Spin-1/2 anisotropic Heisenberg antiferromagnet with Dzyaloshinskii-Moriya interaction via mean-field approximation

Walter E. F. Parente

Universidade Estadual de Roraima, Av. Senador Helio Campo, s/n - Centro, Caracara - RR, 69360-000

J. T. M. Pacobahyba

Departamento de Física, Universidade Federal de Roraima, BR 174, Km 12. Bairro Monte Cristo. CEP: 69300-000 Boa Vista/RR

Minos A. Neto *

Universidade Federal do Amazonas, Departamento de Física, 3000, Japiim, 69077-000, Manaus-AM, Brazil

Ijanílio G. Araújo

Departamento de Física, Universidade Federal de Roraima, CEP: 69300-000, Boa Vista/RR.

J. A. Plascak

Universidade Federal da Paraíba, Centro de Ciências Exatas e da Natureza - Campus I, Departamento de Física - CCEN Cidade Universitária 58051-970 - João Pessoa-PB, Brazil and Department of Physics and Astronomy, University of Georgia, 30602 Athens GA, USA

(Dated: February 21, 2018)

* Corresponding author.
E-mail address: minos@pq.cnpq.br (Minos A. Neto)
Contact number: 55-92-3305-4019
Abstract

ABSTRACT

The spin-$1/2$ anisotropic Heisenberg model with antiferromagnetic exchange interactions in the presence of a external magnetic field and a Dzyaloshinskii-Moriya interaction is studied by employing the usual mean-field approximation. The magnetic properties are obtained and it is shown that only second-order phase transitions take place for any values of the theoretical Hamiltonian parameters. Contrary to previous results from effective field theory, no anomalies have been observed at low temperatures. However, some re-entrancies still persist in some region of the phase diagram.

PACS numbers: 64.60.Ak; 64.60.Fr; 68.35.Rh

PACS numbers:
I. INTRODUCTION

The theoretical study of quantum magnetic systems has gained increased attention in the last decades not only because of their quite interesting intrinsic quantum phase transitions, which are induced by quantum fluctuations, but because these magnetic systems can also be well suited to describe some superconducting materials. For instance, the cuprate La$_2$CuO$_4$ compound has been shown to exhibit metamagnetic behavior [1, 2] and, when doped with Sr, forming the La$_{2-x}$Sr$_x$CuO$_4$ compound, it becomes a high-temperature superconductor for $x > 2.5\%$ [3].

On the theoretical point of view, the spin-1/2 antiferromagnetic Heisenberg model (AHM) has been one of the most studied model in order to try to understand the role played by the quantum fluctuations in the CuO$_2$ planes of these cuprates superconductors. The interest in the AHM comes from the early Anderson suggestion that these quantum fluctuations should be responsible for the superconductivity in this class of compounds [4]. Therefore, the AHM has been treated from several different techniques and some aspects of its phase diagram are well established (see, for instance, references [5, 6] and references therein). However, in real materials, anisotropies are expected, not only regarding the exchange interactions but also from spin-orbit couplings, which may lead to the Dzyaloshinskii-Moriya interaction. In this sense, the AHM in the presence of an external field and a Dzyaloshinskii-Moriya interaction turns out to be a very interesting model with applications in several experimental realizations, going from cuprates superconductors to spin-glass behavior in magnetic systems [5–7].

The AHM in the presence of an external field has been treated by the effective-field theory (EFT) [5] and the phase diagram in the temperature versus external field presents a reentrant behavior at low temperatures. This same model with an external longitudinal field and an extra Dzyaloshinskii-Moriya interaction has also been studied by employing the EFT. The results show that the phase diagram also exhibits re-entrances and, in addition, some anomaly behavior at low temperatures [6, 8]. As no exact solution is still available for this model, the results obtained by the EFT are still questionable and, in some way, controversial.

Our purpose in this work is thus to study the thermodynamic behavior of the AHM with XXZ exchange anisotropy in the presence of a longitudinal external magnetic field and a
Dzyaloshinskii-Moriya interaction placed in the $z$ direction. We employ the usual mean-field approximation, based on Bogoliubov variational approach using a two-spin cluster, in order to analyze the order parameter and the corresponding phase transition. A two-spin like approximation has been proven to be quite efficient in treating the transverse Ising model [9] and the Blume-Capel model in a transverse crystal field [10]. Although still being a mean-field approach, it would be very interesting to compare the results so obtained in treating the AHM with external field and Dzyaloshinskii-Moriya interactions with the previous ones from EFT.

The plan of the paper is as follows. In the next section, the model and the variational procedure formalism are presented. The results are discussed in Section III and some final remarks are commented in the last section.

II. MODEL AND FORMALISM

The model studied in this work is the anisotropic antiferromagnetic Heisenberg model in a magnetic field and with a Dzyaloshinskii-Moriya interaction, which can be described by the following Hamiltonian

$$
\mathcal{H} = J \sum_{\langle i,j \rangle} \left[ (1 - \Delta) \left( S_i^x S_j^x + S_i^y S_j^y \right) + S_i^z S_j^z \right] - \sum_{\langle i,j \rangle} \mathbf{D} \cdot (\mathbf{S}_i \times \mathbf{S}_j) - \sum_{i=1}^{N} \mathbf{H} \cdot \mathbf{S}_i,
$$

where the first term represents the nearest-neighbors anisotropic exchange interaction, with $\Delta$ being the anisotropy parameter, the second term represents the nearest-neighbors antisymmetric Dzyaloshinskii-Moriya (DM) interaction placed along the $z$ direction ($\mathbf{D} = \mathbf{D}_{ij} = -\mathbf{D}_{ji} = D\mathbf{\hat{z}}$), the third term corresponds to the Zeeman interaction with an external magnetic field $\mathbf{H} = H\mathbf{\hat{z}}$, and finally $S_i^\nu (\nu = x, y, z)$ are the spin-$1/2$ Pauli matrices at $i$-sites in a hypercubic lattice of $N$ spins. On such a lattice, one has coordination number $c$ given by $c = 2, 4, 6, \cdots$ for, respectively, the one-dimensional lattice, square two-dimensional lattice, simple cubic three-dimensional lattice, and so on. This model has no exact solution and the topology of the phase diagram in the $H - D$ plane, as a function of the anisotropy $\Delta$, still remains a fundamental problem. For $\Delta = 0$ one has the isotropic Heisenberg model, while for $\Delta = 1$ we recover the spin-$1/2$ Ising model, both with DM interaction.

We will employ a variational method based on Bogoliubov inequality (an inequality that is mainly based on arguments of convexity, as can be seen, for instance, in reference [11]),
which can be formally written, for any classical or quantum system, as

\[
F(\mathcal{H}) \leq F_0(\mathcal{H}_0) + \langle \mathcal{H} - \mathcal{H}_0 \rangle_0 \equiv \Phi(\eta),
\]

(2)

where \(F\) and \(F_0\) are the free energies associated with two systems defined by the Hamiltonians \(\mathcal{H}\) and \(\mathcal{H}_0(\eta)\), respectively, the thermal average \(\langle \ldots \rangle_0\) should be taken in relation to the canonical distribution associated with the trial Hamiltonian \(\mathcal{H}_0(\eta)\), with \(\eta\) standing for variational parameters. The approximated free energy \(F\) is given by the minimum of \(\Phi(\eta)\) with respect to \(\eta\), i.e. \(F \equiv \Phi_{\text{min}}(\eta)\).

With \(D\) and \(H\) defined above, the hamiltonian \(H\) in eq. (1) can be rewritten as

\[
H = J \sum_{\langle i,j \rangle} \left[ (1 - \Delta) \left( S_x^i S_x^j + S_y^i S_y^j \right) + S_z^i S_z^j \right] - D \sum_{\langle i,j \rangle} \left( S_x^i S_y^j - S_y^i S_x^j \right) - H \sum_{i=1}^{N} S_z^i.
\]

(3)

Otherwise, for the trial Hamiltonian \(\mathcal{H}_0\), we have chosen the simplest cluster for this model, which corresponds to a sum of \(N/2\) disconnected pairs of spins. As we are dealing with an antiferromagnetic system, each spin of the pair belongs to one particular \(A\) or \(B\) sub-lattice. We then have

\[
\mathcal{H}_0 = \sum_{\ell=1}^{N/2} \left\{ J \left[ (1 - \Delta) \left( S_x^A S_x^B + S_y^A S_y^B \right) + S_z^A S_z^B \right] - D \left( S_x^A S_y^B - S_y^A S_x^B \right) - \left( \eta_A + H \right) S_z^A - \left( \eta_B + H \right) S_z^B \right\},
\]

(4)

where \(S_x^A\) and \(S_x^B\) are the spins of the \(\ell\)-th pair on the \(A\) and \(B\) sub-lattices, respectively, and \(\eta_A\) and \(\eta_B\) are variational parameters, which are different in each sub-lattice.

It is not difficult to diagonalize the above trial Hamiltonian and to obtain the corresponding free-energy \(F_0\). The same holds for the mean value \(\langle \mathcal{H} - \mathcal{H}_0 \rangle_0\), where we still have \(Nc/2 - N/2\) remaining pairs in \(\mathcal{H}\). Thus, after minimizing the right hand side of Eq. (2) with respect to the variational parameters \(\eta_A\) and \(\eta_B\) we obtain the approximated mean-field Helmholtz free energy per spin, \(f = \Phi/N\), which can be written as

\[
f = -\frac{1}{2\beta} \ln \left\{ 2e^{-K} \cosh \Delta_1 + 2e^K \cosh 2K \Delta_2 \right\} - \frac{J}{2} (c - 1)m_A m_B,
\]

(5)

with

\[
\Delta_1 = 2h - (c - 1)(m_A + m_B)K,
\]

(6)

\[
\Delta_2 = \sqrt{(1 - \Delta)^2 + (c - 1)^2 (m_A - m_B)^2 + d^2}
\]

(7)
and the corresponding sub-lattice magnetizations $m_A$ and $m_B$ given by

$$m_A = \frac{\sinh \Delta_1 + e^{2K} \Delta_3 \sinh K \Delta_2}{\cosh \Delta_1 + e^{2K} \cosh K \Delta_2}$$ (8)

and

$$m_B = \frac{\sinh \Delta_1 - e^{2K} \Delta_3 \sinh K \Delta_2}{\cosh \Delta_1 + e^{2K} \cosh K \Delta_2},$$ (9)

where

$$\Delta_3 = (c - 1)(m_A - m_B)/\Delta_2.$$ (10)

In the above expressions, we have defined the reduced quantities $K = J/k_B T$, $h = H/J$, $d = D/J$, and $\beta = 1/k_B T$, where $k_B$ is the Boltzmann constant.

In order to analyze the criticality of this system, it will be more convenient to define an order parameter that characterizes the antiferromagnetic phase transition. The two new quantities that we will use here are the total ($m$) and staggered ($m_s$) magnetizations (the latter one being the desired order parameter of the antiferromagnetic transition), which are given by

$$m = \frac{1}{2}(m_A + m_B)$$ (11)

and

$$m_s = \frac{1}{2}(m_A - m_B).$$ (12)

Substituting Eqs. (8) and (9) in (11) and (12) we have

$$m = \frac{\sinh \tilde{\Delta}_1}{\cosh \tilde{\Delta}_1 + e^{2K} \cosh 2K \tilde{\Delta}_2},$$ (13)

and

$$m_s = \frac{\tilde{\Delta}_3 e^{2K} \sinh 2K \tilde{\Delta}_2}{\cosh \tilde{\Delta}_1 + e^{2K} \cosh 2K \tilde{\Delta}_2},$$ (14)

where now

$$\tilde{\Delta}_1 = 2K[h - (c - 1)m],$$ (15)

$$\tilde{\Delta}_2 = \sqrt{(1 - \Delta)^2 + (c - 1)^2 m_s^2 + d^2},$$ (16)

and

$$\tilde{\Delta}_3 = (c - 1)m_s/\tilde{\Delta}_2.$$ (17)

Accordingly, the free energy defined in (5) can be written in terms of the new order parameter as

$$f(m, m_s) = -\frac{1}{2\beta} \ln \left\{ 2e^{-K} \cosh \tilde{\Delta}_1 + 2e^K \cosh 2K \tilde{\Delta}_2 \right\} - \frac{J}{2}(c - 1)(m^2 - m_s^2).$$ (18)
Thus, for a given value of the set of Hamiltonian parameters, namely the reduced exchange anisotropy $\Delta/J$, the reduced Dzyaloshinskii-Moriya interaction $d$, and the reduced external field $h$, all in units of the exchange interaction $J$, we can obtain the temperature dependence of $m$ and $m_s$ by simultaneously solving the two nonlinear coupled equations (13) and (14). Below the antiferromagnetic phase transition the magnetizations of sub-lattices A and B are opposite and nonzero, while above the transition temperature one has $m_s = 0$ and $m = m_0$, which is the paramagnetic phase. In this paramagnetic phase one has

$$m_0 = \frac{\sinh(2h - 2(c - 1)Km)}{\cosh(2L - 2(c - 1)Km) + e^{2K}\cosh 2K\sqrt{(1 - \Delta)^2 + d^2}}$$

(19)

and

$$f(m_0) = -\frac{1}{\beta^2} \ln \left\{ 2e^{-K}\cosh(2h - 2(c - 1)Km) + 2e^K \cosh 2K\sqrt{(1 - \Delta)^2 + d^2} \right\} - \frac{J}{2}(c - 1) m_0^2.$$  

(20)

Close to the second-order transition line, one has $m_s << 1$ and the corresponding free energy (18) can be expanded in a Landau type so we can obtain a closed form equation for the Néel transition temperature $T_N$ (in fact $k_BT_N/J$) as a function of the Hamiltonian parameters. We can also obtain the criticality by noting that at the transition $m_s = 0$ and from relations (13) - (17) we obtain two coupled equations

$$m = \frac{\sinh \tilde{\Delta}_1}{\cosh \tilde{\Delta}_1 + e^{2K}\cosh 2K\tilde{\Delta}_4},$$

(21)

and

$$1 = \left( \frac{c - 1}{\tilde{\Delta}_4} \right) \frac{e^{2K}\sinh 2K\tilde{\Delta}_4}{\cosh \tilde{\Delta}_1 + e^{2K}\cosh 2K\tilde{\Delta}_4},$$

(22)

where $\tilde{\Delta}_4 = \sqrt{(1 - \Delta)^2 + d^2}$. Thus, given the values of $\Delta$, $d$, $h$, and $c$, these two equations furnishes $m$ and $k_BT_N/J$.

In order to seek for first-order transitions, we have to compare the antiferromagnetic free energy with $m_s \neq 0$ and the paramagnetic one with $m_s = 0$. The first-order phase transition is located when they have the same value. However, for the present model, as discussed in the next section, no first-order transitions have been detected.
III. RESULTS

The reduced critical transition temperature $k_B T_c / J$, as a function of the Hamiltonian parameters, is shown in Fig. 1 for the simple cubic lattice and the isotropic Heisenberg model ($\Delta = 0$) in the presence of external field and DM interaction. All the transition lines are second order and we have no indication of any first-order transition lines in these diagrams. We can see that the increase of either the external field or the DM interaction tends to decrease the corresponding transition temperature.

![Fig. 1: Critical transition temperature $k_B T_c / J$ of the simple cubic lattice $c = 6$ and isotropic Heisenberg model $\Delta = 0$ as a function of: (left) external field $h$ and several values of the DM interaction $d$; and (right) DM interaction $d$ and several values of the external field $h$.](image)

We can see that phase diagram in the temperature versus external field presents a reentrancy for DM interactions $d \lesssim 2.5$ while no re-entrancies are found in the phase diagram in the temperature versus DM interaction for any value of $h$. In addition, at $T = 0$, the value of the critical external field is given by $h_c = c$ and is independent of the DM interaction. On the other hand, from Eqs. (21) and (22) it can be shown that the critical value of the DM interaction $d_c$ is given by

$$
d_c = \sqrt{(c - 1)^2 - (1 - \Delta)},
$$

and is independent of the external field.
The critical temperature at zero external field, namely $k_B T_N/J(H = 0)$ = 5.78, is also comparable to those obtained from different methods, such as EFRG-12 $k_B T_N/J = 4.09$ obtained by de Sousa and Araujo [12], $k_B T_N/J = 3.54$ from Monte Carlo simulations [13], high-temperature expansion $k_B T_N/J = 3.59$ [14], variational cumulant expansion $k_B T_N/J = 4.59$ [15], EFT-2 $k_B T_N/J = 4.95$ and EFT-4 $k_B T_N/J = 4.81$ [5].

![FIG. 2: The same as Fig. 1 for $c = 8$.](image)

The same sort of picture can be seen in Fig. 2 for higher dimensions, which is an example for the case $c = 8$. For this value of the coordination number, at zero field, our results coincide with those by Bublitz et al. MFA-2 $k_B T_N/J = 7.83$ [16]. This numerical result is also comparable to other different methods, such as high-temperature expansion $k_B T_N/J = 5.53$ [17], EFT-2 $k_B T_N/J = 6.94$, and EFT-4 $k_B T_N/J = 6.89$ [5].

For the particular case $\Delta = d = h = 0$ we have the Ising limit. In this way $m = 0$ from Eq. 21, as expected, and the Eq. 22 provides exactly the equation of the pair approximation for Ising model [18] which is given by

$$2K(c - 1)e^{2K} = 1 + e^{2K}. \quad (24)$$

As a final comment, it should be stressed that the qualitative behavior of the phase diagrams are also the same for different values of the anisotropy $\Delta$, even in the limit of the Ising case $\Delta = 1$ [8].
IV. FINAL REMARKS

We have studied the anisotropic antiferromagnetic Heisenberg model, in an external magnetic field and with a Dzyaloshinskii-Moriya interaction, using a mean-field procedure based on Bogoliubov inequality for the free energy by employing a cluster of two spins. We have obtained the phase diagram as a function of the Hamiltonian parameters.

When comparing our results to those obtained from the effective field theory, which are, up to our knowledge, the only results for this system, we notice that there is no anomalous behavior of the transition lines at low temperature, although some re-entrancies are still present in some region of the phase diagram.

Of course, this treatment is still a mean field one. It is in some sense different from the EFT, although the latter one having also an intrinsic mean field character. The present results strongly suggest that the behavior of the thermodynamic properties of the anisotropic Heisenberg model with Dzyaloshinskii-Moriya interaction is far from having a complete understandable behavior.

ACKNOWLEDGEMENTS

This work was partially supported by FAPEAM and CNPq (Brazilian Research Agencies).

[1] T. Thio, et al., Phys. Rev. B 38 905 (1988).
[2] S. W. Cheong, et al., Phys. Rev. B 39 4395 (1989).
[3] J. G. Bednorz, K.A. Muller, Z. Phys. B 64 89 (1986).
[4] P. W. Anderson, Science 235 1196 (1987).
[5] Minos A. Neto, J. Roberto Viana, J. Ricardo de Sousa, J. Magn. Magn. Mater. 324 2405 (2012).
[6] Walter E. F. Parente, J. T. M. Pacobahyba, Ijanfilio G. Araújo, Minos A. Neto, J. Ricardo de Sousa, Ümit Akinci J. Magn. Magn. Mater. 355 235 (2014).
[7] Yunzhou Sun, Lin Yi, Xige Zhao, Huiping Liu, Solid State Commun. 144 61 (2007).
[8] Walter E. F. Parente, J. T. M. Pacobahyba, Ijanfilio G. Araújo, Minos A. Neto, J. Ricardo de Sousa, Physica E 74 287 (2015).
[9] J. A. Plascak, Phys. Stat. Sol. B 120 215 (1983).
[10] D. C. Carvalho and J. A. Plascak, Physica A 432, 240 (2015).
[11] H. Falk, Am. J. Phys. 38, 858 (1970).
[12] J. Ricardo de Sousa, I. G. Araujo, J. Magn. Magn. Mater 202, 231 (1999).
[13] He-Ping Ying et al., Phys. Lett. A 183, 441 (1993).
[14] G. S. Rushbrooke and P. J. Wood, Mod. Phys. 11, 409 (1967).
[15] Hong Li and T. L. Cheng, Phys. Rev. B 52, 15979 (1995).
[16] E. Bublitz Filho, J. Ricardo de Sousa, J. Magn. Magn. Mater. 269, 266 (2004).
[17] K. K. Pan, Phys. Lett. A 244, 169 (1998).
[18] J. W. Tucker, T. Balcerzak, M. Gzik, A. Sukiennicki, J. Magn. Magn. Mater. 187 (1998) 381.