

Metastability in a four-spin Ising model

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2000 J. Phys. A: Math. Gen. 33 4451

(<http://iopscience.iop.org/0305-4470/33/24/304>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.123

The article was downloaded on 02/06/2010 at 08:22

Please note that [terms and conditions apply](#).

Metastability in a four-spin Ising model

Adam Lipowski^{†‡} and Des Johnston[†]

[†] Department of Mathematics, Heriot-Watt University, Edinburgh EH14 4AS, UK

[‡] Department of Physics, A Mickiewicz University, 61-614 Poznań, Poland

Received 27 July 1999, in final form 14 March 2000

Abstract. Slow dynamics and metastability are often seen in models with quenched disorder, but rather harder to find in situations where no such disorder is present and energy or entropy barriers must be generated dynamically. Using Monte Carlo simulations we show that the 3D four-spin interaction Ising model, which possesses no quenched disorder, exhibits rather strong metastability in a broad range of temperatures around its first-order transition point, due to the shape dependence of excitations in the model and the resulting largeness of the associated critical droplets.

1. Introduction

Although models which do *not* contain quenched disorder and display slow dynamics and metastability are rarer than those displaying metastability which do have quenched disorder, some examples are known. One such interesting model exhibiting slow dynamics and metastability, which is three dimensional, contains short-range interactions and does not have any quenched disorder, was proposed some years ago by Shore *et al* [1, 2], who studied the dynamics of a 3D ferromagnetic Ising model with antiferromagnetic next-nearest-neighbour interactions (the SS model)

$$H = J_1 \sum_{\langle ij \rangle} \sigma_i \sigma_j - J_2 \sum_{\langle\langle ij \rangle\rangle} \sigma_i \sigma_j. \quad (1.1)$$

They showed that the low-temperature coarsening of a random quench asymptotically becomes very slow and the characteristic length scale increases logarithmically in time. They also showed that in their model the transition into the slow-dynamics regime is induced by a corner-rounding transition at which the energy barriers should vanish. In the SS model the high-temperature phase (liquid) cooled below the critical point T_c but above the corner-rounding transition relatively quickly evolves toward the low-temperature crystalline phase. In more physically realistic models one would expect that when brought to this temperature range, liquid should not immediately crystallize or polycrystallize but, at least for some time, should remain in a metastable state of supercooled liquid.

Recently it has been shown that a 3D four-spin Ising model (FSIM) with plaquette interactions[†]

$$H = \frac{1}{2} J_1 \sum_{[i,j,k,l]} \sigma_i \sigma_j \sigma_k \sigma_l \quad (1.2)$$

[†] Where $\sigma_i = \pm 1$ and summation is performed over all elementary plaquettes (i, j, k, l) of a simple cubic lattice of linear size L with spins placed at the *sites* of the lattice.

also displays metastability without quenched disorder [3]. In particular, it was shown that in this model certain configurations are very long lived due to large energy barriers arising from the shape dependence of excitations.

The FSIM is a special case ($\kappa = 0$) of the so-called gonihedric models, which have recently been studied in the context of the lattice field theory [4,5]

$$H = J_1 \left[2\kappa \sum_{\langle i,j \rangle} \sigma_i \sigma_j - \frac{\kappa}{2} \sum_{\langle\langle i,j \rangle\rangle} \sigma_i \sigma_j + \frac{1-\kappa}{2} \sum_{[i,j,k,l]} \sigma_i \sigma_j \sigma_k \sigma_l \right]. \quad (1.3)$$

It is also noteworthy that for the particular ratio of couplings $(J_1/J_2) = \frac{1}{4}$ the SS model falls into the gonihedric family (this time with $\kappa = 1$). The ratio of terms in the gonihedric model is chosen specially to give no area contribution from the boundary of spin domains, in antithesis to the usual 3D Ising model. Closely related models have been studied with the aim of using the boundaries of their spin domains to model random surfaces and a very rich phase structure mapped out [6,7].

In this paper we investigate the FSIM model further. Firstly, we show that in the low-temperature regime the characteristic length $l(t)$ increases very slowly in time. We argue that this increase is likely to be logarithmic, namely $l(t) \sim \ln t$. Although the origin of the very slow dynamics in our model is basically the same as in the SS model, the nature of the observed transition to the slow-dynamics regime is quite different. Above the transition the model does not enter a fast-dynamics regime (as the SS model does) but remains trapped in a supercooled liquid phase. In addition, our estimation of the relevant characteristic time shows that energy barriers exist even above the transition point. This strongly suggests that the transition to the slow-dynamics regime in our model is not induced by a corner-rounding transition and that energy barriers persist even in this regime.

There are other properties of the FSIM which are very interesting. Our simulations show that in this model in the temperature range $3.4 < T < 3.9$, depending on the initial conditions, the model might be either in the liquid or the crystal phase. Using the thermodynamic integration method we calculated the free energies of both phases and, as expected, the crossing point (i.e., the first-order phase transition) appears approximately in the middle of the region of metastability. Such metastable effects (hysteresis) frequently accompany first-order phase transitions [8,9]. A distinctive feature of the metastability in the FSIM is that it is an extremely strong effect. We show that even for temperatures close to the limits of hysteresis only a large droplet of the stable phase injected into the metastable phase can divert the evolution of the system into the stable phase. Spontaneous nucleation of such large droplets is an extremely improbable event, and is well beyond the range of our simulations.

This paper is organized as follows. In section 2 we introduce the model, review its basic properties and study the evolution of random quench. In section 3 we calculate the free energy and the specific heat and present the time evolution of internal energy. In section 4 we discuss metastability properties of our model. Section 5 contains our conclusions.

2. Basic properties and domain coarsening

The basic properties of the FSIM which are already known can be briefly described as follows. The ground state is strongly degenerate with the degeneracy $\sim 2^{3L}$ (the ground state entropy per site is thus zero). Monte Carlo simulations show [3,5] that upon heating of an arbitrary ground state (crystal) configuration, the model appears to undergo a discontinuous phase transition into the disordered phase (liquid) around $T \sim 3.9$; the temperature scale is set as in [3] with the Boltzmann constant put to unity. An important feature of the FSIM is the shape dependence of excitations [3]: it is not only the size of the excitation which determines its energy (as in the

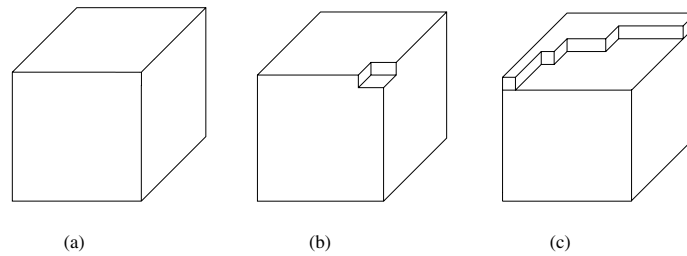


Figure 1. In the FSIM the energy of an excitation (e.g., ‘down’ spins surrounded by ‘up’ spins) is proportional to the total length of edges of the boundary of that excitation. To remove a cubic excitation (a), the system is likely to proceed through configurations like those shown in (b) and (c). It is easy to realize that in (b) and (c) the total length of edges and thus the energy of such configurations is larger than that in (a). In the case (c) the energy increase is proportional to the linear size of the excitation. In contrast, in a two-spin Ising model all configurations would have the same energy (since the area of all configurations is the same) and removal of excitations would proceed without climbing any energy barriers.

ordinary two-spin Ising model) but also its shape (see figure 1). This property, which holds also for the SS model, gives rise to energy barriers which are in turn responsible for the very slow dynamics of both models.

To study the evolution of the random configuration quenched to low temperature, we measured the energy excess $\delta E(t) = E(t) - E_0$ over the ground state energy $E_0 = -3$. One expects [2] that the inverse of this quantity sets the characteristic length scale $l(t)$ of the system, which roughly corresponds to the average size of domains. Moreover, there is convincing evidence [10] that in many systems with nonconservative dynamics and a scalar order parameter (i.e., conditions which are satisfied in our approach) $l(t)$ increases asymptotically in time as $l(t) \sim t^n$ and $n = \frac{1}{2}$. However, in some systems $l(t)$ is known to increase logarithmically, $l(t) \sim \log(t)$. These exceptional systems include some random (at the level of the Hamiltonian) systems [11, 12], and the SS model for temperatures below the corner-rounding transition[†]. Energy barriers developing in the non-random systems during the coarsening cause the slow increase of $l(t)$.

We performed standard [14] Monte Carlo simulations using the Metropolis algorithm with a random sequential update. Unless stated otherwise, periodic boundary are imposed throughout. The log–log plot of $1/\delta E(t)$ as a function of time for the FSIM is shown in figure 2. The presented results were obtained for $L = 40$ but very similar behaviour was observed for $L = 30$. From figure 2 it is clear that for $T = 1.5$ and 2.8 the asymptotic slopes of the curves are much smaller than $\frac{1}{2}$ and there is a tendency for these curves to bend downwards. Taking into account the absence of models with n considerably smaller than $\frac{1}{2}$, and the existence of energy barriers in the FSIM of basically the same nature as in the SS model, suggests that for the examined temperatures the characteristic length asymptotically increases logarithmically in time. We cannot exclude, however, that in this temperature regime the increase of $l(t)$ is even more exotic, with neither logarithmic nor power-law increase. It would appear that such a slow increase of $l(t)$ takes place even for $T = 3.3$ and 3.4, but the behaviour of $l(t)$ for these temperatures is obscured by the metastability effects, since before collapsing into the glassy phase the system remains in the liquid state for some time.

The difference between our model and the SS model becomes clear when we approach the lower boundary of the metastable region which we roughly estimate to lie at $T = T_1 \sim 3.4$ by

[†] For additional confirmation of logarithmically slow growth of $l(t)$ in the SS model see [13].

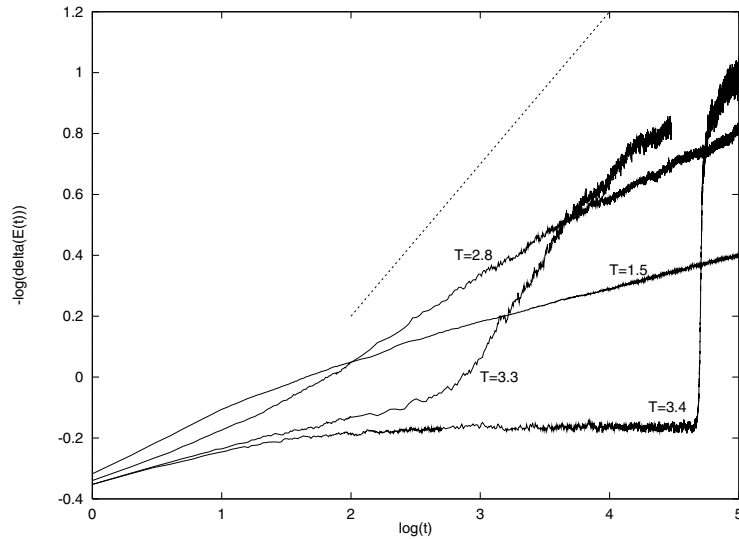


Figure 2. The log–log plot of $1/\delta E(t)$ as a function of time t ($L = 40$). The dashed line has a slope $\frac{1}{2}$.

increasing the temperature. In the SS model for temperatures below the critical point but above the corner-rounding transition thermal fluctuations roughen corners of domains and energy barriers are no longer relevant. Consequently, the ‘ordinary’ dynamics with $n = \frac{1}{2}$ is restored and the system rapidly evolves toward the low-temperature phase. In contrast, in the FSIM for $3.4 < T < 3.9$ the random quench does not even evolve toward the low-temperature phase but remains disordered [3]. Since the low-temperature phase does exist at these temperatures (as we have already mentioned, the transition from the low-temperature phase to the disordered phase takes place around $T = T_u \sim 3.9$), there should be some barriers which prevent the liquid from collapsing. We conjecture that these barriers are of entropic origin and may be related to the strong degeneracy of the ground state, which would explain why the behaviour of our model is different from the SS model[†]. This phenomenon is discussed further in section 4.

3. Free energy and specific heat

The free energy encodes all the important thermodynamic information about a system. In equilibrium statistical mechanics this quantity is defined as

$$f = -T/N \ln \left[\sum e^{-H/T} \right] \quad (3.1)$$

where N is the number of particles (lattice sites) and H is the Hamiltonian of the system with the Boltzmann constant put to unity. However, calculation of the above-defined free energy using Monte Carlo simulations is not straightforward and requires thermodynamic integration [14]. To calculate the free energy of our model in the liquid and crystal phases we used the following equations:

$$f_{\text{cryst}} = u - T \int_0^T \frac{c}{T} dT \quad f_{\text{liq}} = -Ts(\infty) + T \int_0^{1/T} u d\left(\frac{1}{T}\right). \quad (3.2)$$

[†] Entropic barriers are known to play an important role in glassy systems (see e.g., [15]).

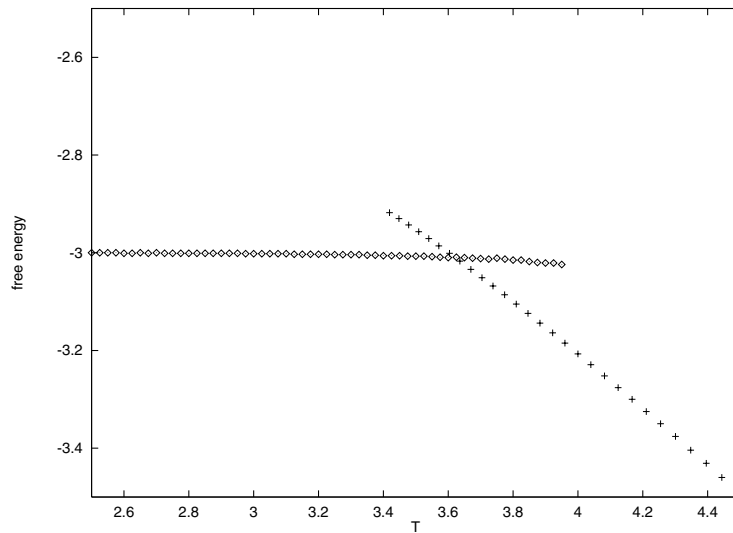


Figure 3. The free energy of liquid (+) and crystal (\diamond). Calculations were done for $L = 30$, and 5000 Monte Carlo steps were used at each temperature. The integration steps were $\Delta T = \Delta(1/T) = 0.025$.

In the above equation c and u denote the specific heat and internal energy, respectively (calculated using standard formulae [14]), and $s(\infty) = \ln(2)$ is the entropy per site at infinite temperature. The results of our calculations are shown in figure 3. We checked the stability of our results with respect to the integration step ΔT (or $\Delta(1/T)$), the system size L and the number of Monte Carlo steps at each temperature.

In figure 3 one can see that the free energies of the crystal and of the liquid cross around $T = 3.6$ and we expect that this is the temperature of the first-order phase transition. The estimation of the transition temperature is in a good agreement with calculations done using the cluster variational/Padé approximant method (CVPAM) [16]. However, due to the strong metastability, which is discussed in more detail in the next section, the thermodynamic transition at this point is very difficult to observe. Indeed, if we heat a crystal sample, we see the boundary of the metastable region at $T_u = 3.9$, while cooling a liquid sample we see the boundary at $T_l = 3.4$, which also agree well with the limits of metastability calculated in [16] using CVPAM methods.

To overcome the metastability and confirm that a first-order transition *does* take place around $T = 3.6$, we simulated the system with a nonuniform initial configuration by preparing the system with one half in the crystal phase (e.g., all spins ‘up’) and the other half in the liquid phase (all spins random); see figure 4. Such a choice facilitates the evolution toward the stable phase (i.e., the one with the lowest free energy), but because both phases are present in the initial configuration the system does not have to nucleate the stable phase. The results of such simulations are shown in figure 5 where one can clearly see that the evolution of the system depends on whether the temperature is above or below $T = 3.6$. For $T < (>) 3.6$ the crystal (liquid) phase gradually expands until the stable phase invades the whole system. The identification of the final state is obtained from a comparison of its internal energy with simulations which use a uniform initial state and confirmed from the visual inspection of snapshot Monte Carlo configurations.

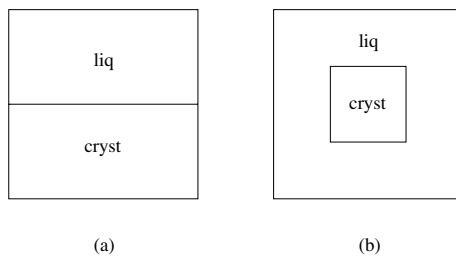


Figure 4. Two-dimensional sections of initial configurations used in our calculations. (a) An initial configuration used in the calculations of internal energy shown in figure 5. (b) An initial configuration with a droplet of crystal phase injected into the liquid phase (see section 4.2). Spins in the crystal/liquid part of the system are initially set 'up'/at random.

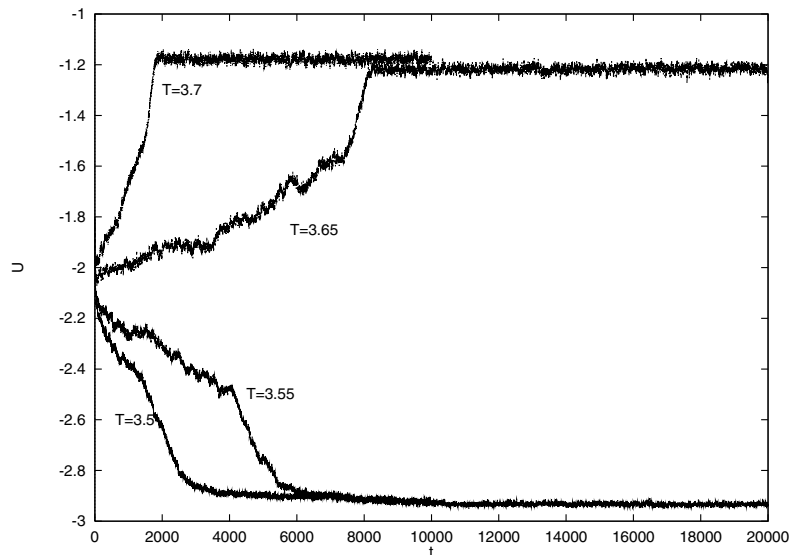


Figure 5. The internal energy U as a function of time for $L = 50$ and an initial configuration composed of 50% of crystal and 50% of liquid (see figure 4(a)). The steady-state values of U for $T = 3.5, 3.55$ and for $T = 3.65, 3.7$ are identical (within error bars) with the internal energy of crystal and liquid at corresponding temperatures.

To provide additional information about the FSIM, we measured the variance of the internal energy and calculated the specific heat [14]. Our data are shown in figure 6. When we start our simulations from the ground-state configuration (heating), the behaviour of the specific heat appears to show a transition around $T_u = 3.9$, in agreement with earlier simulations [3,5]. However, under cooling this peak is shifted toward much lower temperature and it seems to coincide with our estimation of T_l . Under cooling we do not observe any singularity in the specific heat until $T = T_l$, which indicates that during cooling the system remains in the liquid phase for $T > T_l$. Let us note that the locations of both peaks are almost unchanged after increasing the system size by almost a factor of two. Moreover, for $T < T_l$ the specific heat is slightly larger upon cooling than upon heating. This is in agreement with the fact that in this temperature range the model has slow dynamics and cannot reach the crystal phase within numerically accessible computing time, for which the specific heat is very small.

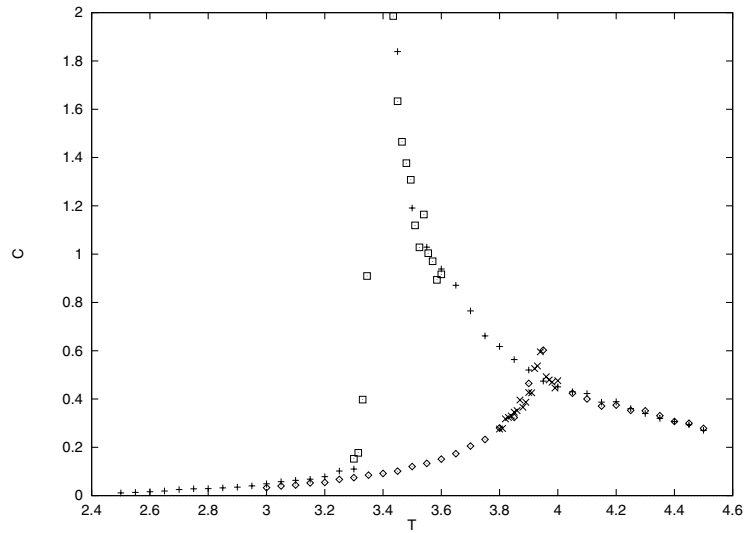


Figure 6. The specific heat calculated during (i) heating for $L = 24$ (\diamond) and $L = 40$ (\times) and (ii) cooling for $L = 24$ ($+$) and $L = 40$ (\square). For each temperature and system size we made runs of 10^4 Monte Carlo steps plus 10^3 Monte Carlo steps for relaxation.

4. Metastability

Results presented in the previous sections suggest that in the temperature range $T_1 < T < T_c$ the system might remain in either the liquid or the crystal phase. In the present section we present some additional results concerning the (meta-) stability of the liquid and crystal phases.

4.1. Characteristic times

We measured various characteristic times imposing different initial and boundary conditions and monitoring the evolution toward a final state. To check the stability of the liquid (τ_{liq}), we used a random initial configuration and simulated the system until the energy reached $E = -2.3\ddagger$. To calculate τ_{liq} we made 100 independent runs. Our results for $T = 3.5$ are shown in figure 7 and they suggest that the escape time increases at least exponentially with the system size.

To check the stability of the crystal, one should measure the time (τ_+) needed for the crystal to be transformed into the liquid. It would be particularly interesting to examine the size dependence of τ_+ for $3.6 < T < 3.9$, i.e., for temperatures where the crystal is metastable. We have found, however, that this quantity increases very rapidly with the system size and in this temperature range it is virtually impossible to increase the system size beyond $L = 6$. The stability of this phase might be also inferred from other measurements we made in which we estimated the time (τ_{+-}) needed to shrink a cubic excitation of size L . This technique parallels that which has already been applied to the SS model [2]: the initial configuration has ‘up’ spins at the boundary of the cube of size $L + 2$ (which are kept fixed) and ‘down’ spins inside this cube. Simulations are performed until the magnetization of the interior of the cube decays to zero and the time needed for such a run is recorded. To calculate τ_{+-} at a given temperature we made 100 independent runs. Our results for $T = 3.6$ (figure 7) suggest that τ_{+-} increases

\ddagger This value is chosen rather arbitrarily, but once the system reaches this energy it does not return to the liquid phase.

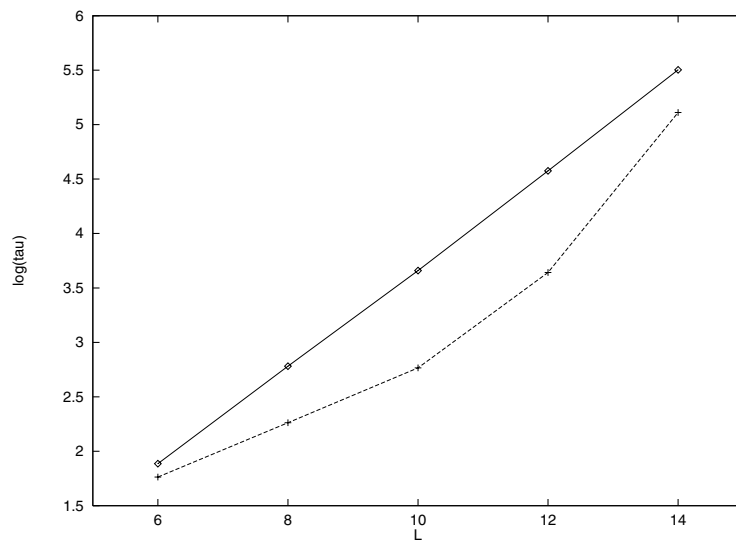


Figure 7. The size dependence of the logarithm of the escape times τ_{liq} (\square) and τ_{+-} ($+$). Calculation of τ_{liq} and τ_{+-} was performed for $T = 3.5$ and 3.6 , respectively.

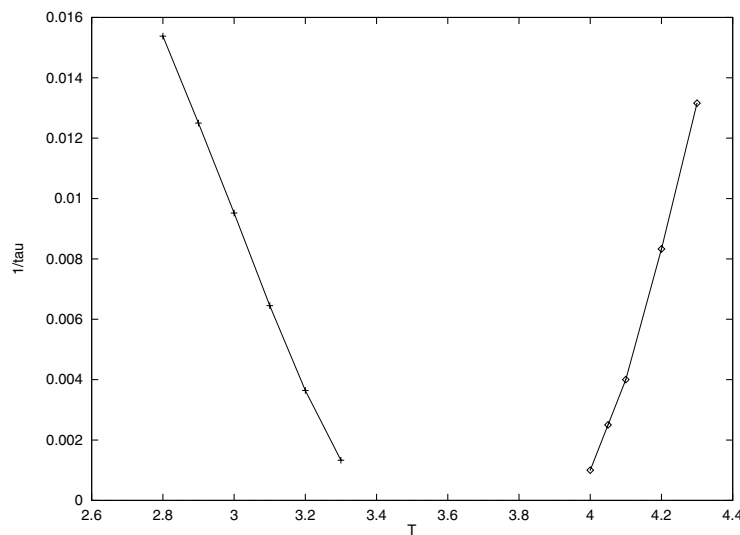


Figure 8. The inverse of the characteristic times τ_{liq} ($+$) and τ_{+} (\diamond) as a function of temperature. The plotted results are obtained by extrapolation of the finite-size data to the thermodynamic limit.

approximately exponentially with L , whereas above the corner-rounding transition in the SS model one expects $\tau_{+-} \sim L^2$ [2], in which case the data in figure 7 would bend considerably downwards. This also confirms the stability of the crystal since it is clear that bringing the crystal (a homogeneous, low-energy configuration) into the liquid is a slower process than shrinking an excitation. Similar size dependence of τ_{liq} and τ_{+-} was also observed for other temperatures in the interval $3.4 < T < 3.9$.

We also measured the characteristic times τ_{liq} and τ_{+} outside the interval $3.4 < T < 3.9$. Simulations were performed for several values of system size L and the results were extrapo-

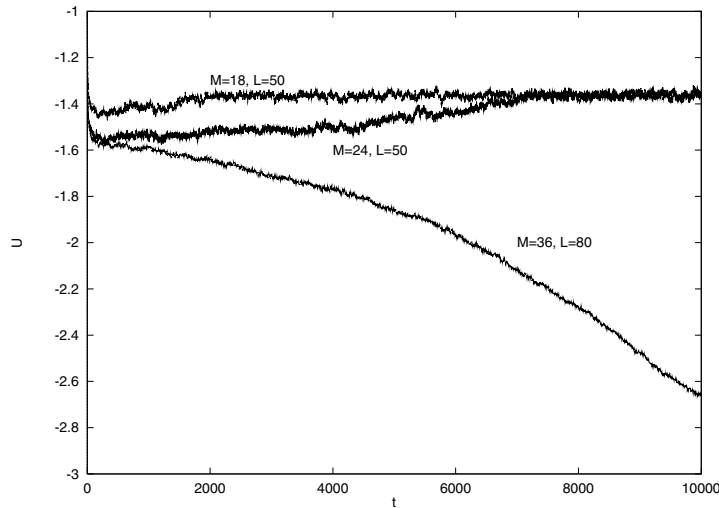


Figure 9. The internal energy U as a function of time for $T = 3.5$. The initial configuration consists of a droplet of crystal phase of size M injected into the liquid phase.

lated to the thermodynamic limit ($L \rightarrow \infty$) using a simple fit[†]. These extrapolated values are shown in figure 8. One can see that outside this temperature range τ_{liq} and τ_+ are definitely finite and they seem to diverge upon approaching $T = 3.4$ from below (τ_{liq}) and $T = 3.9$ from above (τ_+).

4.2. Droplets of a stable phase

The numerical data presented in the previous section suggest that for $3.4 < T < 3.9$ the model has two different phases of effectively infinite lifetime. Such a result would be in disagreement with the result that in short-range interacting systems metastability is only a quantitative effect [8, 9]. In this section we show, however, that data presented in figures 7 and 8 are misleading and in the thermodynamic limit ($L \rightarrow \infty$) the characteristic times τ_{liq} for $T < 3.6$ and τ_+ for $T > 3.6$ should be finite. The timescale of these metastable effects is, however, enormously long in comparison with the length of our simulations.

One expects that metastable phases have only a finite lifetime due to droplet nucleation. When a sufficiently large droplet of stable phase nucleates inside a metastable phase, it diverts evolution of the system toward a stable phase. Since the critical (i.e., minimal) droplet size is finite, there is a finite probability of spontaneous nucleation of such droplets and thus the lifetime of a metastable phase is also finite.

To check whether such a mechanism operates in the FSIM, we monitored the evolution of the system with droplets introduced by hand into the initial configuration (see figure 4). Our results for $T = 3.5$ are shown in figure 9. One can see that when a droplet of the crystal is sufficiently small (of linear size $M = 18, 24$), the system after some transient ends up in the liquid phase. However, a large droplet of size $M = 36$ diverts evolution of the system toward the more stable phase. We performed similar simulations to examine the (meta-) stability of the crystal phase. Setting $T = 3.8$ we observed that droplets of liquid of size $M \geq 24$ divert evolution of the crystal phase toward the stable liquid phase.

[†] We plotted the results for finite L as a function of $x = 1/L$ and then used a parabolic fit to extrapolate the value at $x = 0$.

The above results show that the droplet-nucleation mechanism is effective in the FSIM and the metastable phases are of finite lifetime. However, the important question is how long this lifetime is. This quantity is determined by the inverse of the probability of the spontaneous nucleation of critical droplets. It is clear that for computationally accessible systems ($L \sim 100$) spontaneous nucleation of crystal droplets of linear size $M \sim 30$ is an extremely unlikely event, which takes place on astronomical timescales. We should emphasize that this does not mean that our model predicts such a lifetime of metastable liquids. Since the nucleation of droplets is basically a local event, its probability for macroscopic systems increases merely due the system size (droplets might nucleate independently in many places).

The radius of critical droplets presumably vanishes upon approaching the limits of hysteresis (i.e., $T = 3.4$ and 3.9). Thus, very close to these limits one should be able to observe finite-lifetime effects such as the spontaneous collapse of liquid into the crystal or disordered phase.

5. Conclusions

In the present paper we have studied the 3D Ising model with four-spin interactions. The Hamiltonian of this model is homogeneous, non-frustrated and contains only short-range plaquette interactions. Nevertheless, we found that this model has very interesting dynamical and thermodynamical properties. In particular, our numerical results suggest that the model displays very slow coarsening dynamics in its low-temperature phase. Moreover, due to very strong metastability in the temperature range $3.4 < T < 3.9$ the model can remain in either a crystal or liquid phase, depending on how it has been prepared. We have shown that a droplet-nucleation mechanism is, however, still effective and thus that metastability in this model is a finite-size, but extremely strong, effect. The timescale of spontaneous nucleation for critical droplets is extremely large and lies well beyond the timescales of our simulations.

References

- [1] Shore J D and Sethna J P 1991 *Phys. Rev. B* **43** 3782
- [2] Shore J D, Holzer M and Sethna J P 1992 *Phys. Rev. B* **46** 11 376
- [3] Lipowski A 1997 *J. Phys. A: Math. Gen.* **30** 7365
- [4] Ambartzumian R V, Sukiasian G S, Savvidy G K and Savvidy K G 1992 *Phys. Lett. B* **275** 99
- [5] Espriu D, Baig M, Johnston D A and Malmini R P K C 1997 *J. Phys. A: Math. Gen.* **30** 405
- [6] Karowski M 1986 *J. Phys. A: Math. Gen.* **19** 3375
- [7] Cappi A, Colangelo P, Gonella G and Maritan A 1992 *Nucl. Phys. B* **370** 659
Colangelo P, Gonnella G and Maritan A 1993 *Phys. Rev. E* **47** 411
Gonnella G and Maritan A 1993 *Phys. Rev. B* **48** 932
Gonnella G, Lise S and Maritan A 1995 *Europhys. Lett.* **32** 735
- [8] Penrose O and Lebowitz J L 1979 *Fluctuation Phenomena* ed E W Montroll and J L Lebowitz (Amsterdam: North-Holland)
- [9] Rikvold P A and Gorman B M 1994 *Annual Review of Computational Physics* vol 1, ed D Stauffer (Singapore: World Scientific)
- [10] Bray A J 1994 *Adv. Phys.* **43** 357
- [11] Lai Z W, Mazenko G F and Valls O T 1988 *Phys. Rev. B* **37** 9481
- [12] Rao M and Chakrabarti A 1993 *Phys. Rev. Lett.* **71** 3501
- [13] Rao M and Chakrabarti A 1995 *Phys. Rev. E* **52** R13
- [14] Binder K 1984 *Applications of the Monte Carlo Method in Statistical Physics* ed K Binder (Berlin: Springer)
- [15] Mohanty U, Oppenheim I and Taubes C H 1994 *Science* **266** 425
Kirkpatrick T R and Wolynes P G 1987 *Phys. Rev. B* **36** 8552
- [16] Cirillo E N M, Gonella G, Johnston D A and Pelizzola A 1997 *Phys. Lett. A* **226** 59