Many-Body Effects in Motility-Induced Phase Separation

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Equilibrium phase separation requires attractive interactions, but introducing motility can profoundly alter collective behavior and drive nonequilibrium phase transitions, even with purely repulsive interactions. Most studies of motility-induced phase separation (MIPS) have considered pairwise additive potentials. Here, we investigate the impact of many-body interactions on MIPS by restricting the number of neighbors each particle can interact with. We find that this implicit introduction of non-additive interactions shifts the MIPS regime toward higher densities and suppresses phase separation at short persistence lengths, where MIPS would otherwise occur, while still allowing phase separation at longer persistence lengths.

I. INTRODUCTION

Motility-induced phase separation (MIPS) is a type of liquid–gas condensation that occurs in the absence of any attractive interactions. MIPS is triggered by a positive feedback loop: if interactions act to slow down active particles, a small aggregate will accumulate more particles, ultimately leading to phase separation. Experimentally, MIPS has been observed in various systems, both biological (e.g., bacteria) and synthetic (e.g., self-propelled colloids) [1],[2],[10].

Active Brownian particles (ABPs) interacting via short-range pairwise repulsive forces—such as excluded-volume interactions—have been shown to undergo MIPS. The transition arises because crowding reduces particle motility, causing further accumulation where particles slow down. This feedback leads to a runaway effect and, eventually, a spinodal instability.

The phase separation can be explained by a kinetic argument [3] that demonstrates how the persistent dynamics of ABPs breaks detailed balance: the influx of particles into a cluster, $J_{\text{in}} \sim v_0$, differs from the outflux, which is governed by the rate at which particles reorient their direction, $J_{\text{out}} \sim \tau_p^{-1}$. A simple estimate for the onset of MIPS is then given by $J_{\text{in}} \sim J_{\text{out}}$, which corresponds to the condition $\tau_p > \tau_{\text{mf}}$, where

$$\tau_{\text{mf}} \sim \frac{1}{\sigma v_0 \rho} \tag{1}$$

is the mean free time between significant collisions. In other words, aggregation occurs when particles do not reorient quickly enough to escape new collisions.[11]

While ABPs interacting via pairwise potentials have been extensively studied, it has been suggested that many-body interactions may be necessary to reproduce some emergent behaviors in active matter systems. For instance, in flocking models of self-propelled particles with alignment, collective motion only arises when particles align with more than one neighbor [?]. A lattice model of run-and-tumble particles with limited occupancy [4] showed that MIPS occurs when the maximum number of particles per site exceeds one; for $n_{\max} = 1$, only finite-size clusters are observed, indicating that single-particle exclusion is insufficient to trigger MIPS.

Another study comparing ABPs with passive Brownian particles [5] concluded that, beyond linear response, active particles display genuinely non-equilibrium behavior that cannot be captured by effective pairwise interactions alone.

Motivated by analogous ideas in the glassy materials community[6]—where models include interactions with randomly displaced images of particles—we propose a new control parameter: limiting the number of interactions per particle. This constraint breaks additivity and introduces effective many-body interactions, as the total interaction energy is no longer a simple sum over all pairs. Instead, it depends on which neighbors are selected and on the local and global densities of the system.

II. NUMERICAL SIMULATION

To examine the behavior of a minimal model with only motility and purely isotropic steric interactions, we simulate a collection of N disk-shaped active Brownian particles (ABPs) in a two-dimensional periodic domain of size $L \times L$, interacting via a multi-particle repulsive interaction. To eliminate boundary effects, all simulations are performed with periodic boundary conditions.

From the mean-field theory [8], the condition $t \gg D/L^2$ is required in order to observe MIPS, where D is the diffusion coefficient. ABPs exhibit ballistic dynamics for $t \ll \tau_p$ and diffusive dynamics for $t \gg \tau_p$, where the persistence time $\tau_p = 1/D_r = \mathcal{O}(10^{-2})$. Therefore, all simulations are run up to $t = 3000$ with $L = 60$. As discussed in the Introduction, when $\tau_p > \tau_{\text{mf}}$, it follows that $\rho > D_r$. Accordingly, we fix the density to $\rho_0 = 0.6$ in all simulations.

The microscale dynamics of each particle is governed

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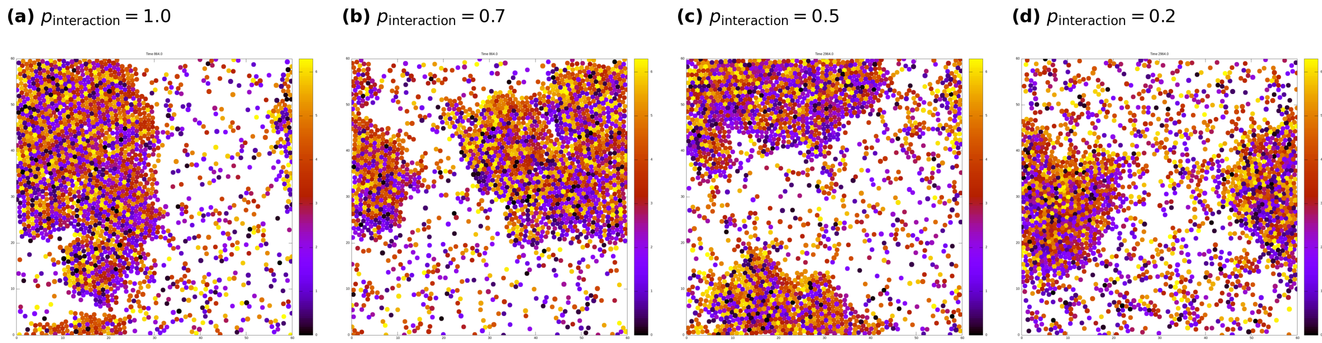

FIG. 1. Snapshots at different values of $p_{\text{interaction}}$, showing phase separation with varying cluster sizes. In all panels, $D_{\text{r}} = 0.03$, corresponding to a persistence length of $l_{\text{p}} = 33$ where we can see MIPS.

by the overdamped Langevin equations:

$$\dot{\mathbf{r}}_i = v_0 \mathbf{v}_i + \mathbf{F}_i, \tag{2}$$

$$\dot{\theta}_i = \sqrt{2D_r}\, \eta_i(t), \tag{3}$$

where $\eta_i(t)$ is Gaussian white noise with zero mean and correlation

$$\langle \eta_i(t) \eta_j(t') \rangle = 2D_r \delta_{ij} \delta(t - t').$$

The total interaction force $\mathbf{F}_i$ on particle i is given by

$$\mathbf{F}_i = \sum_{j \neq i} \mathbf{F}_{ij}, \quad \text{with} \quad \mathbf{F}_{ij} = -\nabla_{\mathbf{r}_i} V(|\mathbf{r}_i - \mathbf{r}_j|),$$

where $V(r)$ is a harmonic repulsive potential:

$$V(r) = \begin{cases} k(\sigma - r)^2, & r < \sigma, \\ 0, & r \geq \sigma. \end{cases}$$

To accelerate simulations involving many interacting particles, we implement spatial hashing [7], a technique that efficiently identifies neighboring particles to reduce computational cost.

To introduce many-body effects, we modify the interaction rule: each particle interacts with a given neighbor within range σ with probability p, drawn from a Bernoulli distribution. Unlike conventional simulations with deterministic, pairwise-additive potentials—where the total force is the sum of two-body forces—this probabilistic rule breaks additivity. The total force now depends on the configuration and number of neighbors, making the system inherently non-additive and many-body in nature.

In the remainder of this paper, we investigate how this probabilistic, many-body interaction alters the MIPS phase diagram. Sample final configurations are shown in Fig. 1, and dynamical behavior is included in the supplementary material.

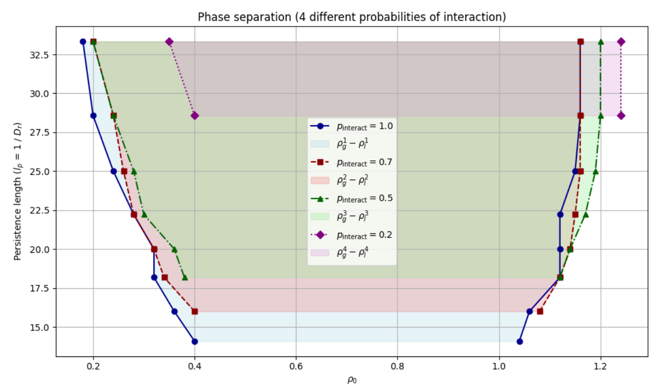

FIG. 2. Phase separation diagram for different values of the interaction probability p_{interact}. Each curve represents the coexistence boundaries between the dilute phase ρ_g (left) and the dense phase ρ_l (right) for a given p_{interact}, plotted as a function of initial density ρ_0 and persistence length $\ell_p = 1/D_r$. As p_{interact} decreases, the binodal lines shift to the right, indicating that both the dilute and dense phases emerge at higher densities. This shift is attributed to an increase in the effective packing fraction: particles that do not experience repulsion can approach more closely than their nominal diameter, effectively behaving like soft spheres. Moreover, MIPS is observed only at longer persistence lengths for lower interaction probabilities, due to a reduced effective density.

III. DISCUSSION

To quantify the densities of the dense and dilute phases, we compute time-averaged histograms of local particle densities after the system's transient period. The presence of bimodal distributions in these histograms is a clear signature of Motility-Induced Phase Separation (MIPS).

Our results show that when the system starts with an initial density ρ_0 between the dilute-phase density ρ_g and the dense-phase density ρ_l, it spontaneously phase separates and stabilizes at these two densities (FIG. 2).

By decreasing the probability of interaction between

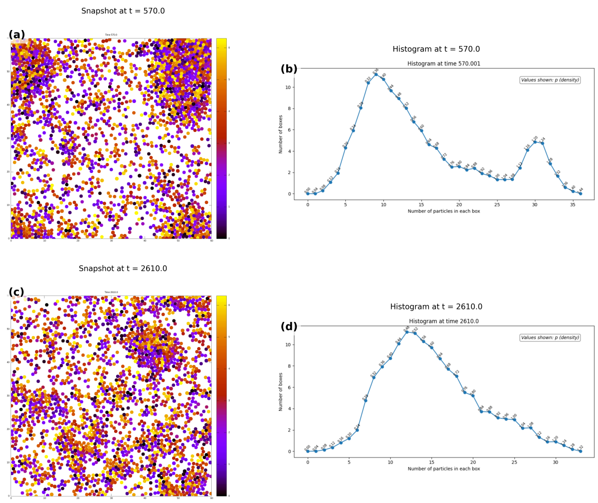

FIG. 3. (a), (b) Snapshots of a system with $D_\mathrm{r} = 0.04$ and $p_\mathrm{interaction} = 0.2$. As can be seen, the system undergoes an unstable phase separation, which eventually dissolves. (c), (d) Histograms of local particle densities. The presence of two peaks indicates the coexistence of distinct dilute and dense phases in the system.

neighboring particles, we observe a rightward shift in the phase separation diagram. This can be naturally explained through the concept of effective packing fraction. When particles interact with only a subset of their neighbors, some particles experience no repulsive forces and are able to come closer than the nominal particle diameter. As a result, lower interaction probability increases the effective packing fraction, thereby shifting both ρ_g and ρ_l to higher values (FIG. 2).

Introducing a finite interaction probability effectively softens the particles: hard spheres with limited interaction among their neighbors begin to behave like soft spheres.

Furthermore, in addition to the rightward shift of the phase boundary, decreasing the interaction probability also modifies the effective density of the system. Consequently, MIPS is only observed at larger persistence lengths. (FIG. 2)

Although stable MIPS is not observed at low persistence lengths, transient phase separation does occur in some periods and then dissolves (FIG. 3).

Moreover, as shown in FIG. 1, decreasing the probability of interaction leads to a reduction in cluster size, despite the global density ρ_0 being held constant across all simulations. This behavior can be attributed to an increase in the effective packing fraction: when fewer interactions are allowed, particles are able to overlap more easily, reducing excluded volume effects and thereby lowering the tendency for large clusters to form.

IV. CONCLUSION

We have investigated phase separation in a system of self-propelled active Brownian particles interacting via a harmonic oscillator pair potential. Motility-induced phase separation (MIPS) is observed whenever the persistence length l_p exceeds approximately 14 particle diameters σ, in the absence of many-body interactions.

We have further shown that by implicitly introducing a multi-particle repulsive interaction, MIPS persists, but the phase diagram shifts upward and to the right. This shift indicates that both the dilute and dense phases occur at higher densities, and that a larger persistence length is required when the number of interactions among neighboring particles is reduced.

This work can be extended by comparing our results with models that include soft interaction potentials, as well as with alternative probabilistic rules where the interaction probability depends on the local density of each particle individually. One possible extension involves introducing a probabilistic interaction rule in which each particle randomly selects a limited number of neighbors—up to a specified maximum—with which to interact.

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