Monte Carlo results for the Ising model with shear

E. N. M. Cirillo

Dipartimento de Metodi e Modelli Matematici, Facoltà di Ingegneria, Universita di Roma "La Sapienza", via A. Scarpa 16, 00161 Rome, Italy

G. Gonnella and G. P. Saracco

Dipartimento di Fisica, Università di Bari and Istituto Nazionale di Fisica Nucleare, Sezione di Bari, via Amendola 173, 70126 Bari, Italy (Received 28 April 2005; published 31 August 2005)

We study the kinetics of domain growth in the Ising model with nonconserved dynamics under the action of a stochastic driving field that mimics the action of a shear flow. At late times, we found multistriped configurations with constant transversal size and linear growth in the direction of the flow. In cases with weak shear, a regime characterized by the decreasing of the transversal size is found that could correspond to previous

theoretical investigations. This behavior is confirmed by the analysis of the structure factor patterns.

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I. INTRODUCTION

When a system in its homogeneous disordered state is suddenly quenched into a multiphase coexistence region, the domains of the ordered phases start to form and grow in reciprocal competition. This process, known as coarsening or phase ordering, is generally characterized by dynamical scaling [1]. The equal-time two-point correlation function C(r,t)behaves like $C(r,t) \sim f(r/R(t))$, where R(t) can be identified as the typical size of domains during coarsening. R(t) generally follows a power-law behavior $R \sim t^{\alpha}$; the existence of several regimes, characterized by different exponents α depending on the particular mechanism operating during phase separation, is well established [1,2].

In cases of practical interest, phase separation often occurs under the action of an external field or, if the system is a liquid mixture, making the liquid flow. In the case of applied shear, which is particularly relevant for applications, the ordering process is known to be profoundly affected by the flow [3]. The most noticeable effect is the alignment of the domains of the different phases along the flow direction. However, given its importance, the comprehension of many features of the kinetics of this process is still poor. The anisotropic growth of domains suggests that the dynamical evolution is described by different exponents α_{\parallel} and α_{\perp} for the growth along the directions parallel and orthogonal to the flow, respectively, [4]. While theoretical arguments, simulations, and experiments suggest that the relation $\alpha_{\parallel} - \alpha_{\perp} = 1$ generally holds [5-8], the determination of the exponents, with the possible existence of dynamical scaling, is still an open problem. Moreover, it is not clear whether the shear, at late times, causes an interruption of coarsening with a stationary state consisting of striped domains of fixed width or whether indefinite growth can be observed at asymptotic times [9].

Previous studies of phase separation in binary fluids also showed the occurrence of less-expected phenomena due to the action of the shear flow. The evolution of structure factor and other related quantities (domain size, stress, etc...) was observed to be characterized by oscillatory patterns with cyclical storage and dissipation of elastic energy [10]. In a self-consistent approximation of a Landau-Ginzburg model, the oscillations were found to persist indefinitely with time [11], even if they were not found in the analytical solution of the model in the limit of infinite time [12]. Simulations of the Landau-Ginzburg model showed that the oscillations can be related with the existence of two typical domain lengths for each space direction [5]. A similar scenario has been found in experiments on binary fluids [13].

In the present work, we study the coarsening dynamics of the d=2 Ising model with a driving stochastic field implemented to mimic the effects of a uniform shear flow. The discrete nature of the model avoids the problems that could arise in the numerical implementation of continuum convection-diffusion equations [14]. The model evolves with a dynamics with nonconserved order parameter, corresponding to model A in the classification of Hohenberg and Halperin [15]. Models with nonconserved dynamics are used to describe the kinetics of twisted nematic liquid crystals [1,16]. Our results can therefore be relevant to understanding the effects of shear in these systems. Model A with shear was studied by Cavagna et al. in the context of the Ohta-Jasnow-Kawasaki approximation [17]. In two dimensions it was found that the typical size of domains in the direction of the flow grows as $R_{\parallel} \sim t(\ln t)^{1/4}$, while the transverse length R_{\perp} experiences an unlimited narrowing, behaving as R_{\perp} $\sim (\ln t)^{-1/4}$. The aim of this work is to test numerically these results and to compare also with the previously described phenomenology of coarsening in systems with conserved dynamics. Simulations of Ising models with shear were also performed in [17], but there a lattice of limited size was used and only one value of shear rate was considered.

We performed simulations in a large interval of shear rate values and different temperatures. We confirm results of previous simulations with domains characterized by a finite transversal size at late times. We also obtained evidence of an intermediate regime with transversal size decreasing with time, as suggested by theoretical predictions [17].

The structure of this paper is as follows: In Sec. II, we introduce the model and the algorithm for the realization of the external flow. Short time evolution will be discussed in Sec. III. Section IV contains our simulation results for different shear rates $\dot{\gamma}$, temperatures, and lattice sizes. Our conclusions are presented in Sec. V.

II. THE MODEL

We will consider the nearest-neighbor two-dimensional stochastic Ising model with a single-spin-flip thermalization dynamics, e.g., the Metropolis dynamics. The driving field will be defined in order to mimic the convective velocity shear profile

$$v_x(y) = \dot{\gamma}y \quad v_y = 0, \tag{1}$$

where the real parameter $\dot{\gamma}$ is called the *shear rate*. If the system is represented as a sequence of layers labeled by y, then $\dot{\gamma}y$ is the displacement of the layer y in a unit of time. If L is the vertical size and v_{max} is the speed of the fastest layer, then $\dot{\gamma}L=v_{\text{max}}$.

The model is defined on a square lattice Λ of side length L with periodic boundary conditions in the horizontal direction and free in the vertical one. More precisely, let $\Omega = \{-1, +1\}^{\Lambda}$ be the space of configurations, and for $\sigma \in \Omega$, let $\sigma_{x,y}$ be the value of the spin associated to the site $(x, y) \in \Lambda$. Then, the Hamiltonian of the model is

$$H_{\Lambda}(\sigma) = J \sum_{y=1}^{L} \sum_{x=1}^{L} \sigma_{x,y} \sigma_{x+1,y} + J \sum_{x=1}^{L} \sum_{y=1}^{L-1} \sigma_{x,y} \sigma_{x,y+1}, \qquad (2)$$

where $\sigma_{L+1,y} = \sigma_{1,y}$ for all y = 1, ..., L, and J is a positive real.

We try to combine the thermalization dynamics with an algorithm introducing the shear in the system. The shear is superimposed to the thermalization dynamics with typical rates not depending on the thermalization phenomenon, but fixed *a priori*. This problem has been faced in [17–19], and different solutions have been proposed therein. In this paper, we use a very ductile generalization of those dynamics aiming to introduce the shear effects in a way that is competitive with respect to the thermalization process.

Let the *time unit* be the time needed for a full thermal update of the entire lattice, e.g., a full sweep of the Metropolis algorithm. The shear algorithm is parametrized with a submultiple τ of L^2 (the period of the shear procedure), a positive integer $\lambda \leq L/2$ (the space a row is shifted when the shear is performed), and a non-negative real $\nu \leq 1/L$. The dynamics of the model that we study in this paper is defined in a precise way via the following algorithm:

(i) Set t=0, choose $\sigma_0 \in \Omega$, and set n=0.

(ii) Set n=n+1, and choose at random with uniform probability $1/L^2$ a site of the lattice and perform the elementary single-site step of the thermalization dynamics.

(iii) If *n* is multiple of τ , a layer is randomly chosen with uniform probability 1/L. Then, if \overline{y} is the chosen layer, all the layers with $y \ge \overline{y}$ are shifted λ lattice spacings to the right with probability νL .

(iv) If $n < L^2$, go to (ii); otherwise, denote by σ_{t+1} the configuration of the system.

(v) Set t=t+1, set n=0, and go to (ii).

We note that if $\nu = 1/L$, the shift at step (iii) is certainly performed—this case will be called *full shear*. The smoothness of the shear profile is ensured by the stochastic character of step (iii) in the algorithm.

We want to express, now, the shear rate $\dot{\gamma}$, introduced in Eq. (1), in terms of the parameters of our dynamics. We have to estimate the typical displacement per unit of time of the row labeled y. Such a row is involved in a shear event, step (iii) of the preceding algorithm, if and only if the extracted row \bar{y} is such that $\bar{y} \leq y$, and this happens with probability y/L. Since the shear event results in a shift with probability νL , the probability that during a shear event the row y does shift is given by

$$\frac{y}{L}\nu L = \nu y.$$

By noting that the number of shift events per unit of time is equal to L^2/τ and recalling that the shift amplitude is λ , we have that the typical shift of the row y per unit of time is given by

$$\frac{L^2}{\tau}\lambda\nu y.$$

By using definition (1), we finally get $\dot{\gamma} = L^2 \nu \lambda / \tau$, which becomes $\dot{\gamma} = L\lambda / \tau$ in the case of full shear.

For completeness, we now show how the dynamics defined by the preceding algorithm can be thought of as a Markov chain $\sigma_t \in \Omega$, with t=0, 1, ... the time variable and σ_t the configuration of the model at time t. To write the associated transition matrix, one has to take into account both the thermal and the shear effects. Let $\sigma, \eta \in \Omega$, and denote by $q(\sigma, \eta)$ and $p(\sigma, \eta)$ the probability that the system jumps from σ to η , respectively, in a single spin flip of the thermalization dynamics [step (ii) of the algorithm] and in a shear event [step (iii) of the algorithm]. Normalize both q and p so that for each configuration σ ,

$$\sum_{\eta \in \Omega} q(\sigma, \eta) = 1 \quad \text{and} \quad \sum_{\eta \in \Omega} p(\sigma, \eta) = 1.$$

Now notice that the transition σ_t to σ_{t+1} is realized by performing the steps (ii) and (iii), respectively, L^2 and L^2/τ times. One can expect that for each $n=1, \ldots, L^2$, the transition σ to σ' happens with probability

$$f_n(\sigma, \sigma') = \begin{cases} \sum_{\sigma'' \in \Omega} q(\sigma, \sigma'') p(\sigma'', \sigma') & n \text{ multiple of } \tau \\ q(\sigma, \sigma') & \text{otherwise.} \end{cases}$$

Finally, can write the transition matrix r of the dynamics resulting from the preceding algorithm. For each $\sigma, \eta \in \Omega$, one has

$$r(\sigma,\eta) = \sum_{\sigma_1 \in \Omega} \cdots \sum_{\sigma_{L^2-1} \in \Omega} \prod_{n=1}^{L^2} f_n(\sigma_{n-1},\sigma_n),$$

where $\sigma_0 = \sigma$ and $\sigma_{L^2} = \eta$.

As usual for a Markov chain, one can consider a continuous time process and write the master equation. Indeed, if we let $W(\sigma, t)$, the probability that at time *t* the process visits the configuration σ , we have that

$$\frac{dW}{dt}(\sigma,t) = \sum_{\eta \in \Omega} \left[W(\eta,t)r(\eta,\sigma) - W(\sigma,t)r(\sigma,\eta) \right].$$
(3)

III. SHORT TIME EVOLUTION

In the absence of driving fields, the growth properties of ordered phases in the Ising model with nonconserved dynamics are the same as those of the Landau-Ginzburg model A [1]. When a shear flow is imposed on the system, model A can be generalized to the convection-diffusion equation

$$\frac{\partial \varphi}{\partial t} + \vec{\nabla} \cdot (\varphi \vec{v}) = -\Gamma \frac{\delta \mathcal{F}}{\delta \varphi} + \eta, \qquad (4)$$

where φ is the order parameter,

$$\mathcal{F}\{\varphi\} = \int d^d x \left(\frac{a}{2}\varphi^2 + \frac{b}{4}\varphi^4 + \frac{\kappa}{2}|\nabla\varphi|^2\right)$$
(5)

is the usual double-well Ginzburg-Landau free energy, and the Gaussian stochastic field η , with zero average and variance proportional to the temperature *T* of the system, describes the thermal fluctuations [17].

The linearized theory developed by Cahn and Hilliard for describing the early stages of spinodal decomposition can be extended to the present case. The approximation consists in neglecting the quartic term in the local part of the free energy, since at the beginning of phase separation, the order parameter is small. It is known that the early regime with domains not yet in local equilibrium is correctly described in this approximation. Therefore, it could be instructive to compare at initial times the evolution of the linearized system (4) with our Monte Carlo results.

The solution of Eqs. (4) and (5) with b=0 gives for the structure factor

$$C(\vec{k},t) \equiv \langle |\varphi_{\vec{k}}(t)|^2 \rangle \tag{6}$$

the expression

$$C(\vec{k},t) = \Delta e^{-\int_0^t [\mathcal{K}^2(z) - 1] dz} + T \int_0^t e^{-\int_0^z [\mathcal{K}^2(s) - 1] ds} dz, \qquad (7)$$

where $\mathcal{K} = (k_x, k_y + \dot{\gamma}k_x z)$, and $\varphi_{\vec{k}}(t)$ is the Fourier transform of $\varphi(\vec{x}, t)$. The symmetry properties of Eq. (4) have been used to rescale parameters to $\Gamma = 1$, a = -1, $\kappa = 1$ [5]. Δ is the initial value of the structure factor, here set to a constant.

In Fig. 1, $C(\vec{k},t)$ is plotted at two different times for the case $\dot{\gamma}=0.1$, $\Delta=1$, T=0. At the beginning ($\dot{\gamma}t=0.45$), when the shear has not yet produced sensible effects, the structure factor has the typical isotropic Gaussian shape observed in nonconserved coarsening. With time, while the extension of $C(\vec{k},t)$ decreases and the height increases as usual in phase separation, the function becomes anisotropic and squeezed along the 45° direction, as can be observed at $\dot{\gamma}t=1.25$ in Fig. 1. Later, the structure factor continues to become nar-



FIG. 1. Time evolution of the structure factor defined in Eq. (7) at T=0. The left plot corresponds to $\dot{\gamma}t=0.45$, and the right plot corresponds to $\dot{\gamma}t=1.25$.

rower in the transversal direction with an orientation that tends to align with the axis $k_x=0$. The profile of the structure factor will not change with time, and this feature, as we will see, differs from the results of the simulations.

IV. RESULTS

We run simulations with different quenching temperatures (measured in units of J/k_B , where J is the coupling constant and k_B is the Boltzmann constant), shear rates, and lattice size up to L=8192. The initial condition consisted of filling randomly one half of the lattice volume with up spins, and then filling the other half with down spins. For each case, we averaged macroscopic quantities over several histories (typically from 3 to 5); results from different histories and initial configurations have been seen to not differ in an observable significant way, showing that the system is self-averaging for the sizes considered.

We start to describe our results from the case with the lowest temperature we considered $(T=0.1J/k_B)$. The effects of shear on the morphology of coarsening can be seen in the sequence of configurations shown in Fig. 2 for the case $\dot{\gamma}$ =1/8, L=4096. After the initial stage, when domains are formed from the mixed initial state, a bicontinuous pattern is observed. As in many experiments and other simulations with shear [4-6,8], an incipient distortion produced by the flow starts to appear from $\dot{\gamma}t \approx 1$ (see the snapshot at $\dot{\gamma}t$ =1.25). At $\dot{\gamma}t$ =12.5, the anisotropy is very pronounced, and the tilt angle between the main direction of domains and the flow is observed to decrease as time passes by, as can be seen at $\dot{\gamma}t=31.25$ and $\dot{\gamma}t=312.5$. At this last time, the interfaces are almost completely aligned with the flow. The increase of anisotropy goes with the development of nonuniformities in the system. Domains with different thickness can be observed in the last times shown. This is different from what occurs in phase separation without shear, where the tendency of domains to order on the same space length is more pronounced. A quantitative description of the morphological properties can be obtained from the structure factor. It is defined as



FIG. 2. Configurations of the system corresponding to different times. From left to right, the upper configurations were taken at $\dot{\gamma}t$ =1.25 and $\dot{\gamma}t$ =12.5, while the lower ones were taken at $\dot{\gamma}t$ =31.25 and $\dot{\gamma}t$ =312.5, respectively. The square system is of size L=4096, but only a portion of size L'=512 is displayed. The parameters of the system are $\dot{\gamma}$ =1/8, T=0.1 J/k_B .

$$C(\vec{k},t) = \frac{1}{L^2} \left| \sum_{x,y} \sigma_{x,y}(t) e^{i\vec{k}\cdot\vec{r}} \right|^2,$$
 (8)

where $\sigma_{x,y}(t)$ is the value of the spin in the position $\vec{r} \equiv (x, y)$ at time *t*.

Figure 3 shows the structure factors corresponding to the configurations of Fig. 2. At $\dot{\gamma}t=1.25$, $C(\vec{k},t)$ is only slightly anisotropic and closely resembles the shape observed in coarsening with nonconserved dynamics without the driving field. The pattern is also similar to the first pattern shown in



FIG. 3. Structure factors corresponding to the configurations of Fig. 2.

Fig. 1. Later, $C(\vec{k},t)$ becomes squeezed along the diagonal $k_x = -k_y$, in agreement with the predictions of the linear theory shown in Fig. 1. With time, the results of the simulation become different, also qualitatively, from the expectations of linear theory. The structure factor, which becomes more and more aligned with the direction $k_x=0$, is not peaked at the origin of the plane $k_x - k_y$ but develops two broad peaks related by $\vec{k} \rightarrow -\vec{k}$. This symmetry, existing in the model defined in Eq. (4), is verified in all the results of our simulations. The shape of the two peaks suggests a broad distribution for the transversal size of domains. The fact that the peaks do not tend to collapse one on the other means that the average transversal length becomes stationary with time.

A standard measure of the average size of domains in the two directions R_x and R_y can be obtained from the first momenta of the structure factor

$$R_{\alpha} = \int d\vec{k} C(\vec{k}, t) \left/ \int d\vec{k} |k_{\alpha}| C(\vec{k}, t) \quad \alpha = x, y.$$
 (9)

We also considered two other measures for the size of domains in terms of correlation function and interface length. The two-point correlation functions are defined as

$$G_x(r,t) = \frac{1}{L^2} \sum_{x,y \in \Lambda} \sigma_{x,y}(t) \sigma_{x+r,y}(t), \qquad (10)$$

and similarly for the transversal direction. Typical lengths can be calculated in the usual way, that is, fixing a cutoff and measuring R_{α} at the intersection point of G_{α} and this cutoff. In terms of the interface length, R_{α} can be defined as [1]

$$R_{\alpha} = L^2 / I_{\alpha}, \quad \alpha = x, y, \tag{11}$$

where I_{α} represents the total amount of interface in the α direction, which can be calculated by the sum of the product of the appropriate neighboring spins.

We see in Fig. 4 that all these quantities show the same behavior and can be equivalently used to describe the growth properties of the system. The evolution of R_{α} is shown in the lower part of Fig. 4 for the case so far discussed with $\dot{\gamma}$ =1/8. After the initial isotropic growth with $R_x \sim R_y, R_y$ tends to a constant value, while R_x grows almost linearly. The snapshots of Fig. 2 confirm that the late-time state of the evolution is a multistriped configuration with average transverse length $R_y \approx 10$.

In the upper part of Fig. 4, we show the results of simulations with weaker shear rate ($\dot{\gamma}$ =1/1024) at the same temperature. We see that also, in this case, the system remains isotropic until times corresponding to $\dot{\gamma}t \sim 1$ with $R_x \sim R_y \sim t^{1/2}$, as expected for systems with nonconserved dynamics (this feature is indicated by the dashed line drawn at the early stages of evolution in this plot). After the maximum, R_y decreases for more than one decade until a regime is reached, where it remains constant. Finite size effects can be observed at the end of evolution. The decrease of R_y occurs in correspondence with the formation of the two peaks of the structure factors at finite k_y . The evolution and shape of the structure factor is similar to the case with stronger shear. The instantaneous slope of $R_x(t)$ is that of R_y augmented by 1, as predicted by a simple scaling analysis [5].



FIG. 4. Evolution of domain sizes in a lattice of size L=4096 at $T=0.1J/K_B$, with different shear rates $\dot{\gamma}$. The upper plot displays the evolution with $\dot{\gamma}=1/1024$; the lower plot shows the evolution with $\dot{\gamma}=1/8$. The open (solid) triangles, circles, and squares indicate the average domain size $R_x(R_y)$ measured using the structure factor [Eq. (9)], the correlation function [Eq. (10)], and the inverse of the interface length [Eq. (11)], respectively. In the upper plot ($\dot{\gamma}=1/1024$), the early stages of evolution show a power-law behavior with exponent 1/2, as indicated by the dashed line. The dashed lines drawn at the final evolution times in both plots indicate the linear growth of the domains.

We also performed simulations at the temperature $T = 0.83J/k_B$ [20]. The behavior of R_x and R_y is shown in Fig. 5 for various $\dot{\gamma}$ and L=4096. Comparing with the results of Fig. 4, one observes that fluctuations accelerate the aniso-



FIG. 5. Evolution of domain sizes in a lattice of size L=4096 at $T=0.83J/k_B$, using the correlation function [Eq. (9)]. The values of shear rates are showed in the legend. The dotted-dashed and the dashed lines indicate that the domains grow with exponents 1/2 and 1, respectively.



FIG. 6. Typical snapshot configuration of the whole system at late times of evolution ($t > 3 \times 10^4$) for $\dot{\gamma} = 1/512$. The system size is L=8192.

tropic evolution of the system. For example, when $\dot{\gamma} = 1/1024$, one can see that the system becomes anisotropic $(R_x \neq R_y)$ before it does in the case of $T=0.1J/k_B$. Also, the regime with R_x growing linearly is reached earlier and is more clearly visible. We recall that, in nondriven binary mixtures, temperature fluctuations favor segregation, increasing the factor A in the expression $R \sim A(T)t^z$ [1].

Simulations of Fig. 5 confirm that the system evolves towards a multistriped configuration, as suggested by the constance of R_y at late times. An example of such configuration is given in Fig. 6 for the case $\dot{\gamma}=1/512$. The existence of a wide distribution of lengths in the transverse direction can be observed also in this case.

Finally, to check that late-time properties are independent of the lattice size, we also run simulations with the same parameters and larger size (L=8192), obtaining results confirming those with L=4096. The behavior of R_x and R_y is shown in Fig. 7. The decreasing regime for R_y is better seen in the case with the weakest shear rate $\dot{\gamma}=1/8192$. R_y in all cases tends to a constant value.

The structure factor, corresponding to a late-time configuration with $\dot{\gamma}=1/512$, $T=0.83J/k_B$, and lattice size L=8192is shown in Fig. 8. Also in this case, $C(\vec{k},t)$ exhibits two broad peaks with the same shape of those at the latest times in Fig. 3.

V. DISCUSSION AND CONCLUSIONS

We studied the kinetics of phase ordering in a driven Ising model. Our results, with different shear rates and temperatures, show that the evolution of domains is characterized at late times by a constant value of R_y and a linear growth of R_x . The asymptotic value of R_y decreases when $\dot{\gamma}$ is increased; our data cannot allow us to extract a quantitative behavior [8,23].

To check that our results do not depend on finite size effects, we performed simulations with lattice sizes up to L



FIG. 7. Time evolution of the average domain sizes R_x and R_y in a lattice of L=8192, $T=0.83J/k_B$, for several values of $\dot{\gamma}$, which are indicated in the inset. The dashed-dotted (dashed) line indicates the slope in the early and long time regimes. The domain sizes were obtained using the correlation function [Eq. (9)].

=8192. Before becoming constant, R_y reaches a maximum that is more evident at weak shear rates. The maximum generally occurs at the end $(\dot{\gamma}t \sim 1)$ of the isotropic part of the evolution of the system $(R_x \sim R_y \sim t^{1/2})$. During the decrease of R_y , the structure factor develops two peaks at finite k_y . The large width of these peaks corresponds to a broad distribution for the domain transversal sizes, as can be seen looking at the configurations.

This scenario is different from that suggested by the calculations of [17], based on Ohta-Jasnow-Kawasaki approximation [21], predicting an unlimited decrease of R_y . Different from previous simulations on smaller lattices, our results show the existence of a decreasing regime for R_y , but also show that this does not correspond to the asymptotic evolution of the system that is characterized by a constant R_y .

We can also compare our results with those coming from studies of systems with conserved dynamics [1]. In that case, without shear, for a two-dimensional system, due to the suppression of the $\vec{k}=0$ mode imposed by the conservation law,



FIG. 8. Structure factor corresponding to the last time regime of the system ($\dot{\gamma}t$ =19.53), in a lattice of *L*=8192, *T*=0.83*J*/*k*_B, for $\dot{\gamma}$ =1/512.

the structure factor has the shape of a volcano with radius decreasing with time. When shear is applied, four peaks develop on the edge of the volcano with the relative heights oscillating with time [11]. The four peaks define two typical lengths for each direction, which is a phenomenon not common in phase-separating systems. These features are not present in our simulations.

To conclude, we have shown that multistriped configurations characterize the asymptotic evolution of the system considered in this work. This is analogous to what happens in other driven statistical models [22]. It would be interesting to see whether similar asymptotic states are obtained also in the three-dimensional version of these models. Previous analytical results correctly describe only an intermediate time regime.

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