On Phase Transition and Vortex Stability in the Generalized XY Models

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We study a recent generalization proposed for the XY model in two and three dimensions. Using both, the continuum limit and discrete lattice, we obtained the vortex configuration and shown that out-of-plane vortex solutions are deeply jeopardized whenever the parameter of generalization, $L$, is increased. The critical temperature for such models is calculated using the self consistent harmonic approximation. In both, two- and three-dimensional cases, such a temperature decreases with raising $L$. Our results are also compared with other approximated methods available in the literature.

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I. INTRODUCTION AND MOTIVATION

The Hamiltonian $H = -J \sum_{<ij>} (S_i^x S_j^x + S_i^y S_j^y)$, where $J$ is a coupling constant, the summation is taken over the nearest-neighbors sites in a square lattice and $S^\alpha_i (\alpha = x, y)$ is a spin component at site $i$, describes two important models in magnetism known as the two-dimensional (2D) planar rotator model (PRM) and the XY model. The difference between these two models lies in the number of spin components. Thus, in the PRM framework we have only two spin components which are subject to the constraint $S_x^2 + S_y^2 = S^2$. On the other hand, XY model also displays the third component with the condition $S_x^2 + S_y^2 + S_z^2 = S^2$. Hence, whenever fixing the spin $S$ of the system, we are led with one and two independent spin degrees of freedom for these models, respectively. Thus we may parametrize the PRM physical spin content by only one scalar field, the azimuthal angle $\varphi_i$, say, $(\vec{S}_i)^{PRM} = S(\cos \varphi_i, \sin \varphi_i)$, while in the XY model, we have two scalar, the azimuthal and polar angles, say, $(\vec{S}_i)^{XY} = S(\sin \theta_i \cos \varphi_i, \sin \theta_i \sin \varphi_i, \cos \theta_i)$. As it is well-known, the 2D PRM and XY models support topological excitations and, although no long range order is established at any finite temperature, they are shown to exhibit phase transition related to the unbinding of vortex--antivortex pairs. Indeed, at low temperatures, the vortex excitations are bound into pairs whose interaction grows logarithmically with the distance between the vortex centers. However, whenever the so-called Berezinskii-Kosterlitz-Thouless (BKT) transition temperature, $T_{BKT}$, is reached, the bound pairs appear to dissociate.

In addition, the static critical behavior of such models, mainly the PRM, in two and three dimensions, has been studied for a long time, using several statistical and Monte Carlo (MC) simulation methods. Among others, such studies have led to the consensus upon the nature of the phase transitions and the values of the critical temperature and exponents. On the other hand, an interesting extension of the 2D PRM was introduced around two decades ago by Domany, Schick, and Swendsen, in which the potential is given by $V(\chi) = 2J(1-|\cos^2(\chi/2)|^p)$, where $\chi \equiv \varphi_j - \varphi_i$. Clearly, the usual PRM is recovered as long as $p = 1$. Nevertheless, as $p$ is raised, an increasingly narrow potential well, with a width around $\pi/p$, is observed in the model. Notice also that whenever we have $\chi = (2n+1)\pi$ (n integer), then the potential gets a constant value, $V((2n+1)\pi) = 2J$. In addition, ordinary spin-wave behavior at low temperatures is ensured by the fact that, near the minimum we do have $V(\chi) \approx Jp^2\chi^2/2$. It was also shown by MC simulation that, for very large $p$ a first-order, rather than a continuous phase transition takes place. In this sense, it seems that the vortex excitations alone are sufficient to account for both continuous and first-order transitions, though in qualitatively distinct ways.

Recently, a generalization of XY model has been proposed by Romano and Zagrebnov, whose potential looks like $-J(\sin \theta_i \sin \theta_j)^L \cos(\varphi_i - \varphi_j)$, with $L \in \mathbb{N}$. In their paper the authors have established rigorous inequalities holding for every $L \geq 1$. Using Mean Field (MF) and Two-Site Cluster (TSC) techniques they have also estimated the critical temperature, in the 3D case, for some values of $L$. In the 2D case, and for arbitrary $L$, they suggested that the above potential produces orientational disorder at all finite temperatures, and supports BKT transition. However, the stability and behavior of the vortex-like solutions in these models are still unclear. Therefore, it would be important to know about the types of vortices present in the system and their roles in such a phase transition. Thus, in this work we present a detailed analysis of the stability of vortex solutions. This is done by applying discrete lattice and usual continuous approximation approaches. The main conclusion is that out-of-plane solutions are deeply jeopardized as long as the anisotropic parameter, $L$, is increased. Furthermore, concerning the problem of phase transitions it would
also be desirable to verify in more details the validity of some approximated methods used to estimate the values of the critical temperatures. For this purpose, we apply here the Self Consistent Harmonic Approximation (SCHA) to the generalized XY model in two and three dimensions. Our results strongly supports the idea that as \( L \) is turned up the critical temperature of the 2D and 3D generalized XY models appears to decrease. However, it is worth noticing that our results predict lower critical temperatures than those obtained by both, MF and TSC methods. Namely, for the case \( L = 1 \), SCHA approach yields the value which is the closest to that found by means of Monte Carlo simulations.

The generalized XY model is defined below like below:

\[
H_{XY}^{Gen} = -J \sum_{<ij>} \left[ 1 - (S_i^z)^2 - (S_j^z)^2 + (S_i^z S_j^z)^2 \right]^{L/2} \left( S_i^x S_j^x + S_i^y S_j^y \right)
= -J \sum_{<ij>} (\sin \theta_i \sin \theta_j)^L \cos(\varphi_i - \varphi_j),
\]

where the spin vector at site \( i \) is defined by \( \vec{S}_i = (S_i^x, S_i^y, S_i^z) \) satisfying the non-linear constraint \( S_i^2 = 1 \), and \( L \in \mathbb{N} \). Clearly, as long as \( L = 1 \) we recover the usual XY-model, while for \( L = 0 \) we get the PRM (with \( S^z = 0 \)). In addition, as long as \( L \) increases the anisotropy of the generalized model is taken up. This Hamiltonian is a function of the spin components of the form \( f(S_i^z, S_j^z) \left[ S_i^x S_j^x + S_i^y S_j^y \right] \), where \( f(S_i^z, S_j^z) = -[1 - (S_i^z)^2 - (S_j^z)^2 + (S_i^z S_j^z)^2]^{L/2} \).

II. THE SOLUTIONS AND THEIR STABILITY

In order to study possible vortex-like and spin-wave configurations, as well as their stability, we need to take into account the continuous version of Hamiltonian \( H_{XY} \). It is not difficult but length to obtain that:

\[
H_{XY}^{Gen} = \frac{J}{2} \mathbb{E} \left[ (1 - m^2)^L (\vec{\nabla} \phi)^2 + L^2 m^2 (1 - m^2)^{L-2} (\vec{\nabla} m)^2 - \frac{4}{a^2} (1 - m^2)^L + \frac{4}{a^2} \right],
\]

where \( m = \cos \theta \), while the constant \( +4/a^2 \) has been introduced in order to renormalize the energy.

The equations of motion for spin-field variables, \( m(x, y; t) = \cos[\theta(x, y; t)] \) and \( \phi(x, y; t) \) read like follows:

\[
\frac{\partial m}{\partial t} = J(1 - m^2)^{L-1} \left[ 2mL(\vec{\nabla} m) \cdot (\vec{\nabla} \phi) - (1 - m^2) \vec{\nabla}^2 \phi \right],
\]
\[
\frac{\partial \phi}{\partial t} = JLm(1 - m^2)^{L-2} \left[ \frac{L(\vec{\nabla} m)^2}{(1 - m^2)} - \frac{L(L-2)m^2(\vec{\nabla} m)^2}{(1 - m^2)^2} + \frac{Lm \vec{\nabla}^2 m}{(1 - m^2)} + (\vec{\nabla} \phi)^2 - \frac{4}{a^2} \right].
\]

Now, we shall pay attention to the possible topological excitations associated to the non-linear equations of motion, as well as their stability. First of all, we notice that genuine static planar vortex-like configurations, \( m = \cos \theta = 0 \) and \( \phi = \arctan(y/x) \), are supported by the generalized model, for every \( L \geq 2 \) \((L \in \mathbb{N}) \). This technique is based upon the discrete lattice, and consists in analyzing the energy of out-of-plane vortex solutions, along with non-zero out-of-plane spin components appearing only in a finite number of sites equidistant from the vortex center. In a first approximation, we consider that only the first four nearest spins of the vortex center have non-zero out of plane components, \( m_1 \neq 0 \), while all the other sites display \( m = 0 \). In order to improve this calculation, we can include more sets of equidistant sites. Considering the first three sets of equidistant spins at radius \( r_1 = 1/\sqrt{2}, r_2 = \sqrt{10}/2 \) and \( r_3 = \sqrt{18}/2 \), with
out-of-plane components $m_1$, $m_2$ and $m_3$ respectively, we then find the effects due to the 40 bond sites nearest to the vortex center:

\[
E_3 = -16J \left[ \frac{(1 - m_2)^{L/2}}{5} + \frac{4(1 - m_2)^{L/2}}{\sqrt{5}} + \frac{(1 - m_1^2 + m_1m_2 - m_2^2)^{L/2}}{\sqrt{5}} \right. \\
\left. + \sqrt{\frac{2}{3}} \frac{(1 - m_2^2)^{L/2}}{2} + \frac{(1 - m_2^2 + m_2m_3 - m_3^2)^{L/2}}{\sqrt{5}} \right] - \frac{5}{2},
\]

(5)

where we have subtracted out the ground state energy $-40J$ (in-plane exchange).

Minimization of the energy with respect to the out-of-plane spin components demands the vanishing of the following derivatives:

\[
\frac{\partial E}{\partial m_1} = -\frac{8JL}{\sqrt{5}} (m_2 - 2m_1)(1 - m_1^2 + m_1m_2 - m_2^2)^{L/2 - 1},
\]

(6a)

\[
\frac{\partial E}{\partial m_2} = -\frac{8JL}{\sqrt{5}} (m_1 - 2m_2)(1 - m_1^2 + m_1m_2 - m_2^2)^{L/2 - 1} + \frac{16JL}{5} m_2(1 - m_2)^{L/2 - 1} \\
+ \frac{64JL}{\sqrt{65}} m_2(1 - m_2)^{L/2 - 1} - \frac{8JL}{\sqrt{5}} (m_3 - 2m_2)(1 - m_2^2 + m_2m_3 - m_3^2)^{L/2 - 1},
\]

(6b)

\[
\frac{\partial E}{\partial m_3} = -\frac{8JL}{\sqrt{5}} (m_2 - 2m_3)(1 - m_2^2 + m_2m_3 - m_3^2)^{L/2 - 1} \\
+ 16JL \sqrt{\frac{2}{3}} m_3(1 - m_3)^{L/2 - 1}.
\]

(6c)

Then, out-of-plane vortex solutions are stable whenever Eqs. (6) identically vanish, while $m_i \neq 0$, for every $i = 1, 2, 3$.

To solve these equations, we assume small amplitudes for $m_i$. In this case, the linearized version of these equations reads like below:

\[
\frac{16JL}{\sqrt{5}} m_1 - \frac{8JL}{\sqrt{5}} m_2 = 0,
\]

(7a)

\[
- \frac{8JL}{\sqrt{5}} m_1 + \left( \frac{16JL}{5} + \frac{32JL}{\sqrt{5}} + \frac{64JL}{\sqrt{65}} \right) m_2 - \frac{8JL}{\sqrt{5}} m_3 = 0,
\]

(7b)

\[
- \frac{8JL}{\sqrt{5}} m_2 + 16JL \left( \frac{1}{\sqrt{5}} + \sqrt{\frac{2}{3}} \right) m_3 = 0.
\]

(7c)

Of course, trivial solutions, $(m_i = 0)$, are always possible (in-plane vortex). Nevertheless, our interest lies in the conditions which could provide non-trivial configurations to show up. The latter ones are possible if and only if the determinant of the matrix coefficients is zero. However, such a determinant takes the following value: \( d \approx 3331.52(JL)^3 \), which implies that non-trivial configurations are possible only for \( L = 0 \) (PRM, which of course, can not support out-of-plane solutions). This result clearly states us that out-of-plane vortex solutions are unstable. Furthermore, we have also performed a similar plain for equidistant sets of spins from \( r_1 = 1/\sqrt{2} \) to \( r_6 = \sqrt{50}/2 \) (six sets of spins), whose conclusion is analogous to the above one. In Ref. [8], Wysin found an accurate value of \( \lambda_c \) (critical anisotropy) for the anisotropic Heisenberg model which is in good agreement with Monte Carlo results, using only three sets of equidistant spins (form \( r_1 = 1/\sqrt{2} \) to \( r_3 = \sqrt{15}/2 \)). Thus, we claim that as long as we have used six sets of equidistant spins, our results can be generalized leading us to conclude that out-of-plane vortex solutions will be unstable in this model, for every \( L \) value.

Analogous conclusion is also obtained if we study the plane-wave (meson) behavior of the model. In order to see that, let us take expressions (8), and suppose the appearance of small time-dependent deviations from the planar vortex-like solution \( m = m_0 = \cos \theta = 0 \) and \( \phi = \phi_0 = \arctan(y/x) \), like below:

\[
m \rightarrow m = m_0 + m_1(\vec{x}; t) = m_1(\vec{x}; t),
\]

(8)

\[
\phi \rightarrow \phi = \phi_0 + \phi_1(\vec{x}; t) = \arctan(y/x) + \phi_1(\vec{x}; t).
\]

(9)
Since \( m_1 \) and \( \phi_1 \) are small, we may neglect higher orders terms proportional to them and their derivatives in the equations of motion. In this case we would be neglecting the spin wave interactions. In addition, taking \( m_1(\vec{x}, t) = m_1(\vec{x}) e^{i\omega t} \) and \( \phi_1(\vec{x}, t) = \phi_1(\vec{x}) e^{i\omega t} \), where \( \omega \) is the frequency of such long wavelength spin-wave excitations, we get the following equations for \( m_1 \) and \( \phi_1 \):

\[
\nabla^2 \phi_1(\vec{x}) = -\frac{i\omega}{J} m_1(\vec{x}),
\]

\[
\dot{m}_1(\vec{x}) = -\frac{i\omega}{JL \left( \frac{1}{r^2} - \frac{1}{4\pi r^2} \right)} \phi_1(\vec{x}),
\]

which imply that:

\[
\nabla^2 \phi_1(\vec{x}) = -\frac{\omega^2}{J^2 L \left( \frac{1}{r^2} - \frac{1}{4\pi r^2} \right)} \phi_1(\vec{x}).
\]

Then, as \( r \to \infty \), we expect that such excitations look like plane-waves, say, \( m_1(\vec{x}) = m_1^0 e^{i\vec{k} \cdot \vec{x}} \) and \( \phi_1(\vec{x}) = \phi_1^0 e^{i\vec{k} \cdot \vec{x}} \), getting:

\[
\omega^2(|\vec{k}|; L) = \frac{-4J^2}{a^2} |\vec{k}|^2 L,
\]

which confirms our earlier conclusion. Hence, for \( L > 1 \) out-of-plane fluctuations appear to spend more and more energy. As \( L \) is increases, the magnon density decreases as \( e^{-\sqrt{|k|^2}} \), while the planar-vortex density is not affected. It may imply in important differences in the thermodynamics of these Generalized XY systems. In fact as has been shown by Currie et al., the phase shift interaction between spin waves and solitons provide the sharing mechanism of energy and degrees of freedom among the nonlinear excitations of the system and therefore is important in the study of the statistical mechanics of the model.

III. PHASE TRANSITIONS IN TWO- AND THREE-DIMENSIONAL GENERALIZED XY MODELS

Romano and Zagrebnov in Ref. [5] have shown that this model supports Berezinskii-Kosterlitz-Thouless (BKT) phase transition in 2D, and ordering transitions in 3D. In this section, we perform an estimative of the critical temperature, in 2D and 3D, by applying the Self Consistent Harmonic Approximation (SCHA), which has been widely appeared in the literature, in connection with isotropic and anisotropic models of the same class of universality of the XY model.

Such a technique works by replacing the original Hamiltonian of the model by a harmonic one, along with the coupling constant, \( J \), by an effective one, \( K \), which takes into account the nonlinearities of the interactions. First, we shall apply this technique to the spatially anisotropic 3D generalized XY model, defined by the following hamiltonian:

\[
H_{3D} = -J \sum_{r,a} \left[ 1 - (S_r^z)^2 - (S_{r+a}^z)^2 + (S_r^x S_{r+a}^x)^2 \right]^{L/2} \cos(\varphi_r - \varphi_{r+a})
\]

\[
- J_z \sum_{r,c} \left[ 1 - (S_r^z)^2 - (S_{r+c}^z)^2 + (S_r^x S_{r+c}^x)^2 \right]^{L/2} \cos(\varphi_r - \varphi_{r+c}),
\]

where \( r + a \) and \( r + c \) represents the nearest-neighbors in the XY plane, and in the \( z \) direction respectively, and \( J_z \) is the inter-plane coupling constant. The harmonic hamiltonian related to the hamiltonian is given by:

\[
H_0 = \frac{1}{2} \sum_r \left[ K \sum_a (\varphi_r - \varphi_{r+a})^2 + K_z \sum_c (\varphi_r - \varphi_{r+c})^2 \right.
\]

\[
+ (4LJ + 2LJ_z)(S_r^z)^2 \right],
\]

where \( K \) and \( K_z \) are given by:

\[
K = J \left[ 1 - (S_r^z)^2 - (S_{r+a}^z)^2 + (S_r^x S_{r+a}^x)^2 \right]^{L/2} \cos(\varphi_r - \varphi_{r+a}),
\]

\[
K_z = J_z \left[ 1 - (S_r^z)^2 - (S_{r+c}^z)^2 + (S_r^x S_{r+c}^x)^2 \right]^{L/2} \cos(\varphi_r - \varphi_{r+c}).
\]
These averages are approximated replacing $\langle \ldots \rangle$ by $\langle \ldots \rangle_0$, i.e., they are calculated using $H_0$ instead $H$. In this case, $\varphi_r$ and $S_r^z$ are decoupled allowing us to write:

$$K \approx J \langle (1 - (S_r^z)^2)^L \rangle \cos(\varphi_r - \varphi_{r+a})$$

$$K_z \approx J_z \langle (1 - (S_r^z)^2)^L \rangle \cos(\varphi_r - \varphi_{r+c})$$

As we have seen in Section II, as $L$ increases, the out-of-plane spins fluctuations decreases. Using this result, we expand $(1 - (S_r^z)^2)^L$ as $1 - L(S_r^z)^2 + \ldots$, keeping only the terms of the order of $(S_r^z)^2$. Then, the first average is easily solved giving:

$$1 - L\langle (S_r^z)^2 \rangle = 1 - \frac{T}{4J + 2J_z}L.$$  (20)

Hamiltonian (13), except for the $L$ term in $(S_r^z)^2$, has the same form of the Hamiltonian of Ref. [15]. So, for a generic value of $L$, we obtain, in the two limits $J_z \approx J$ and $J_z \ll J$, the following expressions:

(a) $J_z \approx J$

$$K = J \left( 1 - \frac{T}{4J + 2J_z}L \right) \exp \left\{ -\frac{T}{16} \left[ \frac{3K + K_z}{2K^2 + KK_z} + \frac{3K + K_z}{2K^2 + 2KK_z} \right] + \frac{1}{2K} \left( 1 - g \tanh^{-1}(1-g)^{1/2} \right) \right\},$$

$$K_z = J_z \left( 1 - \frac{T}{4J + 2J_z}L \right) \exp \left\{ -\frac{T}{16} \left[ \frac{2K + 2K_z}{K_z^2 + 2KK_z} + \frac{2K + 2K_z}{(K_z + K)^2} \right] + \frac{1}{K} \left( \tanh^{-1}(1-g)^{1/2} - \frac{1}{1-g} \right) \right\},$$

where $g = K/K_z$.

(b) $J_z \ll J$

$$K \approx J \left( 1 - \frac{T}{4J + 2J_z}L \right) \exp \left\{ -\frac{T}{16K} \left[ \frac{5}{2} + \frac{1}{1 + K_z/K} + \frac{1}{2 + K_z/K} \right] + \left( \frac{\pi^2 + 12}{24\pi} \right) \left( \frac{K_z}{K} \right) \ln \left( \frac{K_z}{K} \right) \right\},$$

$$K_z \approx J_z \left( 1 - \frac{T}{4J + 2J_z}L \right) \left( \frac{K_z}{K} \right)^{d/16K} \exp \left\{ -\frac{T}{16K} \left[ \frac{2}{1 + K_z/K} + \frac{1}{2 + K_z/K} + c \right] \right\},$$

where $d = (\pi^2 + 12)/12\pi$ and $c = (\pi/12) \ln(4/\pi) + (1/\pi) \ln \pi$.

These self-consistent equations for the coupled variables $K$ and $K_z$ gives the effective coupling at each value of the temperature. The critical temperature is reached whenever these equations admit only the trivial solutions, say, $K = 0$ and $K_z = 0$. In this case, numerical data obtained from these equations can be approximately fitted by

$$T_c \approx \frac{4 + 2\lambda}{e + L},$$

where $\lambda = J_z/J$.

For $L = 0$ and $L = 1$ we recover previous results from Refs. [15,16], for the PRM and XY models, respectively, which are known to be in good agreement with those obtained via Monte Carlo. In Table I results from Monte Carlo simulations for the PRM and XY models and those obtained by Romano and Zagrebnov via MF and TSC techniques are compared with those calculated by SCHA, for the isotropic case. It is worth noticing that our results generally yields critical temperatures lower than those predicted by MF and TSC techniques. Moreover, for the $L = 1$ case (usual XY model) for which we have a more detailed study, our result is the closest to that obtained by MC simulation.

On the other hand, whenever $J_z = 0$, we get the 2D XY model. In this case, the effective coupling constant, $K$, representing the stiffness or superfluid density $\rho_s$, is given by

$$K = J \left( 1 - \frac{T}{4J}L \right) \exp \left( -\frac{T}{4K} \right).$$

(26)
TABLE I: Mean-Field, Two-Site Cluster, Monte Carlo and SCHA results for the critical temperature of the isotropic 3D generalized XY model.

| \( L \) | Monte Carlo | Mean Field | Two-Site Cluster | SCHA |
|-------|-------------|------------|------------------|------|
| 0     | 2.2 ± 0.05  |            |                  | 2.2073 |
| 1     | 1.54 ± 0.01 | 2.0000     | 1.7130           | 1.6136 |
| 2     | 1.6000      | 1.4389     |                  | 1.2716 |
| 3     | 1.3741      | 1.2827     |                  | 1.0493 |
| 4     | 1.2190      | 1.1779     |                  | 0.8931 |

FIG. 1: Stiffness as a function of the temperature for \( L = 1 \) (a), \( L = 2 \) (b), \( L = 3 \) (c) and \( L = 4 \) (d) in the two dimensional case.

Similarly, the critical temperature is obtained whenever the self-consistent equation for \( K \) is solved only by taking \( K = 0 \). Then, we found that the critical temperature, as function of \( L \), is \( T = 4/(e + L) \), which is quite above Monte Carlo results for PRM and XY models\(^{15,16}\). This occurs because the SCHA approach attributes an excessive energetic cost to topological excitations, such as vortex, causing an overestimation of the Berezinskii-Kosterlitz-Thouless transition temperature\(^{11,15}\). In Fig. 1, we show the stiffness \( K \) as a function of \( T \) for some values of the parameter \( L \).
IV. CONCLUSIONS

In summary, we have obtained the continuum limit for the Generalized XY-model, defined by Hamiltonian (1) and studied the vortex stability. Calculations using the discrete lattice confirmed the results obtained by the continuum approach. Out-of-plane fluctuations, and as a consequence, the magnon density, decrease as the parameter of generalization $L$ increases. The phase transition temperature as a function of $L$ was estimated using the self consistent harmonic approximation. Our results seem to be more realistic than other approximated methods available in the literature, such as two-site-cluster and mean field. However, it has to be shown numerically and is beyond the scope of this letter. We would like to consider in a future paper some Monte Carlo simulations to calculate the critical temperature for the Generalized XY-model in order to confirm our assertion.

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