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Aggregation of Flexible Chainlike Walkers in Off-Lattice Space

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Abstract: Two-dimensional off-lattice behavior of chainlike self-driven objects is numerically studied. The objects undergo spontaneous, irreversible aggregation, irrespective of their deformability, in contrast with the on-lattice case in which aggregation is observed only when the objects are deformable. Also, we found that the tendency of aggregation increases with the decrease in the degree of deformability of each object or with the increase in the degree of fluctuation.

Keywords: **s**elf-driven objects, multi-body system, simulation.

1. Introduction

Multi-body systems of self-driven objects have attracted considerable attention of researchers, and vast knowledge has been accumulated [1]. In most of the previous studies, each object has been mimicked by a point-like particle (with minimal excluded-volume effect), or at most by a rigid body (with size/shape effects). Numerical simulations based on the flexible chainlike walker (FCW) model [2] elucidated that the deformability of each object causes peculiar collective motions, such as the spontaneous, irreversible aggregation [2], freezing transition to a completely jammed state [3], and flow enhancement by a countercurrent [4]. Here we extend the FCW model and perform numerical simulations to study the collective behavior of FCWs in an off-lattice space.

2. Model and Simulation

An FCW of length l is modeled as l serially concatenated particles of diameter 1. Representing the position vector of ith particle as $\boldsymbol{r}_i$ $(1 \le i \le l)$, the relative position vector between adjacent particles is given by $\boldsymbol{d}_i = \boldsymbol{r}_{i-1} - \boldsymbol{r}_i$ $(i \ge 2)$, where $|\boldsymbol{d}_i| = 1$ (Fig. 1(a)). The movement of an FCW at one time unit $t \to t+1$ is executed in two steps as follows.

First, the head particle ($i = 1$) moves from $\boldsymbol{r}_1$ to $\boldsymbol{r}_1' = \boldsymbol{r}_1 + \boldsymbol{d}_1$, where the displacement vector $\boldsymbol{d}_1$ is randomly determined so that the angle θ between $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$ should satisfy $|\theta| \le \theta_{max}$, with θ_{max} being a control parameter. The following particles ($i \ge 2$) move to the previous positions of the previous particles, $\boldsymbol{r}_i' = \boldsymbol{r}_i + \boldsymbol{d}_i = \boldsymbol{r}_{i-1}$, and now the new relative position vector is given by $\boldsymbol{d}_i' = \boldsymbol{r}_{i-1}' - \boldsymbol{r}_i'$ (Fig. 1(b)). If the head particle at the new position $\boldsymbol{r}_1'$ overlaps another particle, the FCW does not move at this time step. It is clear that deformability is introduced if and only if $l \ge 3$. In the on-lattice model [2], the position of each particle was limited to a lattice point, with θ being an integral multiple of $\pi/2$. Here in the off-lattice model, we allow the coordinates to take any real numbers. We define "flexibility" $F \equiv \theta_{max}/\pi$ $(0 \le F \le 1)$, as an index of the degree of deformation, where $F = 0$ and 1 correspond to the ballistic motion and fully random-walk-like motion, respectively.

As the second step, we introduce the fluctuation of the form, by rotating the vector $\boldsymbol{d}_i'$ $(i \ge 2)$ by an angle φ_i, with $|\varphi_i| \le \varphi_{max}$, to make a new vector $\boldsymbol{d}_i''$. Here the rotation is conducted sequentially from $i = 2$ to l, and skipped for i that would lead to overlapping of particles. The final positions of particles are given by $\boldsymbol{r}_1'' = \boldsymbol{r}_1'$ and $\boldsymbol{r}_i'' = \boldsymbol{r}_{i-1}'' - \boldsymbol{d}_i''$ $(i \ge 2)$ (Fig. 1(c)). The "perturbation" $P \equiv \varphi_{max}/\pi$ $(0 \le P \le 1)$ is defined as an index of the degree of fluctuation. Note that while F is related to the movement of the head particle, P is related to that of the following particles. If $P = 0$, the movement of the following particles are determined only by that of the head particle.

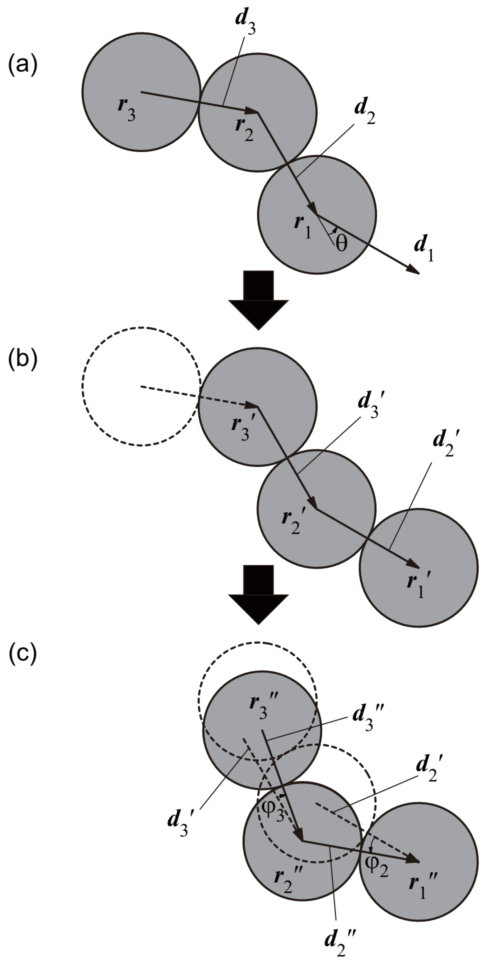

Figure 1. Movement of an $l = 3$ FCW.

The simulations are conducted as follows. At t = 0, N FCWs of length l are placed at random positions on a square of W (= 100) on a side with periodic boundaries. Each FCW is put straight (*i.e.*, $\boldsymbol{d}_2 = \cdots = \boldsymbol{d}_l$) but at a random direction. Then the FCWs are updated following the above-mentioned rule in a fixed order at every time step.

To describe the collective behaviors of FCWs, we define the density of particles by $\rho = lN/W^2$, corresponding to the on-lattice case [2]. Also, the mobility of FCWs at time t is defined as $M(t) = N_{\mathrm{mov}}(t)/N$, where $N_{\mathrm{mov}}(t)$ is the number of FCWs that have succeeded in moving at t.

3. Results and Discussion

3.1 Effect of Lattice Elimination

In general, the mobility M turned out to decrease with time, to an asymptotic value $M_\infty = M(t\rightarrow\infty)$. Typically, $t \sim 50000$ was enough for M to reach M_∞. In this paper, M_∞ is averaged over 50000 time steps in the asymptotic state (*e.g.*, t = 50001 - 100000) and typically over 30 simulation runs.

First, we show in Fig. 2 the plots of M_∞ as a function of ρ for the on-lattice case for comparison. The main results are as follows [2]. We see that the larger ρ, the less M_∞, which is quite intuitive. Also, we notice that the larger l, the less M_∞. For l = 1 and 2, linear relationship between M_∞ and ρ is observed, which agrees well with the theoretical predictions of $M_\infty = 1 - \rho$ for l = 1 and $M_\infty = (3/4)*(1 - \rho)$ for l = 2. For l = 3 and 4, a sharp drop from the higher-M_∞ state to the zero-M_∞ state can be seen, which suggests a transition from a moving state to an aggregated state at a critical density. And the critical density for l = 4 is smaller than that for l = 3. For $l \geq 5$, FCWs settle down in the aggregated state ($M_\infty \sim 0$) even when ρ is low. In our previous work [2], these results were explained in terms of the "mutual locking" of FCWs, which is possible only for deformable FCWs (*i.e.*, $l \geq 3$), and the aggregation mechanism was compared with that of the traditional models such as the diffusion-limited aggregation [5], ballistic deposition [6, 7], and the Eden model [8].

Next, we show in Fig. 3 the M_∞-ρ plots obtained in the off-lattice simulations for F = 0.5 and P = 0.0. We can see that the larger ρ, the less M_∞, and that the larger l, the less M_∞. Also, a sharp transition from the moving state to the aggregated state is observed for l = 3 and 4, while $M_\infty \sim 0$ is observed for $l \geq 5$. All these results are the same as in the on-lattice case. However, the results for $l \leq 2$ are remarkably different. The FCWs of $l \leq 2$ (without deformability) undergo the transition to the aggregated state (see Fig. 4), as the deformable FCWs of $l \geq 3$ do.

This is due to the difference in the situation of collisions of FCWs. Typical collision patterns of four l = 2 FCWs are illustrated in Fig. 5 for the on-lattice and off-lattice cases. In the on-lattice case, such patterns are only temporary, because some of the nearest-neighbor sites of the head particles are vacant and hence the FCWs can move again (Fig. 5(a)). Irreversible aggregation is possible only if FCWs are deformable, via mutual locking [2]. In the off-lattice case, however, the collision pattern can be unresolvable when the distance between the FCWs is small and the turning angle (*e.g.*, $|\theta| \leq \pi/2$ for F = 0.5) is not sufficiently large (Fig. 5(b)). Then the FCWs concerned cannot move again, which nucleates the spontaneous, irreversible aggregation.

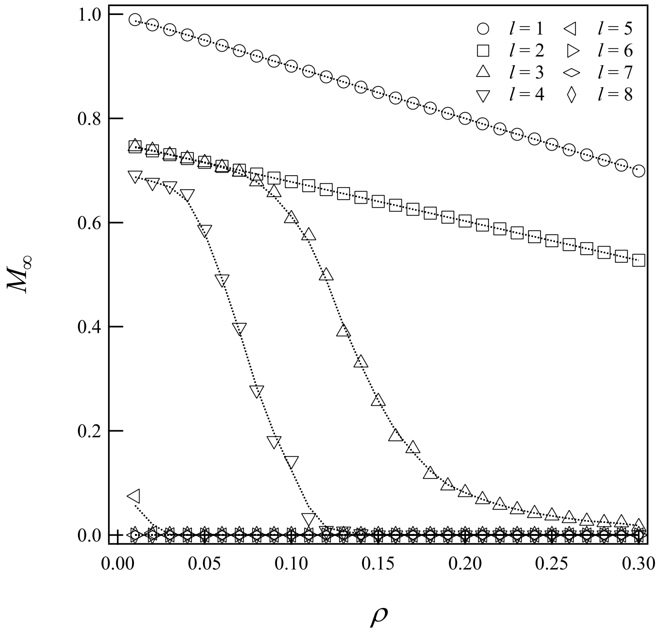

Figure 2. M_∞ as a function of ρ for l = 1-8 (on-lattice).

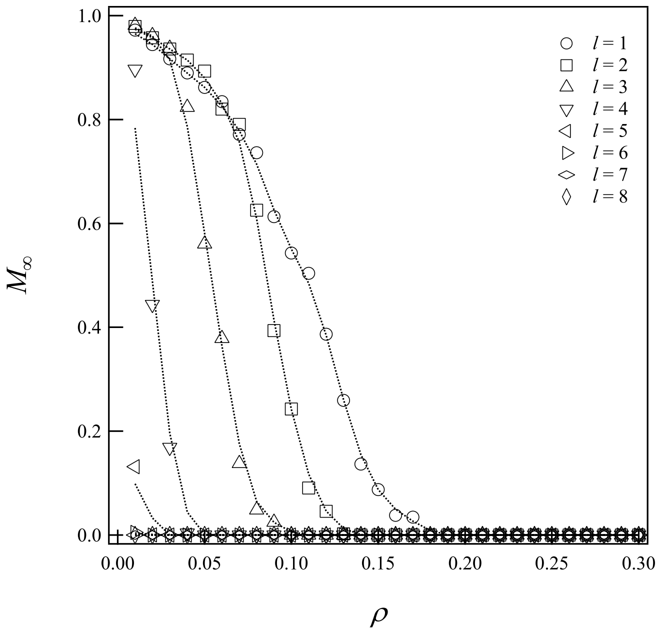

Figure 3. M_∞ as a function of ρ for l = 1-8 (F = 0.5, P = 0.0).

3.2 Effect of Flexibility *F*

Now we discuss the effect of the flexibility F on the mobility M_∞. As a typical result, we show in Fig. 6 the M_∞-ρ plots of l = 2 for different values of F with P = 0.0 (similar results are obtained for l = 1). For $F \leq 0.3$, we see that the FCWs settle down in the aggregated state even when the density ρ is low. This is because when F and thus the turning angle θ are small, the FCWs have less ability to get out of the above-mentioned collision patterns, and are easy to get trapped into the aggregated state. For F = 0.4 and 0.5, a sharp transition can be seen, which means that when ρ is low, aggregation is evaded because the FCWs become able to get out of the collision as F is increased. For $F \geq 0.6$, linear M_∞-ρ relationship is observed, which means that the aggregated state is avoided even for higher ρ. We also notice that M_∞ decreases as F increases in the range $F \geq 0.7$. This is because for $F \geq 2/3$ (*i.e.*, $\theta_{max} \geq 2\pi/3$), the movement of an FCW can be disabled by the overlap of its head particle at the tentative new position $\boldsymbol{r}_1'$ with its own second particle (see Fig. 1), and the probability of this disablement increases with F.

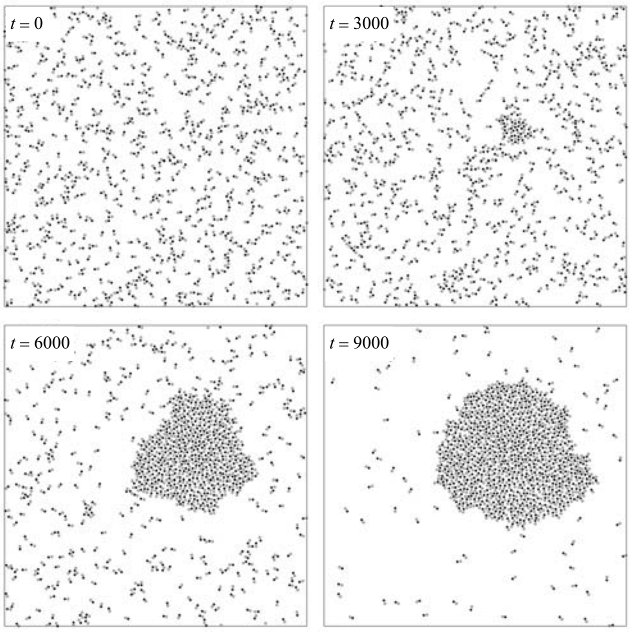

Figure 4. Typical time variation of $l = 2$ FCW distributions at $\rho = 0.15$ ($F = 0.5$, $P = 0.0$).

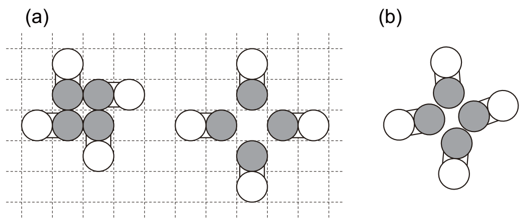

Figure 5. Typical collision patterns of four $l = 2$ FCWs; (a) on-lattice case, (b) off-lattice case.

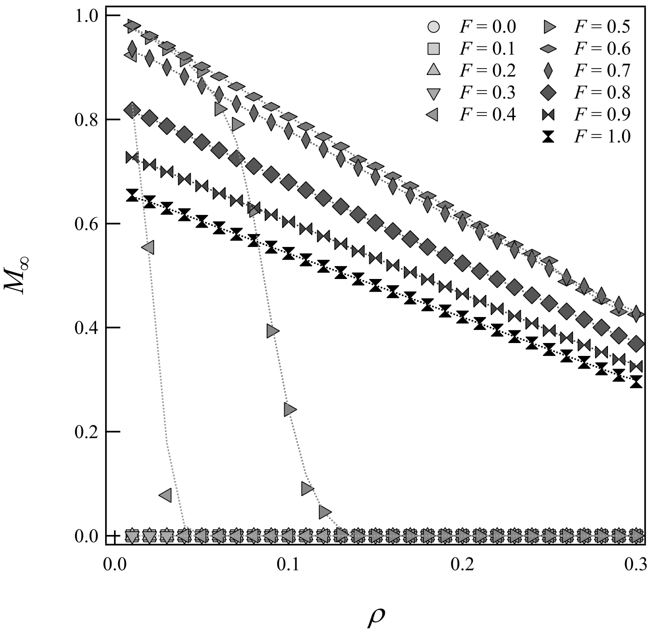

Figure 6. M_∞ as a function of ρ for $l = 2$ ($F = 0.0$-1.0, $P = 0.0$).

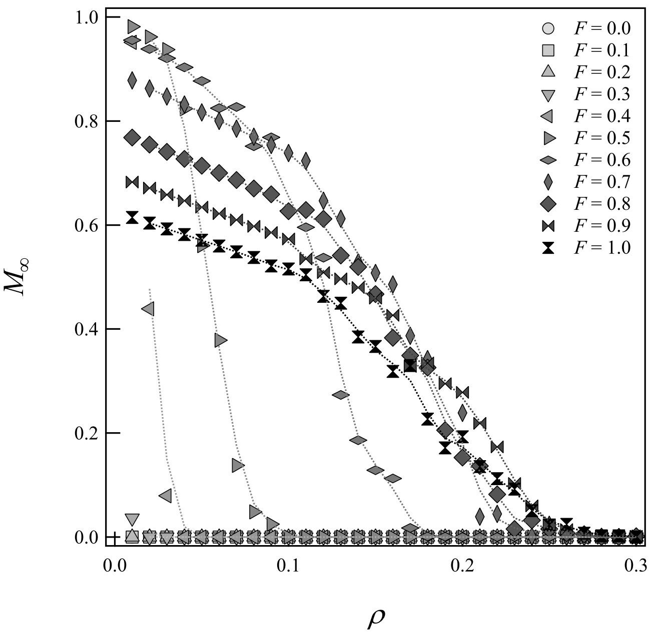

Figure 7. M_∞ as a function of ρ for $l = 3$ ($F = 0.0$-1.0, $P = 0.0$).

Likewise, Fig. 7 shows the M_∞-ρ plots for $l = 3$ (similar results are obtained for $l = 4$ and 5). While only the aggregated state is observed for $F \leq 0.3$, the moving state is possible for $F \geq 0.4$; the transition from the moving state at lower ρ to the aggregated state at higher ρ is observed. Furthermore, the critical density at which the transition occurs becomes larger as F is increased, at least up to $F = 0.6$, which means that the increase in the flexibility of each FCW enhances the mobility. On the other hand, the mobility tends to decrease when the flexibility is further increased ($F \geq 0.7$). These can be explained similarly to the results for $l = 2$. But the decrease in M_∞ with the increase in F is rather an artificial effect which depends on the details of the model including the definitions of F and M_∞. In essence, the individual deformability increases the collective mobility of FCWs.

For $l \geq 6$, only the aggregated state ($M_\infty \sim 0$) was observed, even when F is increased (data not shown). This is due to the length effect. That is, the mobility decreases as FCWs become longer (see Fig. 3), because they become more likely to entangle each other and get immobile, as discussed in the on-lattice case [2]. In short, although the mobility is enhanced by the increase in F, it is suppressed by the increase in l.

3.3 Effect of Perturbation *P*

Here the effect of the fluctuation of the form is discussed. Figure 8 shows the M_∞-ρ plots of $l = 2$ for different values of P, with $F = 0.5$ fixed (similar results are obtained for other values of l, although only the aggregated state was observed for $l \geq 6$). We see that all the plots are qualitatively the same in the sense that they show the transition from the higher-M_∞ state to the zero-M_∞ state. However, the critical density decreases with the increase in P, and at a certain density (*e.g.*, $\rho = 0.08$), M_∞ is larger for smaller P ($M_\infty > 0.6$ for $P = 0.0$) and smaller for larger P ($M_\infty < 0.1$ for $P = 1.0$). This means that the random fluctuation of each object decreases the collective mobility and enhances the tendency of aggregation, which is reminiscent of the "freezing-by-heating" effect [9].

The reason of the decrease in M_∞ with the increase in P is considered as follows. In a collision such as the one shown in Fig. 5(b), FCWs sometimes get locked and become unable to move again, especially when l is large or F is small, as already discussed. That is, the first step of the movement in a unit time (Figs. 1 and 9, (a) → (b)) is disabled. This nucleates the aggregation of FCWs. Otherwise, the FCWs can move and the nucleation of aggregation is tentatively avoided. However, except for $P = 0.0$, in which case only the first step is conducted, the FCWs then experience the second step (Figs. 1 and 9, (b) → (c)). Here it is possible that they come to face each other again, which may lead to an unresolvable collision. The larger the rotation angle φ (see Fig. 1), the more likely this re-collision occurs. In summary, as P is increased, the probability of the nucleation of aggregation increases due to the fluctuation-induced re-collisions, even if the original collisions have been resolved, and consequently, the mobility M_∞ is decreased.

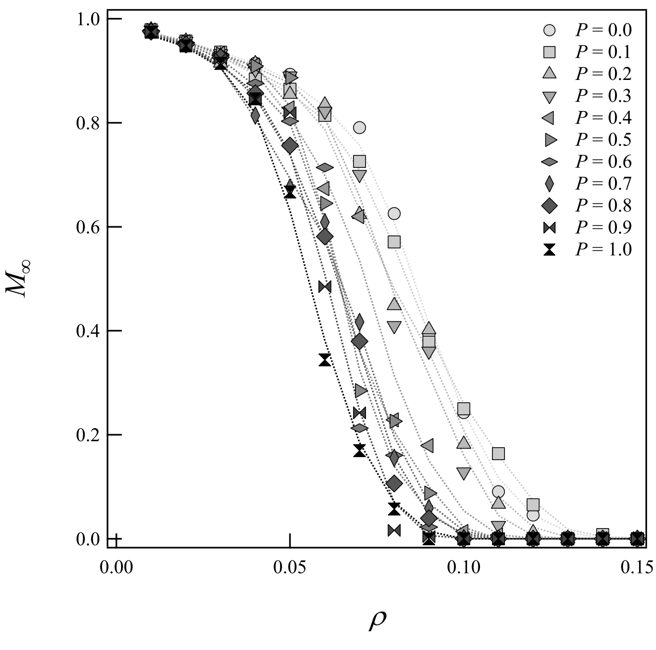

Figure 8. M_∞ as a function of ρ for $l = 2$ ($F = 0.5$, $P = 0.0$-1.0).

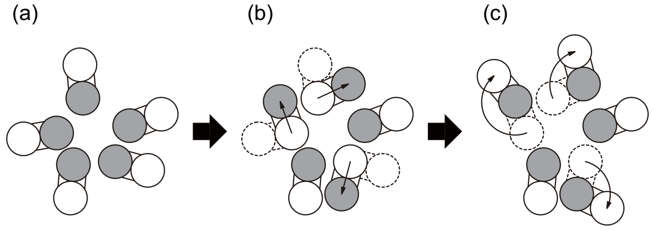

Figure 9. Effect of perturbation on collision.

4. Conclusion

We extended the FCW model and conducted numerical simulations in an off-lattice space. It turned out that aggregation of FCWs without deformability is enabled by lattice elimination. The tendency of aggregation was found to increase with the decrease in the flexibility or the increase in the perturbation of each FCW, and these results were discussed.

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