Letter

Soliton-like behavior of traveling bands in self-propelled soft particles

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We have found through numerical simulations of interacting self-propelled deformable particles in two dimensions that traveling bands of ordered state are not destroyed upon a head-on collision just like solitons in integrable systems. Quite recently, Kuwayama and Ishida have reported experiments of non-chemotactic Dictyostelium discoideum mutants in which density waves of migrating cells exhibit a soliton-like behavior upon collision. We investigate properties of the traveling bands to clarify the similarities and differences between the theoretical and experimental results.

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1. Introduction

The dynamics of interacting self-propelled particles have been studied for almost two decades since Vicsek et al. published a seminal paper [1]. Theories based on a particle picture and coarse-grained hydrodynamic approaches [2] have been developed—see, for example, the review articles [3,4]. Numerical simulations of the Vicsek-type model of point particles have revealed non-equilibrium transitions of the system from a disordered state to an ordered state by increasing the particle density and/or decreasing the intensity of random noise. In a fully ordered state, all the particles travel coherently in a certain direction at a constant velocity as average. However, Chaté and his coworkers [5] have found by numerical simulations of the Vicsek-type point particles that the homogeneous ordered state is not stable near the discontinuous order–disorder transition point. Thin traveling bands inside which particles are dense and ordered evolve in a matrix of the disordered low density state. Properties of traveling bands have also been investigated by hydrodynamic formulations [6,7] and by a kinetic description [8]. Experimentally, traveling concentration waves have been observed in dense actin motility assay [9].

The inhomogeneous dynamical state is one of the characteristic features in out-of-equilibrium systems since such a state does not exist in phase transitions in equilibrium. Therefore, investigation of traveling bands is of fundamental importance in elucidating transitions far from equilibrium. In our previous paper [10], we reported the collective dynamics of deformable self-propelled particles with a Gaussian soft potential and found that, if we impose a condition that the migration velocity of each particle is an increasing function of local density around the particle, traveling bands as observed...
in point particles are easily formed spontaneously. Furthermore, we found a remarkable property that those bands survive collisions just like solitons in integrable systems. These are obtained by numerical simulations in two dimensions.

Interestingly, quite recently, an apparently similar phenomenon has been reported by Kuwayama and Ishida [11] in experiments of non-chemotactic Dictyostelium discoideum mutants in which propagating density waves emerge spontaneously on a substrate and behave like solitons upon collision. The purpose of the present article is to compare our theoretical results and the experimental ones to elucidate the properties of such robust waves.

This paper is organized as follows. In the next section, we explain our model equations. The results of numerical simulations in two dimensions are presented in Sect. 3. Comparison with the experiments is given in Sect. 4, and discussion of the findings is presented in Sect. 5.

2. Time-evolution equations

The time-evolution of the $i$th particle is represented in terms of the position of the center of mass $r^{(i)}$, velocity $v^{(i)}$, and deformation tensor $S^{(i)}$. We consider the coupled set of equations in two dimensions [12,13],

\[ \frac{d}{dt} r^{(i)} = v^{(i)}, \]

\[ \frac{d}{dt} v^{(i)}_\alpha = \gamma v^{(i)}_\alpha - (\vec{v}^{(i)})^2 v^{(i)}_\alpha - a S^{(i)}_{\alpha\beta} v^{(i)}_\beta + f^{(i)}_\alpha, \]

\[ \frac{d}{dt} S^{(i)}_{\alpha\beta} = -\kappa S^{(i)}_{\alpha\beta} + b \left( v^{(i)}_\alpha v^{(i)}_\beta - \frac{1}{2} v^{(i)}_\nu v^{(i)}_\nu \delta_{\alpha\beta} \right), \]

where $\kappa$, $a$, and $b$ are positive constants. The coefficient $\gamma$ depends on the local density, which will be explained below. The deformation tensor is defined by

\[ S^{(i)}_{\alpha\beta} = s^{(i)} \left( n^{(i)}_\alpha n^{(i)}_\beta - \frac{1}{2} \delta_{\alpha\beta} \right), \]

where $s^{(i)}$ denotes the magnitude of deformation around a circle shape and $n^{(i)}$ is the unit vector along the long axis of an elliptically deformed particle. The set of equations (2) and (3) without the $f^{(i)}$ term were introduced for isolated deformable particles in Ref. [14]. The force $f^{(i)}$ acting on the $i$th particle takes the form

\[ f^{(i)} = K \sum_{j=1}^{N} F_{ij} Q_{ij}, \]

where $K$ is a positive constant, $N$ is the total number of particles, and

\[ F_{ij} = -\frac{\partial U(r_{ij})}{\partial r_{ij}}, \]

with $r_{ij} = r^{(i)} - r^{(j)}$. We employ a Gaussian soft potential for $U(r_{ij})$:

\[ U(r_{ij}) = \exp \left[ -\frac{r_{ij}^2}{2\sigma^2} \right]. \]

The other factor $Q_{ij}$ in eq. (5) represents an alignment mechanism of the particles and is given in two dimensions by

\[ Q_{ij} = 1 + \frac{Q}{4} \left[ (s^{(i)} - s^{(j)})^2 + 4s^{(i)}s^{(j)} \sin^2(\theta^{(i)} - \theta^{(j)}) \right]. \]
where the angle $\theta^{(i)}$ is defined through $n^{(i)} = (\cos \theta^{(i)}, \sin \theta^{(i)})$. This indicates that the repulsive interaction is weak when two elongated particles are parallel to each other compared to the case where they are perpendicular.

The coefficient $\gamma$ takes the form [10],

$$\gamma(\rho^{(i)}) = \gamma_0 + \gamma_1 \left( \frac{\rho^{(i)}(t)}{\rho_*} - 1 \right),$$

where the constants $\gamma_0$, $\gamma_1$, and $\rho_*$ are positive. Throughout the present paper, we fix $\rho_*$ as $\rho_* = 0.06$.

The local density $\rho^{(i)}(t)$ is defined by the number of the particles around the $i$th particle within the distance $R_D$. Experiments in swimming bacteria have shown that the average migration velocity increases with density [15]. In the opposite case that the migration velocity decreases with local density, traveling bands do not exist [16].

3. Numerical results

Equations (1), (2), and (3) are solved numerically in a rectangular area under periodic boundary conditions. In what follows, we show the results for the parameters $\kappa = a = \sigma = 1$, $b = 0.5$, $K = R_D = 5$, and $Q = 50$. The average density $\rho_0$ is defined by $\rho_0 = N/(L_x L_y)$, where $L_x$ and $L_y$ are the linear dimensions of a rectangular system, and is fixed as $\rho_0 = 6.00 \times 10^{-2}$ with $N = 8192$, $L_x = 640$, and $L_y = 213.33$. That is, we consider the case $\rho_0 = \rho_*$. The leap-frog method [17] is used for numerical integration with the iteration time step $\Delta t = 1/64$.

In order to quantify the degree of order, we have evaluated the order parameter defined by

$$\Phi = \left| \frac{1}{N} \sum_{j=1}^{N} e^{2\pi i \theta^{(j)}} \right|. $$

This is an apolar order parameter. One may define a polar order parameter by using the migration velocity [13]. When two bands with the same size are traveling in opposite directions, the apolar order parameter $\Phi$ is finite while the polar order parameter is equal to zero and it is impossible to distinguish the traveling state from the uniform disordered state.

We have solved the time-evolution equations for fixed values of $\gamma_0$ and $\gamma_1$ starting from random initial conditions, and have checked whether the system becomes ordered or not [10]. When $\gamma_0 = 0.5$ and $\gamma_1 = 0$, the system reaches a homogeneous ordered state asymptotically in time. By increasing $\gamma_1$, the magnitude of $\Phi$ decreases and eventually the system becomes disordered for $\gamma_1 > 1.5$. The homogeneous ordered state does not appear for $0.7 < \gamma_1 < 1.5$. Many thin traveling domains of the high density ordered state grow by absorbing the surrounding particles. The accumulated particles in the front area move laterally due to the high pressure in the accumulated region. As a result, the domains are elongated perpendicularly to the traveling direction. The domain size in the lateral direction eventually becomes comparable to the shorter system size $L_y$. Then each domain constitutes a band traveling along the $x$-axis. Thicker bands grow further at the expense of thinner bands since the traveling velocity of a thicker band is larger than that of a thinner one. When the bandwidth becomes too large, orientational fluctuations are excited in the rear region of the band and these strong fluctuations or random waves cause splitting of the band, emitting a daughter band traveling in the opposite direction.

Traveling bands produced in this way undergo head-on collisions with other bands because of the periodic boundary conditions. Surprisingly, these bands are very robust. Particles in a band are
Fig. 1. Snapshots of a pair of colliding traveling bands at (a) \( t = 5865 \), (b) \( t = 5905 \), (c) \( t = 5945 \), and (d) \( t = 5985 \). The bars represent elongated particles. The arrows indicate the propagating directions. The dot shows the location of a tagged particle.

disturbed during a collision but the band is not destroyed completely and survives the collision. Furthermore, a smaller band increases its width during collision so that a pair of bands traveling in opposite directions become a comparable size after several collisions. Snapshots during a collision are displayed in Fig. 1. The location of a tagged particle is also indicated by the black dot. Clearly, the individual particles follow the traveling bands only transiently and are left behind, indicating that the traveling bands are a kind of compressional wave.

We have carried out numerical simulations in a rectangular system whose size along the \( x \)-axis is much larger than the bandwidth to eliminate finite size effects. The results described in this section, that is, formation of traveling bands and their soliton-like behavior, are also obtained in a square system with a sufficiently large system size.

4. Comparison with experiments

We compare our numerical results obtained in the preceding section with the experiments on non-chemotactic Dictyostelium discoideum mutants [11]. When these cells are put in a starved condition on a substrate, density waves or high-density band-like structures elongated perpendicular to the propagating direction are spontaneously formed, and move around—see Fig. 1b in Ref. [11]. A pair of waves traveling in opposite directions can be seen in Fig. 2. The bandwidth is of the order of 100 \( \mu m \), which is much larger than the cell size. Figure 2 shows a head-on collision of two waves. Clearly, the waves do not undergo pair-annihilation upon collision. We note, however, that the waves after collision at \( t = 180 \) min are thinner than those at \( t = 0 \) min. According to the authors of Ref. [11], the reason is that the cells in the experiments in Fig. 2 were in a starved condition for a long period. Collisions of more vital cells and waves can be seen in Supplementary Video S12 or in the initial period of Supplementary Video S3 in Ref. [11].

Kuwayama and Ishida call the waves biological solitons. Since the traveling velocity of the waves is about twice as large as that of the individual cells, the waves catch up the dispersed cells in the front area and leave the cells at the rear. This is essentially the same behavior as happens in our traveling bands. The cell density inside the waves is about two or three times higher than that in the surrounding matrix, indicating that cells in a wave overlap each other. Since our model is two-dimensional, direct comparison is not possible, but the ratio of the density inside an isolated band to that of the outside disordered state is about 2.5 for the present set of parameters.
Fig. 2. Collision of the density waves. This is reproduced, with permission, from Fig. 1c in Ref. [11].

We have introduced an alignment mechanism as Eq. (8) such that the magnitude of the repulsive interaction depends on the relative angle of the elongation directions of two particles. In the experiments, on the other hand, the mutants have a strong adhesion at the head and the tail so that they constitute necklace-like structures which may be regarded as semi-flexible self-propelled rods—see Fig. 5a in Ref. [11]. This means that the aspect ratio $\alpha$ of the migrating object, defined by the width divided by the length, is effectively small, which can be $\alpha \approx 0.13 \sim 0.3$ depending on the cell number constituting a necklace structure. On the other hand, the aspect ratio in our deformable particles is much larger, about $\alpha \approx 0.79$ in a traveling band, which was obtained from the averaged value $s = \langle s^{(i)} \rangle \approx 0.23$. In this derivation, we have used the definition $\alpha \equiv (2 - s)/(2 + s)$ for an elliptically deformed particle.

As mentioned above, both the traveling bands in our model system and the waves in the living cells exhibit soliton-like behavior upon collision. However, there are differences in the behavior of individual objects during a collision, as illustrated in Fig. 3. In our model, a particle in the band traveling to the left before collision, as in Fig. 3(a), stays either (b) in the middle area or (c) in the band traveling to the right just after the collision. Of course, the configurations (c) and (d) are transient. As the band moves further, the tagged particle is left behind. Similar analysis is possible experimentally by using red fluorescent protein-expressing cells [11]. The experiments show that the cases (c) and (d) are observed with almost equal (50%) probability [11]. In our numerical simulations, the case (d) is quite rare. This is the most distinct difference between the experiment and the theory.

One of the origins of the abovementioned difference is probably due to the difference in the aspect ratio. Self-propelled slender rods propagating in opposite directions can interpenetrate upon collision without changing their traveling directions. In other words, they constitute lanes [18]. Particles with larger aspect ratio, as in our model, have a larger impact parameter and hence they easily change the magnitude and direction of the velocity upon collision. In fact, the picture of interpenetration of the living cells during a collision of waves is not inconsistent with the experimental observation (H. Kuwayama and S. Ishida, unpublished). Extension of the present model to particles with smaller aspect ratios [19] to study the dynamics of traveling bands is an interesting future problem.
Fig. 3. Possible positions of a tagged particle (dot) which is in the right band before collision: (a). (b)–(d) illustrate three possible configurations just after collision. The arrows indicate the traveling direction of the bands.

5. Discussion

We have shown that traveling bands in deformable self-propelled particles with a Gaussian repulsive soft potential and with density-dependent migration velocity exhibit a soliton-like behavior upon collision. As far as we are aware, non-destruction of traveling bands upon collision, as shown here and in Ref. [10], has not been reported in any other theoretical studies of self-propelled objects. We have found that two bands survive a head-on collision but, when a large band catches up a smaller band moving in the same direction, only the larger band survives upon collision, absorbing the smaller one. It is noted that the Galilean invariance does not hold in our model system.

In Sect. 3 we described the splitting of a traveling band. This is a quite rare event. It seems that a band with an extremely large width is unstable and a daughter band is emitted from the tail. However, the mechanism for this phenomenon is unclear at present. Soliton-like behavior has also been confirmed for head-on collisions which are realized by setting two bands traveling in opposite directions as an initial condition.

There are several properties which are necessary for the robustness of traveling bands. First of all, the fact that the set of Eqs. (1), (2), and (3) is non-variational is definitely responsible. Second, we expect that the soft potential in Eq. (7) is a favorable factor for the soliton-like behavior since it does not totally exclude overlapping of particles. Third, we introduced the local density dependence of the migration velocity as Eq. (9). If this condition is removed, traveling bands as observed in Vicsek-type particles [5] do not appear in the present model in the absence of stochastic noise [13]. Therefore, we expect that the third condition is mostly relevant to the robust traveling bands. On the other hand, it is unclear at present whether or not the deformability is a necessary condition for the preservation of bands. Further investigations are necessary to clarify the origin of the soliton-like behavior of traveling bands and to compare with the biological solitons revealed in the living cells.

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