Dynamic correlations in the three-dimensional Ising model

Robert B. Pearson
Physics Department, University of California, Irvine, California 92717

John L. Richardson
CHI Systems, 100 Burns Place, Goleta, California 93117

Doug Toussaint
Physics Department, University of California at San Diego, La Jolla, California 92093
(Received 17 December 1984)

We have used Monte Carlo simulation to measure the equilibrium correlation times for finite-sized Ising lattices at the bulk critical temperature. The measured value of the dynamic critical exponent z is 1.99 ± 0.02.

We have measured the equilibrium correlation times for the magnetization, energy, and magnetization squared in a Monte Carlo simulation of the three-dimensional Ising model. Our interest in these measurements is to explore the dynamics of this model, and in particular to measure the dynamical exponent z which describes the dependence of correlation time on correlation length.

To control the correlation length we use the idea of finite-size scaling[1,2] in its crudest form. The idea is that in a finite-size system the correlation length is limited by the size of the system, and if we simulate finite-sized lattices at the critical temperature of the bulk system we will see behavior corresponding to a correlation length proportional to the lattice size. The extension of this idea to dynamic critical phenomena was made by Suzuki,[3] and basically states that the time scale for a finite lattice is the time scale for a bulk system with correlation length proportional to L.

The dynamics in this model is defined by our Monte Carlo updating method. To be specific, we are doing a "heat-bath" Monte Carlo updating of the Ising spins, moving sequentially along the rows of the lattices. Actually, we have sixteen "updating machines" spread out through the lattice, each moving along rows. Our lattices have skewed boundary conditions, so when an updating machine goes off the end of one row in the x direction it begins immediately on the row displaced by one in the y direction. This particular choice of updating algorithm is dictated by the hardwired logic in the special purpose processor used for the simulations.[4] The measured correlation times will depend on the updating algorithm and hence cannot be directly compared to other Monte Carlo measurements using different updating algorithms.[5,7] However, we expect the dynamical exponent to be universal and hence independent of the updating algorithm. Henceforth, when we speak of time we mean the number of Monte Carlo sweeps using this particular algorithm.

To measure the dynamical exponent we make measurements of the correlation times on different size lattices at the bulk critical temperature. We use the critical temperature obtained in our earlier study of the static properties of the Ising model,

$$K_c = 1/T_c = 0.221\,650 \pm 0.000\,005$$

(Ref. 8). We do expect the correlation times to be sensitive to errors in our estimate of K_c. For this reason we have not used the largest lattices possible in our machine, instead reserving them for determining K_c. To check on the sensitivity of our results to errors in the determination of K_c we made some measurements on a 64^3 lattice at $K=0.221\,660$. (We expect the dependence on K to increase rapidly with size, so it suffices to check only the largest lattice used.) In Ref. 7 we found that corrections to finite-size scaling behavior are small for lattices larger than 24^3, so we have used 24^3, 40^3, and 64^3 lattices in this work.

The quantity we study is the autocorrelation function

$$C_Q(t) = \frac{\langle Q(0)Q(t)\rangle - \langle Q(0)\rangle^2}{\langle Q^2(0)\rangle - \langle Q(0)\rangle^2}\ , \tag{1}$$

where Q is some measurable quantity and t is the time separating two measurements. In our measurements we measured $C_Q(t)$ by taking blocks of 10 000 measurements. Each of these measurements was separated by 250 sweeps in the cases of the 40^3 and 64^3 lattices, and by 100 sweeps in the case of the 24^3 lattices. Thus each block contained 2 500 000 or 1 000 000 sweeps, depending on lattice size. Before each block of measurements we made 100 000 warmup sweeps to bring the lattice to equilibrium. The experimental data consisted of 143 such blocks of 64^3 data, 87 blocks of 40^3 data, and 246 blocks of 24^3 data. In addition there were 43 blocks of 64^3 data taken at $K=0.22\,166$. Within each block we then approximated $C(t)$ by

$$C_j = \frac{1}{D_1 D_2}\left[\frac{1}{N-j}\sum_{i=1}^{N-j} Q_i Q_{i+j} - \frac{1}{(N-j)^2}\sum_{i=1}^{N-j} Q_i \sum_{i=j+1}^{N} Q_i\right] \tag{2}$$

where

$$D_1=\left[\frac{1}{N-j}\sum_{i=1}^{N-j}Q_i^2-\frac{1}{(N-j)^2}\left[\sum_{i=1}^{N-j}Q_i\right]^2\right]^{1/2}, \quad (3)$$

$$D_2=\left[\frac{1}{N-j}\sum_{i=j+1}^{n}Q_i^2-\frac{1}{(N-j)^2}\left[\sum_{i=j+1}^{N}Q_i\right]^2\right]^{1/2}.$$

In this expression t is $250\times j$ or $100\times j$ depending on the lattice size. This somewhat forbidding expression has a simple interpretation: Let the vector $\bar{v}_1$ be the first N-j elements of the N consecutive measurements and let $\bar{v}_2$ be the last N-j measurements. Subtract the average of the elements of $\bar{v}_1$ from each element of $\bar{v}_1$, and similarly for $\bar{v}_2$. Then normalize each vector, and take the dot product, or the cosine of the angle between them. Thus C_j is kinematically restricted to lie between -1 and 1.

Although the data blocks are many correlation times long, there is a small but systematic error introduced because the $\langle Q(0)\rangle$ subtracted in Eq. (1) should be the true expectation value, rather than the average of our sample of data. In the case of the magnetization correlations this is not a problem because we know the expectation value of the magnetization exactly—it is zero on a finite lattice. (We, of course, check that the sample average is consistent with zero.) If we had used the sample mean for each block rather than zero for the expectation value of the magnetization, we would have measured a magnetization correlation time 1% too small for the 64^3 lattice. Since the energy and magnetization squared correlation times are about 0.15 times the magnetization correlation time while the runs contain the same number of sweeps, the systematic error will be much smaller for these measurements.

We measured the autocorrelation functions for the total magnetization of the finite-sized lattice, the total energy of the lattice, and the square of the total magnetization. The magnetization autocorrelation function $C(t)$ for the 64^3 lattice is shown in Fig. 1, and the energy and magnetization squared autocorrelation functions are displayed in Fig. 2. The error bars represent estimates of the error on each single point. The different points are not statistically independent; in fact, their correlation is almost unity. Therefore the points lie on a much smoother curve than would be expected from the size of the statistical errors.

We expect that for asymptotically large times these correlation functions will fall off as

$$C(t)=Ae^{-\Gamma t}, \quad (4)$$

where the correlation time τ is $1/\Gamma$. It can be seen from Figs. 1 and 2 that this is a good approximation. To extract the rate Γ we measure the logarithmic derivative of the correlation functions; that is, if we look at two times t_1 and t_2,

$$\Gamma=\frac{\ln[C(t_2)]-\ln[C(t_1)]}{t_1-t_2}. \quad (5)$$

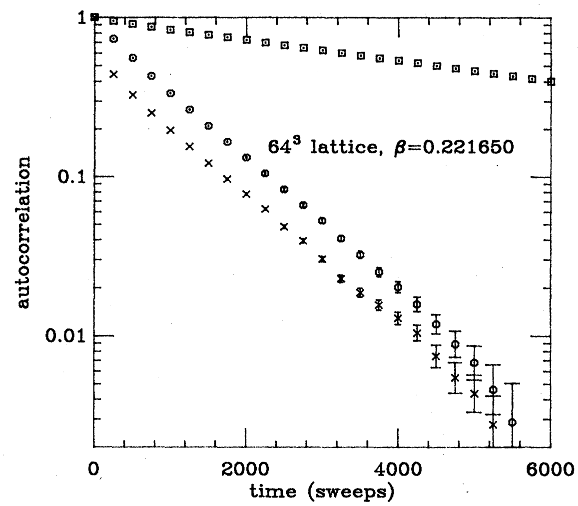

FIG. 2. Energy autocorrelation function (crosses) and the magnetization squared autocorrelation function (octagons) on the 64^3 lattice. The magnetization autocorrelation function is also shown (squares) to emphasize its different decay rate.

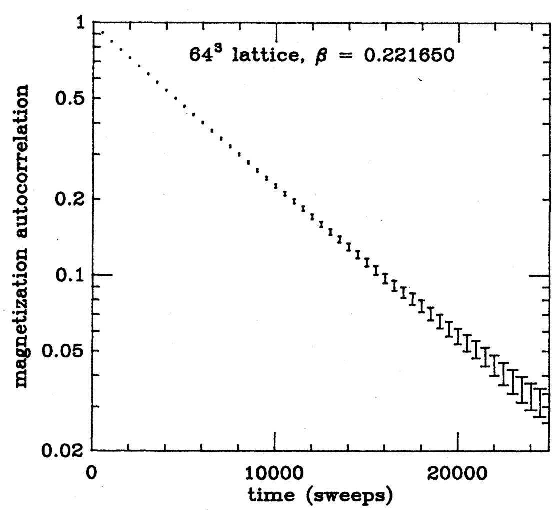

FIG. 1. Magnetization autocorrelation function on a 64^3 lattice at the bulk critical temperature. The y axis is logarithmic.

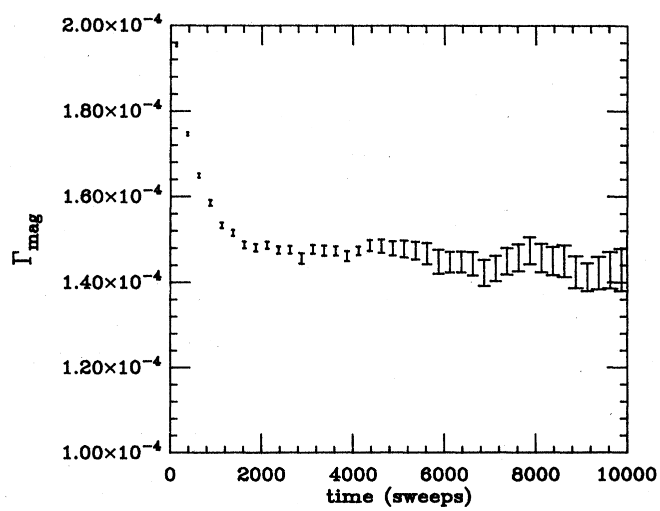

FIG. 3. Decay rate for the 64^3 autocorrelation function, computed as described in the text using $\Delta t=250$.

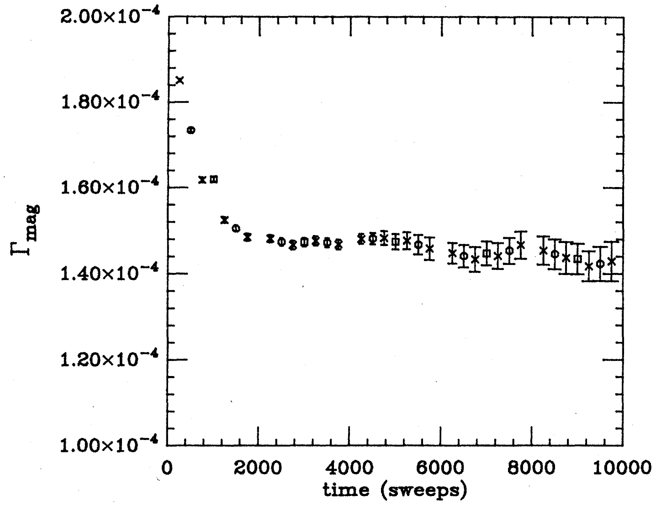

FIG. 4. Same decay rate, using $\Delta t=500$ (crosses), $\Delta t=1000$ (octagons), and $\Delta t=2000$ (squares). Note the near independence of the sizes of the error bars on Δt.

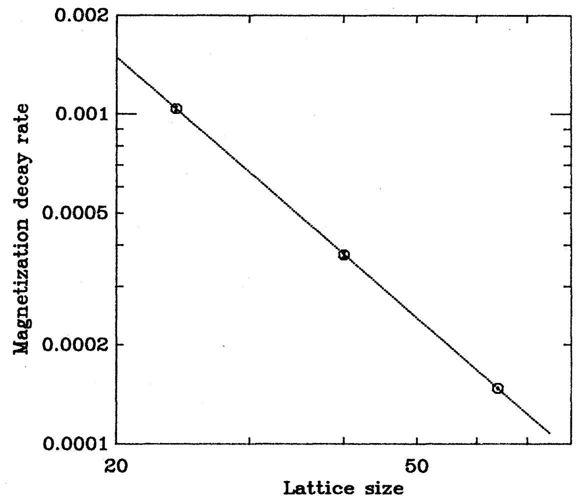

FIG. 5. Magnetization decay rates for the 24^3, 40^3, and 64^3 lattices, together with the least-squares fit. The error bars are visible inside the octagons marking each point.

In Fig. 3 we show the Γ extracted from the magnetization autocorrelation function on a 64^3 lattice. In this case we used the difference between successive measurements, or $t_1-t_2=250$ sweeps. The decay time measured in this way clearly has large corrections for small time, then levels off, then becomes lost in statistical errors for very large time. We must therefore estimate Γ from the portion of the figure where the measurements appear to have leveled off but the errors are not yet large.

The error bars in Fig. 3 were obtained by the following procedure. Take the 143 measurements of the correlation (recall that each of these measurements covered 2 500 000 sweeps) and average them in groups of 10 or 11 blocks, thus producing 14 partial averages. Then extract Γ from each partial average, and use the standard deviation of the mean of this set as the error estimate. The values of Γ itself were obtained by averaging all the correlation measurements for each time and then extracting Γ from this grand average.

It might be expected that the statistical fluctuations in the measurements of Γ are large because Γ involves a small difference between $C(t_1)$ and $C(t_2)$, and that the statistical error could be reduced by taking t_2-t_1 larger. Empirically this proves not to be true. If the fluctuations in the decay rate were uncorrelated from one 250 sweep time step to the next, doubling the size of Δt would cut the statistical error on Γ by a factor of 2. In fact the statistical error obtained by using $\Delta t=500$, 1000, or 2000 are almost the same as the errors obtained by using $\Delta t=250$, as can be seen in Fig. 4. This tells us that the evolution of the magnetization in one 250 sweep interval is correlated with the evolution in the next 250 sweep interval in the sense that if the magnetization changes rapidly in one interval it is likely to change rapidly in the next, while if it is almost steady in one interval it is likely to be steady in the next. In other words we suppose that the time history of an individual lattice is characterized by periods when the magnetization is almost constant separated by periods when the magnetization evolves relatively rapidly. The above periods would have to be long compared to 250 sweeps. We do not have any direct evidence for this picture, only the unexpected behavior of the statistics of our correlation measurements. Unfortunately, this results in measurements of the correlation time that are not nearly as accurate as we had hoped.

To estimate Γ from Fig. 3 we observe that the rate appears to have leveled off around $t=3000$. We therefore choose the value for Γ using $t_1=2000$ and $t_2=5000$, which is $\Gamma_{\text{mag}}=1.476\times10^{-4}\pm9.6\times10^{-7}$. The error estimate here comes from the previously described procedure of making several estimates of the decay rate from subsets of the sample and taking the standard deviation of the mean of these estimates. Similar estimates were made for the energy and squared magnetization, and for the other lattice sizes. These estimates are tabulated in Table I.

TABLE I. Autocorrelation decay rates.

Size	Γ_{mag}	Γ_{energy}	Γ_{mag^2}
24	0.001 039 ±0.000 017	0.007 13 ±0.000 20	0.007 15 ±0.000 11
40	0.000 374 1±0.000 007 6	0.002 590±0.000 044	0.002 436±0.000 015
64	0.000 147 6±0.000 001 0	0.000 921±0.000 030	0.000 920±0.000 020
64	0.000 144 7±0.000 001 2	(at $K=0.221\,166$)	

The two "even operators," energy and squared magnetization, have the same correlation times, which are about 0.15 times the correlation time for the "odd" magnetization.

The dynamic critical exponent z is defined by $\tau = C\xi^z$, where ξ is the correlation length. At the critical temperature we expect that the effective ξ which controls the physics should be proportional to the lattice size. Therefore z can be estimated by the slope in a fit of $\ln(\Gamma) = \text{const} - z \ln(L)$. If we make a least-squares fit of this form to the magnetization decay rates for the three lattice sizes, we find $z = 1.99 \pm 0.02$, and since the other decay rates are proportional to the magnetization decay rate the same exponent applies. This critical exponent is lower than the Monte Carlo estimates in Ref. 5, $z = 2.08$, and Ref. 6, $z = 2.11 \pm 0.03$, but is closer to an earlier estimate from ϵ expansions,[9] $z = 2.02$. The three data points for the magnetization decay rate, together with the fitted form, are shown in Fig. 5. It can be seen that the fit is very good, with a χ^2 of 0.05 for one degree of freedom. The sensitivity of this exponent to the value of K_c can be estimated by recomputing the fit using the decay rate measured at $K = 0.221\,660$ on the 64^3 lattice. This gives an overestimate of the effect, since the 24^3 and 40^3 decay rates would also decrease, although to a lesser extent. If we were to use this value for the 64^3 decay rate, the fit for z would be 2.01 ± 0.02. Recall that our earlier measurement of K_c was $0.221\,650 \pm 0.000\,005$. A recent estimate from high-temperature series is $K_c = 0.221\,655 \pm 0.000\,005$,[10] while another Monte Carlo study gave $K_c = 0.221\,654 \pm 0.000\,006$.[11]

ACKNOWLEDGMENTS

This work was supported by NSF Grant No. PHY77-27084, supplemented by funds from NASA, NSF Grant No. DMR80-01492, and DOE Grant No. DEAT03-81ER40029. We would like to thank Michael Barber for reading the manuscript.

[1]M. E. Fisher, in *Critical Phenomena, Proceedings of the 51st Enrico Fermi Summer School, Varenna, Italy,* edited by M. S. Green (Academic, New York, 1971).

[2]For a recent review, see M. N. Barber, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. L. Lebowitz (Academic, New York, 1983).

[3]M. Suzuki, Prog. Theor. Phys. **58**, 1142 (1977), or see Sec. V.G. of Ref. 2.

[4]R. B. Pearson, J. L. Richardson, and D. Toussaint, J. Comp. Phys. **51**, 241 (1983).

[5]M. C. Yalabik and J. D. Gunton, Phys. Rev. B **25**, 534 (1982).

[6]B. K. Chakrabarti, H. G. Baumgärtel, and D. Stauffer, Z. Phys. B **44**, 333 (1981).

[7]J. C. Angles d'Auriac, R. Maynard, R. Rammal, J. Stat. Phys. **28**, 307 (1982).

[8]M. N. Barber, R. B. Pearson, J. L. Richardson, and D. Toussaint, Phys. Rev. B (to be published).

[9]C. De Dominicis, E. Brezin, and J. Zinn-Justin, Phys. Rev. B **12**, 4945 (1975).

[10]J. Adler, J. Phys. A **16**, 3585 (1983).

[11]G. Pawley, R. H. Swendsen, D. J. Wallace, and K. G. Wilson, Phys. Rev. B **29**, 4030 (1984).