A variational approach for the classical anisotropic Heisenberg model in a crystal field

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ABSTRACT

The variational approach based on the Bogoliubov inequality for the free energy is used to study the three-dimensional anisotropic Heisenberg XXZ model with a crystal field. The magnetization and the phase diagrams are obtained as a function of the parameters of the Hamiltonian. Limiting cases, such as isotropic Heisenberg, XY, and planar rotator models in two and three dimensions, are analyzed and compared to previous results obtained from analytical approximations as well as to those obtained from more reliable approaches such as series expansion and Monte Carlo simulations. A parametric procedure has been used in order to simplify the solutions of the self-consistent coupled equations.

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1. Introduction

Since the discovery of exchange interaction by Heisenberg [1] and Dirac [2] in 1926, which occurred just a year after Ising solved the one-dimensional version of the Ising model [3,4], the study of spin systems has attracted considerable attention. The analytical treatment of such systems is indeed, even nowadays, a real challenge from the theoretical point of view, because it requires complex applications of quantum mechanics, statistical mechanics, and electromagnetism. In particular, regarding the Heisenberg model, it is also suitable for describing the properties of pure and diluted real insulating magnetic materials [5–7]. Although this model has been widely studied and employed in both classical and quantum contexts, analytical exact solutions are available only in a few limiting cases. The spin-1/2 quantum version in one dimension has been treated by Bethe [8], and a theorem by Mermim and Wagner [9] shows that this model, even in two dimensions, has no spontaneous long-range order. The same applies also to the classical version of the model, with the one-dimensional lattice being exactly treated by Fisher [10].

Recently, due to the discovery of high-$T_c$ (critical temperature) superconductors, the interest in the two-dimensional Heisenberg model has substantially increased, due to the layered structure in these compounds. However, it is known that most quasi-two-dimensional magnetic materials exhibit some kind of anisotropy. So, the analysis of anisotropic Heisenberg models turns out to be quite important because, from the experimental point of view, the presence of some degree of anisotropy in the structural arrangements of the atoms is to be expected in nearly all cases. Besides, the atomic structure and asymmetry of the density of charges can further induce anisotropies in the exchange interactions as well.

It is also known that the quantum character of the spin variables should play an important role in these systems. However, the study of classical models with continuous spin variables continues to be an important subject of research. There are

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several physical realizations such as Rb$_2$MnF$_4$ [11,12] and K$_2$MnF$_4$ and Mn(HCOO)$_2$ - 2H$_2$O [13] which, besides being quasi-two-dimensional, present Mn atoms with spin $s = 5/2$, allowing then a classical treatment.

On the other hand, the antiferromagnetic Heisenberg model has been shown to exhibit a rich phase diagram when in the presence of an external field [14,15]. It has also been shown that such an antiferromagnet in an external field behaves like an anisotropic ferromagnet, with the external field term replaced by an effective crystal field-like interaction [16]. Thus, motivated by these former ideas, we study in this work the anisotropic ferromagnetic Heisenberg model with a crystal field interaction in a three-dimensional lattice. We employ a variational approach based on the Bogoliubov inequality for the free energy. In this case, a simpler analytical approach can be easily implemented according to the procedure recently suggested by Castro et al. [17].

The plan of the paper is the following. In Section 2, we present the model and the theoretical approximation for getting the thermodynamic quantities. In Section 3, we present the results, and some concluding remarks are given in Section 4.

2. Hamiltonian and variational approach for the free energy

2.1. Hamiltonian

In this work, we study the classical anisotropic XXZ model with a crystal field interaction described by the following Hamiltonian:

$$
\mathcal{H} = -J \sum_{\vec{r}, \vec{r}'} \left\{ S^x_{\vec{r}} S^x_{\vec{r}'} + S^y_{\vec{r}} S^y_{\vec{r}'} + \lambda S^z_{\vec{r}} S^z_{\vec{r}'}, \right\} - J_z \sum_{\vec{r}, \vec{r}'} \left\{ S^x_{\vec{r}} S^x_{\vec{r}'} + S^y_{\vec{r}} S^y_{\vec{r}'} + \eta S^z_{\vec{r}} S^z_{\vec{r}'}, \right\} + D \sum_{\vec{r}} (S^z_{\vec{r}})^2,
$$  (1)

where $J$ is the exchange interaction between spins in the layers parallel to the $xy$ plane and $J_z$ the exchange interaction between spins in different adjacent layers along the $z$ direction. $D$ is the crystal field and $S^2_{\vec{r}}$ are the $\alpha = x, y, z$ components of a classical unitary spin vector $| \vec{S} | = 1$. The parameters $\lambda$ and $\eta$ measure the degree of the spin interaction anisotropy within and between layers, respectively. The first sum runs over nearest-neighbor spins $\langle \vec{r}, \vec{r}' \rangle$ within the layers, the second sum is over nearest-neighbor spins $\langle \vec{r}, \vec{r}' \rangle$ between layers, and the last sum is made over the entire $N$ spins on a simple cubic lattice. For $J = J_z$ and $D = 0$, the above system reduces to the three-dimensional isotropic Heisenberg model for $\lambda = \eta = 1$ and to the $XY$ model when $\lambda = \eta = 0$. For $J_z = D = 0$, we have the two-dimensional anisotropic Heisenberg model, with no phase transition for $\lambda = 1$ and a Berezinsky–Kosterlitz–Thouless transition for $\lambda = 0$ [18,19].

By means of the usual polar representation for the spins [20,21], one has

$$
\vec{S}_{\vec{r}} = (S^x_{\vec{r}}, S^y_{\vec{r}}, S^z_{\vec{r}}) = (\sin \theta_{\vec{r}} \cos \phi_{\vec{r}}, \sin \theta_{\vec{r}} \sin \phi_{\vec{r}}, \cos \theta_{\vec{r}}),
$$

$$
\vec{S}_{\vec{r}} = \left( \sqrt{1 - (S^z_{\vec{r}})^2} \cos \phi_{\vec{r}}, \sqrt{1 - (S^z_{\vec{r}})^2} \sin \phi_{\vec{r}}, S^z_{\vec{r}} \right),
$$

(2)

where $\theta_{\vec{r}}$ and $\phi_{\vec{r}}$ are the spherical angles of the spin at site $\vec{r}$. In this representation, the Hamiltonian given by Eq. (1) can be written in the form

$$
\mathcal{H} = -\frac{J}{2} \sum_{\vec{r}, \vec{a}} \left\{ \sqrt{1 - (S^z_{\vec{r}})^2} \sqrt{1 - (S^z_{\vec{r} + \vec{a}})^2} \cos (\phi_{\vec{r} + \vec{a}} - \phi_{\vec{r}}) + \lambda S^z_{\vec{r}} S^z_{\vec{r} + \vec{a}} \right\},
$$

$$
-\frac{J_z}{2} \sum_{\vec{r}, \vec{c}} \left\{ \sqrt{1 - (S^z_{\vec{r}})^2} \sqrt{1 - (S^z_{\vec{r} + \vec{c}})^2} \cos (\phi_{\vec{r} + \vec{c}} - \phi_{\vec{r}}) + \lambda S^z_{\vec{r}} S^z_{\vec{r} + \vec{c}} \right\} + D \sum_{\vec{r}} (S^z_{\vec{r}})^2,
$$

(3)

where $\vec{a}$ labels the four nearest-neighbor sites of $\vec{r}$ in the $xy$ plane and $\vec{c}$ the two nearest-neighbor sites of $\vec{r}$ along the $z$ direction.

2.2. Variational approach

We employ a variational approach based on the Bogoliubov inequality for the free energy

$$
F \leq F_0 + \langle \mathcal{H} - \mathcal{H}_0(\gamma) \rangle_0 \equiv \Phi(\gamma),
$$

(4)

where $\mathcal{H}$ is the Hamiltonian under study (1), and $\mathcal{H}_0(\gamma)$ is a trial Hamiltonian which can be exactly solved and depends on variational parameters designated by $\gamma$. $F$ is the free energy of the system described by $\mathcal{H}$, $F_0$ is the corresponding free energy of the trial Hamiltonian $\mathcal{H}_0$, and the thermal average $\langle \cdot \cdot \cdot \rangle_0$ is taken over the ensemble defined by $\mathcal{H}_0$. The approximate free energy is then given by the minimum of $\Phi(\gamma)$ with respect to $\gamma$, i.e., $\Phi \equiv \Phi_{\text{min}}(\gamma)$.

It is desired that the trial Hamiltonian resembles, in several aspects, the one under study. As for the $XY$ model [17], in the present case, $\mathcal{H}_0$ can be chosen as a sum of two parts,

$$
\mathcal{H}_0 = \mathcal{H}_0^0 + \mathcal{H}_0^2,$$

(5)
where the first term is a kind of a planar Hamiltonian component,

\[ H^\phi_0 = \frac{\gamma}{4} \sum_{\vec{r},\vec{a}} (\phi_{\vec{r}+\vec{a}} - \phi_{\vec{r}})^2 + \frac{\gamma_2}{4} \sum_{\vec{r},\vec{c}} (\phi_{\vec{r}+\vec{c}} - \phi_{\vec{r}})^2, \tag{6} \]

and the second term is an axial Hamiltonian,

\[ H^\phi_z = -\frac{J_z}{2} \sum_{\vec{r},\vec{a}} S^2_{\vec{r}+\vec{a}} - \frac{J_z \eta}{2} \sum_{\vec{r},\vec{c}} S^2_{\vec{r}+\vec{c}} + (D + 2J_z) \sum_{\vec{r}} (S^2_{\vec{r}}), \tag{7} \]

where \( \gamma \) and \( \gamma_2 \) stand for the two variational parameters. This harmonic choice has the same motivation as the one discussed for the anisotropic XY model by Castro et al. [17]. It is valid in the low-temperature region because, for an almost ordered system, the difference in the planar angles in Eq. (3) are very small and one keeps just second-order terms in the expansion of the cosine functions. An improvement on the approach could be realized by taking high-order terms. However, as was reported in the previous work, Monte Carlo (MC) results were close to this variational approach for the XY model even close to the transition temperature. We expect the same holds for the present anisotropic Heisenberg model.

To see that \( H_0 \) can be exactly solved, we first note that the planar Hamiltonian \( H^\phi_0 \) can be diagonalized in reciprocal space through the Fourier transform \( \phi_{\vec{q}} \)

\[ \phi_{\vec{q}} = \frac{1}{\sqrt{N}} \sum_{\vec{r}} e^{i\vec{q}\cdot\vec{r}} \phi_{\vec{r}}, \tag{8} \]

which, for a translationally invariant system, gives

\[ H^\phi_0 = \frac{1}{2} \sum_{\vec{q}} \left( \gamma \sum_a (1 - e^{-i\vec{q}\cdot\vec{a}}) \phi_{\vec{q}} \phi_{-\vec{q}} + \gamma_2 \sum_{\vec{c}} (1 - e^{-i\vec{q}\cdot\vec{c}}) \phi_{\vec{q}} \phi_{-\vec{q}} \right). \tag{9} \]

Summing now over the vectors \( \vec{a} \) in the \( xy \) plane and \( \vec{c} \) along the \( z \) direction, and rearranging terms, we obtain the diagonal form of the planar trial Hamiltonian,

\[ H^\phi_0 = \sum_{\vec{q}} (\gamma_q + \gamma_{qz}) |\phi_{\vec{q}}|^2, \tag{10} \]

where \( \gamma_q = \gamma(2 - \cos q_a a - \cos q_c c), \gamma_{qz} = \gamma_z(1 - \cos q_z z), a = |\vec{a}|, c = |\vec{c}|, \) and \( |\phi_{\vec{q}}|^2 = \phi_{\vec{q}} \phi_{-\vec{q}}. \)

By introducing the corresponding Fourier transform of the \( z \) component of the spins \( S^z_{\vec{r}} \),

\[ S^z_{\vec{q}} = \frac{1}{\sqrt{N}} \sum_{\vec{r}} e^{i\vec{q}\cdot\vec{r}} S^z_{\vec{r}}, \tag{11} \]

one can diagonalize the axial term of the harmonic Hamiltonian (7):

\[ H^\phi_z = \sum_{\vec{q}} \Omega_{\vec{q}} |S^z_{\vec{q}}|^2, \tag{12} \]

where

\[ \Omega_{\vec{q}} = (D + 2J_z) - 2\lambda J y_{\vec{q}} - \eta \gamma_{q} y_{\vec{q}}. \tag{13} \]

As the planar and the axial parts of the harmonic Hamiltonian are independent, its partition function \( Z_0 \) can be written as

\[ Z_0 = \text{Tr} e^{-\beta H_0} = \text{Tr} e^{-\beta (H^\phi_0 + H^\phi_z)} = Z_0^\phi Z_0^z. \tag{14} \]

Moreover, since both \( H^\phi_0 \) and \( H^\phi_z \) are quadratic in their variables, one has

\[ Z_0^\phi = \text{Tr} e^{-\beta H^\phi_0} = \prod_{\vec{q}} \left[ \frac{\pi}{\beta(\gamma_q + \gamma_{qz})} \right]^\frac{1}{2}. \tag{15} \]

and

\[ Z_0^z = \text{Tr} e^{-\beta H^\phi_z} = \prod_{\vec{q}} \left[ \frac{\pi}{\beta \Omega_{\vec{q}}} \right]^\frac{1}{2}. \tag{16} \]
The corresponding free energy $F_0$ is then given by

$$ F_0 = -\frac{k_BT}{2} \sum_q \left\{ \ln \frac{\pi}{\beta(q_4 + q_{2q})} + \ln \frac{\pi}{\beta\Omega_q} \right\}. \tag{17} $$

Using the equipartition theorem, the mean value $\langle \mathcal{H}_0 \rangle_0$ can be easily evaluated, resulting in

$$ \langle \mathcal{H}_0 \rangle_0 = \frac{Nk_BT}{2} + \frac{Nk_BT}{2} = Nk_BT. \tag{18} $$

The mean value $\langle \mathcal{H} \rangle_0$ is, however, not so straightforward to compute. It can be written as

$$ \langle \mathcal{H} \rangle_0 = -\frac{J}{2} \sum_{r,a} \left( \sqrt{1 - (S_z^a)^2} \sqrt{1 - (S_z^{r,a})^2} \right) \langle \cos(\phi_{r+a} - \phi_r) \rangle_0 $$

$$ - \frac{J_z}{2} \sum_{r,c} \left( \sqrt{1 - (S_z^c)^2} \right) \langle \cos(\phi_{r+c} - \phi_r) \rangle_0 $$

$$ + D \sum_{r} (\langle S_z^r \rangle^2) - \frac{J}{2} \sum_{r,a} (\langle S_z^{r,a} \rangle) - \frac{J_z}{2} \sum_{r,c} (\langle S_z^{r,c} \rangle). \tag{19} $$

Since $(\phi_{r+a} - \phi_r)$ and $(\phi_{r+c} - \phi_r)$ are Gaussian variables, we can write

$$ \langle \cos(\phi_{r+a} - \phi_r) \rangle_0 = e^{-\frac{1}{2}((\phi_{r+a} - \phi_r)^2)_0}, \tag{20} $$

where the mean value of the exponential argument is given by

$$ \langle (\phi_{r+a} - \phi_r)^2 \rangle_0 = \frac{2}{\lambda_q} \sum_q (1 - \lambda_q) (\langle \phi_q \rangle_0^2), \tag{21} $$

with $\lambda_q = \frac{1}{2} (\cos q_x a + \cos q_y a)$ and

$$ \langle \phi_q \rangle_0^2 = \frac{k_BT}{2(y_q + y_{2q})}. \tag{22} $$

Analogously, for the Gaussian variable $(\phi_{r+c} - \phi_r)$, we have

$$ \langle \cos(\phi_{r+c} - \phi_r) \rangle_0 = e^{-\frac{1}{2}((\phi_{r+c} - \phi_r)^2)_0}, $$

and

$$ \langle (\phi_{r+c} - \phi_r)^2 \rangle_0 = \frac{2}{\lambda_{qc}} \sum_q (1 - \lambda_{qc}) (\langle \phi_q \rangle_0^2). \tag{23} $$

where $\lambda_{qc} = \cos q_y c$. Thus, Eq. (19) assumes the form

$$ \langle \mathcal{H} \rangle_0 = -\frac{J}{2} \sum_{r,a} (1 - \langle (S_z^a)^2 \rangle_0) e^{-\frac{1}{4} \sum_q (1 - \lambda_q) (\langle \phi_q \rangle_0^2)} $$

$$ - \frac{J_z}{2} \sum_{r,c} (1 - \langle (S_z^c)^2 \rangle_0) e^{-\frac{1}{4} \sum_q (1 - \lambda_{qc}) (\langle \phi_q \rangle_0^2)} + \sum_q \Omega_q (\langle S_z^q \rangle^2)_0, \tag{24} $$

where we have used the additional assumptions that $S_z^a \approx S_z^{r+a}$ and $S_z^c \approx S_z^{r+c}$. The last term can again be computed from the equipartition theorem and, since the terms in the sums do not depend on the respective indexes, we have

$$ \langle \mathcal{H} \rangle_0 = -2JN(1 - \langle (S_z^a)^2 \rangle_0) e^{-\frac{1}{4} \sum_q (2 - (\cos q_x a + \cos q_y a)) (\langle \phi_q \rangle_0^2)} $$

$$ - \frac{J_z}{2} N(1 - \langle (S_z^c)^2 \rangle_0) e^{-\frac{1}{4} \sum_q (2 - \cos q_y c) (\langle \phi_q \rangle_0^2)} + \frac{Nk_BT}{2}. \tag{25} $$

The right-hand side of Eq. (4) can then be written as

$$ \Phi(y', y'_z) = -\frac{k_BT}{2} \sum_q \ln \frac{\pi}{\beta(y_q + y_{2q})} - \frac{k_BT}{2} \sum_q \ln \frac{\pi}{\beta\Omega_q} - 2JN(1 - \langle (S_z^a)^2 \rangle_0) e^{-\frac{1}{4} \sum_q (2 - (\cos q_x a + \cos q_y a)) (\langle \phi_q \rangle_0^2)} $$

$$ - \frac{J_z}{2} N(1 - \langle (S_z^c)^2 \rangle_0) e^{-\frac{1}{4} \sum_q (2 - \cos q_y c) (\langle \phi_q \rangle_0^2)} - \left( 2 - \frac{D}{\Omega} \right) \frac{Nk_BT}{2}. \tag{26} $$
An upper bound limit for the free energy can be obtained by minimizing the above equation with respect to the variational parameters. They are determined from the conditions
\[
(a) \quad \frac{\partial \Phi(\gamma, \gamma_z)}{\partial \gamma} = 0 \quad \text{and} \quad (b) \quad \frac{\partial \Phi(\gamma, \gamma_z)}{\partial \gamma_z} = 0. \tag{27}
\]

The mathematical expressions for Eq. (27) are rather lengthy to be reproduced here. However, factoring terms that can be canceled out and defining
\[
\delta_{xy} = \frac{1}{2N} \sum_q \left[ 2 - (\cos q_x a + \cos q_y a) \right] \langle |\phi_q|^2 \rangle_0, \tag{28}
\]
\[
\delta_z = \frac{1}{N} \sum_q (1 - \cos q_z c) \langle |\phi_q|^2 \rangle_0, \tag{29}
\]
we arrive at the following expression:
\[
\left[ 1 - \langle (S^z_f)^2 \rangle_0 \right] \left( 2J \delta_{xy} e^{-\delta_{xy}} + J_z \eta_z e^{-\delta_z} \right) = \frac{k_B T}{2}. \tag{30}
\]

It should be stressed that equation is obtained from either Eq. (27)(a) or (b). This means that both variational parameters cannot be obtained from this equation alone. However, from the Gaussian variable definitions (20)–(23), one can deduce the following additional relation for the fluctuations \( \delta_{xy} \) and \( \delta_z \):
\[
2 \gamma \delta_{xy} + \gamma_z \delta_z = \frac{k_B T}{2}. \tag{31}
\]

Comparing now Eqs. (30) and (31), we find the following identifications:
\[
\gamma = J \left[ 1 - \langle (S^z_f)^2 \rangle_0 \right] e^{-\delta_{xy}}, \tag{32}
\]
\[
\gamma_z = J_z \left[ 1 - \langle (S^z_f)^2 \rangle_0 \right] e^{-\delta_z}, \tag{33}
\]

which are now two parametric equations from which the two variational parameters can be obtained. These equations can be put in a more convenient form by noting that
\[
e^{-\delta_{xy}} = \exp \left\{ -\frac{1}{N} \sum_q \frac{k_B T (1 - \lambda_q)}{2 \gamma \left( 1 - \lambda_q \right) + \gamma_z (1 - \lambda_{qz})} \right\}. \tag{34}
\]

Taking the continuum limit of the above equation in cylindrical coordinates \( \frac{1}{N} \sum_q \rightarrow \frac{2 \pi}{2 \pi} \int_0^{2 \pi} \int_0^{\pi} dq \, dq \, \int_0^{\pi} d\theta \int_0^{\pi} \frac{1}{2} \Gamma \frac{\phi_0}{g} \right\} \]
\[
e^{-\delta_{xy}} = \exp \left\{ -\frac{k_B T}{2 \gamma} \left[ \frac{\arctan g^\frac{1}{2}}{3g^{\frac{1}{2}}} + \frac{1}{6} - \frac{g}{6} \ln \left( 1 + \frac{1}{g} \right) \right] \right\}, \tag{35}
\]
where \( g = \frac{\gamma_z}{\gamma} \). Analogously, we find that
\[
e^{-\delta_z} = \exp \left\{ -\frac{k_B T}{2 \gamma} \times \left[ \frac{1}{g} - \frac{1}{3g^{\frac{1}{2}}} \left( 2 \arctan g^\frac{1}{2} + g^\frac{1}{2} - g^\frac{3}{2} \ln \left( 1 + \frac{1}{g} \right) \right) \right] \right\}, \tag{36}
\]
so the variational parameters are finally obtained from
\[
\gamma = J \left( 1 - \langle (S^z_f)^2 \rangle_0 \right) \exp \left\{ -\frac{k_B T}{2 \gamma} \left[ \frac{\arctan g^\frac{1}{2}}{3g^{\frac{1}{2}}} + \frac{1}{6} - \frac{g}{6} \ln \left( 1 + \frac{1}{g} \right) \right] \right\}, \tag{37}
\]
\[
\gamma_z = J_z \left( 1 - \langle (S^z_f)^2 \rangle_0 \right) \exp \left\{ -\frac{k_B T}{2 \gamma} \left[ \frac{1}{g} - \frac{1}{3g^{\frac{1}{2}}} \left( 2 \arctan g^\frac{1}{2} + g^\frac{1}{2} - g^\frac{3}{2} \ln \left( 1 + \frac{1}{g} \right) \right) \right] \right\}. \tag{38}
\]

The above equations are the same as those obtained for the XY model studied in Ref. [17] and can also be obtained by employing the usual self-consistent harmonic approximation. However, in the present case, the out-of-plane fluctuation is given by
\[
\left( \langle S^z_f \rangle \right)_0 = \frac{2k_B T}{\pi \lambda (J_z \eta^2)} \left[ \sqrt{\Delta + J \lambda \pi^2 \arctan \left( \frac{\pi (J_z \eta)^2}{\sqrt{\Delta + J \lambda \pi^2}} \right)} - \sqrt{\Delta \arctan \left( \frac{\pi (J_z \eta)^2}{\sqrt{\Delta}} \right)} \right]
+ \frac{\pi (J_z \eta)^2}{2} \ln \left( 1 + \frac{J_z \lambda \pi^2}{\Delta + \pi^2 J_z \eta} \right). \tag{39}
\]
where $\Delta = 2D + 4J(1 - \lambda) + 2J_\perp(1 - \eta)$, and which, as will be seen below, results in a new physical behavior of the system. Thus, for a given value of the reduced quantities $t = k_B T/J, D/J,$ and $J_\perp/J$ one can solve the nonlinear system (37) and (38) to get $\gamma / J$ and $\gamma_z / J$, and from them all the desired thermodynamics of the model. For instance, by taking the continuum limit in the long-wavelength regime, the $x$ component of the magnetization is given by

$$m = \left( 1 - \frac{1}{2} \langle (S_x^z)^2 \rangle_0 \right) \exp \left\{ -\frac{k_B T}{2\pi^2 2\gamma} \left[ \arctan(g^2) + \frac{1}{2} \ln \left( 1 + \frac{1}{g^2} \right) \right] \right\}. \tag{40}$$

The transition temperature is obtained when the only solution of Eqs. (37) and (38) is $\gamma = \gamma_z = 0$.

3. Numerical results

Before discussing some of the results, it is worthwhile exploring possible simpler solutions of Eqs. (37) and (38), and also presenting the results at some known limiting cases, where a comparison can be made with other works employing different approaches.

3.1. Parametric procedure

A parametric procedure has been proposed in Ref. [17], where a simpler procedure for getting the thermodynamical properties of the present model can be used. The idea is to assume that $\delta_z = \delta_{xy}$ (Assumption 2 in that reference), meaning that the quadratic fluctuations are not very different in vertical or in-plane bonds. This provides one more equation, allowing us to get all the parameters from Eq. (30) alone. In the following, this parametric procedure will be compared to the present solution obtained from the coupled equations (37) and (38).

3.2. Limiting cases

For $\lambda = \eta = 0$, we get the $XY$ model, and all limits discussed by Castro et al. [17] are also valid here. For completeness, the corresponding results for the $XY$ system are reported in Table 1. It should be said that the BKT transition is not completely described in a qualitatively way, since vortex corrections are not taken into account in this variational approach. On the other hand, for $J = J_z$ and $D = 0$, the above system reduces to the three-dimensional isotropic Heisenberg model for $\lambda = \eta = 1$. In this case, although one does not get the same results from solving Eqs. (37) and (38), and following the parametric procedure from Eq. (30), they are indeed quite close and comparable to the MC estimate [22], as can be seen from Table 1.

3.3. Phase diagrams

In Fig. 1, we show the reduced transition temperature $t_z = k_B T_z / J$ as a function of $\lambda$ in the region of the easy-plane anisotropy for the two-dimensional model, i.e., $J_z = 0$. It should be said that for $J_z = 0$ one gets the same equations, either from the complete present approach or from the simpler parametric procedure. At $D = 0$ it is noted that for $\lambda = 0$ one recovers the result obtained for the two-dimensional $XY$ model [17] (see also Table 1), and in the limit $\lambda \to 1$ the transition temperature drops to zero. This is the expected behavior, because the two-dimensional isotropic Heisenberg model does not exhibit long-range order. One can also notice an anisotropic crossover as soon as $D$ is positive and different from zero (even very small), since the transition temperature is finite for $\lambda = 1$. Thus, for positive values of $D$, the temperature increases as the crystal field increases. This can be understood from the fact that the $z$ component of the spins decreases as the crystal field is enhanced, implying a stronger magnetization on the $xy$ plane which needs, as a consequence, a higher temperature to disorder. In the limit $D \to \infty$, one completely suppresses the $z$ component of the spins. In this case, we recover the planar rotator model, which should have a transition temperature (given in Table 1) independent of the value of $\lambda$. On the other hand, for negative values of $D$, the $z$ component of spin is enhanced, implying a decrease of the plane magnetization and, as a consequence, a lowering of the transition temperature. Finally, for $D/J < -2$, there is no more ordering on the $xy$ plane. The corresponding ordering in the perpendicular Ising-like component is not done in this procedure.

Fig. 2(a) and (b) display the out-of-plane fluctuations and the reduced transition temperature (the latter on a finer scale) as a function of anisotropy $\lambda$ for $J_z = 0$ and $D = 0$. Since the out-of-plane fluctuations are also responsible for driving

<table>
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<tr>
<th>$D \to \infty, J_z = 0, \lambda = \eta = 0$</th>
<th>MC</th>
<th>Present</th>
<th>Parametric</th>
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<tbody>
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<td>$D \to \infty, J_z = J, \lambda = \eta = 0$</td>
<td>0.89 [23]</td>
<td>1.472</td>
<td>1.472</td>
</tr>
<tr>
<td>$D = 0, J_z = 0, \lambda = \eta = 0$</td>
<td>2.202 [24]</td>
<td>2.190</td>
<td>2.207</td>
</tr>
<tr>
<td>$D = 0, J_z = J, \lambda = \eta = 0$</td>
<td>1.54 [1] [26]</td>
<td>1.605</td>
<td>1.613</td>
</tr>
<tr>
<td>$D = 0, J_z = J, \lambda = \eta = 1$</td>
<td>1.443 [22]</td>
<td>1.458</td>
<td>1.465</td>
</tr>
</tbody>
</table>

Table 1 Reduced transition temperatures $t_z$ for the present model in some isotropic limiting cases according to the Monte Carlo approach (MC), the present approach (Present), and the parametric procedure (Parametric).
Fig. 1. Reduced transition temperature $t_r = k_B T_r / J$ as a function of $\lambda$ for $J_z = 0$. The numbers for each line refer to the reduced value $D/J$.

Fig. 2. (a) Out-of-plane spin fluctuation $\langle (S_z^r)^2 \rangle_0$ and (b) the reduced transition temperature on a finer scale for $D = 0$ and $J_z = 0$. The reduced critical temperature is shown in (c) for $\lambda = 0$ and in (d) for $\lambda = 1$. The system to disorder, one can clearly relate the maximum of $t_r$ to being due to the minimum of $\langle (S_z^r)^2 \rangle$ as a function of $\lambda$. (In fact they happen at the same value of $\lambda$.) Such slight increase of $t_r$ with $\lambda$ also happens for other values of the crystal field. Fig. 2(c) and (d) show the transition temperature of Fig. 1 as a function of the crystal field at $\lambda = 0$ and $\lambda = 1$, respectively. In (c), one notes that for $D/J < -2$ there is no longer any transition (the number 2 coming from the dimensionality of the lattice) while, in (d), for the isotropic exchange $\lambda = 1$, the transition happens only for positive crystal fields, which are the only anisotropic breaking parameters.

We show in Fig. 3 the transition temperature for $J_z = J$ and $\eta = \lambda$, as a function of $\lambda$, for several values of the reduced crystal field. The dashed lines correspond to the simpler parametric procedure and the full line to the complete coupled equations approach. One can see that on that scale the results for the phase diagram are qualitatively the same, and also quantitatively comparable to each other. As for the two-dimensional model, in the limit $D \to \infty$ one gets the three-dimensional planar rotator model, and the results do not depend on $\eta$ and $\lambda$ since the $z$ component of the spin is suppressed. For $D/J < -3$ (again, in this case, the number 3 comes from the three-dimensional lattice) there is no longer any transition. On the other hand, in the present model, for $D < 0$, the curves end at some value of $\lambda$, and there are no solutions for the transition temperatures. From other approaches, such as the phenomenological mean field renormalization group [27], this can be inferred as an indication of a possible tricritical point. However, for the present case, we think that this is not the case, and that it may be an artifact of the procedure.

Similar phase diagrams are obtained for different values of the ratio $J_z/J$ as well as for $\eta \neq \lambda$. In all cases, the minimum of the out-of-plane fluctuation corresponds to the maximum of the transition temperature, when plotted as a function of $\lambda$. The minimum of $\langle (S_z^r)^2 \rangle$ occurs now for higher values of $\lambda$ as the crystal field increases. As for $\lambda < 1$ and $\eta < 1$ we have the easy-plane model, it is possible to find pairs of $(\eta, \lambda)$ such that the transition temperature is the same as that
Fig. 3. Reduced transition temperature $t_r = k_B T_r / J$ as a function of $\lambda$ for $J_z = J$ and $\eta = \lambda$. The numbers for each line refer to the reduced value $D/J$. The full line comes from the present complete approximation and the dashed line from the simpler parametric procedure.

Fig. 4. Results for $(\eta, \lambda)$ at which the XXZ anisotropic model has the same temperature as the XY model for some values of the Hamiltonian parameters.

for the XY model. In Fig. 4, there are some examples for which the present XXZ anisotropic model has the same transition as the XY model. It should be stressed that in this case only the non-universal quantity $T_r$ is the same for the easy-plane anisotropic Heisenberg model and the XY model, their critical exponents belonging to a different universality class. This variational approach, however, does not provide the critical exponents for the model, because the magnetization does not vanish continuously at the transition temperature (which still makes it difficult to characterize first-order transitions). On the other hand, for discrete quantum and classical Hamiltonians, the critical exponents are always mean-field like, regardless of the trial Hamiltonian [28].

Fig. 5 depicts the magnetization as a function of the reduced temperature for several values of the Hamiltonian parameters. In Fig. 5(a), we have the plane rotator model, which is independent of $\lambda$ and $\eta$. The behavior of the magnetization is quite different from that of the present coupled equations and the parametric solution in the quasi-two-dimensional model $J_z / J = 0.1$, and they are almost equal in the isotropic three-dimensional lattice $J_z = J$. Despite that, the corresponding transition temperatures are almost the same. In 5(b) and (c), we show, for two distinct values of the ratio $D/J$, the quasi-two-dimensional model for $\eta = 0$, respectively for the isotropic Heisenberg plane interaction $\lambda = 1$ and the XY plane $\lambda = 0$. Again, in this case, the transition temperatures are comparable. In Fig. 5(d), both approaches are practically identical in the isotropic Heisenberg limit.

4. Concluding remarks

The anisotropic Heisenberg model with a crystal field interaction has been studied according to the Bogoliubov variational approach for the free energy. This system is a generalization of the planar rotator model and the anisotropic XY model.
previously treated in the literature [17,26,29]. We have obtained a satisfactory picture of the thermodynamic behavior of the model as a function of its parameters in both the complete procedure solving two coupled equations and a simpler parametric approach with just one transcendental equation.

It should be stressed that the approximation employed in this work is valid only at low temperatures. It is therefore rather surprising that the values for the transition temperatures, shown in Table 1, for the three-dimensional model are quite comparable to those coming from more reliable methods. On the other hand, the agreement with the two-dimensional model is not so good. This is, however, justifiable, since in two dimensions we expect vortex effects, which are not taken into account in the present approach.

As a final remark, something should be said about the maximum of the transition temperature when plotted as a function of the anisotropic parameter $\lambda$. We are not sure whether this is a proper physical behavior of the model or just a consequence of the approximation. The same holds for the ending of the transition temperatures in the three-dimensional model. Monte Carlo simulations would be very welcome. We also expect that improvements to the present approach should clarify such points.

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**References**