Spontaneous stable rotation of flocking active swarms

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Cluster rotation discussed in many active matter systems, as interpreted by many existing theoretical models, is transient. Yet in nature there exists spontaneous stable rotation of cluster in many active swarms such as flocking worms or sheep. In this paper we present a four-node flexible worm model to study the collective motion of two-dimensional active worms, and confirm that there exists a spontaneous stable rotation of clusters synchronized with a chirality produced by the flexibility under the impetus of the active force. The angular velocity of such a rotation is found to be generated via a competition between the individual flexibility, the diffusion coefficient, the cluster size and the active force. The conclusions well explain the spontaneous stable rotation of clusters that exists in many flexible active matters, like worms or sheep, once flocking together.

I. INTRODUCTION

Since the publication of the Vicsek model [1], studying the collective motion of self-propelled agents has become an important topic in physics [2–5]. Emergence of rotating structures from the collective motion of active agents is a fascinating phenomenon observed in nature, from swimming bacteria in the micro-meter scale [6–9], to flocks of worms [10], processory caterpillars [11], ants [12], tadpoles [13], daphnias and fish in the meters scale [14–17]. Such an emergent collective rotation is typically associated with confined geometry [18–20]. In a dense suspension of active particles, if alignment interaction exists, a vortex structure is favored to maximize the entropy[21]. Rotational motion was also common in synthetic systems made of magnetic or dielectric colloidal particles.

By introducing one or a group of flexible structures into the matrix of active matters, the flexible structure can demonstrate spontaneous stable rotation. It was reported that an aster-like structure with flexible arms placed in the matrix of self-propelled particles, the arms can bend and form a spiral structure and spontaneously rotate under the collective collision of the active particles [22]. When placing long bacteria in a bath of short bacterial, the long bacteria were found to fold themselves under the collision of the short bacteria, and wrap around into a clockwise or anticlockwise coil, or double coils with both types [23]. In these studies, the rotation of a large flexible structure is typically associated with chiral symmetry breaking due to its interaction with a population of small hard particles. Introducing external field is another way to produce rotational motion. In the presence of an alternating electric field, experiments found that spherical particles with dipole moment can be self-propelled and form a transient/stable rotating cluster [24–26]. Similar phenomena were also observed with magnetic rollers [27–30]. Hydrodynamic interaction plays an important role in vortex formation in these artificial roller systems.

If the active particles are intrinsically chiral, the large-scale rotation exhibits novel phenomena[31]. For instance, a collection of self-spinning particles can form topologically protected edge flows that circulate around the boundary[32, 33]. Simulations have found that such a dense suspension of L-shaped particles exhibits a chirality-triggered oscillation phase, in which transient vortex is assembled and disassembled in a periodic manner [34].

In nature, even flexible individual agents that are achiral in their natural form, like worms [10], ants [12], can spontaneously form a stable rotating cluster once flocking together even under no spatial constraints in the absence of hydrodynamic interactions. Vortex structure has been observed in colonies of bacteria due to the alignment pressure generated by dividing cells in a crowded environment [35–39]. However, the current existing models for active matter, which can only generate transient rotation of clusters, fail to explain such a stable rotation. The mechanism that how a group of achiral active particles form a stable rotating cluster spontaneously without any spatial confinement and hydrodynamic interactions remains to be elucidated.

In this paper, as a theoretical attempt, we present a four-node flexible worm model to study the collective motion of a group of achiral but flexible particles. It is found that a spontaneous stable rotation of the cluster can be generated as a result of the self-organization of the flexible worms into a chiral structure.

II. MODEL OF CHAIN-LIKE ACTIVE WORMS

Our model is designed to simulate the collective motion of chain-like active worms. Each worm consists of 4 spheres (nodes) of radius r = σ connected by harmonic
springs, as shown in Fig. 1. A total number of $N$ worms are placed in a square of length $L$ with periodic boundary conditions implemented at the four edges. The overdamped dynamic equation of the worm’s four nodes is given by

$$\xi \partial r_{i,\alpha}/\partial t = \delta_{i,\alpha} f_i(N_i) p_i - \nabla r_{i,\alpha}(E_{i,\alpha}^r + E_{i,\alpha}^b + E_i^s),$$

(1)

where $\xi$ is the viscosity coefficient, and $i,\alpha$ denotes the position of the $\alpha$-th node in the $i$-th worm. Hereafter, the Roman letters and the Greek letters are used to label the worm and the node in the worm, respectively. The first term on the right hand side of Eq. (1) is the active force with its magnitude $f_i$ inversely proportional to the number $N_i$ of the surrounding nodes within a circle of a cutoff radius $R_c$,

$$f_i = f_{\text{max}}/N_i.$$  

(2)

Here $f_{\text{max}}$ denotes the maximum active force generated by the worm head, i.e., the first node. The direction $p_i$ of the active force is the unit vector pointing from tail to head, i.e.,

$$p_i = \frac{r_{i,1} - r_{i,4}}{||r_{i,1} - r_{i,4}||}.$$  

(3)

The second term describes the interaction force between nodes. The steric interaction between node $\alpha$ in the $i$-th worm and node $\beta$ in the $j$-th worm is described by the repulsive energy $U_{WCA}(r_{i,\alpha}^{j,\beta})$ with a distance $r_{i,\alpha}^{j,\beta} = ||r_{i,\alpha} - r_{j,\beta}||$ between them. Here $U_{WCA}(r)$ is the Weeks-Chandler-Anderson (WCA) potential energy given by

$$U_{WCA}(r) = \begin{cases} 4\varepsilon([\sigma/r]^{12} - [\sigma/r]^{6}) + \varepsilon, & r < 2^{1/6}\sigma \\ 0, & \text{otherwise}, \end{cases}$$

(4)

where $r = 2^{1/6}\sigma$ is a cutoff length, and $\varepsilon$ is the strength of the steric interaction. The total steric energy experienced by the $\alpha$-th node in the $i$-th worm reads

$$E_{i,\alpha}^s = \sum_{j=1}^{N} \sum_{\beta=1}^{4} U_{WCA}(r_{i,\alpha}^{j,\beta}).$$

(5)

Note that the summation here should exclude the term when $i = j$ and $\alpha = \beta$ simultaneously hold. To describe the flexibility of the worm, we introduce the bending energy of the $i$-th worm as

$$E_i^b = \lambda(s_{i,1} \cdot s_{i,2} + s_{i,2} \cdot s_{i,3}),$$

(6)

where $s_{i,\alpha} = (r_{i,\alpha} - r_{i,\alpha+1})/||r_{i,\alpha} - r_{i,\alpha+1}||$ denotes the orientation of $\alpha$-th segment in the worm and $\lambda$ denotes the bending stiffness of the worm. The harmonic elastic energy accounting for the bond connecting two neighboring nodes in the $i$-th worm reads

$$E_i^s = \frac{k}{2} [(r_{i,1}^2 - r_0)^2 + (r_{i,2}^2 - r_0)^2 + (r_{i,3}^2 - r_0)^2],$$

(7)

where $k$ is the elastic constant, and $r_0$ is the equilibrium length of the bond.

In our simulations, to describe the rotation of the cluster, we define an angular velocity

$$\omega = \frac{1}{N} \sum_{i=1}^{N} \frac{\arcsin|q_i(t) \times q_i(t + \delta t)|}{\delta t},$$

(8)

where

$$q_i = \frac{r_i - r_c}{||r_i - r_c||}.$$  

(9)

is the unit orientation vector pointing from the position of the $i$-th worm $r_i = \sum_{\alpha=1}^{4} r_{i,\alpha}/4$ to the geometric center of all the worms

$$r_c = \frac{1}{N} \sum_{i=1}^{N} r_i.$$  

(10)

Meanwhile, we also introduce a chirality parameter

$$c = \frac{\sum_{i=1}^{N} (r_i - r_c) \times p_i}{N}$$

(11)

to describe the spiral structure of cluster. For a cluster with all the worms precisely oriented towards the center, the chirality $c$ vanishes.

| Table I. Parameters used in simulations |
|---------------------------------------|
| Variable   | Meaning                      | Typical value | Range              | Unit |
| $\lambda$  | Bending stiffness            | 0.25          | [0, 2]             | $\varepsilon/\sigma$ |
| $D$        | Diffusion coefficient        | $10^{-6}$     | $[10^{-6}, 10^{-4}]$ | $\varepsilon/\xi$ |
| $N$        | Number of worms              | 80            | [80, 168]          | –    |
| $f_{\text{max}}$ | Maximum active force         | 5             | –                  | –    |
| $R_c$      | Cutoff radius                | 6             | [5, 80]            | $\varepsilon/\sigma$ |

### III. RESULTS AND DISCUSSIONS

We start our simulations with a configuration formed by worms strictly positioned along a series of concentric circles with their orientation $p_i$ all pointing radially towards the circle center. The parameters used in our simulations are shown in Table I. It is found that as time evolves, both the angular velocity $\omega$ and the chirality $c$
reach a plateau quickly, and synchronizing as well, as shown in Fig. 2. During this process, a rotating cluster is formed with its constituent worms bending their body either clock-wisely or counter-clock-wisely in a synchronizing way to form a spiral structure (insets in Fig. 2). The simulations were repeated for 144 times and each simulation ends up with a different angular velocity $\omega$ and a chirality $c$ due to the randomness of the dynamics.

Figure 3 shows the correlations between angular velocity and chirality, and their corresponding probability distribution functions (PDFs) by changing one parameter while fixing others as listed in Table I. It is found that the scatter plots of $(c, \omega)$ at steady state fall into a single straight line regardless of the bending stiffness $\lambda$ (Fig. 3 (a) left). The PDFs for the angular velocity $\omega$ and the chirality $c$ with a kernel-density-estimation method demonstrates a bimodal distribution with two peaks almost symmetrically located with respect to 0. The absolute peak positions for $\omega$ and $c$ are both found to decrease with increasing $\lambda$ (Fig. 3 (a) middle and right), indicating that the cluster formed by flexible worms rotates faster than that formed by rigid worms due to the chirality of the individual structure created by bending.

Besides the individual mechanical feature, we also explore the influence of diffusion on the angular velocity of the cluster. As shown in the left figure of Fig. 3, all the $(c, \omega)$ points at steady state, once again, collapse into a single straight line for different diffusion coefficients. The absolute peak positions of the bimodal histogram distributions for chirality $c$ and angular velocity $\omega$ slightly increase even by increasing diffusion coefficient $D$ two orders of magnitude each time (Fig. 3 (b) middle and right). This is reasonable because a larger diffusion coefficient $D$ gives more room for the worms to bend their bodies so as to become more chiral structurally.

By varying the total number of worms $N$, we find that a larger $N$ results in a smaller slope of the straight line in the $(c, \omega)$ plane (Fig. 3 (c) left), obeying
\[
\frac{\omega}{c} \propto N^{-1}.
\] (12)

This can also be confirmed by the absolute peak positions in the histogram of $\omega$ and $c$ (Fig. 3 (c) middle and right), which show opposite dependence on the worm number $N$, i.e., increasing the worm number $N$ enhances the chirality $c$, but reduces the angular velocity $\omega$. This arises from the fact that in the definition of the chirality $c$, a larger $r$ in the summation contributes to a larger $c$. A larger number of worms tend to form a larger cluster which has a larger chirality $c$.

In a similar way, it is found that increasing the maximum active force $f_{\text{max}}$ will proportionally increase the slope of the $(c, \omega)$ straight lines at steady state, i.e.,
\[
\frac{\omega}{c} \propto f_{\text{max}}.
\] (13)

The PDF for the chirality $c$ is slightly dependent of the the active force $f_{\text{max}}$, a behavior quite different from that of the angular velocity $\omega$. As shown in the right figure of Fig. 3(d), with the increase of $f_{\text{max}}$, the PDF becomes more dispersed as the absolute peak positions of angular velocity increase.

By summarizing all the results above and using dimensional analysis, we obtain an empirical formula for the slope of the $\omega$-$c$ curve,
\[
\frac{\omega}{c} = A \frac{f_{\text{max}}}{R_c^2 \xi N},
\] (14)
where $A$ is a dimensionless prefactor determined roughly as 1/7 by fitting the data. To rationalize this empirical formula, we propose a simplified model (see the APPENDIX) by assuming that the density of worms in the cluster is a constant and the cluster performs a rigid body rotation. The angular velocity $\omega$ is determined by a torque balance between the active part and the dissipative part (see the Appendix). The prefactor $A$ turns out to be equal to 1/8 in the simplified model. The tiny difference between the empirical value and the analytical value is due to the fact that in the simplified model the number of worms $N_c$ within the cutoff radius $R_c$ is assumed to be a constant, but in the simulations, the worms near the boundary apparently have less neighbors than those do in the central parts. A comparison between the empirical formula (14) and the analytical model in the APPENDIX shows an excellent agreement (Fig. 4).

To check out the influence of the initial orientational distribution, we let each worm in its initial state be randomly oriented within a angle range of $[-\pi/8, \pi/8]$. As expected, we still see the linear relationship between angular velocity and chirality, as shown in Fig. 5.

The spiral structure formation in our model is due to the alignment interaction between worms as a result of the steric interactions between the nodes. When two chain-like worms collide, they tend to align their bodies in the same direction. Given the initial condition we impose, the worms tend to tilt their directions in
Figure 3. Scatter plots of $\omega - c$, and probability distribution functions PDF $- c$ and PDF $- \omega$ at steady state as a result of repeated simulations for different (a) stiffness $\lambda$, (b) diffusion coefficient $D$, (c) number of worms $N$, and (d) maximum active force $f_{\text{max}}$. The straight lines in $\omega - c$ plots denote the fitting results.

The same manner (clockwise or anti-clockwise) while they move towards the center, thus forming a spiral structure in which all the worms have their tail-to-head direction $p_i$ deviate from pointing towards the center $r_i - r_c$. In this way, the active force $f_i p_i$ generates an active torque $(r_i - r_c) \times (f_i p_i)$, which in turn rotates the cluster. We stress that the flexibility of the worm plays an important role but not an essential role in generating spontaneous rotation. A soft worm can generate a faster rotation because a worm can bend its body more, such that the tail-to-head direction $p_i$ has a larger deviation from $r_i - r_c$, thus generating a larger torque. However, even the worm is exactly straight, the alignment interaction still holds and spontaneous rotation still exists. This effect can be used to make soft rotation for the robot swarm, a swarm pattern of the drone swarm, or even microbial devices, using microorganisms. It also provides a possible explanation for the vortex, turbulence, under the microbial...
IV. CONCLUSIONS

In summary, in this paper we present a model to study the collective motion of chain-like worms. Our model differs from previous studies in the direction of the active force, which is chosen to point from tail to head rather than one undergoing Brownian rotation in the traditional ABP models. Our choice of the active force direction reflects certain intelligence of the worm that actively tunes its direction based on the geometry of the worm itself, instead of being indecisively influenced by its neighbors as assumed in the classical Vicsek model [1]. A steady rigid-body-like rotation of the cluster is observed to be synchronized with the formation of a spiral structure, which well explains the spontaneous stable rotation existing in nature formed by worms or sheep, once flocking together. The three important factors that influence the stable rotation are the active force, stiffness, and active force related to the body orientation. The active force provides the driving element for the cluster, which turns out to become an inherent angular momentum due to its chirality generated by flexibility and collectively enhanced by alignment interaction between worms. The application of spontaneous stable rotation under the microbial system has always been a presence to be excavated. It also provides new insights into rotational ordering in soft matter systems: bending stiffness produces chirality, and initiation in active systems leads to spontaneous stable rotation.

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VI. APPENDIX

A. Kernel density estimation

We use the kernel density estimation (KDE) method to calculate the probability density function (PDF) of the angular velocity $\omega$ and the chirality $c$. The idea is to regard each sampling as a kernel function $K(x)$, and obtain the PDF through the superposition of the kernel functions

$$f(x) = \frac{1}{Nh} \sum_{i=1}^{N} K\left(\frac{x - x_i}{h}\right),$$

where $1/Nh$ is the normalization factor, $x_i$ is the data of the $i$-th experiment, $N$ is the total number of experiments, and $h$ is the window width. Here $h = 1.06\eta N^{-1/5}$ is chosen by the rule of thumb, where $\eta$ is the standard deviation of all experimental data and $N_{exp}$ represents the number of repeated simulations. In order to make the estimated function smooth, the standard normal distribution function is used as the kernel function $K(x)$.

When we apply KDE to the entire data set of $\omega$ which typically demonstrates a bimodal distribution, the fitting PDF is much wider than the true distribution around each peak. We therefore apply KDE to the positive $\omega$ and...
negative \( \omega \) separately and combine the two distributions to form the final PDF based on the ratio of the two data sets.

**B. A simplified rigid-body rotation model**

In the simulation, we observe that when the cluster rotates, the relative positions of the worms are almost unchanged and the rotation can be approximated as a rigid body rotation. The movement of each worm therefore obeys

\[
\dot{r}_i = \omega \times r_i ,
\]

where \( z \) is the unit vector pointing to the \( z \)-axis perpendicular to the motion plane. The force balance equation of each worm in the cluster reads

\[
4\xi \dot{r}_i = F_i^\alpha ,
\]

where \( 4\xi \dot{r}_i \) is the damping force of the 4 nodes in a worm and \( F_i = (f_{\text{max}}/N_i)p_i \) is the active force generated by the head node. By substituting Eq. (16) into Eq. (17) and taking the cross product of both sides with \( r_i \), we obtain

\[
\omega = \frac{\sum_{i=1}^{N} r_i \times (f_{\text{max}}/N_i)p_i}{\sum_{i=1}^{N} 4\xi \dot{r}_i^2} = \frac{M}{\Gamma} .
\]

Assuming the worm density of the cluster is a constant \( \rho \), the number of nodes within the cutoff radius is \( N_i = 4\pi \rho R_i^2 \), where the prefactor 4 comes from the 4 nodes in a worm. The nominator \( M \) in Eq. (18) represents the active torque and can be reduced to

\[
M = \frac{cN f_{\text{max}}}{4\pi R_c^2 \rho} .
\]

The denominator \( \Gamma \) in Eq. (18) represents the dissipative torque. We replace the summation \( \sum_{i=1}^{N} \) with the integral \( \rho \int_0^R 2\pi rd \) and find

\[
\Gamma = \int_0^R 8\pi \xi \rho \omega^2 dr = 2\pi \xi \rho R^4
\]

Using the equation \( \rho R^2 = N \) to replace \( R \) in Eq. (20), we obtain Eq. (14) in the main text.

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