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METASTABILITY AND NUCLEATION IN ISING MODELS WITH SWENDSEN–WANG DYNAMICS

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The cluster numbers of stable phase droplets in the metastable state and nucleation rates for the three-dimensional Ising model with Swendsen–Wang dynamics are measured for $T = 0.59 T_c$ and compared with previous Metropolis results. Both dynamics appear to give the same metastable properties. When the external field is small the results agree with classical nucleation theory. No evidence is found for the existence of a spinodal line.

1. Introduction

Recently, there has been a growing interest in various aspects of stochastic dynamics employed in Monte Carlo simulations. The efficiency of a given simulation is strongly dependent upon the dynamics. This is especially true near critical points where the correlation length is large [1]. However, a good understanding of dynamical properties is useful not only for developing efficient simulations; it also aids in the general understanding of dynamical phenomena as a whole. For example, by examining the behavior of different types of dynamics under nonequilibrium conditions, one can gain insight into how robust certain features are and how much variation is allowed in the correlation between successive configurations.

The dynamics introduced by Swendsen and Wang (SW) is a novel system for studying general dynamical behavior [2]. Since the dynamics deals with clusters rather than individual spins, it appears to be quite different than other conventional dynamics like Metropolis. It would be interesting to know to what extent this is true. Several papers have given evidence that the functional time dependence is different although the basic qualitative behavior is the same [3–5].

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In one of these papers, the behavior of a metastable Ising model in two dimensions governed by SW dynamics was investigated [5]. The system was observed to decay from the metastable state via the formation of nucleating droplets. Nucleation rates were measured which were roughly consistent with classical nucleation theory. The nucleating droplets appeared to have a bulk consisting of the stable phase and, at low temperatures, a distinct surface. Once formed, the droplets grew along their surface radially outwards. This same type of qualitative behavior was also observed in a metastable Ising system governed by Metropolis dynamics. It is also consistent with classical nucleation theory (CNT), the standard phenomenological theory for the decay of metastable states [6]. The differences between SW and Metropolis dynamics appear in the growth rate of nucleating droplets and in the prefactor of the nucleation rate J (the rate of formation of nucleating droplets). For temperatures far below T_c, both the nucleation rate and the nonequilibrium growth of nucleating droplets after formation are slower for the SW system than for the Metropolis system. Close to T_c, the opposite is true.

The present paper studies this problem more carefully and quantitatively for a three dimensional nearest-neighbor Ising system. The results are then compared to those from previous work with the same system governed by Metropolis dynamics [7]. Since classical nucleation theory assumes a specific form for the droplets (i.e. the free energy can be written as the sum of a bulk term and a surface term) it is important to verify this. By means of cluster numbers, these properties are investigated. Nucleation rates are also measured and compared to the Metropolis results.

The surface tension between the metastable and equilibrium phase is also measured and found to be close to that obtained from Metropolis dynamics. Since the surface tension is an equilibrium property this is an expected result. However, the data of Meyer-Ortmanns and Trappenberg suggests that this is not necessarily true in SW dynamics [3]. Their measurements of the surface tension between the two degenerate phases ($H = 0$) in the $d = 3$ Ising model gives two significantly different results for SW and Metropolis. In their work the authors assume a form for the tunneling time T which is the same as that assumed in CNT when the external field goes to zero:

$$T \propto \exp(2\sigma L^2) . \tag{1}$$

Here σ is the surface tension and L is the length of the system. The temperature in their simulations is quite close to the critical point ($T = 0.955 T_c$) and the authors are suspicious of finite size effects in their SW results.

The implementation of the SW dynamics in a metastable Ising system has been previously described [5]. For completeness, the procedure is outlined here:

(1) Initialize the system with all spins opposed to the external field.

(2) Between all pairs of parallel, neighboring spins place a bond with probability $p_b = 1 - \exp(-2J/kT)$.

(3) Between all spins which are aligned with the external field H and the ghost spin place a bond with probability $p_g = 1 - \exp(-h)$. Here $h = 2H/kT$ is the dimensionless field standardly used in cluster statistics.

(4) Flip all clusters of spins not connected to the ghost spin with probability $\frac{1}{2}$ *except for the largest cluster which remains antiparallel to the external field.*

Step (1) is necessary so that the system can relax into the metastable state. All other steps except for the italicized portion of step (4) constitute the normal implementation of SW for an Ising system with an external field and are described elsewhere [8, 9]. Since the spanning cluster is always kept opposed to the field, the system will not trivially flip into the equilibrium state. Instead it must initially relax into the metastable state before decaying to equilibrium.

All of the simulation results reported in this paper are for the three-dimensional nearest-neighbor metastable Ising model. Helical boundary conditions were used and all measurements were done at $T = 0.59T_c$. The simulations were run on SUN 4 workstations and on a Transputer containing four units. A Hewlett-Packard mainframe was used to run the $L = 80$ systems.

2. Cluster measurements

Instead of using the "Fisher droplet" definition of clusters (i.e. a group of positive spins surrounded by a sea of negative spins) as in the Metropolis simulations [7], it is natural to use the "Coniglio–Klein" clusters generated in step (2) of the above procedure [10]. All measurements presented here will be in terms of these latter clusters. The two definitions are significantly different only near the critical point. All of the data is taken at $T = 0.59T_c$ so that a comparison between it and previous work with Metropolis dynamics [7] which used the Fisher droplet definition is valid.

The cluster number n_s is defined to be the number of clusters consisting of s spins per unit volume. Only spins aligned with the external field are included and their connectivity now ignores the ghost spin. According to classical nucleation theory,

$$n_s \propto \exp(-F_s/kT) \tag{2}$$

with

$$F_s/kT = \Gamma s^{2/3} - hs\,. \tag{3}$$

Here F_s is the free energy of a droplet consisting of s spins. The first term is the contribution due to the surface energy of the droplet and the second from the bulk. Apart from a geometric factor, Γ is the ratio of bulk surface tension per unit area to kT.

When h is positive, the system is metastable and the droplet free energy has a maximum at the critical droplet size s^*. If the droplet exceeds this size it has a tendency to grow so that the system decays from the metastable state.

It is important to verify that the droplets have the free energy which is assumed in the above equations. This can be done by measuring the average values of the cluster numbers n_s. In fig. 1, the logarithm of the observed n_s minus h_s is plotted against $s^{2/3}$ for several values of the field. According to eqs. (2) and (3), this should give a straight line with slope equal to $-\Gamma$. The system used had a linear size $L = 40$ and the results were averaged over $\sim 10^4$ SW steps. For small sizes $s < 5$, some deviation from the predicted behavior is seen. For larger s, the results are consistent with the classical theory. In this region, the slope of the curve gives $\Gamma = 3.2 \pm 0.1$, which agrees well with previous Metropolis results. This indicates that the droplets have a well-defined surface. Also, the surface tension is the same as that measured in Metropolis systems [7]. This last result is expected since the surface tension is an equilibrium quantity.

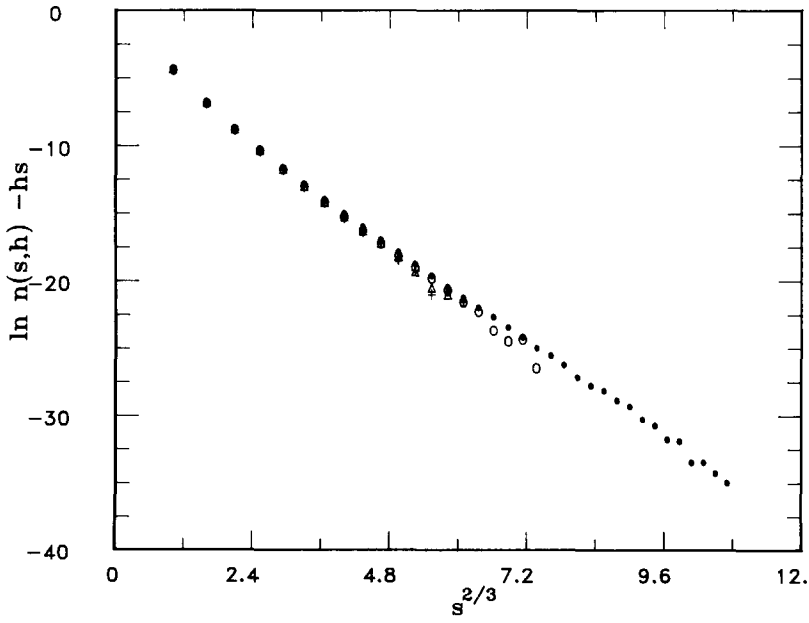

Fig. 1. Log of cluster number n_s versus $s^{2/3}$ for different values of the external field. For $h = 0$, 0.1, 0.2 and 0.4 the data is indicated by triangles, pluses, circles and bullets, respectively.

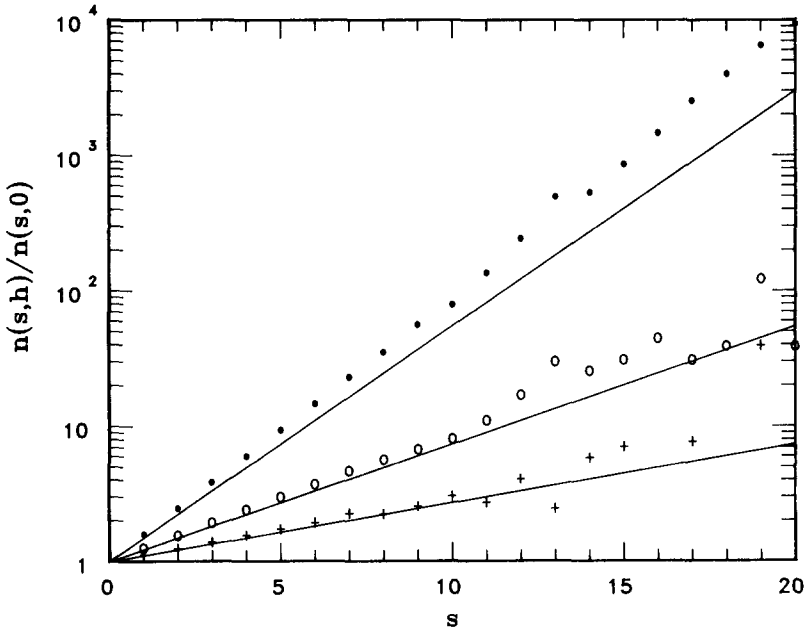

Fig. 2. Log of the ratio of cluster numbers $n_s(h)$ to $n_s(0)$ versus cluster mass s. For $h = 0.1$, 0.2 and 0.4 the data is indicated by pluses, circles and bullets, respectively. The lines drawn in the figure have the slopes assumed in classical nucleation theory.

The bulk properties of the clusters have been similarly investigated. In fig. 2, the ratio of n_s for field h to n_s for zero field is plotted against s on a semilog plot for three values of h. Eqs. (2) and (3) indicate that the plots should be straight lines having slopes equal to h as long as Γ remains constant (fig. 1 suggests that this last assumption is valid).

The lines drawn in the figure have the predicted slopes. For the two smaller values of h, the data is roughly consistent with the classical theory. A least square fits for the slopes taking the data from $s = 1$ to 10 agrees to within statistical error. However, at $h = 0.4$, the slope is measured to be about 10% larger than expected. Although not large, this deviation seems to be significant. The cluster numbers with $s > 14$ for $h = 0$ have been extrapolated from the behavior of the smaller clusters. This could introduce systematic error.

3. Nucleation rates

The nucleation rate J is defined to be the average number of nucleating droplets formed per unit volume per unit time. Classical nucleation theory

predicts that this quantity is given by the equation

$$J = P_k P_s \exp(-c/h^{d-1}) . \tag{4}$$

Here c is a constant which depends upon the surface tension and the dimension of space d. The prefactors P_k and P_s are governed by the details of the dynamics and by time averaged properties independent of the dynamics, respectively. When h is small, the exponential dependence dominates the prefactors. This is usually taken to be the signature of the CNT regime.

Two separate methods have been used to measure the J values in the SW simulations. According to the first criterion, the system is allowed to evolve until a droplet with more than 70 spins forms. This is identified as the first nucleating droplet. Then J is defined to be the inverse of the average time for formation divided by the volume of the system.

The J values defined according to this criterion for system sizes $L = 10$, 20, 40 and 80 are graphed as a function of $1/h^2$ on a semilog plot in fig. 3. Also shown is the nucleation data for Metropolis dynamics presented by Stauffer et al. [7]. According to eq. (3) this plot should give straight line behavior when J is dominated by the exponential. The figures shows that each system has two regimes. When h is large, there is a regime in which J decreases slowly as h

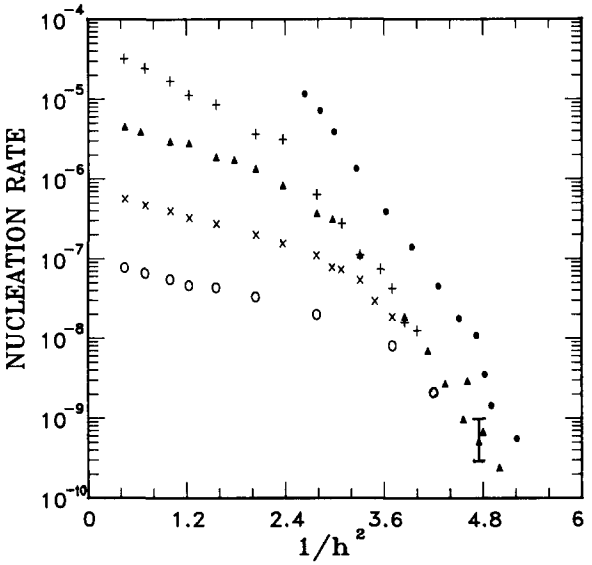

Fig. 3. Nucleation rates for first criterion (see text) versus $1/h^2$ for different system sizes. Pluses, triangles, crosses and circles are for systems with lengths $L = 10$, 20, 40 and 80, respectively. Also shown in bullets is the nucleation data for Metropolis dynamics taken by Stauffer et al. [7] ($L = 168$).

decreases. The extent of this regime increases with system size. For small h the curve enters a second regime where the results appear to be independent of system size. Here, the slope predicted by CNT is consistent with the data. It is also close to the slope of the Metropolis data. The two dynamics appear to differ only by a factor in this regime.

The statistics were quite good for the data with nucleation rates greater than $\sim 2 \times 10^{-9}$; each point is averaged from 16 runs. The points for rates lower than 2×10^{-9} were averaged over only 3 runs. One of the calculated error bars is displayed. Assuming CNT it is possible to show that the nucleation events are governed by an exponential distribution. This means that the standard deviation is equal to the mean value, and is probably the reason that the error bars are so large. This suggests that the drop off in the Metropolis data for low nucleation rates is probably not significant.

Much of the dependence of J on system size for large h in fig. 3 is probably due to the simultaneous formation of nucleating droplets. A criterion for J which takes this into account was used to take the data in fig. 4. Here the system is allowed to evolve for a fixed number of steps. Then all droplets above the size of 70 are counted. The number of these droplets is then divided by the time and by the volume of the system. The first 22 Monte Carlo steps were subtracted from the total time in order to allow for the initial relaxation of the

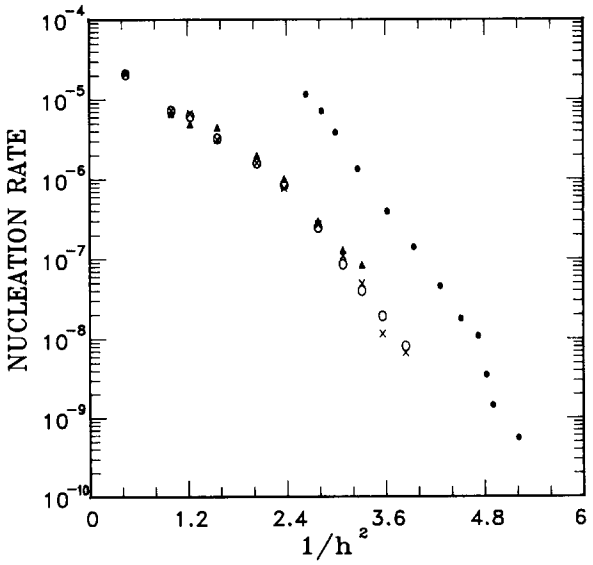

Fig. 4. Nucleation rates for second criterion (see text) versus $1/h^2$ for different system sizes. Triangles, crosses and circles are for systems with lengths $L = 20$, 40 and 80, respectively. Also shown in bullets is data from Metropolis simulations of Stauffer et al. [7] ($L = 168$).

system into the metastable state. The choice for the initial time only affects the first data point significantly. This second criterion is close to the one used by Stauffer et al. for the Metropolis data [7].

The data has been taken for three different system sizes ($L = 20$, 40 and 80) and shows that J measured according to this criterion does not have much dependence on the system size. The Metropolis data from Stauffer et al. [7] is again plotted for comparison.

For small h, this second criterion is difficult to implement. Since the nucleation events are presumably governed by an exponential distribution, the droplets are likely to form at times which are far apart from one another. This means that the first droplet that forms will, on average, have a significant amount of time to grow before the next one appears. Since most of the system will be in the interior of the first droplet, the second will not have much in which to form. This will effectively reduce the measured value of J. Because of this problem no data was taken for small nucleation rates.

Although the results shown in fig. 4 seem to be independent of system size, there is still a regime for large h where the slope of the data is smaller than the predicted value from CNT. For small h, the system crosses over to the expected classical behavior. The regime of h for which CNT applies is consistent with the Metropolis data. The SW and Metropolis results in the CNT regime seem to differ only by a prefactor. The prefactor for SW at $T = 0.59T_c$ is smaller than Metropolis by about an order of magnitude. This is very close to the behavior found at this temperature in two dimensions [5].

In mean-field theories the metastable and unstable regimes are divided by a sharp line called the *spinodal* [6]. Neither of the nucleation criteria appear to show any evidence for the existence of a spinodal. If such a feature existed, the nucleation rate would have to decrease as h becomes larger. Instead, the rates are observed to monotonically increase as a function of h. In addition, the mean cluster size shows no evidence of a divergence. This is consistent with the two-dimensional data [5] and with the work of Coniglio et al. [11].

4. Conclusion

The behavior of metastable states in SW dynamics appears to be quite similar to that observed in Metropolis dynamics. At $T = 0.59T_c$, the clusters in the metastable background have a well-defined surface and volume. The cluster numbers seem to have the functional dependence on h, s, and the surface tension as predicted by classical nucleation theory. In addition, the measured value of the surface tension is consistent with that measured in the Metropolis work. The surface tension between the metastable and stable

phases appears to be the same in both SW and Metropolis. Finally, there is no evidence observed for the existence of a sharp spinodal line dividing the metastable and unstable regimes.

The reason why the two dynamics decay from the metastable state in the same manner is probably due to the fact that the clusters are governed by equilibrium and quasiequilibrium properties (at least for small h). Since both SW and Metropolis are designed to sample states according to their weight in the equilibrium distribution, all bulk properties such as surface tension and free energies must be the same. The CNT regime is defined to be the one in which the system remains metastable for times large enough for the statistical averages to be quite accurate. Eq. (3) predicts a value of J which depends on the bulk properties up to the kinetic prefactor P_k. As is the case with the two-dimensional data, this seems to be the only difference between SW and Metropolis.

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