Monte Carlo study of the critical behavior of the two-dimensional biquadratic planar rotator model

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We present an analysis of the critical properties of the two-dimensional rigid rotor model with a biquadratic interaction $H=-J\Sigma_{i,j}\vec{S}_i\cdot\vec{S}_j+D\Sigma_{i,j}(\vec{S}_i\cdot\vec{S}_j)^2$. We use a self-consistent harmonic approximation and a Monte Carlo calculation to study the Hamiltonian. The results for the specific heat, susceptibility, fourth order Binder's cumulant and helicity modulus obtained by Monte Carlo suggest that the model has a critical BKT line $-\infty<D/J<D_c/J$, where $D_c/J=0.96(9)$.

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I. INTRODUCTION

Magnetic systems with reduced dimensionality have provided a basis for a great number of insights into the varying roles thermal fluctuations play in driving phase transitions.[1] The planar rotator (PR) model represents a particularly important example of such a system, impacting problems in disciplines ranging from particle field theory to material sciences. Some of the notable properties of the PR model are the absence of long-range order, the presence of topological defects called vortices and the Berezinkii-Kosterlitz-Thouless (BKT) transition. The low temperature phase has only bound vortex-antivortex pairs and the BKT transition is associated with the unbiding of the vortex-antivortex pairs.[2,3] A lot of research, both analytically and numerically, has been done on the BKT transition. For instance, just to mention some Monte Carlo (MC) simulations performed in the PR-like systems: The phase diagrams and critical behavior of the anisotropic model have been extensively studied by Landau and Binder[5] using Monte Carlo simulations and the coupling between planes has been considered by Costa *et al.*[6]

Here we are going to study the planar rotator model with a biquadratic interaction (PR4) described by the Hamiltonian

$$H=-J\sum_{i,j}\ \vec{S}_i\cdot\vec{S}_j+D\sum_{i,j}\ (\vec{S}_i\cdot\vec{S}_j)^2. \tag{1}$$

For $J=0$ we have a disordered ground state and no BKT transition. The biquadratic term D is ordinarily small in systems where the orbital motion is quenched, but can be large in systems where the orbital motion is important and where a pseudospin formalism is used to describe the energy levels.[7] The Hamiltonian (1) with $J=0$ may be used to describe the interaction between atoms in liquid crystals.

In this work we present a Monte Carlo simulation for the PR4 model for several values of the parameter D and compare the results with a self-consistent harmonic approximation (SCHA).[4] Our results strongly suggest that the model has a BKT transition over the region $-\infty<D/J<D_c/J$, where $D_c/J0.96(9)$, in this case the ground state is ferromagnetic. For $D>D_c$ the system loses the ground state ferromagnetic order.

II. SELF-CONSISTENT HARMONIC APPROXIMATION

Writing the Hamiltonian (1) in terms of the polar representation for the spin at site j, $\vec{S}=(\cos\phi,\sin\phi)$ we find

$$H=-\sum_{i,j}\ [\cos(\phi_i-\phi_j)-\delta\cos^2(\phi_i-\phi_j)], \tag{2}$$

where $\delta=J/D$. The ground state is obtained by putting $\vec{S}_i\cdot\vec{S}_j=\cos\phi$ in the Hamiltonian (1) and minimizing the energy with respect to ϕ. We find

$$E=-J\cos\phi+D\cos^2\phi. \tag{3}$$

The condition $dE/d\phi=0$, leads to

$$\sin\phi(-J+2D\cos\phi)=0. \tag{4}$$

We have two solutions: (1) $\phi=0$ which is the lowest energy solution for $\delta<0.5$. We remark that for $J=0$ we have a disordered ground state but any finite value of J stabilizes the ferromagnetic ground state. (2) $\cos\phi=J/2D$ with $D/J>0.5$. We show the ground state for $D/J=1.0$ in Fig. 1. In region (1) $\phi_i-\phi_j$ is small and the long wavelength limit of the Hamiltonian (2) can be written as

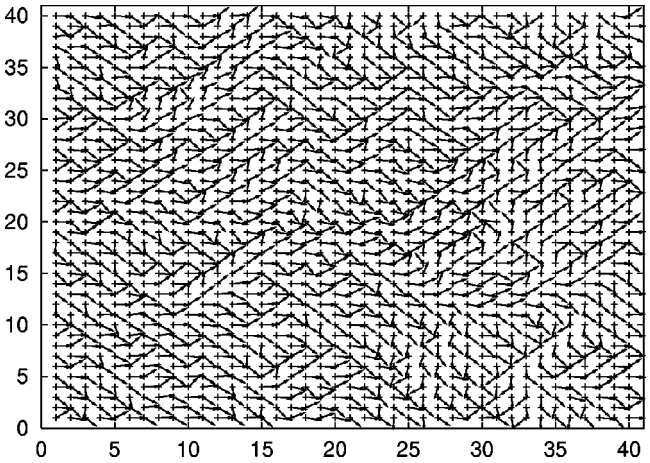

FIG. 1. Ground state of the Hamiltonian obtained by simulated annealing for a $L=40$ lattice and $D=0.70$.

$$H=\int \mathcal{H}\, dx\, dy, \tag{5}$$

where

$$\mathcal{H}=\left(\frac{J}{2}-D\right)a^2(\nabla\phi)^2-\frac{1}{3}\left(\frac{J}{8}-D\right)a^4(\nabla\phi)^4,$$

here a is the lattice spacing. In the standard treatment of the planar rotator model the second term in the right-hand side of Eq. (5) is much smaller than the first term and can be neglected. Here, however, this is not the case. For instance for $D=J/2$ we have

$$\mathcal{H}=\frac{J}{8}(\nabla\phi)^4. \tag{6}$$

Then a spin-wave treatment can be used only if $D\ll J/2$. In this case we can use the SCHA (Ref. 5) and write the Hamiltonian (2) as

$$H_0=\frac{J}{4}\sum_{r,a}\left[\rho_1(\phi_r-\phi_{r+a})^2-2\,\delta\rho_2(\phi_r-\phi_{r+a})^2\right], \tag{7}$$

where ρ_i are the effective spin stiffnesses given by

$$\rho_1=\langle\cos(\phi_r-\phi_{r+a})\rangle,\quad \rho_2=\langle\cos^2(\phi_r-\phi_{r+a})\rangle. \tag{8}$$

Now in order to apply the SCHA the averages $\langle\cdots\rangle$ in Eq. (8) are approximated by $\langle\cdots\rangle_0$ (all averages are then evaluated in an ensemble defined by H_0). Following Ref. 4 we obtain

$$H_0=\frac{J}{4}\rho_{\rm eff}\sum_r\,(\phi_r-\phi_{r+a})^2, \tag{9}$$

where

$$\rho_{\rm eff}=J(\rho_1-2\,\delta\rho_2),$$

$$\rho_2=\rho_1^4,\quad \rho_1=\exp\left[-\frac{T}{4J\rho_{\rm eff}}\right].$$

We have to solve Eq. (9) self-consistently. The BKT temperature can be determined by the crossing between the curve $\rho_{\rm eff}(T)$ and the line $\gamma=(\pi/2)T$. For details see Ref. 4. The SCHA has its limitation and it should be expected to work only around $\delta=0$. However, it gives around this point, the correct behavior of $T_{\rm BKT}$ as compared to the simulation data. In region (2) we have $\phi_i-\phi_j+\alpha$ small, where $\cos\alpha=J/2D$ and we obtain

$$\mathcal{H}=\left(D-\frac{J^2}{4D}\right)a^2(\nabla\phi)^2+\frac{J}{2}\sin\alpha a^3(\nabla\phi)^3+\left(\frac{7}{48}\frac{J^2}{D}-\frac{D}{3}\right)a^4(\nabla\phi)^4. \tag{10}$$

For $D\gg J$ the first term dominates, and a spin-wave treatment can again be used. Equations (5) and (10) show that, although a spin-wave technique can be applied only in limited regions (where the harmonic term dominates), the equation of motion in the continuum limit [obtained by calculating $\partial\mathcal{H}/\partial(\nabla\phi)=0$] has always a vortex solution $\tan\phi=y/x$, indicating the possibility of a BKT transition.

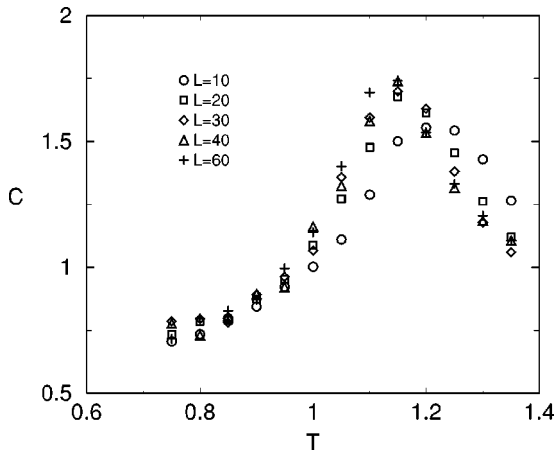

FIG. 2. Specific heat for lattice sizes $L=10,20,30,40,60$ and $\delta=0.25$. The peak height does not depend on L suggesting a BKT transition.

III. SIMULATION

The precise determination of the temperature for a BKT transition is a difficult task due to absence of sharp peaks in the thermodynamic quantities. One way to extract $T_{\rm BKT}$ was suggested by Weber and Minnhagen[8] by calculating the helicity modulus defined as

$$\Upsilon=-\frac{1}{2}\langle E\rangle-\frac{J}{TL^2}\left\langle\sum_{\langle i,j\rangle}\right\rangle\,\sin(\theta_i-\theta_j-A_{i,j})^2x_{i,j}, \tag{11}$$

where $x_{i,j}=x_i-x_j$ and $\langle E\rangle$ is the mean energy per spin. The finite size scaling for the helicity modulus is given by the Weber and Minnhagen's relation

$$\frac{\Upsilon_L\pi}{2T_{\rm BKT}}=1+\frac{1}{2(\ln L+l_0)}, \tag{12}$$

where l_0 is a parameter to be determined. Some care must be taken using this relation, since the scaling relation is obeyed only for large lattices. Another quantity we can study is the BKT susceptibility which must be of the form

$$\chi_{\rm BKT}=e^{c(T-T_{\rm BKT})^{-1/2}}. \tag{13}$$

To characterize the BKT transition we can calculate the specific heat C

$$C=\frac{1}{T^2}(\langle E^2\rangle-\langle E\rangle^2) \tag{14}$$

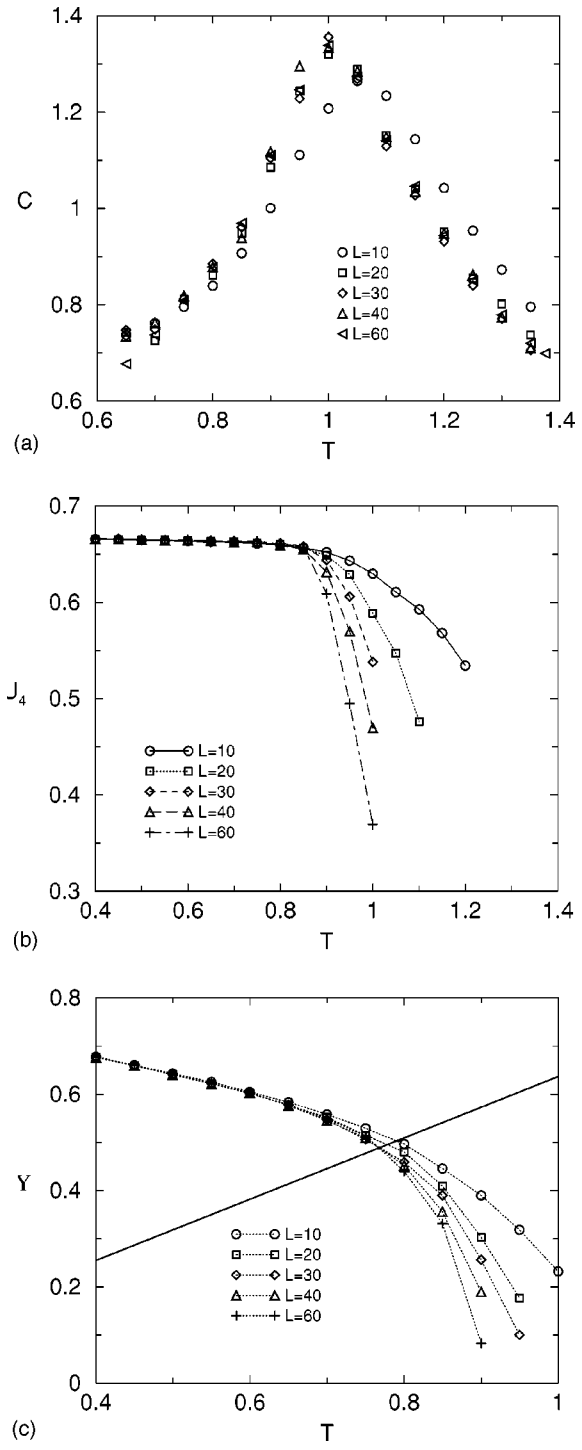

FIG. 3. Binder's cumulant as a function of T for $\delta=0.25$. The lattice sizes are the same as in Fig. 2.

for several lattice sizes. It is well known that C is independent of the lattice size and its maximum is dislocated from the BKT temperature. Another indication of the BKT transition character is the Binder's cumulant defined as

$$U=1-\frac{\langle M^4\rangle}{3\langle M^2\rangle^2}, \quad M=\frac{1}{L^2}\left[\sum_i^{L^2}(S_i^x)^2+\sum_i^{L^2}(S_i^y)^2\right]^{1/2} \tag{15}$$

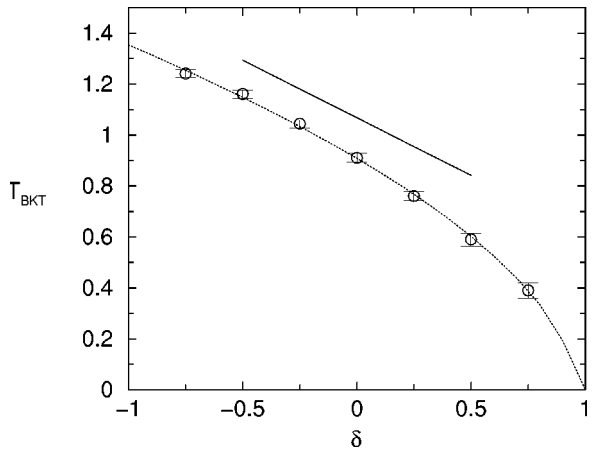

FIG. 4. Helicity as a function of T for $\delta=0.25$. The lattice sizes are the same as in Fig. 2.

which should be independent of the lattice size L at the critical region.

The simulations were carried out using the standard Metropolis algorithm combined with over relaxation updates. We used lattices of size $L\times L$ with $L=10,20,30,40,60$ and periodic boundary conditions. Each Monte Carlo (MC) step is a combination of 8 Metropolis steps and 1 over relaxation. We varied the temperature in steps of size $\Delta T=0.05$ and the parameter $-1.0<\delta<0.75$ in steps of size $\delta=0.25$. In order to reach thermodynamical equilibrium we performed long runs of size $100\times L\times L$. After this procedure we started to store the energy and magnetization values separated by 5 MC steps which was enough to break correlations between successive configurations. Each point in our simulation is the result of the average over 2×10^5 independent configurations. We then use the single histogram technique to study the interesting regions. In our simulations, when not indicated, the error bars are smaller than the symbols.

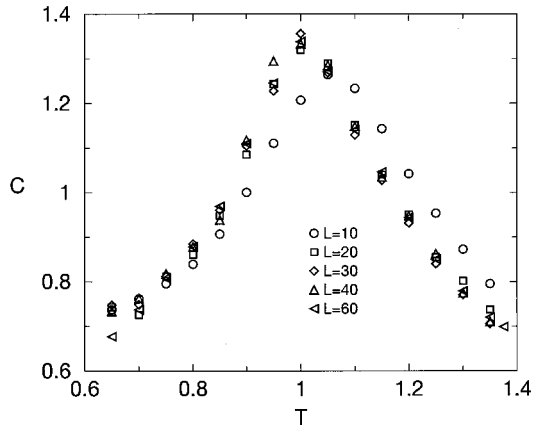

FIG. 5. BKT as a function of the parameter δ. Open circles are simulation results. The dotted line is the best χ^2 adjust using $T_{BKT}=A(\delta-\delta_c)^\alpha$ with $A\approx 0.93$, $\delta_c\approx 0.96$, and $\alpha\approx 0.56$ and the solid line is the SCHA.

IV. RESULTS

In Figs. 2 to 4 we show typical results obtained in our MC simulations. In Fig. 2 we show the results obtained for the specific heat as a function of temperature for several lattice sizes. It is quite evident that the peak height does not depend on L indicating a BKT phase transition. The Binder's cumulant results (Fig. 3) also show a typical BKT behavior with all curves coming parallel to each other with no single point interception. Following Eq. (12) we plot the helicity modulus Υ as a function of T for several lattice sizes. Figure 4 shows the result for $\delta=0.25$. The dotted lines are guides to the eye. The solid line is the $(2/\pi)T$ curve. The crossing between the dotted lines and the solid line give estimates of the BKT temperature. This estimate gets more accurate with increasing lattice size. The extrapolated values for the BKT temperature as a function of the parameter δ is plotted in Fig. 5. At the same figure we show the SCHA result as a solid line. The dotted line is the best χ^2 adjust using $T_{\mathrm{BKT}}=A(\delta-\delta_c)^{\alpha}$ with $A=0.93(4)$, $\delta_c=0.96(9)$ and $\alpha=0.56(6)$. The rapid decay of T_{BKT} with δ_c prevents us going further in the MC simulation since the computer time for equilibration of the system beyond $\delta\approx 0.75$ becomes prohibitive.

V. CONCLUSION

The two-dimensional planar rotator model with a biquadratic interaction has been investigated by using a self-consistent harmonic approximation and Monte Carlo computer simulations. We have found a Berezinskii-Kosterlitz-Thouless transition for values of the biquadratic exchange interaction less than $D/J<\delta_c$ with $\delta_c=0.96(9)$, where δ_c is the value of D/J where the Berezinskii-Kosterlitz-Thouless transition temperature goes to zero. The value of δ_c is not well determined due to the severe slowing down which appears for very low temperatures.

We hope this paper can stimulate further research both analytically and numerically in this model. For instance, an accurate estimate of δ_c should be interesting.

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