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MONTE CARLO STUDIES OF DYNAMIC CRITICAL PHENOMENA

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Abstract. We review the current state of knowledge of dynamic critical phenomena in simple magnetic models and present high statistics Monte Carlo data for critical slowing down in Ising and Potts models in two and three dimensions. By fitting the relaxation functions to multi-exponential decays at the critical temperature and applying finite size scaling we are able to extract very accurate estimates for the dynamical critical exponent $z$. Our results are compared with previous numerical estimates and with the predictions of renormalization group theory.

1. Introduction

During the past several decades there has been an enormous improvement in our understanding of static critical phenomena including not only the development of the concept of universality but also the appearance of very accurate numerical results for specific critical exponents for different models. In contrast, although certain basis ideas have been formulated about dynamic critical behavior [1], progress in obtaining accurate values for the dynamic exponent $z$ has been very slow. As the critical point $T_c$ is approached, the characteristic relaxation time $\tau$ is expected to diverge as

$$\tau \sim \xi^z$$

(1)

where $\xi$ is the correlation length and $z$ is the dynamic critical exponent. Expressed in terms of the reduced distance from $T_c$ equation (1) becomes

$$\tau \sim |1 - T / T_c|^\Delta$$

(2)

with $\Delta = z \nu$ where $\nu$ is the exponent which describes the divergence of $\xi$. Interest in obtaining precise numerical estimates for $z$ has been increasing and such estimates should lead to an understanding of dynamic universality classes.

In this paper we shall limit ourselves to one of the simplest, but still unsolved, cases of models with relaxational time dependent behavior with no conserved quantities (model A in the nomenclature of Ref. [1]). Here we shall consider $q$-state Potts models [2] with Hamiltonian

$$\mathcal{H} = -J \sum_{nn} \delta_{\sigma_i \sigma_j}, \quad \sigma_i = 1, 2, ..., q$$

(3)

for which the Ising model is the special case of $q = 2$.

At the upper and lower critical dimensions for the kinetic Ising model ($d = 4$ and $d = 1$, respectively) $z = 2$ and for intermediate dimension a Padé estimate suggests that $(z - 2)$ is always positive [3]. As table I shows, however, some numerical results suggest that $z = 2$.

Table I. Survey of estimates for the dynamic exponent $z$ for $q$-state Potts models in two dimensions.

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<td>2.19</td>
</tr>
</tbody>
</table>

(*) This work "best estimates".

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2 Present Address: Kontron Elektronik, 8057 Eching, F.R.G.
z < 2. (Numerical work on the Ising model prior to 1981 is reviewed in Ref. [26]; a wide range of exponent estimates are quoted ranging from 1.4 to 2.22.) In many studies, including the most recent ones, small error bars are given and many results obtained by different authors differ by far more than allowed by the quoted errors.

A second important question is that of dynamic universality. Existing numerical data and theory suggest that for \( d = 2 \), \( z \) may vary strongly with \( q \)-value. (In three dimensions there appear to be first order transitions for \( q > 2 \) and hence no critical slowing down.) The goal of our work has been to extract higher precision estimates for \( z \) than currently exist to resolve current discrepancy between various numerical results and theory.

2. Method

The kinetic evolution of these models is governed by a master equation for the probability function \( P(\{\sigma\};t) \) which gives the probability that a spin configuration \( \{\sigma\} \) occurs at time \( t \):

\[
\frac{\partial P(\{\sigma\}; t)}{\partial t} = \sum_{\{\sigma\}'} \left[ P(\{\sigma\}'; t) W(\{\sigma\} \to \{\sigma\}') - P(\{\sigma\}; t) W(\{\sigma\} \to \{\sigma\}') \right]
\]

\( W(\{\sigma\}' \to \{\sigma\}) \) is the transition probability per unit time that the system undergoes a transition from state \( \{\sigma\} \) to state \( \{\sigma\}' \). The solution to the discretized master equation is a Markov chain of states produced using a transition rate which satisfies the condition

\[
\frac{W(\{\sigma\} \to \{\sigma\}' )}{W(\{\sigma\} \to \{\sigma\} )} = \exp(-\Delta H / kT).
\]

Our Monte Carlo simulation generates successive spin configurations using “sublattice decompositions” in which entire sublattices composed of mutually non-interacting sites are updated in a single vector loop. For the Potts models, we used a checkerboard decomposition with a memory-to-register swapping technique to increase the speed. For the \( d = 3 \) Ising model a special multispin coding technique was developed which produced as many as \( 4 \times 10^7 \) spin-flip trials per second. In all cases, fully periodic boundary conditions were used. All computations were carried out on the Cyber 205 at the University of Georgia. The kinetic behavior was extracted from the decay of the time-displaced correlation function \( \phi(t) \) where for the magnetization

\[
\phi(t) = \frac{1}{t_{\text{max}} - t} \sum_{t'=0}^{t_{\text{max}}-t} \frac{m(t + t') m(t') - \langle m \rangle^2}{\langle m^2 \rangle - \langle m \rangle^2}
\]

where \( m(t) \) is the magnetization at time \( t \).

A suitable number of MCS/site were first discarded to ensure that equilibrium was reached before data were retained for analysis. Typically \( 2.3 \times 10^6 \) MCS/site were retained for the averages for \( d = 2 \) Potts models and between \( 3 \times 10^6 \) and \( 20 \times 10^6 \) MCS/site were used for the \( d = 3 \) Ising model.

The time dependence of \( \phi(t) \) can be written in general

\[
\phi(t) = \sum_{i=1}^{n} A_i e^{-t/\tau_i} \quad (\tau_1 > \tau_2 > \cdots \tau_n > 0)
\]

where \( \tau_i \) denote the inverse eigenvalues of the Liouville operator of the kinetic model in question. In the past a characteristic relaxation time was often extracted from the integral of \( \phi(t) \), but we fitted \( \phi(t) \) explicitly to equation (7) and extract the longest relaxation time \( \tau_1 \).

Theoretically the dynamical critical exponent is defined by the relation between the typical length scale of the system, i.e. the correlation length \( \xi \) (see Eq. (1)). According to finite size scaling theory for lattices of linear dimension \( L \) at \( T_c \) the correlation length is replaced by \( L \) and

\[
\tau \sim L^z
\]

for sufficiently large \( L \).

3. Results

3.1 \( d = 2 \). - The qualitative behavior of \( \phi(t) \) was similar for all lattice sizes: the magnetization correlation function decayed almost completely as a single exponential decay with only very small corrections for the very short time behavior, whereas the energy correlation function showed pronounced contributions from the non-leading exponential decays. As shown in figure 1, the magnetization could be fitted essentially exactly by the sum of just two exponentials decays with the inclusion of the second, faster decay providing only a small change in the value of \( \tau_1 \) obtained by use of a single exponential decay for the data at longer times. In contrast, the decay of the energy could only be fitted for values of \( \phi(t) \) below approximately 0.6 even with the use of a two exponent decay, and when a two exponential fit was used the sum of the two terms only accounted for 90% of the correlation function at \( t = 0 \). For any further improvement, additional exponential decay terms would have to be added; although the relaxation times are quite similar for the magnetization and energy, the amplitudes of the terms are quite dissimilar. Our best fit for \( q = 2 \) (Ising model), shown in figure 2, is obtained with \( z = 2.14 \pm 0.05 \). This value agrees well with several recent studies and with \( \varepsilon \)-expansion predictions but is outside the error estimates of other recent work. In figure 2, we show the final estimates for the relaxation times obtained from the magnetization for all three values of \( q \) versus lattice size \( L \) on a log-log scale. These data show a very nice power law increase, as predicted by finite size scaling theory, with slopes for all three being al-
The exponents describing the divergence of $\tau_1$ and $\tau_2$ for the energy correlation function $\phi$ are virtually the same as for $\phi_M$. As mentioned earlier, the most significant difference is that high order relaxation terms are far more important for the energy relaxation than for the magnetization.

Final estimates for $z$ based on both $\phi_M$ and $\phi_E$ are shown in Table I. There are still sufficiently large errors ($\sim \pm 3\%$) that it is not really possible to determine if all three values of $z$ are identical, however, these is sufficient accuracy to show that the values are much closer than predicted by theory [15] or suggested by earlier numerical work (See Tab. I).

3.2 $d = 3$. – The three dimensional Ising model has been studied less often than its two dimensional counterpart [14, 27-30]. Since the “best” existing numerical work [14, 28] yielded value of $z$ which were less than 2, and came perilously close to violating a lower bound [31], we obtained very high statistics data for even larger lattices than for $d = 2$. The qualitative features of these results were the same as for $d = 2$, so we shall not show any raw data. The very high speed of the $d = 3$ program allowed us to carefully search for possible systematic as well as statistical errors. For example, we compared data for fully periodic boundaries and for screw periodic boundaries and did indeed find a systematic difference which becomes negligible only for very large $L$. We also carefully examined the effects of finite run length to remove effects of biased sampling [30]. (Runs of length $> 10^8\tau_1$ are needed to effectively eliminate this effect.) An analysis of $\phi(t)$ based on fitting to multiple exponential decays shows

most identical. Very recent independent simulations [22] support all three estimates.

The second relaxation time $\tau_2$ extracted from the fits is subject to a relatively large error; it also diverges but with an effective exponent which is some 10-20% smaller than $z$.

Fig. 1. – Time displaced correlation functions for the $q = 4$ Potts model on an $L = 64$ lattice. The dashed lines show single exponential fits to the long time behavior and the solid curves show two exponential fits.

Fig. 2. – Log-log plot of the longest relaxation time $\tau_1$ for the magnetization vs. lattice size for $q$-state Potts models on $L \times L$ square lattices.

Fig. 3. – Log-log plot of the longest relaxation time $\tau_1$ for the magnetization vs. lattice for the Ising model on $L \times L \times L$ simple cubic Ising models.
that the magnetization correlation function was well described by a single decay for almost all times and the inclusion of a second, faster decaying exponential decay provided only a relatively small correction to our estimate for $\tau_1$. A log-log plot of $\tau_1$ vs. $L$ (obtained from two exponential fits) showed very good linear behavior for $L \geq 12$ and yielded an exponent estimate of $z = 2.03 \pm 0.04$. This is in very good agreement with the theoretical $\varepsilon$-expansion prediction. The decay of $\phi_E$ was much more rapid and gave smaller values of $\tau_1$ than did $\phi_M$, but the resulting estimate for $z$ was the same. We thus conclude that no discrepancy exists with the $\varepsilon$-expansion prediction [3].

4. Discussion

Within the last year or two there has been substantial progress in understanding dynamic behavior of kinetic spin models, but clearly much remains to be done. Simulations still tend to underestimate errors caused by both systematic and statistical sources, e.g.: 

1. finite sampling;
2. corrections to the asymptotic decay;
3. corrections to asymptotic finite size behavior;
4. boundary conditions,

and further progress will require careful analysis as well as better data. Important theoretical questions remain. Is the true spectrum of relaxation times discrete or continuous? What does the dynamic exponent look like for the non-leading decays? Substantial improvement in our computational power is needed to provide the answers.

More experiments are also needed to untangle the confusion of existing experimental results. Neutron scattering data yield a very low value of $z = 1.69 \pm 0.05$ for pseudo-two-dimensional Rb$_2$CoF$_4$ [32] and $\Delta = 1.04 \pm 0.09$ (i.e., $z = 1.65 \pm 0.15$) for Ni$_2$Mn [33] whereas electrical resistivity measurements on Cu$_3$Au [34] give $\Delta = 1.20 \pm 0.16$ (i.e., $z = 1.90 \pm 0.25$). Only this latter result can be said to possibly be consistent with theory and simulation; however, Cu$_3$Au actually has a weakly 1st order transition!

5. Conclusions

The various analyses of our Monte Carlo data show clearly that very high quality data and careful analysis are necessary to produce reliable exponent estimates. Our study shows rather conclusively that the $\varepsilon$-expansion accurately predicts the dimension dependence of $z$ for Ising models. The lack of any strong dependence of the number of states ($q$) of the $d = 2$ Potts model supports the dynamic extension of Suzuki’s weak universality [33]. Simulation studies of other kinetic models will have to be carried out quite carefully to avoid both systematic and statistical errors.

Acknowledgments

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[22] de Alcantara Bonfim, O. F. (to be published).