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Zero-temperature dynamics of 2D and 3D Ising ferromagnets

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Abstract

We consider zero-temperature, stochastic Ising models σ^t with nearest-neighbour interactions in two and three dimensions. Using both symmetric and asymmetric initial configurations σ^0 , we study the evolution of the system with time. We examine the issue of convergence of σ^t and discuss the nature of the final state of the system. By determining a relation between the median number of spin flips per site ν , the probability p that a spin in the initial spin configuration takes the value $+1$, and lattice size L , we conclude that in two and three dimensions, the system converges to a frozen (but not necessarily uniform) state when $p \neq 1/2$. Results for $p = 1/2$ in three dimensions are consistent with the conjecture that the system does not evolve towards a fully frozen limiting state. Our simulations also uncover ‘striped’ and ‘blinker’ states first discussed by Spirin *et al* (2001 *Phys. Rev. E* **63** 036118), and their statistical properties are investigated.

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1. Introduction

Consider the stochastic process σ^t corresponding to the zero-temperature limit of Glauber dynamics for a ferromagnetic Ising model with Hamiltonian

$$\mathcal{H} = - \sum_{\langle x,y \rangle} \sigma_x \sigma_y. \quad (1)$$

Here $\langle \cdot \rangle$ denotes a sum over nearest-neighbour sites only and $x, y \in \mathbf{Z}^d$, the d -dimensional hypercubic lattice. So σ^t takes values in $\mathcal{S} = \{-1, +1\}^{\mathbf{Z}^d}$, the space of infinite-volume spin configurations on \mathbf{Z}^d . The process σ^t can be interpreted as modelling the nonequilibrium dynamical evolution of a classical Ising ferromagnet following a deep quench.

Perhaps the most basic question that can be asked is whether the process σ^t settles down to a limit as $t \rightarrow \infty$. Knowledge of this fundamental long-time property is a prerequisite for studying persistence properties [2–7], and useful for the understanding of domain formation and evolution, spatial and temporal scaling properties, and related questions (for a review, see [8]), as well as ageing phenomena (see, e.g., [9–13]).

Given the fixed lattice type and dynamics under consideration, the convergence of σ^t can depend only on dimension d and on the starting spin configuration σ^0 . (Other lattice types were considered in [14, 15].) Rigorous results exist for symmetric σ^0 (i.e., for all x , $\sigma_x^0 = \pm 1$ with equal probability, independently of all other spins, corresponding to a quench from infinite to zero temperature in zero external field) in $d = 1, 2$; here every spin flips infinitely often [14, 15]. Numerical studies by Stauffer [2] indicate that this result may hold up to $d = 4$, beyond which σ^t could have a limit. There are few numerical studies [16] of the long-time behaviour of σ^t given *asymmetric* σ^0 (corresponding to a deep quench in nonzero external field) in dimensions greater than one.

In this paper we present the results of numerical studies that examine the question of convergence of σ^t for $d = 2$ and 3 with both symmetric and asymmetric initial conditions. It is known that the magnetization per spin at zero temperature

$$M(t) = \lim_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} \sum_{x \in \Lambda_L} \sigma_x(t), \quad (2)$$

where Λ_L is an L^d cube centred at the origin, is independent of time in one dimension for any initial magnetization [17]. This time invariance of the magnetization under Glauber dynamics at zero temperature does not hold in higher dimensions; indeed, it is easy to see, using the independence of the spins in σ^0 , that in 2D at time $t = 0$ the sign of dM/dt is that of the initial magnetization. For $d = 2$ our results indicate that the long time behaviour of the symmetric case is unstable to small perturbations in the following sense: for any deviation from up–down symmetry in the initial state, σ^t flows towards the uniform final state which is magnetized in the direction of the initial asymmetry. While this result is not surprising, it settles the question of whether the nonexistence of σ^∞ could persist for a nonzero range of asymmetry in σ^0 . Our results for 2D are summarized in figure 1. For a 2D lattice of finite size, a non-uniform final state called the frozen stripe state is also possible. Such a configuration occurs when the spins are aligned parallel to the axes and cease to flip thereafter.

In addition to the frozen stripe state, a finite size 3D lattice can evolve towards a ‘partially frozen’ state (called ‘blinker states’ in [16]) when a subset of the spins continue to flip ceaselessly, without any change in energy, while the remainder of the spins do not flip any more. Our results for the symmetric case in 3D agree with those of Stauffer [2]. For $p = 1/2$, we find, in agreement with [16], frozen stripe states and blinker configurations, to be discussed in the following sections.

We also discuss the question of extrapolation of results on finite size lattices to those of infinite extent.

2. Definitions and previous results

So far we have defined the problem informally: following a quench from infinite to zero temperature, in zero or nonzero external magnetic field, and subsequently evolving through standard Glauber dynamics in zero field, will the spin configuration eventually settle down to a final state, or will it continue to evolve forever (and if so, in what sense)?

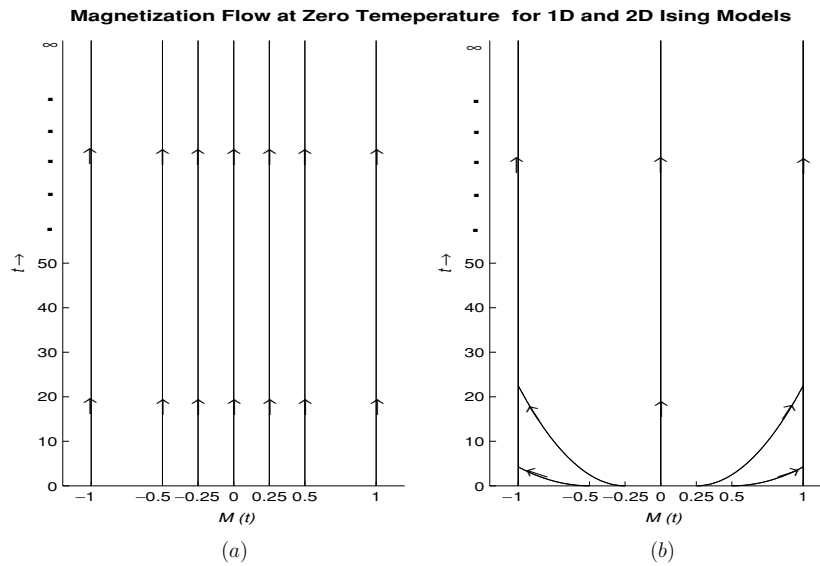


Figure 1. Sketch of magnetization flow at zero temperature under the Glauber dynamics discussed in the text. (a) One dimension. (b) Two dimensions.

We now state the problem more precisely. The initial spin configuration σ^0 is chosen from a Bernoulli product measure (denoted P_{σ^0}), with each spin independently having value $+1$ with probability p and -1 with probability $1 - p$. The initial magnetization $M(0) = 2p - 1$. The symmetric case corresponds to $p = 1/2$ and has $M(0) = 0$; any other P_{σ^0} will be called asymmetric.

The (single-spin-flip) dynamics will be taken to be continuous time, given by independent rate 1 Poisson processes at each x corresponding to those times t_x (which can be thought of as clock rings at x) when a spin flip ($\sigma_x^{t+0} = -\sigma_x^{t-0}$) is considered. If the resulting change in energy is negative, then the flip occurs with probability 1, and if positive, with probability 0. If there is a ‘tie’, i.e., the resulting change in energy would be zero, then the flip occurs with probability $1/2$, as determined by a fair coin toss. We denote by P_ω the probability distribution on the realizations ω of the dynamics.

So there are two sources of randomness, in the dynamics ω and in the initial spin configuration σ^0 . The joint distribution of ω and σ^0 will be denoted P . All results to be discussed below are to be understood as occurring with probability one in P .

The question posed in the introduction is whether σ^t has a limit, with P -probability one, as $t \rightarrow \infty$. This is equivalent to σ_x^t flipping only finitely many times for every x . Using the same nomenclature as in [15], we call such an x an \mathcal{F} -site (\mathcal{F} for finite); if σ_x^t flips infinitely often it is an \mathcal{I} -site (\mathcal{I} for infinite). By translation ergodicity, the collection of \mathcal{F} -sites (resp., \mathcal{I} -sites) has (with P -probability one) a well-defined non-random spatial density $\rho_{\mathcal{F}}$ (resp., $\rho_{\mathcal{I}}$). The densities $\rho_{\mathcal{F}}$ and $\rho_{\mathcal{I}} (= 1 - \rho_{\mathcal{F}})$ can depend on both d and p . A particular model will be said to be of type \mathcal{F} , \mathcal{I} or \mathcal{M} (for mixed) according to whether $\rho_{\mathcal{F}} = 1$, $\rho_{\mathcal{I}} = 1$ or $0 < \rho_{\mathcal{F}}, \rho_{\mathcal{I}} < 1$, respectively.

In one dimension the analysis is particularly simple, and it is fairly straightforward to show that, for any $0 < p < 1$, the model is type- \mathcal{I} [14]. (The proof given there is for $p = 1/2$ only, but the result is not hard to extend to asymmetric models.) In [14] it was also shown that the homogeneous ferromagnet with $p = 1/2$ on \mathbf{Z}^2 is type- \mathcal{I} ; essentially the same argument

holds for the homogeneous antiferromagnet on \mathbf{Z}^2 with symmetric initial conditions. No results were obtained for asymmetric initial conditions.

We note for completeness that the $\pm J$ spin glass on \mathbf{Z}^2 with symmetric initial conditions was shown to be type \mathcal{M} [19]; the proof is far more involved than those for the homogeneous cases. These are models in which couplings are chosen *a priori* from a symmetric Bernoulli distribution, with values $+1$ or -1 , and are thereafter quenched. (In fact a much wider class of related models was also shown to be type- \mathcal{M} , but these are less relevant to the models studied here.)

Under periodic boundary conditions, convergence to a final $+1$ or -1 state is not guaranteed: the lattice can form *domain walls* parallel to the lattice axes. These walls are stable under the dynamics (hence referred to as the frozen ‘stripe’ states), so any state with one or more such walls (non-intersecting, i.e., all in either the x - or the y -direction) is a final state. A simple example of a domain wall in a 4×4 lattice is shown below:

```

+ + + +
+ + + +
- - - -
- - - -

```

Investigations into this freezing phenomenon for a zero-temperature Ising ferromagnet having single-spin flip Glauber dynamics indicate that the system need not always evolve into the uniform state. Studies investigating the final state of zero-temperature Ising ferromagnets [16] by Spirin *et al* indicate that when $d = 2$, the system reaches either a frozen ‘striped’ state (i.e., with one or more domain wall pairs) with probability $\approx 1/3$ or the uniform state with probability $\approx 2/3$. (Striped phases have also been seen in certain driven diffusive systems [18].) Moreover their study indicates that these frozen states persist with positive probability as $L \rightarrow \infty$. When $d > 2$, persistent configurations other than the striped or uniform state are also observed. In these, the system wanders through a series of iso-energy partially frozen states. These metastable states are called *blinkers* in [16] and consist of localized sets of spins that flip forever with zero energy cost, surrounded by frozen spins. These blinkers become more numerous as the lattice size increases and the system is more likely to be trapped in one of these states. Presence of blinkers in the infinite system would indicate that it is of type- \mathcal{M} . These results will be discussed further in section 4.

3. Simulation results

Zero-temperature Glauber dynamics has been implemented by each spin independently chosen to flip through a Poisson process having rate parameter $\mu = 1$. When a particular site is selected, it assumes the sign of the majority of its neighbours. In the case of a tie, the sign of the spin is determined by a fair coin toss.

Results depicting the median value of spin flips, \mathcal{N} , for 2D and 3D Ising models of different lattice sizes are shown in figures 2 and 3, respectively. For those runs in which the system converges to a final uniform state, \mathcal{N} has been computed by averaging several independent (both in choice of initial spin configuration and in dynamical realization) runs.

Our simulations in 3D also uncovered blinker states. When such a state appeared, the ‘unfrozen’ spins (i.e. those that continued to flip) were tracked.

From the simulation data for the 2D lattice, we observe that the number of spin flips is symmetric about a maximum at $p = 1/2$ irrespective of the lattice size. We also observe that the slope of this curve is sharpest near $p = 1/2$, while it remains relatively constant for very

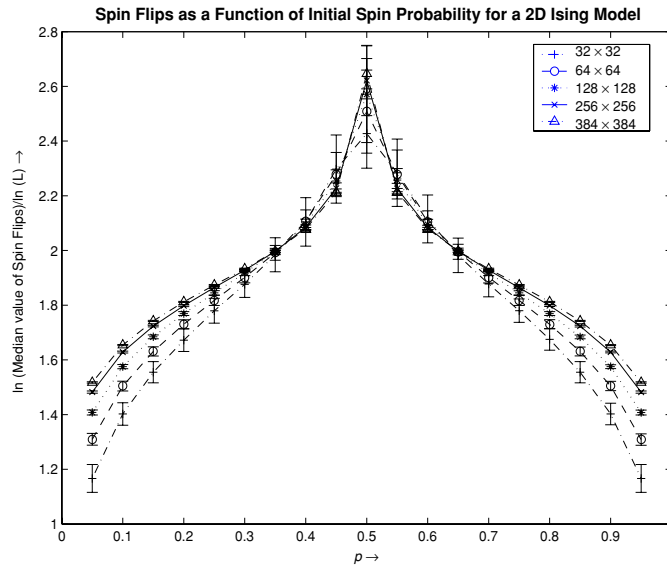


Figure 2. $\ln \mathcal{N} / \ln L$, as a function of p in a 2D Ising Model. At least 10^3 independent runs have been considered for $L < 256$, and at least 5×10^2 independent runs for $L \geq 256$.

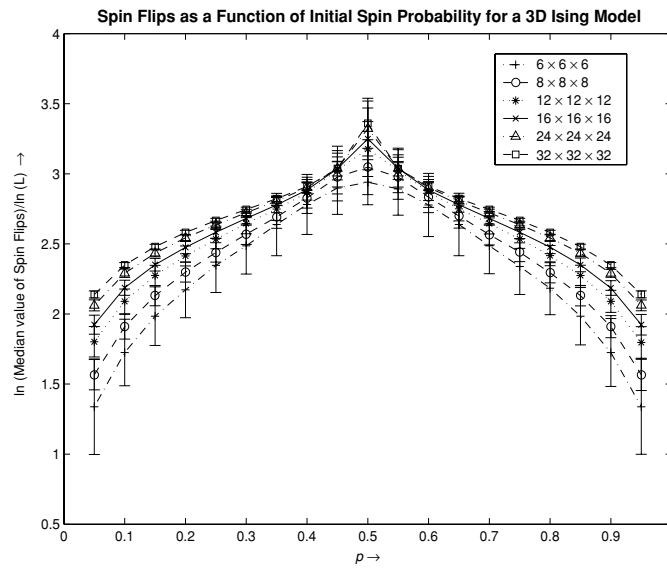


Figure 3. $\ln \mathcal{N} / \ln L$, as a function of p in a 3D Ising Model. At least 10^3 independent runs have been considered for all values of L , and only configurations that settle down to a fully frozen final state are included.

small or large values of p . For both the 2D and 3D models, the family of curves corresponding to different lattice sizes collapses to a single curve when $\ln \mathcal{N} / \ln 2L$ is plotted versus p . For very large lattice sizes, we have observed that the system almost always converges to a ± 1 state even for small departures from $p = 1/2$.

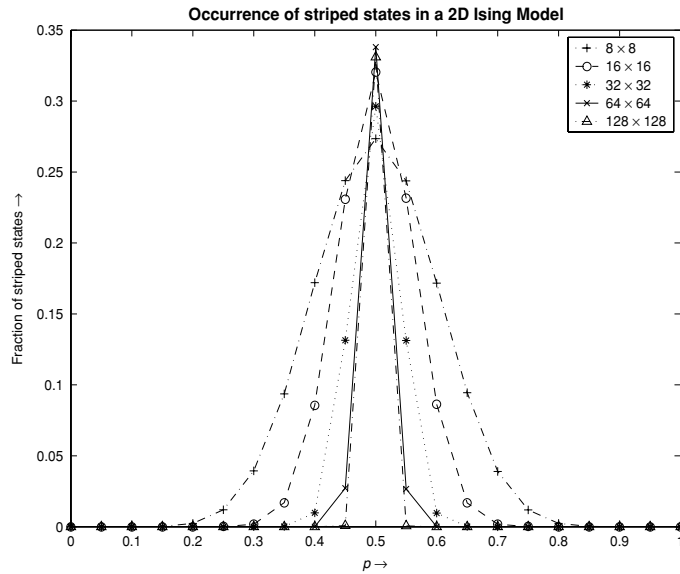


Figure 4. Occurrence of striped states as a function of p for a 2D Ising model. At least 10^6 independent runs have been considered for $p \neq 1/2$, and at least 10^3 runs for $p = 1/2$.

It is interesting to study the fraction of striped states as a function of p and lattice size L . This has been studied for a 2D model shown in figure 4. We observe that when $p = 1/2$, as the lattice size increases, the fraction of the spins converging to a final striped state asymptotically tends towards $1/3$, in agreement with the results in [16]. When $p \neq 1/2$, the fraction of final spin configurations in the striped state decreases as lattice size increases; i.e., the uniform state is increasingly favoured. No blinker configurations are present in the 2D lattice. These results are consistent with the known result [15] that the infinite square lattice is type- \mathcal{I} for $p = 1/2$, and they indicate that otherwise the lattice is type- \mathcal{F} .

Figure 3 shows results for the 3D cubic lattice; the data collapse similarly to the 2D case. As expected, the maximum number of spin flips occurs when $p = 1/2$. Figure 5 shows the occurrence of striped states as a percentage of the total number of final states while figure 6 depicts the occurrence of blinker states. Comparison of figures 5 and 6 clearly shows that, as L increases, the fraction of blinker states increases at the expense of the frozen striped states, in agreement with [1]. These trends suggest that for larger lattices, even small deviations from $p = 1/2$ causes the system to converge to the uniform state, while for $p = 1/2$, most final states are blinkers. In the latter case it seems likely that as $L \rightarrow \infty$, almost every final configuration is a blinker state (but see the discussion in section 4).

The median number of spin flips per site, $\nu = \mathcal{N}/L^d$, was studied in 2D and 3D models for different system sizes and different p (0.45, 0.50, 0.55), when the system converged to either a striped or a uniform state. For $p = 0.45$ and 0.55, ν increases with L for small system sizes, but rapidly levels off after (roughly) $L \sim 100$ in 2D and $L \sim 20$ in 3D. Interestingly, these correspond to samples with approximately equal numbers of spins. Significantly, in both 2D and 3D the rise of ν with L continued steadily only at $p = 1/2$, where it increased monotonically as a linear function of L (cf figures 7 and 8) up to the largest sizes considered. The rate of increase of ν with L was, to within numerical accuracy, virtually identical in 2D and 3D. This evidence indicates that, in terms of the overall classification of long-time

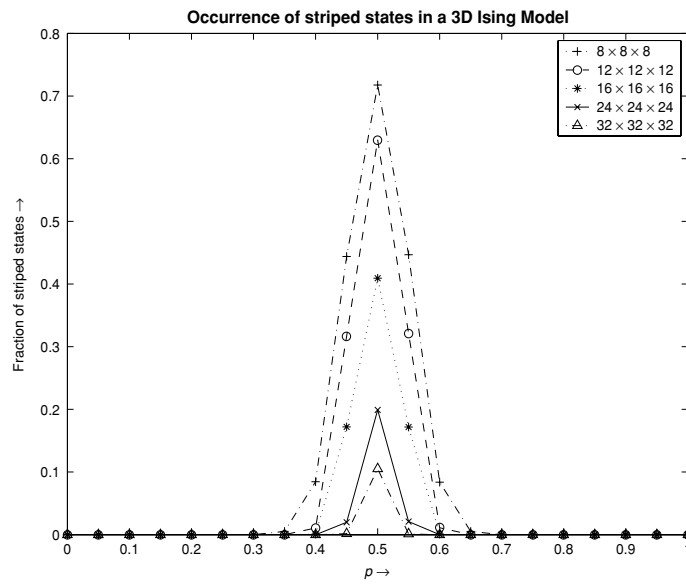


Figure 5. Occurrence of striped states as a function of p for a 3D Ising model. At least 10^6 independent runs have been considered for $p \neq 1/2$, and at least 10^4 runs for $p = 1/2$.

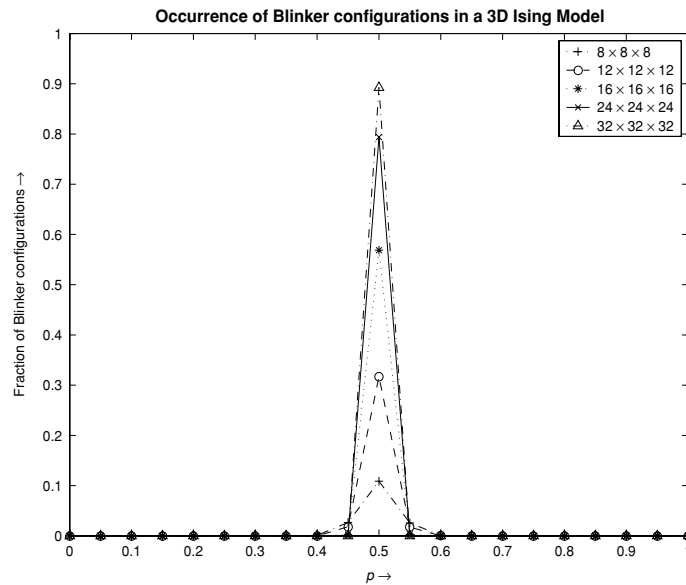


Figure 6. Occurrence of blinker states as a function of p for a 3D Ising model. At least 10^6 independent runs have been considered for $p \neq 1/2$, and at least 10^4 runs for $p = 1/2$.

dynamical behaviour presented in section 2, the Ising ferromagnet on \mathbf{Z}^d behaves similarly for $d = 2$ and $d = 3$ as a function of p . In particular, both are type- \mathcal{F} when $p \neq 1/2$, while for $p = 1/2$ the 3D lattice is either type- \mathcal{I} as in 2D [14] or possibly type- \mathcal{M} . These data, however,

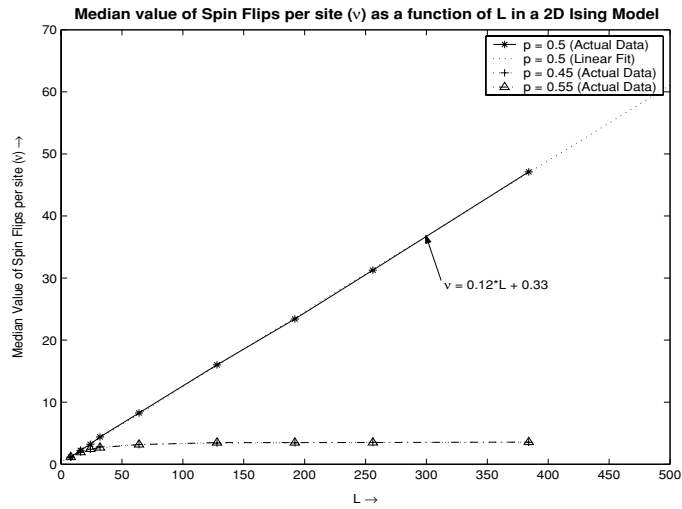


Figure 7. Median value of spin flips per site, v , as a function of L in a 2D Ising model.

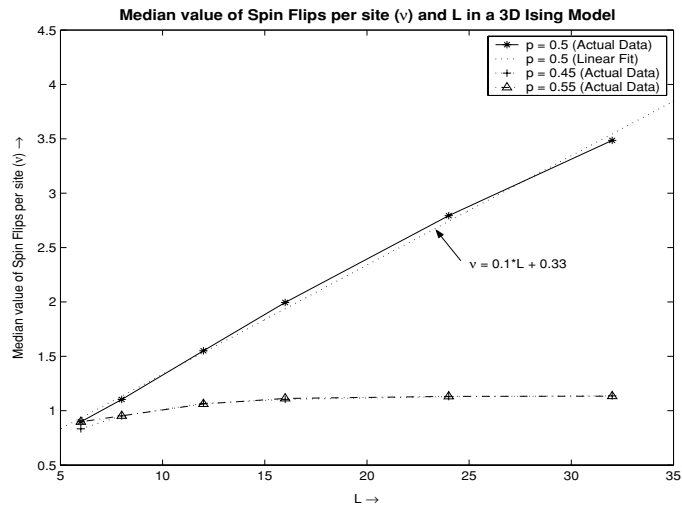


Figure 8. Median value of spin flips per site, v , as a function of L in a 3D Ising model.

do not reveal the nature of the final state(s) for large finite L ; this will be discussed further below.

We now study other aspects of the system evolution for p near $1/2$. One important quantity of interest is the convergence time to a final state (for $p \neq 1/2$) as a function of (p, d) . Figure 9 shows the result when $p = 0.45, 0.50$ and 0.55 , for a 16×16 lattice. Times shown are in units of μ^{-1} , the inverse Poisson rate parameter (here set equal to one). Each simulation consists of 10^5 independent runs where a final uniform or striped state was reached.

For the 2D Ising model, when $p = 0.45$, 66.92% of the runs have final magnetization -1 . In a smaller percentage of cases (9.79%) the minority spin prevails, i.e., the final magnetization is $+1$. The remaining 23.29% are in the striped state. The average time to reach the -1 state

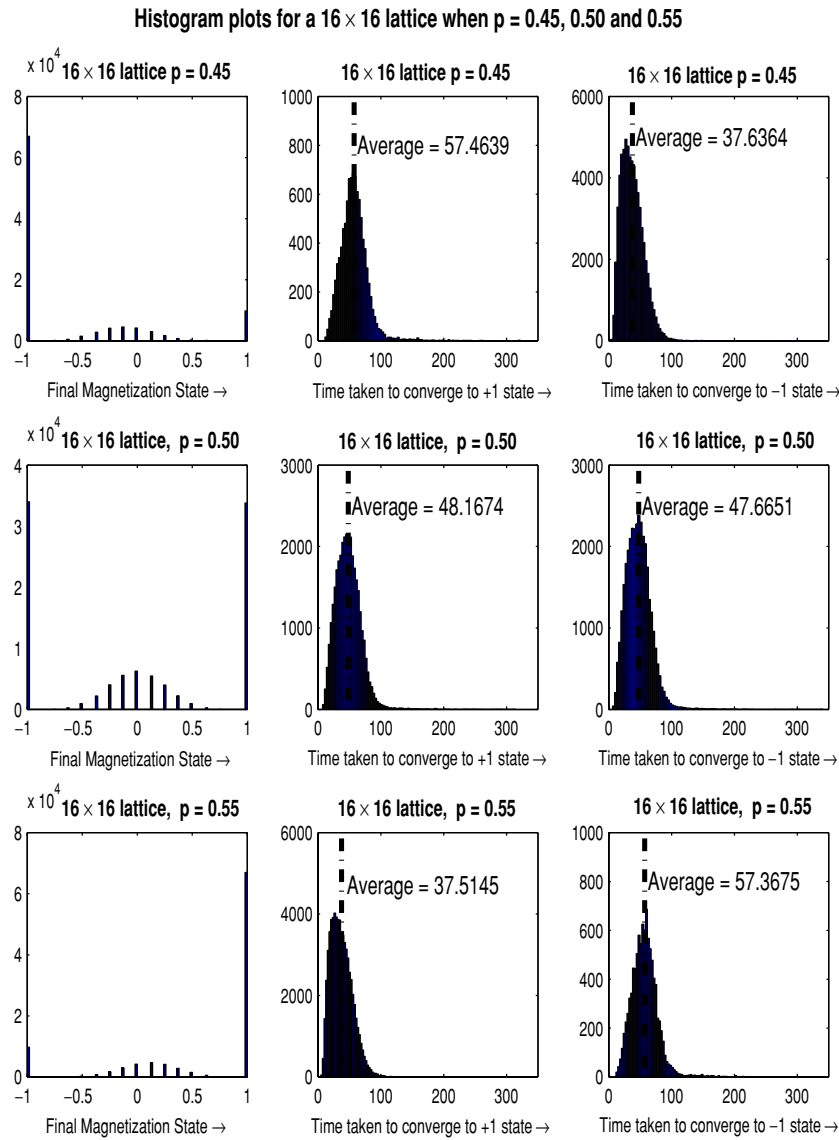


Figure 9. Convergence time as computed by histogram plots for the 16×16 lattice when $p = 0.45, 0.50$ and 0.55 . In all the plots the y -axis represents the frequency of occurrence. All the histograms are divided into 100 equally spaced bins and shown on a linear scale. The first row shows final magnetization states and the time taken to converge to the -1 and $+1$ states when $p = 0.45$. The second and third rows show the results for $p = 0.50$ and 0.55 , respectively. The results along the first and third rows are similar indicating symmetry around $p = 0.50$.

is, not surprisingly, significantly smaller (37.64) than that taken to reach the $+1$ state (57.46). This extra time corresponds to large fluctuations that take the system from the majority to the minority spin state. For the case when $p = 1/2$, the fraction of runs leading respectively, to the uniform $+1$ and -1 final states are remarkably close (33.98% and 33.76%, respectively) to the fraction $1/3$. The system reaches a final striped state with a probability also close to $1/3$, in good agreement with the results found by Spirin *et al* [16]. The corresponding time

Histogram plots comparing the final magnetization states for a 64×64 lattice and $16 \times 16 \times 16$ lattice

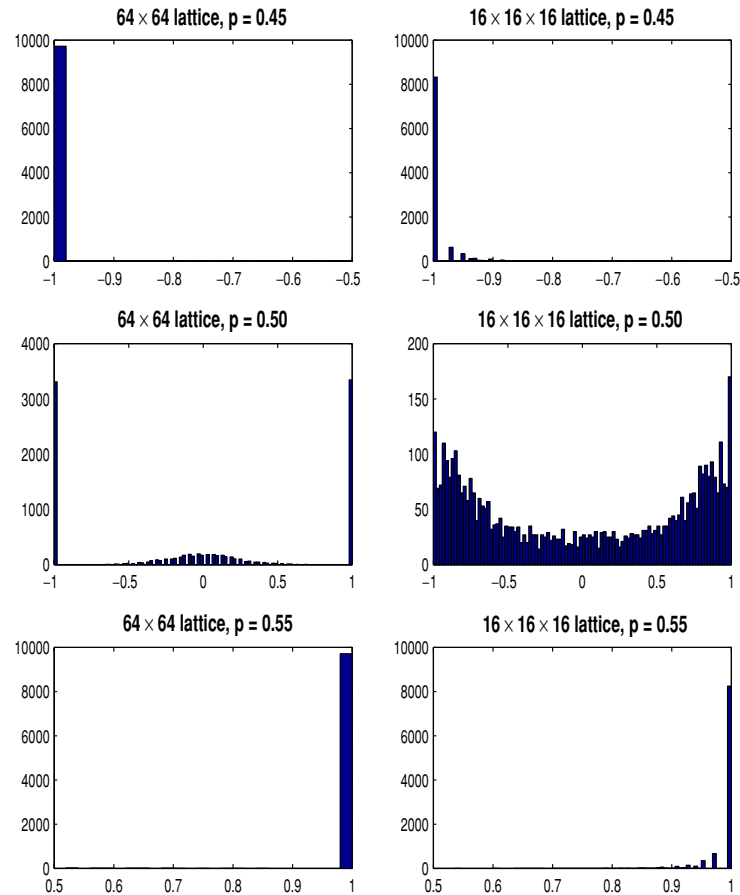


Figure 10. Histogram plots comparing the final magnetization states for a 64×64 lattice with a $16 \times 16 \times 16$ lattice for $p = 0.45, 0.50$ and 0.55 . In all plots the y-axis represents the frequency of occurrence while the x-axis represents the final magnetization states. All the histograms are divided into 100 equally spaced bins and shown on a linear scale. The symmetry for the $p = 0.45$ and 0.50 cases are evident from the first and last rows of the graph.

averages to reach these states are likewise very close (48.17 and 47.67, respectively). The results for $p = 0.55$ mimic those of $p = 0.45$, with the relative roles of the $+1$ and -1 states switched. In this case 66.96% reach the $+1$ final state while 9.66% reach the -1 state. The corresponding time averages are 37.51 and 57.37, respectively.

These tendencies are confirmed using larger lattices, as the next few figures show. In these, we compare results between a (2D) 64×64 lattice and a (3D) $16 \times 16 \times 16$ lattice, which have the same total number of spins. The results are based on 10^4 independent runs for either case. Graphs displaying final magnetization states and convergence times for the two cases when $p = 0.45$ and $p = 0.50$ are displayed in figures 10 and 11, respectively.

Comparing these two cases, we observe that for the 3D Ising model, whenever convergence occurs, there is an overwhelming tendency for the majority spins to prevail in the final state. For $p = 0.45$, none of the 10^4 runs in the 3D case converged towards the $+1$ state compared to 11 instances in the 2D case where the minority spin prevailed in the final state. For a

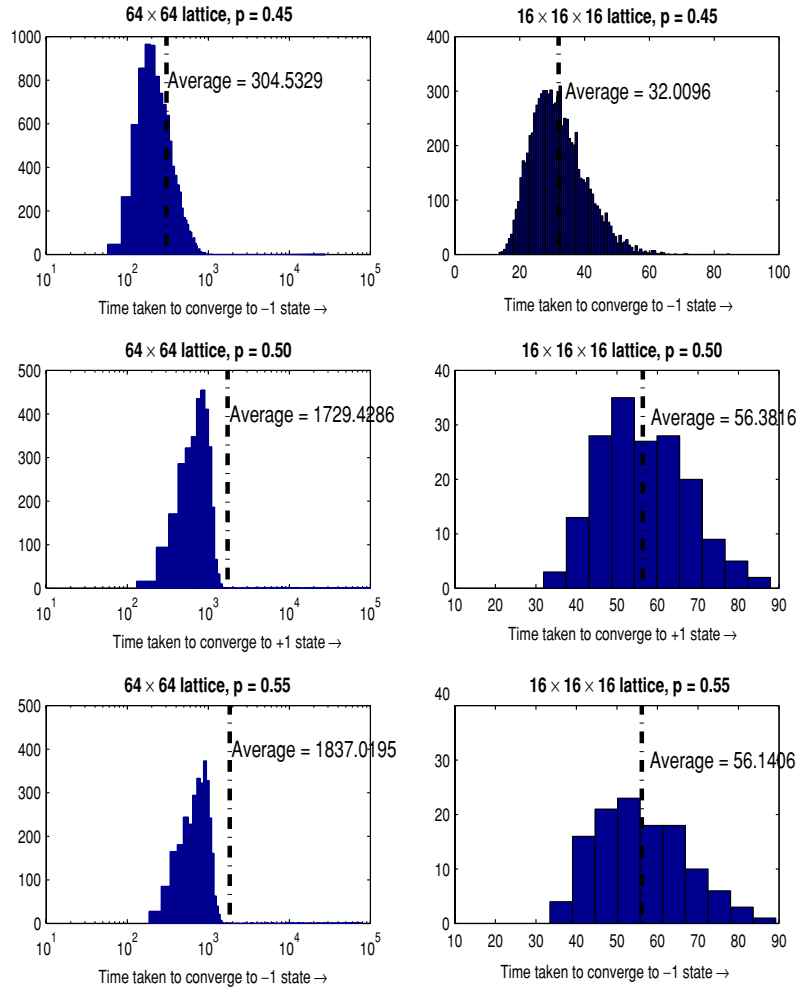
Histogram plots comparing time taken to reach ± 1 state for a 64×64 and $16 \times 16 \times 16$ lattice

Figure 11. Histogram plots comparing the time taken to reach a final ± 1 state for a 64×64 lattice with a $16 \times 16 \times 16$ lattice for $p = 0.45, 0.50$ and 0.55 . In all plots the y-axis represents the frequency of occurrence while the x-axis represents the time taken. Note that the time bins are depicted on a logarithmic scale for the 2D lattice and linear scale for the 3D case. All the histograms are divided into 100 equally spaced bins.

64×64 lattice, 97.18% converged to the -1 state, 0.11% converged to the $+1$ state and the rest (2.21%) were striped states. Similarly, for the $16 \times 16 \times 16$ lattice, 83.24% converged to the -1 state, 16.54% evolve into striped states and the remainder (0.11%) into blinker states. The average convergence time is smaller and more predictable for the 3D model than for the 2D case. For the $16 \times 16 \times 16$ lattice with $p = 0.45$, the average time taken to converge to the -1 state is 32.00 compared to 304.53 for the 64×64 lattice for the same p . When $p = 0.50$, results are symmetric, as expected. Average times taken to reach the $+1$ and -1 states in the $16 \times 16 \times 16$ lattice were 56.38 and 56.14, respectively, while they were 1729.43 and 1837.02 for the 64×64 lattice. Compared to the 2D case, there is a smaller fraction of

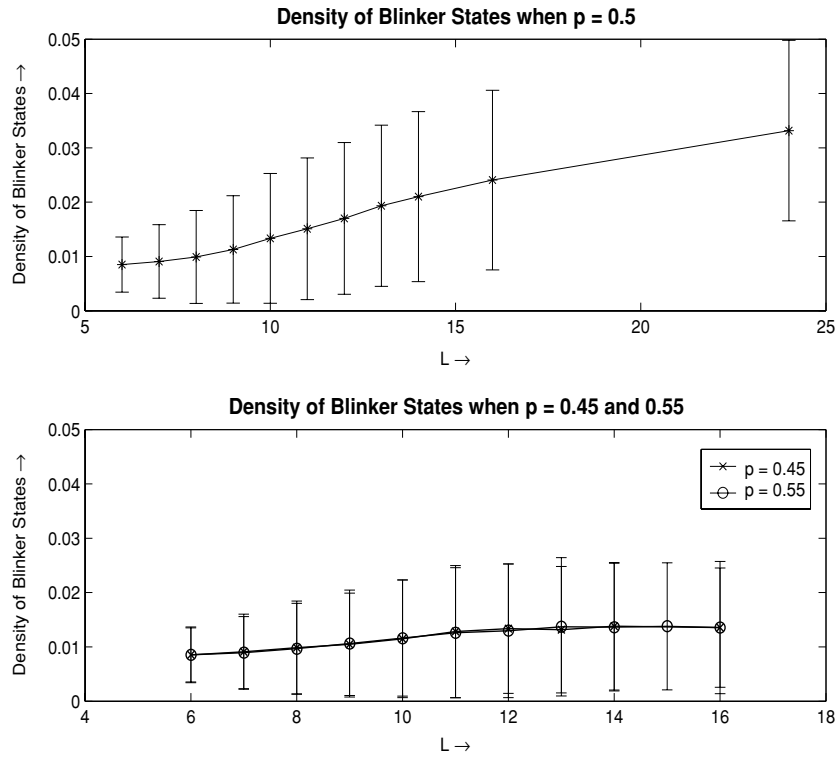


Figure 12. Plots showing the blinker density (that is, the fraction of blinker spins in a given blinker configuration) for a 3D lattice as a function of lattice size when $p = 0.45, 0.50$ and 0.55 . In these plots the y-axis represents the mean number of blinker spins per blinker configuration, while the x-axis represents lattice size.

the spins converging to the final uniform state in the 3D case (2.9%) and this probability only decreases as L increases. Also when $p = 0.50$ in the 3D lattice, configurations that have not converged to the uniform $+1$ or -1 configurations tend to be closer to one of those two states than in the 2D lattice (cf figure 10).

Figure 12 displays the nature of the blinker states in 3D. Typically, the number and position of blinker spins fluctuates greatly from one configuration to another, hence the relatively large error bars. In these simulations, we considered at least 10^4 runs for $L < 16$ and 10^3 runs for $L \geq 16$. Two conclusions can be drawn from these data: first, at the lattice sizes studied the density of blinker spins is quite small; and second, there is a qualitative difference between the symmetric and asymmetric cases. In particular, when $p = 1/2$ the blinker density *may* be increasing with lattice size L , while it appears to remain flat for asymmetric initial conditions. More work needs to be done for larger L to determine whether this trend persists.

4. Discussion and conclusions

From our simulations for the evolution of the 2D and 3D Ising models with random initial conditions and evolving under zero-temperature Glauber dynamics, we draw the following conclusions:

- For $d = 2$, the median number of spin flips is symmetric about a maximum at $p = 1/2$. The median number of spin flips per site, ν , increases with lattice size but the rate of increase is significant only when $p = 1/2$ (cf figure 7), when $\nu = 0.12L + 0.33$. At $p = 1/2$ and large L , the system evolves respectively towards the uniform $+1$ state, the uniform -1 state and the striped state with equal probability $1/3$ (over initial configurations and dynamical realizations).
- However, it was proven in [14] that the infinite lattice with $p = 1/2$ is type- \mathcal{I} . This may suggest that the $L \rightarrow \infty$ limit, which distinguishes between striped and uniform states in a clear limiting sense, differs from the $L = \infty$ case. It is interesting to note that in the infinite square, at almost every sufficiently large time, any large region will *locally* resemble one of the two uniform phases or a domain wall phase. But this same region will continually approximate each of these three possible states infinitely often, separated (probably) by increasingly larger time intervals. On the infinite lattice, this state of affairs results from an unending supply of domain walls coming into any fixed region ‘from infinity’—a state of affairs that cannot occur for a finite lattice, no matter how large. These results and considerations demonstrate that caution needs to be exercised in extrapolating numerical results to infinite lattices in two or more dimensions.
- For $d = 3$, we again found the median number of spin flips to be symmetric about a maximum at $p = 1/2$. For this model the number of spin flips per site again increased linearly with L : $\nu = 0.1L + 0.33$. It seems very likely that, as in the 2D case, a 3D lattice for $p = 1/2$ is not type- \mathcal{F} . The rate of increase of the median number of spin flips per site is, within the accuracy of the simulations, close to that of the 2D case.

As L increases at $p = 1/2$, the fraction of final spin configurations in the blinker state increases rapidly (cf figure 6). For the lattice sizes considered, however, the fraction of spins that are unfrozen in each of these ‘blinker states’ remains quite low. This is not surprising—it seems reasonable that every spin, or small connected cluster of spins, that cycles endlessly through a small number of states requires a significantly larger number of surrounding frozen spins to supply the ‘boundary conditions’ needed for this cycling to occur.

It is unclear at this stage whether, as L increases, the fraction of ‘unfrozen’ spins in a typical final configuration levels off to a limiting value strictly less than (and probably considerably smaller than) one, as required for a blinker state, or continues to increase to one. The former case corresponds to type- \mathcal{M} and the latter to type- \mathcal{I} . Either way, these data are consistent with the conjecture that the symmetric case in 3D is not type- \mathcal{F} . Our data indicate that the symmetric case *may* be type- \mathcal{M} when $L = \infty$; however, the previous example of the 2D case leaves open the possibility that the $L \rightarrow \infty$ limit is type- \mathcal{M} while the $L = \infty$ case, i.e., the infinite cubic lattice, is type- \mathcal{I} , and there is a corresponding dynamical singularity in the $L \rightarrow \infty$ limit.

- For $p \neq 1/2$, our results strongly suggest that the system is type- \mathcal{F} when $L = \infty$ and $d = 2$ or 3 , given that the average number of spin flips per site does not appreciably change with increasing lattice size.
- Both L and d influence the probability of the minority spin prevailing in the final converged state. For any given $p \neq 1/2$, this probability decreases as L or d increases, thereby suggesting that the occurrence of a final minority spin ground state has zero probability when $L = \infty$.
- As might be expected, the average time taken to converge to a final majority state is smaller than that needed to converge to a minority state. For the same number of sites and any given p , dynamics on the 3D lattice shows a tendency to converge faster than in

the 2D case. When $p = 1/2$, the times taken to reach the +1 or -1 final state is almost the same for both 2D and 3D.

Acknowledgments

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