Critical behavior of the Ising model on the four-dimensional cubic lattice

P. H. Lundow*
Department of Theoretical Physics, KTH, SE-106 91 Stockholm, Sweden

K. Markström†
Department of Mathematics and Mathematical Statistics, Umeå University, SE-901 87 Umeå, Sweden
(Received 8 April 2009; published 3 September 2009)

In this paper we investigate the nature of the singularity of the Ising model of the four-dimensional cubic lattice. It is rigorously known that the specific heat has critical exponent $\alpha=0$ but a nonrigorous field-theory argument predicts an unbounded specific heat with a logarithmic singularity at T_c. We find that within the given accuracy the canonical ensemble data are consistent both with a logarithmic singularity and a bounded specific heat but that the microcanonical ensemble lends stronger support to a bounded specific heat. Our conclusion is that either much larger system sizes are needed for Monte Carlo studies of this model in four dimensions or the field-theory prediction of a logarithmic singularity is wrong.

DOI: 10.1103/PhysRevE.80.031104 PACS number(s): 05.50.+q, 12.38.Gc

I. INTRODUCTION

In dimension $D \geq 5$ it is known from [1,2] that the Ising model on the cubic lattice exhibits mean-field critical exponents at the critical temperature. Even earlier it was shown [3] that the specific heat obeys the mean-field exponent $\alpha=0$ for $D \geq 4$ and that for $D \geq 5$ the specific heat is in fact bounded at the critical point. For $D=4$ the rigorous results which determine that $\alpha=0$ are not strong enough to show that the specific heat is bounded. In fact methods from field and renormalization theory predict that the specific heat should diverge as $(\ln|T-T_c|)^{1/3}$, but this has not been possible to prove rigorously. There are thus, at least, two possibilities here, either the specific heat is bounded in $D=4$ as well or it diverges logarithmically.

Earlier studies of the critical behavior in four dimensions include [4–6] using Monte Carlo methods and [7] using series expansion and extrapolation. There has also been some recent controversy [8–10] regarding the consistency of field theoretical predictions and Monte Carlo data.

Using a standard Monte Carlo approach to detect a divergence of the form $(\ln|T-T_c|)^{1/3}$ is difficult since the quantity will remain quite small for a large range of the lattice size L, thereby making it difficult to use sampled data to clearly distinguish between different asymptotic behaviors.

In an attempt to get around this problem we have instead studied the microcanonical density of states of the model, following the methods used in, e.g., [11,12]. The finite-size effects of the canonical ensemble have two components; that coming from the fact that only a certain discrete set of energies are available in finite discrete systems and that coming from finite-size effects of the density of states. The microcanonical ensemble is affected by only the latter effect.

A divergence in the specific heat means that the second derivative of the density of states must become zero at the critical point. The surprising simulation result is that this value is in fact *increasing* with the lattice size at the critical point and the best fit to the data is that it converges to a nonzero value, thereby also giving a bounded specific heat in the limit.

In order to make sure that this was not an artifact caused by our simulation software we wrote two separate programs, one for the Metropolis algorithm and one using the Wolff-cluster algorithm [13], to sample at interleaving lattice sizes; but no systematic differences could be seen. We also tried to push the simulations to large lattices, reaching $L=80$. Our simulations give estimates for the critical exponents which agree well with the rigorous mean-field values and a value for the critical temperature which agrees well with earlier studies.

Hence our conclusion is that either lattice sizes larger than $L=80$ are needed to see the asymptotic behavior of the specific heat or the specific heat is in fact bounded at the critical point. Finding a way to settle this issue is of prime importance since, as discussed in, e.g., [10], this would have consequences for the renormalization techniques used to bound the Higgs mass.

II. NOTATION AND BASIC DEFINITIONS

The lattice studied here is the Cartesian graph product of four L cycles, that is, an $L\times L\times L\times L$-lattice with periodic boundary conditions on $n=L^4$ vertices and $m=4L^4$ edges. We have collected sampled data using the sampling scheme described in [11] for linear orders: $L=4,6,8,10,12,16,20,24,32,40,48,56,60,64,80$. For most orders we used the Metropolis single-spin-flip method with measurements of local energies after every sweep. Since the flip rate near the critical temperature is about 63% there will be no strong dependency between measurements of local energies. For comparison we also employed the Wolff-cluster method for the cases $L=10,20,40,60$, flipping clusters until an expected L^4 spins were flipped.

The energy E of a state $\sigma=(\sigma_1,\ldots,\sigma_n)$, with $\sigma_i=\pm 1$, is defined as $E(\sigma)=\Sigma_{\{i,j\}}\sigma_i\sigma_j$, with the sum taken over all the edges $\{i,j\}$, and the magnetization M is defined as

*phl@kth.se
†klas.markstrom@math.umu.se

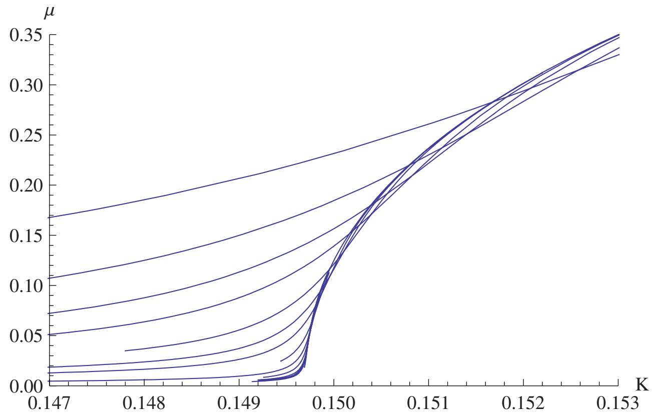

FIG. 1. (Color online) Magnetization $\bar{\mu}(K)$ for lattice sizes $L=6,8,10,12,16,20,24,32,40,48,56,60,64,80$.

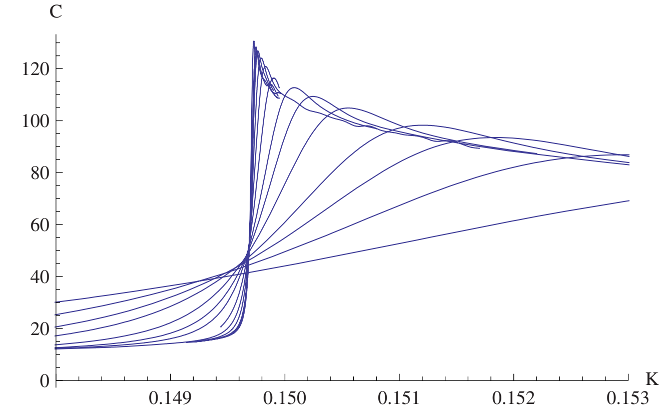

FIG. 2. (Color online) Specific heat $\mathcal{C}(K)$ for lattice sizes $L=6,8,10,12,16,20,24,32,40,48,56,60,64,80$.

$M(\sigma)=\Sigma_i\sigma_i$ with the sum taken over all the vertices.

We have two classes of quantities. First the combinatorial quantities from the microcanonical ensemble which depend on the energy U. Especially the coupling K is of interest here, defined as $K(U)=-\partial S/\partial U$ where $S(U)=[\ln a(E)]/n$ for $U=E/n$ and $a(E)$ denotes the number of states σ at energy E. How to obtain the coupling from sampled data is described in detail in [11] and error estimation in [14].

The canonical or physical quantities are obtained as cumulants, or derivatives of $\ln \mathcal{Z}(K,H)$ with respect to K or H (the external field), where $\mathcal{Z}$ is the partition function. All quantities are measured with the external field switched off, i.e., $H=0$ after the relevant derivative is taken.

At this point we introduce the notation $c_i=\langle(X-\langle X\rangle)^i\rangle$ for the ith central moment of a random variable X, where $\langle X\rangle$ is the mean value. The kth cumulant of E is then the kth derivative of $\ln \mathcal{Z}$ with respect to K, where $\mathcal{Z}$ is the partition function. Recall that the first cumulant is $\langle X\rangle$, the second is $c_2(X)=\mathrm{Var}(X)$, the third is $c_3(X)$ and the fourth is $c_4(X)-3c_2^2(X)$. The internal energy is then $\mathcal{U}(K)=\langle E\rangle/n$ and the specific heat is $\mathcal{C}(K)=\mathrm{Var}(E)/n$. Note also that the susceptibility $\chi=\mathrm{Var}(M)/n=\langle M^2\rangle/n$ has no local maximum, whereas the (spontaneous) susceptibility $\bar{\chi}=\mathrm{Var}(|M|)/n$ does. Analogously we define the magnetization as $\mu=\langle M\rangle/n$ and the spontaneous magnetization as $\bar{\mu}=\langle|M|\rangle/n$.

III. PHYSICAL QUANTITIES

Let us begin by showing some plots of a few physical quantities near the critical coupling. Figure 1 shows the magnetization $\bar{\mu}(K)$. In Fig. 2 we show the specific heat $\mathcal{C}(K)$ for several lattice sizes.

A. Critical points and exponents

First we establish a high-precision estimate of the critical coupling K_c. This is done by determining the critical points for a number of different quantities, listed below, for each system size. The critical points in question are, with one exception, the locations of various maxima or minima of, e.g., cumulants. To these points we fitted a simple scaling law of the form $c_0+c_1L^{-\lambda}$. By selecting points for $L\geq L_{\min}$ for different $L_{\min}$ we can then obtain several (for $L_{\min}=24,32,40$, with a few exceptions) different estimates of the fitting parameters. As a rule we received very good fits deeming a higher-order correction term unnecessary. The sought parameter is of course c_0. Taking the median of these gives a final estimate of K_c for that particular quantity. Repeating this for all quantities, a grand total of 15, allows us to make a statistical analysis of them. We have used the median as the estimate, with the first and third quartile as error estimates. In short, we take the median of the medians, very much like in [12].

The points scale very nicely with the linear order using only the simple expression above, see Fig. 3. The resulting estimate is $K_c=0.149\,694\,7\pm5\times10^{-7}$. This falls inside the by now rather old estimate $K_c=0.149\,65\pm5\times10^{-5}$ found in [15] and agrees with the estimate from [4].

The critical points in question are the locations of the following: the maximum of the specific heat $\mathcal{C}$ and susceptibility $\bar{\chi}$, maximum and minimum of the cumulants $c_3(E)/n$, $c_3(|M|)/n$, $[c_4(E)-3c_2(E)]/n$, and $[c_4(|M|)-3c_2^2(|M|)]/n$, maximum of $\partial\bar{\mu}/\partial K$, $\partial\ln\bar{\mu}/\partial K$, $\partial\ln\chi/\partial K$, and $\partial\mathcal{Q}/\partial K$, where $\mathcal{Q}$ is the Binder cumulant $1-\langle M^4\rangle/3\langle M^2\rangle^2$ and finally the crossing point between $\mathcal{Q}_L$ and $\mathcal{Q}_{L/2}$. See, e.g., [16] for a discussion of the last four quantities.

The expression above also provides us with estimates of the exponent ν. The location of a critical point K_L^* should

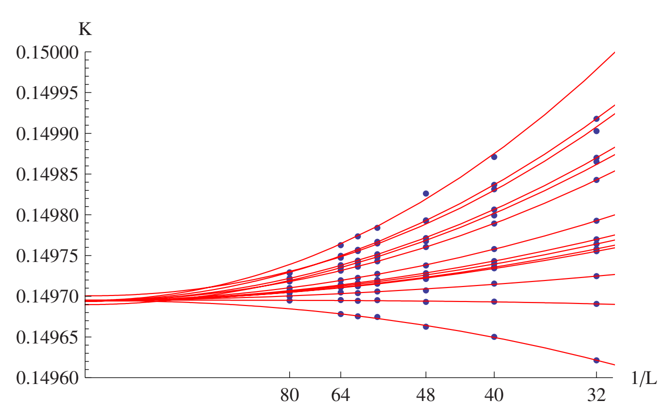

FIG. 3. (Color online) The critical points vs $1/L$ with fitted curves.

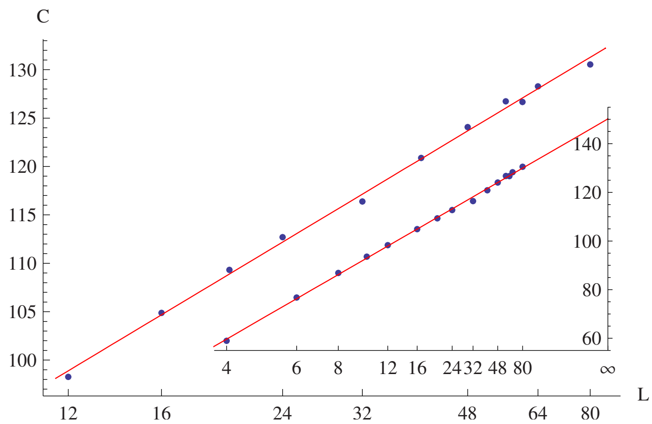

FIG. 4. (Color online) $\mathcal{C}_{max}$ vs $\sqrt[3]{\ln L}$ and $L^{-0.496}$ (inset) together with the fitted curves.

deviate from K_c as roughly $K_L^* - K_c \sim L^{-1/\nu}$, again see [16]. Repeating the median-of-the-medians approach gives $\lambda = 1/\nu = 2.00 \pm 0.03$ where the bounds are again based on the first and third quartiles, thus rendering us $\nu = 0.50 \pm 0.01$. The Josephson inequality tells us that $\alpha \geq 2 - D\nu$, and hence our midpoint estimate gives $\alpha \geq 0 \pm 0.04$ for $D=4$ since $\alpha = 0$ [3] our data are in good agreement with the rigorous results. Similarly an estimate of $\beta = 0.50$ is found, and the mean-field value is $\beta = \frac{1}{2}$.

Having established an estimate of K_c we can now estimate the internal energy $\mathcal{U}_L(K_c)$ and again fit the scaling formula above to these data for $L_{min} = 24, 32, 40$. The different c_0 and thus the asymptotic values of $\mathcal{U}_c$ end up inside the interval $0.770\,53 \pm 4 \times 10^{-5}$.

B. Critical values

Our aim is now to try to distinguish between the two possible scenarios, either we have a logarithmic singularity or the specific heat is bounded at T_c. We attempt to do this by making least-squares fits to the data for two different forms of the fitting function.

According to scaling theory, see [17], the maximum specific heat $\mathcal{C}_{max}$ is proportional to $\sqrt[3]{\ln L}$. For $L \geq 12$ this seems plausible given our data. In Fig. 4 we show $\mathcal{C}_{max}$ versus $\sqrt[3]{\ln L}$ together with a fitted straight line, $y = 115x - 56.7$, and indeed they line up rather convincingly. The reader should note that $\mathcal{C}_{max}$ grows very slowly indeed.

For the bounded scenario we try a fit where $\mathcal{C}_{max}$ is proportional to a power of L. A least-squares fit of both constant and exponent gives $150.49 + 180.5L^{-0.496}$. We show this in the inset of Fig. 4. The fact that the exponent is negative would of course mean that the specific heat is finite in the limit.

For both models there is some variation in the coefficients and the exponent if one makes the fit to different subsets of the data points but no drastic changes. An attempt with evaluating the specific heat and the susceptibility at the asymptotic K_c for each linear size instead gave a very similar behavior to that of their maximum value.

To the eye both fitting functions work reasonably well, and we simply find that the canonical ensemble data cannot strongly distinguish the two scenarios.

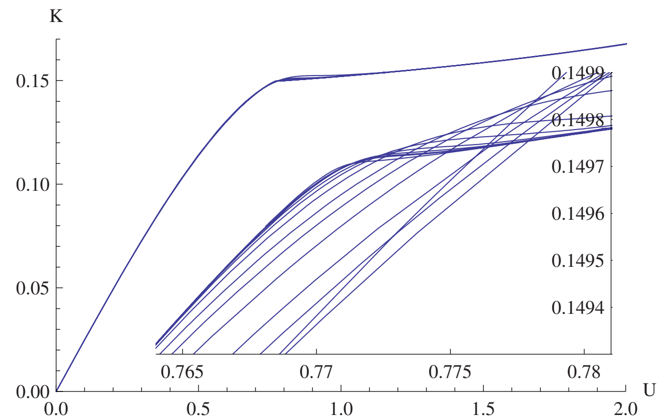

FIG. 5. (Color online) Coupling $K(U)$ for $L \geq 6$.

IV. COMBINATORIAL QUANTITIES

With regards to the microcanonical ensemble the two scenarios will be that either $K'(U)$ goes to 0 at U_c or it converges to a finite positive value

Figure 5 shows the microcanonical quantity $K(U)$ and in Fig. 6 its derivative is shown, both together with zoomed-in versions near the critical energy U_c. Most of the sampling was done for energies close to the critical one for the given value of L so the curves become noisier further away from U_c.

The minima do not at all seem to approach zero as they do for $d=2$ [18] and $d=3$ [12]. In fact the behavior here is qualitatively different in that the values are actually increasing rather than decreasing.

It is known, see, e.g., [11], that the specific heat corresponds to $1/K'(U)$. Thus $\lim_{U \to U_c} K'(U) = 0$ if and only if $\lim_{K \to K_c} \mathcal{C}(K) = \infty$. Figure 7 shows the minima versus $1/L$ together with a fitted line $y = 0.004\,19 - 0.0151x$, suggesting that the minimum approaches a maximum 0.004 19.

The optimal exponent of $1/L$, naturally, depends to some extent on which data points are used. Using a least-squares fit to different subsets of the data for $L \geq 6$ gives exponents between (roughly) 0.9 and 1.5. More specifically, if we check all subsets of the data with $L \geq 6$ on between 10 and 12 points a median exponent of 1.25 is received and for c_0 the median value was 0.004 06 with first and third quartiles

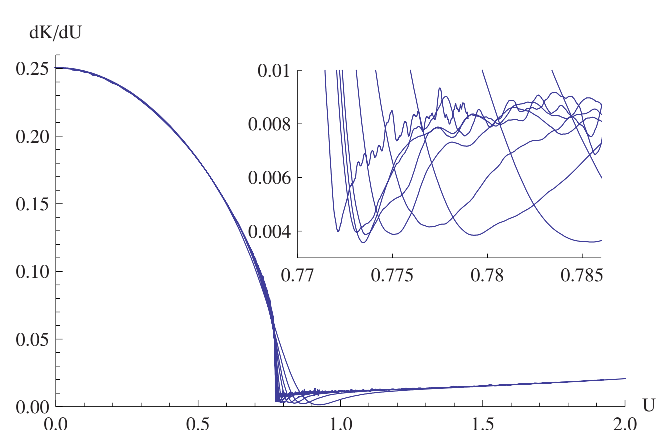

FIG. 6. (Color online) Coupling $K'(U)$ for $L \geq 6$.

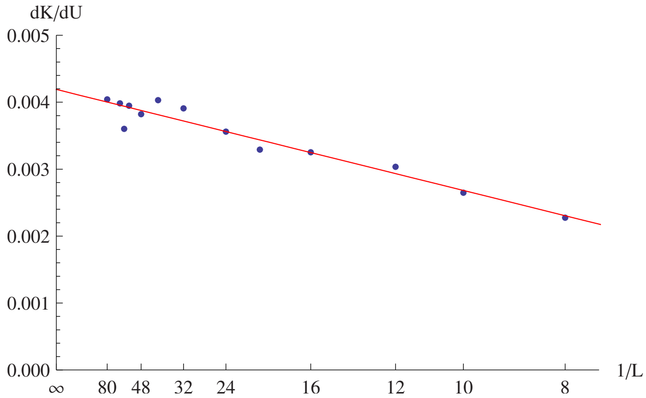

FIG. 7. (Color online) The minimum of $K'(U)$ vs $1/L$, together with the fitted curve.

0.004 02 and 0.004 13, respectively. The extremal values for c_0 are 0.0038 and 0.0044. If we instead use all the data points for $L\geq 8$ we obtain the exponent $\lambda=1.147$ and $c_0=0.004\,11$.

V. CONCLUSIONS

We have studied the two proposed scenarios for the critical behavior of the specific heat of the four-dimensional Ising model. This has been done in both the canonical and the microcanonical ensembles. We have found that for the given lattice sizes the canonical ensemble cannot conclusively distinguish between the two scenarios, and in an attempt to circumvent this we have instead turned to the microcanonical ensemble.

There are two reasons for why the microcanonical ensemble could give clearer results in this situation, the first predicted and the second unexpected. First, the canonical ensemble is expected to have larger finite-size effects than the microcanonical ensemble. To see this we may consider an idealized example where, for a finite system, $S(U)$ at each energy U is identical to the limit as $n\to\infty$. Here the density of states has no finite size effects at all, apart from only being defined at certain discrete set of values of U. However because of the discrete energies there will still be finite-size effects in the corresponding canonical ensemble.

Second, a divergent specific heat means that $K'(U)$ goes to 0 at U_c, and as we have found the minimum value of $K'(U)$ is actually increasing rather than decreasing. This gives us a qualitative signal, rather than a weak quantitative one, that the specific heat actually converges to a finite value.

Our conclusion is that either much larger systems are needed to see the asymptotic behavior of this model, and this possibility can only be ruled out by a rigorous convergence result or the specific heat is in fact bounded at U_c, thus contradicting the renormalization theory prediction.

ACKNOWLEDGMENTS

This work was conducted using the resources of High Performance Computing Center North (HPC2N) and the Center for Parallel Computers (PDC). Thanks are also due to the referees for their constructive criticisms.

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