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Equilibrium and dynamical behavior in the Vicsek model for self-propelled particles under shear

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Abstract: The effects of an externally imposed linear shear profile in the Vicsek model of self-propelled particles is investigated via computer simulations. We find that the applied field changes in a relevant way both the equilibrium and dynamical properties of the original model. Indeed, short time dynamics analysis shows that the order-disordered phase transition disappears under shear, because the flow acts as a symmetry breaking field. Moreover, the coarsening of particle domains is arrested at a characteristic length-scale inversely proportional to shear rate. A generalization of the original Vicsek model where the velocity of particles depends on the local value of the density is also introduced and shows to affect the domain formation.

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1. Introduction

The study of systems of self-propelled particles (SPP) is a topic that has attracted a very large number of physicists in the last decade or so. This is mainly because SPP particles are self-driven systems which are out of, and often far from, thermodynamic equilibrium, as they continuously burn energy from their surroundings or from internal sources, typically in order to move. The non-equilibrium nature of SPP greatly enriches their physics with respect to that of their passive counterparts [1–4]. Examples of systems of SPP abound, both in nature and in the lab, and span a wide range of length scales. Microscopical examples of SPP systems are microbial or bacterial fluids, while macroscopical examples are fish schools, or synthetic swimming micro-robots [1, 5, 6].

The prototypical model to investigate SPP is the Vicsek model [7], which was introduced in 1995. This model studies an ensemble of particles that tend to align their velocity locally to that of their neighbours in a stochastic way. A random noise is added to the average orientation angle playing a role similar to that of temperature in the more familiar case of an equilibrium thermodynamic model (such as the Ising model). By decreasing the strength of noise in the Vicsek model, one observes a transition from a disordered phase to an ordered one in which flocks of particles form and move coherently. Such flocks display long-range order even in 2 dimensions, thus not respecting the Mermin-Wagner theorem stated for passive systems [8].

The main goal of this work is to study the Vicsek model in the presence of a shear flow, complementing our previous direct numerical results in [9] with an analysis of the short time dynamics in this system. We will show that the short time dynamics further supports the conclusion from our previous work that a shear flow changes quite dramatically the physics of the unsheared Vicsek model, in particular washing away the order-disorder transition which characterises it. Our study can provide a theoretical framework to understand the generic, and possibly universal, properties of sheared active microbial suspensions [10], a remarkable physical system which is far from equilibrium because of both the self and the external driving. Even in passive materials an imposed flow may lead to flow-sustained non-equilibrium steady states. For instance, wormlike micelles and liquid crystals form bands when sheared [11, 12], whereas a sheared binary fluid arrests spinodal decomposition, leaving domains of a well-defined size, provided that hydrodynamic coupling between the order parameter and the velocity field is retained [13–16]. The self-driving characteristics of SPP suspensions is likely to add even more richness to this already fascinating physics.

In our work we also consider a variant of the (unsheared) Vicsek model where the velocity of the particles can attain two different values according to the local density. This gives another example in which the velocity of particles varies locally in space, but now such variations are governed by the local neighbourhood of each particle rather than by the overall position in the externally imposed velocity flow. As we shall show this generalised Vicsek model is also of interest as it points to an interesting transient phase separation which it may be intriguing to look for in suspensions of microbial swimmers.

This paper is organized as follows. In section 2, the sheared Vicsek model is described, and its the phase behavior is analyzed. In section 3 we investigate the lack of coarsening due to the shear field. In section 4 the density-dependent movement rule is introduced, an its consequences are exhibited. Finally, the conclusions are stated in section 5.

2. The model and the phase behavior

The Vicsek model is defined in terms of N point-like, off-lattice particles, with positions $\vec{x}_i$, and velocities, having fixed magnitude v_0, denoted by $\vec{v}_i$ $i = 1, \ldots, N$. In two dimensions, to which we restrict hereon, the direction of motion of the $i-$th particle can be described via a single angle, θ_i, so $\vec{v}_i = (v_0 \cos\theta, v_0 \sin\theta)$. To explore the effect of shear, we have generalised the Vicsek update rules to include an imposed linear velocity profile along the x direction, $\vec{v}_s = \dot{\gamma} y \hat{e}_x$ where $\dot{\gamma}$ is the field magnitude and y labels the velocity gradient direction. The dynamics of the particle positions and directions are thus given explicitly by the following formulas:

$$\vec{x}_i(t+\Delta t) = \vec{x}_i(t) + (\vec{v}_i(t) + \dot{\gamma} y \hat{e}_x)\Delta t \tag{1}$$

$$\theta_i(t+\Delta t) = \text{Arg}\left[\sum_{j\sim i} \exp(i\theta_j(t))\right] + \eta\psi_i(t), \tag{2}$$

where t and $t+\Delta t$ denote two successive time steps. The function Arg returns the argument of a complex variable, the parameter $\eta > 0$ measures the noise strength, and $\psi_i(t)$ is a uniform random variable between 0 and 2π. The sum in Eq. (2) is performed over j particles which are within a distance up to r_0 from the $i-th$ SPP particle. Note that in the quiescent limit, $\dot{\gamma} = 0$, we recover the *backward update* rule, which was originally employed by Vicsek *et al.* This model exhibits an ordered-disordered phase critical transition, whose properties have been the subject of some debate [17–19]. In the original Vicsek model standard periodic boundary conditions in all directions were applied. Here, in order to account for the imposed laminar flow, we have implemented Lees-Edwards boundary conditions at the top and bottom surfaces of the system [20]. In order to illustrate how the external field works, we performed a simulation with a large value of shear and initial condition consisting of a single band of particles, placed in the middle of a square lattice, with initial random angles. The value of shear is large in the sense that the maximum flow on the boundary $\dot{\gamma}L$ is larger than the intrinsic particle velocity v_0 [21]. The resulting evolution at short times is exhibited in Fig. 1. As it can be observed, the anisotropy introduced by the shear field progressively shifts and tilts the band along its axis, i.e. the horizontal axis. Then, when the lattice periodic boundaries are reached the configuration of the system is similar to a "barber pole", and the band becomes more aligned with the flow axis. The process continues until the band is spread over the whole lattice; the further morphological evolution will depend on the value of $\dot{\gamma}$ as discussed in section 3.

As it was mentioned before, the system in the quiescent limit undergoes an order-disorder phase transition. We want to study what happens when shear is applied, also comparing with results found in other models with external drive [22]. The order parameter for this system is the modulus of the macroscopic mean velocity normalized to v_0, φ, which is explicitly given by

$$\varphi(t) \equiv \frac{1}{N v_0}\left|\sum_i \vec{v}_i'(t)\right| \tag{3}$$

where the sum extends to all particles, and $\vec{v}_i' \equiv \vec{v}_i - \vec{v}_s$ is the average of the velocities after the imposed shear has been subtracted away. In our simulations, we set, without loss of generality, $\Delta t = 1$ and $r_0 = 1$ [7]. A quantity that is also employed to study critical phase transitions is the variance of φ, given by

$$\chi(t) = L^2\left[\langle\varphi^2(t)\rangle - \langle\varphi(t)\rangle^2\right], \tag{4}$$

which it is analog to the susceptibility in magnetic systems.

In this work, at variance with our previous analysis in [9], we will study the critical-dynamic behavior of the model at the early stages of the evolution. The analysis of such *short time dynamics* (STD) has proved to be

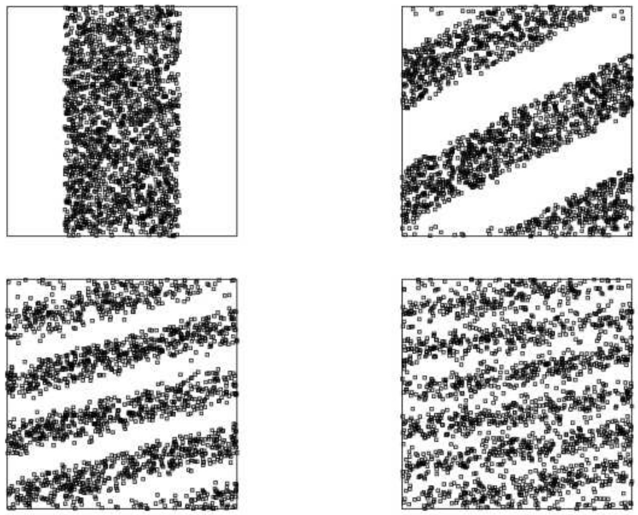

Figure 1. Snapshot configurations showing the evolution of an ordered configuration under shear. More details are given in the text. The system parameters are $N = 2048$, $\rho = 2$, $\eta = 0.1$, $v_0 = 0.5$ and $\dot{\gamma} = 0.2$.

a very useful tool to study phase transitions, as it allows an accurate estimate of both the critical point and the critical exponents characterizing a phase transition [23]. In a typical STD analysis, the time series of the observables chosen to study the transition exhibits a power law behavior if the system is just at the critical point, and deviates from it otherwise, mainly due to modulations in the scaling function.

In our system, two different initial configurations can be chosen: either (i) a fully disordered configuration (FDC), made up by placing particles at random position and with velocities along random angles, or (ii) a ground state configuration (GSC, see Fig. 1, first snapshot) where all the particles start up in a band with the same velocity, chosen along a random angle. Both are in principle suitable to study the behaviour of sheared SPP. Following Baglietto and Albano [24], we focused on the FDC initial condition and measured $\chi(t)$ only for such runs. It is expected that $\chi(t)$ will behave as $\chi(t) \sim t^{g/z\nu}$, where g is the susceptibility critical exponent, z and ν are the dynamical and equilibrium correlation-length critical exponents, respectively. Fig. 2 shows the time evolution of χ for the cases with noise equal to $\eta = 0.070$, 0.093 and 0.100, with other parameters given by $\rho = 1/8$ ($N = 1058$) and $v_0 = 0.1$, *in the absence of shear*. The expected power-law behavior can be clearly distinguished at $\eta = 0.093$, in good agreement with previous results [24]. This is an indication that the parameters are tuned so that the system is at the critical point. For different parameter choices, the time evolution shows upwards and downwards deviations, since the power-law is modulated by scaling functions that depend on the distance to the critical point [23]. Both these behaviours are clear from Fig. 2.

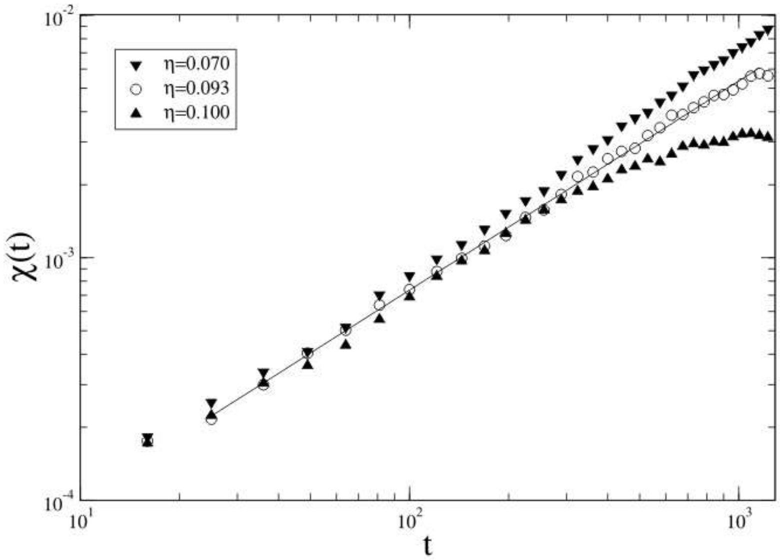

Figure 2. Time evolution of χ defined in equation (4) for a system with $\rho = 1/8$ ($N = 1058$), $v_0 = 0.1$, starting from a fully disordered configuration (FDC). The best power-law obtained, fitted by a linear regression, can be observed at $\eta = 0.093$ that can be identified as the critical value for the noise at the considered density. Upwards and downwards deviations outside the critical point can be also observed.

On the other hand, when the external shear field is applied, the situation changes dramatically. The left panel of Fig. 3 shows the time evolutions of $\chi(t)$ for a system with the same parameters as before, but when a shear field is applied with magnitude $\dot{\gamma} = 1 \times 10^{-5}$. In spite of the small value of $\dot{\gamma}$ and of the wide range of noises explored, $0.1 \leq \eta \leq 0.5$, the evolution is markedly different from that shown in Fig. 2. One can first observes that $\chi(t)$ does not show a power-law behavior at $\eta = 0.1$, which is close to the critical value for the Vicsek model at zero shear. In order to better understand the results at larger values of η – data in the range $0.2 \leq \eta \leq 0.3$ could not exclude power-law behaviour, we performed more simulations by increasing N for the case with $\eta = 0.2$ and $\eta = 0.3$. The power-law regime would broaden with N in the case of a critical dynamics.

From the right panel of Fig. 3 it can be seen that the evolution of $\chi(t)$ for $\eta = 0.2$ flattens as N is increased, and the same happens for the case with $\eta = 0.3$. The power-law regime actually *shrinks* by increasing the system size, rather than broadening. Our data thus suggest that there are no values of the noise strength leading to a critical power-law behaviour. Therefore we can conclude that there is no evidence of a phase transition in the presence of shear, in agreement with the conclusions reached in Ref. [9] by a different analysis.

The absence of a phase transition in the presence of an applied linear shear may be qualitatively understood by recalling that at $\dot{\gamma} = 0$ the transition in the Vicsek model occurs via spontaneous symmetry breaking: a flock forms by selecting, via random fluctuations, a direction for its motion, leading to a violation of total momentum

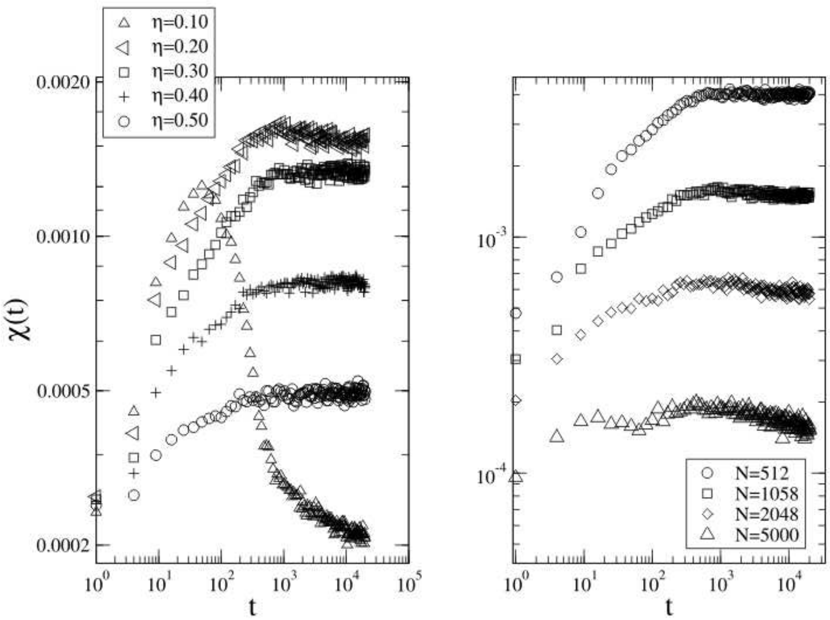

Figure 3. Left panel: Time evolution of χ defined in Eq.(4) for a system with $\rho = 1/8$ ($N = 1058$), $v_0 = 0.1$, $\dot{\gamma} = 1 \times 10^{-5}$, and $0.1 \leq \eta \leq 0.5$ (indicated in the legend). The initial configuration was a FDC. Right panel: Time evolution of χ for $\eta = 0.2$, $\dot{\gamma} = 1 \times 10^{-5}$, $\rho = 1/8$, and four different values of N as indicated in the legend.

conservation. One may then view a shear flow as an external symmetry-breaking field, akin to a magnetic field in a thermal Ising or XY model. Just as there is no finite-temperature transition in a bulk equilibrium Ising model with a field, this argument then suggests that there may be no flocking transition in the Vicsek model under shear, as the imposed laminar flow leads to a natural, preferred direction for the collective motion. Therefore, shear drastically alters the critical behaviour of the Vicsek model in steady state, by *de facto* removing the disordered phase.

3. Arrest of coarsening

Another interesting question regards the effect of the external flow on the *dynamics* of flocking in the Vicsek model at low values of the noise starting from a disordered state [9].

For $\dot{\gamma} = 0$, the flocking, ordered state is characterized by the presence of clusters, which form and coarsen until eventually one single flock remains; the exact domain morphology strongly depends on parameters such as the density and the noise strength. The dynamics also entails a good deal of transient breaking and reforming of the domains during coarsening. An example of the coarsening dynamics at $\dot{\gamma} = 0$ is shown in Fig. 4, for $\rho = 1$. Fig. 5 instead shows the corresponding coarsening when a linear shear is applied ($\dot{\gamma} = 10^{-5}$). We considered a rectangular system in order to exclude possible finite size effects that could be more relevant in the direction of

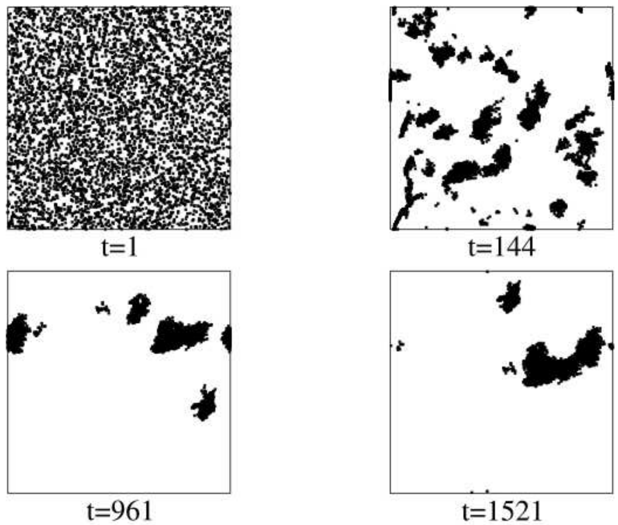

Figure 4. Snapshots at different times of the evolution of a system, initially in a disordered configuration, evolving with parameters corresponding to an ordered state. The system consists of 5184 Vicsek particles with $\dot{\gamma} = 0$, $v_0 = 0.1$, $\eta = 0.01$ and density $\rho = 1$.

the flow. While the very early stages (not shown) are comparable to the quiescent state, it can be seen that the imposed shear elongates the domains by creating a preferential direction (i.e. it breaks the isotropy), aligns them at a small angle with respect to the shear axis, and selects a well-defined size in steady state, as configurations of the systems at late times suggest. Therefore even a *linear* velocity profile is able to arrest coarsening in suspensions of SPP particles.

The arrest of coarsening in the long time limit, when the system has reached a non-equilibrium steady state, can also be characterised quantitatively. In fact, by measuring the time series of the second moment of the instantaneous structure factor, it has been shown that after a transient regime the parallel and perpendicular domain sizes saturate around a well defined value, stabilize and remain constant [9]. Fig. 6 shows that the typical size of the domains decreases when the magnitude of the field is increased [9]. The configurations are taken after that the system has reached a stationary state at a time of order of $t = 10^5$ time steps, when single time observables have been shown to be stationary.

4. Density-dependent movement

In this Section we consider a variation of the Vicsek model, in which again the velocity is non-uniform through the sample. Rather than being due to an externally imposed flow, such inhomogeneities in the propulsion velocities

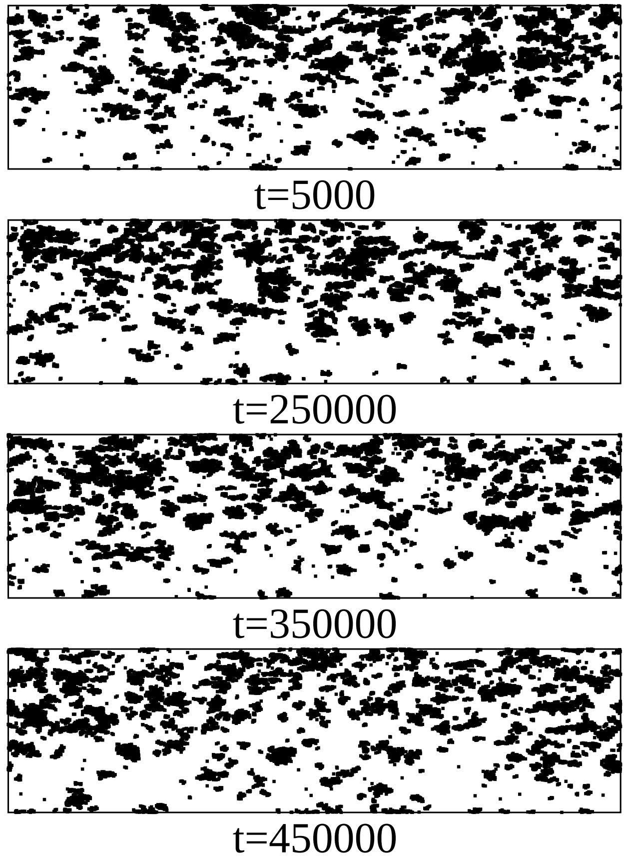

Figure 5. Snapshots at different times of the evolution under shear of a system initially in a disordered configuration. The system consists of $N_p = 20736$ Vicsek particles with $\dot{\gamma} = 10^{-5}$, $v_0 = 0.1$, $\eta = 0.01$, density $\rho = 1$, $L_x = 288$, $L_y = 72$.

are this time due to the local density of the SPP: specifically we imagine that the velocity decreases where the SPP are more crowded. The new algorithm works as follows: for each particle we compute the density in a circle with radius r_0: if such a density is low the particle moves at a "free speed" v_0, whereas, if the density exceeds a threshold ρ_{local}, then the velocity of the SPP is set to $v_{slow} < v_0$. Our rule is simpler than but related to that used in the models in [25, 26], where the dependence of the velocity on the density is continuous. In a real suspension of self-propelled active particles or bacteria, a density-dependent speed may be due to steric interactions [27] or to biochemical signalling [25].

We performed simulations for a system with $N_p = 1024$, $L = 32$, overall density $\rho = 1$, $v_{slow} = 0.02$ and $\rho_{local} = 5.5$. The snapshots exhibited in Fig. 7 show the time evolution of the systems described above for the case of low noise, $\eta = 0.1$. We observe that due to the small noise, the particles tend to form large clusters with velocity magnitude v_{slow}, except at domain edges where the local density takes smaller values. There is also some evidence of a phase separation between "slow" and "fast" SPP, in analogy with the results found in [28] for a mixture of SPP with different speeds. Unlike the domains found in the shear simulations, though, the slow and fast clusters later on merge into a giant cluster of slow particles and some isolated clusters of faster v_0. Therefore

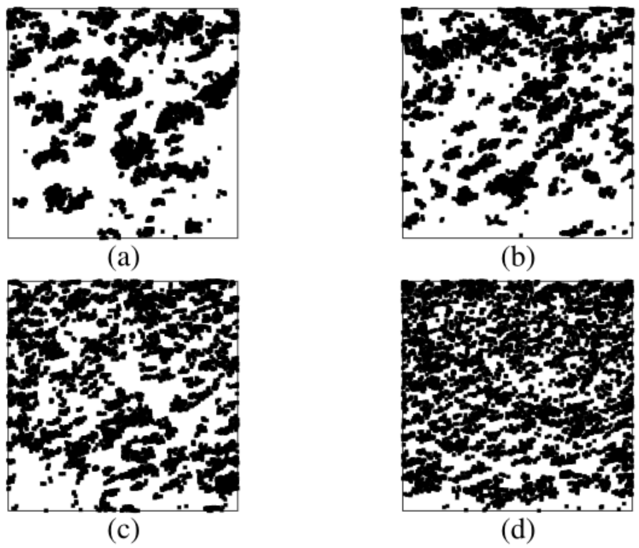

Figure 6. Configurations of the Vicsek model at $t = 10^5$ time steps in a stationary regime with shear fields of different magnitude: (a)$\dot{\gamma} = 5 \times 10^{-5}$, (b)$\dot{\gamma} = 10^{-4}$, (c) $\dot{\gamma} = 2 \times 10^{-4}$ and (d)$\dot{\gamma} = 5 \times 10^{-4}$. Other parameters are the same as in Fig. ... The decrease of the size of domains in the transversal and longitudinal directions can be observed. In these simulations $N_p = 5184$, $\rho = 1$, $\eta = 0.01$, $v_0 = 0.2$.

at small noise the density-dependent kinetic rule favors aggregation in few clusters with slow particles. When the noise is raised, to $\eta = 0.8$, the isolated clusters are stable for longer, however the final configuration $t = 10^5$ is similar to the last one in Fig. 7, albeit there are now less small clusters with fast particles.

Although the morphology of the domain may seem to be relatively insensitive to the phase the SPP are in (ordered or disordered), looking at the intracluster orientational order reveals that the aggregates move coherently at low noise and diffuse randomly at large noise. These motion are of course, independent of both v_0 and v_{slow}. In order to illustrate this, we plotted in Fig. 9 the velocities of small portions of the last configurations in Figs. 7 and 8. In the left panel, the noise is $\eta = 0.1$, and it can be observed that all particles in the clusters have approximately the same direction of motion, while this does not happen in the right panel at $\eta = 0.8$.

5. Conclusions

In conclusion, we have studied the effect of an imposed linear shear flow on a suspension of Vicsek self-propelled particles, and compared it with the model without external fields. We have numerically shown that shear plays havoc with the physics of the Vicsek model. Most notably, via an analysis of the short time dynamics of the model we found that shear removes the order-disorder transition found at zero shear rate, $\dot{\gamma} = 0$, in agreement with what

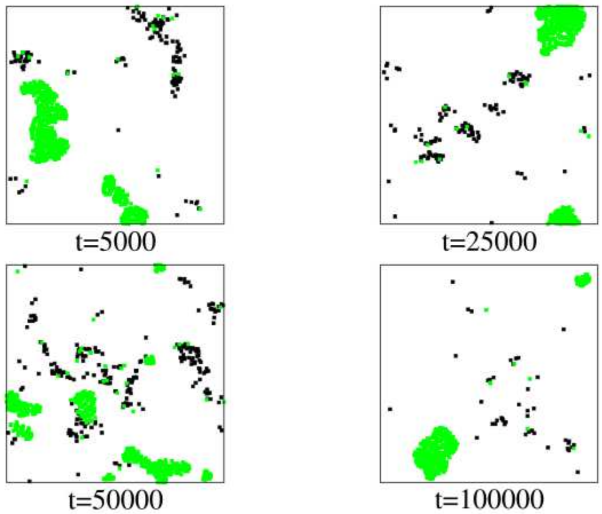

Figure 7. (Color online) Time evolution of the Vicsek model ($N_p = 1024$, $\rho = 1$) with a density-dependent velocity, starting from a disordered configuration (see upper right panel in Fig. 4), and $\eta = 0.1$. The black squares repesent particles with $v_0 = 0.2$ while the light green ones have $v_0 = 0.02$. More details in the text.

we found in Ref. [9] with a different method. We have also shown that shear arrests the coarsening of domains into a single flock, leaving a steady state made up of smaller clusters with a well defined size. This provides another important example in which the physics of active matter qualitatively differs from that of its passive counterpart, as a linear shear is not enough to stop coarsening as it does in, e.g., a binary mixture quenched below the critical temperature.

We have also studied the physics of another variant of the Vicsek model, in which again the velocity varies from particle to particle, but in response to the local density rather than to the external shear. In particular we have considered a case in which the velocity is a binary function of the density: large for a particle in a dilute environment, and slower (but non-zero) for a particle in a locally crowded environment. This rule is simpler than but related to that used in the recent models in [25, 26]. We found that also this inhomogeneity opposes coarsening, leading to the formation of clusters of slow and fast particles. However this arrest is only transient and eventually a giant cluster of slow particles is formed, irrespective of the noise employed, i.e. of the phase the SPP are in. The motion in the clusters in the ordered phase is coherent, and all particles in the same cluster point in the same direction. On the other hand, in the disordered phase there is no clear direction of motion, not even within the same cluster, as the orientational order drops to zero.

We believe that our study should be relevant to rheological experiments on suspensions of bacterial or microbial swimmers, and to the large scale behaviour of social animals, such as birds flocks and insect swarms, which are

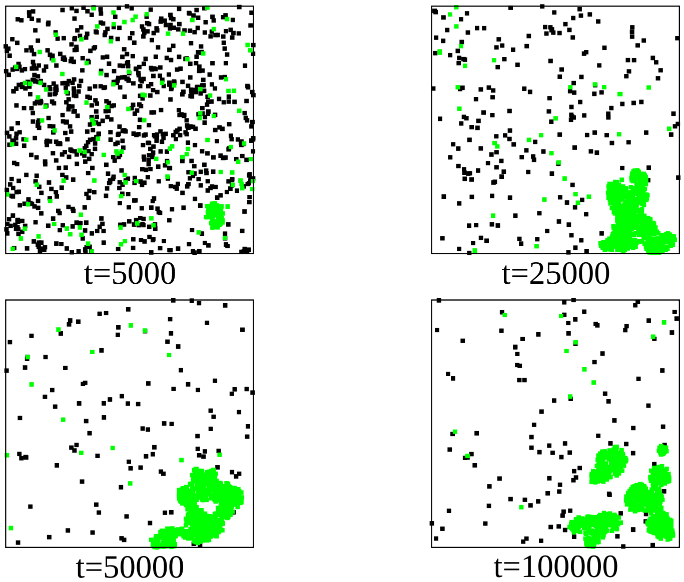

Figure 8. (Color online) Time evolution of the Vicsek model ($N_p = 1024$, $\rho = 1$) with a density-dependent velocity, starting from a disordered configuration a … he light green ones have $v_{slow} = 0.02$. More de

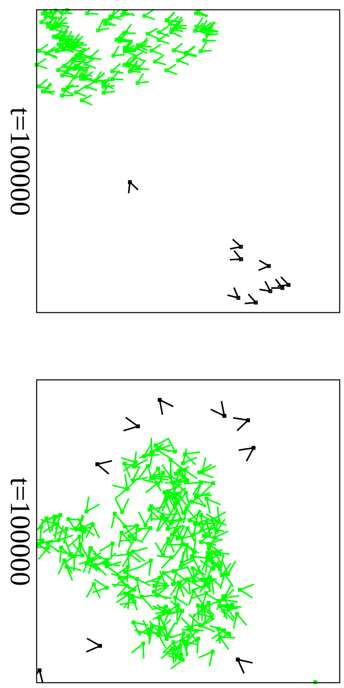

Figure 9. Small portion of the last configurations at $t = 10^5$ time steps of figures 7 (left panel) and 8 (right panel), indicating the coherence and lack of global motion in the case of low noise, $\eta = 0.2$, and high noise, $\eta = 0.8$, respectively.

known to be fragmented or dispersed by strong winds.

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