Phase transitions in the two-dimensional anisotropic biquadratic Heisenberg model

Antônio R. Moura,1∗ Antônio S. T. Pires,2 and Afrânio R. Pereira3

1Universidade Federal de Uberlândia
2Universidade Federal de Minas Gerais
3Universidade Federal de Viçosa

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In this paper we study the two-dimensional anisotropic biquadratic Heisenberg model (ABHM) on the square lattice at zero and finite low temperatures. The model presents many phases due to both biquadratic and anisotropic terms. Its features in one-dimensional systems are well-documented. For the two-dimensional case, however, there are regions which are not so clear and, therefore, more investigations are necessary. In special, we have analyzed the quantum phase transition due to the single-ion anisotropic constant $D$. For values below a critical anisotropic constant $D_c$ (i.e., for $D < D_c$), the energy spectrum is gapless and, at low finite temperatures, the order parameter correlation has an algebraic decay (quasi long-range order). There are a transition temperature where the quasi long-range order is lost and the decay becomes an exponential, similar to the Berezinski-Kosterlitz-Thouless (BKT) transition. For $D > D_c$, the excited states are gapped and there is no long-range order (LRO), even at zero temperature. Using Schwinger bosonic representation and Self-consistent Harmonic Approximation (SCHA), we have studied the quantum and thermal phase transitions as a function of the bilinear and biquadratic constants.

Keywords: Anisotropic Biquadratic Heisenberg Model; Phase Transitions; Schwinger Bosons; SCHA

I. INTRODUCTION

The subject of low-dimensional magnetic models has received a lot of attention since Haldane discovered the intriguing physics of the quantum spin chains. In one dimension, spin models present completely different behavior if the spin value is integer or semi-integer due purely to quantum effects [1]. While semi-integer spin chains have a gapless energy spectrum, the corresponding integer spin chain presents the famous Haldane gap. Other important effects have also been predicted (not only in the condensed matter physics) and observed firstly in the spin 1/2 spin chain presents the famous Haldane gap. Other important effects have also been predicted (not only in the condensed matter physics) and observed firstly in the spin 1/2 spin chain presents the famous Haldane gap. Other important effects have also been predicted (not only in the condensed matter physics) and observed firstly in the spin 1/2 spin chain presents the famous Haldane gap. Other important effects have also been predicted (not only in the condensed matter physics) and observed firstly in the spin 1/2 spin chain presents the famous Haldane gap. Other important effects have also been predicted (not only in the condensed matter physics) and observed firstly in the spin 1/2 spin chain presents the famous Haldane gap. Other important effects have also been predicted (not only in the condensed matter physics) and observed firstly in the spin 1/2 spin chain presents the famous Haldane gap. Other important effects have also been predicted (not only in the condensed matter physics) and observed firstly in the spin 1/2 spin chain presents the famous Haldane gap. Other important effects have also been predicted (not only in the condensed matter physics) and observed firstly in the spin 1/2 spin chain presents the famous Haldane gap. Other important effects have also been predicted (not only in the condensed matter physics) and observed firstly in the spin 1/2 spin chain presents the famous Haldane gap. Other important effects have also been predicted (not only in the condensed matter physics) and observed firstly in the spin 1/2 spin chain presents the famous Haldane gap. Other important effects have also been predicted (not only in the condensed matter physics) and observed firstly in the spin 1/2 spin chain presents the famous Haldane gap. Other important effects have also been predicted (not only in the condensed matter physics) and observed firstly in the spin 1/2 spin chain presents the famous Haldane gap. Other important effects have also been predicted (not only in the condensed matter physics) and observed firstly in the spin 1/2 spin chain presents the famous Haldane gap. Other important effects have also been predicted (not only in the condensed matter physics) and observed firstly in the spin 1/2 spin chain presents the famous Haldane gap. Other important effects have also been predicted (not only in the condensed matter physics) and observed firstly in the spin 1/2 spin chain presents the famous Haldane gap. Other important effects have also been predicted (not only in the condensed matter physics) and observed firstly in the spin 1/2 spin chain presents the famous Haldane gap. Other important effects have also been predicted (not only in the condensed matter physics) and observed firstly in the spin 1/2 spin chain presents the famous Haldane gap.

In the present paper we have investigated the thermal and quantum phase transitions in the anisotropic biquadratic Heisenberg model (ABHM) on a two-dimensional square lattice, defined by the following Hamiltonian:

$$H = \sum_{\langle ij \rangle} [J_1 (S_i \cdot S_j) + J_2 (S_i \cdot S_j)^2] + \sum_i D(S_i^z)^2, \quad (1)$$

where $J_1$, $J_2$ and $D$ are the bilinear, biquadratic and single-ion anisotropy constants, respectively. The first sum is taken over the nearest neighbors while the second one is over all the sites. It is important to note that the above Hamiltonian only makes sense for spins larger than 1/2 due to the anisotropic term. The spin-1/2 case is degenerated and both up and down states have the same energy. Obviously, a magnetic field could break the degeneracy separating the energy spectrum. Thus, here we have considered the more relevant case with spin-1 where there are three energy bands: $S_i^z = \pm 1$ and $S_i^z = 0$. The same model on a triangular lattice has recently been studied by Serbyn et al. [5] through a fermionic representation. These authors have obtained the phase diagram as well as the specific heat and susceptibility.

The biquadratic term arises from fourth-order perturbations in the exchange interaction and normally its value is smaller than the bilinear term (although there are cases where the biquadratic prevails over bilinear interaction). The model studied has a very rich set of phases as a function of constants $J_1$ and $J_2$. It is common to write $J_1 = J \cos \theta$ and $J_2 = J \sin \theta$ and for the one-dimensional case, many phases for $\theta$ are very well known [3, 4]. Indeed, the points $\theta = \pi$ and $\theta = 0$ correspond to the pure ferromagnetic (FM) and antiferromagnetic (AFM) models respectively. In the interval $\pi/2 < \theta < 5\pi/4$ one has a stable ferromagnetic regime with long-range order (LRO); in $-3\pi/4 < \theta < -\pi/4$ a dimerized phase arises while $-\pi/4 < \theta < \pi/4$ leads to an antiferromagnetic phase with Haldane gap (for spin-1) and for
\(\pi/4 < \theta < \pi/2\) there is a trimerized phase. Some points have an exact solution as \(\theta = \pm \pi/4\), which are resolved by the Bethe ansatz. On the other hand, the two-dimensional case is more complicated and still, there are regions not yet understood. By using a continuous model, similar to non-linear sigma model, Ivanov et al. have shown the existence of a nematic phase for \(\theta > 5\pi/4\) while for \(\theta \lesssim 5\pi/4\) there are a disordered nematic phase. Rodrigues et al. have also determined the many phases of the biquadratic anisotropic model to Mott insulators (at unit filling). Using an effective field model (similar to that used by Ivanov et al.) and other methods, they have studied the model in the interval \(-0.9\pi \lesssim \theta \leq 0.5\pi\) for many dimensions. For \(\theta < -3\pi/4\), there is an XY ferromagnetic state for small positive values of \(D\) and a disordered phase for large positive \(D\), while for negative values of \(D\) one has an Ising-FM state. When \(\theta > 3\pi/4\) there is a XY nematic phase if \(D < 0\) and an Ising nematic phase for \(D > 0\). The case \(J_1 = J_2\) in a Mott insulator with 1/3 filling was also analyzed by Tóth et al.[13]. These authors have shown the existence of a three-sublattice long-range order on the square lattice in favor to the two-sublattice (Néel state) at zero temperature while at finite temperatures, the thermal fluctuations stabilize the two-sublattice state.

The single-ion anisotropy (expressed by constant \(D\)) has an important role in the model investigated here. It is present in materials as \(\text{N}_i(C_2H_8N_2)_2 \rightarrow 2\text{NO}_2(\text{ClO}_4)\) (NEMP) and it is responsible for quantum phase transitions\[16, 22\]. For instance, there are two distinct regions separated by a critical value \(D_c\) of the anisotropic constant, each one with unique properties\[16, 22\]. Below the critical point, the system has a gapless spectrum energy and a quasi long-range order (LRO) with an algebraic decay for the order-parameter correlation at low finite temperature. Above a critical transition temperature, the order-parameter decays exponentially and there is no more LRO. This phenomenon is similar to the Berezinsky-Kosterlitz-Thouless (BKT) transition which occurs in the two-dimensional XY-model, where there are bound and unpaired vortex-antivortex phases separated by a finite temperature\[24\]. As \(D\) increases, the transition temperature decreases (it vanishes at zero temperature for \(D = D_c\)). For values of the anisotropic constant above \(D_c\) (the so-called large-\(D\) phase), the system has a different behavior. The ground state is unique and associated to \(S^z = 0\) sector while the excited states are gapped, belonging to \(S^z = \pm 1\) sector. In the large-\(D\) phase, there is no LRO even at zero temperature (the order is totally lost), while the excitations have spin one and an infinite lifetime at low energies. The system suffers a quantum phase transition at zero temperature from a gapless to a gapped energy state. In the present paper we have adopted the antiferromagnetic bilinear model with \(J_1 > 0\) and small biquadratic constant, \(-J_1 < J_2 < J_1\). Once we are interested in the phase transition for large values of \(D\), we have considered only positive values for the anisotropic constant.

To investigate the behavior of the ABHM, we have applied two different methods at zero temperature: the first method is used for the case \(D < D_c\) and the second for the large-\(D\) phase. Below the critical point, we have used the Schwinger bosonic representation\[25–27\] which indicates a phase transition close to \(D_c\), although it does not provide the exact transition point. Better results are found analyzing the large-\(D\) phase, where we have used the bond operator formalism at zero temperature\[22\]. For finite temperatures, the most appropriate spin-wave method is the Self-Consistent Harmonic Approximation (SCHA)\[5, 28–31\]. Using the SCHA, we have determined the transition temperature for many combinations of the bilinear, biquadratic and anisotropic constants. Extrapolating to zero temperature, the SCHA also provides the values of the critical points \(D_c\) close to that one obtained from bond operator formalism. In the next section, we present the results for the phase \(D < D_c\), while in section \[11\] we present the results for the large-\(D\) phase. The section \[14\] is dedicated to finite temperatures analysis and finally, the conclusion is given in section \[15\].

II. SMALL-\(D\) PHASE AND THE SCHWINGER BOSONIC REPRESENTATION

In the phase with \(D < D_c\), the ground state is ordered at zero temperature and without LRO at finite temperatures as dictated by the Mermin-Wagner theorem\[52\]. The lowest energy excitations are the gapless Goldstone bosons that emerge with any amount of energy. We have used the \(SU(2)\) Schwinger bosonic formalism to describe this phase. The spin in each site \(i\) is represented by two bosonic operators \(a_i, b_i\). Forgetting the anisotropic term for a while, the action for the model is given by:

\[
\mathcal{Z} = \int \mathcal{D}[\mathbf{S}] e^{-i \int \mathcal{H} dt}, 
\]

where:

\[
\mathcal{H} = \sum_{\langle i,j \rangle} \left[ 2J_2 \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle - J_2 \langle \mathbf{S}_i \rangle^2 + J_1 \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle \right].
\]

In the above equations we have applied the Hubbard-Stratonovich transform\[33, 34\] to decouple the biquadratic term in favor to the mean-field parameter \(\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle\). In the limit \(J_2 = 0\), we recover the traditional Heisenberg model. The mean-field parameter will be determined by the minimum of the Helmholtz free energy. The spin operators are written as \(\mathbf{S}_i^+ = a_i^\dagger b_i\), \(\mathbf{S}_i^- = b_i^\dagger a_i\) and \(\mathbf{S}_i^z = (a_i^\dagger a_i - b_i^\dagger b_i)/2\), where \(a_i\) and \(b_i\) are the two Schwinger bosons on site \(i\). The bosonic operators keep the spin commutation relation and to fix \(\mathbf{S}^2 = S(S + 1)\) we have to impose the local constraint

\[
\sum_i (a_i^\dagger a_i + b_i^\dagger b_i) = 2S,
\]

which fix the total number of
bosons on each site. Therefore, in the bosonic formalism, the bilinear term is written as

$$S_i \cdot S_j = \frac{1}{2} A_{ij}^\dagger A_{ij} + S^2,$$

(4)

with the bond operator $A_{ij} = a_i a_j + b_i b_j$ (here we make a rotation by $\pi$ around the $y$-axis on sublattice B as usually), while the biquadratic interaction is given by:

$$\sum_i (S_i^z)^2 = \frac{1}{4} \sum_i \left( a_i^\dagger a_i - b_i^\dagger b_i \right)^2 = -\sum_i a_i^\dagger a_i b_i b_i,$$

(5)

where we used the constraint $\sum_i (a_i^\dagger a_i + b_i^\dagger b_i) = 2S$ to simplify the expression and a constant term was discarded by a redefinition of the ground state energy. Both interactions, the bilinear and the biquadratic ones, are fourth order terms in the action and they are decoupled again by using the Hubbard-Stratonovich transform:

$$\tilde{A}_{ij}^\dagger A_{ij} \rightarrow -A(\tilde{A}_{ij}^\dagger + A_{ij}) - A^2$$

(6)

and

$$a_i^\dagger b_i a_j b_i \rightarrow B(a_i b_j + a_j b_i^\dagger) - B^2,$$

(7)

where we have introduced the real mean-fields $A = \langle \tilde{A}_{ij} \rangle = \langle A_{ij} \rangle$ and $B = \langle a_i^\dagger b_i \rangle = \langle a_i b_i \rangle$. The values of $A$ and $B$ are also determined by minimizing the Helmholtz free energy. Thus, the second-order Hamiltonian to the ABHM is:

$$H = H_0 + \sum_i \left[ \frac{1}{2} \lambda (a_i^\dagger a_i + b_i^\dagger b_i) - BD(a_i b_i + b_i a_i) + h.c. \right] +$$

$$+ \hat{A} \sum_{\langle i,j \rangle} \left( a_i a_j + b_i b_j + h.c. \right)$$

(8)

with the constant term

$$H_0 = \left( -\frac{J_1}{2} A^2 + J_2 S^2 A^2 - \frac{3}{4} J_3 A^4 \right) \frac{N^2}{2} + NDB^2 -$$

$$-2N\lambda \left(S + \frac{1}{2} \right)$$

(9)

and $\hat{A} = -\left( \frac{d}{2} A + J_2 S^2 A - \frac{d}{2} A^3 \right)$. Here, a constraint was added by a local Lagrange multiplier $\lambda$ on each site and after that, we have adopted a mean value $\lambda = \langle \lambda_i \rangle$. According to Auerbach [25], the use of a mean value for $\lambda$ causes an incorrect prediction of $S^2$ and some related quantities. The predict value is smaller than the correct one by a factor of $3/2$. The correction can be done by a perturbation expansion around the mean value but we have, however, used the ordinary method of adding a $3/2$ factor when it is necessary. Takahashi has shown that this factor does not appear in a theory based on the Holstein-Primakoff representation [26, 30]. He has naturally obtained the same corrected equations as in the Schwinger formalism; however, this work is substantially simpler in the Schwinger representation and for our purposes, this is an acceptable method. After a Fourier transform, the Hamiltonian in momentum space is given by:

$$H = H_0 + \frac{1}{2} \sum_k \beta_k^\dagger H_k \beta_k,$$

(10)

where the vector $\beta_k^\dagger = (a_k^\dagger b_k^\dagger a_{-k} b_{-k})$ and the matrix is:

$$\breve{H} = \begin{pmatrix} \lambda & 0 & 4\tilde{A}\gamma_k & -BD \\ 0 & -\lambda & -BD & 4\tilde{A}\gamma_k \\ 4\tilde{A}\gamma_k & -BD & \lambda & 0 \\ -BD & 4\tilde{A}\gamma_k & 0 & \lambda \end{pmatrix}$$

(11)

in which $\gamma_k = \sum_\delta e^{ikr_\delta} = \frac{1}{2} (\cos k_x + \cos k_y)$ is the structure factor and $\delta$ designates the four neighboring sites (we have assumed an unitary lattice parameter, $a = 1$). The diagonalization is done by using the Bogoliubov method in order to keep the bosonic nature of the operators. The energy eigenvalues are given by $E_{k\downarrow} = \sqrt{\lambda^2 - (4\tilde{A}\gamma_k + BD)^2}$ and $E_{k\uparrow} = \sqrt{\lambda^2 - (4\tilde{A}\gamma_k - BD)^2}$ while the Hamiltonian assumes a quantum harmonic oscillator format

$$H = H_0 + \sum_{k,m} \left( c_{km}^\dagger c_m + \frac{1}{2} \right) E_m,$$

(12)

in which $c_{km}$ ($m = 1, 2, 3$) are the new bosonic operators. The Helmholtz free energy ($F = -\beta^{-1} \ln \text{Tr} e^{-\beta H}$) is therefore:

$$F = H_0 + \frac{1}{2} \sum_{k,m} \left\{ \ln \left[ \frac{\text{sech} \left( \beta E_m \right)}{2} \right] \right\}$$

(13)

where the sum is taken over the first Brioullin zone. By optimization of the Helmholtz free energy, $\partial F/\partial A = \partial F/\partial B = \partial F/\partial \lambda = 0$, one obtains three integral self-consistent equations. In the continuous limit and at zero temperature, they become:

$$A = -\frac{1}{4} \int \frac{d^2 k}{4\pi^2} \left[ \frac{4\tilde{A}\gamma_k + BD}{E_{k\downarrow}} - \frac{4\tilde{A}\gamma_k - BD}{E_{k\uparrow}} \right] \gamma_k,$$

(14a)

$$B = \frac{1}{4} \int \frac{d^2 k}{4\pi^2} \left[ \frac{4\tilde{A}\gamma_k + BD}{E_{k\downarrow}} - \frac{4\tilde{A}\gamma_k - BD}{E_{k\uparrow}} \right] \gamma_k,$$

(14b)

$$S + \frac{1}{2} = \frac{1}{4} \int \frac{d^2 k}{4\pi^2} \left[ \frac{1}{E_{k\downarrow}} + \frac{1}{E_{k\uparrow}} \right].$$

(14c)

Obviously, an exact solution for $A$, $B$ and $\lambda$ mean-field parameters is a hard task to be obtained and numerical methods must be used. However, we can have a general idea of the system behavior from the existence or not of solutions. According to Takahashi and Arovas, at finite temperatures, the self-consistent equations have a solution and it is associated with an unbroken symmetry. The ground state is disordered and the exponential decay of the spin-spin correlation at large distances can be demonstrated explicitly. At zero temperature, there is no solution to the integral equations because the bosons
condensate in a state with zero energy; the equations are divergent. The absence of solution is a feature of an ordered ground state, i.e., a state with broken symmetry. Similar to the Bose-Einstein condensation, the divergence is countered by separating the term with zero energy from the integral equations. In our case, $E_{k,1}$ vanishes at point $k^* = (\pm \pi, \pm \pi)$, while $E_{k,2}$ reaches the minimum at $k^* = (0, 0)$; so $\lambda = |4A\gamma k + BD|$ in the condensate state. Close to the minimum energy point, we have a massless relativistic dispersion relation $E_k = |k - k^*| c$, where $c$ is the spin-wave velocities. The excited states are the gapless Goldstone modes that emerge from any amount of energy in order to try to restore the broken symmetry. After separating the divergent term of the integral equations, we introduce a new parameter $\rho$ that measures the condensate density as following:

$$\rho = \left(S + \frac{1}{2}\right) \frac{1}{4} \frac{1}{4\pi^2} \int \frac{d^2k}{4\pi^2} \left( \frac{\lambda}{E_{k,1}} + \frac{\lambda}{E_{k,2}} \right). \quad (15)$$

Therefore the equations for $A$ and $B$ are given by:

$$A = 2\rho - \frac{1}{4} \int \frac{d^2k}{4\pi^2} \left( \frac{4\tilde{A}\gamma k + BD}{E_{k,1}} + \frac{4\tilde{A}\gamma k - BD}{E_{k,2}} \right) \gamma_k \quad (16)$$

and

$$B = 2\rho + \frac{1}{4} \int \frac{d^2k}{4\pi^2} \left( \frac{4\tilde{A}\gamma k + BD}{E_{k,1}} - \frac{4\tilde{A}\gamma k - BD}{E_{k,2}} \right). \quad (17)$$

Now the self-consistent equations can be numerically solved. The results for the condensate density are shown in Figures [1] and [2]. In both graphics, the anisotropic and biquadratic constants are given in units of $J_1$. The bosons are highly condensed to small values of the anisotropic constant $D$. At $D = 0$, the level is around 85% for different biquadratic constants but close to $D = 5$, it is approximately 60%, while it does not suffer a notable influence for small values of the biquadratic interaction constant $J_2$. For the Heisenberg model, the condensate density is around 81%, so our results for $J_2 = 0$ and $D = 0$ are only slightly bigger than the expected ones. For $D > 1$ the condensate density decays almost linearly for all $J_2$ values analyzed. When $\rho = 0$, the system exists in the condensate phase and enters in the disordered regime. The bosons do not condensate anymore in a null energy state and the spectrum becomes gapped at zero temperature. Figure [2] suggests us that exist a point where occurs a quantum phase transition from the ordered state to the unbroken symmetry phase at zero temperature. If we extrapolate the results for $\rho \rightarrow 0$ and by assuming the linear behavior, we discover the critical point $D_c \approx 10J_1$, which is bigger than the real value obtained in next sections. The theory is not appropriated when the condensate density is much lower than 1 and the results at $D \approx D_c$ are not accurate. The better way to obtain the critical point is shown in the next section. We begin in the gapped phase with $D > D_c$, lowering the anisotropic constant to the gapless region.

III. LARGE-D PHASE AND BOND OPERATOR

For anisotropic constant bigger than a critical value $D_c$, the physical properties are distinct from those studied in previous section. In the so-called large-$D$ phase, the energy spectrum is gapped and the symmetry is restored for a disordered phase. A phase transition occurs at point $D_c$ even at zero temperature, which characterizes a quantum phase transition. In this section, we analyze the large-$D$ phase by using a $SU(3)$ Schwinger bosonic representation, the so-called bond operator. The critical anisotropic constant $D_c$ is found as a function of the biquadratic constant $J_2$ (in units of $J_1$). We begin representing the eigenstates of $S_i^2$ as a function of three boson operators: $|m_i = -1\rangle = a_{i,-1}^\dagger |0\rangle$, $|m_i = 0\rangle = a_{i,0}^\dagger |0\rangle$ and $|m_i = +1\rangle = a_{i,+1}^\dagger |0\rangle$, where $|0\rangle$ is the vacuum state. The boson operator $a_{i,m}^\dagger$ creates a particle with $m = m$ on site $i$. The commutation relations $[S_i^+, S_j^-] = 2S_i^z \delta_{ij}$ and $[S_i^z, S_j^\pm] = \pm S_i^\pm \delta_{ij}$ are valid and to keep $S_i^2 = S(S + 1)$ we have to impose again a constraint $\sum_{\mu} a_{i,\mu}^\dagger a_{i,\mu} = S$ on each site. A condensation...
occurs in the \(|m = 0\) state, once this is the smaller band energy (the \(|m = \pm 1\) states are degenerate). Therefore the number of particles is \(N_0 = \langle a_{i,0}^\dagger a_{i,0} \rangle \gg 1\) and we can consider the approximation \([N_0, a_{i,0}^\dagger] = 0\) and \([N_0, a_{i,0}] = 0\), which allows to treat the \(a_{i,0}\) operators as real numbers. Thus, in the next equations, we have adopted the mean values \(\langle a_{i,0}^\dagger a_{i,0} \rangle = \langle a_{i,0} \rangle = a_0\). In the SU(3) bosonic representation, the bilinear and biquadratic spin interactions are written as:

\[
(S_i \cdot S_j) = a_0^2 \left( a_{i,-1} a_{j,1} + a_{i,-1} a_{j,-1} + a_{i,1} a_{j,1} + a_{i,1} a_{j,-1} + a_{i,-1} a_{j,-1} + a_{i,-1} a_{j,1} + a_{i,1} a_{j,1} + a_{i,1} a_{j,-1} \right) + \\
+ \left( a_{i,1} a_{j,1} a_{j,1} - a_{i,1} a_{j,1} a_{j,-1} - a_{i,-1} a_{j,-1} a_{j,1} + a_{i,-1} a_{j,1} a_{j,-1} \right),
\]

(18)

and

\[
(S_i \cdot S_j)^2 = \left( a_{i,1} a_{j,1} - a_{i,-1} a_{j,-1} \right)^2 = 1 - a_0^2.
\]

(20)

The Hamiltonian is composed by fourth-order terms and we have applied again the Hubbard-Stratonovich transform. After decoupling, we obtain the following second-order Hamiltonian:

\[
H = (1 - \rho_0) N D + (1 + \rho_0^2) J_2 \frac{N z}{2} + N \lambda (\rho_0 - S) + J_1 (1 - \rho_0)^2 \frac{N z}{2} - 4 \Lambda^2 (J_2 - J_1) \frac{N z}{2} + \lambda \sum_i \left( a_{i,1}^\dagger a_{i,1} + a_{i,-1}^\dagger a_{i,-1} \right) + \\
+ \sum_{(i,j)} \left[ \rho_0 \left( a_{i,1}^\dagger a_{j,1} + a_{i,-1}^\dagger a_{j,-1} + a_{i,1} a_{j,1}^\dagger + a_{i,-1} a_{j,-1}^\dagger \right) - \rho_0 (J_2 - J_1) \left( a_{i,1}^\dagger a_{j,-1}^\dagger + a_{i,-1}^\dagger a_{j,1}^\dagger + a_{i,1} a_{j,-1}^\dagger + a_{i,-1} a_{j,1}^\dagger \right) + \\
+ 2 (J_2 - J_1) \Lambda \left( a_{i,1}^\dagger a_{j,-1} + a_{i,-1}^\dagger a_{j,1} + a_{i,1} a_{j,-1} + a_{i,-1} a_{j,1} \right) \right],
\]

(21)

in which we have introduced the real mean-field \(\Lambda = \langle a_{i,1} a_{j,-1} \rangle = \langle a_{i,1}^\dagger a_{j,-1} \rangle\) and defined the level condensate \(\rho_0 = a_0^2\). Performing a Fourier transform, we obtain in the momentum space:

\[
H = H_0 + \frac{1}{2} \sum_{\mathbf{k}} \beta_\mathbf{k}^\dagger \tilde{H} \beta_\mathbf{k},
\]

(22)

where \(H_0\) are the constant term of equation (21) and the \(\tilde{H}\) matrix is given by:

\[
\tilde{H} = (\lambda + 4 \rho_0 J_1 \gamma_0) I_{4 \times 4} + (4 J' \gamma_0) M_{4 \times 4}
\]

(23)

where \(I\) is the identity matrix, \(M\) is the anti-diagonal matrix, \(J' = (J_1 - J_2)(\rho_0 - 2\Lambda)\) and \(\gamma_0\) is the structure factor, identical to that given in the previous section. The eigenvalues of the above equation are \(E_\mathbf{k} = \sqrt{(\lambda + 4 J_1 \rho_0 \gamma_0)^2 - (4 J' \gamma_0)^2}\). The energy has a minimum at point \(\mathbf{k}^* = (\pm \pi, \pm \pi)\) and close to this, we have a dispersion relation \(E_\mathbf{k}^2 = m^2 c^4 + |\mathbf{k} - \mathbf{k}^*|^2 c^2\), where \(m\) is the mass of the excitations and \(c\) is the spin-wave velocities. Unlike the region in which \(D < D_c\), in the large-\(D\) phase, the energy gap \(\Delta = mc^2\) is not null and so, there is no long-range order even at zero temperature and the magnetization is zero in this phase. The \(\rho_0, \lambda\)
and $\Lambda$ parameters are determined by the self-consistent equations obtained from the minimum of the Helmholtz free energy. At zero temperature they are given by:

$$\rho_0 = 2 - \int \frac{d^2k}{4\pi^2} \frac{\lambda + 4J_1\rho_0\gamma_k}{E_k},$$

$$\Lambda = -2 \int \frac{d^2k}{4\pi^2} \frac{(J_1 - J_2)\rho_0 - 2\Lambda(J_1 - J_2)}{E_k} \gamma_k^2,$$

$$\lambda = -4 \int \frac{d^2k}{4\pi^2} \left( \frac{\lambda + 4J_1\rho_0\gamma_k}{E_k} J_1 - (4J'\gamma_k)(J_1 - J_2) \right) \gamma_k^2 + D + 4J_1 - 4\rho_0(J_1 + J_2),$$

where we applied the continuous limit and the integrals are evaluated over the first Brillouin zone $-\pi < k_x, k_y < \pi$. At finite temperatures, the integrand is multiplied by $\coth\left(\frac{\beta E_k}{2}\right) = 2(n_k + 1)$, where $n_k = (e^{\beta E_k} - 1)^{-1}$ is the Bose-Einstein distribution. The analysis at finite temperature is done in the next section, where we have used the SCHA so, for while, we have considered only the $T = 0$ case. Once the lowest energy is finite, there is no divergence in the above equations and they can be directly solved. The $\rho_0$ term measures the boson condensation in the $|n = 0\rangle$ state and it is expected a high level ($\rho_0 \approx 1$) in the large-$D$ phase followed by a decreasing near the critical value $D_c$. On the other hand, the mean-field parameter $\Lambda$ is close to zero in the large-$D$ phase and it increases for $D \approx D_c$. Figure 3 shows the $\rho_0$ parameter for some biquadratic constants as a function of $D$ in the large-$D$ phase. At $D = D_c$, $\rho_0$ presents a discontinuity and there is no more condensation in $|n = 0\rangle$ state. For $D < D_c$, the system goes to a gapless region with an ordered ground state as described in the previous section.

![FIG. 3. The condensate density as a function of the anisotropic constant $D$ (in units of $J_1$) in the large-$D$ phase.](image)

We can use the self-consistent equation to estimate analytically the transition point $D_c$ as a function of the biquadratic constant. Following Ref. [23], we adopt $\Lambda \approx 0$ and thus:

$$\rho_0 = 2 - \int \frac{d^2k}{4\pi^2} \frac{1}{\sqrt{1 - \frac{1}{E_k}}},$$

$$D = \int \frac{d^2k}{4\pi^2} \frac{4J_1\gamma_k - \frac{1}{g} + 4(J_1 - J_2)}{\sqrt{1 - \frac{1}{E_k}}},$$

in which the dimensionless ratios were defined as $g = \frac{\omega}{\Lambda}$ and $\Gamma_k = \frac{4(1 + 4J_1\gamma_k)}{1 + 4J_1\gamma_k}$. At the transition point, $E_k = 0$ and, therefore, $\Gamma_k = \pm 1$. The critical ratio $g$ is $g_c = \frac{1}{4(1 + 4J_1\gamma_k)}$ for $J_2 < 0.5J_1$ and $g_c = \frac{1}{J_1}$ for $J_2 > 0.5J_1$. Thus we have found the following equation for $D_c$:

$$D_c = \int \frac{d^2k}{4\pi^2} \frac{4J_1\gamma_k - 4J_2 - g_c^{-1} - 4(J_1 - J_2)\gamma_k\Gamma_k}{\sqrt{1 - \frac{1}{E_k}}} + \frac{1}{g_c} + 8J_2.$$

Although the above equation provides a simple method to determine $D_c$, it is only a first approximation. For $|D - D_c| \approx 0$, the condensate level $\rho_0$ becomes smaller than 1 and hence, $\Lambda \approx 0$ is not a good consideration. In the large-$D$ phase, the condensation is almost total and decreases close to $D_c$ (the graphic is not valid for $D < D_c$). The better results are obtained analyzing the point where the gap vanishes for different values of $J_2$. We begin with a large anisotropic constant (approximately 10$J_1$), decreasing its value until the gapless phase. The point where the gap vanishes is taken as $D_c$. In Fig. 4, we show the gap energy as a function of the anisotropic constant $D$ and in Fig. 3 the critical points $D_c$ as a function of the biquadratic constant $J_2$ (all constants are given in units of $J_1$), obtained numerically and through the approximate analytical method described by equation (26). We have evaluated the quantum phase transition in the interval $-1 \leq J_2 \leq 1$ (in units of $J_1$) and both results are similar, presenting an almost linear behavior for $D_c$. The difference between the numeric and approximate analytical results is smaller for $J_2 \approx 0$ where the consideration $\Lambda \approx 0$ is valid and drastically increases for negative values of the biquadratic constant. As argued earlier, Eq. (26) is only an approximation and the numeric results are closer to those obtained by SCHA (see next section).

**IV. SELF-CONSISTENT HARMONIC APPROXIMATION**

Now we analyze the Anisotropic Biquadratic Heisenberg Model (ABHM) by using the Self-consistent Harmonic Approximation[6, 23, 31]. This is the most appropriate method to treat the system at finite temperatures. The bosonic formalisms used in the last sections provide reasonable results at zero temperature but,
as argued by Yoshida [37], for $T > 0$, they present divergences with known results. As we have demonstrated, the model studied has a QPT associated with the single-ion anisotropy $D$. There are a critical value $D_c$ in which one separates an ordered phase ($D < D_c$) from a disordered ($D > D_c$) phase. At finite temperatures the system is always disordered as dictated by the Mermin-Wagner theorem; however, there is a thermal phase transition from a disordered state with algebraic decay to a disordered state with exponentially decay for the correlation order-parameter. This is a transition phase, similar to the BKT transition present on the planar magnets. Using the SCHA, we have determined both quantum and thermal transition to the ABHM.

Starting with Hamiltonian (1), we decouple the bi-quadratic term by using the Hubbard-Stratonovich transform $(S_i \cdot S_j)^2 \rightarrow 2\zeta (S_i \cdot S_j)$, where $\xi = \langle S_i \cdot S_j \rangle$ measures the correlation between the nearest neighbor sites. Therefore, the uncoupled Hamiltonian is given by:

$$H = \frac{1}{2} \sum_{\langle i,j \rangle} (J_1 + 2J_2\xi)S_i \cdot S_j + D \sum_i (S_i^z)^2,$$

in which $i$ runs over the square lattice and $j$ indicates the four nearest neighboring spins (the half-integer factor is included to avoid double counting). Following the standard procedures, we written the spin operator using the Villain’s representation:

$$S_i^+ = e^{i\phi_i} \sqrt{S(S+1) - S_i^z(S_i^z + 1)}$$

$$S_i^- = \sqrt{S(S+1) - S_i^z(S_i^z + 1)} e^{-i\phi_i},$$

where $\phi_i$ is the angle of the parametrization:

$$S_i = (-1)^i \left( \sqrt{S^2 - 1 - \left( \frac{S_i^z}{S} \right)^2} \cos \phi_i, \sqrt{S^2 - 1 - \left( \frac{S_i^z}{S} \right)^2} \sin \phi_i, S_i^z \right)$$

with $\tilde{S} = S(S+1)$. In order to avoid divergences, we choose the angle operator $\phi_i$ relative to the direction of the instantaneous total spin ($\langle \phi_i \rangle$ is not well defined to angles measured relative to a fixed axis). Thus, we make the replacement:

$$S_i \cdot S_j \rightarrow -\frac{\tilde{S}^2}{2} \sqrt{1 - \left( \frac{S_i^z}{S} \right)^2} \sqrt{1 - \left( \frac{S_j^z}{S} \right)^2} \cos (\phi_i - \phi_j) + S_i^z S_j^z.$$

At low temperatures (in the ordered phase), the spin field assumes a configuration with a small angular difference between neighboring sites and, hence, we can consider $|\phi_i - \phi_j| \ll 1$. Therefore, expanding the above equation into powers of $(S_i^z/\tilde{S})^2$ and $(\phi_i - \phi_j)^2$, we have the quadratic Hamiltonian:

$$H = \sum_k \left[ 2g\xi \tilde{S}^2 (1 - \gamma_k) \phi_k \phi_{-k} + (\phi_k - \phi_{-k}) \right] + D \sum_i (S_i^z)^2,$$

where $g = (J_1 + 2J_2\xi)$. The $\xi$ parameter inserted before the $\phi$ operators takes into account nonharmonic terms neglected when the original Hamiltonian is written in the quadratic form [24, 38, 39] and by definition, it has the same form of $(S_i \cdot S_j)$. After a Fourier transform, the Hamiltonian is given by:

$$H = \sum_k \left[ \frac{1}{\sqrt{2}} \frac{2g(1 + \gamma_k) + D}{2g\tilde{S}^2(1 - \gamma_k)} \right]^{1/4} (a_k^\dagger a_{-k}) \quad (32a)$$

$$S_k^z = \frac{i}{\sqrt{2}} \left[ \frac{2g\xi \tilde{S}^2 (1 - \gamma_k)}{2g(1 + \gamma_k) + D} \right]^{1/4} (a_k^\dagger a_{-k}) \quad (32b)$$

where $a_k^\dagger$ and $a_k$ are boson creation and annihilation operators, respectively. After a straightforward calculation, we find in the continuous limit:

$$\left\langle \left( \frac{S_i^z}{\tilde{S}} \right)^2 \right\rangle = \frac{1}{2} \int \frac{d^2k}{4\pi^2} \frac{2g\xi \tilde{S}^2(1 - \gamma_k)}{2g(1 + \gamma_k) + D} \coth \left( \frac{\beta E_k}{2} \right) \quad (34)$$
and
\[ \langle \phi_k \phi_{-k} \rangle_0 = \frac{1}{2} \sqrt{\frac{2g(1 + \gamma_k) + D}{2g\xi^2(1 - \gamma_k)}} \coth \left( \frac{\beta E_k}{2} \right), \] (35)
in which \( E_k = 2\sqrt{2g\xi^2(1 - \gamma_k)[2g(1 + \gamma_k) + D]} \) are the eigenvalues of the energy, \( \langle \ldots \rangle_0 \) means a thermal average calculated through the quadratic Hamiltonian and the integral is evaluated over the first Brillouin zone. The \( \xi \) parameter is given by:
\[ \xi = \sqrt{1 - \left( \frac{S^z}{S} \right)^2} \left[ 1 - \left( \frac{S^z}{S} \right)^2 \cos(\phi_i - \phi_j) \right], \] (36)
where the exact average is taken by considering the original harmonic Hamiltonian (37). To evaluate the above expression, we approximate the average by applying the diagonalized harmonic Hamiltonian. Once \( \phi_i \) and \( S^z_i \) are uncoupled operators and \( \phi_i \) has a Gaussian distribution, we have:
\[ \xi \approx \left[ 1 - \left( \frac{S^z}{S} \right)^2 \right] e^{-\frac{1}{2}((\phi_i - \phi_j)^2)} \] (37)
with
\[ \langle (\phi_i - \phi_j)^2 \rangle_0 = \int \frac{d^2k}{2\pi^2} (1 - \gamma_k) \langle \phi_k \phi_{-k} \rangle_0. \] (38)

Equation (37) is solved self-consistently and the solutions are used to determine the critical point \( D_c \). At zero temperature, a correlation between nearest neighboring spins is finite for \( D < D_c \) (the ordered phase) and abruptly vanishes when \( D \) tends to \( D_c \), characterizing the quantum phase transition. In the large-\( D \) region, the correlation \( \xi \) is null and the system falls into a disordered regime. The critical points are numerically evaluated and the results are shown in Fig. (6). As found in the bond operator method, the behavior of the critical point is almost linear as a function of the biquadratic constant but its value is around 10\% bigger (compared with the numeric results). The finite temperature analysis also is done by Eq. (37). At finite temperatures, the system is disordered but the correlation order-parameter has a different behavior below and above a critical temperature \( T_c \). For \( 0 < T < T_c \), the correlation has an algebraic decay while it falls exponentially for \( T > T_c \). It is important to highlight that it is not a transition associated with a broken symmetry as that considered by Mermin-Wagner theory and so, it is more similar to the BKT transition. Therefore, the temperature where \( \xi \to 0 \) is taken, in first order, as the transition temperature. In Fig. (7), we show the results obtained for \( T_c \) as a function of the biquadratic constant.

V. CONCLUSION

We have studied the Anisotropic Biquadratic Heisenberg Model using some different techniques. As we have shown, there is a quantum phase transition associated with the single-ion anisotropy similar to a thermal phase transition. At zero temperature and for small values of \( D (D < D_c) \), the system is in a gapless ordered state while for \( D > D_c \) there is no long-range order. Using the SU(2) Schwinger formalism, we have found a decreasing behavior for the condensate density, which indicates a phase transition close to \( D = 10 \). Analyzing the large-\( D \)
FIG. 8. The transition temperature as a function of $J_2$ (in units of $J_1$).

region (where the ground state is gapped and disordered)

we have determined the critical points $D_c$ as a function of the biquadratic constant $J_2$. The critical values of $D_c$ have an almost linear behavior with $J_2$ and within the interval $-1 \leq J_2 \leq 1$, there is always a QPT. Finally, applying the SCHA method, we have obtained similar results for the critical points and also, the transition temperature between a disordered phase with algebraic decay and the regime with exponential decay of the order-parameter correlation, including the dependence with $D$ and $J_2$.

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