Critical properties of non-equilibrium systems without global currents: Ising models at two temperatures

1990 J. Phys. A: Math. Gen. 23 3799

(http://iopscience.iop.org/0305-4470/23/16/025)

J. Phys. A: Math. Gen. 23 (1990) 3799–3808. Printed in the UK

Critical properties of non-equilibrium systems without global currents: Ising models at two temperatures

H W J Blöte†, J R Heringa†, A Hoogland† and R K P Zia‡

† Laboratorium voor Technische Natuurkunde, Technische Universiteit Delft, PO Box 5046, 2600 GA Delft, The Netherlands

‡ Physics Department, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061, USA

Received 22 March 1990

Abstract. We study two two-dimensional Ising models with a non-Hamiltonian spin dynamics. The models consist of two sublattices at different temperatures. The steady state properties are investigated by means of Monte Carlo simulations on the Delft Ising System Processor. We find that the phase transition between the disordered and ordered phases persists when a temperature difference between the sublattices is introduced. The critical properties of these non-equilibrium systems fit well within the Ising universality class.

Considerable knowledge exists about the critical properties of statistical mechanical models in equilibrium. One of the most important developments over the last two decades is our understanding that such properties fall into universality classes, to which widely distinct systems belong [1]. In comparison, much less is known about phase transitions in non-equilibrium systems. In particular, there is no reason to expect that the critical properties of a system are unchanged, if indeed such a transition survives the introduction of non-Hamiltonian dynamics.

Recently, Kanter and Fisher [2] gave specific examples of ferromagnetic systems, with Glauber [3] dynamics, in which a phase transition is absent. Prior to that, Grinstein *et al* [4] found that, under certain conditions, the transition survives and argued that critical properties should fall into the Ising class. On another front, there are studies [5–8] of the lattice-gas representation of the Ising model with Kawasaki [9] dynamics, in which a homogeneous electric field is applied to establish a steady state with a non-zero current. If the (nearest-neighbour) interparticle interaction is attractive, the (second-order) phase transition persists for all non-vanishing fields [5], but the critical behaviour has been concluded to lie *outside* the Ising universality class [6, 7]. On the other hand, if the interaction is repulsive, the system *does* display Ising-like properties whenever the transition remains second order [8].

Other studies [10, 11] of this model involve a dynamics which conserves energy rather than particle number. The non-equilibrium steady state is set up by a temperature difference between the opposing boundaries of the sample. As in the previous examples, there is a non-zero global current, associated with internal energy. Most of the accurate data are gathered for systems far away from criticality. Little is known

0305-4470/90/163799+10$03.50

about the critical properties, since both simulations and measurements are difficult to perform.

In this paper, we report our studies on the same model with a non-Hamiltonian dynamics which is *free* from the constraints of a conservation law. Using Glauber [3] dynamics and the spin representation, we couple spins on two sublattices ($i = 1,2$) of the square Ising system to thermal baths at different temperatures T_i. In comparison with the examples given above, the resulting non-equilibrium steady state has a different character. On a microscopic scale, there are no explicitly conserved quantities. There is a steady energy flow from one sublattice to the other. This flow does not correspond with a global current, i.e. on a macroscopic scale it has no vector but a scalar character. Also the average current associated with particle number (i.e. number of + spins) is zero. Thus the spatial inversion symmetry of the Ising model is not broken. Although the energy of our models is adequately described by a Hamiltonian, the transition probabilities are not consistent with a single reduced Hamiltonian; i.e. the dynamics can be characterised as non-Hamiltonian. Our data indicate that, provided one of the T's (say, T_1) is set below a certain value T_o, there is a second-order phase transition at some value of T_2. Further, the critical properties fall into the Ising universality class.

Noteworthy are two other studies on the Ising model with two temperatures. One [12] employed the same model as ours with *competing* dynamics at each site, i.e. *each* spin is coupled to *both* baths, but with probability p and $1 - p$. For temperature differences of 2%, no observable deviations from equilibrium properties are seen. On the other hand, when this difference is ten times larger, no *quantitative* comparisons with the equilibrium case were given. The other study concerns the effects of a combination of Glauber and Kawasaki dynamics [13, 14]. These models have transitions, and, for small probability of the Kawasaki dynamics, no significant deviations from Ising-like behaviour were observed. For large probability of the Kawasaki dynamics, the transition was found to turn first order.

The remainder of this paper is devoted to a brief description of our model and the results. We considered two types of sublattices on the square lattice: 'checkerboard' and 'zebra'. (In the latter, every other column belongs to the same sublattice.) For simplicity, we studied a system with nearest-neighbour ferromagnetic interactions only. To specify a dynamics in a Monte Carlo simulation, we must define a procedure for choosing spins for updating and the transition probabilities for the chosen spin. For the latter, we adopt the transition rates according to Yang [15], i.e. a spin s on a site of sublattice i is assigned a value $s(= \pm 1)$ with probability

$$P(s) = \exp(JsS/kT_i)/2\cosh(JS/kT_i) \qquad (1)$$

where S is the sum of the spin values of the four nearest neighbours. Note that P is not explicitly dependent on the previous value of that spin. For the former, we adopt a random site selection procedure. We should emphasise that the behaviour of the model will depend on this selection procedure. For instance, if the sublattice at the higher temperature is visited more frequently than the other sublattice, then the nearest-neighbour correlation function will be smaller than in our case.

With these rules, the system is found to reach a steady state. We expect the stationary properties of the model to be functions of the parameters J/kT_i only. We first discuss some special cases.

(i) $T_1 = T_2$. This is Onsager's model.

(ii) $T_1 = \infty$. Even when T_2 is zero, the spins on sublattice 1 will be uncorrelated, and therefore correlations between spins on sublattice 2 will be severely limited. In particular, for the checkerboard model, they vanish for separations exceeding two lattice units. Similarly, spins on sublattice 2 of the zebra model are correlated only to those in the same or next columns.

(iii) $T_1 = 0$. In the checkerboard case, sites within a sublattice are not coupled to each other. Thus, we expect a disordered phase for large T_2. The spins on sublattice 1 will be only weakly correlated, counteracting the possibility of long-range order. The zebra case is less obvious, since all spins have two neighbours belonging to the same sublattice. Still, random fields due to the neighbouring spins at a sufficiently high temperature T_2, are sufficient to prevent a divergence of the correlation lengths in the chains of sublattice 1. Therefore we expect also in this case a disordered phase for sufficiently large T_2.

If we alter our model to include anisotropy, i.e. the vertical bonds being stronger than the horizontal ones, then each column in sublattice 1 will have a much stronger tendency to order independently so that we may expect global ordering for much larger values of T_2 in comparison with the isotropic case.

For cases other than these special ones, we have investigated these models by means of Monte Carlo simulations on the DISP (Delft Ising System Processor), a special-purpose computer for the simulation of Ising models [16, 17]. Its spin updating algorithm is able to select sites randomly. The presence of two temperatures did not pose special problems because only transition probabilities need to be stored in the processor's look-up table. While the DISP was originally designed for translationally invariant (over one lattice unit) models, the presence of two zebra sublattices could simply be accounted for by including one extra address bit, namely the least significant bit of the X coordinate of the spin, into the look-up-table address. In the checkerboard case, we took the modulo 2 sum of the least significant bits of the X and Y coordinates instead.

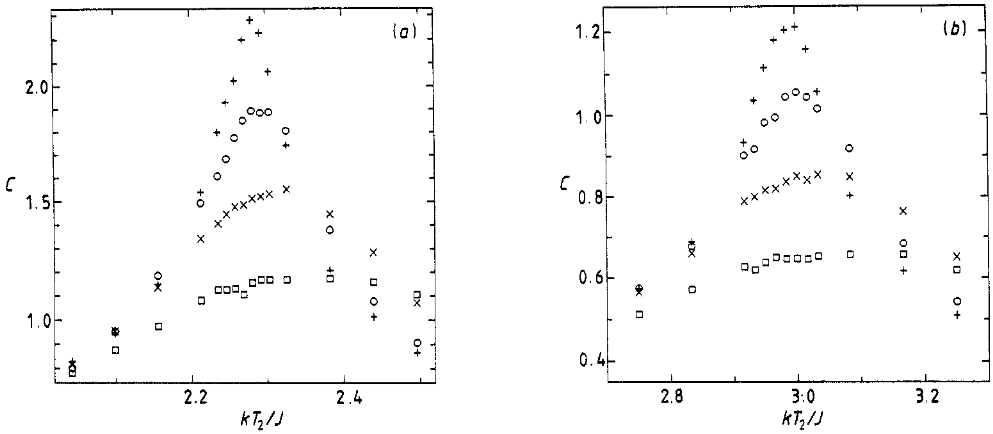
The simulations were performed at three different temperature ratios $\alpha \equiv T_1/T_2$, namely 1, 2 and ∞. We include the equilibrium case ($\alpha = 1$, Onsager's model) for purposes of comparison with the non-equilibrium results. The cases $\alpha = \infty$ were simulated by choosing $J/kT_1 = 12$ which excludes, after truncation of the transition probabilities to the machine precision, spin flips costing energy. We used square systems of $N = L \times L$ spins, with $L = 8, 16, 32$ and 64, with periodic boundaries. We present the data for the checkerboard systems with $\alpha = 1$, 2 and ∞ in some detail here. This is thought to be sufficient for a qualitative picture of our models. The data for the zebra systems are sufficiently similar and we will only limit ourselves to some numerical data and comments at the end.

Figures 1(a), (b) and (c) show the quantity C_L defined via the energy fluctuations of a system with size L as

$$C_L \equiv (1/Nk^2T_2^2)(\langle E_L^2\rangle - \langle E_L\rangle^2) \tag{2}$$

as a function of T_2, with $\alpha = 1$, 2 and ∞ respectively. In (2), E_L is the energy, i.e. $-J$ times the sum over the nearest-neighbour spin products. The data points represent runs up to 4×10^6 sweeps. The energy (as well as other data) was recorded at intervals of twenty sweeps.

For an equilibrium system, (2) is also the dimensionless specific heat, $c \equiv \mathrm{d}U/\mathrm{d}T$, where $U \equiv \langle E_L\rangle$. For non-equilibrium systems, the fluctuation dissipation theorem



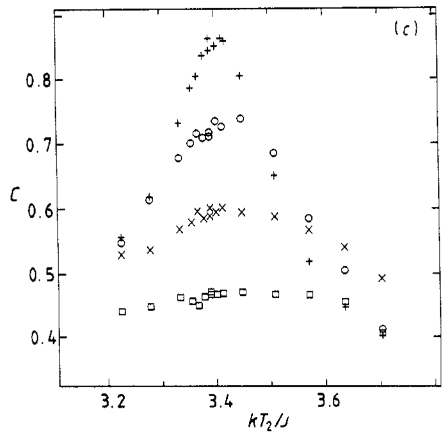
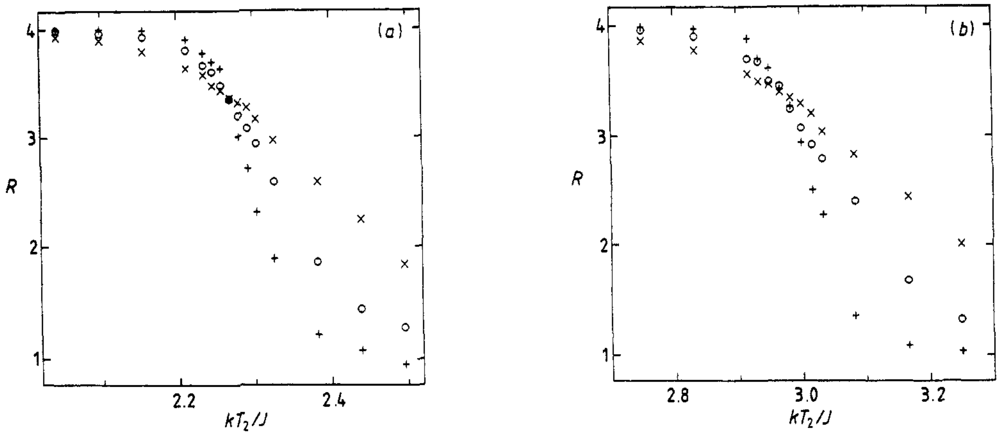


Figure 1. The quantity C_L defined via the energy fluctuations (see text) of the $\alpha = 1$ (a), the $\alpha = 2$ (b), and the $\alpha = \infty$ (c) checkerboard models. The data are shown as a function of the temperature parameter kT_2/J, for four values of the finite-size parameter: $L = 8$ (□); $L = 16$ (×); $L = 32$ (○); and $L = 64$ (+). Error bars are not shown because they do not exceed the symbol size in most cases.

does not apply so that, in general, the two are not identical. A dramatic example was reported in the driven diffusive system with attractive interactions, where c diverges at the transition while C remains finite [7]. By a numerical differentiation of the energy against temperature T_2 (for fixed ratio $\alpha = 1$ and 2), we obtain a 'specific heat' $c = \mathrm{d}\langle E\rangle/\mathrm{d}T_2$. Unfortunately, the results for c are less accurate than those for C. Nonlinearity of $\langle E\rangle$ near the critical point imposes narrow temperature intervals for the numerical differentiation, leading to larger statistical errors. However, it is still clear from the data that the quantities c and C behave very similarly; there appears to be an approximate linear relation. In particular we find again evidence for a logarithmic finite-size divergence of the maximum. For these reasons, we are encouraged to analyse our models using methods developed for equilibrium systems.

Exact results for equilibrium Ising models show that the maximum in the specific heat scales as the logarithm of the system size L: $c \simeq A + B \log L$. This corresponds to a temperature exponent $y_t = 1$, which is generally believed to be a universal property of a large set of two-dimensional Ising models. This behaviour is clearly exhibited in figure 1(a): the differences between subsequent maxima are approximately constant, while subsequent values of L differ by a constant factor 2. Remarkably, the non-equilibrium checkerboard systems display a very similar behaviour as shown in figures 1(b) and (c). These data are strongly suggestive of a phase transition, with the



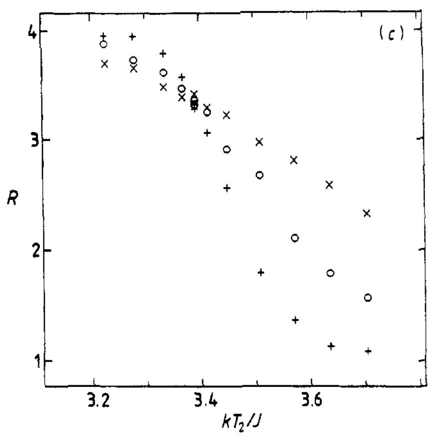


Figure 2. Ratios R_L defined via the magnetisation fluctuations (see text) of the $\alpha = 1$ (a), the $\alpha = 2$ (b), and the $\alpha = \infty$ (c) checkerboard models. The data are shown as a function of the temperature parameter kT_2/J, for three values of the finite-size parameter: $L = 8$ (×); $L = 16$ (○); and $L = 32$ (+). Error bars (not shown) do not exceed the size of the symbols in most cases.

quantity C logarithmically diverging as a function of the system size. Note that the phase transition for $\alpha = \infty$ (figure 1(c)) indeed occurs at a finite value of T_2.

During the simulations, the total magnetisation M was sampled also. Its fluctuations enable the calculation of the quantity

$$X_L \equiv (\langle M_L^2 \rangle - \langle M_L \rangle^2)/N. \tag{3}$$

For an equilibrium system, (3) is also the magnetic susceptibility, χ. The asymptotic finite-size dependence at the Ising critical point is

$$X_L \simeq L^{2y_h - 2} \tag{4}$$

for asymptotically large L, with another universal exponent $y_h = \frac{15}{8}$. Thus, at a critical point, we expect

$$R_L \equiv X_{2L}/X_L \simeq 2^{2y_h - 2}. \tag{5}$$

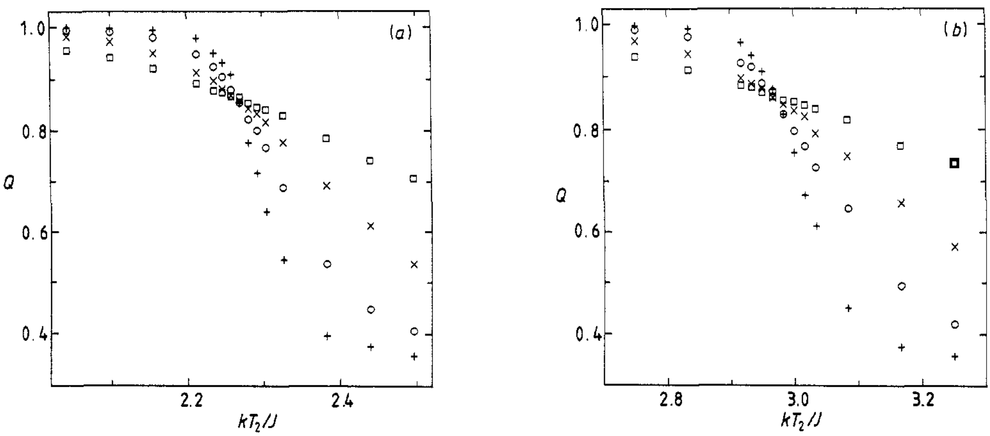
Again, we emphasise that X_L need not be related to χ for non-equilibrium systems. However, we have numerically differentiated M_L with respect to the magnetic field, and observed that the resulting susceptibility χ_L was approximately proportional to X_L, although the statistical errors were larger.

Data for R_L against temperature are shown in figures 2(*a*), (*b*) and (*c*), for $\alpha = 1$, 2 and ∞ respectively. The intersections of subsequent $R_L(T)$ curves yield estimates of the critical point and of y_h. For each ratio α we observe good agreement with the Ising exponent which corresponds with $R_L = 2^{7/4} \approx 3.364$. Again, the non-equilibrium results fail to show any deviations from Ising universality.

A third universal quantity [18] of critical Ising models is the large L limit of

$$Q_L = \langle M_L^2 \rangle^2 / \langle M_L^4 \rangle \tag{6}$$

which takes, according to Bruce [19], and Burkhardt and Derrida [20] the value $Q_c = 0.856$ for square systems with periodic boundaries. Intersections of the Q_L against temperature curves may thus serve as estimates of the critical points of the equilibrium models. Numerical results for Q_L are shown in figures 3(*a*), (*b*) and (*c*). These data show that the Q_L curves intersect at one point, giving credibility to the presence and location of the critical points for the non-equilibrium models. More strikingly, the Q_L values at the intersections for the $\alpha \neq 1$ models are consistent with that for Onsager's system.



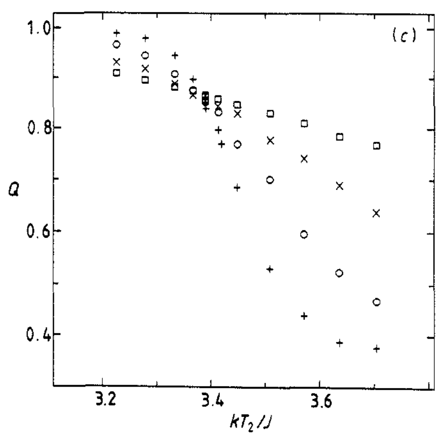


Figure 3. Ratios Q_L defined via the magnetisation fluctuations (see text) of the $\alpha = 1$ (*a*), the $\alpha = 2$ (*b*), and the $\alpha = \infty$ (*c*) checkerboard models. The data are shown as a function of the temperature parameter kT_2/J, for four values of the finite-size parameter: $L = 8$ (□); $L = 16$ (×); $L = 32$ (○); and $L = 64$ (+). Error bars (not shown) do not exceed the size of the symbols in most cases.

The results obtained for the zebra systems show a qualitatively similar behaviour. No obvious deviations from Ising universality are seen. For a closer examination, the data for the checkerboard and zebra systems are also subjected to various fitting procedures. In particular we try to determine y_t, y_h, and Q_c more precisely. Expanding the finite-size scaling functions in $T - T_c$, where T stands for one of the T_i, we expect the following behaviour near a critical point:

$$Q_L = Q_c + pL^{-y_i} + a_1(T - T_c)L^{y_t} + a_2(T - T_c)^2 L^{2y_t} + \dots \tag{7}$$

$$C_L = C_1 + \log(L)L^{2y_t - 2}[c_0 + c_1(T - T_c)L^{y_t} + c_2(T - T_c)^2 L^{2y_t} + \dots] \tag{8}$$

$$X_L = X_0 + L^{2y_h - 2}[b_0 + b_1(T - T_c)L^{y_t} + b_2(T - T_c)^2 L^{2y_t} + \dots] \tag{9}$$

where Q_c, p, C_1, X_0, the a_i, b_i and the c_i are (in principle) unknown parameters. The logarithmic factor was inserted in (8) in order to avoid numerical problems associated with the divergence of the amplitude when y_t approaches 1. The terms shown here were actually used during the least-squares fitting procedures: they were found to be the minimal sets leading to satisfactory residuals. For the irrelevant exponent y_i in (7) we have chosen the 'analytic' value -2. Since simultaneous determination of all unknowns leads to some loss of accuracy, we have used the following procedure. Since it is already known that $y_t \approx 1$ from the foregoing, we have fixed $y_t = 1$ in the formula for Q_L and solved for the remaining unknowns, including Q_c and T_c (see table 1). The results depend only weakly on this choice of y_t. Next, the results for T_c were fixed in the expression for C_L. The results for y_t from subsequent fits (also shown in table 1) confirm the choice made above for y_t. Finally, we have inserted these T_c and y_t results in the formula for X_L and solved for y_h (see table 1). We observe that the results for y_t and y_h lie close to universal Ising values. We conclude that there is strong numerical evidence that our non-equilibrium systems belong to the universality class of the two-dimensional Ising model. The fact that the Q_c results are also close to the known value for square, periodic Ising systems provides an additional consistency check for the checkerboard systems. Note that the situation for the zebra systems is somewhat different because the zebra pattern has a lower symmetry than the underlying square lattice.

Table 1. Numerical results for the critical point, y_t, y_h, and Q_c, for three values of the temperature ratio α. Data are given for the 'checkerboard' (c) as well as for the 'zebra' (z) model, see first column. Estimated uncertainties in the last decimal places are given in parentheses. These data agree well with known results for the equilibrium Ising model, namely the exact values $y_t = 1$ and $y_h = \frac{15}{8}$, and $Q_c = 0.856$ as found in [19, 20] for square systems. The critical point obtained for the case $\alpha = 1$ lies close to the exact value $\log(1 + \sqrt{2})/2 = 0.440\,69\ldots$.

Model	α	$(J/kT_2)_c$	y_t	y_h	Q_c
c,z	1.0	0.4408(3)	0.997(12)	1.874(3)	0.857(3)
c	2.0	0.3362(4)	0.990(10)	1.876(4)	0.853(4)
c	∞	0.2954(2)	0.989(12)	1.875(3)	0.859(2)
z	2.0	0.3303(4)	0.992(10)	1.876(4)	0.861(4)
z	∞	0.2714(3)	0.995(12)	1.872(3)	0.860(3)

During the simulations, we made the additional observation that the spontaneous magnetisation of both sublattices as a function of temperature behaves quite similarly, but the amplitudes near the critical point are obviously different when $\alpha \neq 1$.

To obtain a qualitative understanding of the phase diagram, we apply the 'mean-field' approach. Thus we replace each interaction of a spin with a neighbour by a contribution to the effective magnetic field (H), proportional to the applicable sub-lattice magnetisation. Then one can use equilibrium methods on each individual spin, leading to independent sublattice magnetisations $m_i = \tanh(H/kT_i)$. Following the spirit of equilibrium mean-field theory, we find the self-consistent equations

$$m_i = \tanh(4Jm_{3-i}/kT_i) \qquad i = 1,2 \tag{10}$$

for the checkerboard model. These equations yield the critical line in the $T_1 - T_2$ plane, ($T_1 T_2 = [4J/k]^2$) as shown in figure 4 (bold curve).

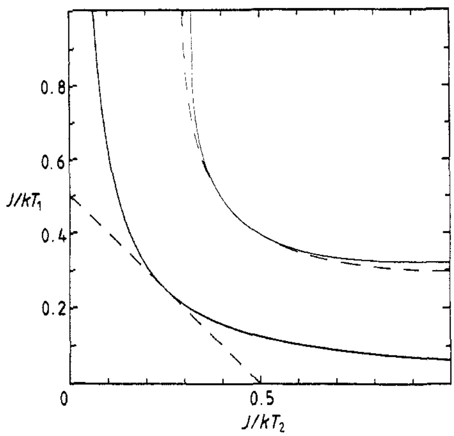


Figure 4. Phase diagram of the checkerboard (full curves) and zebra (broken line and curve) models. The bold lines represent the mean-field predictions for the critical lines of these models (see text). Also shown are smooth curves (fine curves) interpolating between our Monte Carlo results at $T_1/T_2 = 1, 2$ and ∞ which apply, by symmetry, also to $T_1/T_2 = \frac{1}{2}$ and 0. Disordered phases occur near the origin, and ordered phases on the other side of the critical lines.

In the zebra case, the self-consistent equations are

$$m_i = \tanh[2J(m_1 + m_2)/kT_i] \qquad i = 1,2 \tag{11}$$

yielding $J/kT_1 + J/kT_2 = \frac{1}{2}$ for the critical line. This result is also shown in figure 4 (broken line), together with smooth curves connecting the numerical results for the checkerboard and the zebra models. Not surprisingly, the figure is symmetric in T_1 and T_2. There is some qualitative agreement between the mean-field and the numerical results except at the extremes. From the data, we see that, when $T_1 = 0$, criticality occurs at *finite* critical values of T_2. The 'mean-field' prediction is, unfortunately, infinity in the checkerboard case; in the zebra case it is even worse: the transition is predicted to be absent. As an amusing contrast, we may use the temperature parameters $K_i \equiv J/kT_i$ and compare this phase diagram with that of an *equilibrium, anisitropic* Ising model. For the latter case, where $K_i \equiv J_i/kT$, the exact critical line is known: $\sinh 2K_1 \sinh 2K_2 = 1$. Our $\alpha = 2$ data place a critical point surprisingly near this line. In this connection, we remark that the mean-field prediction for the anisotropic model ($K_1 + K_2 = \frac{1}{2}$) also fares poorly at the extremes, where the effects of fluctuations are too strong to be ignored.

Before closing, we point out a special case of our checkerboard system, for which it appears possible to find a mapping onto an *equilibrium* Ising model with an effective Hamiltonian consisting of strictly local interactions. This case is reminiscent of the fast rate limit of the driven diffusive lattice gas, introduced by van Beijeren and Schulman [21]. We change the dynamics such that sublattice 2 is visited much more frequently (infinitely more, in the limit) than sublattice 1. Now, we can express the probability distribution of a type-2 spin in the four surrounding type-1 spins. When the updating algorithm hits a type-1 spin, we are thus able to express the resulting probability distribution of that spin in a 3×3 block of type-1 spins. This means that the stationary set of configurations of sublattice 1 is generated by an effective Hamiltonian with only short-range interactions. Thus, we should expect also this special case to display the universal Ising critical properties.

In conclusion, we have performed Monte Carlo simulations on Ising models out of equilibrium. These systems are without uniform, *global* currents, and have a spin dynamics without a local conservation law. The steady state energy currents are all *local*, i.e. they flow from one sublattice to the other. Our results provide strong evidence that the models belong to the universality class of the equilibrium Ising model. At first sight, this conclusion appears to support the results of Grinstein *et al* [4]. On closer examination, however, our dynamics does not satisfy some of the restrictions it imposed, e.g. homogeneity of the transition probabilities. It may be possible to generalise their arguments and enlarge the Ising class. In any case, much work will be needed before we can answer the most intriguing question, namely, is the existence of a symmetry-breaking global current density a necessary (though perhaps not a sufficient) condition for critical properties of non-equilibrium phase transitions to fall *outside* the universality class of their equilibrium counterparts?

Acknowledgments

We are indebted to J M J van Leeuwen, H van Beijeren, H J Hilhorst, J L Lebowitz and B Schmittmann for valuable discussions. The hospitality of J M J van Leeuwen and the Lorentz Institute at Leiden, where some of this work was performed, is gratefully acknowledged. We thank A Compagner for essential contributions to the performance of the DISP. This research is supported in part by the US National Science Foundation through the division of materials research.

References

[1] Kadanoff L P 1971 *Critical Phenomena* ed M S Green (New York: Academic)
[2] Kanter I and Fisher D S 1989 *Phys. Rev.* A **40** 5327
[3] Glauber R J 1963 *J. Math. Phys.* **4** 294
[4] Grinstein G, Jayaprakash C and He Y 1985 *Phys. Rev. Lett.* **55** 2527
[5] Katz S, Lebowitz J L and Spohn H 1983 *Phys. Rev.* B **28** 1655; 1984 *J. Stat. Phys.* **34** 497
[6] Janssen H K and Schmittmann B 1986 *Z. Phys.* B **64** 503
Leung K-t and Cardy J L 1986 *J. Stat. Phys.* **44** 567
Gawadzki K and Kupiainen A 1986 *Nucl. Phys.* B **269** 45
[7] Valles J L and Marro J 1987 *J. Stat. Phys.* **49** 89
[8] Leung K T, Schmittmann B and Zia R K P 1989 *Phys. Rev. Lett.* **62** 1772
[9] Kawasaki K 1972 *Phase Transitions and Critical Phenomena* vol 2, ed C Domb and M S Green (New York: Academic)

[10] Creutz M 1986 *Ann. Phys., NY* **167** 62
[11] Harris R and Grant M 1988 *Phys. Rev.* B **38** 9323
[12] Garrido P L, Labarta A and Marro J 1987 *J. Stat. Phys.* **49** 551
[13] Gonzalez-Miranda J M, Garrido P L, Marro J and Lebowitz J L 1987 *Phys. Rev. Lett.* **59** 1934
Wang J S and Lebowitz J L 1988 *J. Stat. Phys.* **51** 893
[14] Garrido P L, Marro J and Gonzalez-Miranda J M 1989 *Phys. Rev.* A **40** 5802
[15] Yang C P 1963 *Proc. Symp. Appl. Math.* **15** 351
[16] Hoogland A, Spaa J, Selman B and Compagner A 1983 *J. Comput. Phys.* **51** 250
[17] Hoogland A, Compagner A and Blöte H W J 1988 *Special Purpose Computers* (*Computational Techniques* **5**) ed B J Alder (New York: Academic)
[18] Binder K 1981 *Z. Phys.* B **43** 119
[19] Bruce A D 1985 *J. Phys. A: Math. Gen.* **18** L873
[20] Burkhardt T W and Derrida B 1985 *Phys. Rev.* B **32** 7273
[21] van Beijeren H and Schulman L S 1984 *Phys. Rev. Lett.* **53** 806