Dynamic path dependence of phase behaviors in dense active system

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There are rich emergent phase behaviors in nonequilibrium active systems. Flocking and clustering are two representative dynamic phases. Their complementary shapes in phase diagrams suggest some subtle relationships, which are still an open problem. By numerical simulation of self-propelled particles with active reorientation, we investigate the time evolution of order parameters under different initial states. This work reveals that the steady-state phase behaviors are strongly dependent on dynamic historical path. The distributions of order parameters of flocking and clustering in the long-time steady states show bi-stable state. The existence of these bi-stable states is due to the change of dynamic paths arising from different initial states. Accordingly, we propose a method to eliminate the bi-stable state by controlling the ordering of the initial state. By increasing (decrease) the initial degree of ordering, the bi-stable state can be shifted to a more ordered flocking (disordered clustering) state. Our work on manipulating emergent behaviors of active system will be contribute to the control and design of robots with novel collective motions.

I. INTRODUCTION

Active systems have been the subjects of intense attention \cite{1,2,3}. The emergence of collective motion appeared in such systems inspires us to consider the dynamics in the evolution process of active system. However, unlike equilibrium system determined by the principle of minimum free energy, these systems are far from equilibrium. So far there is a lack of widely acknowledge theory to describe the steady-state phase behaviors since nonequilibrium evolution is usually dependent on their dynamic paths, which is an interesting property widespread existing in many living and inanimate systems \cite{5,6}.

In the past few decades, extensive work has been performed towards dynamic path in network, natural and social systems \cite{10,11}. A series of intriguing behaviors emerge along with different dynamic paths, and the evolution of the system exhibits rich diversity. It is also found that the processing routes or transition pathways give rise to different structures, states, and properties of materials \cite{16,17}. In particular, one of the main manifestation of history dependence is initial-state dependence \cite{23}. In recent years, many studies have shown that initial velocity distributions can influence the formation of coherent structures \cite{24}, nonequilibrium criticality of magnetic systems \cite{25} and alignment of block copolymer micro\cite{26}. However, there is few research specifically concerning the interplay between the collective motion and path-dependent clustering and flocking phases which is related to self-organization in the active system. Consequently, it is worth to understand deeply the mechanisms controlling the key characteristics of specific phase behaviors which are sensitive to the history.

In this work, we focus on the impact of dynamic path on the phase behaviors in the active system, which is consisted of self-propelled particles with active reorientation. The rotations of self-propelled particles are common in active matter by assigning a torque \cite{27,28} or adding angle transformations \cite{29,30}. In our current work, we propose a more natural active rotation inspired by experiment, in which each colliding particles spontaneously reorient and make it easier to separate. The coupling between self-propulsion and active reorientation produces richer dynamics compared with previous models merely involving translation or rotation. As a result, these particles may collectively aggregate to dynamic clusters or self-organize into alignment. By exploring evolution processes under different parameters, we reveal the complementary nature of clustering and flocking. We further study history-dependent property in the active system, and explore how the initial states reshape dynamic path and then affect the steady state of the system. We observe the discrepancy of steady states of the flocking and clustering phase under different initial states. The phase boundary is considered to comes from the competition between active reorientation and noise. It is sensitive to initial particle position and velocity distribution. Interesting, the system could evolve into one of two nonequilibrium stable states by manipulating initial states. All these findings offer a new way to control collective behaviors by adjusting dynamic paths.

The rest of paper is organized as follows. In Sec.II, we introduce an active model and present possible phases in such system. In Sec.III, we quantitatively characterize the flocking and clustering as well as their complementary relationship. In Sec.IV, we try to figure out the effect of history in the phase behaviors of the system. First we explore the effect of initial state on phase diagrams. Then we reveal the influence of initial states on the evolutionary process and steady states. Through further analyzing the distribution of the order parameters of flocking and clustering in steady states, we show that the initial stats can affect the occurrence of bi-stable states. Finally, the

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We numerically solve Eqs. (1) and (2) using periodic boundary conditions. In our simulation, we set time-step $\Delta t = 1$, displacement $\Delta s = 0.1d$, and packing fraction $\phi = 0.3$. We have performed simulations with particle number $N = 100$ to 25,000 particles little difference is observed for systems with 1000 or more particles. Hence, we explore the kinetic properties of system by running simulation with 1000 disks.

III. PHASE BEHAVIORS

The dynamics of the system is controlled by three parameters: $\sigma$ of the Gaussian Noise, self-propulsion speed $\Delta s = 0.1d$, and active reorientation step size $\alpha$. We have tested that the influence of self-propulsion speed on our system is mainly associated with the formation of cluster or living crystal states, such as the emergence of hexatic and solid order in [37], which has little effect on dynamics. However, a certain amount of noise is necessary as well to induce a non-equilibrium phase separation. And the balance among noise, self-propulsion and particle interactions are is the key to demixing in an active Brownian particle [38]. So in this paper, we focus on the effects of noise and active reorientation combined on the phase dynamic behaviors of the system. In the mean time, if noise is big enough, the system goes into random states no matter how big or small active reorientation is. So next, we discuss the dynamics and interactions among these phases that appear in our system in detail.

For each given set of $\sigma$ and $\alpha$, we take random positions and directions of the particles as initial states to simulate the evolution of the system. Fig. 2(a-d) present some possible collective behaviors that arise from different evolutionary processes. As directions of particles evolve by actively reorienting themselves and rotating diffusion, which breaks the local balance and leads to the formation of cluster and related to the broken orientational symmetry. As directions of particles evolve by actively reorienting themselves and rotating diffusely, the local balance and orientational symmetry of system are broken, which leads to the formation of cluster Fig. 2(a). Fig. 2(b) is a flocking state in which the orientations of all particles are approximate aligned while the position distribution is uniform. Fig. 2(c) and (d) represent two kinds of disordered phases. The first one includes small clusters even though the orientations of particles are random. The second one is totally disordered since the orientation and position of particles are all almost random.

A. Order parameters

We introduce two order parameters in order to characterize the steady states of system mentioned above. Flocking appeared in our system is described by an or-
FIG. 2. (color online) Representative steady states: (a) clustering; (b) flocking; (c) partly disordered phase; (d) totally disordered phase. Blue arrows indicate the direction of particle velocity.

entational order parameter,

\[ M = \sqrt{\langle \cos \theta \rangle_N^2 + \langle \sin \theta \rangle_N^2} \]  

(3)

where the average \( \langle \rangle_N \) is taken over all \( N \) particles. \( M \approx 1 \) indicates perfect flocking phase and \( M \approx 0 \) disordered phase. To quantitatively identify the phase of system that separates into dense clustered and dilute gas-like state, we measure the local area density of each particle as \( a_l \):

\[ a_l = \frac{A}{A_v} \]  

(4)

Here \( A \) is the area of each disk, \( A_v \) is the area of Voronoi cell of each disk. The larger size of cluster is, the more particles of larger \( a_l \) there are. By numerical simulation, we found that when \( a_l \) is greater than a certain threshold, the disk is located in the dense cluster. So in our work, we set the threshold as 0.7 and we introduce another order parameter \( \rho_c \), the fraction of particles with \( a_l > 0.7 \), to describe clustering. These two order parameters can give a good description of flocking and clustering, for example, in Fig.2(a)-(d), \( (M \approx 0, \rho_c \approx 0.92), (M \approx 1, \rho_c \approx 0), (M \approx 0, \rho_c \approx 0.26), (M \approx 0, \rho_c \approx 0) \) respectively. In order to explore the dynamics of flocking and clustering, we analyzed a time series of \( M \) and \( \rho_c \). Fig. 3(a) shows time series under parameter \( \alpha = 0.01 \) and \( \sigma = 0.01 \). \( M \) grows slowly first, then sharply increases and eventually reaches flocking state with \( M \) close to 1. \( \rho_c \) grows slowly at the beginning, then it reaches a transient plateau. Concurrent with the sharp increase of \( M \), the transient plateau of \( \rho_c \) collapses. The snapshots of the configurations are shown below Fig.3(a). When the system starts from a disordered state, small condensation clusters appear in the system, and phase separation is triggered. Then the condensation nuclei come together and aggregate into a large cluster. Also, the nonequilibrium clustering appeared in the system were observed in other active models [40–42]. Next, as particles collide with each other, scattering with active reorientation competes with the self-diffusion process. As a result, the cluster gradually disintegrates and disperses. The final state of the system is highly flocking, similar to the flocking state in vicsek model [43]. In contrast, as shown in Fig.3(b), under the parameter \( \alpha = 0.01, \sigma = 0.04 \), \( \rho_c \) increases on a time scale similar to that in Fig.3(a) and finally saturate around 0.8, whereas \( M \) remains low value throughout the simulation. The evolution of configuration is relatively simpler. Particles interact with each other and gradually form stable clusters. There is no orientational order in the steady state.

FIG. 3. (color online) Temporal evolution of order parameters and configurations. The system eventually evolved to (a) flocking state under \( \alpha = 0.01, \sigma = 0.01 \) and (b) clustering state under \( \alpha = 0.01, \sigma = 0.04 \).
FIG. 4. (color online) The dependence of $M$ and $\rho_c$ on $\sigma$ with $\alpha = 0.01, 0.04, 0.08, 0.10$.

B. Phase diagrams

The value of order parameters would fluctuate little for long enough time. In our model, the system keeps stable after a several thousand time-steps. So in order to characterize steady states, we measured the order parameters at 10,000 time-steps under different sets of \{\alpha, \sigma\}. We take random initial states and run simulations. We find that the system eventually evolves to be flocking state with $M \approx 1$ when the values of $\alpha$ and $\sigma$ are in certain region. But in the other region, the system can not reach the flocking state at all. In Fig. 4 we present the dependence of $M$ and $\rho_c$ on $\sigma$ with $\alpha = 0.01, 0.04, 0.08, 0.10$. As shown in In Fig. 4(a), when $\alpha$ is fixed, the system finally presents order or disorder state, which depends on the intensity of noise. With the increase of $\alpha$, the value of $\sigma$ at critical phase transition point also increases. As shown in In Fig. 4(b), similar behavior also manifests in the aggregation of clusters. In particular, the value of $\sigma$ at critical phase transition point for flocking and clustering is the same.

We draw the phase diagram according to the value of $M$ in the steady state in Fig. 5(a). The dash line in the figure is the contour line of $M$ equals to around 0.3. When $\sigma$ is relative small, the system would reach a steady flocking state because active reorientation is dominant so that it promotes local velocity alignment and the formation of global flocking as in the domain below the black dash line. We also found both large active reorientation and random noise weaken the local velocity alignment, so that the system would be in disorder state as in the domain upon the dash line, in which there is basically no global flocking. The phase diagram of $\rho_c$ is depicted in Fig. 5(b), and the white dash line in the figure is the contour line of $\rho_c$ equals to around 0.1. And final clustering states are concentrated in the domain which surrounded by white lines. The overall phase behavior can be understood by considering the competition between the absorption rate of particles to clusters and escape rate of particles from clusters. When a particle collides with a cluster, it has a probability either entering or es-

FIG. 5. (color online) Phase diagram of flocking and clustering. Contour map of flocking and clustering measured from simulations evaluated at the steady state from the initial conditions with a random distribution of particles (a-b).
FIG. 6. (color online) Phase diagrams of steady states starting from highly alignment condition. (a) Phase diagram of $M$. (b) Phase diagram of $\rho_c$. (c) The difference of $M$ between Fig.5(a) and Fig.6(a). (d) The difference of $\rho_c$ between Fig.5(b) and Fig.6(b).

capping from the cluster due to active reorientation and noise. In the diagram of $\rho_c$, the regions with a high degree of clustering correspond to the regions where global alignment can not be formed in the diagram of $M$. High global flocking and large cluster can not coexist with each other.

IV. THE EFFECT OF INITIAL STATES ON CLUSTERING AND FLOCKING

In equilibrium systems, the phase transition is usually independent of the initial state. But this argument may not hold for non-equilibrium systems. So in this session, we explore the influence of initial states such as velocity distribution on the phase diagram, evolutional process and the distribution of order parameter in the steady state.

A. The effect of initial state on phase diagrams

We denote the value of initial orientational order parameter as $M_0$. We change initial states of the system from the homogeneous state ($M_0=0$) to the highly flocking state ($M_0=1$). We thought no matter starting from a random configuration or from perfect alignment configuration, the final steady state would be the same. However, we strikingly find that this is not always the case. Fig.5(a) and (b) represent phase diagrams of $M$ and $\rho_c$ in the steady state under the initial state from highly alignment condition. Comparing phase diagram of $M$ in Fig.5(a) with Fig.6(a), we can see there are differences between them. The phase separation line obviously shifts when $\alpha$ is relative small. And the flocking domain is bordered in Fig.5(a) than it in Fig.6(a). As for the phase diagram of $\rho_c$, on the contrary, the clustering domain in Fig.5(b) becomes smaller than the domain in Fig.6(b).

Next we quantitively characterize the difference between these diagrams. Fig.6(c) shows the difference between orientational order parameters in the steady states under two different initial states mentioned above. The differences are concentrated in the dark area. Likewise, we present the difference between $\rho_c$ under the same condition in Fig.6(d). We observe that they are quite similar to each other, basically matching up in the same domain. Then we define the correlation $C_{\text{cor}}$ as

$$C_{\text{cor}} = \frac{\int \Delta \rho_c \Delta M \, d\alpha d\sigma}{\sqrt{\int (\Delta \rho_c)^2 \, d\alpha d\sigma \int (\Delta M)^2 \, d\alpha d\sigma}}$$

By calculating the correlation between the two phase diagrams, we find that the correlation is about 60.43%, which suggests a strong correlation between flocking and clustering.

B. The influence of initial states on the evolutionary process and steady states

In order to study how initial states affect the evolution of system, we choose two sets of parameters in different regions. One set of parameters is $\alpha = 0.01$ and $\sigma = 0.01$, which belongs to the region that the steady state is not sensitive to the initial state. And the other set is $\alpha = 0.01$ and $\sigma = 0.04$, which belongs to the region that the steady state is sensitive to the initial state. Fig.7(a) and (b) are the evolution of $M$ with time under
different initial states, and Fig. 7(c) and (d) are $\rho_c$ likewise. Fig. 7(a) and (c) reveal that with the increase of $M$, $\rho_c$ accumulates gradually. When $M$ of the system is small, the cluster promotes $M$ and increases the growth of $M$. With $M$ getting larger, $\rho_c$ also increases. This is a positive correlation between $M$ and $\rho_c$. When $M \approx 0.5$, the whole system is in the state of the strongest clustering state. And then as $M$ continues to increase, $\rho_c$ begins to disintegrate. In Fig. 7(a), we observe that initial states influence the growth of $M$, that is to say, the growth rate of $M$ decreases from disorder to highly aligned states under the same time. The behavior of $dM/dt$ synchronizes with $\rho_c$ which is shown in Fig. 7(c). Meanwhile, the ability of clustering decreases with the increase of $M_0$. So we can understand that it is initial states that affect the evolution of the system, reflecting on the change of cluster formation and local alignment.

In the case above, the initial state affects the evolution of the system, but does not affect steady states at all. Further, we explore the other case $\alpha = 0.01, \sigma = 0.04$ which is in the domain sensitive to initial states. From Fig. 7(b) and (d), we obviously observe that the system finally stabilizes at different amplitudes with different initial states when the system reaches steady states. We realized that different initial states of the system lead to distinctly non-equilibrium steady states in the certain critical domain.

C. Distribution of order parameter in the steady-state

Whether the final state of the system is completely maintained in a middle-flocking state, or a result of ensemble average is the key to understanding this non-equilibrium self-organization phenomenon. Thus we explore the distribution of $M$ and $\rho_c$ in the steady states evolved from different initial states. As for the steady states in the domain which is insensitive to initial states, Fig. 8(a) and (b) reveal that the distribution of $M$ and $\rho_c$ in the steady states is totally located at around 1 and 0, respectively. However, in the domain which is sensitive to initial states, according to the distributions shown in Fig. 8(c) and (d), we see that it is possible to move from the bistable regime into the only disordered regime or ordered regime by decreasing or increasing $M_0$. We would like to emphasize that such behaviors only appear in the specific domain of the phase diagrams.

So far, we bring out the existence of a metastability regime which is affected by initial states. However, we still need a understanding of phase-ordering kinetics because the absence of a well-defined notion of temperature and free energy of these systems far from equilibrium makes us difficult to get insights from a theoretical point of view.

V. SUMMARY

We have investigated the influence of dynamic path on the evolution process and steady state of the active system based on a model with active reorientation. The system displays rich phase behaviors including global flocking, clustering and disordered phases. We observe an interesting interplay between flocking and clustering. We notice that the boundary of flocking phase and clustering phase rely on the choice of initial states. Although clustering is like a high nucleation barrier that prevents the system from escaping from metastable states [44], the increasing of the order degree of initial states would suppress clustering during the process of self-organization evolution. In our work, the collision avoidance property makes the active system tend to reach different steady states. This is the reason for history-dependency feature emerged in the system, which was not observed in the previous Vicsek Model or active brownian particles with velocity alignment model. In the work by Chvykov et al [14], the possible future state of active robots can be controlled by adjusting the initial state of the system. Our work provide a theoretical evidence for the experiment mentioned above. Since dynamic path can influence evolution behaviors of self-organizing system, this means that active matter or active robots may be controlled to allow the system to grow towards an expected state from the perspective of regulation. This finding has a wide range of applications in improving designs of collective migration and navigation strategies.
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