Collective motion in repulsive self-propelled particles in confined geometries

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Abstract. We study the collective dynamics of a simple model of repulsive self-propelled particles in three different geometries bounded by reflecting walls. Order-disorder transition is observed in all three cases and the behavior of the phase diagram is similar to that of a system with periodic boundary conditions, which supports a view that the coherent motion of particles is induced by a microscopic mechanism. We also find that some interesting quasi-stable dynamic patterns may appear during the ordering process. The long lifetime of the transient structures indicates that the boundaries hinder the propagation of correlations.

1. Introduction

Much efforts have been devoted to understand the universal feature of collective behaviors seen in biological systems over the last two decades. One of the earliest computational models is the Vicsek model [1], which assumes ferromagnetic-like alignment interactions between self-propelled point particles. Despite its minimal feature, the model exhibits characteristic dynamical patterns, such as a spontaneous transition to collective motion, a long wavelength instability at the onset of order, and so-called “giant” density fluctuations [2,3]. Alignment with neighbors, however, is not always the origin for the collective behavior empirically observed. In fact, many experimental results suggest that the repulsion and excluded volume play an important role in bacterial colonies and cellular aggregates [4–6]. Pedestrian movement in human crowds is also influenced by socio-psychological repulsion from others [7,8]. Collective dynamics with pure repulsion or hard steric interaction (without alignment) has been investigated for quite some time [9–13]. However, only a few studies [14,15] have explored the full phase diagram with a focus on ordering behavior. In our previous work [15], we argued that repulsive active particles may undergo a transition from disorder to coherent motion, based on the results from numerical simulations with periodic boundary conditions (PBCs).

The PBCs gain a long-standing popularity in the field of computational statistical physics because they are useful for approximating the bulk properties from finite size simulations. However, they have a limitation that an artificial order may be imposed that can lead to abnormal results for structural and dynamical properties. In equilibrium systems, finite size scaling analysis provides a convenient way to infer the asymptotic behavior in the thermodynamic limit. However, the method may neither be justifiable nor come in handy when applied to systems strongly out of equilibrium. In such systems, the effect of geometry and of

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boundaries on the dynamics must be examined by direct simulations. In the context of self-propelled particles, some geometries are particularly important because of their analogy with physical systems. In the embryonic development process, for example, collective cell migration often takes place in certain spatial confinements surrounded by extracellular matrix [16, 17]; similarly, pedestrian movement responds to spatial structure of the environment, which is defined by walls and obstacles [18]. In this paper, we analyze the dynamics of the self-propelled particles in systems with three basic geometries: a pipe or a corridor has periodic boundaries in the \( x \) direction while bounded by two reflecting walls in the \( y \) direction; a box or a room is a rectangular area surrounded by walls at all four sides; a disk is a circular surface also enclosed by a reflecting boundary.

2. Repulsive self-propelled particle model

We consider disk particles \( i \) of radius \( a \), driven by self-propelling force of constant magnitude \( \alpha \) in the direction of polarity \( \psi_i \). The dynamics is damped both in the translational and rotational degrees of freedom: a particle is subject to a friction proportional to the velocity with coefficient \( \beta \), and a torque which is proportional to the angular difference between the velocity and the polarity with coefficient \( \gamma \), which rotates the polarity. The overall dynamics is described by the following equations of motion:

\[
\frac{dv_i}{dt} = \alpha \hat{e}(\psi_i) - \beta v_i + \sum_{j \neq i} f_{ij} + \sum_W f_{iW} ,
\]

\[
\frac{d\psi_i}{dt} = \gamma (\theta_i - \psi_i).
\]

Here, \( \hat{e}(\cdot) \) indicates an unit vector in the direction of the argument, and \( \theta_i \) is the direction of the velocity. The interaction with another particle \( j \) is a Hookean contact force,

\[
f_{ij} = \begin{cases} 
-k(2a - |r_{ij}|) \frac{r_{ij}}{|r_{ij}|} & \text{if } |r_{ij}| < 2a \\
0 & \text{otherwise},
\end{cases}
\]

where \( r_{ij} = r_i - r_j \). We assume a similar interaction with a reflecting boundary \( W \)

\[
f_{iW} = \begin{cases} 
-k(a - |r_{iW}|) \frac{r_{iW}}{|r_{iW}|} & \text{if } |r_{iW}| < a \\
0 & \text{otherwise},
\end{cases}
\]

where \( r_{iW} \) denotes the normal vector from the position of the particle to the boundary. The stiffness \( k \) is constant and the same for both types of interactions.

In our previous work [15], we fixed values of \( \alpha \), \( \beta \), and \( k \) so the only control parameter left for microscopic dynamics will be the rotational damping coefficient \( \gamma \), and performed simulations in a square box with PBCs. An ordered motion spontaneously emerges from an initially random configuration for small values of \( \gamma \). The system tends to remain longer in an isotropic and disordered state before the transition for larger \( \gamma \); the waiting time eventually exceeds the finite simulation time. We showed that this behavior stems from iteration of binary collision between particles. In this paper, we examine the dynamics with different geometries and boundary conditions.

3. Pipe geometry

First, we discuss the behavior of the system in a pipe, of which the vertical boundaries (perpendicular to the \( x \) axis) are periodic while the horizontal ones (perpendicular to the \( y \) axis) are reflecting. Typical snapshots are shown in the left column of Fig. 1. The most significant difference from the full-periodic case is the aggregation along the walls. A configuration with
Figure 1: Snapshots of repulsive self-propelled particles at successive times in three different geometries. Colors represent the direction of the polarity. From left to right: time development in a pipe, in a box, and in a disk, respectively. The parameters are $N = 5000$, $\Phi = 0.2$ and $\gamma = 1$ for all figures.

two streams moving in the opposite directions at the reflecting borders is stable, and a fully ordered motion over the entire system cannot be achieved once this structure is formed. A single stream or multiple lanes, moving parallel to the $x$ axis, are also stable. The directions of streams and the number distribution of the aggregates do not depend on the parameter values.

In order to quantify the degree of coherence, we adopt an order parameter following the previous studies on lane formation of colloidal particles [19]. First, we classify the particles into two groups, those who are pointing in the positive direction and those pointing in negative direction, based on the sign of $\mathbf{e}(\psi_i) \cdot \mathbf{x}$. Then we assign each of them an order parameter $\phi^\text{pipe}_i$, which is equal to 1 if the distance along the $y$ axis, $|y_i - y_j|$, to all the particles $j$ in the other group is larger than the sum of the radius of the two particles and equal to 0 otherwise. Finally, the global order parameter $\phi^\text{pipe}$ is defined as the fraction of “ordered” particles,

$$\phi^\text{pipe} = \frac{1}{N} \sum_{i=1}^{N} \phi^\text{pipe}_i. \tag{5}$$

The phase diagram as a function of volume fraction $\Phi$ and $\gamma$, as shown in Fig. 2(a), is generated by averaging the values of the order parameter for the first 5000 time steps. It is in good agreement with the phase diagram for the full-periodic case in Ref. [15].
Figure 2: Phase diagrams for $N = 5000$ system (a) with the pipe geometry, and (b) with the disk geometry. The dots are shaded from black to white proportional to the time average of the order parameter over 5000 time units.

Figure 3: Snapshots of transient states. (a) The coexistence of “gaseous” state at the top and “solid” state at the bottom in a pipe. The parameters are $N = 3000$, $\Phi = 0.4$, and $\gamma = 30$. (b) A transient state with two vortices, observed in a box confinement. $N = 3000$, $\Phi = 0.5$, and $\gamma = 10$.

In some runs near the phase boundary, we observe a transient state where particles are ordered and densely packed in one part while disordered in the rest of the system, as shown in Fig. 3(a). This coexistence between a “crystallized” region and a “gaseous” region is not a stationary state; particles in the gaseous region are eventually absorbed into the ordered stream. However, the relaxation tends to be much slower than that in a full-periodic system, where nucleation is followed by quick growth of clusters which results in the global polarization. We suppose this is due to the difference between the two geometries in capability of propagating the particle-particle correlations. The reflecting boundaries prevent the correlations to spread from one side to another.

4. Enclosed geometries: box and disk
Next we turn to the box geometry, where the reflecting walls are placed at all four sides of the simulation box. In contrast to the periodic and pipe cases, the entire system cannot move in a coherent direction because there is no inflow nor outflow. The “ordered” state in this geometry is a whirling motion along the boundary, as shown in the center column of Fig. 1. A state with two vortices, rotating in the direction opposite to each other, is a quasi-stable transient state (Fig. 3(b)). We emphasize that although this structure is not stationary it survives for a considerably long time compared to the rapid ordering in a system with PBCs. This is again supposed to be due to the bounded propagation of correlations.

Although the transition to coherent motion is evident from the snapshots, a suitable order
parameter is difficult to construct for the box geometry. Instead of a rectangular box, we resort to another, more symmetric confinement: a simulation area enclosed by a circular reflecting wall. As one would expect, coherent circular motion is observed as an ordered state under this geometrical condition as well (Fig. 1, right column). We detect the transition to the circular flow by monitoring an order parameter $\phi_{\text{disk}}$, which is defined as

$$\phi_{\text{disk}} = \frac{1}{N} \left| \sum_{i=1}^{N} \frac{v_i \cdot \mathbf{T}_{\omega_i}}{|v_i|} \right|,$$

where $\mathbf{T}_{\omega_i} = -\sin \omega_i \mathbf{x} + \cos \omega_i \mathbf{y}$ is an unit tangent vector at the polar angle $\omega_i$ whose pole is located at the center of the disk. $\phi_{\text{disk}} = 1$ is attained when all the particles rotate along the concentric circles in the same direction. Again, we perform simulations for various pairs of parameter $(\Phi, \gamma)$ and depict the phase diagram as shown in Fig. 2(b). The fact that the phase boundary traces almost the same curve as those in the periodic and pipe cases leads to a conclusion that the phase transition is not affected by the change of boundary conditions and that the intrinsic mechanism behind the ordering behavior is indeed the correlations propagated by iteration of binary collisions.

5. Summary
We investigate behaviors of simple repulsive self-propelled particle systems with three different geometries, namely, the pipe, the box, and the disk. Since the microscopic mechanism leading to the coherent motion is universal regardless of the geometry, we can predict the behavior of the phase diagrams from that of the system with periodic boundary conditions. However, transient states, where particles are locally aligned but the entire system has not yet reached a stationary state, tend to have longer lifetimes in the systems bounded by reflecting walls, because they prevent the velocity correlations from being transmitted. These transient states include coexistence between gaseous and crystallized phase and convective patterns with multiple vortices. The numerical results we present here illustrate analogies as well as differences between experimental active matter systems, such as bacteria, in which the localization along the border is rarely observed. Bridging this gap would be an interesting future direction.

Acknowledgements
This work was supported by CREST, JST.

References
[1] Vicsek T, Czirok A, Ben-Jacob E, Cohen I and Shochet O 1995 Phys. Rev. Lett. 75 1226–1229
[2] Grecoire G and Chaté H 2004 Phys. Rev. Lett. 92 025702
[3] Chaté H, Ginelli F and Raynaud F 2008 Phys. Rev. E 77 046113
[4] Zhang H, Be'er A, Florin E L and Swinney H L 2010 Proc. Natl. Acad. Sci. 107 13626–13630
[5] Starruf J, Perun F, Jakovljevic V, Sogaard-Andersen L, Deutsch A and Bär M 2012 Interface Focus 2 774–785
[6] Helbing D and Molnár P 1995 Phys. Rev. E 51 4282–4286
[7] Karamouzas I, Skinner B and Guy S J 2014 Phys. Rev. Lett. 113 238701
[8] Perun F, Deutsch A and Bär M 2006 Phys. Rev. E 74 030904
[9] Grossman D, Aranson I S and Ben Jacob E 2008 New J. Phys. 10 023036
[10] Henkes S, Fily Y and Marchetti M C 2011 Phys. Rev. E 84 040301
[11] Fily Y and Marchetti M C 2012 Phys. Rev. Lett. 108 235702
[12] Bislett J, Löwen H and Speck T 2013 EPL 103 30008
[13] Hanke T, Weber C A and Frey E 2013 Phys. Rev. E 88 052309
[14] Hiraoka T, Shimada T and Ito N 2016 Phys. Rev. E 94 062612
[15] Haas P and Gilmour D 2006 Dev. Cell 10 673–680
[16] Cetera M, Ramírez-San Juan G R, Oakes P W, Lewellyn L, Fairchild M J, Tanentzapf G, Gardel M L and Horne-Badovinac S 2014 Nat. Commun. 5 5511
[17] Helbing D, Buzna L, Johansson A and Werner T 2005 Transp. Sci. 39 1–24
[18] Dzubiella J, Hoffmann G P and Löwen H 2002 Phys. Rev. E 65 021402