory. I calculate the critical properties, at zero temperature, for values of the single ion anisotropy parameter D above a critical value D_C, where a quantum phase transition takes place from a higher D disordered phase to a lower D ordered phase.

1. Introduction

The study of frustrated magnetic systems has experienced a burst of theoretical and experimental activity in the last decade since it presents an excellent ground to discover new states and new properties of matter [1–3]. In this context, the synthesis of new materials has motivated a lot of theoretical studies in the two dimensional $S=1$ Heisenberg antiferromagnet on the triangular lattice [4–11]. The triangular lattice antiferromagnet is of interest because of its potential to exhibit exotic phases, and because there are many real materials with this structure. The inclusion of a single ion anisotropy and a biquadratic exchange interaction leads to a model exhibiting a complex phase diagram. Interest in spin-quadrupolar ordering has been raised recently by experimental findings in the layer compound $NiGa_2S_4$, where the Ni^{2+} ions are in the $S=1$ state, and form a two-dimensional triangular lattice [1]. In this paper I will study the model described by the following Hamiltonian:

$$H=J\cos\theta\sum_{\langle n,m\rangle}S_nS_m+J_2\sum_{\ll n,m\gg}S_nS_m+J\sin\theta\sum_{\langle n,m\rangle}(S_nS_m)^2+D\sum_n(S_n^z)^2, \tag{1}$$

where $\langle\,\rangle$ sums over the nearest-neighbors and $\ll\gg$ over the next-nearest neighbors. It is usual to write $J_1\equiv J\cos\theta$, $K=J\sin\theta$, where the parameter θ control the ratio of these two couplings. Here J_1 and J_2 denote the antiferromagnetic exchange coupling between spins located in the nearest neighbor and next-nearest neighbor sites respectively, and K is the coupling for the biquadratic interaction between nearest neighbor spin pairs. Although a negative K can be obtained from a large U expansion of the multi-orbital Hubbard model, or from coupling to phonons, both signs of K are possible.

A negative biquadratic exchange K tends to drive the spins to a collinear state, while a positive biquadratic term induces a state which is minimized with mutually perpendicular spins.

Let us first mention what is known about Hamiltonian (1) when $J_2=0$, $D=0$. This model has been extensively studied in the literature [8,10], where it has been shown that it has four different phases at zero temperature. The ferromagnetic (FM) phase for $\pi/2<\theta<-3\pi/4$. The ferroquadrupolar (FQ) phase, with collinear ferro-nematic order, i. e. nematic order that does not break lattice translational symmetry, for $-3\pi/4<\theta<\Theta$. In this phase the O(3) spin symmetry is broken but $\langle \boldsymbol{S}_n\rangle=0$. The 120° antiferromagnetic (AFM) phase for $\Theta<\theta<\pi/4$, and finally the antiferroquadrupolar (AFQ) phase for $\pi/4<\theta<\pi/2$, where the ground state is described by an antiferro-nematic order, and the director vectors $\mathbf{d}_n$ on three different sublattices are orthogonal to each other, thus breaking lattice translation symmetry. A mean field variational calculation gives $\Theta=\arctan(-2)\approx-1.099$,while a finite-size exact-diagonalization strongly renormalizes this value to $\Theta=-0.3456$ ($K/J_1\approx-0.4$).

For $D\gg J_1, J_2, |K|$, the ground state is a trivial product of states of $|S^z=0\rangle$ on all sites (corresponding to the trivial single-site ferro nematic order) separated by a gap from the first excited states, which lie in the sectors $S^z_{\text{total}}=\pm1$. Therefore, there exists a critical D_C denoting a quantum phase transition from the large-D phase to the small D-phase [12–14].

The introduction of a competitive second-neighbor interaction J_2 leads, at intermediate values of this parameter, to the existence of a disordered phase. In this paper, I will be interested in the case where D is above D_C, this is, in the nematic phase. In Section 2, I present a SU(3) Schwinger boson formalism that is adequate to treat spin-1 systems with competing bilinear J_1 and J_2 exchanges

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http://dx.doi.org/10.1016/j.jmmm.2013.03.037

interactions, biquadratic exchange interaction K, and single ion anisotropy. In Section 3, I describe an approximation to the above formalism convenient to treat the disordered phases. Finally, in Section 4, I present the results of my calculations.

2. SU(3) Schwinger boson formalism

It is impossible to describe the spin nematic phase using the standard SU(2) Schwinger boson (SB) formalism as a boson condensate, because a nonzero condensate $z=\langle a\rangle$ (where a is one of the Schwinger bosons) necessarily produces a nonzero magnetic dipole moment with size $|m|=|z|^2/2$. To avert this shortcoming of the SB formalism, Papanicolaou [15] derived a theory where one additional boson was introduced. The new theory is a generalization SU(3) of the SU(2) Schwinger boson-mean field theory where both, magnetic order and spin nematic order can be described by a boson condensate.

In this formalism, we start by choosing the following basis:

$$|x\rangle = i(|1\rangle - |-1\rangle)/\sqrt{2}, \quad |y\rangle = (|1\rangle + |-1\rangle)/\sqrt{2}, \quad |z\rangle = -i|0\rangle, \tag{2}$$

where $|n\rangle$ are eigenstates of S^z, and representing the spin operators via a set of three boson operators t_α (α=x, y, z) defined by

$$t_x^+|v\rangle = |x\rangle, \quad t_y^+|v\rangle = |y\rangle, \quad t_z^+|v\rangle = |z\rangle, \tag{3}$$

where $|v\rangle$ is the vacuum state, with the constraint

$$t_x^+t_x + t_y^+t_y + t_z^+t_z = 1, \tag{4}$$

for single site occupancy on each site. In terms of the t operators we can write

$$S^\alpha = -i\varepsilon_{\alpha\beta\gamma}t_\beta^+t_\gamma. \tag{15}$$

As pointed out by Li and Shen [5], one may choose the operators t´s as either bosons, or fermions. In principle, the bosons tend to condense to the lowest energy state at low temperatures and form a quantum ordered state, while the fermions tend to form a Fermi sea and a quantum-disordered state. It can easily be verified that

$$[S^\alpha, S^\beta] = i\varepsilon_{\alpha\beta\gamma}S^\gamma. \tag{16}$$

The states $t_x^+|v\rangle$ and $t_y^+|v\rangle$, both consist of $S^z = \pm 1$ eigenstates and have the average $< S^z > = 0$. This property will preserve the disorder of the ground state.

It should be noted that Wang et al. [16] arrived at the same representation starting from the bond operator representation of S=1/2, proposed by Sachdev and Bhatt [17], with the singlet state projected out.

To study the disordered phase, it is convenient to introduce another two bosonic operators u^+ and d^+ given by [12]

$$u^+ = -\frac{1}{\sqrt{2}}(t_x^+ + it_y^+), \quad d^+ = \frac{1}{\sqrt{2}}(t_x^+ - it_y^+), \tag{7}$$

so that

$$|1\rangle = u^+|v\rangle, \quad |0\rangle = t_z^+|v\rangle, \quad |-1\rangle = d^+|v\rangle, \tag{8}$$

with the constraint $u^+u + d^+d + t_z^+t_z = 1$. There is no new physics involved here; this replacement only makes easy the calculations. The spin operators can now be written as

$$S^+ = \sqrt{2}(t_z^+d + u^+t_z), \quad S^- = \sqrt{2}(d^+t_z + t_z^+u), \quad S^z = u^+u - d^+d. \tag{9}$$

Writing the operators t´s as a vector $\mathbf{t}=(t_x, t_y, t_z)^T$, we have

$$S_n = -i\mathbf{t}_n^+\mathbf{t}_n. \tag{10}$$

Using the t´s operators, the Hamiltonian (1) can be rewritten as

$$H = \sum_{<n,m>}[J_1\mathbf{t}_n^+(\mathbf{t}_n\mathbf{t}_m^+)\mathbf{t}_m + (J_1 - K)(\mathbf{t}_n^+\mathbf{t}_m^+)(\mathbf{t}_n\mathbf{t}_m) + K] + J_2\sum_{\ll n,m \gg}[\mathbf{t}_n^+(\mathbf{t}_n\mathbf{t}_m^+)\mathbf{t}_m + (\mathbf{t}_n^+\mathbf{t}_m^+)(\mathbf{t}_n\mathbf{t}_m)] + \sum_n[\mu(1-n_n) + D(1-n_{n\alpha})], \tag{11}$$

where $n_{n\alpha} = t_{n\alpha}^+t_{n\alpha}$ is the particle number operator for bosons of type α on site n, and $n_n = \sum_\alpha n_{n\alpha}$.

To discuss quadrupolar order, it is useful to introduce the quadrupole operators [8,10]

$$\begin{aligned}
Q_n^{(0)} &= (S_n^z)^2 - \frac{2}{3} = \frac{1}{3}(t_{nx}^+t_{nx} + t_{ny}^+t_{ny} - 2t_{nz}^+t_{nz}),\\
Q_n^{(2)} &= (S_n^x)^2 - (S_n^y)^2 = -(t_{nx}^+t_{nx} - t_{ny}^+t_{ny}),\\
Q_n^{xy} &= S_n^xS_n^y + S_n^yS_n^x = -(t_{nx}^+t_{ny} + t_{ny}^+t_{nx}),\\
Q_n^{yz} &= S_n^yS_n^z + S_n^zS_n^y = -(t_{ny}^+t_{nz} + t_{nz}^+t_{ny}),\\
Q_n^{zx} &= S_n^zS_n^x + S_n^xS_n^z = -(t_{nz}^+t_{nx} + t_{nx}^+t_{nz}).
\end{aligned} \tag{12}$$

The nematic order parameters $Q^{\alpha\beta}$ describes the anisotropy of spin fluctuations, not static moment, and can be nonzero only if $S\geq 1$ [6].

Joshi et al. [7] have used the SU(3) Schwinger boson formalism, condensing the bosons associated with the ordering, to study the FQ phase (with J_2=0, D=0). For instance, to describe a state with all directors pointing in the y direction, they let the y bosons condense and replace t_y^+ and t_y by $\sqrt{1-t_x^+t_x-t_z^+t_z}$.

Peng Li et al. [4] studied the region $\pi/4<\theta<\pi/2$ (for D=0, J_2=0) starting from Eq.(11) and doing a decoupling using two real mean-field parameters, just like in the SU(2) Schwinger boson mean field theory. They found that the condensation of the SU (3) bosons led to a gapless nematic phase. In this phase the spin moments vanish, i. e. the nematic state is non-magnetic, whereas the uniform quadrupole moment $< Q_n^{xy} >$ is nonzero at zero temperature, which indicates the existence of a quadrupolar long-range order.

Serbin et al. [18], using a fermionic representation within a mean field theory, studied the Hamiltonian (1), with J_2=0, in the antiferromagnetic phase, $-0.4\leq K/J_1 \leq 1$, for small values of D. In addition to a fully gapped spin-liquid ground state, they found a state where one gapless triplon mode coexists with topological gapped spin excitations. Spin liquid phases for spin-1 system on a triangular lattice were recently found by Xu et al. [9].

The aim of this paper is to investigate the influence of the next nearest neighbor exchange interaction J_2 and the single ion anisotropy D, in the disordered phase, to the biquadratic model on the triangular lattice. The effect of the J_2 term, as far as I know, has not been studied before. The contribution of the single ion term was considered by Serbin et al. [18], but only for small values of D ($|D|, |K| < J_1$). Therefore, the results presented here, even for η=0, are new ones. In this sense, my calculations complement those performed in Ref. [18].

3. The large *D* phase

An adequate approximation to the SU(3) SB formalism in the disordered phase is to suppose that the t_z bosons are condensed [12,16], i. e. $\langle t_z\rangle = t$. I remark that when $< t_z < 1$, this condensation does not mean that every spin is in the eingenstate of S^z=0, although $\langle \sum_n S_n^z\rangle = 0$.The Hamiltonian (11) can be written as

$$H = H_0 + H_1 + H_2^{mf} \tag{13}$$

where

$$H_0 = (1-t^2)DN + \frac{zNK}{2}(1+t^4) + \mu\sum_n(u_n^+u_n + d_n^+d_n + t^2 - 1) \tag{14}$$

$$\begin{aligned}
H_1 = {} & J_1t^2\sum_{\langle n,m\rangle}(u_n^+u_m + d_n^+d_m + h.c.)\\
& + (J_1 - K)t^2\sum_{\langle n,m\rangle}(u_n^+d_m^+ + d_n^+u_m^+ + h.c.)\\
& + J_2t^2\sum_{\ll n,m \gg}(u_n^+u_m + d_n^+d_m + u_n^+d_m^+ + d_n^+u_m^+ + h.c.),
\end{aligned} \tag{15}$$

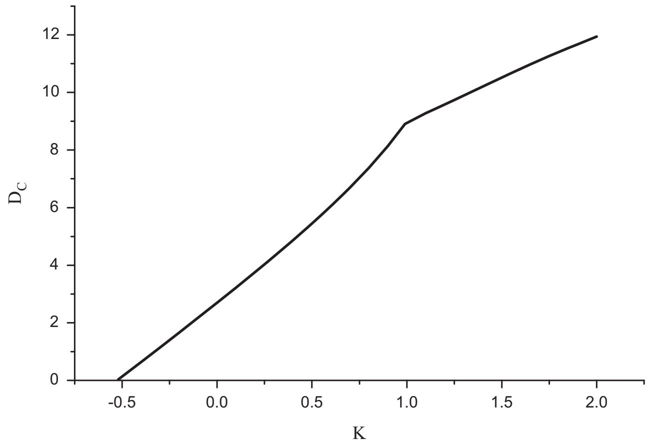

Fig. 1. The critical parameter D_C as a function of K, for $\eta=0$.

and after a mean-field decoupling to the four operator terms H_2^{mf} is given by

$$H_2^{mf} = -2(J_1-K)\sum_{\langle n,m\rangle}[p(u_n^+d_m^+ + d_n^+u_m^+) + h.c.] + \frac{zN}{2}\left[J_1(1-t^2)^2 + 4(J_1-K)p^2\right]. \quad (16)$$

here $p=\langle u_n d_m\rangle$ and $\tilde{p}$ has the same expression, but connect the next nearest neighbor spins. I have found that both terms are very small and can be neglected, but I present the equation for these terms below.

After a Fourier–Bogoliubov transformation we get the final result

$$H = \sum_q \omega_q(\alpha_q^+\alpha_q + \beta_q^+\beta_q) + \sum_k(\omega_q-\Lambda_q) + \text{constant}, \quad (17)$$

with

$$\omega_q = \sqrt{\Lambda_q^2-\Delta_q^2} \quad (18)$$

$$\Lambda_q = \lambda + 6t^2 g_q, \quad \Delta_q = 6(g_q-\gamma_q K)t^2, \quad g_q = \gamma_q + \eta\tilde{\gamma}_q, \quad \eta = J_2/J_1. \quad (19)$$

$$\gamma_q = \frac{1}{3}\left\{\cos q_x + 2\cos\left(\frac{q_x}{2}\right)\cos\left(\frac{\sqrt{3}q_y}{2}\right)\right\}, \quad (20)$$

$$\tilde{\gamma}_q = \frac{1}{3}\left\{\left[\cos(\sqrt{3}q_y) + 2\cos\left(\frac{3q_x}{2}\right)\cos\left(\frac{\sqrt{3}q_y}{2}\right)\right]\right\} \quad (21)$$

The energy gap in the disordered phase ($D \geq D_C$) occurs at a wave vector $\mathbf{q}_0$, which is directly related to the ordered state introduced by the Bose-Einstein condensation of magnons. For small values of η and $K \leq J_1$, $\mathbf{q}_0$ is given by, $\mathbf{q}_0=(4\pi/3, 0)$. At $\mathbf{q}_0$ a quantum phase transition takes place from the disordered large D phase to the ordered small D phase.

Following Ref. [14] and extending their calculations to my case, I obtain the saddle-point equations at $T=0$

$$t^2 = 2-\frac{1}{N}\sum_q\frac{\Lambda_q}{\omega_q}, \quad (22)$$

$$D-\lambda-6Kt^2 + 6(1+\eta)(1-t^2) = \frac{6}{N}\sum_q\frac{(\Lambda_q-\Delta_q)g_q + K\Delta_q\gamma_q}{\omega_q}, \quad (23)$$

$$p = -\frac{1}{2N}\sum_q\frac{\gamma_q\Delta_q}{\omega_q}, \quad \tilde{p} = -\frac{1}{2N}\sum_q\frac{\tilde{\gamma}_q\Delta_q}{\omega_q}. \quad (24)$$

The self-consistent equations can then be written as

$$t^2 = 2-\frac{1}{N}\sum_q\frac{1}{\sqrt{1-\Gamma_q^2}}, \quad (25)$$

$$-D + \frac{2}{g} + 12K = \frac{1}{N}\sum_q\frac{6[(g_q-K\gamma_q)\Gamma_q-g_q] + 1/g + 6K}{\sqrt{1-\Gamma_q^2}}, \quad (26)$$

where

$$\Gamma_q = \frac{6(g_q-K\gamma_q)g}{1+6gg_q}, \quad \text{and} \quad g = t^2/\lambda. \quad (27)$$

here I have set $J_1=1$. The $\eta=0$, $K=1$ case is special: one finds $t^2=1$, meaning that all spins occupy the state $|S^z=0\rangle$.

At the phase transition point D_C, the energy gap goes to zero and the minimum gap appears at $\mathbf{q}=(4\pi/3, 0)$. We find at this point

$$D_C = \frac{2}{g_c} + 12K - \frac{1}{N}\sum_q\frac{6K + 1/g_c + 6(g_q-K\gamma_q)\Gamma_q-g_q]}{\sqrt{1-\Gamma_q^2}}. \quad (28)$$

where g_c is given by

$$g_c = \frac{1}{6[2(1/2-\eta)-K/2]}, \quad (29)$$

for $K \leq 1$. While for $K>1$ it takes the value, $g_c=1/3\ K$.

4. Results and conclusions

In Fig. 1, I show the critical parameter D_C, below which a quantum phase transition to an ordered phase takes place, as a function of the biquadratic interaction K, for $\eta=0$, up to $K=2$. D_C vanishes at $K_C=-0.52$ signaling a transition to the FN phase. This value should be compared with $K_C=-0.4$ obtained by Lauchli et al. [8] using a finite-size exact diagonalization calculation. In Fig. 2, I present the gap m, which is Eq. (16) evaluated at $\mathbf{q}=(4\pi/3,0)$, as a function of K, for $D=10$ and $\eta=0$, and $\eta=0.1$. As one can see, the gap decreases linearly with K. Figs.3 and 4 show the critical parameter D_C as a function of η, for $K=-0.1$ and $K=0.3$ respectively. D_C vanishes at the points $\eta_c=0.0885$ and $\eta_c=0.103$ respectively. The biquadratic exchange drives the critical point η_c toward lower values of η for $K<0$, and toward higher values of η for $K>0$.

To show the behavior of the nematic order in the large D region, I present some calculations for $Q=-Q_n^{(0)}$. In Figs. 5 and 6, it is shown Q as function of K, for $\eta=0$, evaluated at $D=D_C$ and $D=10$ respectively. For large values of D, $<(S^Z)^2>$ tends to be zero, as it should, and $Q\to 0$.

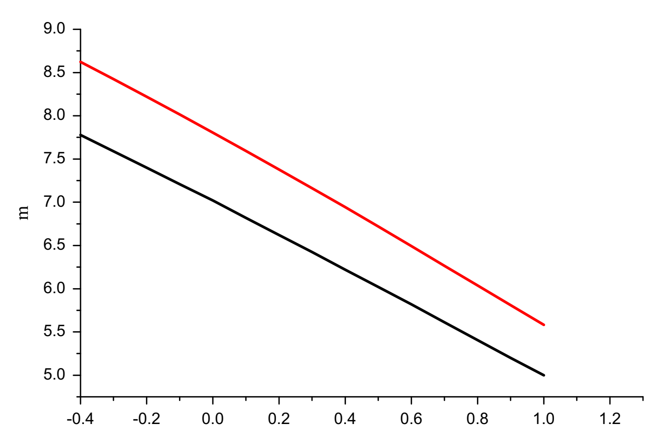

Fig. 2. The gap as a function of K, for $D=10$, and $\eta=0$ (lower line), $\eta=0.1$ (upper line).

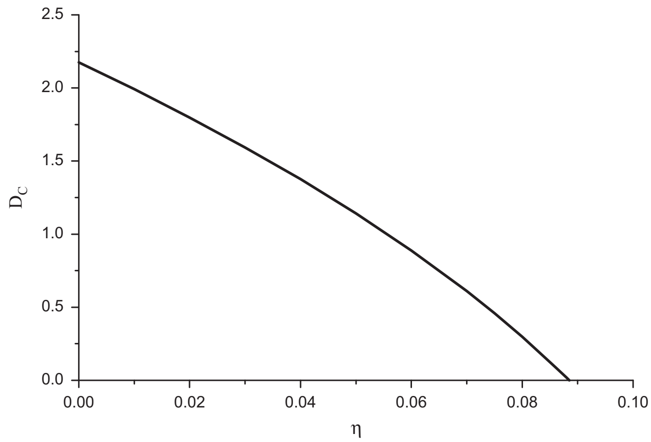

Fig. 3. The critical anisotropy parameter D_C as a function of η for $K=-0.1$.

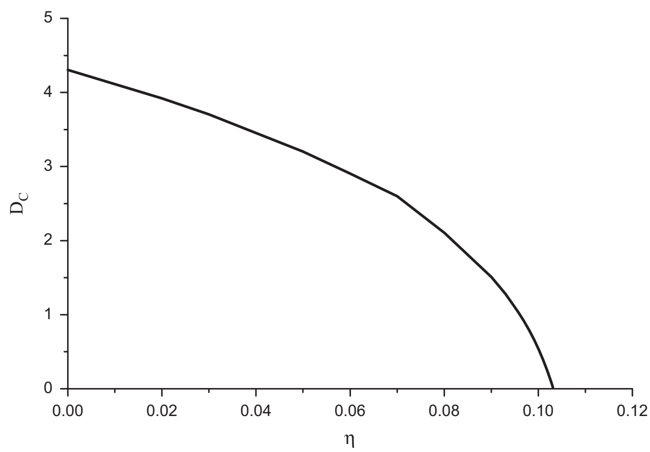

Fig. 4. The critical anisotropy parameter D_C as a function of η for $K=0.3$.

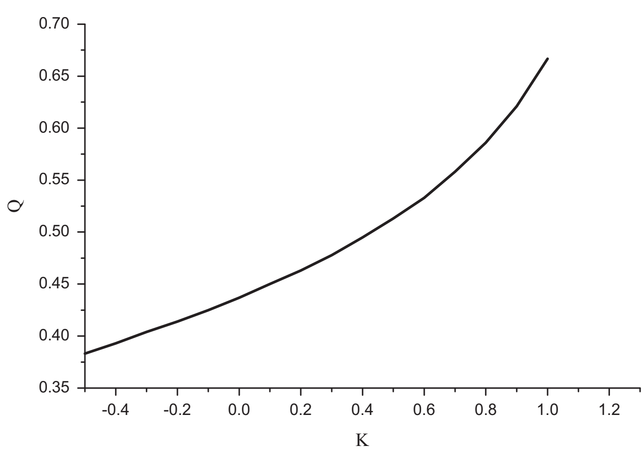

Fig. 5. Q as a function of K, for $\eta=0$, evaluated at D_C.

In Fig. 7, I show Q as a function of D, for $K=0$ and $\eta=0.12$. For this value of η we have $D_C=0$ and so the ground state is disordered. However, $Q=0.243$ at $D=0$, indicating the presence of a nematic phase, and not of a spin liquid state. Wang et al. [16], using the same formalism that I have used here, also found a non zero value for Q for the spin -1 antiferromagnetic chain. Fig. 8 shows the gap m as a function of η, for $K=0$. It vanishes at the critical point $\eta_c=0.098$, and increases linearly with η for $\eta>\eta_c$.

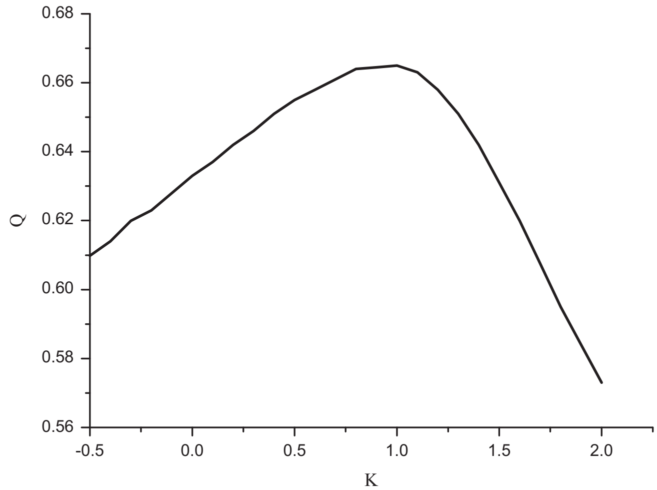

Fig. 6. Q as a function of K, for $\eta=0$, and $D=8$.

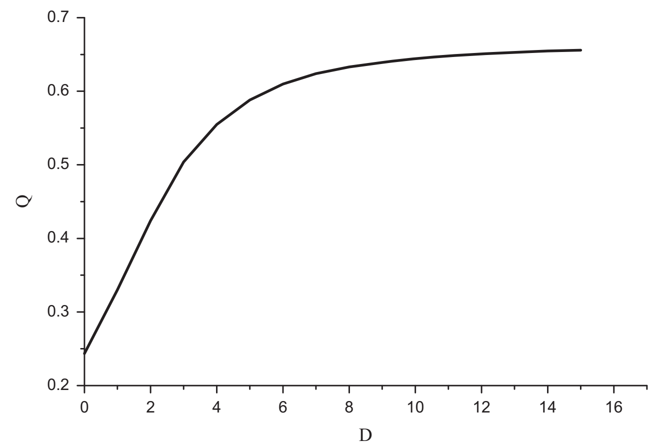

Fig. 7. Q as a function of D, for $K=0$, in the disordered region $\eta=0.12$.

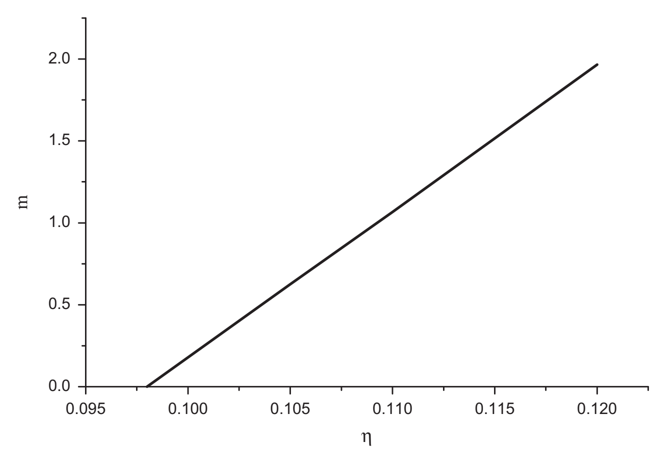

Fig. 8. The gap m in the disordered region as a function of η, for $K=0$.

To provide a general qualitative overview, I plot in Figs. 9 and 10 the spin wave dispersion for $\eta=0$, $D=5$, $K=-0.4$, and $\eta=0$, $D=8$, $K=0.5$, respectively.

The purpose of this paper was to enlarge the study of the two-dimensional $S=1$ Heisenberg antiferromagnet on a triangular lattice. In this context, I have studied the nematic region where the single ion

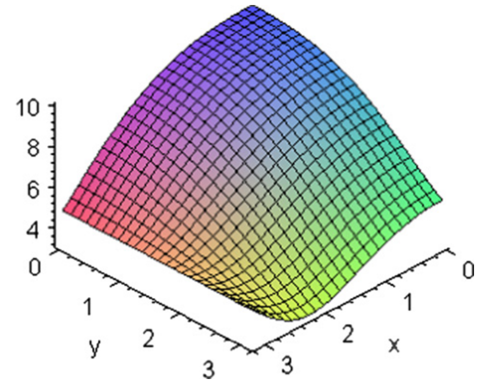

Fig. 9. The spin wave dispersion ω_q is shown for $\eta=0$, $D=5$, $K=-0.4$.

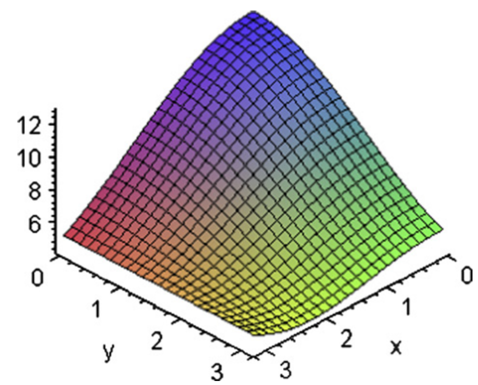

Fig. 10. The spin wave dispersion ω_q is shown for $\eta=0$, $D=8$, $K=0.5$.

anisotropy parameter D is above the critical value D_C where a quantum phase transition takes place to a low D phase. I assumed that one kind of boson was condensed and studied the ground-state properties of the model using a mean field approximation. Kaul [19] using quantum Monte Carlo simulations, has confirmed that the $S=1$ biquadratic model on a triangular lattice has a spin nematic ground state. As pointed out by Perc et al. [10], up to now unambiguous experimental evidence for spin-nematic phases in real materials is still lacking, but given the numbers of system currently been studied, it is expected that such evidence will emerge in the near future.

Acknowledgments

This work was partially supported by Conselho Nacional de Desenvolvimento Cientifico e Tecnologico (CNPQ) and Fundação de Amparo a Pesquisa do Estado de Minas Gerais (FAPEMIG).

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