Eur. Phys. J. B **5**, 571–575 (1998)

THE EUROPEAN PHYSICAL JOURNAL B

Nucleation and hysteresis in Ising model: classical theory versus computer simulation*

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Received: 21 January 1998 / Accepted: 17 March 1998

Abstract. We have studied the nucleation in the nearest neighbour ferromagnetic Ising model, in different (d) dimensions, by extensive Monte-Carlo simulation using the heat-bath dynamics. The nucleation time (τ) has been studied as a function of the magnetic field (h) for various system sizes in different dimensions ($d = 2, 3, 4$). The logarithm of the nucleation time is found to be proportional to the power ($-(d-1)$) of the magnetic field (h) in d dimensions. The size dependent crossover from coalescence to nucleation regime is observed in all dimensions. The distribution of metastable lifetimes are studied in both regions. The numerical results are compared and found to be consistent with the classical theoretical predictions. In two dimensions, we have also studied the dynamical response to a sinusoidally oscillating magnetic field. The reversal time is studied as a function of the inverse of the coercive field. The applicability of the classical nucleation theory to study the hysteresis and coercivity has been discussed.

PACS. 05.50.+q Lattice theory and statistics; Ising problems

1 Introduction

The dynamical aspects of Ising models is an active area of modern research. How does the magnetisation relax towards its equilibrium value, if we start the dynamics with all spins parallel? How long is the lifetime of a metastable state if a magnetic field is antiparallel to the initial spin orientation? Can one answer all these questions in the light of growing and shrinking droplets?

What happens if all spins are up in presence of a small opposite magnetic field and the system is below its critical temperature (T_c)? The magnetisation first settles to a metastable state, and then a droplet (of overturned spins) larger than a critical size is formed. As the time passes, this droplet grows radially and the magnetisation jumps to a negative value. Classical nucleation theory (CNT) [1] predicts the logarithm of the nucleation rate (number of supercritical droplets formed per unit time and per unit volume) to be asymptotically proportional to h^{1-d} in d dimensions, where h is the magnetic field. This has been verified in the three-dimensional Ising model by Monte-Carlo simulation [2]. There are some difficulties in measuring the nucleation rates by checking how long the magnetisation takes to leave its metastable value. In the asymptotic limit of field (h) going to zero for a finite lattice size, only one supercritical droplet will be formed and it grows to cover the whole lattice. This is the proper nucleation regime and the nucleation rate is the reciprocal of the product of nucleation time and lattice volume. On the other hand, in the coalescence regime, with the lattice size going to infinity at fixed field (h), many such supercritical droplets will be formed at a time and they grow and coalesce and as a consequence the magnetisation switches sign. This effect, already discussed by Binder and Müller-Krumbhaar [3] and mathematically shown by Schonmann [4], was demonstrated by Ray and Wang [5] for Swendsen-Wang dynamics.

In this paper, we have studied the nucleation in the Ising system by extensive Monte-Carlo simulation (with geometric parallelization) using heat-bath dynamics. We have also studied the system size dependent crossover (from nucleation regime to coalescence regime) and compared the simulational results with the results of classical nucleation theory. Here, we mainly reexamine (following the earlier works [6,2]) the validity of classical nucleation theory by extensive Monte-Carlo simulation and obtained better results by applying modern parallel computational techniques.

Recently, the *hysteresis* in the kinetic Ising model has gotten much attention in research. Extensive Monte-Carlo simulation [7,8] shows that the hysteresis loop area behaves as a power law with the frequency in the low frequency ($\omega \to 0$) limit. But for very low frequency, the hysteresis loop area (approximately equal to four times the coercive field) should vary logarithmically [9] with the

* Dedicated to J. Zittartz on the occasion of his 60th birthday

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frequency as a consequence of classical nucleation theory. To explore the reason of this mismatch (between theoretical prediction and numerical results) we have studied the dynamical behaviour (coercivity and reversal time) in the two-dimensional Ising model in presence of a sinusoidally oscillating magnetic field for sufficiently small frequencies (as far as possible now) and compared the results with the theoretical predictions (CNT). This is the main motivation of our present study.

2 Classical nucleation theory

We review briefly the results of classical nucleation theory (CNT) far below T_c. The equilibrium number (per site) n_s of droplets, containing s spins is

$$n_s \sim \exp(-E_s/K_BT)$$

where E_s is the formation free energy of the droplet of size s and K_B is the Boltzmann constant. CNT assumes a spherical droplet shape and takes (in d-dimension)

$$E_s = -2hs + C_d s^{\frac{d-1}{d}}\sigma(T)$$

where h is the absolute value of the applied magnetic field and σ is the temperature dependent surface tension. The critical size s^* of a droplet which maximises the free energy, is

$$s^* = \left(\frac{(d-1)C_d\sigma}{2dh}\right)^d$$

and

$$E_{max} = \frac{K_d\sigma^d}{h^{d-1}}$$

where K_d and C_d are d-dependent constants. The number n_{s^*} of supercritical droplets

$$n_{s^*} \sim \exp(-E_{max}/K_BT) \sim \exp(-\frac{K_d\sigma^d}{K_BTh^{d-1}}),$$

where the symbol $\sim$ stands for asymptotically proportional for small fields. The nucleation rate I is proportional to n_{s^*}. In the nucleation regime, where only one supercritical droplet grows and engulfs the whole system, the nucleation time (τ; the time required by the system to leave the metastable state) is inversely proportional to the nucleation rate I,

$$\tau \sim I^{-1} \sim \exp(\frac{K_d\sigma^d}{K_BTh^{d-1}}).$$

In the coalescence regime, many such supercritical droplets form at about the same time, coalesce and ultimately form a system-spanning big droplet. The radius ($\sim s^{1/d}$) of a supercritical droplet grows linearly with time (t), consequently, the number of spins (s) in a supercritical droplet will grow as t^d. For a steady rate of nucleation, the rate of change of magnetisation is It^d, for a fixed change (Δm) in magnetisation during the nucleation time τ,

$$\Delta m \sim \int_0^\tau It^d dt \sim I\tau^{d+1}.$$

So, in the coalescence regime,

$$\tau \sim I^{-1/(d+1)} \sim \exp(\frac{K_d\sigma^d}{(d+1)K_BTh^{d-1}}).$$

In an infinitely large system only this coalescence regime is seen. In this paper, we have performed large-scale simulation (using geometric parallelization) of ferromagnetic nearest neighbour Ising model (in 2, 3 and 4-dimensional hypercubic lattices) to verify the prediction of classical nucleation theory described above, in the generalization of earlier works [6,2].

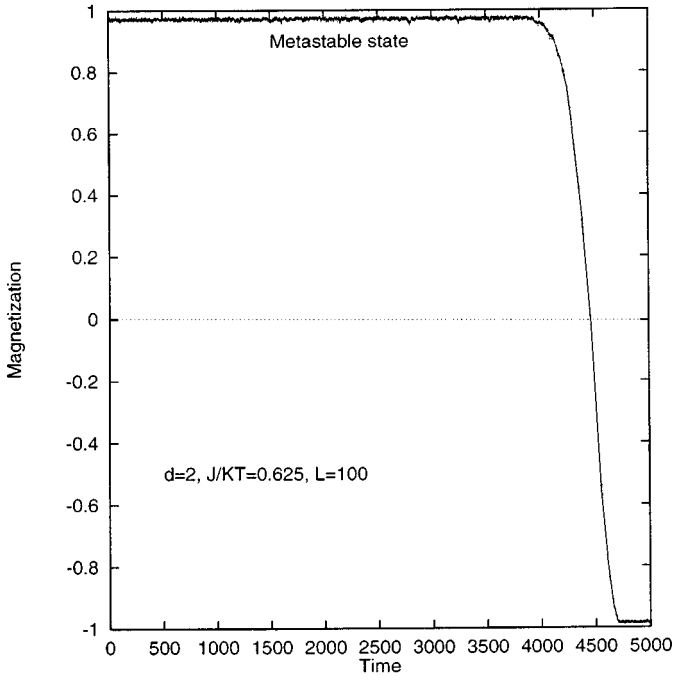

Fig. 1. A typical decay of metastable state.

3 Model and simulation scheme

We have used the standard heat-bath technique to orient the spins (Glauber kinetics) and started with all spins up in a down field. Initially the system relaxes towards a metastable state. It remains for a long time (if the field is quite small) in the metastable state and then jumps to the other stable state. One such time variation of the magnetisation is depicted in Figure 1. We have measured the lifetime of this metastable state and studied it as a function of the applied field for various system sizes.

The multispin coding technique has been applied to simulate this updating process. We have used CRAY-T3E supercomputer having 64 bits per word. We have stored

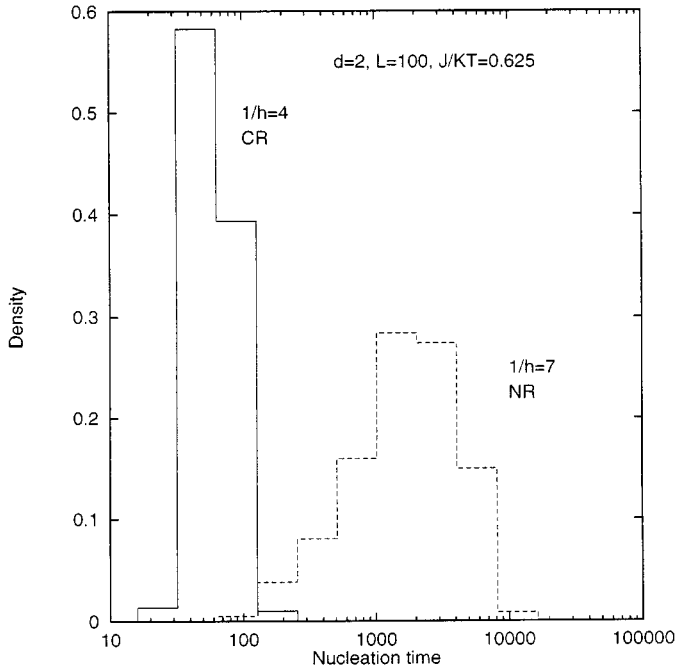

Fig. 2. Distribution of nucleation times in coalescence regime (CR, $1/h = 4$) and in nucleation regime (NR, $1/h = 7$). The results are obtained for $L = 100$ in $d = 2$.

16 spins in a computer word (64 bits) and updated a computer word (16 spins) by a single command. In this sense the updating is parallel and saves computer memory and time. To improve the efficiency of the updating process we have used geometric parallelization, where the whole lattice is distributed over N_p processors. Each processor updates a rectangular strip ($L \times L/N_p$) of a square lattice (in $d = 2$). The updated values of the upper and lower lines of the nth strip (by nth processor) were passed *via* message passing. In periodic boundary conditions, this was done through a ring-type topology. We have simulated systems of smaller sizes in SUN workstation. To produce the strong field regime, coalescence regime and nucleation regime for a fixed system size, one needs to simulate a large enough system and allow it to nucleate for a wide range of fields. In an earlier study in two dimension [6], due to smaller system size and nucleation time these three regimes were less clearly observed.

In the nucleation regime, the true nucleation time is quite large and fluctuates enormously. We have checked the range of metastable values for the corresponding range of fields used (in this study) at a fixed temperature. We define the nucleation time as the time required by the system to have the magnetisation below a cut-off value (chosen below the lowest metastable magnetisation). This choice is quite arbitrary and the results do not depend considerably on the choice of this cut-off value. Due to the huge fluctuations in the nucleation time, to avoid the waste of computer time we have taken the *median* nucleation time instead of taking the (algebraic) mean. One such distribution of nucleation time is shown in Figure 2. The fluctuation (width of the distribution) in the nucleation regime is much larger than that in the coalescence regime.

We have also studied in the same system (in two dimensions only), how the coercive field (value of the field for which the magnetization changes sign) varies with the reversal time (the time taken to change the sign of the magnetization) , when the system is placed in a sinusoidally ($h(t) = h_0 \cos(\omega t)$) varying magnetic field. In a small lattice (80×80) we have carried out this simulation and calculated the coercive field and the reversal time for various frequencies. Since in the first quarter of the cycle the field is positive and becomes negative after that, the reversal time will be much higher than the nucleation time defined above. However, in the static limit ($\omega \to 0$), the reversal time should be equal to the nucleation time. Since in the nucleation regime, the nucleation time is very high in comparison with the inverse of the frequency used, these two times will be same. This will give some idea about the value of the frequency below which the usual classical nucleation theory can be safely applied to study the hysteresis and coercivity [7–9]. A crossover theory from hysteresis (large ω) to nucleation (low ω) is given in reference [6c].

4 Results

In our simulation in two dimensions, at $J/K_BT = 0.625$, we have obtained the results for various system sizes ranging from $L = 80$ to $L = 2048$. In Figure 3 these results are displayed. Three different regimes, the strong field regime (SFR), the coalescence regime (CR) and the nucleation regimes (NR) are clearly identified. The median nucleation time τ (in log scale) is plotted against the inverse of applied magnetic field. In the coalescence regime the fluctuations are very small and $\log(\tau)$ behaves linearly with $1/h$ as predicted by the classical nucleation theory. We have also estimated the slope from the linear best fit. In the nucleation regime, the fluctuations are quite high. From the prediction of CNT, the slope ($\log(\tau) \sim 1/h$) in this regime should be three times higher than that in the coalescence regime. Our data show good agreement with this. From the estimated slope, we have calculated the surface tension $\sigma(T)$ and compared it with the previous estimates.

In two dimensions, at the same temperature, also the reversal time (in logscale) is plotted against the inverse of coercive field in the same plot (Fig. 3). The range of frequencies we have used is from 6.28×10^{-2} to 1.57×10^{-6}. The topmost datum in Figure 3 corresponds to the lowest frequency. Here also, the coalescence regimes are shown. The slope (for very small frequencies) is same with that for the static case. The nucleation regime is not very clear, however the data show a tendency towards the nucleation regime and in the long run, we believe, it could merge with the static nucleation regime. However, with the present available computer this regime is not fully accessible to us. From the figure it is quite clear for smaller lattices (80×80), that one has to go below the frequency range $\omega \simeq 10^{-6}$, to get the results for hysteresis which will be comparable with that obtained from classical nucleation

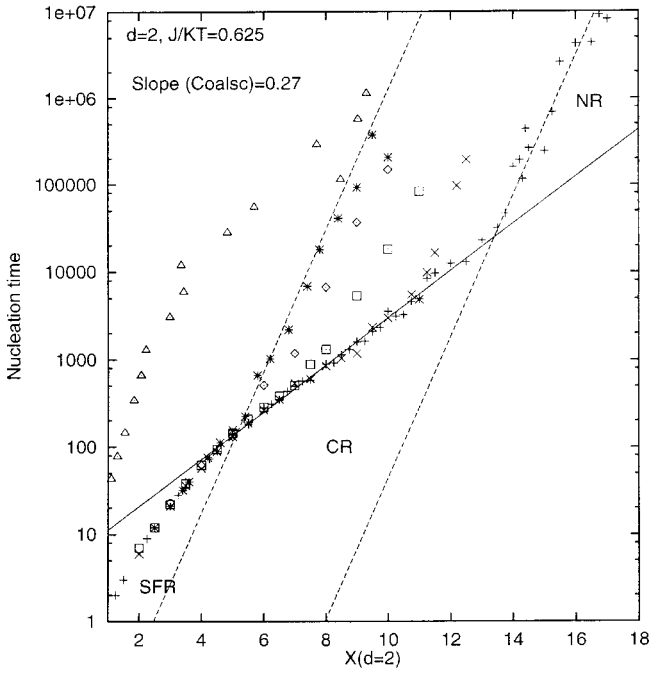

Fig. 3. Nucleation time (τ) (in logscale) plotted against $X(d = 2) = 1/h$ in $d = 2$. Different symbols correspond to different system sizes. $L = 80$ (star), $L = 100$ (diamond), $L = 400$ (box), $L = 1200$ (cross) and $L = 2048$ (plus). The solid line is the linear best fit in the coalescence regime (CR). The dashed line has a slope three times higher than that of the solid line. The reversal time (triangles for $L = 80$; in logscale) is also plotted against the inverse of the coercive field in the same plot. The nucleation regime is also shown here by another dashed straight line. In the low field regime, the reversal time and the nucleation time follow the same behaviour and are expected to agree. The intercepts of the straight lines depend on L.

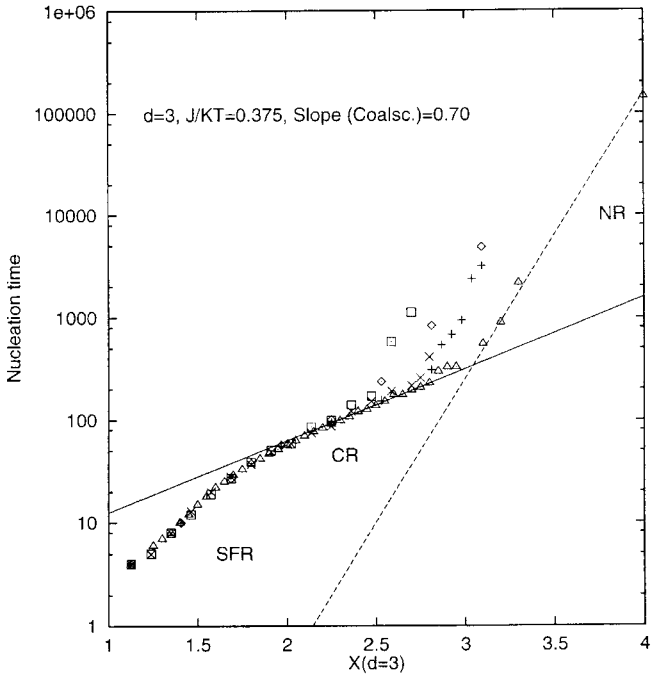

Fig. 4. Nucleation time (τ) (in logscale) plotted against $X(d = 3) = 1/h^2$ in $d = 3$. Different symbols correspond to different system sizes. $L = 60$ (box), $L = 64$ (diamond), $L = 90$ (cross), $L = 128$ (plus) and $L = 256$ (triangle). The solid line is the linear best fit in the coalescence regime (CR). The dashed line has a slope four times higher than that of the solid line.

theory. For the large lattice sizes, this value of the frequency will be much smaller. For example, if $L = 1200$, one can see (from extrapolation) that the crossover might be at $\omega \simeq 10^{-7}$. For shorter times (high frequency), the simulation results and the theoretical prediction (from CNT) for the coercive field (or loop area) with respect to frequency will disagree with each other. Due to this reason, the recent simulation results [8] show a power law variation of the coercive field with respect to frequency which is not in agreement with the theoretical prediction [9] obtained from CNT.

The simulations (for static field) are also done in $d = 3$ and 4. The results are depicted in Figures 4 and 5 respectively. Here also we observed the results are consistent with that of CNT. In Table I, all the results are summarised. The computational time for the largest lattices in all three dimensions are also given there. The surface tensions, calculated from the simulation (σ_{Sim}) are compared with the previous estimates (σ_{Prev}).

In Table 1 σ_{Hor}, the surface tension (in units of J) for horizontal direction, has been calculated from reference [11] and agrees nearly with the surface tension for

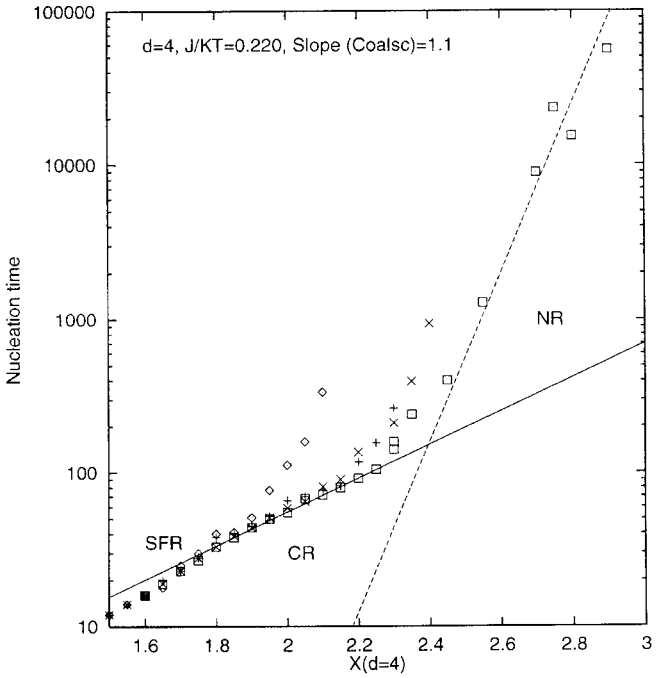

Fig. 5. Nucleation time (τ) (in logscale) plotted against $X(d = 4) = 1/h^3$ in $d = 4$. Different symbols correspond to different system sizes. $L = 17$ (diamond), $L = 31$ (plus), $L = 32$ (cross) and $L = 48$ (box). The solid line is the linear best fit in the coalescence regime (CR). The dashed line has a slope five times higher than that of the solid line.

Table 1.

d	L_{max}	τ_{max}	N_p	Time (CPU)	J/K_BT	Slope (in coalsc. regime)	σ_{Sim}	σ_{Prev}
2	2048	9160000	512	5293.3 s	0.625	0.27	1.378	$\sigma_{Hor} \simeq 1.06$
3	256	144250	32	5864.8 s	0.375	0.70	1.60	$\simeq 1.3$, Ref.[10]
4	48	55750	16	2602.9 s	0.220	1.10	1.363	–

45° direction with respect to the horizontal line. See reference [6a] for a discussion of the discrepancy between σ_{Sim} and σ_{Prev}.

5 Summary

We have studied nucleation in the two-, three- and four-dimensional Ising system by Monte-Carlo simulation with heat-bath dynamics. The logarithm of the nucleation time is found to be proportional to the $(-(d-1))$ power of the magnetic field. The size-dependent crossover from coalescence to nucleation is observed clearly in all dimensions. The surface tensions have been estimated from the proportionality constants (related to the surface tension) and are compared with the previous bulk estimates. The results are roughly consistent with the prediction of classical nucleation theory.

In two dimensions, the dynamical responses of the system are studied in a sinusoidally oscillating magnetic field. The reversal time has been studied as a function of the coercive field. For low enough frequency the logarithm of the reversal time is found to be proportional to the inverse of the coercive field. These results are compared with the nucleation results for static field; in the nucleation regime, the reversal time and the nuclation time become identical for low enough frequency.

However, for intermediate frequencies, the Monte-Carlo results [7,8] for the frequency variation of the dynamic coercivity and the hysteresis loop area do not agree with the theoretical predictions [9] obtained from classical nucleation theory.

In a recent study [12] the spin reversal transition was found in the two dimensional kinetic Ising model in a short-duration pulsed magnetic field. The phase boundary was drawn in the plane formed by the strength and duration (of activity) of the field. This is nothing but the variation of nucleation time as a function of field-strength. However, in that study, the results are mostly confined to strong fields and the coalescence regime. The asymptotic ($\Delta \to \infty$) functional form of this phase boundary can also be predicted from the classical nuclation theory and it will be $\ln(\Delta t) \sim 1/h_p$ for very large Δt and small h_p.

Recently [13] a similar crossover from nucleation regime to coalescence regime has been observed by Monte-Carlo simulation in three-dimensional anisotropic (large) Heisenberg model by tuning the temperature.

Sonderforschungsbereich 341 is gratefully acknowledged by one of us (MA) for financial support. MA would like to thank Bikas Chakrabarti, Deepak Dhar and Per Rikvold for important discussions. Authors would like to acknowledge the computational facilities provided by HLRZ, Jülich, Germany.

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