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The magnetic properties of a quasi-two-dimensional spin 1 easy axis Heisenberg antiferromagnet with competing interactions

Griffith Mendonça A. Sousa *, A.S.T. Pires

1,2-Departamento de Física, Universidade Federal de Minas Gerais, CP702, Belo Horizonte 30123-970, MG, Brazil

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ABSTRACT

The Neel and collinear ordered phases of the two-dimensional $S=1$ antiferromagnet with next and next near neighbor exchange interactions and easy axis single ion anisotropy, on the square lattice, are studied at low temperature using a Modified Spin Wave Theory. We calculate the low-temperature quantities as a function of the temperature, frustration and anisotropy. We calculate also the phase diagram at $T=0$. We found a disordered phase separating the Neel and collinear phases.

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1. Introduction

Magnetic materials with spin $S=1$ ions have been of interest for many years. The two-dimensional 2D Heisenberg antiferromagnet K_2NiF_4 was studied in the 1970s [1]. In the 1980s a number of weakly coupled linear chain systems were investigated, including $CsNiCl_3$ [2], which has a weak axial anisotropy, $CsFeBr_3$ [3], which has strong planar anisotropy, and the complex materials NENP $Ni(C_2H_8N_2)_2NO_2(ClO)_4$ [4] and NENC $Ni(C_2H_8N_2)_2Ni(CN_4)$ [5], which have weak and strong planar anisotropy, respectively.

The square lattice antiferromagnet (AF) with next and next nearest neighbor exchange interactions, the so called J_1–J_2 model, has been the subject of intense research, since it can present the behavior of a frustrated system. The frustration destroys the Neel order, and an extremely important question is what kind of states can emerge.

Properties of this model for spin $S=1/2$ in two-dimension have been studied by a variety of methods [6–28], such as the spin wave theory [10], exact diagonalization (ED) [13,15,21], series expansion [19,23–26] large-N expansion [27], functional renormalization group [22], Green's function method [18], and projected entangled pair states [28]. In all of these methods, it is believed that for $\eta = J_2/J_1 \leq 0.4$ the ground state of the model is Neel.

However for $\eta \geq 0.6$ the spins arrange in a collinear phase (CL), where adjacent spins in one spatial direction are aligned and parallel, while they are aligned parallel in other spatial directions. The disordered intermediate phase $0.4 < \eta < 0.6$ is believed to be a quantum paramagnetic (QP) without magnetic long-range order. It is believed that the ground state of this intermediate phase can be a columnar dimer state, [24,28] a plaquette valence bond solid order, [15,20,29] or a quantum spin liquid (QLS) [12,30]. The precise determination of the value of the critical points η_{1c} and η_{2c}, where the magnetization goes to zero, is also not conclusive. Recently the exact diagonalization method [18], using results up to $N=40$, to perform a finite-size extrapolation, estimates the transition points at $\eta_{1c}=0.35$ and $\eta_{2c}=0.66$. Due to the minus signal problem, the Monte Carlo simulation is not applicable in this frustrated system. Recently, using the Density Matrix Renormalization Group (DMRG) method, Jiang et al. [31] found $\eta_{1c}=0.41$ and $\eta_{2c}=0.62$ at zero temperature.

There are few numerical results for the J_1–J_2 model with spin $S > 1/2$. An exception is the two-step density-matrix renormalization group studied by Moukouri [32,33] and an analysis with spin wave expansion [34]. It has also been observed that quantum fluctuations can destabilize the classic ground state, even for spin $S > 1/2$, for large enough values of the frustration. Of particular relevance to the case with spin 1 are the very recent first-principles calculations [35] showing that the undoped material LaOFeAs is well described by the spin 1 J_1–J_2 model on the square lattice with $J_1 > 0$, $J_2 > 0$, and $J_2/J_1 \approx 2$. Recently, these systems have received interest motivated by the discovery of Fe-based superconducting materials [36], where a weakened AF order can be described by this model with spin $> 1/2$ [37–39].

A generalization of the frustrated J_1–J_2 model is the J_1–J_1'–J_2 model where J_1 is the exchange interaction in the x direction, J_1' in the y direction and J_2 is the interaction between second neighbors

* Corresponding author.
E-mail address: griffith_mas@hotmail.com (G.M.A. Sousa).

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[40–45]. This model is not purely of academic interest since there are several vanadium phosphate material systems ($Pb_2VO(PO_4)_2$, $SrZnVO(PO_4)$, $BaZnVO(PO_4)$ and $BaCdVO(PO_4)_2$) in which extensive band structure calculations show a spatially anisotropic exchange interaction along the x and y directions [46]. Bishop [45] studied this model and found the surprising and novel result that for the spin 1/2 case there is a quantum triple point below which there is a second-order phase transition between the Neel and the collinear phases.

In the case of spin 1, Bishop et al. [45] found no evidence for an intermediate phase between the (AF) and (CL) phases, as compared with all previous results for the corresponding spin 1/2 case. However, they found a quantum tricritical point at $J_1'/J_1 \approx 0.66$ and $J_2/J_1 \approx 0.35$, where a line of second-order phase transitions between the (AF) and (CL) phases (for $J_1'/J_1 \leq 0.66$) meets a line of first-order phase transitions between the same two states (for $J_1'/J_1 \geq 0.66$).

A significant single-ion anisotropy is believed to be present in materials with spin 1 (as for instance, in solid molecular oxygen (O_2) either in bulk or in monolayers adsorbed on graphite [47]), and has been included in the analyses of the experimental data. In this context, various approaches have been used, including mean-field type theories, [48], [49] spin–wave approximations, [50,51] a coupled cluster calculation [52], and a bosonic mean-field approach [53]. At low temperatures the standard spin-wave theory works satisfactorily for the easy axis model. Recently, using the Linear Spin Wave Theory, You et al. [54] studied the J_1–J_2 model with spin $S=1$ and single ion anisotropy. They discussed the effects of frustration and single-ion anisotropy on the low-temperature magnetic properties, such as the staggered magnetization and the specific heat. Corrections due to the spin–wave interactions at higher temperatures (but without competitive interactions) were treated self-consistently many years ago using a variational approach [55].

In this paper we study the two-dimensional spin 1 J_1–J_1'–J_2 Heisenberg antiferromagnet model with single ion anisotropy D, using a Modified Spin Wave Theory (MSW) at zero and finite temperature. One drawback of the spin wave theory is that since it is based on the assumption of long range order and therefore it cannot account for the disordered phases.

2. Modified Spin Wave Theory

For small values of the parameter η, we suppose that the classical ground state of the antiferromagnet is Neel ordered, with two sublattices "a" and "b", as it is shown in Fig. 1a. We have two different kinds of the next-near-neighbor (NN) interaction. The exchange interaction in the x direction is denoted by J_1 and that along the y direction by J_1'. The exchange interaction of the next-nearest-neighbor (NNN) is denoted by J_2. In Fig. 1a, spin up and down are represented by "+" and "−" in the z direction. We can see that, spins on sublattice "a" interact with the spins on sublattice "b" in the x direction with exchange interaction J_1, while the spins in sublattice "a" interact with spins on sublattice "b" in the y direction with J_1.

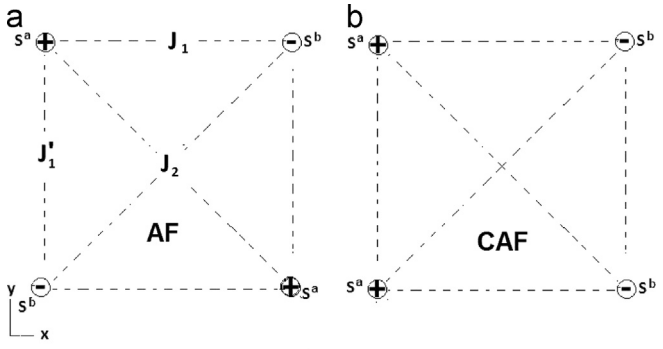

Fig. 1. AF and CL ordered phases of the square lattice. (a) In the AF phase all a-sublattice spins are in the direction "up" while in the b-sublattice spins point in the opposite direction "down". (b) For the CL phase there are two interpenetrating Neel states.

Whereas, the next-nearest interaction (NNN) J_2 connects only spins on sublattice "a" with spins on sublattice "a", and spins on sublattice "b" with spins on sublattice "b" along the diagonal direction. We can therefore write the Hamiltonian for this phase as

$$H^{(AF)} = J_1 \sum_{\langle i,j\rangle} S_i^a S_j^b + J_1 \sum_{\langle i,j\rangle} S_i^a S_j^b + \frac{J_2}{2} \sum_{\langle\langle i,j\rangle\rangle} \left[S_i^a S_j^a + S_i^b S_j^b\right] - D\sum_i (S_i^z)^2. \quad (1)$$

Here $D>0$ is the easy axis anisotropy. The indices on $\langle\ldots\rangle$ and $\langle\langle\ldots\rangle\rangle$ represent the sum over (NN) and (NNN) sites respectively.

We study the Hamiltonian (1) using the standard Dyson–Maleev (DM) representation where the spin operators are replaced by the bosonic operators as

$$\begin{aligned} S_i^+ &= \sqrt{2S}\left(1-\frac{a_i^+ a_i}{2S}\right) a_i \\ S_i^- &= \sqrt{2S} a_i^+ \\ S_i^z &= S - a_i^+ a_i, \end{aligned} \quad (2)$$

for the "a" sublattice, and by

$$\begin{aligned} S_i^+ &= \sqrt{2S} b_i^+ \left(1-\frac{b_i^+ b_i}{2S}\right) \\ S_i^- &= \sqrt{2S} b_i \\ S_i^z &= -S + b_i^+ b_i, \end{aligned} \quad (3)$$

for the "b" sublattice. Here $a_i^+(a_i)$ and $b_i^+(b_i)$ represent the creation (annihilation) operator on site i in the "a" and "b" sublattices respectively. Replacing Eqs. (2) and (3) into Eq.(1), and using the Fourier transform

$$a_i = \sqrt{\frac{2}{N}} \sum_k e^{ikR_i} a_k, \quad b_i = \sqrt{\frac{2}{N}} \sum_k e^{-ikR_i} b_k \quad (4)$$

we get

$$H^{(AF)} = H^{(0)} + H^{(2)} + H^{(4)}. \quad (5)$$

The classical energy ($H^{(0)}$), and the quadratic Hamiltonian ($H^{(1)}$) can be written as

$$H^{(0)} = -z_1 N J_1 S^2 \left(1 + \lambda - \frac{z_2}{z_1}\eta + \overline{D}\right) \quad (6)$$

$$H^{(2)} = J_1 \sum_k A_{0k}(a_k^+ a_k + b_k^+ b_k) + C_{0k}(a_k^+ b_k^+ + a_k b_k) \quad (7)$$

where the coefficients A_{0k} and C_{0k} are given by

$$\begin{aligned} A_{0k} &= z_1 S[1+\lambda] + z_2 S\eta[\gamma_k^{(2)} - 1] + S\overline{D} \\ C_{0k} &= z_1 S \gamma_k^{(1)} \end{aligned} \quad (8)$$

With

$$\overline{D} = \frac{D}{J_1}, \quad \lambda = \frac{J_1'}{J_1}, \quad \eta = \frac{J_2}{J_1}, \quad z_1 = 2 \quad \text{and} \quad z_2 = 4.$$

where we have defined the structure factors for the first and second neighbors as

$$\gamma_k^{(1)} = \cos(k_x) + \lambda \cos(k_y) \gamma_k^{(2)} = \cos(k_x)\cos(k_y) \quad (9)$$

The quadratic terms in $H^{(AF)}$ are given by

$$H^{(4)} = -J_1 \sum_{k_1,k_2,k_3} \{z_1[\gamma_{k_1}^{(1)} a_{k_2+k_3-k_1}^+ a_{k_2} a_{k_3} b_{k_1}$$

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