Coarsening Dynamics of a Quasi One-dimensional Driven Lattice Gas

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We study domain growth properties of two species of particles executing biased diffusion on a half-filled square lattice, consisting of just two lanes. Driven in opposite directions by an external “electric” field, the particles form clusters due to steric hindrance. While strictly one-dimensional systems remain disordered, clusters in our “quasi 1D” case grow until only a single macroscopic cluster survives. In the coarsening regime, the average cluster size increases ∼ t^0.6, significantly faster than in purely diffusion-controlled systems. Remarkably, however, the cluster size distribution displays dynamic scaling, following a form consistent with a diffusion-limited growth mechanism.

Introduction. The dynamics of a system undergoing phase segregation when quenched below the transition temperature has been of interest for many years. Starting from a homogeneous state, domains of the co-existing phases form and grow. Nearly all existing studies of such coarsening processes are devoted to systems subjected to dynamical rules which eventually take them to equilibrium states [1]. Our interest is coarsening in systems which are evolving toward nonequilibrium steady states (NESS): The underlying dynamics of our systems violates detailed balance and time reversal invariance. In particular, our main focus will be the remarkable characteristic of dynamic scaling. In this letter, we report the presence of this behavior in a simple model of biased diffusion of two species. In stark contrast to similar phenomena in other systems where the growth exponent is typically 1/2 or 1/3 [2–4], we find it to be at least 0.6! This large, anomalous value rules out diffusion-controlled growth mechanisms. Surprisingly, however, the scaling function for the cluster-size distribution resembles that of diffusion-dominated growth quite well. Since our system is essentially one-dimensional, we may also exploit a reduced description, in terms of coalescing random walkers on a line. To account for the faster growth, we introduce interactions between neighboring walkers. Apart from small deviations, the “cluster-size” distributions in this picture are in good agreement with the data. In the following, we briefly describe the model, present the data from Monte Carlo (MC) simulations, discuss the coalescence picture, and conclude with some open questions. More details will be left to [6].

Biased Diffusion of Two Species. Motivated by the physics of fast ionic conductors [7], Katz, et.al. [8] generalized the well-known Ising lattice gas to include a uniform bias affecting all particles. With periodic boundary conditions, the system settles into a NESS rather than a simple equilibrium state. In addition to a non-trivial particle current, many novel collective phenomena emerge, some of which remain unexplained [9]. A natural extension of such “driven diffusive systems” involves two species. When these are driven in opposite directions, the system displays a phase transition in d = 2, even if the only interparticle interaction is an excluded volume constraint [10]. In d = 1, however, one can prove [11] that phase transitions cannot occur. Since such a system consists of particles on a line, it may be used to model traffic flow [12], and we will use the term “single lane” for this d = 1 case. Remarkably, when a second “lane” is introduced, the system again displays a phase transition [13]. We briefly describe this study.

A fully periodic 2 × L square lattice is randomly filled with equal numbers of two types of particles (labeled by “charge” + or −), subject to an excluded volume constraint. When not driven, the particles diffuse according to the following rules. Two nearest neighbor (NN) sites are chosen at random, and attempts to exchange their contents are (a) always allowed for particle-hole pairs and (b) accepted with probability γ for particle-particle pairs. Under this dynamics, the two species are just diffusing randomly. The system obviously remains homogeneous, with trivial collective properties. Next, we impose an external “field” which drives the two species along the “ring” in opposite directions, by simply forbidding all exchanges which result in, say, +/− particles moving clockwise/anticlockwise. In [14], γ is fixed at 0.1 while systems up to L = 10^4 are evolved for as many as 4 × 10^6 MC steps (1 MCS corresponds to 2L exchange attempts). For early times (10-20 MCS), small blockages form everywhere, due to the mutual obstruction of the opposing species. These clusters coarsen until, at late stages when NESS is essentially established, only a single macroscopic cluster remains. The characteristics of this cluster are notable. (a) It contains almost no holes. (b) It exhibits a non-trivial “charge” profile. (c) Its size (number of particles connected as NN’s) is gaussian distributed around 0.94L, so that its “length” is about L/2. (d) A low-density region spans the remainder of the system, consisting of particles (“travellers”) which leak out of the cluster at one end and later rejoin it at the other. By contrast, for the “single lane” case, the system remains homogeneous, and the cluster size distribution is known exactly [14] to decay exponentially (with weak 1/L corrections). In this sense, we believe that it is justifiable to use the terms “long range order” and
“phase segregation” to characterize the two-lane system in steady state. Of course, if the overall particle density is reduced sufficiently, there must be a phase transition to re-establish homogeneity. In an effort to understand why a two-lane system orders while the single-lane version remains disordered, we turn to a study of how long-range order builds up in the latter case.

Simulations, Characterizations, and Results. To study the time dependence of our stochastic system, we carry out many runs with the same random initial distribution of particles. Typically, data from 100 – 1000 runs are used to build histograms. In addition, with finite size effects in mind, we exploit a range of system sizes, from $2 \times 100$ to $2 \times 1000$. At half filling, local blockages appear everywhere soon after the run starts, a phenomenon reminiscent of homogeneous nucleation. Though small, these blockages share some characteristics of the terminal cluster, having few holes inside and growing through accretion of particles from the inter-cluster region. In a relatively short time ($\sim 100$ MCS), a rough balance between accretion and loss is established so that both the density of travellers and their total number remain relatively constant for the rest of the run. The associated values, $\sim 5\%$ and $\sim 0.06L$ respectively, can be understood qualitatively [4]. Thus, we may characterize this initial stage as one in which local densities quickly reach their (approximate) final values. For later, intermediate times (the “growth” regime), the larger clusters grow at the expense of smaller ones, a mechanism reminiscent of Lifshitz-Slyosov growth. However, the similarity is deceptive, as we will show next.

To characterize domain growth in our model, we monitor the cluster size distribution since it carries very detailed information. The most natural definition of the size of a cluster, $s$, is just the number of particles (regardless of their charge) connected via NN bonds. We collect data at various times, $t$, to construct histograms of such cluster sizes: $\tilde{p}(s, t)$. Since this distribution is sensitive to both the growing clusters and the travellers, we refer to it as the microscopic cluster distribution. Clearly, $\tilde{p}$ is not conserved, decreasing when clusters merge, etc. Instead, we consider $p(s, t) \equiv \tilde{p}(s, t)$, which, counting just the total number of particles, is conserved. Known as the “residence distribution” in percolation studies, $p(s, t)$ is proportional to the probability of any site belonging to a cluster of size $s$ at time $t$. For the $2 \times L$ case, $p$ displays two peaks from an early time, one at $s = 1$ (followed by a sharp drop to nearly zero) and another moving to higher $s$ with $t$. As mentioned above, the first is relatively constant, so that we focus only on the behavior of the second peak. To this end, we devise a coarse-grained (CG) description of the clusters, which has the added advantage of tolerating the occasional hole in a cluster. For any configuration on the $2 \times L$ lattice, we construct another one, with occupation numbers 0 or 1 on a line of $L$ sites, as follows. At each site $i$, we assign 0 if there are five or less particles in the ten sites around the $i^{th}$ column of the original lattice; and 1 otherwise (cf. Fig. 1.)

![FIG. 1. Illustration of the coarse-graining procedure for a configuration in a $L = 12$ periodic lattice. An example of the microscopic configuration is shown with ± particles and holes. The CG version shows only {0,1}’s.](image)

In the CG configuration, a cluster is simply a consecutive sequence of 1’s and its “size” ($\ell$) is just the length of this string. Histograms for these cluster sizes, $\tilde{p}(\ell, t)$, can be compiled easily. Note that clusters in the traveller region are usually quite small ($s \leq 5$), so that $\tilde{p}(\ell, t)$ has only one peak, associated with the growing clusters. Again, we consider the residence distribution: $p(\ell, t) \equiv \tilde{p}(\ell, t)$, from which a natural definition of an average cluster length arises: $\bar{\ell}_C(t) \equiv \sum_{\ell} p(\ell, t) / \sum_{\ell} \tilde{p}(\ell, t)$. In Fig. 2, we present a log-log plot of this quantity for various $L$ (solid points). Clearly, there is good data collapse in the growth regimes. For the two smaller systems, our runs are long enough for saturation ($\lim_{t \to \infty} \bar{\ell}_C(t) \approx 0.47L$) to occur. More significantly, the effective power in the growth (i.e., $d \ln \bar{\ell}_C / dt$) appears to be still increasing for the largest system at the latest times. In the figure, we provide two straight lines, corresponding to $t^{1/2}$ and $t^{2/3}$, to guide the eye. From these lines, we estimate that the effective exponent is about 0.6 at the latest stage. Unless a mysterious slow-down sets in at even later times, we are confident that the power of 1/2 is ruled out. Finally, we turn to the distributions and, to check for dynamic scaling, construct the normalized scaled form, $f(x, t) \equiv \bar{\ell}_C(t)p(x/t, t)$ with $x = \ell / \bar{\ell}_C(t)$. As we see in Fig. 3a, $f(x, t)$ is largely independent of $t$ (and $L$) in the growth regime. Thus, we conclude that, despite the possible absence of pure power law growth, the distribution displays, remarkably, dynamic scaling. Further, the scaled distribution is well approximated by the solid line in Fig. 3a, a distribution (cf. Eqn. 2 below) well known from diffusion-limited coalescence. This suggests casting our MC dynamics in terms of an effective model, involving coalescing random walkers (RW).

Coalescing random walkers in $d = 1$. Since the density of travellers is relatively constant, a good macroscopic picture focuses on the sizes (lengths) of the clusters only, with the main dynamics being particle exchange between neighboring clusters. To describe this sequence of clusters, points (“walkers”) are placed on a ring of $N$ sites, with spacings corresponding to the cluster-lengths [3]. Particle exchanges translate into walkers taking steps. When two walkers meet, they “coalesce,” representing the disappearance of a cluster. The number, $n$, maps into the number of clusters, while $N$ represents the sum of all cluster lengths. At the end, there is only
one walker, i.e., one macroscopic cluster. For simplicity, we set $N = L/2$ which well approximates the observed 0.47L. In our simulations, RW time ($\bar{t}$) increases by 1 when every walker has had, on average, a chance to make one step.

If the random walkers were free (apart from coalescence), the problem is exactly soluble in $d = 1$ \cite{3}. Denoted by $P_0(\ell, \bar{t})$, the (unnormalized) frequency of finding two adjacent walkers separated by a distance $\ell$, at time $\bar{t}$, satisfies a diffusion equation in the continuum limit. With absorbing boundary condition at $\ell = 0$ to model coalescence, the solution is standard. To compare with the MC data, consider the normalized "residence" distribution, $\bar{P}_0(\ell, \bar{t}) \equiv \ell P_0(\ell, \bar{t})$. Its first moment, $\bar{\ell}_0$, should correspond to $\bar{\ell}_C$. Clearly, $\bar{\ell}_0$ grows diffusively: $\bar{\ell}_0(\bar{t}) \propto \bar{t}^{3/2}$. Further, dynamic scaling prevails (in the limit $\bar{t} \to \infty$, $\ell \to \infty$ at fixed $x = \ell/\bar{\ell}_0(\bar{t}))$:

$$\bar{\ell}_0(\bar{t}) P_0(\ell, \bar{t}) \equiv F_0(x) = \frac{32}{\pi^2} x^2 \exp\left(-\frac{4}{\pi} x^2\right), \quad (1)$$

which serves as a good benchmark (solid line in Figs. 3a and b) for scaling plots of the data. Unfortunately, the growth exponent (1/2) of this simple model is unequivocally ruled out by our data (Fig. 2). Its deficiencies can be traced, by monitoring the evolution of our clusters, to the rapid, systematic disintegration of small ones. To model this bias towards larger clusters, we introduce a model of interacting random walkers (IRWs), where neighboring walkers experience stronger attraction with decreasing separation. Specifically, consider a walker and its two nearest neighbors. Letting $\ell_R (\ell_L)$ be the distance to its right (left) neighbor, and $q_R, q_L, q_S (= 1 - q_R - q_L)$ be the probabilities for moving to the right, left, and staying, respectively, we choose:

$$\frac{q_R}{q_S} = 1 + \left(\frac{C}{\ell_R}\right)^2 \quad \text{and} \quad \frac{q_L}{q_S} = 1 + \left(\frac{C}{\ell_L}\right)^2 \quad (2)$$

where $C$ is an amplitude giving the best fit to the data.

![FIG. 2. Coarse-grained MC (solid symbols) and interacting random walk (open symbols) data for the average cluster size vs time, for $L = 10000$, 1000, and 500.](image)

![FIG. 3. Scaled residence distributions for CG MC, $f(x)$, and IRW, $F(x)$. For comparison, the "benchmark," $F_0$, is shown as a solid line in both plots. In (a), $\bullet$, $\blacksquare$, $\blacktriangle$ and $\blacklozenge$ are data from a $2 \times 2000$ lattice at $t = 1096, 2981, 8103$, and 2207, respectively. Open symbols are data from $2 \times 500$ at $t = 403, 1096, 2981$, and 8103. In (b), this set of solid (open) symbols correspond to $N = 1000 (500)$, at scaled times.](image)
value 0.06, we note that this is also the traveller density, but can offer no insight into this coincidence.

This choice for $C$ renders our rates time-dependent (through $n(\ell)$), so that the exact solution of this dynamics remains elusive. Fortunately, our IRW is easily simulated. At time $t = 0$, walkers are distributed randomly over the ring, with an initial density of 0.4, and then updated according to (5). We measure the normalized residence distribution $P(t, \tilde{t})$ and its first moment, $\ell(t)$. Adjusting a single scale parameter to match sizes. The success of our effective model is quite spectacular (in Fig. 2) both with residence distribution updated according to (2). We measure the normalized size of $\ell(t)$ approach a final value of $F$. The scaling plot: $F(x) \equiv \ell(t) P(\ell, t)$ vs $x = \ell(\ell(t))$ (Fig. 3b). Within statistical noise, the data collapse is quite satisfactory. Most remarkably, this $F(x)$ also closely follows $F_0(x)$ of the free RW!

There are, however, small deviations from scaling, revealed only by close inspection. We first note that, in both cases, the late-time data tend to deviate systematically from $F_0(x)$. In Fig. 3a, the data lie slightly above $F_0$ for $x \leq 0.5$, and slightly below $F_0$ for $x > 0.5$ near its maximum. In Fig. 3b, the trend is reversed. For $x > 1$, there are no perceptible deviations in either case. While we cannot offer any rigorous understanding, it is conceivable that the lengthening domains of travellers - which are neglected in the IRW dynamics - play a role here. Another possible mechanism is described in (10). Much more remarkable, however, is how close both $F$ and $F$ follow Eqn. (1), i.e., the free RW scaling function, even though neither $\ell_C$ and $\ell_t$ are consistent with the diffusion equation leading to $F_0$! It appears as if the complexity of our full dynamics can be absorbed into a single “renormalization” of time, $t \propto \tau^\sigma$, such that simple diffusion-controlled coalescence emerges in $\tau$. Matching $t^{1/2} \sim \ell(\ell(t))$ then requires $\sigma = z/2$. Clearly, formalizing this scenario poses a serious theoretical challenge.

Summary and Outlook. To conclude, we summarize our findings and end with some speculations. We consider a lattice gas with two species of particles driven in opposite directions on a “single-lane road” vs. a “two-lane highway.” Allowing a small amount of particle-particle exchange, both systems are ergodic but display drastically different final states: While the one-lane system remains homogeneous, the two-lane case exhibits a macroscopic cluster which scales with system size. In an effort to probe the surprisingly different outcomes, we study the growth of clusters in the two-lane case in some detail, measuring the average cluster size, $\ell(t)$, and the full residence distribution. We discover that $\tilde{t}(t)$ grows much faster than typical domains in similar models. At late times, the growth law may be characterized by an effective exponent of about 0.6. We end with a speculative note. In ordinary Lifshitz Slyosov growth, which leads to the power 1/3, the mechanism for transport (of material from smaller clusters to larger ones) is diffusion. Here, particles suffer biased diffusion, so that the motion is ballistic instead. Can the difference of a factor of two between these different mechanisms transform the power 1/3 to a 2/3? Needless to say, to arrive at definitive conclusions, we need not only a deeper analytic understanding but also a better Monte Carlo study of this simple, yet intriguing, model system.

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