Anisotropic Lattice Gases

J. Marro¹ and A. Achahbar^{1, 2}

Received October 29, 1996; final September 4, 1997

We have studied lattice gases with a particle-conserving dynamic rule that involves two principal parameters. One of them has two limiting values that correspond, respectively, to a large, saturating constant field, which induces a positive particle current, and to a random field (zero net current). Varying the other parameter, either particle attractions or repulsions perpendicular to the field are simulated. The nature of ordering is shown to be independent of the value for the field parameter. In particular, the two indicated limiting cases of the latter lead to the same order-parameter critical behavior, consistent with $\beta \simeq 1/3$, in the presence of a linear interface for attractions in two dimensions. Some qualitative features of the time relaxation are briefly described.

KEY WORDS: Nonequilibrium phase transitions; anisotropic dynamics; interphases; driven lattice gases.

Universality is well established in equilibrium critical phenomena. The asymptotic behavior at critical points is determined by a few, essentially geometrical properties of the system and its order parameter, and simplified mathematical models, such as lattice systems and their continuum analogs play an important role. Equilibrium is a very special case, however, in which dynamics becomes irrelevant. Concluding about nonequilibrium steady states, which may—by contrast—be determined by dynamics, is a challenging problem. Consider lattice, Ising-like systems that, under dynamic rules violating detailed balance, evolve irreversibly with time towards nonequilibrium steady states. They may often (but not always) be considered as perturbed equilibrium systems. For non-conservative cases with the up-down symmetry, the dynamic Ising fixed point is predicted to

¹ Instituto Carlos I de Física Teórica y Computacional, and Departamento de Física Aplicada, Facultad de Ciencias, Universidad de Granada, 18071-Granada, Spaín.

² Present address: Laboratoire de Physique de la Matière Condensée, Faculté des Sciences, B.P. 133, 14000 Kenitra, Morocco.

^{0022-4715/98/0200-0817\$15.00/0 © 1998} Plenum Publishing Corporation

Marro and Achahbar

be locally stable.⁽¹⁾ Although many examples of such simple behavior have been reported (even beyond the intended range of validity of the argument),⁽²⁾ this is not expected to hold in general. At the present time, the latter assertion has a rather phenomenological basis; i.e., the limits of influence of the dominant, pervasive Ising fixed point are far from clear cut.^(2, 3) This is so because the role of symmetries for non-Hamiltonian systems, e.g., which symmetries (of the lattice, configurations, forces, order parameter, and dynamics) are the relevant ones, and how they influence the emergent critical behavior, is not yet well enough understood.

We introduce in this letter a class of anisotropic lattice gas automata (ALGA) that provide a simple scenario to analyze the influence of anisotropies on phase transitions. Time evolution proceeds by nearest-neighbor particle-hole exchanges as induced by superposition of a longitudinal *field* mechanism and transverse thermal processes. Implementing this in the computer by sequential updating-the only case we consider here-can be made efficient enough as to conclude about the influence of the system parameters on critical properties, and to describe the whole system evolution from an arbitrary disordered configuration to the final steady state. The behavior of the ALGA is reminiscent of that reported for the driven lattice gas (DLG) and its variations; cf. refs. 2 and 3, for instance. Therefore, our study bears also some relevance concerning the DLG critical behavior, which is presently under debate.⁽³⁻⁸⁾ In fact, a main motivation to study the ALGA was trying to confirm a changeover from classical to non-classical critical behavior which is predicted by field theory for the DLG as the driving field is modified. Another interesting feature of the ALGA is that it exhibits non-trivial behavior while it involves rather simple microscopics. In particular, the ALGA is characterized by the simplest thermal process one can imagine; this is important because different rate functions are known to induce (arbitrary) fluctuations in the DLG whose detailed influence on the steady state is not yet well-understood.

The ALGA consist of the simple "cubic" lattice in d > 1 dimensions with toroidal boundary conditions. Occupation variables at the lattice sites have two states, $\sigma_r = 1$ or 0, corresponding to the presence or not of a particle at site r; the particle density is n. The repeated rule inducing changes with time of the configuration is as follows: A particle is selected at random (and the time counter is increased by 1/N, with N the number of sites); then, also at random, one selects one of its nearest-neighbor sites. If this is occupied, the process commences again. Otherwise, the exchange between the particle and the (nearest-neighbor) hole is considered. Exchanges that transfer a particle a distance $+\hat{x}$ or $-\hat{x}$ apart, where \hat{x} is one of the principal unit vectors of the lattice, are accepted with probability p or 1 - p, respectively. Transverse particle-hole exchanges have probability b if the

Anisotropic Lattice Gases

second neighbor in the direction of the attempted jump is a particle, and 1-b if it is a hole. Table 1 lists all the possible transitions for d=2. The process is repeated as necessary (a minimum of 10^7 time units in practice). Detailed balance is not satisfied by this rule in general. We mainly report here on d=2 and n=1/2 (i.e., the half-filled square lattice) for p=1, 3/4 and 1/2, and varying values of b. Some details not included here, and other cases of the parameters are reported elsewhere.^(2, 9)

The parameter $b \in [0, 1]$ controls a tendency of the jumping particle either to approach its neighbor along any of the transverse directions (for b > 1/2) or to separate from it (for b < 1/2). Consider a generalization of the above system in which one samples the $\pm \hat{x}$ directions with a priori probability q, as compared to 1-q for transverse directions.⁽²⁾ The limits $q \rightarrow 0, 1$ allow for two well-separated time scales for the field and thermal processes, respectively. Assuming $q \equiv 0$ reduces the system to independent chains acted on by the thermal processes only. The study of this case indicates that b-1/2 plays indeed a role similar to the (inverse) temperature parameter for the ordinary Ising chain. For $q \equiv 1$, the system reduces to independent one-dimensional exclusion processes-quite asymmetric for p = 1.⁽¹⁰⁾ We shall only deal hereafter with q = 1/2, i.e., no a priori bias exists. (Note that investigating the influence of q on emergent properties is interesting.⁽⁹⁾ The parameter $p \in [1/2, 1]$ plays the role of a field driving particles along $\hat{\mathbf{x}}$. For p = 1, particles do not jump backwards, $-\hat{\mathbf{x}}$; therefore, the steady state exhibits a positive, saturating particle current. For p = 1/2, the simulated field is random, i.e., displacements $\pm \hat{\mathbf{x}}$

Table 1. The Rate for the Two-DimensionalSystem (With No A Priori Bias), AssumingThat the Preferred Direction, +x̂,Is Vertical Upwards^a

Transition	Rate	
	b b b $1 - b$ $1 - b$ p $1 - p$	

^a The symbols ■ and □ stand for occupied and vacant sites, respectively.

are produced with equal probability, and there is no net current on the average.

Figure 1 illustrates the evolution with time. For large enough b, namely $b > b_c(p)$, where $b_c(p)$ appears to correspond to a line of critical points for the infinite lattice, the system segregates by developing first clusters elongated along the $\hat{\mathbf{x}}$ axis, which transform then into several strips that finally coalesce into a single one. That is, the steady state exhibits linear interfaces parallel to $\hat{\mathbf{x}}$ separating rich- from poor-particle phases. A natural way of revealing the presence of one or more strips is by monitoring the anisotropic magnetization, defined $m = |M_x - M_y|^{1/2}$, where $M_{x(y)}$ is the ensemble average (computed in practice as a time average during the steady state) of

$$N^{-1} \sum_{x(y)} \left[\sum_{y(x)} (1 - 2\sigma_{x,y}) \right]^2$$

The steady, single-striped states are better analyzed by computing the *local* density, φ , defined as the ensemble average of

$$\frac{1}{2\sqrt{N}}\sin\left(\frac{\pi}{\sqrt{N}}\right)\left|\sum_{x,y}\left(1-2\sigma_{x,y}\right)e^{i\mathbf{k}\cdot\mathbf{r}}\right|$$

 $\mathbf{k} = (0, 2\pi N^{-1/2})$. We have monitored $m, \varphi, \psi \propto m\varphi$, and φ corresponding to each phase; no essential differences are noticeable.

The observed nature of processes such as those in Fig. 1 deserve comment, even though we cannot conclude definitely about (obtaining sufficiently good statistics with this aim is far beyond our objectives here). Studying m and ψ suggests that time relaxation occurs discontinuously by steps, as caused by repeated "avalanches" of "all" sizes. Concluding about it would require careful coarsening to avoid disturbing noise due to smallscale cutoffs; e.g., our study is hampered by changes involving a few



Fig. 1. Typical evolutions with time of the 64^2 lattice for n = 1/2, b = 0.9, and (from left to right, respectively) $t = 10^2$, 10^3 , 10^4 , and 10^6 time units. The field parameter here is p = 1/2, but one obtains apparently the same configurations for p = 1.⁽²⁾ The preferred axis, $\hat{\mathbf{x}}$, is vertical.

820

Anisotropic Lattice Gases

particles, and by the fact that the sizes investigated are small for the purpose. Another interesting fact we should mention is that the time variation of the pair correlation function appears to exhibit self-similarity properties⁽¹¹⁾ if scaled using the mean width of strips as the relevant measure of time. Again a definite conclusion in this regard would required much more data than available, i.e., monitoring the whole evolution of *very* large systems. We concentrate below on steady properties, for which reasonably conclusions can be reached in practice for $N \gtrsim 10^4$.

The behavior in Fig. 1 is reminiscent of that exhibited by different variations of the DLG.⁽²⁾ The differences between the two systems are important, however. First, the DLG is a perturbed equilibrium system, whereas the ALGA has no limiting equilibrium counterpart. Second, the relevant symmetries are essentially similar in both cases, except that the ALGA, unlike the DLG when the lattice is half-filled, does not have the up-down symmetry along the transverse direction. It has some important consequences, e.g., non-complementary densities for the rich- and poorparticle phases (which is often clear by direct inspection of configurations). However, such a difference is quite irrelevant to the main conclusion below (i.e., a comparison between the cases p = 1 and p = 1/2), and it does not seem critical in other respects. (The latter belief is consistent with the transverse process showing up in the simulations as a true thermal one, and with the fact that various measures of order applied to the two phases did not result into any noticeable difference.) Also important is that the ALGA simplicity makes it much more convenient for numerical studies. On one hand, the ALGA dynamics is given once for all whilst the rate function for the DLG is left arbitrary-in fact, most known DLG properties concern the Metropolis rate, the only one studied systematically so far. On the other hand, the ALGA rule leads more efficiently to the steady state than the DLG dynamics. In part, this is a consequence of the fact that the ALGA algorithm requires one to check the state of only one nearest neighbor of the particle-hole to be exchanged, as compared to six for the 2d DLG. Also noticeable is that the mean probability of any transverse move in the latter can be approximated (for the Metropolis case at high enough temperature, using familiar notation) by $2^{-6} \sum_{\text{cluster conf.}} \min\{1,$ $\exp(-\Delta H/T)$, which is always larger than 2/3, and goes to unity as $T \rightarrow \infty$, so that much larger fluctuations than for the ALGA case are allowed. In fact, unlike for the DLG in a comparable experiment, it turns out relatively simple to observe—within reasonable computer time—the whole time decay of the ALGA from a random configuration, as in Fig. 1 (which might also indicate a somewhat different phase space in which sates with several strips are more unstable than for the DLG). Finally, as a consequence of the above, the ALGA rule has also turned out to be efficient in approaching the critical point rather closely for the standards.^(4, 6) For example, we have obtained rather good data (corresponding to stationary averages over 10^8 independent configurations) for the 128^2 lattice with p = 1 at 13 different values of b > 1/2 within the range $0.001 \le \varepsilon$ ($\equiv b/b_c - 1$) < 0.07. This technical detail happens to be important, as it somewhat strengthens some of the conclusions in this letter.

Our key result is that the parameter p is rather irrelevant for ordering, even though a net current is only measured for $p \neq 1/2$. This is suggested, for instance, by the comparison in Fig. 2 between steady-state configurations for different p values at (approximately) the same distance from the corresponding critical point. The behavior of the order parameter for the 128^2 lattice is presented in Fig. 3. On the scale of the figure, the set for p = 1 cannot be distinguished from the one for p = 1/2. We have generated data for other sizes, and estimated b_c^L , which locates the transition for each $L \equiv \sqrt{N}$, from analysis of the order-parameter susceptibility. The result of this analysis is in Fig. 4. (It may be mentioned that, assuming v = 0.7, as suggested by the DLG behavior,⁽²⁾ when extrapolating to the infinite system, gives $b_c = 0.855$, 0.857 for p = 1, 1/2, respectively, which equal the

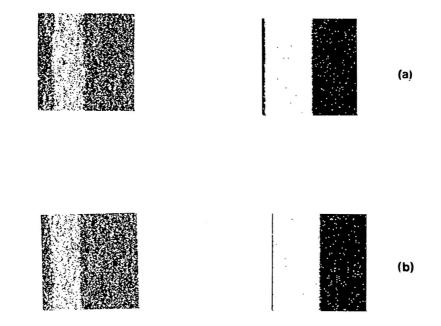


Fig. 2. Typical steady state configurations of the 128^2 lattice for p = 1/2 (a), and p = 1 (b). The graphs are for $\varepsilon \equiv b/b_c - 1 = 0.011$ (left) and 0.144 (right). The axis $\hat{\mathbf{x}}$ is vertical.

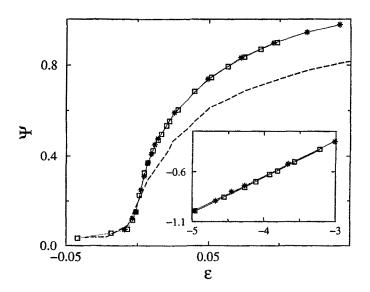


Fig. 3. The variation with $\varepsilon = b/b_{c} - 1$, where $b_{c}(p)$ is given in the main text (cf. Fig. 4), of the density φ for $N = 128^{3}$, and p = 1 (squares) and 1/2 (asterisks). The dashed line is for the corresponding two-dimensional DLG of the same size. The inset is a ln-ln plot of the data for the ALGA in the critical region which gives slope $\beta \simeq 1/3$ for any p.

values we obtained independently from the cumulant method.⁽¹²⁾) Figure 3, and its inset, involve ε defined using the value of b_c^L for L = 128 in Fig. 4, namely, $b_c^{128}(1) = 0.856$ and $b_c^{128}(1/2) = 0.858$. The inset in Fig. 3 thus reveals that not only b_c , but also the thermodynamic amplitude differs from one case to the other: the differences are small but systematic. In any case, the same value for the order-parameter critical exponent, β , is suggested for any p.

An important question is critical behavior at $b_c(p) > 1/2$. We have presented in the inset of Fig. 3 some evidence that the critical exponent for the order parameter is independent of p, and consistent with $\beta \simeq 1/3$ rather close to the critical point, namely, for $0.001 \le \varepsilon \le 0.05$. The following remarks are in order. This result concerns a finite lattice with $N = 128^2$; we have avoided using here finite-size scaling formulas, because no definite theory exists for these anisotropic cases yet.⁽²⁾ It should be noted, however, that one may prove consistency with $\beta = 1/8$ by analyzing data for the 128^2 -equilibrium–Ising model within a similar critical region.⁽¹³⁾

We wish to remark that, besides observing the true asymptotic regime, one needs an accurate estimation of the critical point before concluding confidently about critical exponents. It was argued recently^(6, 7) that failing to do so was the cause to observe $\beta \simeq 1/3$ for the DLG (instead of $\beta = 1/2$

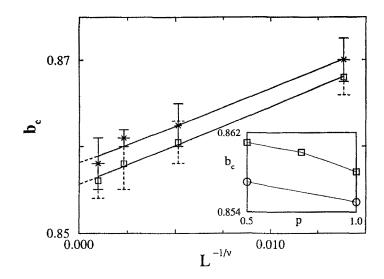


Fig. 4. The critical value b_c , for p = 1 (squares) and 1/2 (asterisks), as a function of the lattice side, $L = \sqrt{N}$. The bars indicate upper bounds for the corresponding errors, as obtained by analysis of the order-parameter susceptibility. We set here (rather arbitrarily) v = 0.7;⁽⁸⁾ this gives $b_c = 0.855$ (p = 1) and 0.857 (p = 1/2) for the infinite system, $N \to \infty$, in accord with the values obtained from the cumulant method.⁽¹²⁾ (The Ising value v = 1 leads instead to $b_c = 0.854$, 0.856, respectively.) The inset shows the variation with p of our b_c estimates for $N = 70^2$ (upper curve) and 128².

which is predicted for attractive forces by field theory.⁽⁵⁾). Therefore, we have submitted our best-quality data to the stringent test illustrated in Fig. 5. For p = 1, the slope in a plot of $\log \psi$ versus $\log \varepsilon$ is observed to vary somewhat within the region $0.001 \le \varepsilon \le 0.1$. In order to make explicit this fact, we have performed a running average; this gives the squares in Fig. 5. That is, the *effective* critical exponent β estimated in this way slightly

System	β	Critical point	Amplitude, A
p = 1	0.34	0.856	2.05
p = 1 p = 1/2	0.34	0.858	2.08
DLG	0.34	1.29	1.63
Ising	1/8	2.28	1.19

Table 2. Parameter Values That Produce Collapsing of Data for the Order Parameter of the Indicated Systems near $\epsilon = 0$.⁽¹³⁾

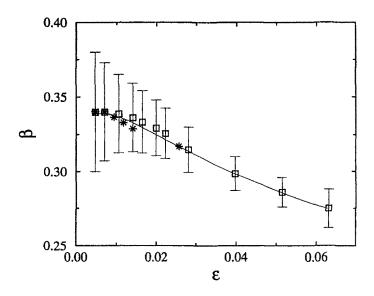


Fig. 5. The temperature variation (very close to the critical point) of the quantity $\beta(\varepsilon)$, defined as the slope, in a running fit, of $\log \psi$ versus $\log \varepsilon$, for p = 1 (squares) and 1/2 (asterisks). The error bars here are a consequence of the ones in Fig. 4.

increases monotonically with decreasing ε before it finally seems to stabilize for $\varepsilon \leq 0.01$. The minimum observed value, around $\varepsilon = 0.06$, is $\beta \approx 0.27$ (which is the value reported before^(4, 8) for the DLG for $0.01 < \varepsilon < 0.3$); this increases up to $\beta \simeq 1/3$. The effect of allowing for variations of the critical parameter within the range $b_c(p=1) = 0.856 \pm 0.002$ (i.e., assuming that our estimate is affected by errors larger than suggested by the corresponding analysis) is also illustrated in Fig. 5. Applying the same method to our data for p = 1/2 (which are admitted to be of slightly poorer quality) gives the same result.

Summing up, the lattice gas automata presented here appear to exhibit for b > 1/2 a line of critical points, $b_c(p)$, where the order parameter behaves $\psi \sim \varepsilon^{\beta}$ as $\varepsilon \to 0$ with $\beta \simeq 1/3$, independent of p. The anisotropic nature of the dynamic rule, and the resulting linear interphase are probably at the origin of such rare bulk property. The situation is similar to the one described before for the DLG,⁽²⁾ which contains fundamentally the same anisotropy and driving field. One is tempted to contrast the behavior of the ALGA with existing field theory for the DLG⁽⁵⁾ (in which, however, the up-down symmetry holds), which predicts classical behavior ($\beta = 1/2$) for a saturating field but $\beta \simeq 1/3$ for a random one.⁽¹⁴⁾ On the other hand, a preliminary study of the ALGA for b < 1/2, i.e., repulsive interactions, reveals that it also exhibits order, apparently independent of p,⁽⁹⁾ which again contrasts the field-theoretic prediction⁽¹⁵⁾ that a saturating driving field washes out any long-range order for the DLG with repulsive forces. Consistent with such disagreements, which we interpret as caused by an essential difference between the discrete DLG and available continuous counterparts, it has been shown⁽³⁾ that the latter might not always take proper account of the microscopic field parameter. The fact that only one relevant correlation length is involved by the present problem, which may be seen as a side result of our study, was recently concluded from other points of view.^(8, 16) The same ensues from the field-theoretic study of the DLG in ref. 3, where it is attributed to the singular lack of Galilean invariance when the driving field becomes infinite.

ACKNOWLEDGMENTS

We acknowledge useful comments by Pedro L. Garrido and Herbert Sphon, and support by the DGICYT under Project No. PB91-0709 and by the Junta de Andalucía of Spain.

REFERENCES

- 1. G. Grinstein, C. Jayaprakash, and Y. He, Phys. Rev. Lett. 55:2527 (1985).
- 2. J. Marro and R. Dickman, Nonequilibrium Phase Transitions in Lattice Models, (Cambridge, Univ. Press Cambridge, 1998).
- 3. P. L. Garrido, F. de los Santos, and M. A. Muñoz, Phys. Rev. E 57:752 (1998).
- 4. A. Achahbar and J. Marro, J. Stat. Phys. 78:1493 (1995).
- 5. B. Schmittmann and R. K. P. Zia, in *Phase Transitions and Critical Phenomena*, C. Domb and J. L. Lebowitz, eds. (Academic Press, New York, 1995).
- 6. J.-S. Wang, J. Stat. Phys. 82:1409 (1996).
- 7. K.-T. Leung and R. K. P. Zia, J. Stat. Phys. 83:1219 (1996).
- 8. J. Marro, A. Achahbar, P. L. Garrido, and J. J. Alonso, Phys. Rev. E 53:6038 (1996).
- 9. J. Marro et al., to be published.
- 10. See, for instance, M. R. Evans and B. Derrida, Acta Physica Slovaca 44:331 (1994).
- 11. J. Marro, J. L. Lebowitz, and M. H. Kalos, Phys. Rev. Lett. 43:282 (1979).
- K. Binder, in *Monte Carlo Methods in Statistical Physics*, K. Binder, ed. (Springer-Verlag, Berlin, 1979).
- 13. In fact, we have explicitly checked that data in such region for the 128^2 lattice with different dynamics, including our rule with p = 1 and 1/2, the DLG, and the Ising model, all can be scaled to a unique behavior by using the parameters given in Table 2. Note also that the main graph in Fig. 3 indicates that the region of interest has approximately the same asymptotic significance for both our model and the DLG, in spite of different definitions for ε .
- 14. B. Schmittmann and R. K. P. Zia, Phys. Rev. Lett. 66:357 (1991).
- 15. K.-T. Leung, B. Schmittmann, and R. K. P. Zia, Phys. Rev. Lett. 62:1772 (1989).
- J. Marro, in *Monte Carlo and Molecular Dynamics of Condensed Matter Systems*, K. Binder and G. Ciccotti, eds., Chapter 32, pp. 843-858, (Italian Physical Society, Bologna, 1996).