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Coarsening in a Driven Diffusive System with Two Species.

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Abstract. – We study the dynamics of a lattice gas with two species of «charged» diffusing particles in the presence of an external field. There are several time scales characterizing the approach of the steady state. At short times diffusion smears out inhomogeneities. For fields such that the density is below the virtual (size-dependent) threshold of jamming, *i.e.* in the flow phase, this is the main relaxation mechanism. In addition, there are kinematic waves arising from the non-linear dependence of the current on the density. Above the threshold there is an instability leading to a *multi*strip structure of blockages: in each strip one type of particle prevents the other type from following the direction of the imposed field. The strips coarsen logarithmically slowly, until finally a single blockage remains.

Driven diffusive systems have attracted much attention [1] as they provide tractable examples of non-equilibrium phenomena. Recently, a simple model with two oppositely «charged» species (with however no interaction other than hard-core exclusion) was shown to exhibit interesting phase-transition–type behaviour [2]. In diffusive dynamics in the presence of a uniform external field, structures develop in the high-density regime—this is the inhomogeneous phase of the system—while at low density particles are uniformly distributed on the lattice in the so-called homogeneous phase. Analogous behaviour is also observed in a deterministic traffic model, where the low-density regime is a flowing phase, while at high densities a «traffic jam» develops [3].

In this paper we investigate the time evolution of the formation of structures in this problem.

The model is defined as follows: consider, for simplicity, the square lattice of size L, with fraction ρ of the sites occupied by particles, half of which have $+$, and the other half $-$ «charge». Particles diffuse to randomly chosen empty neighbouring sites. An external field E (pointing diagonally, north-east) introduces a bias and each type of particle acquires a preferred direction, in which it preferentially hops with probability $a = x/(1+x)$ with $x = \exp[E/k_B T]$. The different types of particles have opposing preferred directions: thus for

+ particles, these are north and east, while for the − particles, south and west are preferred. The probability of hopping in the less preferred direction is $b = 1 - a$. Periodic boundary conditions are imposed both parallel and perpendicular to the field. There are three parameters in the problem: the system size, L, the density, ρ, and the difference of probabilities to hop in the preferred or opposite directions, $\Delta = a - b$.

It has been noted in earlier studies [2,3] that for given system size there is apparently a phase transition as a function of particle density ρ and applied field (which determines the asymmetry, Δ). For large values of ρ and Δ the asymptotic density becomes spatially inhomogeneous on the lattice, and particles build up a blockage perpendicular to the field. In the other phase which occurs for low ρ, the asymptotic density is homogeneous and no structures emerge. We denote the threshold for the transition as ρ_c, and note that it depends strongly on the system size and applied field. However, based on the scaling solutions of the mean-field results, it was argued [4] that in the thermodynamic limit, for any fixed non-zero field and density, the stationary state is inhomogeneous, and consequently the phase *transition* disappears.

Simulation of the model in the high-density phase shows interesting temporal evolution of the blockage structures. Starting from random initial conditions, in the early stages, one sees that patches develop: these later form «clouds» which grow and coarsen [5] until finally one blockage spans the lattice. (Depending on the shape of the lattice, helical strips can be formed [6].)

This is typical of a coarsening phenomenon [7], and our aim here is to understand its mechanism. For this purpose we study the mean-field theory of this model numerically.

The mean-field equations of the model [4,8] reflect the translational symmetry in a direction perpendicular to the field, which reduces the problem to one dimension. Here we focus on the lattice version [4]. Letting the density of + particles at position i at time t be $p_i(t)$ and that of − particles $m_i(t)$, the equations are

$$\dot{p}_i = -ap_i(1 - p_{i+1} - m_{i+1}) - (1-a)p_i(1 - p_{i-1} - m_{i-1}) + \\ + (1-a)p_{i+1}(1 - p_i - m_i) + ap_{i-1}(1 - p_i - m_i) \quad (1)$$

and

$$\dot{m}_i = -am_i(1 - p_{i-1} - m_{i-1}) - (1-a)m_i(1 - p_{i+1} - m_{i+1}) + \\ + (1-a)m_{i-1}(1 - p_i - m_i) + am_{i+1}(1 - p_i - m_i) . \quad (2)$$

In addition, periodic boundary conditions are assumed:

$$p_{L+1} = p_1 , \qquad m_{L+1} = m_1 , \qquad p_0 = p_L , \qquad m_0 = m_L . \quad (3)$$

We solve these equations numerically with random initial conditions: at time $t = 0$, both m_i and p_i are taken from a uniform random distribution around the average density $\rho/2$, with width $\min(\rho/2, 1 - \rho/2)$. After random filling, the initial densities are corrected to maintain charge neutrality. Numerical integration was carried out with time step 0.1 (in natural units).

A typical series of density plots for one type of species is shown in fig. 1, where the density and field strength are taken deep in the blocked phase, $\rho = 0.9$, $\Delta = 0.4$ and $L = 300$. (This size is used only for displaying the density plots; the results of the paper were obtained with $L = 1024$.) The formation of the multistrip structure, as well as the coarsening with time are clearly observable. Obviously, there is more than one time scale involved in this problem. In fig. 1*a*), at time $t = 100$ the blockages have just emerged; at later times, say by $t = 10^4$, the strip is quite well-formed, with particle density nearly 1 in the entire width of the strip.

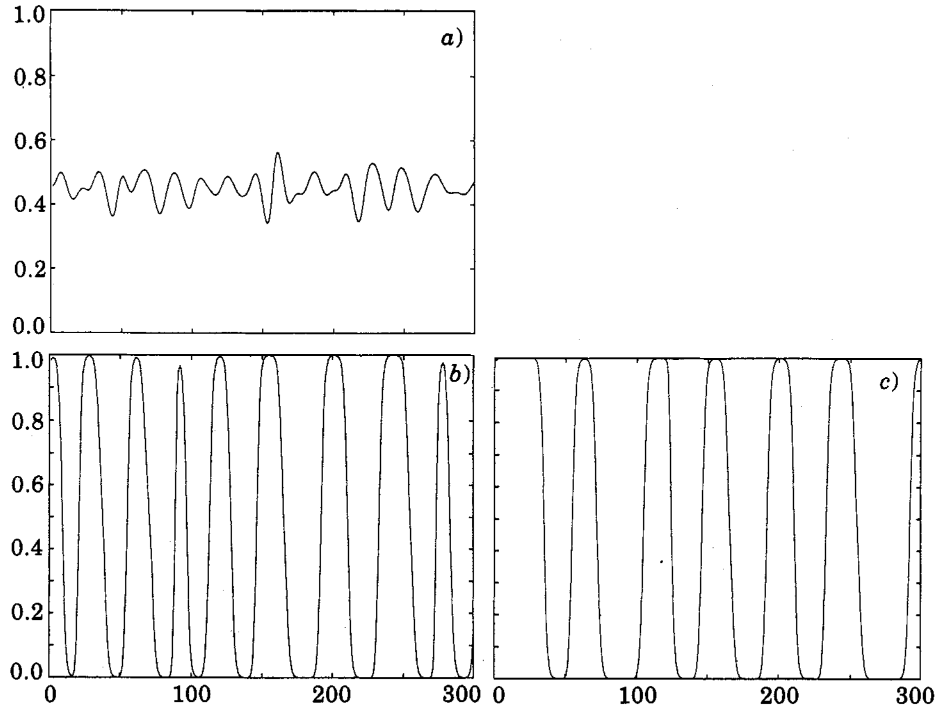

Fig. 1. – Density of one of the species as a function of the space coordinate at different times: *a*) $t = 10^3$, *b*) $t = 10^5$, *c*) $t = 10^7$. The total density of particles is $\rho = 0.9$ and the difference in the jumping probabilities in the preferred (*a*)) and opposite (*b*)) directions is $\Delta = 0.4$. Note that in this and all other figures the units of time are 0.1 (in natural units).

In order to monitor the development of these structures at early times, we examine density fluctuations $w^2(t) = 1/L \sum_i (m_i(t) - \rho/2)^2$. Shown in fig. 2 are three different regimes, which we now describe. For the considered size ($L = 1024$) and field $\Delta = 0.2$ the critical density is $\rho_c \approx 0.47$. Below ρ_c the initial fluctuations decay exponentially: this is characterized by a diffusion time which is set by the effective diffusion coefficient of the system. An interesting structure emerges even in this phase: the decay is non-monotonic, showing well-defined oscillations (see the inset in fig. 2) which have their origin in kinematic waves [9] arising from the non-linear dependence of the current J on the density ρ. For exclusion processes, this is basically of the form $J \sim \rho(1 - \rho)$, and the speed of the kinematic wave is $u = \mathrm{d}J/\mathrm{d}\rho$. Measurement of the characteristic time of the oscillations shows a linear dependence on $1/(1 - 2\rho)$. Direct simulation of the microscopic model also shows the typical shock-wave–type patterns in the particle configurations. Both mean-field and simulation results concerning the kinematic waves will be presented in a forthcoming publication [10].

Above ρ_c, inhomogeneities start to decay by diffusion. However, this is only the short-time behaviour in this case, since growth of the blockages, which is governed by the intrinsic instability of the system, takes over. The characteristic time τ for this process determines the rapid growth of the density fluctuations. We defined τ as the time needed to reach the half-value of the maximum of the density fluctuations and observed from numerical simulations that, as may be expected, τ is large for large densities and close to ρ_c and it has a minimum at medium densities (see fig. 3*a*)). The slowing-down at ρ_c is the consequence of the

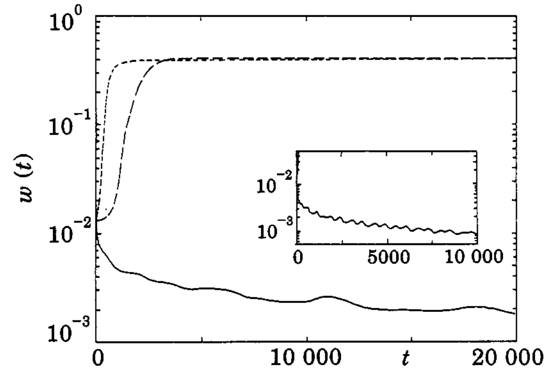

Fig. 2. – Density fluctuations as a function of time t for different total densities ρ: 0.4 (full line), 0.5 (short dashes) and 0.6 (long dashes) at fixed $\Delta = 0.2$. The inset shows the fluctuations at density $\rho = 0.4$ for a longer time. The system size is $L = 1024$.

competition between the homogeneous and the inhomogeneous «phases» while for ρ close to 1 the $(1 - m_i - p_i)$ factors in (1) and (2) become small and hinder the motion.

The low-density limit is rather complicated because of the finite-size dependence of the threshold, while at high densities the characteristic time is proportional to $(1 - \rho)^{-1}$. On the other hand, the dependence of τ on the parameter Δ is monotonic (fig. 3*b*)). An estimate of τ may perhaps be obtained from a linear-stability analysis; however, this seems to be somewhat non-trivial for this problem [5].

After the initial rapid growth of the blockages, a *much* slower process becomes dominant. The multistrip structure coarsens in time, until finally a single strip remains in the system: this will be the steady state. The coarsening can be characterized by the average distance d between the blockages. Shown in fig. 4 is the dependence of d^2 on $\log t$. (The d *vs.* $\log t$ plot has a pronounced downward curvature.) This result indicates that the characteristic length d in this coarsening process (at least in the mean-field approximation) has the form

$$d \propto \log^\alpha t\,, \tag{4}$$

with α close to $1/2$.

In the following we describe how the pattern formation proceeds in time and what the mechanism leading to the slow coarsening is: particles interact through exclusion and thus they have to overcome effective barriers of increasing difficulty.

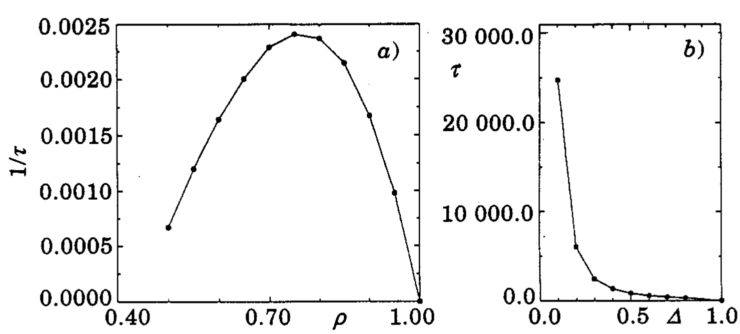

Fig. 3. – Characteristic time τ of the instability as a function *a*) of the average density ρ with $\Delta = a - b = 0.2$ and *b*) of Δ at density $\rho = 0.9$. The system size is $L = 1024$.

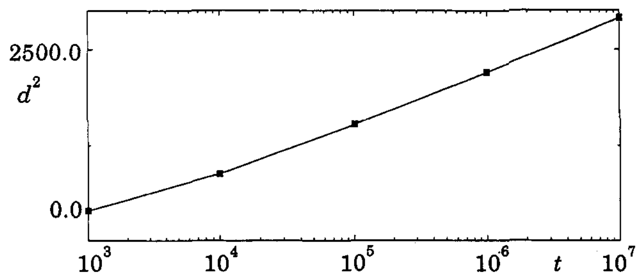

Fig. 4. – The square of the characteristic length d (distance between the blockages) as a function of the logarithm of time t. Parameter values are $\rho = 0.9$, $\Delta = 0.4$ and $L = 1024$.

In the high-density jammed phase, a number of strips are formed after the initial stage when transients have died out. Each strip consists of two substrips of approximately equal numbers of + and − particles mutually hindering each other. The interstrip region is almost empty, and the distance between strips d is thus linearly related to the width of each substrip δ. As time goes to infinity, the distance between the strips goes to infinity as well and so does δ because of the conservation of the particles. (At stationarity $\delta \propto L$ [4,8].) In the one-dimensional mean-field version of the model, the density profile for + and − particles is, therefore, for finite times like a train of two square waves which are out of phase, of width δ and varying amplitude.

Consider one such strip. The substrip on the left is composed of + particles. We assume that their density p is uniform in this width. Similarly, on the right there are − particles, with uniform density m. The way in which this strip will vanish is if all the + particles manage to move rightwards, and the − particles leftwards. The probability for a + particle to cross all the − ones on its right is $p(1-m)^{\delta}$ which gives the time scale for a strip to vanish as $t \propto \exp[A\delta]$, where $(1-m) = \exp[-A]$, and thus $d \propto \log t$. As the particles get more segregated, $m \approx 1$, and thus this time gets extremely long. Furthermore, as the surviving strips get thicker, they pose even more of a barrier to transport (as δ increases). This simple argument ignores the shape of the barriers and the fact that the density of particles is strictly not uniform in the substrips. These fluctuations may well lead to an exponent $\alpha \neq 1$.

It has not been possible here to study the scaling behaviour of the characteristic length d with all the parameters of the problem, since the transient time τ also depends strongly on them. As in the mean-field calculations [4,8], lengths occur in the form $x\Delta$; we expect $d \sim 1/\Delta$ and for late times we have seen signatures of this type of scaling.

In the mean-field approximation, fluctuations originate in initial conditions: in this sense the present system is a further example of deterministic coarsening [11]. In the microscopic model, however, the presence of the second spatial dimension enables the formation of finite clusters («clouds»). The transient time described above can probably be identified with the time needed for the finite clouds to merge into strips. Of course an additional difference is the presence of fluctuations but, as is usual for coarsening phenomena, they presumably do not influence the scaling significantly. We therefore expect that the overall asymptotic picture suggested by our results concerning logarithmically slow relaxation will remain valid in this case as well.

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REFERENCES

[1] SCHMITTMANN B. and ZIA R. K. P., preprint for *Phase Transitions and Critical Phenomena*, edited by C. DOMB and J. L. LEBOWITZ, Vol. **17** (Academic Press, New York, N.Y.).
[2] SCHMITTMANN B., HWANG K. and ZIA R. K. P., *Europhys. Lett.*, **19** (1992) 19.
[3] BIHAM O., MIDDLETON A. and LEVINE D., *Phys. Rev. A*, **46** (1992) R6124.
[4] FOSTER D. and GODRÈCHE G., to be published in *J. Stat. Phys.*
[5] ZIA R. K. P. and SCHMITTMANN B., private communication.
[6] BASSLER K. E., SCHMITTMANN B. and ZIA R. K. P., *Europhys. Lett.*, **24** (1993) 115.
[7] GUNTON J. D., SAN MIGUEL M. and SAHNI P. S., in *Phase Transitions and Critical Phenomena*, edited by C. DOMB and J. L. LEBOWITZ, Vol. **8** (Academic Press, New York, N.Y.) 1983.
[8] VILFAN I., ZIA R. K. P. and SCHMITTMANN B., preprint (1994), VPI.
[9] LIGHTHILL M. J. and WHITHAM G. B., *Proc. R. Soc. London, Ser. A*, **229** (1955) 281, 317. See also WHITHAM G. B., *Linear and Nonlinear Waves* (J. Wiley, New York, N.Y.) 1974.
[10] RAMASWAMY R. and KERTÉSZ J., in preparation.
[11] BRAY A., DERRIDA B. and GODRÈCHE C., preprint (Newton Institute, Cambridge) 1994.