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Non-equilibrium stationary states in the $1-d$ BEG model: first- and second-order phase transitions

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Abstract. Monte Carlo simulations and finite-size scaling were used to study the one-dimensional BEG (Blume–Emery–Griffiths) model under the influence of two competing dynamics: single spin flip (Glauber dynamics at finite temperature T) and random exchange of two spins (Kawasaki dynamics at infinite temperature). The phase diagram shows first- and second-order phase transitions. The critical exponents are obtained for different values of the rates and the range of the exchanges. We find $\beta = 0.325 \pm 0.020$, $\gamma = 0.996 \pm 0.004$ and $\nu = 1.71 \pm 0.01$ for long-range exchanges and equal intrinsic rates. However, for different rates and nearest-neighbour exchanges we obtain $\beta = 0.07 \pm 0.03$, $\gamma = 1.60 \pm 0.06$ and $\nu = 1.53 \pm 0.08$, thus exhibiting non-universal behaviour.

1. The model

Recent years have witnessed a growing interest in non-equilibrium systems. These are often referred to as probabilistic cellular automata [1] or interacting particle systems [2] respectively in the physics or mathematical literature. The statistical mechanics of non-equilibrium stationary states is still an open problem, in marked contrast to equilibrium systems. The main difference is that the steady-state probability distribution is not known *a priori*. Analytical studies are at present restricted to infinitely fast exchanges [3]. For the other cases, simulation methods are used.

One way to obtain non-equilibrium stationary states is through competition between two dynamics, e.g. two Glauber dynamics at different temperatures [4] or Glauber (T finite) competing with Kawasaki dynamics at infinite temperature [5]. Here we will report a study of the one-dimensional Blume–Emery–Griffiths (BEG) model, which presents a rich variety of phase transitions and non-universal critical behaviour.

Our system is a simple one-dimensional lattice, at each site of which there is a three-state spin $\sigma_i = \pm 1, 0$, where $i \in \mathbb{Z}^1$. Denoting the general configuration of the system by $\sigma = \{\sigma_i : i \in \mathbb{Z}^1\}$, the reduced Hamiltonian is defined as

$$-\beta\mathcal{H}(\sigma) = \sum_{i=1}^{N}[J\sigma_i\sigma_{i+1} + K\sigma_i^2\sigma_{i+1}^2 - D\sigma_i^2]. \tag{1}$$

We consider two mechanisms by which a configuration of the lattice σ evolves in time:

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(i) Glauber dynamics in which a spin flips at a site i, $\sigma_i \to \sigma_i'$, with a rate W_i^{G},

$$W_i^{\mathrm{G}}(\sigma) = W^{\mathrm{G}}(\sigma_i \to \sigma_i') = \frac{1}{\tau_{\mathrm{G}}}\left\{1 - \tanh\left[\frac{Jx}{2}(\sigma_i - \sigma_i') + \frac{Ky - D}{2}(\sigma_i^2 - \sigma_i'^2)\right]\right\}$$

where $x = \sigma_{i-1} + \sigma_{i+1}$ and $y = \sigma_{i-1}^2 + \sigma_{i+1}^2$. This rate obeys detailed balance with respect to a heat bath at temperature β^{-1}. We notice that, as $D \to -\infty$, configurations with spins in the state 0 are forbidden; therefore, in this limit we recover the results for the (two-state) Ising model. More generally, this same limit is obtained, particularly at low temperatures, when the model parameters are such that only transitions between the ± 1 states are allowed.

(ii) The exchange Kawasaki dynamics at infinite temperature ($T = \infty$) in which two distinct spins in the lattice i, j exchange, with a rate $W_{i,j}^{\mathrm{K}}$. The two selected spins i, j may be nearest neighbours ($|i - j| = 1$) or arbitrarily distant. These two cases are studied here. The rate $W_{i,j}^{\mathrm{K}}(\sigma)$ may be defined in the following way

$$W_{i,j}^{\mathrm{K}}(\sigma) = W^{\mathrm{K}}(\sigma_i, \sigma_j \to \sigma_j, \sigma_i) = \hat{P}_{i,j}(\sigma)$$

where $\hat{P}_{i,j}$ is an operator that exchanges the spins at sites i and j. We shall denote by $\epsilon = \tau_{\mathrm{G}}/\tau_{\mathrm{K}}$ the ratio of the intrinsic microscopic rates. Since we were not able to perform an exact analysis of the time evolution for the magnetization m and quadrupolar average q in the case of finite ϵ, we applied the Monte Carlo method to study this system. We first considered the same weight for the bare rates ($\epsilon = 1$) but long-range exchanges (random mixing). It is well known that the Ising version of these competing dynamics shows no phase transition (at finite temperature) [6]. The evolution equation for the magnetization is linear and therefore the stationary state presents only the trivial solution. A phase transition is, however, observed [6] for Ising spins if the Glauber rate is modified to include nonlinear terms for the order parameter. It is argued by some authors [7] that under these conditions the $1-d$ Ising model exhibits mean-field behaviour, because the random mixing is expected to play the role of infinite-range interactions in the equilibrium Ising model. We here observe that the Glauber rate for the BEG model is intrinsically nonlinear (although it reduces to the linear form in the appropriate $D \to -\infty$ limit) and perhaps for this reason it leads to phase transitions even in the $1 - d$ systems.

The second case we studied corresponds to nearest-neighbour exchanges and arbitrary ϵ. The system also presents a phase transition in the stationary state, but the exponents are different from the ones found before. We therefore conclude that there are strong violations of universal behaviour in these non-equilibrium systems.

2. Second-order phase transitions

2.1. Long-range exchanges

The model we simulated consists of a linear chain with size varying from $L = 100$ up to $L = 5000$ sites. Periodic boundary conditions were always assumed in order to minimize finite-size effects. Up to 10^6 MCS were accepted, particularly for the largest samples. Furthermore, the initial evolution was discarded until a stationary distribution was reached. We accepted that stationarity was obtaineed when the following quantities were found to be independent of time:

$$M_L = \langle |m| \rangle = \left\langle \left| \frac{1}{L} \sum_{i=1}^{L} \sigma_i \right| \right\rangle$$

$$Q_L = \langle q \rangle = \left\langle \frac{1}{L} \sum_{i=1}^{L} \sigma_i^2 \right\rangle$$

$$\chi_L = L\{\langle m^2 \rangle - \langle m \rangle^2\}$$

which are, respectively, the magnetization, quadrupolar average and susceptibility. It is important to analyse finite-size effects carefully. A powerful tool for this purpose is the finite-size theory, first introduced by Fisher [8]; for a recent review see Privman [9]. We assumed that the finite-size theory for equilibrium systems can also be applied to this non-equilibrium model. We define a *critical temperature* for the finite system $T_c(L)$ as the one corresponding to the peak of the susceptibility. According to the finite-size hypothesis it follows that

$$1 - \frac{T_c(L)}{T_c} \simeq aL^{-1/\nu}(1 + \cdots) \tag{2}$$

where T_c is the value of $T_c(L)$ when $L \to \infty$. This *ansatz* arises from the assumption that there is a characteristic correlation lenght ξ in the system. Furthermore if we admit that a certain quantity, $A_L(T)$, presents algebraic singular behaviour when $L \to \infty$, then it should have the following scaling behaviour $A_L(T) = L^{\sigma/\nu}\tilde{A}(L^{1/\nu}t)$, where $t = (T - T_c)/T_c$ and $\tilde{A}(x)$ must be constant for small x and $\tilde{A}(x) \approx x^{-\sigma}$ for large enough values of x. One obtains the critical temperature T_c from the *Binder* number [10], which measures deviation from a Gaussian distribution,

$$U_L = 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2}.$$

This quantity goes to zero at high temperature and to $\frac{2}{3}$ at low temperatures. When U_L is plotted against temperature for different system sizes the curves should intersect at a fixed point value U^* and $T = T_c$. This quantity U^* is universal for equilibrium systems ($U^* = 0.611 \pm 0.001$, for $d = 2$ [11]). In our simulations (figure 1) we also obtain (within numerical accuracy) a universal value ($U^* = 0.357 \pm 0.005$).

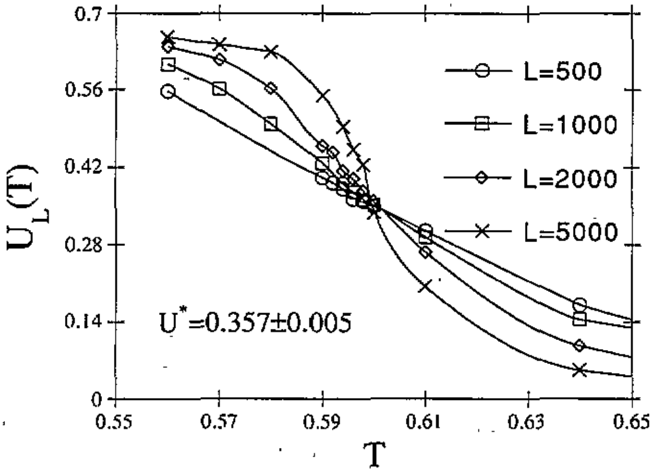

Figure 1. The 'Binder number', U_L, against temperature for different system sizes.

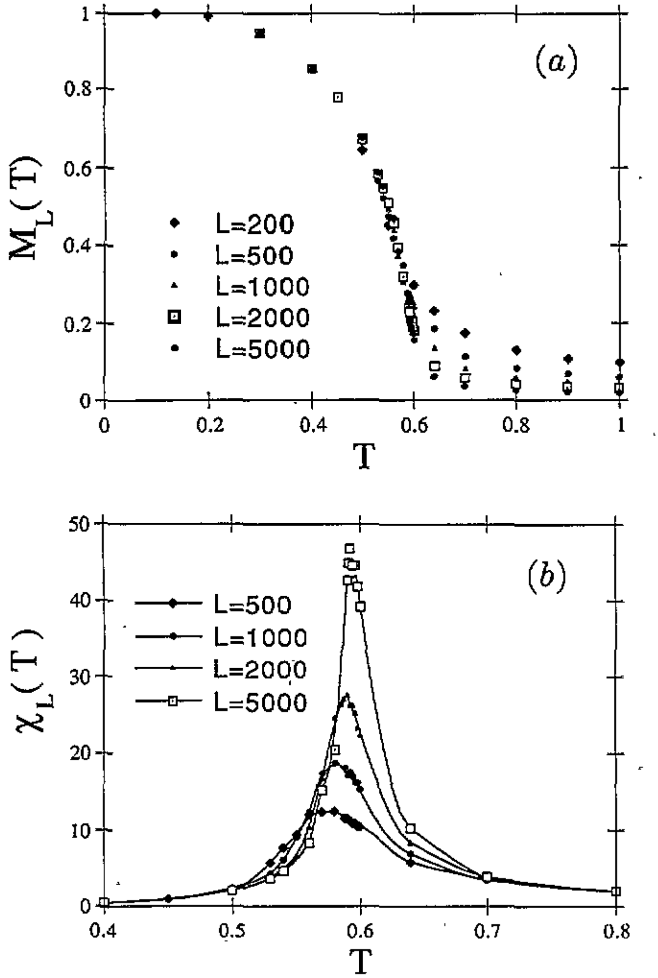

Figure 2. (a) Plot of the magnetization ($M_L = \langle |m| \rangle$) for different values of L. (b) Plot of the susceptibility χ_L for different values of L.

The previously defined quantities are therefore expected to obey the following finite size relations

$$M_L(T) = L^{-\beta/\nu} \tilde{M}(L^{1/\nu} t) \tag{3}$$

$$\chi_L(T) = L^{\gamma/\nu} \tilde{\chi}(L^{1/\nu} t) \tag{4}$$

$$U_L(T) = \tilde{U}(L^{1/\nu} t). \tag{5}$$

Using these relations the critical exponents may be obtained. We illustrate the method for long-range exchanges and equal microscopic rates. Figures 2(a) and (b) show the data obtained for the order parameter M_L and for the susceptibility χ_L as a function of temperature for different sample sizes. From the position of the peak we obtain $T_c(L)$ which when plotted (figure 3) against $L^{-1/\nu}$ yields T_c and this may be compared with the estimate from Binder's number. At the same time, the best value of ν is obtained when a linear fit is achieved. Our results are $T_c = 0.5974 \pm 0.0020$ and $\nu = 1.709 \pm 0.004$. The

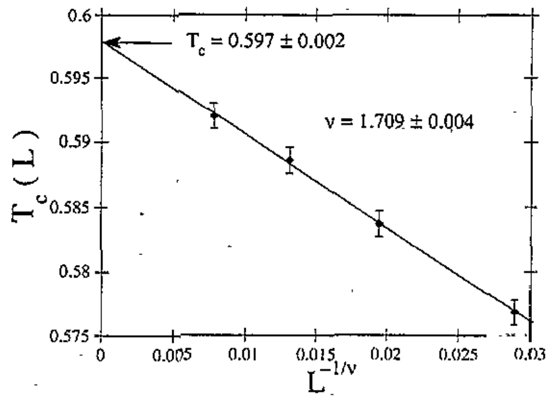

Figure 3. Plot of $T_c(L)$ against $L^{-1/\nu}$. The values of $T_c(L)$ correspond to the peak of the susceptibility. The exponent ν is obtained when the data are fitted to a straight line.

exponent β ($\beta = 0.325 \pm 0.020$) is obtained from a linear fit of $\ln M_{L=\infty}$ against $\ln(T - T_c)$ (figure 4). Figure 5 shows that we can again rule out the mean-field value ($\beta = \frac{1}{2}$) as well as the $2d$ Onsager value ($\beta = \frac{1}{8}$). Also, the exponent γ was extracted from the susceptibility peak $\chi_L(T_c(L))$ and also at T_c, $\chi_L(T_c)$ (figure 6), $\gamma = 0.996 \pm 0.004$. Finally, from a plot of $M(L)L^{\beta/\nu}$ againt $L^{1/\nu}t$ (figure 7) we obtained a scaling of the data, using for exponents γ, ν the values found previously; the exponent β may be independently found from a linear fit. Within numerical error (approximately 4%), we therefore find that these critical exponents obey the relation $2\beta/\nu + \gamma/\nu = d = 1$. We have not analysed possible biased systematic errors. Our error bars arise from the unavoidable dispersion of the numerical results due to the many different runs we performed. We can only claim that the *hyperscaling* relation is obeyed within numerical accuracy. Simulations were also performed at seven different points in phase space. Although the critical temperature is found to depend on the model parameters (figure 8) the exponents are the same, in agreement with universality.

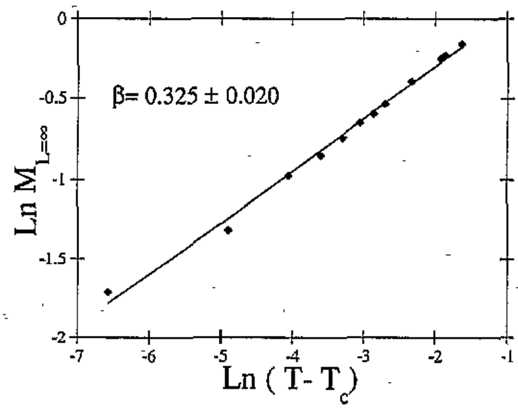

Figure 4. Plot of $\ln M_{L=\infty}$ against $\ln(T - T_c)$.

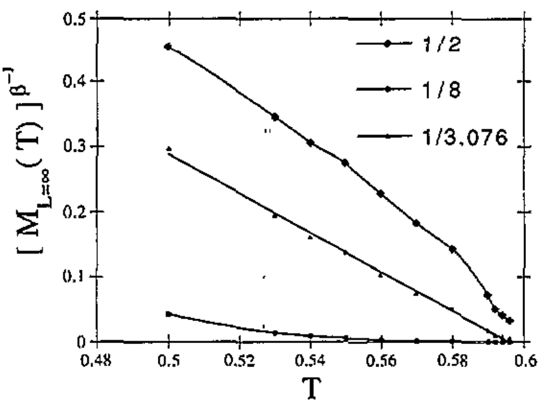

Figure 5. The data for the extrapolated order parameter M corresponding to the infinite lattice are plotted for different values of β. The case $\beta = 0.325$ produces the best straight line over the expected temperature range and extrapolates to a value T_c consistent with the one obtained by a different analysis.

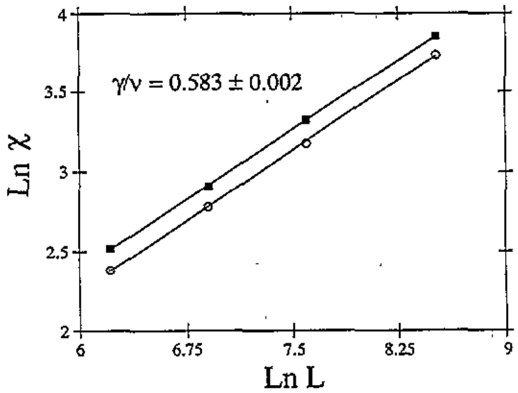

Figure 6. Plot of $\ln \chi$ for the susceptibility in the peak (squares) and at T_c (circles), against $\ln L$.

2.2. *Short range exchanges*

In contrast to the previous case, here we will consider different intrinsic microscopic rates and nearest-neighbour exchanges in order to study the effect of the range of the exchanges. A similar analysis was done in the $1-d$ Ising case where phase transitions were only observed for some values of the rates [12]. In our case, however, we observed phase transitions for different values of ϵ (figure 9) and for different points in the phase space (in fact the ones previously considered). In figure 9 we show a plot of $T_c(L, p)$, where $p = 1/(1+\epsilon)$, against $L^{-1/\nu}$. The slope of the fits gives the exponent ν and this appears to be the same within the numerical error for the different rates.

Figure 10 shows plots of the susceptibility against temperature for different system sizes. The critical exponents appear to be universal for all phase-space points where the transition is second-order. The critical exponents were found $\beta = 0.07 \pm 0.03$, $\gamma = 1.60 \pm 0.06$

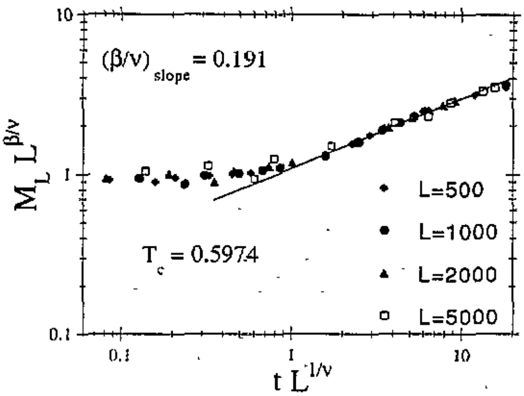

Figure 7. Plot of $M_L L^{\beta/\nu}$ against $tL^{1/\nu}$, using $\beta/\nu = 0.20$, $1/\nu = 0.58$, $T_c = 0.5974$. From the slope of the linear fit, we obtain $\beta/\nu = 0.191$.

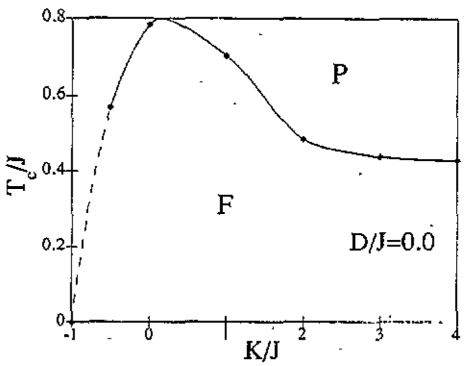

Figure 8. Plot of T_c against K/J (for $D/J = 0$). The curve passing through the data points is a guide to the eye. The broken curve extrapolates to the origin, where we should recase the results for the two-state Ising model.

and $\nu = 1.53 \pm 0.08$. The model now belongs to a completely different universality class. The exponents γ and ν were determined with a reasonable accuracy, however for the mean values found, γ/ν is a little larger than one, which seems to be in disagreement with the *hyperscaling* relation, but we believe that they have to obey as before and also in other non-equilibrium problems. The exponent β is small and affected by a big error because the magnetization decreases more rapidly at temperatures near T_c.

3. First-order phase transitions

In this section we will show in a qualitative way the existence of first-order phase transitions for some values of the parameters in the phase space $(D/J, K/J)$. We have considered $\epsilon = 1$ and long-range exchanges. The model was simulated in a way analogous to the previous one. However, in order to observe the different phases we repeated the simulations for each point in phase space with different initial configurations (figure 11). For $T > T_c^*$ (critical temperature) all initial configurations go to the same fixed point corresponding to

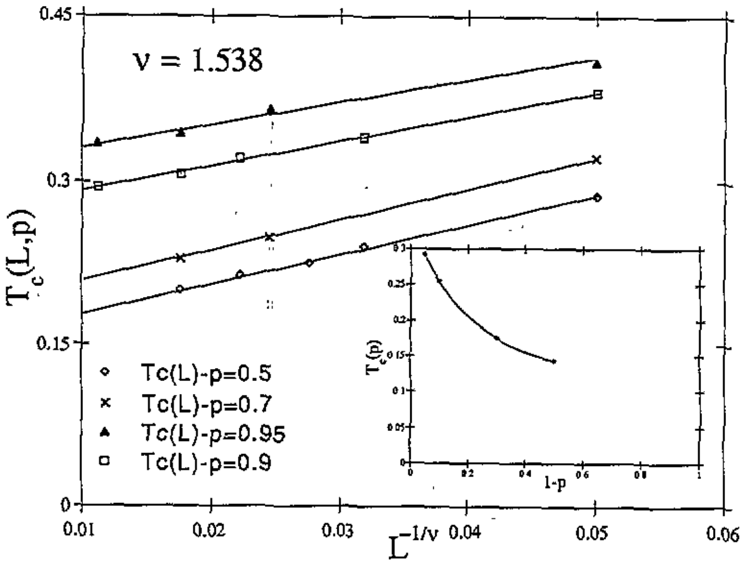

Figure 9. Plot of $T_c(L, p)$ for different values of $p = (1+\epsilon)^{-1}$ against $L^{-1/\nu}$.

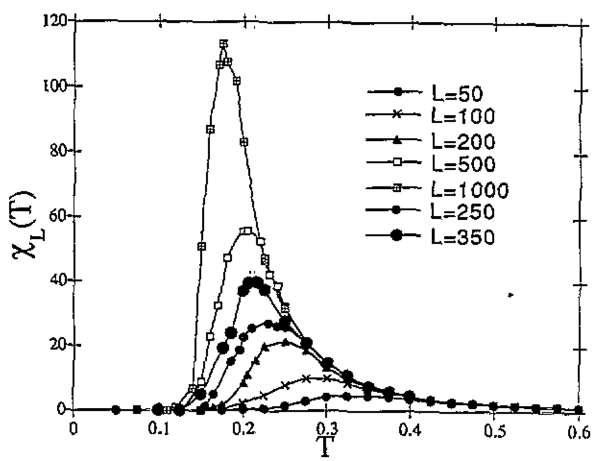

Figure 10. Plot of the susceptibility χ_L against temperature for $p = 0.5$.

the quadrupolar phase, where $M_L \sim 0$ and Q_L is different from zero. But for $T < T_c^*$ the system bifurcates and for each temperature we observe two distinct values of M_L and Q_L, corresponding to the phases $\cdots + + + + + \cdots$ or $\cdots - - - - - \cdots$ ($M_L = Q_L = 1$) and $\cdots 00000 \cdots$ ($M_L = Q_L = 0$). The phase with $M_L = 0$ and $Q_L = 0$ is not a paramagnetic phase but an ordered phase with all spins equal to zero. The phase diagram is therefore very rich and presents an interesting problem about the relative stability of the phases when first-order phase transitions are observed in non-equilibrium systems.

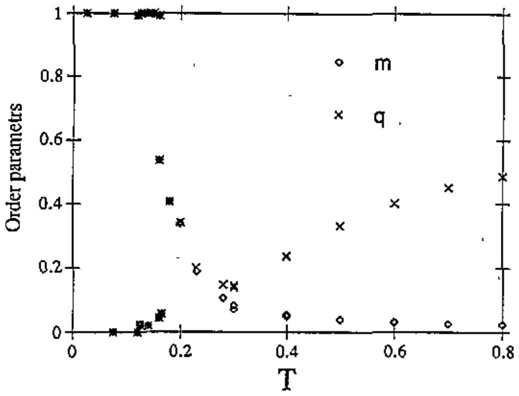

Figure 11. Typical plot of a first-order phase transition.

4. Conclusion

Using Monte Carlo simulations and finite-size scaling have we studied the $1-d$ BEG model under the influence of two competing dynamics, one Glauber and the other Kawasaki. The main scope of this study was to understand the effect of the ratio of intrinsic microscopic rates and the range of the exchanges. We obtained the critical exponents β, γ and ν in two distint cases: $\epsilon = 1$ and long-range exchanges; and $\epsilon \neq 1$ and short-range exchanges. In each of these cases we found different critical exponents, though they apppear to be universal within the respective phase-space diagrams. Furthermore, the exponents are not classical although mean-field behaviour is obtained for infinitely fast exchanges†. We conclude that the range of exchanges is a decisive factor in the definition of universality classes at least for these simple non-equilibrium systems. For the one-dimensional non-equilibrium Ising model it is known that the range of the spin exchanges yields a critical behaviour which depends on the assumed power law (Lévy flight) for the space decay of the microscopic rates [13]. This behaviour is similar to the well known behaviour found for the one-dimensional equilibrium Ising model and it interpolates between the short- and infinite-range models.

Similar, possibly richer behaviour may be expected for the non-equilibrium, one-dimensional BEG model. In this paper we have just considered the two extreme limits—infinite-range and nearest-neighbour spin exchanges. Our results were obtained after approximately 5000 h of CPU time in WorkStations HP 720 and CDC 4680. It is anticipated that a thorough examination of the whole phase space or the influence of the range of the spin exchanges will take much more CPU time than we can afford at the moment. Therefore, the important questions about the other possible universality classes in this model are beyond the scope of this paper and will hopefully be considered for future research.

References

[1] Vichniac G 1984 *Physica* D **10** 117
[2] Liggett T M 1985 *Interacting Particle Systems* vol 296 (Berlin: Springer)
[3] De Masi A, Ferrari P A and Lebowitz J L 1986 *J. Stat. Phys.* 44 589

† An analytical study of this model in the limit of infinitely fast exchanges showing a rich phase diagram with first-and second-order phase transitions will be published in the near future.

[4] Blote H W, Heringa J R, Hoogland A and Zia R K P 1990 *J. Phys. A: Math. Gen.* **23** 3799
[5] Droz M, Rácz Z and Schmidt J 1989 *Phys. Rev.* A **39** 2141
[6] De Masi A, Ferrari P A and Lebowitz J L 1985 *Phys. Rev. Lett.* **55** 1947
[7] Droz M, Rácz Z and Tartaglia P 1991 *Phys. Rev.* A submitted
[8] Fisher M E 1972 *Critical Phenomena Proc. 51st Enrico Fermi Summer School (Varenna)* ed M S Green (New York: Academic)
[9] Privman V 1990 *Finite Size Scaling and Numerical Simulation of Statistical Systems* (Singapore: World Scientific)
[10] Binder K 1981 *Z. Phys.* B **43** 119
[11] Bruce A D 1985 *J. Phys. A: Math. Gen.* **18** L873
[12] Gonzaléz-Miranda J M, Garrido P L, Marro J and Lebowitz J L 1987 *Phys. Rev. Lett.* **59** 1934
[13] Bergensen B and Rácz Z 1991 *Phys. Rev. Lett.* **67** 3047