PHYSICAL REVIEW B VOLUME 52, NUMBER 17 1 NOVEMBER 1995-I

Finite-size scaling study of the vortex-free three-dimensional XY model

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(Received 21 July 1995)

Monte Carlo simulations have been used to study a version of the XY model without vortex loops for $J/T=0$ on simple cubic and face-centered-cubic lattices. Finite-size scaling of data from $L\times L\times L$ lattices with L up to 32 is used to obtain values for the order parameter $|\mathbf{M}|$ and a $1/L$ finite-size correction on each lattice. The order-parameter susceptibility is found to be diverging as $L^{0.8}$. We then study the crossover from three-dimensional to one-dimensional behavior on $L\times W\times W$ simple cubic lattices, with $W=4$ and 8, and L up to 1024.

I. INTRODUCTION

In 1955 Feynman[1] argued that it should be possible to analyze the superfluid transition of three-dimensional liquid helium in terms of the behavior of vortex loops. As is well known, this phase transition is in the universality class of the XY model, and its critical properties are believed to be understood in terms of a renormalization group based on spin-wave theory.[2] Despite efforts by several authors,[3–7] the connection between the vortex line description and the spin-wave description remains far from complete.

Halperin[4] pointed out that in the absence of vortices the phase of the order parameter cannot relax, except at the boundaries. He argued that this implies that the presence of vortex loops is necessary in order for the spin stiffness to vanish. This suggestion motivated Kohring, Shrock, and Wills[5] (KSW) to perform Monte Carlo calculations on an XY model with an additional vortex fugacity term. We write the KSW Hamiltonian as

$$H=-J\sum_{\langle ij\rangle} \mathbf{S}_i\cdot\mathbf{S}_j+g\sum_{\text{plaq}} |\mathbf{v}|, \quad (1)$$

where $\langle ij\rangle$ is a sum over neighbor pairs, each $\mathbf{S}$ is a classical unit length two-component spin, and $\mathbf{v}$ is the (quantized) vorticity of a plaquette.

Denote the direction in spin space defined by each $\mathbf{S}_i$ to be θ_i. Then $\mathbf{v}$ is defined on the lattice by the following procedure. Let $\theta_{ij}=\theta_i-\theta_j+2\pi n_{ij}$, where n_{ij} is the integer which puts θ_{ij} into the range $(-\pi,\pi]$. Now the sum of the θ_{ij} around a plaquette is defined to be $2\pi\mathbf{v}$, and $\mathbf{v}$ is an integer. KSW found that in the limit $J/T\to 0$ (where T is temperature) this model remains ferromagnetic for $g/T>0.55$. When vortices were completely removed from the model by making g infinite, then an $8\times 8\times 8$ simple cubic lattice with periodic boundary conditions retained a magnetization of $|\mathbf{M}|\approx 0.47$ for $J/T=0$.

Here we will examine this phenomenon in more detail, using a similar Monte Carlo technique. We perform numerical simulations of the KSW model in the limit $J/T=0$ and $g/T=\text{inf}$ on $L\times L\times L$ simple cubic (sc) and face-centered-cubic (fcc) lattices with periodic boundary conditions, as a function of L. We will also study the crossover from three-dimensional (3D) to one-dimensional (1D) behavior, by using $L\times W\times W$ sc lattices with $L>W$. Although there is no critical point for the vortex-free model in three dimensions, this crossover function takes us from a ferromagnetic state to a paramagnetic state. A finite-size scaling analysis of the ordinary XY model near its critical point has been performed by Li and Teitel.[8]

It should be noted that the topological nature of the vortex fugacity term is not really an essential element of this problem. Any isotropic interaction between the four spins of each plaquette of the sc lattice which causes the spins to align more ferromagnetically than a sum of pairwise exchange interactions, e.g., $-J_4|\mathbf{S}_1+\mathbf{S}_2+\mathbf{S}_3+\mathbf{S}_4|^4$ with $J_4>0$, will have a similar effect. For the fcc lattice we could use an interaction between the four spins at the corners of each elementary tetrahedron of the lattice. This is a well-known example of universality. The fact that for an XY model we have a choice between analyzing the model in terms of vortices or four-spin couplings has been discussed in detail for the two-dimensional case by Jose *et al.*,[9] and the essentials remain true in the three-dimensional case.

II. MONTE CARLO PROCEDURE

All lattices were studied using classical planar spins of unit length and periodic boundary conditions. To improve the efficiency of the computer program, a Z_{256} discretization was used. This means that each spin variable θ_i was allowed to take on the values $\pi n/128$, with $n=0,1,\ldots 255$, rather than any value in $[0,2\pi)$. For such a Z_p model, the finite p effects on $|\mathbf{M}|$ are of order $1/p^2$. Thus for $p=256$ the finite p effects are negligible compared to out statistical errors. A similar discretization was used by Li and Teitel.[8]

The Monte Carlo procedure used in this work was straightforward. Each lattice was initialized to a fully aligned state. The program then proceeded through the lattice, attempting to reorient each spin in turn. The proposed new state of each spin was chosen using a multiplicative linear congruential random number generator,[10] and the new state was accepted whenever the change did not create a vortex loop. After discarding the initial part of each run for equilibration, the remainder of the data were averaged to obtain the statistical properties.

Small lattices were run for 163 840 Monte Carlo steps per spin (MCS), with sampling every 10 MCS. This was increased by a factor of 2 for most of the larger lattices, and by even more when necessary. It is difficult to characterize the

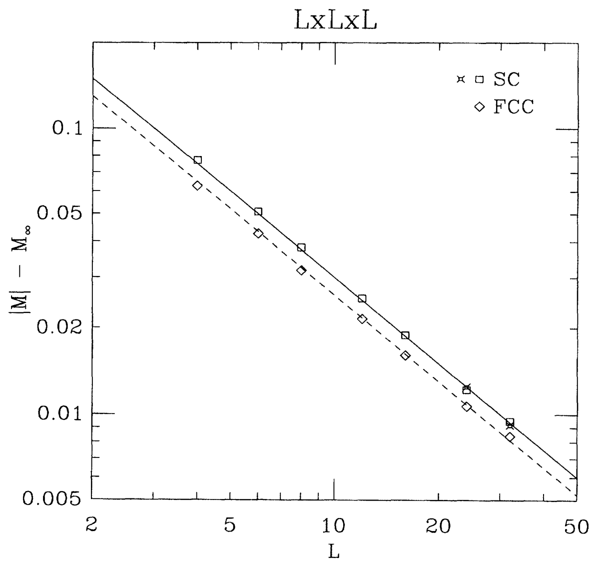

FIG. 1. Finite-size scaling of the order parameter for $L\times L\times L$ sc and fcc lattices. The axes are scaled logarithmically. The solid line show Eq. (3), and the dotted line shows Eq. (4). The spiked symbols show data obtained using the improved random number generator.

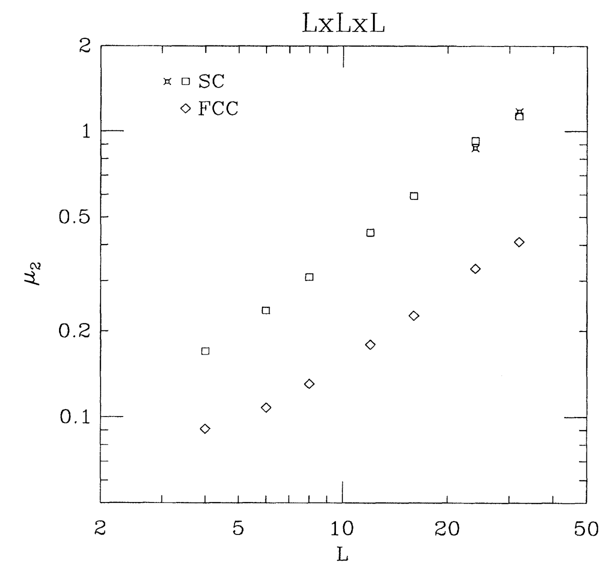

FIG. 2. Size dependence of the second moment of the distribution for the order parameter for $L\times L\times L$ sc and fcc lattices. The axes are scaled logarithmically. The spiked symbols show data obtained using the improved random number generator.

size of the errors precisely, because the algorithm is sensitive to nonideal behavior of the "random" numbers. An examination of the power spectrum of the magnetization fluctuations showed clear evidence of peaks due to correlations in the "random" numbers. Some runs were repeated with an improved random number generator.[11] This made the large peaks in the power spectrum disappear. The differences between the results for the two different random number generators are not large, and may be assumed to give the scale of the errors. The author is reasonably confident that the numerical results given here are accurate to the quoted precision.

III. THREE-DIMENSIONAL SCALING

The only input parameters in the model are the size, shape and type of lattice. The order parameter for the model is the average magnetization per spin, defined on finite lattices by

$$|\mathbf{M}|=N^{-1}\left[\left(\sum_{i=1}^{N}\mathbf{S}_i^x\right)^2+\left(\sum_{i=1}^{N}\mathbf{S}_i^y\right)^2\right]^{1/2}, \qquad (2)$$

where N is the number of sites on the lattice. In Fig. 1 we display the average of $|\mathbf{M}|$, for $L\times L\times L$ sc and fcc lattices, with $4\leqslant L\leqslant 32$. For the sc case the data are well described by the form

$$\langle|\mathbf{M}|\rangle=0.430+0.30/L, \qquad (3)$$

and for the fcc case (where $N=L^3/2$) we find

$$\langle|\mathbf{M}|\rangle=0.542+0.26/L. \qquad (4)$$

The $\langle\ \rangle$ brackets indicate a time average. Note that for $L=8$ on the sc lattice we are in complete agreement with KSW.

A finite-size effect proportional to L^{-1} indicates that the free energy of long-wavelength spin fluctuations is proportional to the square of the wave number. This means that hydrodynamic spin-wave theory[12] is still a useful approximation for our model, despite the absence of the usual ferromagnetic exchange energy. The helicity modulus[13] will, as usual, be proportional to $|\mathbf{M}|^2$. From this we infer that the net entropy of domain formation of the vortex-free XY model is negative. This must be true for the model to be ferromagnetic at all temperatures on three-dimensional lattices. A partial explanation of this effect is that, because the "coarse-grained" local value of θ changes slowly, due to the absence of vortex loops, the leading order contribution to the domain-related entropy coming from fluctuations in the position of localized (topological) defects is absent here. A similar phenomenon has been found in computer simulations of an isotropic three-component spin model with exclusion of hedgehog defects.[14] In that case the $L\rightarrow\infty$ magnetization of a sc lattice was estimated to be only 0.15. The reader who finds these effects bizarre or pathological should recall the more familiar problem of the hard-sphere system, where, in the absence of any interaction other than excluded volume, a crystalline phase is found to be stable over a range of densities.[15]

We characterize the shape of the distribution of $|\mathbf{M}|$ by its normalized second moment:

$$\mu_2(|\mathbf{M}|)=N[\langle|\mathbf{M}|^2\rangle-\langle|\mathbf{M}|\rangle^2]. \qquad (5)$$

Values of μ_2 for the sc and fcc $L\times L\times L$ lattices are shown in Fig. 2. From these data it appears that on both lattices μ_2 grows like $L^{0.8}$ for large L. The transverse spin fluctuations, on the other hand, grow approximately as N, as expected for an isotropic ferromagnetic.

As pointed out by Halperin and Hohenberg,[12] the hydrodynamic behavior of an XY model in the broken symmetry phase is essentially similar to that of the two-fluid model of a Bose liquid. Our vortex-free condition corresponds to the absence of rotons in the Bose superfluid. In this case, a physical manifestation of the divergence of μ_2 as seen in Fig. 2 would be an anomalous contribution to the damping of second sound. This anomaly is not large enough to invalidate the essential correctness of the hydrodynamic description, however.

The dynamical behavior of $\mathbf{M}(\omega)$ appears to be Debye-like, with a relaxation time τ that depends on L, being approximately proportional to L^2. (The reader is reminded that our results for the dynamical behavior are somewhat unreliable, due to the sensitivity of the algorithm to the quality of the random number generator.) As L grows, the transverse spin-diffusion time diverges much more rapidly than the relaxation time of $|\mathbf{M}|$. For $L=32$ on the sc lattice, the transverse spin-diffusion time is about 10^5 MCS, but $|\mathbf{M}|$ achieves its equilibrium value within 100 MCS. The calculated spectral density function, $S(\omega)=\chi''(\omega)/\omega$, for the $L=32$ sc lattice is shown in Fig. 3(a). It behaves approximately as L^2/ω^2, as expected for Debye-like behavior. The spectral density of $|\mathbf{M}(\omega)|$, shown in Fig. 3(b), is almost independent of ω, for fixed L.

The observation that $P(\omega)$ is Fig. 3(b) is almost independent of ω is consistent with the predictions of Debye-like theories. It demonstrates that the growth of μ_2 with L, as shown in Fig. 2, is not a mean-field spin-wave theory effect. The possibility of this type of non-mean-field behavior has been discussed qualitatively in Sec. 10 of the paper by Halperin and Hohenberg,[12] and in earlier work cited by them. It is hoped that these data will stimulate additional quantitative work, both theoretical and experimental.

IV. 3D TO 1D CROSSOVER SCALING

Working with lattices of size $L\times W\times W$, we can study the crossover from an ordered three-dimensional lattice behavior to a disordered one-dimensional lattice behavior by varying the ratio of L and W. Within a spin-wave theory, the spin stiffness, and therefore the value of $|\mathbf{M}|$, for a finite lattice can be related to the conductance of an equivalent resistor network.[16,17] Therefore we should expect the crossover to be a function of the scaling variable L/W^2. Note that this variable is *not* dimensionless. L and W must be measured in units of the lattice constant. We are not studying a critical point, so there is no requirement of scale invariance. For any fixed value of the aspect ratio, L/W, we will approach the three-dimensional broken-symmetry fixed point as we let the size of the system become large.

This geometry was discussed by MacKinnon and Kramer[18] for the Anderson localization problem. For the localization problem there is an additional length scale, the mean free path λ, which comes from the disorder. The length scale which has "disappeared" from our problem is the distance between vortex loops. A scaling function similar to the one found here probably applies to the Anderson localization problem when $W\ll\lambda$.

In Fig. 4 we demonstrate that our scaling hypothesis is essentially correct for the sc lattice. There are corrections to scaling for small L and W, as required by Eq. (3). The dominant behavior, however, is seen to be that $|\mathbf{M}|$ remains close to its three-dimensional value for $L/W^2<1$, while for $L/W^2>1$ it rapidly approaches the form

$$|\mathbf{M}|=0.40W/\sqrt{L}. \tag{6}$$

The fact that the long-range order is seen to disappear as we take L to infinity while holding W fixed demonstrates that the order we find in the three-dimensional thermodynamic limit is a true equilibrium effect.

Equation (6) means that for a long cylinder the correlation length for variations in θ along the cylinder is proportional to the cross-sectional area W^2. Thus in this limit the Debye time τ becomes proportional to W^2, and independent of L. Because the system can now be approximated as a set of independently fluctuating domains (subject to the constraint

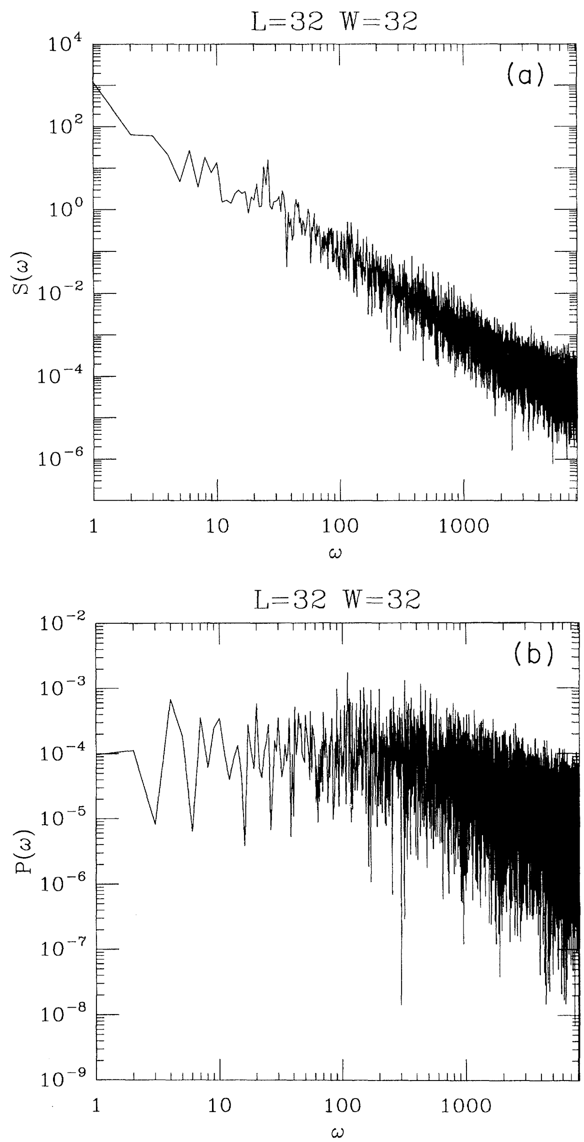

FIG. 3. (a) Spectral density $S(\omega)$ of $\mathbf{M}$ for a $32\times32\times32$ sc lattice. (b) Spectral density $P(\omega)$ of $|\mathbf{M}|$ for the same data set. The axes are scaled logarithmically. Data shown were obtained using the improved random number generator, sampling every 20 MCS.

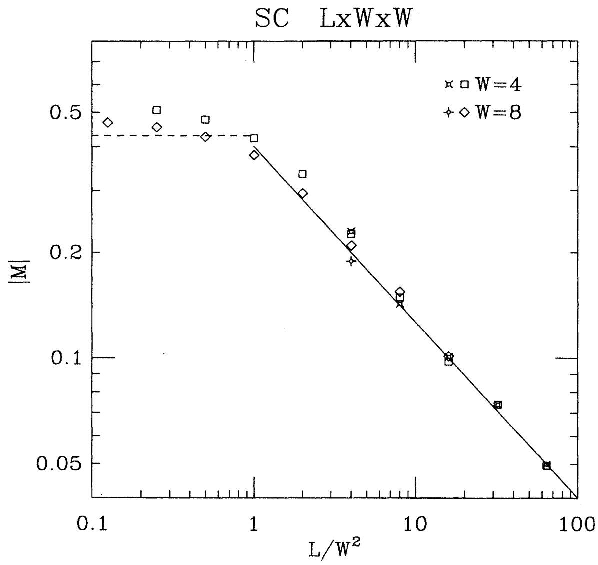

FIG. 4. Crossover scaling function of the order parameter for $L\times W\times W$ sc lattices. The axes are scaled logarithmically. The solid line shows Eq. (6), and the dotted line shows M_∞ from Eq. (3). The spiked symbols show data obtained using the improved random number generator.

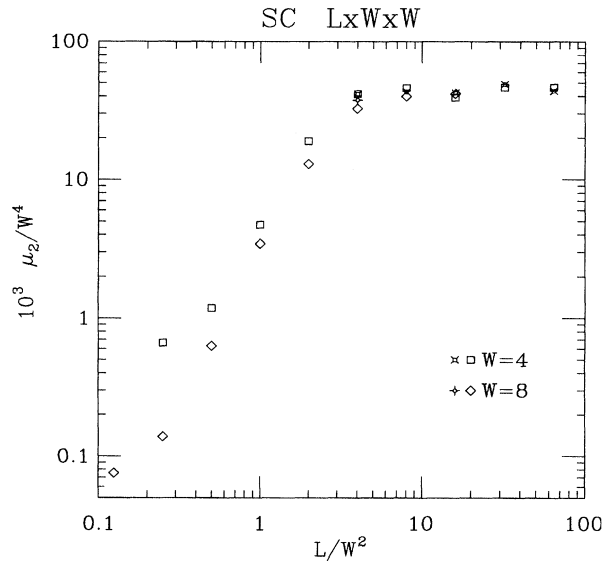

FIG. 5. Crossover scaling function for the second moment of the order-parameter distribution for $L\times W\times W$ sc lattices. The axes are scaled logarithmically. The spiked symbols show data obtained using the improved random number generator.

that the coarse-grained value of θ changes smoothly as we move along the cylinder), the relaxation time for $|\mathbf{M}|$ is now equal to τ.

From this we anticipate that plotting μ_2/W^4 versus L/W^2 should also exhibit a scaling behavior. The data for $W=4$ and 8, and L up to 1024 are shown in Fig. 5. For $L/W^2>4$, this crossover function is essentially independent of L, but in the range $2W\leqslant L\leqslant 2W^2$ it is approximately proportional to $L^{2.2}$. This is a reasonable result, since 2.2 is the difference between 3 and 0.8, as found in Fig. 2.

V. SUMMARY

In this work we have performed a more detailed Monte Carlo study of the vortex-free three-dimensional XY model, with the exchange coupling set to zero. On $L\times L\times L$ lattices the model behaves like a long-range ordered three-dimensional XY ferromagnet. The transverse susceptibility has the usual spin-wave theory divergence, proportional to L^3, while the longitudinal susceptibility diverges like $L^{0.8}$. We have also studied $L\times W\times W$ lattices, and calculated crossover functions between three-dimensional long-range ordered and one-dimensional short-range ordered behavior.

ACKNOWLEDGMENTS

The author thanks James Beatty for the use of a DEC3000/600 workstation, and Jonathan Katz for a helpful remark.

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