Journal of Statistical Physics, Vol. 60, Nos. 5/6, 1990

Properties of Metastable Ising Models Evolving under the Swendsen–Wang Dynamics

T. S. Ray[1] **and P. Tamayo**[2]

Received March 19, 1990

The behavior of the metastable nearest neighbor Ising model governed by Swendsen–Wang dynamics (SW) is investigated in $d=2$. The results are compared to those obtained in standard Metropolis dynamics. Both the SW and Metropolis systems are observed to decay from the metastable state via the formation of nucleating droplets. Nucleation rates are measured and found to agree with those predicted by classical nucleation theory. The growth rates of the droplets are observed to differ between the two dynamics. In addition, the dynamic critical exponent z is measured in a mean-field (Curie–Weiss) metastable Ising model at the spinodal. It is found that for SW dynamics, $z=2$. Since this is the same value as that obtained in the Metropolis case, this result shows that SW does not change the dynamical universality class at the spinodal.

KEY WORDS: Nucleation; metastability; Ising model; Metropolis; Swendsen–Wang; spinodal point; critical dynamics.

1. INTRODUCTION

Recently Swendsen and Wang proposed a new dynamics (SW) for Ising-like systems[(1)] which has several novel features. One of these which is particularly interesting and potentially useful is that the value of the dynamic critical exponent z is reduced. In fact, due to the nonlocal nature of the dynamics, z is found to be smaller than the lower bound γ/ν calculated by Kawasaki for local dynamics.[(2)]

As is the case with local dynamics, SW obeys detailed balance. This condition ensures that a given dynamics will sample states in accordance with the thermodynamic equilibrium distribution.[(3)] However, the correlation between successive configurations as a function of their separation in

[1] HLRZ c/o Forschungszentrum Jülich, D-5170 Jülich 1, Federal Republic of Germany.
[2] Center for Polymer Studies and Department of Physics, Boston University, Boston, Massachusetts 02215.

0022-4715/90/0900-0851$06.00/0

time is, to a certain degree, arbitrary. This allows the value of z, for example, to vary according to the particular dynamics. A natural question which arises is the following: How much of a constraint does the requirement of detailed balance impose upon the dynamic evolution of the system? This is interesting for both the equilibrium and nonequilibrium cases. One would like to know whether different types of dynamics cause the system to take statistically dissimilar paths in phase space, how the growth rates of distinct features differ, and whether or not these features even have the same structure.

Because it is in many important respects different than conventional dynamics, SW is a good system in which to study these questions. Already there has been some work in this area. Meyer-Ortmanns and Trappenberg investigated the behavior of finite Ising systems below T_c with no external field.[4] They found that the flipping rate (i.e., the average time for the magnetization to reverse its sign when the spanning cluster is held fixed) under SW dynamics had a behavior different from that of Metropolis. In addition, Burkitt and Heerman investigated continuous ordering under rapid quenching with Ising models governed by SW dynamics.[5]

In this paper, the evolution of metastable Ising systems under SW dynamics is investigated. The metastable state is good to work with since it gives both quasiequilibrium (formation of nucleating droplets) and nonequilibrium (growth of droplets) phenomena. Also, the theory of nucleation is understood reasonably well, so that the results can be compared to theoretical relations for nucleation rates and Metropolis data.

In addition, the metastable Ising system is used to test the lower bound α/ν for the dynamic critical exponent z calculated by Li and Sokal for SW dynamics.[6] This relation has been found to hold for Ising models at the critical point, where it differs considerably from the lower bound on z for local dynamics calculated by Kawasaki (γ/ν).[2] However, at the spinodal or limit of metastability for a mean-field Ising model, both of these lower bounds are equal to the value 2. This is also the exact value for standard Metropolis dynamics. If the above bound is correct, SW dynamics does not reduce the value of z from that of Metropolis at the spinodal. Simulation of a Curie–Weiss Ising model, where all pairs of spins interact with equal strength, indicates z is indeed not reduced.

2. IMPLEMENTATION OF SW IN THE METASTABLE ISING MODEL

The Ising models simulated in this work are governed by the usual Hamiltonian:

$$\mathscr{H} = -\mathscr{J} \sum_{\langle ij \rangle} s_i s_j - H \sum_i s_i \tag{1}$$

Here $\mathcal{J} > 0$, so that all the system is ferromagnetic. The spins s_i have the values ± 1. The first term is a sum over all pairs of interacting spins. The second term is the energy due to the coupling between all spins and the external field H. The external field is constant with respect to the position on the lattice of s_i and of the time.

For temperatures less than T_c with the external field set to zero, the Ising system has two degenerate ground states. Under a naive implementation of SW dynamics, the system will flip between these two states. This is because the spanning cluster of spins, which corresponds to the instantaneous magnetization, will be flipped with a probability of 1/2 during every SW step. In several different papers, it has been noted that the system will correctly sample one of the ground states if the spanning cluster is held fixed in one orientation.[4,7,8] Detailed balance ensures that configurations where the majority of spins point in the particular direction chosen will be sampled according to the equilibrium distribution. All thermodynamic quantities will therefore be correct. Surface tension between the two phases guarantees that an infinite system will remain in the chosen ground state.

Suppose that the field is increased to a small positive value and that the temperature remains fixed ($T < T_c$). One of the former ground states having a bulk magnetization with the same sign as the external field will become the equilibrium state. The other, where the bulk magnetization has a sign opposite to the external field, will become the *metastable* state. If the spanning cluster of spins is held fixed (opposed to the external field), the system should initially relax into the metastable state.

Following the above line of thinking, the SW dynamics is modified according to the following procedure:

1. Initialize the system so that all spins are opposed to the external field.
2. Between all pairs of interacting spins with the same orientation, place bonds with probability $p_b = 1 - e^{-2\beta\mathcal{J}}$.
3. Between every spin which is aligned with the external field and the ghost spin, place bonds with probability $p_g = 1 - e^{-2\beta H}$. (The ghost spin is an auxiliary spin aligned with the external field.)
4. Flip all clusters of spins not connected to the ghost spin with 50% probability *except for the spanning cluster, which must remain opposed to the external field.*

Step 1 is done in order to allow the system to relax into metastable configurations; in the equilibrium implementation of SW dynamics one could also start with this initial condition. Steps 2 and 3 along the non-italicized portion of step 4 are the standard ones used for an Ising model with an external field and are described elsewhere.[1,9] The only modification is the last part of step 4; rather than flipping the spanning cluster with 50% probability, it is kept fixed.

The above procedure is justified by recalling that the metastable state is in *quasiequilibrium*; i.e., it exists for time which is long enough so that bulk properties can be measured with a reasonable degree of accuracy. Although this idea is difficult to define mathematically, it is commonly realized in real experiments and in simulations. As long as the system remains in the metastable state, it will sample configurations according to their weight in the partition sum. This means that any dynamics which obeys detailed balance, in addition to giving the correct equilibrium properties, will also give the correct quasiequilibrium properties for the metastable state. This has been observed in different simulations using several local dynamics[10–12] and it is also expected for SW dynamics. To confirm this conjecture, the quasistatic energy and magnetization were measured in the metastable SW system and compared to those obtained from standard Metropolis. Both dynamics gave values which were identical up to four significant figures.

This procedure was used to study a two-dimensional nearest-neighbor Ising model and a mean-field Ising model (i.e., *all* pairs of spins interact with equal strength). In the $d=2$ case, the simulations were run on a Connection Machine (Thinking Machines, Inc.) located at Boston University. This device is an "SIMD" (Single Instruction Multiple Data) computer nominally containing 64K processing units. The processors are connected together in hardware by means of a hypercube geometry, but they can be configured in the software to form a square lattice of arbitrary size. The Ising systems consisted of 256×256 spins and ran on 8K or 16K of the processors. The parallel algorithm used to determine the connectivity of the clusters will be described elsewhere.[13] It should be possible to adapt this algorithm to vector machines. The entire program, although quite sufficient for our purposes, is not impressively fast (5 μsec per spin). However, with appropriate "fine tuning" of the parameters, much improvement is expected.

The mean-field system was run on an IBM 3090 at Boston University, and on a Sun workstation at KFA Jülich, West Germany. The algorithm used was a slightly modified version of the one described in previous work.[8]

3. RESULTS AND DISCUSSION

3.1. Nearest-Neighbor $d=2$ Ising Model

Under both Metropolis and SW dynamics, this system was observed to decay from the metastable state via the formation of nucleating droplets.

For the sake of completeness, a brief discussion of the features of nucleation theory relevant to the present work follows.

In both experiments and simulations, metastable systems are found to decay to equilibrium by means of the phenomenon of *nucleation*.[14] In a homogeneous system, this can qualitatively be described as the formation of centers of the stable phase due to spontaneous fluctuations of the metastable background. These centers, called *nucleating droplets*, proceed to grow and take the system to equilibrium.

One of the quantities which is of theoretical interest in the field of metastability is the *nucleation rate* J. This quantity is defined to be the number of nucleating droplets formed per unit time per unit volume. The phenomenological droplet model of Becker and Döring (see ref. 14) has been found to give results for J which agree quite well with simulations.[10] Other work has shown that this model becomes exact as one approaches the coexistence curve ($H=0$) as long as the temperature is kept fixed.[15] The predicted dependence of J according to the droplet model in d dimensions is

$$J = P_k P_s e^{-c/H^{d-1}} \tag{2}$$

Here, d is the dimension of space and c is a constant which depends upon the temperature and the surface tension between the phases. The two prefactors P_k and P_s also depend upon these variables and upon the external field H. They are referred to as the kinetic and static prefactors, respectively. The static prefactor P_s depends upon the averaged properties of the metastable state, whereas the kinetic prefactor P_k is governed by the dynamics. Usually the dependence of J on H is dominated by the exponential for small enough H.

The $d=2$ Ising model was run both with Metropolis and SW dynamics. Two temperatures were chosen. One of these was far below the critical point ($T=0.59T_c$) and the other was chosen to be quite close ($T=0.975T_c$). At both values of the temperature, nucleation was observed in the SW metastable system as well as the Metropolis system. Qualitatively, the nucleating droplets in both dynamics appeared to have the same structure, although the nucleation rates were much different. The nonequilibrium growth of the droplets after their formation was also found to be quite different.

In order to measure the nucleation rates, the metastable systems were first run at each value of the field in order to determine a good criterion for the size and time of formation of nucleating droplets. Next, according to the criterion, the system was run for a set number of time steps and then stopped. The nucleating droplets were then counted. Finally, the nucleation rate J was determined by dividing the number of nucleating droplets by the number of time steps and by the system size. Each data point was averaged over at least 15 such runs. Although this procedure is somewhat subjective, the J values were found to be reasonably insensitive to the actual criterion for the range of H displayed in the plots. However, when the external field was too large, it was difficult to establish a criterion, since no metastable state could clearly be defined and even very small clusters of spins aligned with H grew rapidly.

The nucleation rate results are shown in Fig. 1 ($T = 0.59T_c$) and in Fig. 2 ($T = 0.975T_c$) for both Metropolis and SW dynamics. The J values are graphed against $\mathcal{J}/H$ on semilog plots. According to Eq. (2), these plots should give straight lines if the behavior is dominated by the exponential. For both temperatures the two dynamics give reasonably straight lines when H is small. The slope at $0.59T_c$ agrees fairly well with what classical nucleation theory predicts. At each temperature the linear regions are roughly parallel for both dynamics. This indicates that the surface tension between the two phases is independent of the dynamics, which is an expected result, since the surface tension is a thermodynamically averaged quantity. The data close to T_c in Fig. 2 have a slope which is much less than that of Fig. 1. This is consistent with the fact that the surface tension should vanish at T_c.

It appears that SW dynamics gives data which are consistent with the droplet model. Since the exponential dependence of the nucleation rate on

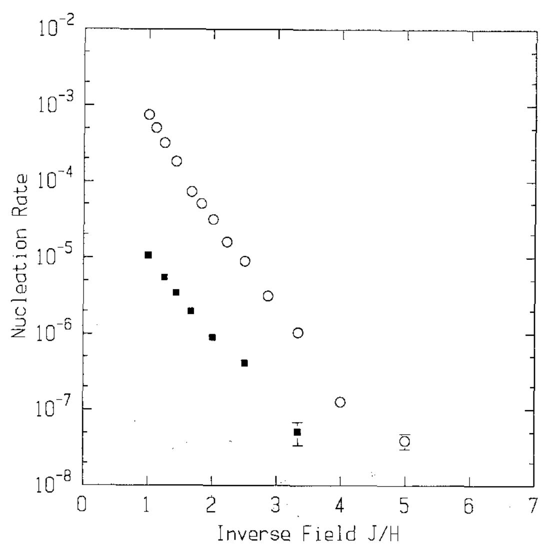

Fig. 1. Nucleation rate versus $\mathcal{J}/H$ for SW (squares) and Metropolis (circles) dynamics at $T = 0.59T_c$.

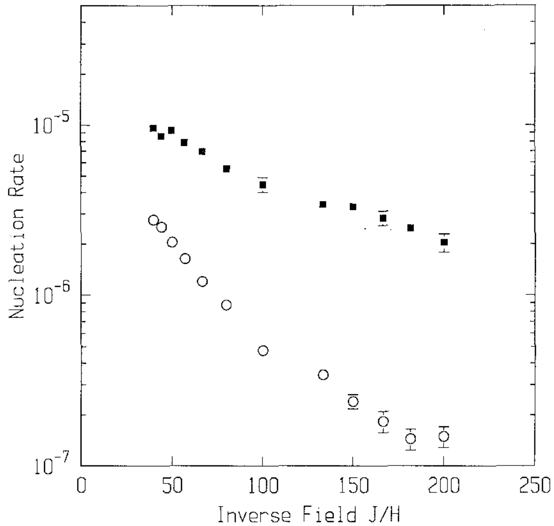

Fig. 2. Nucleation rate versus $\mathscr{J}/H$ for SW (squares) and Metropolis (circles) dynamics at $T = 0.975 T_c$.

the field and the static prefactor P_s depend only on thermodynamically averaged properties, this is a reasonable result. The difference between SW and Metropolis should occur in the kinetic prefactor P_k, since this is the part of the nucleation rate which depends upon the dynamics. Figures 1 and 2 show that the behavior of P_k for SW dynamics is much different than Metropolis. At $T = 0.975 T_c$ the nucleation rate for SW is greater than Metropolis ($J_{\text{SW}} > J_M$), while at $T = 0.59 T_c$ it is smaller ($J_{\text{SW}} < J_M$). Qualitatively, this occurs because SW clusters become increasingly larger near T_c. The nonlocal nature of the dynamics allows all of the spins in a single large cluster to align with the external field at once, whereas Metropolis can only flip individual spins. When two or more of these clusters which border one another align with H, their composite mass is large enough so that the probability of their being connected to the ghost spin (i.e., remaining aligned with H) is close to unity. At temperatures far below T_c, the SW clusters are small and the dynamics is effectively local. The only large cluster is the spanning cluster which forms the metastable background.

Once nucleating droplets have formed, they grow in a highly non-equilibrium manner. The growth properties depend strongly upon the dynamics and the temperature. Near T_c, the SW droplets grow rapidly, since large clusters of spins the size of the correlation length may be added in one time step. Metropolis, on the other hand, grows one spin at a time, so that when the correlation length is much larger than the lattice spacing, it is significantly probable that the spin near the border of a nucleating droplet will not remain aligned with the external field. Far from T_c, the SW droplets grow very slowly. Since the bond probability is close to unity, it takes a long time for a spin on the border of a droplet which is not aligned with H to become detached from the spanning cluster and become part of the droplet. However, in the Metropolis dynamics, it is very probable for a spin just outside a droplet to become aligned with the external field; accordingly, the droplets grow rapidly.

3.2. The Mean-Field Metastable Ising Model (Curie–Weiss)

In this system, all pairs of spins interact ferromagnetically and with equal strength. Because every spin is a nearest neighbor of all others, there is no geometrical measure of length. This means that it is impossible for interesting local entities, like nucleating droplets, to form. However, the system is still useful for studying properties of the *spinodal*, which is the sharp boundary between the metastable and unstable regimes. In previous work, the spinodal has been shown to behave like a critical point in the mean-field approximation.[12]

One of the characteristics of the spinodal is that it exhibits the phenomenon of critical slowing down. Autocorrelation functions of bulk quantities are expected to be governed by the slowest mode according to the exponential $e^{-t/\tau}$. The value of τ diverges at the spinodal as a power law, and a dynamic critical exponent z can be defined in the usual manner:

$$\tau \sim \xi^z \tag{3}$$

Here τ is the relaxation time for the slowest mode and ξ is the correlation length. For this system, ξ is defined through the exponent ν as

$$\xi \sim (\Delta H)^{-\nu} \tag{4}$$

where ΔH is the reduced distance to the spinodal. The temperature is held fixed.

Recently, Li and Sokal calculated a lower bound for z in SW dynamics.[6] They found $z_{\mathrm{SW}} \geqslant \alpha/\nu$. This bound has been determined to hold at the Ising critical point in several different dimensions as well as in the Curie–Weiss system. The spinodal in the Curie–Weiss Ising model is a good test for this bound, since $\alpha/\nu = 2$, which is the same value as that obtained from Metropolis dynamics. If the bound holds in this case, it implies that SW dynamics does not reduce the dynamic critical exponent from that of Metropolis at the spinodal.

The longest decay mode was measured at the spinodal using the autocorrelation function for the magnetization $A(t)$:

$$A(t) = \langle m(t+t')\, m(t') \rangle_{t'} - \langle m(t') \rangle_{t'}^2 \tag{5}$$

for a system of $N = 10^4$ spins. The averages were taken over 60,000 SW steps. The system always remained in the metastable state during this time, so that these averages were over metastable configurations. Each value of τ was determined from a linear fit of $A(t)$ to t on a semilog plot.[16]

In Fig. 3, the data for τ are shown as a function of ΔH on a log–log plot. The rapid initial rise for ΔH close to 1 is typical for quantities measured at the spinodal. At small ΔH, the curve is approaching asymptotic power-law behavior. According to Eqs. (3) and (4), the asymptotic slope should have the value $-\nu z$. Since $\nu = 1/4$ for the spinodal, the slope should be equal to $-1/2$ if $z_{SW} = 2$. The dashed line on the plot has the expected slope and is in close agreement with the last few data points.

From a geometrical point of view this result is reasonable because the connectedness length of the clusters does not diverge at the spinodal. The success of recent algorithms like SW in accelerating the dynamics seems to be based on the proper matching between the connectedness length in the embedded percolation problem and the correlation length in the thermal

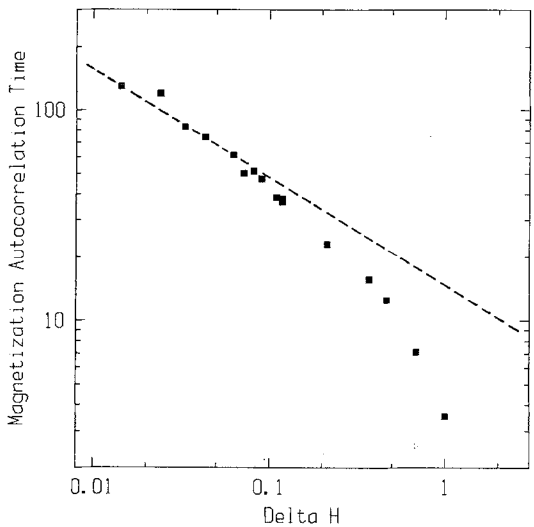

Fig. 3. Autocorrelation data for the magnetization near the spinodal. The dashed line has the predicted asymptotic slope of $-1/2$ with $z_{SW} = 2$.

problem.[17,18] Since at the spinodal the percolation clusters are finite while the correlation length diverges, the SW dynamics is effectively local (This mismatch of lengths at the spinodal has recently been reported by Coniglio *et al.*[19]).

4. CONCLUSIONS

The $d=2$ metastable Ising model has been observed to decay from the metastable state via the formation of nucleating droplets. Differences between SW and Metropolis dynamics have been observed in the growth and formation of droplets, but not in their structure. The nucleation rates have been compared to those predicted by the droplet model of Becker and Döring and have been found to agree fairly well for small values of the external field. The nucleation rates for SW are smaller than Metropolis at $T=0.59T_c$ and larger than Metropolis at $T=0.975T_c$. This is thought to be a consequence of the nonlocal nature of SW dynamics near T_c.

It appears that all properties which are functions of equilibrium or quasiequilibrium bulk quantities are the same in both SW and Metropolis. This includes surface tension between the metastable phase and the droplets and the exponential dependence of nucleation rates on the external field. Since the condition of detailed balance guarantees all of these properties to be independent of the dynamics, this is not unexpected. The non-equilibrium growth phenomena, while different in SW and Metropolis with respect to actual rates, shares the same qualitative behavior. There is no evidence observed as radical as, for example, the existence of a spinodal line in the $d=2$ system. A more detailed paper on these effects in $d=3$ will be published shortly.

The Curie–Weiss simulations near the spinodal give evidence that $z_{SW}=2$, which is consistent with the lower bound calculated by Li and Sokal. This is thought to result from the fact that although the Ising correlation length diverges at the spinodal, the percolation connectedness length does not.

ACKNOWLEDGMENTS

The authors wish to thank R. Brower, A. Coniglio, D. Considine, W. Klein, L. Monette, D. Stauffer, and J. S. Wang for many enlightening discussions.

REFERENCES

1. R. Swendsen and J. S. Wang, *Phys. Rev. Lett.* **58**:86 (1987).
2. K. Kawasaki, *Phys. Rev.* **145**:224 (1966).

3. K. Binder, ed., *Monte Carlo Methods in Statistical Physics* (Springer-Verlag, 1979).
4. H. Meyer-Ortmanns and T. Trappenberg, *J. Stat. Phys.* **58**:185 (1985).
5. A. N. Burkitt and D. W. Heermann, *Comp. Phys. Commun.* **54**:201 (1989).
6. X. Li and A. Sokal, *Phys. Rev. Lett.* **63**:827 (1989).
7. Z. Alexandrowicz, *Physica A* **160**:310 (1989).
8. T. S. Ray, P. Tamayo, and W. Klein, *Phys. Rev. A* **39**:5949 (1989).
9. J. S. Wang, *Physica A* **161**:249 (1989).
10. D. Stauffer, A. Coniglio, and D. W. Heermann, *Phys. Rev. Lett.* **49**:1299 (1982).
11. L. Monette, W. Klein, M. Zuckermann, A. Khadir, and R. Harris, *Phys. Rev. B* **38**:11607 (1988).
12. T. S. Ray and W. Klein, *J. Stat. Phys.*, submitted.
13. R. C. Brower, P. Tamayo, and B. York, *J. Stat. Phys.*, submitted.
14. J. Gunton and M. Droz, *Introduction to the Theory of Metastable and Unstable States* (Springer, Berlin, 1983).
15. J. Langer, *Ann. Phys.* (N.Y.) **14**:108 (1967).
16. S. Tang and D. P. Landau, *Phys. Rev. B* **36**:567 (1987).
17. R. C. Brower and P. Tamayo, *Phys. Rev. Lett.* **62**:1087 (1989).
18. U. Wolff, *Phys. Rev. Lett.* **62**:361 (1989).
19. A. Coniglio, F. de Liberto, G. Monroy, and F. Peruggi, *J. Phys. A* **22**:L837 (1989).

Communicated by D. Stauffer.