KL-TH-94/8
CERN-TH.7290/94

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

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Abstract

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 in the free energies of a system with periodic and a system with antiperiodic boundary conditions in the neighbourhood 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.

KL-TH-94/8
CERN-TH.7290/94
June 1994

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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 interface free energy. In the case of $O(N)$-invariant vector models with $N \geq 2$, such as the XY model ($N = 2$) and the classical Heisenberg model ($N = 3$), however, the continuous symmetry of the model prevents the creation of a sharp interface and ΔF becomes rather 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 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 [4, 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, 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 "favourable" and "unfavourable" boundary conditions for the 3D AF 3-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], which is not consistent with the exponent $\nu = 0.669(2)$ [11] of the 3D 2-component $(\phi^2)^2$-theory. This result has to be compared with recent high-precision studies of the 3D AF 3-state Potts model [12, 13], where the XY exponents and critical amplitudes where recovered to high accuracy. To clarify this point we discuss how antiperiodic boundary conditions can be implemented for the 3D AF 3-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 neighbour plane of the lower-most plane. An analogous identification is done for the other two lattice directions. The $O(N)$ model is defined by the classical Hamiltonian

$$H(\vec{s}, bc) = -\sum_{<ij>} J_{<ij>} \vec{s}_i \cdot \vec{s}_j \ , \tag{3}$$

where $\vec{s}_i$ are unit-vectors with N components. When periodic (p) boundary conditions (bc) are employed, then $J_{<ij>} = 1$ for all nearest-neighbour pairs. When antiperiodic

(ap) boundary conditions are employed, then $J_{<ij>} = -1$ for bonds $< ij >$ connecting the lower-most and uppermost plane of the lattice, while all other nearest-neighbour pairs keep $J_{<ij>} = 1$. The free energy difference is now given by

$$\Delta F = F_{ap} - F_p = -\ln \frac{Z_{ap}}{Z_p}, \tag{4}$$

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_{ap}/Z_p we consider a system that allows both periodic and antiperiodic boundary conditions. The partition function of this system is given by

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

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

$$\begin{aligned} \frac{Z_{ap}}{Z} &= \frac{\prod_{i \in \Lambda} \int_{S_{N-1}} ds_i \exp(-KH(\vec{s}, ap))}{Z} \,, \\ &= \frac{\sum_{bc} \prod_{i \in \Lambda} \int_{S_{N-1}} ds_i \exp(-KH(\vec{s}, bc)) \delta_{bc,ap}}{Z} \,, \\ &= \langle \delta_{bc,ap} \rangle \,, \end{aligned} \tag{6}$$

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

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

which 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

$$p_d = \exp(-K(|s_i s_j| + J_{<ij>} s_i s_j)). \tag{8}$$

or else frozen. After deleting or freezing the bonds 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 $J_{<ij>}$ connecting top and bottom are flipped simultaneously. This is a valid update, since the bonds in the interface are deleted and the value of $J_{<ij>} s_i s_j$, for i in the lowermost and j in the uppermost plane, is not changed when we alter the sign of $J_{<i,j>}$ and s_i.

In order to apply this algorithm to $O(N)$ models, each component of the spin must be considered 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 do 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, with 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-neighbour 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 a 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 favourable value of the neighbouring spin instead of two. Hence changes in the free energy would also arise from a local distortion of the system. However, when one adds or removes one layer from the lattice, so 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

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

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 adds or removes 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 The 3D XY model

On lattices of 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 i^{th} configuration, and x must 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 neighbourhood of the simulation coupling K_0. This range shrinks with increasing volume of the lattice. However, fig. 1 shows that in a sufficiently large neighbourhood 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 towards 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

$$K_{cross}(L) = K_c\ (1 + const.L^{-(\omega+1/\nu)} + \ldots), \tag{13}$$

where ω is the correction to scaling exponent [2, 17]. We performed a two-parameter fit with fixed $\nu = 0.669$ and $\omega = 0.780$ [11]. 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 reanalysed $K_c = 0.45419(2)$ [13]) from the crossing of the fourth-order cumulant. From the scaling behaviour 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

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

In table 1 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

1. 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 2, are stable within the error bars, when we discard data with small L from the fit. We take as our final result the fit including the lattice sizes $L = 16, 32$, and 64, i.e. $\nu = 0.679(7)$, where the error due to the uncertainty in 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 $\nu = 0.669(2)$ obtained [11] from resummed perturbation theory.

5.2 The 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

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

where V is the number of lattice sites. Hence

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

at $K = 0$. For $L = 4$ we measured ΔE at 83 different values of K, starting at $K = 0.01$ and 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 values of K, starting at $K = 0.50$ and going up in steps of $\Delta K = 0.005$ until we reached $K = 0.83$. For $L = 16$ we measured ΔE at 52 different values of K, starting at $K = 0.70$ and 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 3. Our

statistical accuracy degrades with increasing lattice size. 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; 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 more than half 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 cubic lattices we used the results of our previous study [13], where 200 000 measurements had been performed. The resulting ΔE are summarized in table 3. We performed fits according to eq. (2) for the ΔE at the critical coupling and at the edges of the error bars. The results are summarized in table 4. The fit including all lattice sizes gives an unacceptably large $\chi^2/degrees\ of\ freedom$, which in the following will be denoted as G. Discarding the $L = 4$ data the value of G becomes acceptable, and when discarding also the $L = 8$ data the result for ν remains stable within the 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, 5] can be applied to $O(N)$ models with $N > 1$. We demonstrated, in the case of the 3D XY model, that its critical properties 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 behaviour 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 this strongly supports the fact that the 3D AF 3-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 3-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 3-state Potts results. A first attempt in this direction you can find in ref.[19].

For a detailed comparison with previous results, see [13].

Acknowledgements

We would like to thank D. Stauffer for many helpful suggestions.

The major part of the numerical simulations was performed on an IBM RISC 6000 cluster of the Regionales Hochschulrechenzentrum Kaiserslautern (RHRK). The simulations took about one CPU-month on an IBM RISC 6000-590 workstation.

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Figure 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 neighbourhood. The dashed lines give the statistical errors obtained by a Jackknife analysis.

Figure 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 1: Results of the ratio Z_{ap}/Z_p and ΔE at the critical coupling $K_c = 0.45415(2)$. The number in the second bracket gives the uncertainty due to the error bar of the critical coupling.

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.(13.)(18.)

Table 2: Estimates of the critical exponent ν obtained from the fit of the surface energy density following eq. (2) at $K_c = 0.45415(2)$. # gives the number of discarded data points with small L and G denotes $\chi^2/degrees\ of\ freedom$.

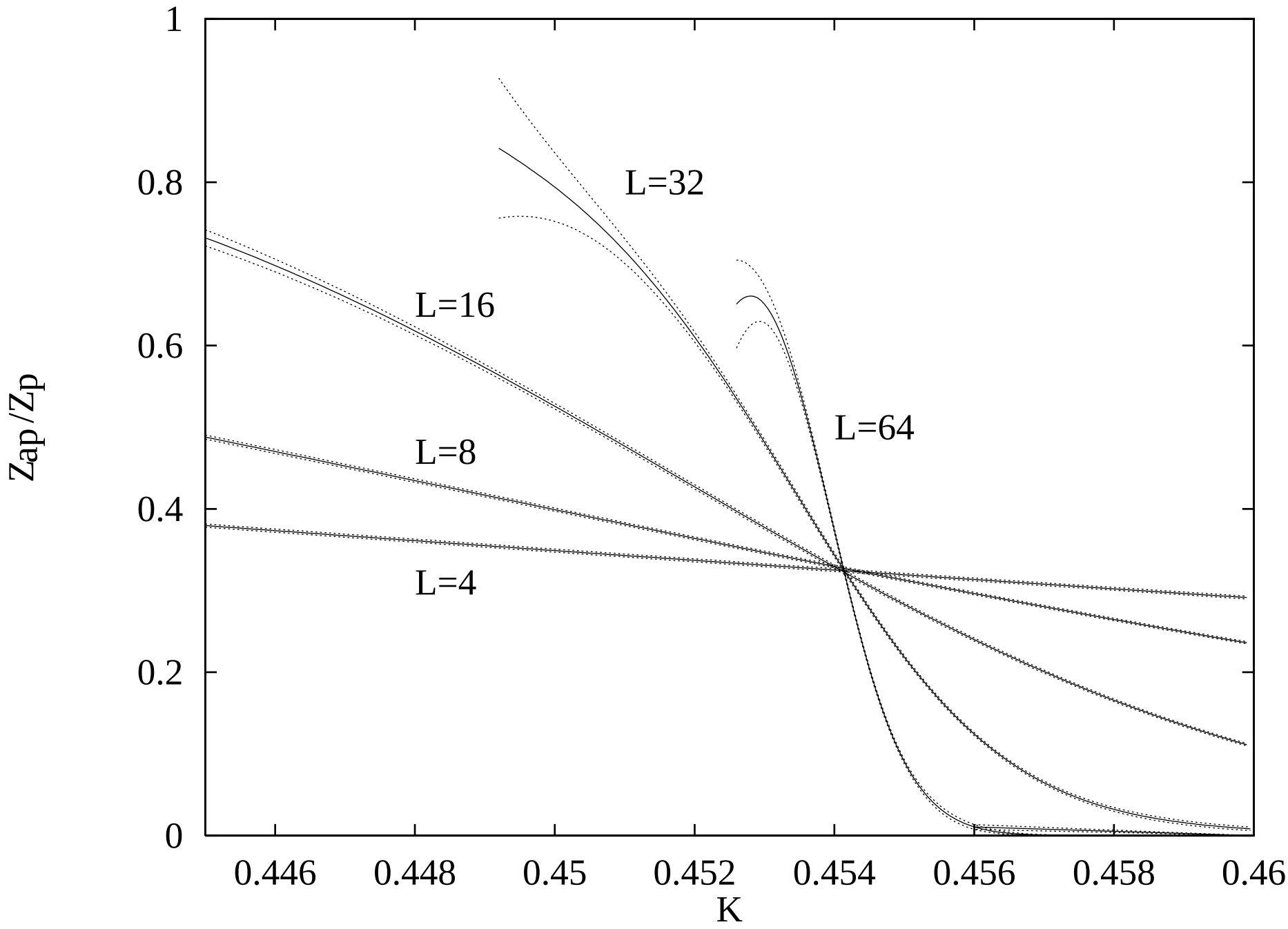
	$K_c - \Delta K_c$		K_c		$K_c + \Delta K_c$	
#	ν	G	ν	G	ν	G
0	0.6771(45)	1.80	0.6756(44)	0.78	0.6741(44)	0.77
1	0.6813(30)	0.96	0.6783(29)	0.53	0.6753(29)	0.32
2	0.6833(50)	1.67	0.6787(49)	1.05	0.6743(48)	0.57

Table 3: ΔF and ΔE for the 3D AF 3-state Potts model at $K = 0.81563(3)$. The number in the second bracket of ΔE gives the uncertainty due to the error bar of the critical coupling.

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)

Table 4: Results for the critical exponent ν obtained from the fit following eq. (2). # denotes the number of discarded data points with small L and G denotes $\chi^2/degrees\ of\ freedom$.

	$K_c - \Delta K_c$		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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Z_{ap}/Z_p
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L=16
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L=8
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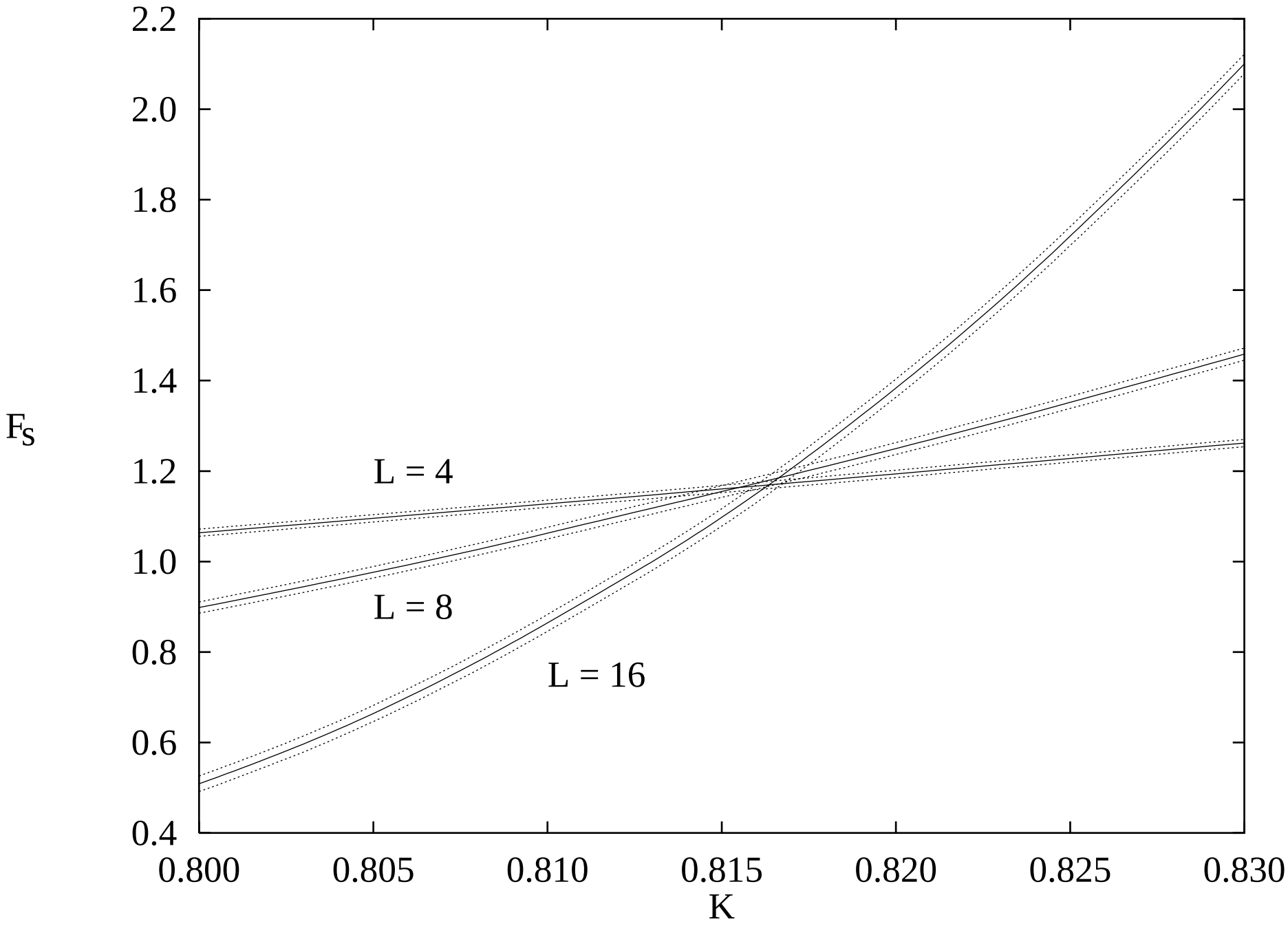
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