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The XY Model and the Three-State Antiferromagnetic Potts Model in Three Dimensions: Critical Properties from Fluctuating Boundary Conditions

Aloysius P. Gottlob[1] **and Martin Hasenbusch**[2, 3]

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We present the results of a Monte Carlo study of the three-dimensional XY model and the three-dimensional antiferromagnetic three-state Potts model. In both cases we compute the difference of the free energies of a system with periodic and a system with antiperiodic boundary conditions in a neighborhood of the critical coupling. From the finite-size scaling behaviour of this quantity we extract values for the critical temperature and the critical exponent ν that are compatible with recent high-statistics Monte Carlo studies of the models. The results for the free energy difference at the critical temperature and for the exponent ν confirm that both models belong to the same universality class.

KEY WORDS: Monte Carlo simulation; three-state antiferromagnetic Potts model; XY model; three dimensions; universality class.

1. INTRODUCTION

Ueno *et al.*[1] pointed out that the differences in the free energy ΔF of systems with different boundary conditions, such as periodic and antiperiodic boundary conditions, might be a powerful alternative to the fourth-order cumulant[2] in the study of critical phenomena. For the Ising model antiperiodic boundary conditions force an interface into the system, and ΔF can be interpreted as the interface free energy. In the case of $O(N)$-invariant vector models with $N \geqslant 2$, such as the XY model ($N=2$) and the classical Heisenberg model ($N=3$), however, the continuous symmetry of

[1] Universität Kaiserslautern, D-67653 Kaiserslautern, Germany.
[2] CERN, Theory Division, CH-1211 Geneva 23, Switzerland.
[3] Present address: DAMTP, Cambridge, CB3 9EW, England.

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the model prevents the creation of a sharp interface and ΔF rather becomes a measure for the helicity modulus.

Ueno *et al.*[1] give, based on previous results,[3] the scaling relation

$$\Delta F = f(tL^{1/\nu}) \tag{1}$$

where $t = (T - T_c)/T_c$ is the reduced temperature, L is the linear extension of the lattice, and the reduced free energy F is given by $F = -\ln Z$, where Z is the partition function of the system. It is important to note that the above relation requires that all directions of the lattice scale with L. It follows that the crossings of ΔF, plotted as a function of the temperature for different L, provide estimates for the critical temperature. Furthermore, the energy difference ΔE, which is the derivative of ΔF with respect to the inverse temperature, scales as

$$\Delta E \propto L^{1/\nu} \tag{2}$$

where ν is the critical exponent of the correlation length ξ.

The drawback of the method outlined above is that in general it is hard to obtain free energies from Monte Carlo simulations. The standard approach is to measure ΔE at a large number of temperatures and perform a numerical integration starting from $T = 0$ or $T = \infty$, where the free energy is known, up to the temperature in question. In refs. 4 and 5, however, one of the authors presented a version of the cluster algorithm[6,7] that gives direct access to the interface free energy of Ising systems ($N = 1$). It was demonstrated that the crossings of ΔF converge even faster than the crossings of the fourth-order cumulant in the case of the 3D Ising model on a simple cubic lattice.

In the present paper we show how the algorithm of refs. 4 and 5 can be generalized to $O(N)$-invariant vector models with $N > 1$ and apply it to the 3D XY model on a simple cubic lattice.

The λ-transition of helium from the fluid He I phase to the superfluid He II phase at low temperature is supposed to share the 3D XY universality class. It is the experimentally best studied second-order phase transition. The superfluid density corresponds to the helicity modulus of the XY model.[8] The quoted error bars of the measured value $\nu = 0.6705(6)$[9] are smaller than that of the theoretical predictions for the 3D XY universality class.

Banavar *et al.*[10] conjectured that the 3D antiferromagnetic (AF) three-state Potts model belongs to the same universality class as the 3D XY model. Ueno *et al.*[1] implemented "favorable" and "unfavorable" boundary conditions for the 3D AF three-state Potts model. They found that the corresponding ΔF is incompatible with that found for the 3D XY model.

They also obtained an estimate for the critical exponent of the correlation length $\nu = 0.58(1)$[1] that is not consistent with the exponent $\nu = 0.669(2)$[11] of the 3D two-component $(\phi^2)^2$-theory. This result has to be compared with recent high-precision studies of the 3D AF three-state Potts model,[12, 13] where the XY exponents and critical amplitudes were recovered to high accuracy. To clarify this point, we discuss how antiperiodic boundary conditions can be implemented for the 3D AF three-state Potts model. Our numerical findings are then compared with the 3D XY results.

2. $O(N)$ MODELS WITH FLUCTUATING BOUNDARY CONDITIONS

We consider a simple cubic lattice with extension L in all directions. The uppermost layer of the lattice is regarded as the lower neighbor plane of the lowermost plane. An analogous identification is done for the other two lattice directions. The $O(N)$ model is defined by the classical Hamiltonian

$$H(\mathbf{s}, \mathrm{bc}) = -\sum_{\langle ij \rangle} J_{\langle ij \rangle} \mathbf{s}_i \cdot \mathbf{s}_j \tag{3}$$

where $\mathbf{s}_i$ are unit vectors with N components. When periodic (p) boundary conditions (bc) are employed, then $J_{\langle ij \rangle} = 1$ for all nearest-neighbor pairs. When antiperiodic (ap) boundary conditions are employed, then $J_{\langle ij \rangle} = -1$ for bonds $\langle ij \rangle$ connecting the lowermost and uppermost planes of the lattice, while all other nearest-neighbor pairs keep $J_{\langle ij \rangle} = 1$. The free energy difference is now given by

$$\Delta F = F_{\mathrm{ap}} - F_{\mathrm{p}} = -\ln \frac{Z_{\mathrm{ap}}}{Z_{\mathrm{p}}} \tag{4}$$

where Z_{ap} and Z_{p} are the partition functions with antiperiodic and periodic boundary conditions, respectively.

In order to obtain the ratio of partition functions $Z_{\mathrm{ap}}/Z_{\mathrm{p}}$ we consider a system that allows both periodic and antiperiodic boundary conditions. The partition function of this system is given by

$$Z = \sum_{\mathrm{bc}} \prod_{i \in \Lambda} \int_{S_{N-1}} ds_i \exp[-KH(\mathbf{s}, \mathrm{bc})] \tag{5}$$

where K is the inverse temperature. The fraction of configurations with antiperiodic boundary conditions is given by the ratio Z_{ap}/Z,

$$\frac{Z_{\text{ap}}}{Z} = \frac{\prod_{i \in \Lambda} \int_{S_{N-1}} ds_i \exp[-KH(\mathbf{s}, \text{ap})]}{Z}$$

$$= \frac{\sum_{\text{bc}} \prod_{i \in \Lambda} \int_{S_{N-1}} ds_i \exp[-KH(\mathbf{s}, \text{bc})]\, \delta_{\text{bc, ap}}}{Z}$$

$$= \langle \delta_{\text{bc, ap}} \rangle \tag{6}$$

where $\delta_{\text{bc, ap}} = 1$ for antiperiodic boundary conditions and $\delta_{\text{bc, ap}} = 0$ for periodic boundary conditions. An analogous result can be found for periodic boundary conditions. Now we can express the ratio $Z_{\text{ap}}/Z_{\text{p}}$ as a ratio of observables in this system,

$$\frac{Z_{\text{ap}}}{Z_{\text{p}}} = \frac{Z_{\text{ap}}/Z}{Z_{\text{p}}/Z} = \frac{\langle \delta_{\text{bc, ap}} \rangle}{\langle \delta_{\text{bc, p}} \rangle} \tag{7}$$

and is hence accessible in a single Monte Carlo simulation.

3. BOUNDARY FLIP ALGORITHM FOR $O(N)$ MODELS

We shall now describe an efficient algorithm to update the system explained above, where the type of boundary condition is a random variable.[4, 5]

The algorithm is based on a standard cluster algorithm.[6, 7] For the Ising model it can be explained as follows. First the bonds are deleted with the standard probability

$$p_d = \exp[-K(|s_i s_j| + J_{\langle ij \rangle} s_i s_j)] \tag{8}$$

or otherwise frozen. After deleting or freezing the bounds of the system one searches for an interface of deleted bonds that completely cuts the lattice in the z direction. If there is such an interface, the spins between the bottom of the system and this interface and the sign of the coupling $J_{\langle ij \rangle}$ connecting top and bottom are flipped simultaneously. This is a valid update, since the bonds in the interface are deleted and the value of $J_{\langle ij \rangle} s_i s_j$ for i in the lowermost and j in the uppermost plane is not changed when we alter the sign of $J_{\langle ij \rangle}$ and s_i.

In order to apply this algorithm to $O(N)$ models, one has to consider each component of the spin as an embedded Ising variable. In the delete probability we just have to replace the Ising spins by a given component of the $O(N)$ spin.

Note that these embedded Ising models to not couple with each other. The above boundary flips can be done independently for any component.

The simplest approach would be to simulate an ensemble that contains also configurations which have different boundary conditions for the different components. However, we avoided these configurations with mixed boundary conditions. We only allowed a flip of the boundary condition when it could be done for all components simultaneously.

In our simulations we alternate this boundary-flip update with standard single-cluster updates.[7]

4. THE ANTIFERROMAGNETIC THREE-STATE POTTS MODEL AND ANTIPERIODIC BOUNDARY CONDITIONS

The three-state AF Potts model in three dimensions is defined by the partition function

$$Z = \prod_{l \in \Lambda} \sum_{\sigma_l = 1}^{3} \exp\left(-K \sum_{\langle i,j \rangle} \delta_{\sigma_i, \sigma_j} \right) \tag{9}$$

where the summation is taken over all nearest-neighbor pairs of sites i and j on a simple cubic lattice Λ, and $K = |J|/k_B T$ is the reduced inverse temperature.

One has to note that a change of the boundary interaction to negative sign is incompatible with the symmetries of the classical Hamiltonian. The change of the sign of J from minus to plus would mean that there is only one favorable value of the neighboring spin instead of two. Hence changes in the free energy would also arise from local distortion of the system. However, when one adds or removes one layer from the lattice, such that the extension in one direction, measured in units of lattice spacings, becomes an odd number, one obtains the global frustration we are aiming at. Hence we define ΔE of an L^3 system by

$$\Delta E(L, L, L) = \tfrac{1}{2}[E(L, L, L+1) + E(L, L, L-1)] - E(L, L, L) \tag{10}$$

where the energy E of the model is given by

$$E = \sum_{\langle i,j \rangle} \delta_{\sigma_i, \sigma_j} \tag{11}$$

We were not able to find an efficient algorithm that allows us to add or to remove a layer of sites from the lattice. Hence we had to rely on the standard integration method to obtain the corresponding ΔF for the Potts model, as opposed to the XY model.

5. NUMERICAL RESULTS

5.1. 3D *XY* Model

On lattices of the size $L=4$, 8, 16, 32, and 64 we performed simulations at $K_0=0.45420$, which is the estimate for the critical coupling obtained in ref. 14. As explained above, we performed single-cluster updates[7] in addition to the boundary updates. We have chosen the number N_0 of the single-cluster updates per boundary update such that N_0 times the average cluster volume is approximately equal to the lattice volume. We performed a measurement after each boundary update. The number of measurements was 100,000 for all lattice sizes.

First we determined the critical coupling K_c using the crossings of Z_{ap}/Z_p. For the extrapolation of $\langle \delta_{bc,\,ap} \rangle$ and $\langle \delta_{bc,\,p} \rangle$ to couplings K other than the simulation coupling K_0 we used the reweighting formula[15]

$$\langle \delta_{bc,\,x} \rangle(K) = \frac{\sum_i \delta_{bc(i),\,x} \exp[(-K+K_0) H_i]}{\sum_i \exp[(-K+K_0) H_i]} \tag{12}$$

where i labels the configurations generated according to the Boltzmann weight at K_0, bc(i) denotes the boundary condition of the ith configuration, and x has to be replaced by either p or ap. We computed the statistical errors from jackknife binning[16] applied to the ratio $\langle \delta_{bc,\,ap} \rangle / \langle \delta_{bc,\,p} \rangle$. The extrapolation gives good results only within a small neighborhood of the simulation coupling K_0. This range shrinks with increasing volume of the lattice. However, Fig. 1 shows that in a sufficiently large neighborhood of the crossings of Z_{ap}/Z_p the extrapolation performs well. The results for the crossings are $K=0.45439(22)$, 0.45412(10), 0.454138(31), and 0.454147(14) for $L=4$ and 8, 8 and 16, 16 and 32, and 32 and 64, respectively.

The convergence of the crossings of Z_{ap}/Z_p toward K_c is excellent. Even with the high statistical accuracy that we reached, all crossings starting from $L=4$ and $L=8$ are compatible within error bars. The convergence of the crossings is governed by

$$K_{cross}(L) = K_c(1 + \text{const} \cdot L^{-(\omega+1/\nu)} + \cdots) \tag{13}$$

where ω is the correction-to-scaling exponent.[2,17] We performed a two-parameter fit with $\nu=0.669$ and $\omega=0.780$[11] being fixed. Taking all crossings, we obtain $K_c=0.454142(13)$ and when discarding the $L=4$ and 8 crossing, we get $K_c=0.454148(15)$, where both times the correction term is compatible with zero. Note that we obtained $K_c=0.45420(2)$[14] (or reanalyzed $K_c=0.45419(2)$[13]) from the crossing of the fourth-order

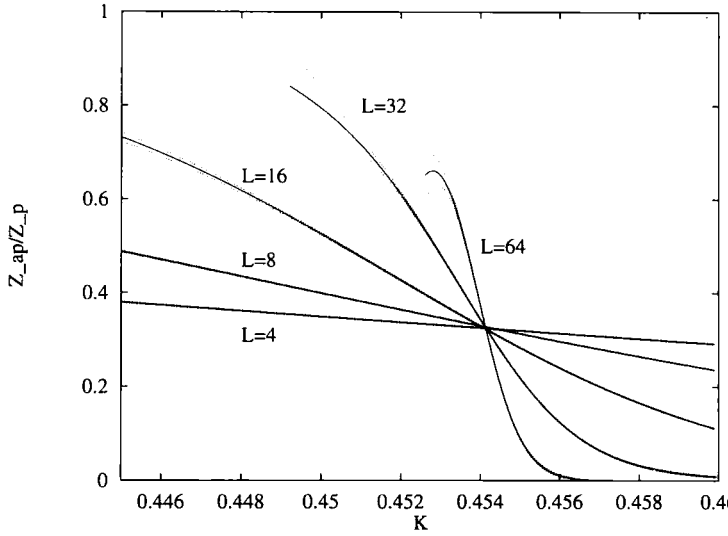

Fig. 1. The ratio Z_{ap}/Z_p for the 3D XY model on lattices of size $L=4$ up to $L=64$. The curves are obtained from simulations at $K=0.45420$ in combination with reweighting to couplings in the neighborhood. The dashed lines give the statistical errors obtained by a jackknife analysis.

cumulant. From the scaling behavior of the magnetic susceptibility in the high-temperature phase we obtained $K_c=0.45417(1)$.[14] All these estimates are consistent within two standard deviations.

At the critical coupling Z_{ap}/Z_p converges with increasing L like

$$\frac{Z_{ap}}{Z_p}(L)=\frac{Z_{ap}}{Z_p}(\infty)(1+\text{const}\cdot L^{-\omega}...) \tag{14}$$

In Table I we give the value of Z_{ap}/Z_p at our estimate of the critical coupling. The result is stable with increasing L. Hence we take the result for $L=64$, $Z_{ap}/Z_p=0.322(8)$, as our final estimate for the infinite-volume limit. Taking the logarithm, we obtain $\Delta F=1.13(2)$.

We extracted the critical exponent ν of the correlation length from the L dependence of the energy difference ΔE. The values for ΔE at the critical coupling are given in Table I. We performed fits according to Eq. (2) for the ΔE at the new estimate of the critical coupling and at the edges of the error bars. The results, which are summarized in Table II, are stable within error bars when we discard data with small L from the fit. We take the fit including the lattice sizes $L=16$, 32, and 64 as our final result $\nu=0.679(7)$, where the error due to the uncertainty in the critical coupling

Table I. Results of the Ratio Z_{ap}/Z_p and ΔE at the Critical Coupling $K_c = 0.45415(2)$[a]

L	Z_{ap}/Z_p	ΔE
4	0.3245(19)(1)	17.64(13)(1)
8	0.3242(19)(3)	52.18(41)(4)
16	0.3234(21)(9)	144.7(1.3)(3)
32	0.3224(20)(27)	407.0(4.6)(2.2)
64	0.3216(25)(72)	1113.0(13.0)(18.0)

[a] The number in the second parentheses gives the uncertainty due to the error bar of the critical coupling.

is taken into account. Performing a similar analysis at our old estimate for the critical coupling $K_c = 0.45419(2)$ leads to $\nu = 0.670(7)$, which is more consistent with the accurate value $\nu = 0.669(2)$[11] obtained from resummed perturbation theory.

5.2. 3D AF Three-State Potts Model

For the 3D AF three-state Potts model we computed ΔF by the integration method. At $K = 0$ the free energy is given by

$$F = V \ln 3 \tag{15}$$

Table II. Estimate of the Critical Exponent ν Obtained from the Fit of the Surface Energy Density Following Eq. (2) at $K_c = 0.45415(2)$[a]

	Estimates for ν from ΔE					
	$K_c - \Delta K_c$		K_c		$K_c + \Delta K_c$	
#	ν	G	ν	G	ν	G
0	0.6771(45)	1.80	0.6756(44)	0.78	0.6741(44)	0.77
1	0.6813(30)	0.96	0.6783(29)	0.53	0.6753(29)	0.32
2	0.6833(50)	1.67	0.6787(49)	1.05	0.6743(48)	0.57

[a] Here # gives the number of discarded data points with small L and G denotes χ^2/*degrees of freedom*.

where V is the number of lattice sites. Hence

$$\Delta F = \tfrac{1}{2}[F(L, L, L-1) + F(L, L, L+1)] - F(L, L, L) = 0 \qquad (16)$$

at $K = 0$. For $L = 4$ we measured ΔE at 83 different K values, starting at $K = 0.01$ going up in steps of $\Delta K = 0.01$ until we reached $K = 0.83$. In the large-L limit, ΔF stays 0 up to the critical point. Therefore we started the integration at a K such that we observed $\Delta E > 0$ within our statistical accuracy for the larger lattices. For $L = 8$ we measured ΔE at 67 different K values, starting at $K = 0.50$ going up in steps of $\Delta K = 0.005$ until we reached $K = 0.83$. And for $L = 16$ we measured ΔE at 52 different K values, starting at $K = 0.70$ going up in steps of $\Delta K = 0.0025$ until we reached $K = 0.83$.

All runs consisted of 10,000 measurements. Per measurement we performed such a number of single-cluster updates that the lattice volume was approximately covered by the average cluster volume. Then we performed the integration using the trapeze rule. The result is given in Fig. 2. The curves for $L = 4$ and $L = 8$ cross at $K = 0.8155(18)$ and the curves for $L = 8$ and $L = 16$ at $K = 0.8166(8)$, which is in good agreement with $K_c = 0.81563(3)$.[13] The values of ΔF at $K_c = 0.81563$ are summarized in Table III. Our statistical accuracy degrades with increasing lattice size.

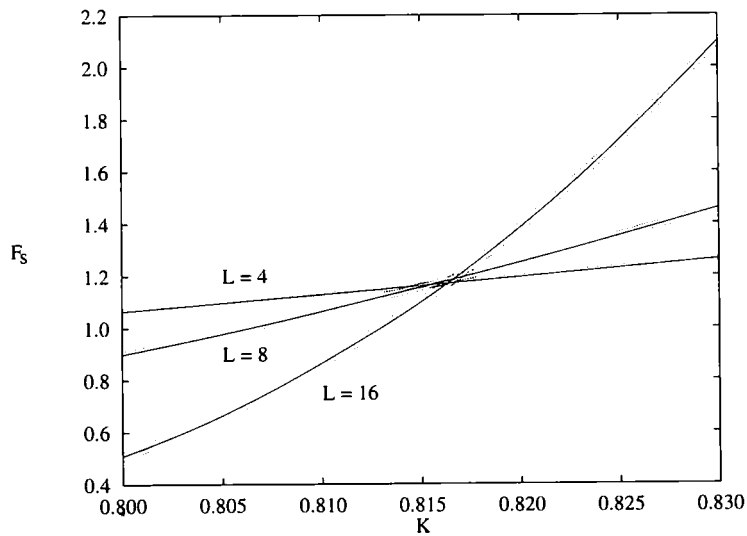

Fig. 2. The free energy difference ΔF for the 3D AF Potts model on lattices of size $L = 4$, 8, and 16. The curves are obtained from numerical integration of ΔE. The dashed lines give the statistical errors obtained by a jackknife analysis.

Table III. ΔF and ΔE for the 3D AF 3-State Potts Model at $K = 0.81563(3)$[a]

L	ΔF	ΔE
4	1.165(8)	6.68(2)
8	1.157(13)	19.10(9)(1)
16	1.130(20)	53.36(30)(6)
32		152.92(92)(48)
64		431.8(2.6)(3.7)

[a] The number in the second parentheses of ΔE gives the uncertainty due to the error bar of the critical coupling.

Hence we skipped the simulations of larger lattice sizes. However, already for the small lattices the results at $K_c = 0.81563$ are rather stable and systematic errors due to corrections to scaling should be small. The result $\Delta F = 1.13(2)$ for $L = 16$ at the critical point nicely agrees with our final result $\Delta F = 1.13(2)$ for the 3D XY model. One should note that for the 3D Ising model one obtains $\Delta F = 0.605(6)$,[5] which is only a little larger than half of the XY value.

At $K_c = 0.81563$ we simulated the $L \times L \times L - 1$ and $L \times L \times L + 1$ lattices for sizes up to $L = 64$ with a statistics of 100,000 measurements. For the cubical lattices we used the results of our previous study,[13] where 200,000 measurements were performed. The resulting ΔE are summarized in Table III. We performed fits according Eq. (2) for the ΔE at the critical coupling and at the edges of the error bars. The results are summarized in Table IV. The fits including all lattice sizes give an unacceptably large

Table IV. Results for the Critical Exponent ν Obtained from the Fit Following Eq. (2)[a]

	$K_c - \Delta K_c$		K_c		$K_c + \Delta K_c$	
#	ν	G	ν	G	ν	G
0	0.8988(49)	2528	0.9130(43)	3392	0.8598(42)	1903
1	0.6681(19)	1.21	0.6664(16)	1.92	0.6650(18)	1.73
2	0.6651(32)	1.10	0.6629(26)	1.04	0.6605(31)	0.45

[a] Here # denotes the number of discarded data points with small L, and G denotes χ^2/*degrees of freedom*.

χ^2/*degrees of freedom*, which in the following will be denoted as G. Discarding the $L=4$ data, we find that the value of G becomes acceptable, and when discarding also the $L=8$ data the result for ν remains stable within error bars. Hence we conclude that systematic errors due to corrections to scaling are smaller than our statistical errors. We take $\nu=0.663(4)$ from the fit including the lattice sizes $L=16$, 32, and 64 as our final result, where the error due to the uncertainty in the critical coupling is taken into account.

6. CONCLUSIONS

In the present work we have shown how the boundary algorithm of refs. 4 and 5 can be applied to $O(N)$ models with $N>1$. We demonstrated in the case of the 3D XY model that critical properties of the model can be nicely extracted from the ratio of the partition functions Z_{ap}/Z_p. The accuracy of the results for the critical coupling and the critical exponent of the correlation length ν are compatible with that obtained from the fourth-order cumulant.

We showed how antiperiodic boundary conditions can be implemented for the 3D AF Potts model. The value of the free energy difference $\Delta F=F_{ap}-F_p$ at the critical coupling is in good agreement with that found for the 3D XY model. The value $\nu=0.663(4)$ obtained from the scaling behavior of the energy difference ΔE at the critical coupling is as accurate as our previous estimate, which we obtained from the slope of the fourth-order cumulant. We conclude that those facts strongly support that the 3D AF three-state Potts model and the 3D XY model belong to the same universality class. The confirmation of the conjecture by Banavar *et al.* also has practical implications. The 3D AF three-state Potts model is simpler to simulate than the 3D XY model. The application of multispin-coding techniques, which have been used to speed up simulations of the Ising model,[18] might also allow further improvements of the 3D AF three-state Potts results.

For a detailed comparison with previous results see ref. 13.

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