Supplementary Information: Collective motion of run-and-tumble repulsive and attractive particles in one-dimensional systems.

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I. OVERDAMPED DYNAMICS WITH INELASTIC COLLISIONS

A. Simulation details

We now consider the case where particles collide inelastically with each other. We simulate a system of particles whose translational equation of motion follows a Brownian dynamics with an additional propulsion force F^p [1]. For each particle,

$$\dot{x} = \beta D(F^p + F^i) + \sqrt{2D}\eta \tag{S1}$$

where F^p is the propulsion force, F^i is the conservative force between particles, η a Gaussian White Noise, β the inverse of the temperature and D the translational diffusion coefficient. The rotational equation of motion is implemented as a one-dimensional run-and-tumble: at every time step, the ith-particle direction d_i is redefined at random with probability α, the tumbling rate.

When dealing with an on-lattice system, independently on the nature of the conservative force (whether repulsive or attractive) particles only perform 1) one-lattice-site jumps when the landing site is empty or 2) do not move when it is occupied. Contrary to its lattice counterpart, particles in the off-lattice model can jump any distance depending on the forces at play. This might lead to jumps beyond their first neighbours. However, such displacements are not allowed as particles cannot overlap. In this scenario, aiming to keep a consistent type of dynamics throughout the different systems considered, we only allow particles to jump close to their neighbour and neglect momentum conservation collisions in the implementation. This type of dynamics, which resembles bacteria behaviour, thus favours aggregation compared to the particle bouncing off its neighbour even in the case where only repulsive interactions are present.

In line with the rest of systems considered in this work, we simulate these dynamics for $T_{max} = 10^8$ time steps with a time step $dt = 0.01$ ($\tau_{\max} = 10^6$), and estimate physical magnitudes when $T > 10^4$ at intervals of $T_{save} = 10^4$ time steps; ensuring proper steady-state relaxation.

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B. Results

Qualitative behaviour. In figure S1 we represent a few particle trajectories of the off-lattice system for a wide set of parameters: the density, ϕ, the tumbling rate, α, and the potential depth, ϵ.
For the repulsive system ($\epsilon = 0$, left column) we detect an overall qualitative behaviour similar to the off-lattice system with Langevin dynamics discussed in section 4.3 of the main text (notice that the time interval displayed in these trajectories is 1/10 of the one displayed in figure 9 of the main text). This suggests that neither inertial nor elastic collisions play any essential role in the system's evolution and steady state.

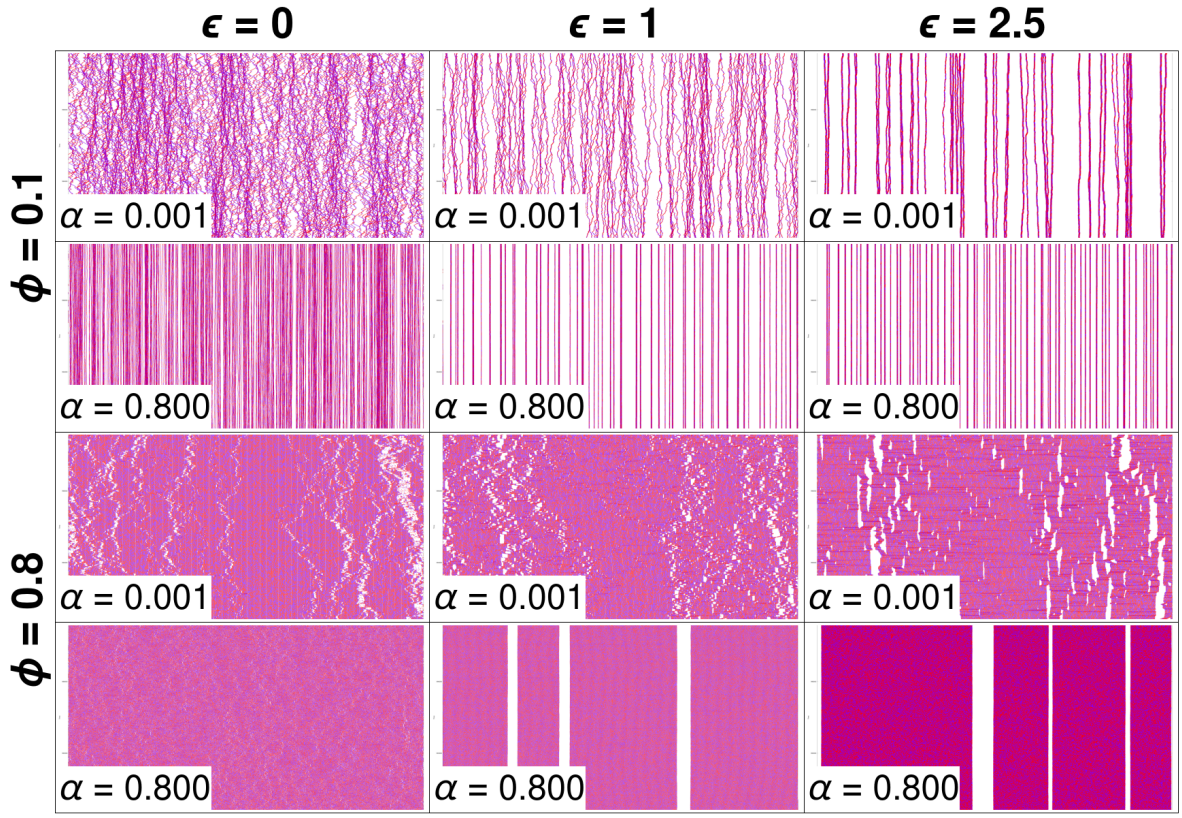

FIG. S1: Particle trajectories of the off-lattice system with inelastic collisions in stationary state for high (0.1) and low (0.8) densities and three values of the potential intensity ϵ: 0 (repulsive-left), 8 (attractive force $\sim$ propulsion force-middle) and 10 (attractive force $>$ propulsion force-right). High/low values for α are shown (some of the high values are different for a better visualisation). In each panel, time flows from bottom to top, and the last 1% of the total time interval is represented.

Cluster size distribution. Overall, the cluster size distribution (figure S2) also supports the fact that this system is similar to the Langevin dynamics discussed in the main text, although some differences are significant.
To start with, for the low density case (top panels in figure S2) we detect the same behaviour as in figure 10 of the main text. However, a slightly lower aggregation is present for the overdamped dynamics (this effect is more pronounced for $\alpha = 10^{-3}$).
In other words, comparing the off-lattice Langevin dynamics without inelastic collisions to the Brownian dynamics with inelastic collisions, we conclude that, contrary to what we expected, the former is slightly more aggregated than the latter but the overall behavior remains unchanged.
The simulation results also show that inelastic collisions do not lead to larger aggregation, even if particles tend to stick to each other. This can be due to he fact that for elastic interactions clusters are more mobile due to momentum conservation between particles inside them, which allows for larger cluster displacements. The resulting effect is that collisions increase clusters motility. This argument supports the fact that the collective behavior of run and tumble particles is essential for aggregation in these

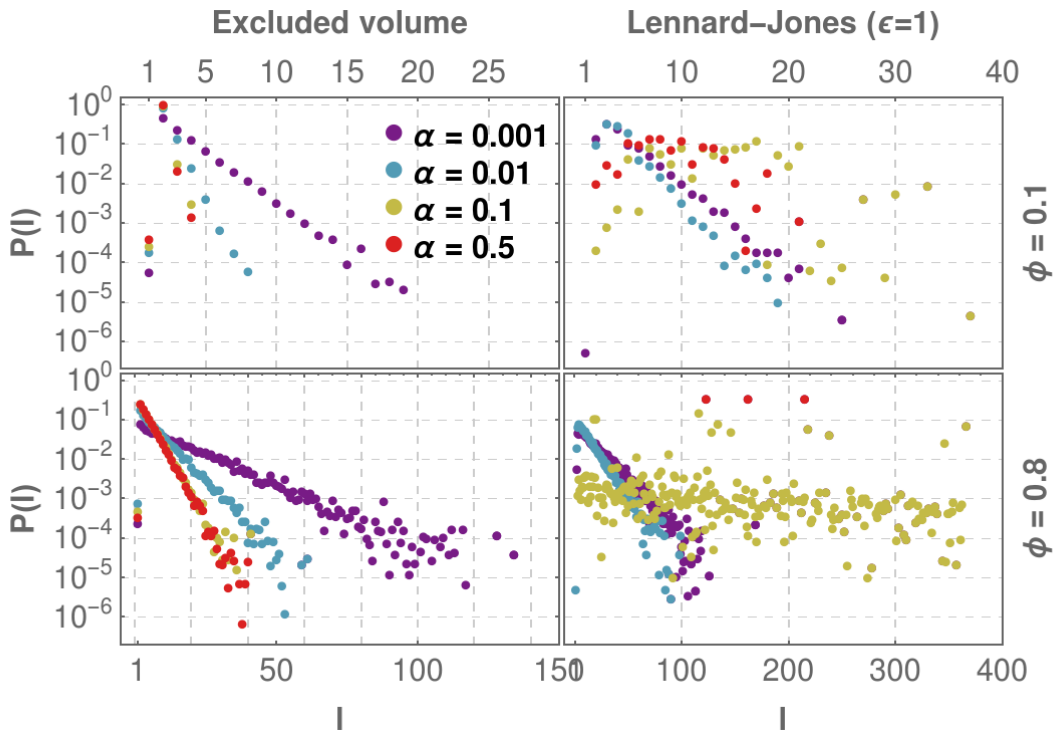

FIG. S2: Cluster size distribution $P(l)$ for the off-lattice system with inelastic collisions where particles interact repulsively (left-hand side) and attractively (right-hand side). Top panels correspond to low density, bottom panels to high density (note that x-axis scale is different for better visualization). Purple points are data for $\alpha = 0.001$, green for $\alpha = 0.1$ and red for $\alpha = 0.5$.

systems, as discussed in the main text.
When analyzing the high density repulsive case (bottom left-panel in figure S2), we detect more aggregation than in the Langevin dynamics for $\alpha = 0.5$. This is consistent with our previous argument since, as already pointed out, for this tumbling rate the system starts resembling a passive one which, in the absence of inter-particle attraction, results in a low aggregation state. However, since particles activity becomes negligible, the *aggregating* effect arising from the inelastic collisions results in an increase in aggregation with respect to the off-lattice Langevin dynamics (see the main text). For high attractive interactions and $\alpha = 0.1$ (bottom right-panel in figure S2) a bimodal distribution is observed, akin to the one obtained for other dynamics.

***J* and *M*.** In figure S3 we report the values of the mean cluster size M (top) and the fraction of jammed particles J (bottom). Overall, the behaviour of the two aggregation variables is quite similar to that observed for Langevin dynamics. For repulsive interactions, the decay of both J and M with the tumbling rate α follows a very similar profile to that observed for the for Langevin dynamics, with slightly larger average cluster size, M. This agreement in the dependency on α indicates that activity drives aggregation in non-attractive scenarios independently of the details of the dynamics. For attractive interactions ($\epsilon > 0$ in figure S3) we again observe a similar dependence of the aggregation (both the fraction of jammed particles J and the mean cluster size M) on the tumbling rate α, with a crossover between two regimes dominated either by free particle capture or clusters merging. Such behaviour is characterised by the initial decay in J followed by an increase and eventual saturation to $J = 1$. Note that an analogous saturation is also observed for the mean cluster size as well. Consequently, the general behaviour of the system is conserved between the two off-lattice implementations, although the latter (inelastic collisions) displays a slightly lower overall aggregation for attractive active particles.

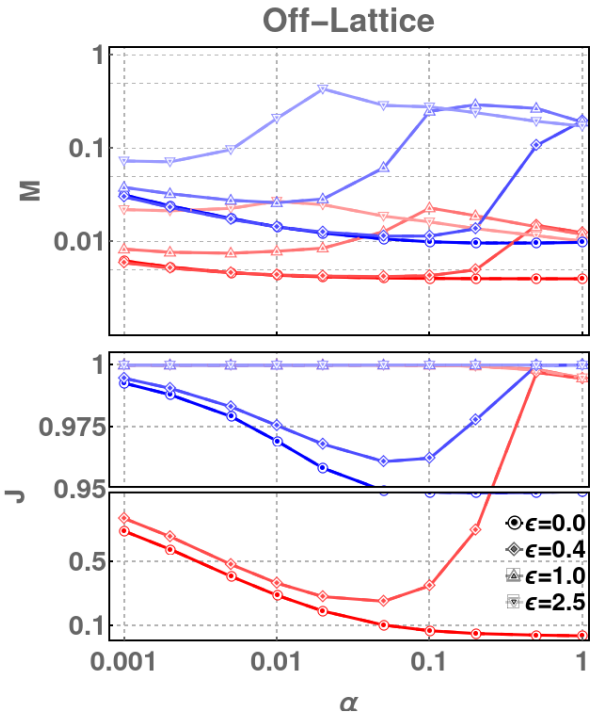

FIG. S3: M and J for the (Langevin overdamped (or Brownian) inelastic off-lattice dynamics.

II. ADDITIONAL TECHNICAL DETAILS

A. Steady state check

As discussed throughout this work, the fact that the system reaches a steady state is of the utmost importance for the reliability of the results. In this section we present different ways we have explored to assert that the results indeed correspond to a steady state regime for the discrete system as well as some numerical issues regarding the relaxation of the continuous system.

On-lattice. The discrete system we work with relaxes relatively fast to its steady state, both for repulsive interactions as well as attractive ones. This claim is supported because the total number of clusters in the system $N_C(t) = \sum_l n_{l,t}$ stabilizes around a constant value before 10^4 time-steps for all explored sets of parameters $\{\alpha, \phi\}$ in different interaction (EV or LJ) and collective dynamics (with or without explicit cluster moves) conditions, as shown in figure S4.
Depending on the values of the different system parameters, $N_C(t)$ will drop for a varying number of iterations but will always end up fluctuating around a constant value. Moreover, the number of clusters in the steady state $N_C = \langle N_C(t \to \infty) \rangle$ presents a consistent behavior with the state of aggregation depending on ϕ and α for the two types of interactions considered in this work. Indeed, for sets of parameter that lead to a clustering state, N_C stays high, while for parameter sets corresponding to a coarsening state, $N_C \sim 1$.
Throughout this work we have presented results based on single-seed statistics (initializing the system only once for each set of parameters and letting it run long enough to have good statistics of the steady state in a single run), assuming initial conditions are *forgotten* quickly enough. This approach is justified by comparing results from single-seed statistics with results from multiple-seed statistics (measuring only once in the steady state and then reinitializing the system with an independent random configuration, thus guaranteeing independent measurement points to average over, data not shown). We observe that independently of the parameter choice (α and ϕ) the cluster size distribution presents consistently the same behavior for all different regimes. One important feature that we observe here is also the fact that single-seed statistics present more noise in the coarsened state. This noise doesn't however justify choosing multiple-seed statistics over single-seed statistics for full parameter sweeps as they are much more costly computationally.

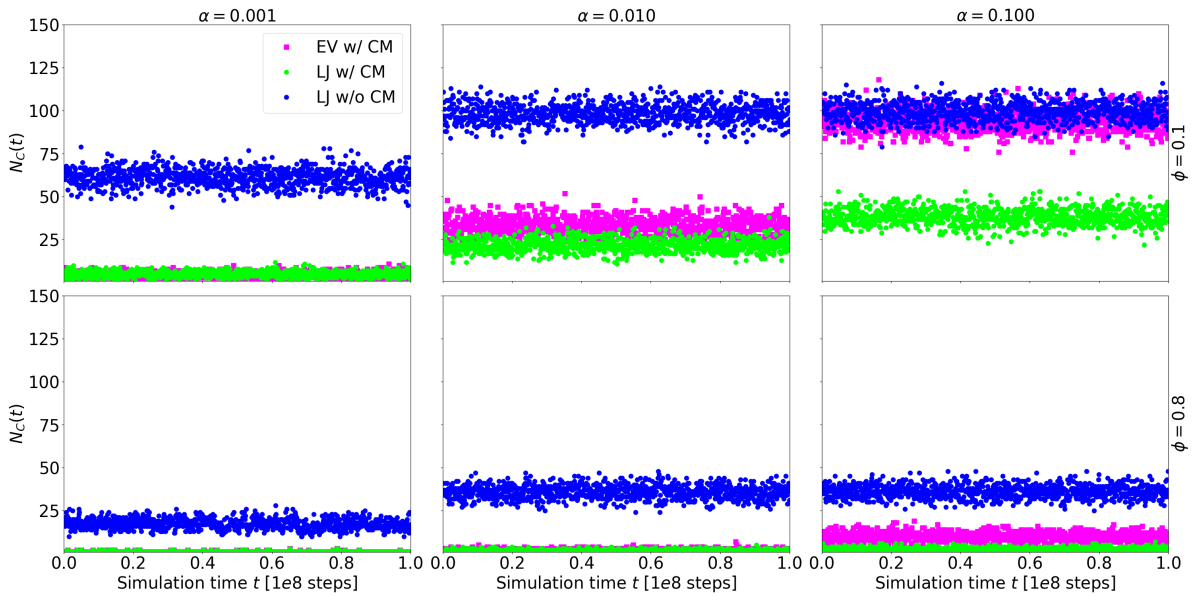

FIG. S4: Time evolution of the total number of clusters in the on-lattice system. The different colors and markers correspond to either purely repulsive (EV) or attractive (LJ) interactions with or without explicit cluster moves as shown in the legend. Each column corresponds to a different value of α for $\phi = 0.1$ (top row) and $\phi = 0.8$ (bottom row). All curves are computed on discrete systems of varying size for a fixed total number of particles.

Off-lattice. Given its continuous nature, the off-lattice system presents slower relaxation dynamics, which are highly dependent on the interplay between activity and attractive interactions. Consequently, even though the system generally reaches its steady state before 10^4 time-steps, some parameter combinations give rise to unexpected behavior. In this section we discuss some of these cases and how to address them.

In broad terms the behavior of the continuous system can be described as either reaching a clustered state or a coarsened state (all particles merging in one or a few clusters), which will depend on the choice of tumbling rate, density and attraction strength. By studying the phase diagram for all parameter combinations (data not shown) we conclude that, as parameters vary, the system evolves from one state of aggregation to the other when it crosses a transition line defined by $\epsilon/log(\alpha) \approx -0.55$. However, we find that for values close to this transition line the relaxation time of the system diverges (as it often happens for thermodynamic transitions). This is due to slow cluster motion (since almost all particles are trapped in clusters, and the system dynamics is mostly the cluster dynamics). Even if clusters move too slowly to merge into one big cluster over the simulation time considered, reaching the coarsening regime is controlled by the fact that clusters do not break apart fast enough, so in the infinite time limit, even if they move only a little, they will eventually merge. Thus, even if the number of clusters is not strictly 1, we can state we are in the coarsening regime.
Nonetheless, this leads to a more difficult analysis of these points, since it is difficult to assess whether the system has reached its steady state regime. In an attempt to overcome this difficulty we have initialized the system for the mentioned points of the parameter space with different configurations, representing varying states of aggregation, ranging from completely diluted to completely aggregated and considering different average cluster sizes. By taking this approach we can compare how the system evolves for the different initial conditions and determine whether its preferred regime is aggregation or dilution.
We thus find that diluted systems remain diluted if their steady state regime corresponds to this state, while the opposite happens for coarsened systems. However, an interesting phenomenon occurs for high attractive interactions strength ϵ. In such cases we find that even though the preferred state of aggregation seems to be clustering (starting from a different diluted and clustered configurations the system always reaches the same average cluster size), if we initialize the system at a higher aggregation than the actual steady state (lower average cluster size or even complete coarsening) the system remains in its initial state. This is likely due to the fact that in this regime of high attraction strength, the

particle's self-propulsion is not sufficient to escape the attractive potential generated at the ends of clusters, thus leading to particles trapping in an artificially aggregated state.

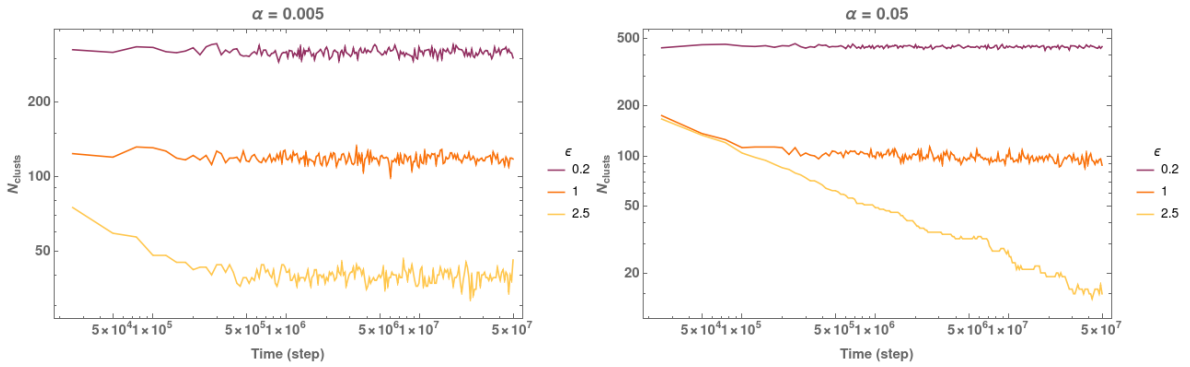

FIG. S5: Time evolution of the total number of clusters for the off-lattice dynamics and low density ($\phi = 0.1$) scenario and for $\alpha = 0.005$ (left) and $\alpha = 0.05$ (right). The different colors correspond to different values of the attractive potential.

B. Finite size analysis

While coarsening is inherently a finite size effect and cannot occur for infinitely large systems, in our work we are interested in checking that the statistics of the different states of aggregation are independent of the system's size. This means that while coarsening for a system of $N = 500$ particles will imply a maximum cluster size two times larger than for $N = 250$, we expect the cluster size distribution (CSD) to follow the same (or similar) law. We thus check that the CSD of the system is independent of its size in the desired range by simulating systems of $N = 250$, $N = 500$, $N = 1000$ and $N = 2000$ particles for different parameter sets $\{\alpha, \phi\}$ for both the continuous *off-lattice* and discrete *on-lattice* systems with different combinations of dynamics (with or without explicit cluster moves) and interactions (EV or LJ) and comparing the resulting steady state CSD.

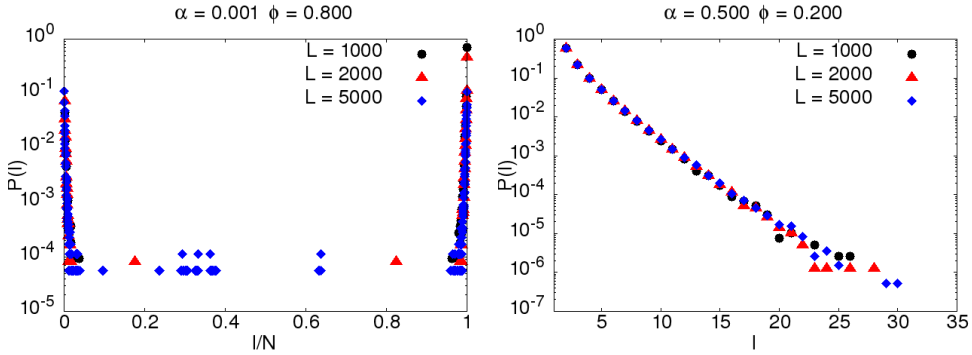

FIG. S6: Cluster size distribution as measured for different sizes of the on-lattice system (see legends) for different combinations of the α and ϕ parameters covering all different regimes. Top panel: coarsening regime. Bottom panel: clustering regime. Note that the x-axis corresponds to the normalized cluster size l/N for the top panel while on the bottom panel it corresponds to the real cluster size l.

In figure S6 we present the resulting cluster size distribution for on-lattice systems of sizes $N = 250$ (black circles), $N = 500$ (red triangles) and $N = 1000$ particles (blue diamonds) and two different combinations of α and ϕ, corresponding to the coarsening (top panel) and clustering (bottom panel) regimes. Note that in the top panel we normalize the cluster size so that the two can overlap, as the maximum cluster size depends on the size of the system. For the bottom panel, however, we plot the distribution function against the real cluster size as the decay should only depend on α and ϕ but not on L. This is indeed what we observe, with a perfect match between the different curves for the clustering

regime and a very similar and overlapping shape for the coarsening regime, with only a few statistical error differences between them (see points for intermediate sizes). We can therefore conclude that the system indeed behaves in the same way independently of N in this range of values. Note however that as the system gets larger the relaxation time for the coarsened states also increases as more particles need to merge together. This explains the higher statistical noise observed for the blue curve in the top panel. For this reason, we choose to work with $N = 500$ and not with larger systems, since the computational cost would be too high to achieve good statistics. We haven't worked with lower system sizes either to guarantee that all typical cluster sizes can be reached with this system for the chosen range of α and ϕ.

Similar analysis for the off-lattice system shows the same size-independent features (data not shown). It is worth noting that for the lowest tumbling rates ($\alpha \sim 0.001$) the swimmers persistence length becomes comparable to the box size so size effects might arise in this case. However, careful comparison across different system sizes for this value of α indicates that such effects only affect the dynamics but retain the same aggregation steady state.

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[1] P. Romanczuk, M. Bär, W. Ebeling, B. Lindner, and L. Schimansky-Geier. Active brownian particles. *The European Physical Journal Special Topics*, 202(1):1–162, Mar 2012.