Finite-size scaling study of the three-dimensional classical XY model

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The three-dimensional classical XY model on a cubic lattice has been studied using Monte Carlo simulations. The finite-size scaling method of the phenomenological renormalization group has been used to calculate the critical exponents ν, v, and β of the correlation length, helicity modulus, and order parameter. Good agreement with series-expansion results is obtained.

I. INTRODUCTION

The three-dimensional classical XY model is of great interest, both as the simplest statistical model with a continuous degree of freedom, and as a model for the phase transition of superfluid ^{4}He and granular superconductors. Critical exponents and T_c have been obtained by using various methods such as high-temperature expansion.[1,2] ϵ expansion,[3] and Monte Carlo renormalization group.[4] Monte Carlo (MC) simulation has also been used in study of the three-dimensional XY model.[5] However, previous MC simulation has been limited to the determination of T_c alone. MC simulation has not been used to calculate the critical exponents.

The Monte Carlo finite-size scaling approach of the phenomenological renormalization group (PRG) (Refs. 6 and 7) has been very successful in analyzing the critical exponents of lower-dimensional models. Great advances in computational power have now made calculations for three-dimensional systems with continuous symmetries feasible,[8] and it is important to see how well the finite-size scaling method works in these cases.

Here, we report the first results of MC finite-size scaling and PRG analysis as applied to the three-dimensional XY model. We have carried out MC simulations on cubic lattices of size ranging from 4^3 to 16^3. An over-relaxation scheme is implemented to reduce critical slowdown near T_c. Data are analyzed to obtain the critical temperature T_c and the critical exponents for the order parameter $M\sim t^{\beta}$, helicity modulus $\Upsilon\sim t^{v}$, and correlation length $\xi\sim t^{-\nu}$. We obtain results which are in good agreement with those determined by previous methods.[1,3,4]

II. MONTE CARLO CALCULATIONS

The three-dimensional classical XY model is given by the Hamiltonian

$$\mathcal{H}=-J\sum_{\langle ij\rangle}\cos(\theta_i-\theta_j)\ , \tag{1}$$

where θ_i is the angle of the planar spin at site i of a cubic lattice, and the summation is restricted to all pairs of nearest-neighbor sites. We have simulated the Hamiltonian (1) with periodic boundary conditions on $L\times L\times L$ cubic lattices using a MC scheme to be described later.[9] The average energy per site $\langle u\rangle$, the helicity modulus Υ, the "order parameter" $|\mathbf{M}|^2$, and the specific heat C were calculated as functions of temperature T and size L. The "order parameter" we take to be the magnetization squared, and it is given by

$$|\mathbf{M}|^2=\frac{1}{N^2}\left\langle\left|\sum_j\exp(i\theta_j)\right|^2\right\rangle,\quad N=L^3\ . \tag{2}$$

The helicity modulus in direction $\hat{\mu}$ is determined by the relation[10]

$$\Upsilon_{\hat{\mu}}/J=\frac{1}{N}\left\langle\sum_{\langle ij\rangle}\cos(\theta_i-\theta_j)(\hat{\mathbf{e}}_{ij}\cdot\hat{\boldsymbol{\mu}})^2\right\rangle - \frac{J}{TN}\left\langle\left[\sum_{\langle ij\rangle}\sin(\theta_i-\theta_j)\hat{\mathbf{e}}_{ij}\cdot\hat{\boldsymbol{\mu}}\right]^2\right\rangle\ , \tag{3}$$

where $\hat{\boldsymbol{\mu}}=\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$ are the bond directions, and $\hat{\mathbf{e}}_{ij}$ is the unit vector connecting nearest-neighboring sites i and j. The Boltzmann's constant k_B has been set to unity. The specific heat is calculated using the usual fluctuation-dissipation relation.

As critical slowing down is a major factor affecting the accuracy of MC data near T_c, we have used in our simulations the standard Metropolis scheme supplemented by the over-relaxation method.[11] The over-relaxation method, which has been used in simulations of gauge theories[11] and spin systems,[12] has been demonstrated to be quite efficient in reducing critical slowing down. Its implementation for the XY model is very simple. At each over-relaxation step, one simply performs the following transformation:

$$\theta_i\rightarrow\theta_i'=2\Phi-\theta_i\ , \tag{4}$$

where Φ is defined as

$$|\mathbf{M}|e^{i\Phi}\equiv\sum_{\hat{\mu}}e^{i\theta_{i+\hat{\mu}}}\ , \tag{5}$$

and the summation is over all nearest-neighbors of the site i. This transformation maps the system from one point in its phase space to another point with exactly the same energy. As these points are separated by a finite distance in phase space, this over-relaxation can prevent the system from getting stuck in a particular local minimum. In our test runs, the particular combination of

over-relaxation and Metropolis schemes reduced the decorrelation time by a factor of 4 for small lattice sizes. It is expected to be more effective for large lattice sizes.

We have simulated the Hamiltonian (1) on lattices of size $L=4$, 6, 8, 10, 12, 14, and 16. Results for helicity modulus Υ, order parameter $|\mathbf{M}|^2$, and specific heat C, are shown in Figs. 1–3, respectively. For temperatures between $2.15J$ and $2.25J$ the data shown in Figs. 1–3 are results averaged over three to four independent runs, while only one run is used in the calculations for temperatures below $2.15J$. Within each independent run, the update of spins is done in combination of eight over-relaxation passes followed by two Metropolis passes. This particular combination of ten passes we refer to as *one* combined MC pass. The first 500 combined MC passes in each independent run at every temperature were dropped to equilibrate the system. The next 2000 to 3500 combined MC passes were used in the calculations of Υ, $|\mathbf{M}|^2$, and C. Since the system is isotropic, the helicity modulus Υ, along the $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ directions should be equal. The helicity moduli along these three directions have been averaged to achieve better statistics. Statistical errors for data (shown as error bars in Figs. 5 and 6) are estimated by standard block averaging. Simulations were carried out on an Alliant FX/8. A typical run at a fixed temperature for $L=10$ took 0.9 CPU hours.

III. ANALYSIS OF DATA

We first use PRG analysis to analyze our MC data. The critical exponent ν is defined as $\Upsilon \sim |T-T_c|^{\nu}$ as T approaches T_c from below. β and ν are the critical exponents for magnetization and correlation length as usual. From the finite-size scaling theory, one can show that Υ and $|\mathbf{M}|^2$ scale for large L as[6]

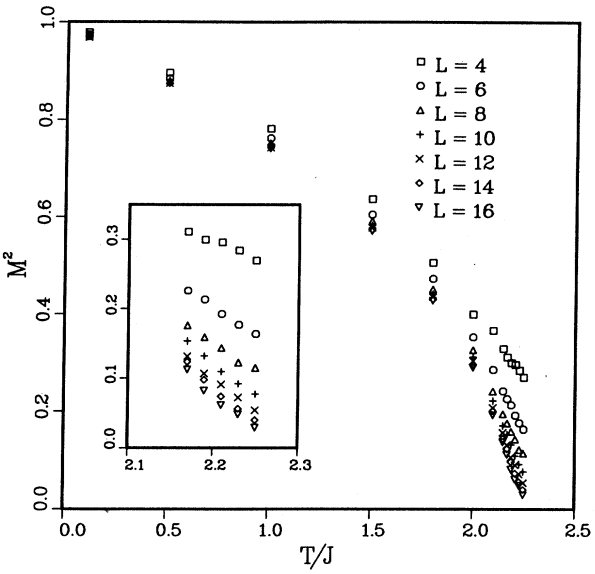

FIG. 2. The temperature dependence of the order parameter $|\mathbf{M}|^2$ for different lattice sizes L. The inset shows the data near T_c on a finer scale.

$$\Upsilon(L,T)=L^{-\nu/\nu}H(L^{1/\nu}\Delta)\ , \tag{6}$$

$$|\mathbf{M}(L,T)|^2=L^{-2\beta/\nu}\Phi(L^{1/\nu}\Delta)\ , \tag{7}$$

where

$$\Delta\equiv\frac{1}{T}-\frac{1}{T_c}\ ,$$

and H and Φ are scaling functions. Let us take the helici-

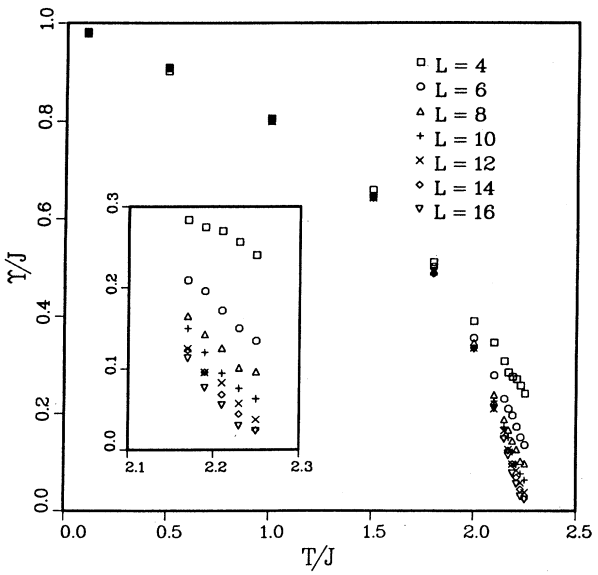

FIG. 1. The temperature dependence of helicity modulus Υ for different lattice sizes L. The inset shows the data near T_c on a finer scale.

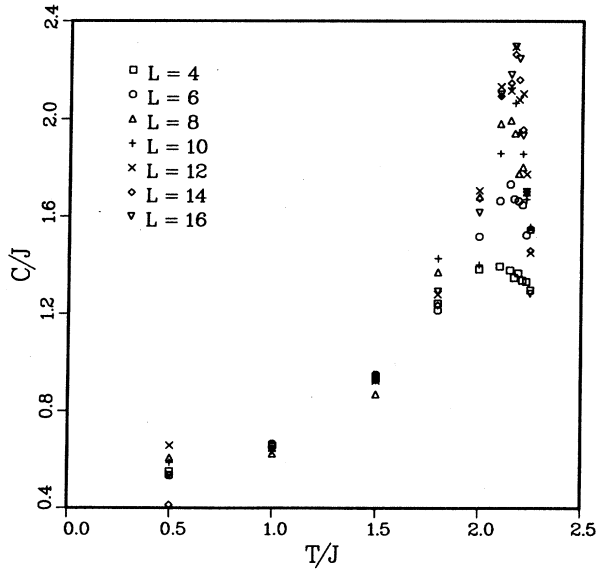

FIG. 3. The temperature dependence of specific heat C for different sizes L. It shows the existence of peak in the specific heat, with weak dependence on size L.

ty modulus as an example to see how to obtain T_c and v/ν using PRG analysis. Following Barber,[6] we use data from two different sizes, L and L', to construct the quantities

$$P_\Upsilon(L,L',T)\equiv\Upsilon(L,T)/\Upsilon(L',T)\ . \tag{8}$$

From the finite-size scaling form Eq. (6), we know that $P_\Upsilon=(L/L')^{-v/\nu}$ when $T=T_c$. So, two curves of $P_\Upsilon(L,L',T)$ versus T for different L and L', but fixed ratio of L/L', should intersect at $[T_c,(L/L')^{-v/\nu}]$.

In Fig. 4, the temperature dependences of $P_\Upsilon(L,L',T)$ for $L/L'=\frac{8}{4}$, $\frac{12}{6}$, and $\frac{16}{8}$ are shown. These three curves intersect at a single point indeed. From Fig. 4, we can estimate $T_c\approx 2.197$ and $v/\nu\approx 1.00$. This result for T_c is in reasonable agreement with that obtained by other methods and the previous MC simulation. The result of $v/\nu=1.00$ is nothing else but confirmation of the Josephson scaling law $v/\nu=d-2$ for the three-dimensional case.[13]

Since this phenomenological renormalization method can yield only the ratio of critical exponents to the correlation length exponent ν, we need another method to determine ν. We follow the analysis of Nightingale and Blöte[8] and fit our MC data to the first-order expansion form of the scaling function to determine ν. Since $v=\nu$, we have

$$\Upsilon L=H_0+H_1L^{1/\nu}(K-K_c)+O(L^{2/\nu}(K-K_c)^2)\ , \tag{9}$$

where $K\equiv 1/T$. This is a four-parameter fitting. We have used the Levenberg-Marquart method[14] to perform the χ^2 fit. Our results are $T_c=2.201\pm0.003$, and $\nu=0.68\pm0.02$. The result of this fitting of the helicity modulus to the MC data is shown in Fig. 5.

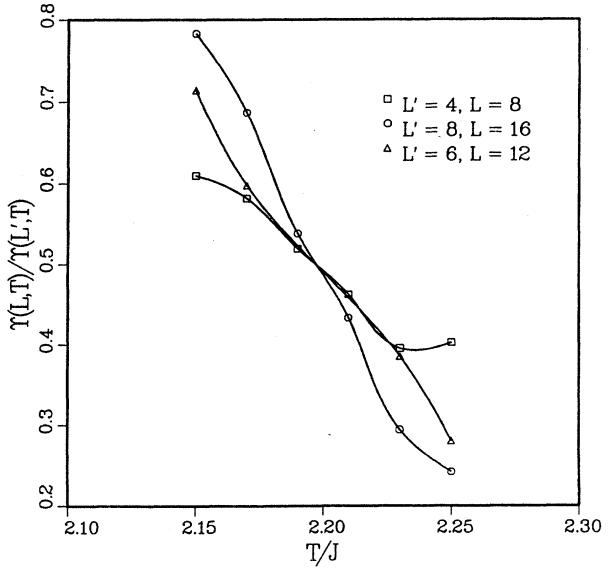

FIG. 4. Plot of the PRG ratio function $\Upsilon(L,T)/\Upsilon(L',T)$ vs temperature T for $L'/L=\frac{4}{8}$, $\frac{6}{12}$, and $\frac{8}{16}$. The intersection of curves falls at the point $(T_c,(L/L')^{v/\nu})$ and enable estimation of $T_c\approx 2.197$ and $v/\nu\approx 1.0$.

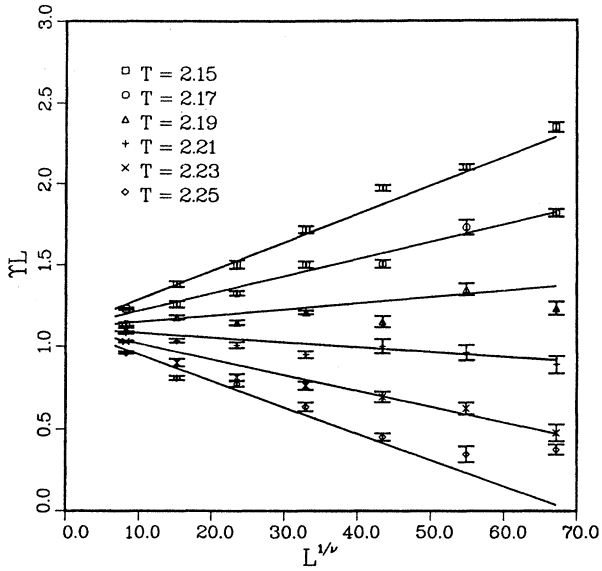

FIG. 5. The finite-size scaling behavior of the helicity modulus Υ. Symbols with error bars represent the MC simulation results. The solid lines represent the results of fitting to Eq. (9) using data from size $L=10$–16. $\nu=0.68$ is used in making horizontal axis of the plot.

To check that we have reached the asymptotic large L limit required by scaling, fits were carried out using data for only $L=L_{\min}-16$. The lower value $L_{\min}$ was increased until no changes in the fitted parameters were observed with further increases in $L_{\min}$. The curves shown in Fig. 5, and the results already cited, come from a fit to the data for $L=10$–16. We have also performed fits to the scaling function expanded to quadratic order (requiring one additional fitting parameter), and have observed no change in our results. The errors we cite are estimated as follows. First, many sets of "fictitious" data are generated by adding Gaussian distributed noise to the original MC data. The width of each Gaussian distribution is set to be the standard deviation of the corresponding original MC data point. These fictitious data are then fitted to Eq. (9). The fluctuation in the results of each fitting parameter is chosen to be the estimated error.

The value of T_c found with this method is in agreement with the one we obtained from the PRG analysis of Fig. 4. It is also in good agreement with the high-temperature series expansion[1] result $T_c=2.203\pm0.006$ and the previous MC simulation[5] result $T_c=2.208\pm0.005$. The value of ν is also in good agreement with that determined by series expansions, $\nu=0.675\pm0.015$ (Ref. 1) and $\nu=0.669\pm0.022$.[3]

We performed a similar χ^2 fitting of our MC data for the order parameter $|\mathbf{M}|^2$ to the first-order expansion form of its scaling function. Expanding the scaling function Φ on the right-hand side of Eq. (7), we have

$$|\mathbf{M}(L,K)|^2=L^{-2\beta/\nu}[\Phi_0+\Phi_1L^{1/\nu}(K-K_c)+O(L^{2/\nu}(K-K_c)^2)]\ . \tag{10}$$

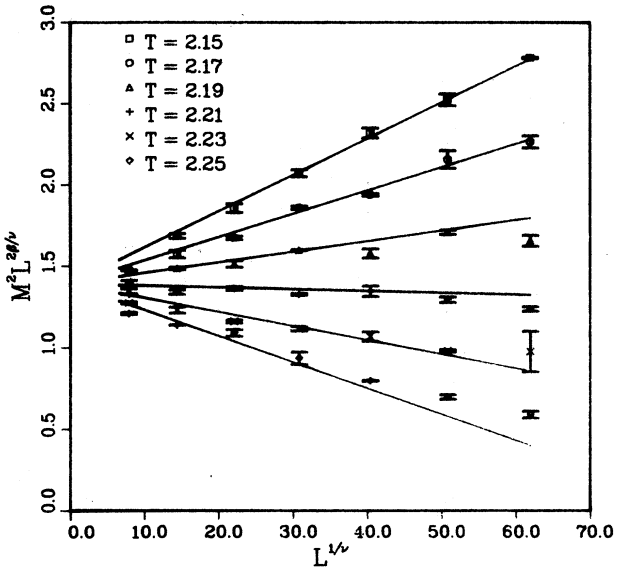

FIG. 6. The finize-size scaling behavior of the order parameter $|\mathbf{M}|^2$. Symbols with error bars represent the MC simulation results. The solid lines represent the results of fitting to Eq. (10) using data from size $L=10$–16. $\nu=0.67$ and $\beta=0.36$ are used in making the axes of the plot.

This is a five-parameter fitting. The ratio $2\beta/\nu$, instead of β itself, is chosen as an independent fitting parameter. With the same fitting procedure as used for Υ, we obtained $\beta=0.36\pm0.01$, $\nu=0.67\pm0.02$, and $T_c=2.206\pm0.003$. The result of this fitting for the order parameter to the MC data is shown in Fig. 6. The values of ν and T_c agree very well with those obtained in the fitting of helicity modulus data. Our result for β agrees well with those found in the series expansions, $\beta=0.367\pm0.02$ (Ref. 1) and $\beta=0.3455\pm0.0020$.[3]

While in the middle of this work, we learned of similar calculations for the three-dimensional (3D) XY model being carried out by Nightingale and Blöte,[15] using the transfer matrix method. Their results are consistent with ours, but they report greater accuracy in T_c.

IV. CONCLUSIONS

We have carried out Monte Carlo simulations for the three-dimensional XY model on cubic lattices. The finite-size scaling and phenomenological renormalization group approaches have been used to analyze the data and extract values for critical temperature T_c and critical exponents ν, β, and v. Good agreement with series-expansion results have been obtained. Our simulations demonstrate that it is feasible to apply these methods to three-dimensional systems with a continuous symmetry, and get reliable results for the critical behavior, using lattice sizes within current computational capability.

Note added in proof: In a recent work,[16] the combination $\beta/(1+\nu)$ has been computed by a scaling analysis of Monte Carlo simulations of a model with a spatially varying coupling.

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[1]M. Ferer, M. A. Moore, and M. Wortis, Phys. Rev. B **8**, 5205 (1978).
[2]K. Ohno, Y. Okabe, and A. Morita, Prog. Theor. Phys. **71**, 714 (1984).
[3]J. C. Le Guillou and J. Zinn-Justin, Phys. Rev. B **21**, 3976 (1980).
[4]R. H. Swendsen, Phys. Rev. B **27**, 391 (1983).
[5]A. Garg, R. Pandit, S. A. Solla, and C. Ebner, Phys. Rev. B **30**, 106 (1984).
[6]M. N. Barber and W. Selke, J. Phys. A **15**, L617 (1982).
[7]M. P. Nightingale, J. Appl. Phys. **53**, 7927 (1982).
[8]M. P. Nightingale and H. W. J. Blöte, Phys. Rev. Lett. **60**, 1562 (1988).
[9]We have in fact simulated a model with θ_i allowed to take only one of 512 discrete states uniformly distributed between 0 and 2π, namely the 512-state clock model. 512 is sufficiently large that we expect no difference between this and the true XY model where θ_i may take continuous values.
[10]S. Teitel and C. Jayaprakash, Phys. Rev. B **27**, 598 (1983).
[11]M. Creutz, Phys. Rev. D **36**, 515 (1987).
[12]R. Gupta, J. DeLapp, G. G. Battrouni, G. C. Fox, C. F. Baillie, and J. Apostolakis, Phys. Rev. Lett. **61**, 1996 (1988).
[13]B. D. Josephson, Phys. Lett. **21**, 608 (1966); M. E. Fisher, M. N. Barber and D. Jasnow, Phys. Rev. A **8**, 1111 (1973).
[14]W. H. Press, B. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes* (Cambridge University Press, Cambridge, 1986), pp. 521-528.
[15]M. P. Nightingale and H. W. J. Blöte (private communication).
[16]P. Muzikar and N. Giordano, Physica A **157**, 742 (1989).