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High precision single-cluster Monte Carlo measurement of the critical exponents of the classical 3D Heisenberg model *

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We report measurements of the critical exponents of the classical three-dimensional Heisenberg model on simple cubic lattices of size L^3 with $L = 12$, 16, 20, 24, 32, 40, and 48. The data was obtained from a few long single-cluster Monte Carlo simulations near the phase transition. We compute high precision estimates of the critical coupling K_c, Binder's parameter U^*, and the critical exponents $\nu, \beta/\nu, \eta$, and α/ν, using extensively histogram reweighting and optimization techniques that allow us to keep control over the statistical errors. Measurements of the autocorrelation time show the expected reduction of critical slowing down at the phase transition as compared to local update algorithms. This allows simulations on significantly larger lattices than in previous studies and consequently a better control over systematic errors in finite-size scaling analyses.

1. INTRODUCTION

The three-dimensional (3D) classical Heisenberg model is one of the simplest spin models, and its critical behavior has been investigated by a variety of approaches. Recently Peczak, Ferrenberg, and Landau [1] (PFL) have undertaken a high statistics Monte Carlo (MC) study of this model on cubic lattices of sizes up to $V = L^3 = 24^3$, using standard Metropolis and multi-histogram techniques [2]. They found a value of $K_c = 0.6929(1)$ that was in disagreement with previous estimates of the critical coupling $K_c = J/k_B T_c$. These estimates were derived from high-temperature series (HTS) expansion analyses [3] based on the Padé ($K_c = 0.6924(2)$) and ratio ($K_c = 0.6925(1)$) method, respectively, and more recent transfer-matrix (TM) MC investigations [4] ($K_c = 0.6922(2)$ and $K_c = 0.6925(3)$). The critical coupling is a non-universal parameter and from this point of view of no particular interest. Most estimates of universal critical exponents, however, are biased and usually depend quite strongly on the precise value of K_c. To clarify the above discrepancy we performed an independent high precision single-cluster MC study on large lattices of sizes up to 48^3. We could confirm PFL's value of K_c and obtained measurements of the critical exponents that are in their accuracy comparable to the best estimates coming from field theory.

2. MODEL AND ALGORITHM

The Metropolis (pseudo) dynamics suffers from the severe problem of critical slowing down, which is the reason why we used as update algorithm the cluster algorithm in its single-cluster version [5]. One update in the single-cluster variant consists of chosing a random mirror plane and a random starting site, which is the germ of a cluster whose members are selected from adjacent sites by a Metropolis-like accept/reject criterion. From studies of related spin models it is known [6] that this variant of the cluster algorithm is extremely efficient in three dimensions.

The classical Heisenberg model is defined by the Hamiltonian

$$\mathcal{H} = J \sum_{\langle i,j \rangle} [1 - \vec{s}_i \cdot \vec{s}_j] \qquad (1)$$

where J is the ferromagnetic coupling ($J > 0$). The sum runs over all nearest neighbour pairs $\langle i, j \rangle$, and $\vec{s}$ are three-dimensional unit spins that

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live on the sites i of a simple cubic lattice with periodic boundary conditions. The continuous energy range $0 \leq E \leq 3V$ was discretized into 90000 bins, which is fine enough to ensure no significant discretization errors. We stored histograms instead of the whole data time series in order to save storage space.

Our simulations were organized as follows. First, we did one run for each lattice size at $K_0 = 0.6929$, the estimate of K_c by PFL, and recorded the energy histogram $P_{K_0}(E)$ and the microcanonical averages $\langle\langle m^k \rangle\rangle(E) \equiv \sum_M P_{K_0}(E,M) m^k / P_{K_0}(E)$, $k = 1, 2, 4$, where $m \equiv M/V = |\vec{m}|$ is the magnetization $\vec{m} = \frac{1}{V}\sum_{\boldsymbol{x}} \vec{s}(\boldsymbol{x})$ of a single spin configuration. The temperature independent averages $\langle\langle m^k \rangle\rangle(E)$ can be computed by accumulating the values of m^k in lists indexed by the associated energy bin of the configuration and normalizing at the end by the total number of entries in each bin, making it thus unnecessary to store the two-dimensional histogram $P_{K_0}(E,M)$.

From the data of the K_0 run we could compute the approximate positions $K_+ > K_0$ and $K_- < K_0$ of the (connected) susceptibility and the specific-heat peak maximum by reweighting techniques [2]. We then performed two more runs at K_+ and K_-, respectively, again recording $P_K(E)$ and $\langle\langle m^k \rangle\rangle(E)$. This choice of the simulation points has the advantage that one automatically stays in the critical region since both K_+ and K_- scale with $L^{-1/\nu}$, where ν is the correlation length exponent. From this data we then computed three estimates $\mathcal{O}_L^{(n)}(K)$, $n = -, 0, +$ for all thermodynamic observables $\mathcal{O}_L$ of interest, and for any K value in the vicinity of K_-, K_0, K_+ by reweighting. The reweighting range was determined by the energy value at which the energy histogram had decreased to a third of its maximum. This ensured a high enough statistics of the histogram to allow the reweighting scheme to produce reliable results. Furthermore we used blocking to compute jackknife errors $\Delta\mathcal{O}_L^{(n)}$ on $\mathcal{O}_L^{(n)}$. To get an optimized average of these three values that minimizes the relative error of the combined $\mathcal{O}_L(K)$ for each observable separately, we added the $\mathcal{O}_L^{(n)}$ with relative weight $1/(\Delta\mathcal{O}_L^{(n)})^2$. All our runs contain at least $10000 \times \tau$ measurements, where τ is the integrated autocorrelation time of the susceptibility. The measured value of τ turned out to be almost independent of the lattice size and to be very small, $\tau < 2$, in units of lattice sweeps that allow direct comparison with the Metropolis algorithm. This is of course expected for the single-cluster update. For the 48^3 lattice we obtain a value of τ which is about three orders of magnitude smaller than for the Metropolis algorithm. This explains why we could study much larger lattice sizes than PFL, and could still afford to have about ten times better statistics.

3. RESULTS

To determine K_c we first concentrated on Binder's parameter

$$U_L(K) = 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2}. \tag{2}$$

Asymptotically for large L, all curves $U_L(K)$ should cross in the unique point (K_c, U^*). The locations of the crossing points of two different curves $U_L(K)$ and $U_{L'}(K)$ depend on the scale factor $b = L/L'$, due to residual corrections to finite-size scaling (FSS). From the crossings with the $L = 12$ and $L = 16$ curves we obtained six and five data points, respectively, whose linear fits shown in Fig. 1 gave us the result

$$K_c = 0.6930 \pm 0.0001, \tag{3}$$

and

$$U^* = 0.6217 \pm 0.0008. \tag{4}$$

The critical coupling is found in excellent agreement with the value quoted by PFL, and also U^* agrees very well with their estimate of 0.622(1). For comparison, a field theoretic ϵ-expansion predicts a 4% lower value of 0.59684... [7].

To obtain an estimate for the correlation length exponent ν we use that at K_c the derivatives dU_L/dK should scale asymptotically with $L^{1/\nu}$. To calculate dU_L/dK from our data, we took the thermodynamic derivative

$$\frac{dU_L}{dK} = (1-U)\left\{\langle E \rangle - 2\frac{\langle m^2 E \rangle}{\langle m^2 \rangle} + \frac{\langle m^4 E \rangle}{\langle m^4 \rangle}\right\}, \tag{5}$$

which is less vulnerable to systematic errors than a finite difference approximation scheme. In a log-log plot we find a perfect straight line fit (with goodness-of-fit parameter $Q = 0.61$ at $K_c = 0.6930$) that yields

$$\nu = 0.704 \pm 0.006. \quad (6)$$

This value is in good agreement with PFL's measurement of $\nu = 0.706(9)$ (determined by the same method, but at $K = 0.6929$), and with the field theoretic estimates derived from the resummed g-expansion [8] or from the resummed ϵ-expansion [9]; see Table 1. The high quality of this fit (as well as of all other fits described below) shows that the asymptotic scaling formula works down to our smallest lattice size $L = 12$, indicating that there is no need for confluent correction terms.

Having now measured ν we can get two more estimates for the critical coupling by assuming the FSS relation $T_{\max} = T_c + aL^{-1/\nu} + \ldots$ for the location of the maxima of the specific heat $C = V^{-1}K^2\left(\langle E^2\rangle - \langle E\rangle^2\right)$, and the connected susceptibility $\chi^c = VK\left(\langle m^2\rangle - \langle m\rangle^2\right)$. Using our value of $\nu = 0.704$ we obtain from the linear fits shown in Fig. 1 the estimates $K_c = 0.6925(9)$ (from $T_{C_{\max}}$ with $Q = 0.80$) and $K_c = 0.6930(3)$ (from $T_{\chi^c_{\max}}$ with $Q = 1.0$), respectively. These values are consistent with the crossing value (3), but have larger statistical errors.

The ratio of exponents β/ν follows from the scaling of the magnetization, $\langle m\rangle \propto L^{-\beta/\nu}$. From the linear least-square fit in a log-log plot of $\langle m\rangle$ versus L at $K_c = 0.6930$ we obtain the estimate

$$\beta/\nu = 0.514 \pm 0.001, \quad (7)$$

(with $Q = 0.68$) that is slightly lower than the value given by PFL, $\beta/\nu = 0.516(3)$ (determined at $K = 0.6929$). To test by how much our result is biased by the value of K_c we have redone our analysis at $K = 0.6929$ ($K = 0.6931$). Here we get the slightly higher (lower) value of 0.519(1) (0.509(1)). The quality of the fits, however, is much worse, namely $Q = 0.30$ ($Q = 0.31$), which we interpret as support for our estimate of K_c. We rely on the goodness-of-fit parameter since visually it is impossible to make a distinction between these fits when plotted on a natural scale.

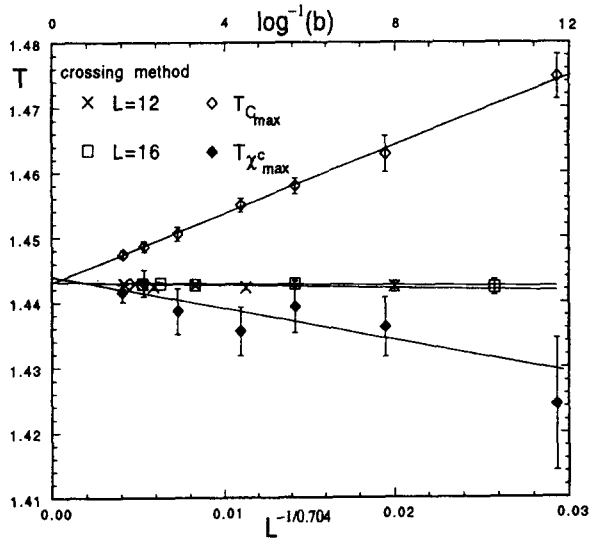

Figure 1. Estimates of the critical temperature T_c, coming from Binder's crossing method and from the scaling of $T_{C_{\max}}$ and $T_{\chi^c_{\max}}$.

It should be emphasized that even these slight variations in the estimate of the critical coupling significantly change the estimate of the exponent ratio in a way that clearly dominates the statistical errors, making it necessary to have an accurate estimate of K_c.

Relying on the scaling law $\eta = 2 - \gamma/\nu = 2\beta/\nu - 1$ we estimate

$$\eta = 0.028 \pm 0.002. \quad (8)$$

One can get independent estimates of η by direct measurements of $\chi = VK\langle m^2\rangle$ and χ^c at our best estimate of $K_c = 0.6930$, where they both should scale like $L^{2-\eta}$. From linear fits we obtained $\eta = 0.0271(17)$ ($Q = 0.78$) and $\eta = 0.0156(44)$ ($Q = 0.69$), respectively. Finally, analyzing the FSS behavior of the susceptibility maximum, $\chi^c_{\max} \propto L^{2-\eta}$, we estimate $\eta = 0.0231(61)$ ($Q = 0.60$). Notice that all MC estimates are lower than the field theory values, which are collected in Table 1.

Similarly, using the hyper-scaling law $\alpha/\nu = 2/\nu - 3$ we obtain for the specific-heat exponent

$$\alpha/\nu = -0.159 \pm 0.024. \quad (9)$$

Table 1
Selected sources for K_c, U^*, and the critical exponents of the classical 3D Heisenberg model.

method	K_c	U^*	ν	β/ν	η	α/ν
g-expansion [8]			0.705(3)	0.517(6)	0.033(4)	−0.163(12)
ϵ-expansion [7, 9]		0.59684	0.710(7)	0.518(11)	0.040(3)	−0.183(28)
HTS [11]	0.6929(1)		0.712(10)	0.513(50)	0.034(42)	−0.191(40)
MC [1]	0.6929(1)	0.622(1)	0.706(9)	0.516(3)	0.031(7)	−0.167(36)
MC (this work)	0.6930(1)	0.6217(8)	0.704(6)	0.514(1)	0.028(2)	−0.159(24)

Measurements of the specific heat are difficult to analyze directly, because α is negative, which implies a finite, cusp-like singularity. We tried a three-parameter fit of the form $C_{\max} = a - bL^{\alpha/\nu}$. The result $\alpha/\nu = -0.33(22)$ ($Q = 0.69$) is compatible with eq. (9), but has large statistical errors. Another way of testing eq. (9) is to assume the predicted value of α/ν and to fit only the parameters a and b. The resulting fit turned out to be of almost equally good quality [10].

To summarize, using the single-cluster MC update for the classical 3D Heisenberg model on simple cubic lattices of size up to 48^3, we obtained high-precision data. Using multi-histogram techniques we optimally combined the data and performed a fairly detailed FSS analysis. Qualitatively, our main result is that the asymptotic FSS region sets in for small lattices sizes, $L \approx 12$. Quantitatively, our value for the critical coupling, $K_c = 0.6930(1)$, is significantly higher than estimates from old HTS expansion analyses and TM MC methods, but is in almost perfect agreement with the MC estimate reported recently by PFL [1], with new analyses of longer HTS expansions [11], and with recent MC simulations in the high-temperature phase [12]. Our results for the two basic critical exponents, $\nu = 0.704(6)$ and $\beta = 0.362(4)$, are in good agreement with field theoretic predictions. Direct measurements of η give good agreement with the scaling prediction when the scaling of χ at K_c is considered. Using χ^c at K_c or $\chi^c_{\max}$, however, the situation is less clear. In the case of α/ν, its negative value causes numerical problems, which result in large statistical errors. Table 1 lists our measured values and their scaling implications for η and α/ν. For comparison, various other sources for the critical exponents are added. More details of this study can be found in refs. [10, 12].

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