Kinetics of motility-induced phase separation and swim pressure

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Active Brownian particles (ABPs) represent a minimal model of active matter consisting of self-propelled spheres with purely repulsive interactions and rotational noise. Here, we examine the pressure of ABPs in two dimensions in both closed boxes and systems with periodic boundary conditions and show that its nonmonotonic behavior with density is a general property of ABPs and is not the result of finite-size effects. We correlate the time evolution of the mean pressure towards its steady state value with the kinetics of motility-induced phase separation. For parameter values corresponding to phase separated steady states, we identify two dynamical regimes. The pressure grows monotonically in time during the initial regime of rapid cluster formation, overshooting its steady state value and then quickly relaxing to it, and remains constant during the subsequent slower period of cluster coalescence and coarsening. The overshoot is a distinctive feature of active systems.

I. INTRODUCTION

Over the past decade, there has been growing interest in the physics of active matter, defined as collections of self-driven particles that exhibit rich emergent behavior [1]. Realizations abound in the living world, from bird flocks [2,3] to epithelial cell monolayers [4,5], and in engineered systems, such as self-catalytic colloids [6,7] and microswimmers [8]. The distinctive property of active systems is that the particles are independently driven out of equilibrium and time reversal symmetry is broken locally, rather than globally as in systems driven out of equilibrium by external fields or boundary forces.

Progress has recently been made in formulating the nonequilibrium statistical mechanics of active matter using a minimal model of active Brownian particles (ABPs) consisting of purely repulsive self-propelled spherical colloids with overdamped dynamics [9]. Perhaps the most remarkable property of this simple system is that it spontaneously phase separates into a dense liquid phase and a gas phase in the absence of any attractive interactions [10,11]. This phenomenon arises from the persistent dynamics of self-propelled particles when the time for particles to reorient after a collision exceeds the mean free time between collisions, hence the name of motility-induced phase separation (MIPS). Additionally, in a sort of reverse MIPS, confined ABPs spontaneously accumulate at the walls of the container [11,12], a behavior which is at odds with fundamental properties of gases and fluids in thermal equilibrium. These findings have raised a lot of interest in understanding whether active matter can be characterized in terms of equilibrium-like properties, such as effective temperature and pressure. A broad class of active particles can exert persistent forces on the walls of a container. These forces have been quantified recently in terms of a new contribution to the pressure, dubbed swim pressure, that measures the flux of propulsive forces across a unit bulk plane of material [13,14]. Remarkably, it has been shown that in generic active systems the mechanical force exerted on the walls of the container depends on the detail of particle-walls interactions, making it impossible to define the pressure of an active fluid as a state function [15].

This result, however, does not apply to the special case of spherical ABPs. For this minimal model it has been shown that the pressure is indeed a state function that characterizes the bulk materials properties of this simple active fluid [16,17]. On the other hand, the behavior of pressure of spherical ABPs is unusual, in that simulations have reported a non-monotonic behavior of pressure versus density, arising from the suppression of motility (and therefore of swim pressure) associated with particle cageing at the onset of phase separation [17,18]. Experimental measurements of pressure of active colloids have similarly shown a strong suppression of pressure at intermediate density [8]. In spite of extensive work, some open question remains concerning the quantitative role of finite-size effects in active systems and the origin and robustness of the non-monotonic behavior of pressure.

In this paper we use molecular dynamics simulations to investigate the pressure of spherical ABPs with soft repulsive forces and correlate its non-monotonic behavior with density with the kinetics of cluster size growth in phase separating systems. By examining both systems bounded by confining walls and ones with periodic boundary conditions, we show that finite-size effects are consistent in both cases with the behavior expected for a rarefied thermal gas. The pressure calculated in confined systems is strongly suppressed by the presence of boundaries if the persistence length of the particles dynamics is comparable to the linear size of the container, with a linear dependence on system size and a behavior that resembles that of a rarefied Knudsen gas. With periodic boundary conditions the convergence to the large system size limit is exponential, again as expected in a thermal system.

The non-monotonic behavior of pressure as a function of density for repulsive ABPs with large persistence lengths was first reported in simulations of systems in closed boxes [17] and has been seen in sedimentation ex-
periments of active colloids. More recently it was confirmed in numerical studies of hard active particles with periodic boundary conditions in three dimensions. Our work provides a systematic study of finite size effects in both bounded and periodic systems and shows that the nonmonotonicity is not a finite size effect, but a bulk properties of ABPs. It arises because in phase separated systems the aggregate effectively provides a bounding wall for the active gas, which suppresses the swim pressure. Additionally, by considering soft repulsive disks, we complement previous work on hard particles and show that this effect does not depend on the details of the interparticle interaction. Finally, we examine the kinetics of coarsening and establish a strong correlation between the aggregate dynamics and the relaxation of the pressure towards its steady state value. We identify two dynamical regimes that control the relaxation of a disordered initial state towards the nonequilibrium steady state of the system. For system parameters that produce a homogeneous steady state, pressure grows monotonically in time to its steady state value, which it reaches on a timescale controlled by the persistence time of the self-propelled dynamics. In contrast, for parameters that produce a phase-separated steady state, the time evolution of the pressure is not monotonic and there are two dynamical regimes. Initially, small clusters form and break up rapidly and the pressure quickly builds up and overshoots its asymptotic value. Eventually, the dynamics crosses over to a coarsening regime with a slower cluster growth and the pressure relaxes to its steady-state value.

The rest of the paper is organized as follows. Section II described the ABP model and provides details of our simulations. Section III examines the swim pressure and its behavior at low and high density. It also discusses the relevance of finite-size effects. Section IV examines correlations between the pressure relaxation and the kinetics of MIPS of swim pressure. Finally, we close in Section V with some concluding remarks.

II. ACTIVE BROWNIAN PARTICLES MODEL

We consider a well-established minimal model of monodispersed ABPs in two dimensions, consisting of $N$ self-propelled disks of radius $a$ in a square box of area $L^2$. Each particle is identified by the position $\mathbf{r}_i$ of its center and a unit vector $\hat{\mathbf{e}}_i = (\cos \theta_i, \sin \theta_i)$ that defines the axis of self propulsion. Assuming the medium only provides friction, the dynamics is governed by Langevin equations, given by

$$\dot{\mathbf{r}}_i = v_0 \hat{\mathbf{e}}_i + \mu \sum_{j \neq i} \mathbf{F}_{ij},$$  

$$\dot{\theta}_i = \eta_i(t),$$

where $v_0$ is the bare self-propulsion speed, directed along $\hat{\mathbf{e}}_i$ and $\eta_i(t)$ a Gaussian random torque with zero mean and variance $\langle \eta_i(t) \eta_j(t') \rangle = 2D_\eta \delta_{ij} \delta(t - t')$, with $D_\eta$ the rate of rotational diffusion. The pair forces $\mathbf{F}_{ij}$ are purely repulsive and harmonic, with $\mathbf{F}_{ij} = k(2a - r_{ij}) \hat{\mathbf{r}}_{ij}$ for $r < 2a$ and $\mathbf{F}_{ij} = 0$ otherwise, where $r_{ij} = r_i - r_j$ is the interparticle separation and $\hat{\mathbf{r}}_{ij} = r_{ij}/|r_{ij}|$. Finally, $\mu$ is the mobility. We neglect here noise in the translational dynamics, which is less important than the orientational one in both synthetic active colloids and swimming bacteria. The nonequilibrium nature of this minimal active model is provided entirely by the propulsive force $\mathbf{F}_i^\lambda = (v_0/\mu) \hat{\mathbf{e}}_i$. After integrating out the angular dynamics, $\mathbf{F}_i^\lambda$ represents a non-Markovian stochastic force correlated over the persistence time $\tau = D_\eta^{-1}$. Since the finite correlation time of the noisy propulsive force is not matched by similar correlations in the friction coefficient $\mu^{-1}$, which is constant, the system does not obey the equilibrium fluctuation-dissipation theorem embodied by the Stokes-Einstein relation.

The persistence time $\tau$ controls the crossover from ballistic to diffusive regime in the single particle dynamics. For $t \gg \tau$, the dynamics of noninteracting ABPs is diffusive, with diffusion coefficient $D_\lambda = v_0^2 \tau/2$. The single particle dynamics can also be characterized by the persistence length, $\ell_p = \frac{\tau}{D_\lambda}$, and the rotational Pécelt number, $P_\eta = \ell_p/\eta$, used in much of the literature.

Our simulations employ a conventional Brownian dynamics algorithm. We take the interaction timescale, $\tau_D = (\eta k)^{-1}$, as the unit time ($\mu = k = 1$) and the particle radius $a$ as the unit of length ($a = 1$). To prevent particles from passing through each other, we
set \( \nu_0 = (\alpha \mu k)/100 \). We choose a time step sufficiently small to handle many-body interactions at high density, \( \delta t \ll \tau_0 \).

As discussed in the introduction, purely repulsive ABPs exhibit macroscopic phase separation, or MIPS, where the dense phase grows to the size of the system and nearly free particles in the gas phase try to explore lengths or order \( \ell_p \). For this reason, ABPs are subject to strong finite-size effects that we quantify here by considering simulation boxes of linear size \( L = 50, 100, 200, 400 \), both in a closed box geometry and with periodic boundary conditions. We tune the packing fraction \( \phi = N \pi a^2 / L^2 \) that sets the total number of particles, \( N \), with \( N \sim 10^5 \) for \( L = 400 \). A schematic representation of the phase diagram explored in the present work is shown in Fig. 1, where the color represents the variance of the magnetic quantities over exponentially increasing time windows. In particular, we use the so-called log\(_2\)-binning procedure by following the evolution of averages in time intervals \( I_n = (2^{-(n+1)} t_i , 2^{-n} t_i ] \). The error bars are estimated from the fluctuations between several independent runs with a jackknife procedure (see, e.g., [24]). We have 500 runs for \( \phi = 0.01 \), 10–20 runs for larger values of \( \phi \).

We also use this time binning procedure to assess convergence to the steady state. We consider the simulation to have reached a steady state if the averages in at least the first three \( I_n \) are compatible with each other within errors. If this condition is not met, we double the simulation time. In particular for parameter values where the system phase separates, simulations have been run for \( 10^7 \) time units.

Finally, we shall denote our estimate of the steady state ensemble average of an observable \( O \) by \( \langle O \rangle \), which we compute by taking the value for the \( I_0 \) time interval (i.e., the last half of the simulations).

### III. Swim Pressure

There has recently been a lot of interest in characterizing the pressure of active systems. Pressure can be defined in terms of the forces transmitted across a unit bulk plane of material. In an active fluid there is a unique contribution to pressure that measures the flux of propulsive forces across a bulk plane of material [17, 21, 22]. This contribution, named swim pressure in recent literature [26], can be expressed via a virial-type formula as [15, 17, 19]

\[
p_{s} = \frac{1}{d L^2} \sum_i F_i^s \cdot R_i,
\]

with \( d \) the spatial dimension (here \( d = 2 \)). In a closed box \( R_i = r_i \), but with periodic boundary conditions \( R_i \) is the position of the particle in an infinite system, accounting for winding numbers as the particle crosses the periodic boundary [23, 28]. The virial expression estimates the swim pressure as the propulsive force carried over a distance of the order of the persistence length, in analogy

![FIG. 2. Time evolution of the pressure of a dilute gas (\( \phi = 0.01 \)) of ABPs for various values of the persistence length for periodic (a) and closed (b) square boxes of linear size \( L = 200 \). At this density the pressure is determined entirely by the swim pressure. The solid lines show the large-\( L \) ideal gas prediction of Eq. (5), which matches the numerical results for periodic boundary conditions even at very large \( \ell_p \). For closed systems the pressure is significantly suppressed by accumulation of particles at the walls as soon as \( \ell_p \) becomes comparable to \( L \). The insets show our estimate for the steady-state pressure (\( p \)) in the dilute limit divided by the ideal gas steady state value \( p_0 = \rho v_0 \ell_p / 2 \mu \) as a function of persistence length for a various systems sizes \( L \). For periodic boundary conditions (a)-inset the system is self-averaging and \( \langle p \rangle^{(\infty)} \approx p_0 \) within errors for \( L = 200 \). For the closed box (b)-inset, there are strong finite-size effects due to the walls. We show that \( \langle p \rangle / p_0 \) versus \( \ell_p / L \) can be fit to \( 1 - A \ell_p / L \) for \( \ell_p / L \leq 0.1 \) (black line) with a result of \( A = 1.78(3) \), \( \chi^2 = 7.16 \) for 6 degrees of freedom (d.o.f.).]
to the kinetic pressure of an ideal gas or the radiation pressure of a photon gas. Note, however, that in spite of the one-body expression given in Eq. (3), the swim pressure depends on interactions that lead to suppression of the persistence length. In addition to the swim pressure, there is also the contribution describing the direct transmission of interaction forces across the bulk plane. For pairwise forces $F_{ij}$, as relevant to our collection of ABPs, this can be calculated from the familiar virial expression

$$p_D = \frac{1}{dL^2} \sum_{i,j} F_{ij} \cdot r_{ij}. \quad (4)$$

Recent work has shown that for the minimal model of spherical ABPs considered here the total pressure $p = p_s + p_D$ defined from Eqs. (3) and (4) coincides with the pressure per unit area on the walls of a container, and represents a state function of the active fluid, independent of the properties of the walls.

In the remainder of this section we examine the importance of finite-size effects in the calculation of the pressure of active systems and demonstrate that the predicted and observed non-monotonicity of pressure versus density is an intrinsic property of these nonequilibrium fluids, not a finite-size effect.

### A. Pressure of a dilute active gas

For a dilute gas of ABPs, the dominant contribution to the pressure comes from the swim pressure $p_s$. Neglecting interactions, and in the large-size limit, Eq. (3) can be calculated exactly, with the result

$$p(t) = p_0 \left(1 - e^{-D_s t}\right), \quad p_0 = \rho\frac{v_0^2}{2\mu D_s}, \quad (5)$$

where $\rho = N/L^2 = \phi/(\pi a^2)$ is the number density. The pressure $p_0$ of an active ideal gas can be naturally interpreted in terms of an active temperature, with $p_0 = \rho k_B T_a$, and $T_a = v_0^2/(2\mu k_B D_s)$. This active temperature also coincides with the one set by the ratio of translational diffusion $D_s = v_0^2/2\tau_s$ to the friction coefficient $\mu^{-1}$, as required for thermal Brownian particles satisfying the Stokes-Einstein relation. Indeed, the stochastic propulsive force becomes $\delta$-correlated in time in the limit $\tau_s \to 0$, with $k_B T_a = \text{constant}$. In other words, noninteracting ABPs behave like thermal colloid at temperature $T_a$ in the limit of vanishing persistence time, $\tau_s$. Here we consider the pressure of active particles for finite values of the persistence time, away from this Brownian limit.

The time evolution of $p_0$ of a dilute active gas ($\phi = 0.01$) is shown in Fig. 2 for a system in a box of linear size $L = 200$ with periodic boundary conditions (a) and one enclosed by bounding walls (b), for various values of the persistence length, $\ell_p$. Flat repulsive walls are implemented using the same harmonic forces that describe interparticle interactions.

For periodic boundary conditions, Eq. (5) provides an excellent fit to the calculated pressure over the entire time range and for all $\ell_p$ considered. In confined systems, however, a second time scale comes into play, that is the time $\tau_L = L/v_0$ it takes an ABP to travel the size of the box. The finite-size corrections to pressure are negligible only when $\tau_L \gg \tau_s$, or equivalently $L \gg \ell_p$ (here with $L = 200$ this only holds for the smallest $\ell_p = 5$). In all other cases the presence of confining walls strongly suppresses the asymptotic long-time value of the pressure as compared to the value $p_0$ given by Eq. (5). To quantify the finite-size corrections, the insets of Fig. 2 show the ratio $(p)/p_0$ of the calculated steady-state pressure to the ideal active gas pressure as a function of $\ell_p$ for various systems sizes $L$. With periodic boundary conditions (a), the finite-size corrections are essentially independent of $\ell_p$ and converge very quickly to $p_0$ with increasing system size—in fact for $L = 200$ $(p(\ell_p))/p_0$ is indistinguishable from 1 with our errors.

In the case of the closed box the finite-size effects are much more pronounced and depend strongly on $\ell_p$, as

![FIG. 3. Pressure as a function of packing fraction for $\ell_p/a = 25$ (a) and $\ell_p/a = 50$ (b) for a system with periodic boundary conditions. The box size must be several times larger than $\ell_p$ to obtain results representative of the large-$L$ limit.](image-url)
shown in the inset of Fig. 2. Our \( p/\rho_0 \) for different \( L \) can be nearly collapsed when plotted versus \( \ell_p/L \). In fact, for \( \ell_p/L \lesssim 0.1 \), the behavior can be fitted by a linear form, \( p/\rho_0 \approx 1 - A \ell_p/L \). This functional dependence supports the idea that the box boundary has a simple surface effect on the pressure for \( \ell_p/L \ll 1 \). At higher persistence lengths, collective effects, such as clustering of particles at the corners of the box, yield further deviations from the linear behavior.

In summary, we find that at low density the swim pressure is clearly suppressed in systems that restrict the mean free path below \( \ell_p \), so that the dynamics remains ballistic at all times. When particles are confined, there are strong boundary effects reminiscent of those seen in a Knudsen gas, where the density is so low that the mean-free path from inter-particle collisions exceeds the box size. Specifically, the convergence to the large-\( L \) limit is exponential for the periodic box and linear for the closed box. This is precisely the type of the finite-size effects one expects in a thermal system whose free energy would have bulk and surface contributions, with the former the only relevant one in periodic systems at large \( L \).

### B. Pressure at finite density

At finite density, both the swim contribution and the direct contribution from interactions are appreciable. The direct contribution form interactions, \( p_D(\phi) \), grows monotonically with density as in passive systems and depends only weakly on self propulsion \[17\]. In contrast the swim pressure is non-monotonic in density and strongly suppressed at intermediate density due to the decrease of particle motility. This leads to an overall non-convex density dependence of the total pressure \( \langle p(\phi) \rangle \), which has been seen in simulations \[17, 20, 22\] and experiments \[5\]. For larger \( \ell_p \) simulations show a non-monotonic \( \langle p(\phi) \rangle \).

When the system phase separates, the macroscopic aggregate effectively provides a bounding wall to the gas phase, leading to strong finite-size effects in the swim pressure even in systems with periodic boundary conditions. This is shown in Fig. 3. Here, the bottom frame \( (\ell_p/a = 50) \) shows a system which undergoes phase separation for intermediate densities, while in the top frame \( (\ell_p/a = 25) \) the phase separation is still incipient (recall Fig. 1). We note that in the former case we need box sizes of \( L \geq 200 \) to achieve convergence \[30\]. All the results reported in the remainder of the paper are for box sizes \( L = 200, 400 \), and are free of finite-size effects within our error bars.

For sufficiently large values of \( \ell_p \) the pressure of the active fluid is non-monotonic with density. This behavior, shown in Fig. 3b, is not a finite-size effect and is associated with the strong suppression of the swim pressure arising from motility-induced aggregation. Ref. \[20\] showed that the suppression of \( p_s \) can be captured by a simple expression, given by

\[
p_s = \rho v_0 v(\rho) \frac{\mu D_r}{2 \mu D_t},
\]

with \( v(\rho) = v_0 + \mu \langle \hat{e}_i \cdot \sum_{j \neq i} F_{ij} \rangle \) the effective velocity of a particle along its direction of self-propulsion. To leading order in the density, this has a linear decay \( v(\rho) = v_0 (1 - \rho/\rho_s) \), where \( \rho_s \equiv \rho_s(\ell_p) \) provides a cutoff, above which \( v(\rho) \) goes to zero. Inserting this form of \( v(\rho) \) into Eq. \[6\] yields a quadratic form for the swim pressure, \( p_s = k_B T_a (1 - \rho/\rho_s) \) \[20\].

As we can see in Fig. 1b, this ansatz works well only for moderate \( \ell_p \) \( (\ell_p/a \lesssim 25 \) with our parameters). For large \( \ell_p \), i.e., for systems exhibiting phase separation (see Fig. 1), the swim pressure displays a much stronger dependence on density and drops abruptly at the onset of phase separation. Phase separating systems always evolve to contain a single large dense region,
obtained for hard repulsive spheres in the onset of phase separation. A similar result has been state value in a time of the order of the persistence time, corresponding to homogeneous steady states, the preservation, which operate on a density-dependent timescale towards the final steady state reveals a non-monotonically, is longest for the lowest densities that exhibit to reach steady state depends on density and, not surprisingly, is longest for the lowest densities that exhibit phase separation. The growth of the dense phase is associated with the formation of clusters of jammed particles. If the reorientation time \( \tau_r \) required for particles to turn and escape from the cluster is longer than the mean free time between collisions, more particles will accumulate and the cluster will grow. This process continues as long as the rate for escaping from the cluster \( (D_r) \), is slower than the rate at which particles absorb at the boundary, which is controlled by the collision rate. Systems with lower densities take a longer time to reach the final state due to lower nucleation and adsorption cross-sections. This is in agreement with recent work examining the kinetics of MIPS in terms of classical nucleation theory.

By comparing the evolution of pressure and of density correlations in our largest phase-separating systems \( (L = 400) \), we can identify two distinct dynamical regimes. Once the pressure reaches its steady state value, clusters begin to coarsen at a slower rate, corresponding to previous observations.

By the time pressure equilibrates, multiple clusters have formed and there is an average zero net flux between phases, shown in Fig. 6 where we additionally quantify the number of particles in the largest cluster \( N_1 \) alongside all clustered particles \( N_c \). At this stage, the dense aggregates move very slowly, having caged the motility of most aggregated particles, only allowing those at the boundary to de-adsorb, while large clusters coalesce into one another until system-spanning phase separation occurs. We find a division in time regimes of growth for \( N_1(t) \) and \( N_1(t) \) and show snapshots of this process in Fig. 6. The largest cluster continues to grow long after the cluster fraction saturates, which corresponds with pressure reaching its steady state.

In particular, for the data shown in Fig. 6, we have fit the number of particles in the largest cluster to

\[
N_1(t) \sim t^\gamma. \tag{7}
\]

In the first time regime (up to and including point B in the figure, that is, for \( tD_r < 20 \)) this fit gives \( \gamma_1 = 1.3(2) \), \( \chi^2 / \text{d.o.f.} = 0.12/1 \). In the coarsening regime, for \( tD_r > 20, \) we obtain \( \gamma_2 = 0.29(4), \chi^2 / \text{d.o.f.} = 1.65/3 \). These fits are plotted with dotted lines in the figure.

We note that the coarsening regime has been studied in previous work using the growth of a length scale computed from the structure factor: \( L(t) \propto t^\alpha, \alpha \approx 0.28 \). If we reproduce the analysis of \( L(t) \) in with our data we obtain \( \alpha = 0.26(2), \chi^2 / \text{d.o.f.} = 1.82/3 \) for \( tD_r > 20 \).

Finally, we compare the approach to the steady state to the dynamics of pressure fluctuations in the steady state by computing the time autocorrelation function of the instantaneous mean pressure, given by

\[
C_p(t) = \frac{\langle p(s)p(s + t) \rangle - \langle p \rangle^2}{\langle p^2 \rangle - \langle p \rangle^2}. \tag{8}
\]

This function is shown in Fig. 6 for \( \ell_p = 25 \) and \( \phi = 0.4 \). The correlation function decays exponentially,
FIG. 6. Time evolution of pressure $p$ (red squares), total cluster fraction $N_c/N$ (blue lines), and largest cluster fraction $N_1/N$ (blue circles) for a system with size $L = 400$, $\phi = 0.35$, and $\ell_p = 50$. $N_c/N$ is shown in (f) for 10 individual runs to emphasize its robust steady state. Snapshots (a–e) show a single run, for times that correspond to the points in the (f), labeled respectively.

The overshoot in pressure results from the onset of clustering, which dampens the swim and total pressure in the long-time limit. The steady state of pressure corresponds with the steady state of $N_c$, while $N_1$ continues to grow as the system coarsens.

allowing us to extract a relaxation time $\tau$, 

$$C_p(t) \simeq e^{-t/\tau},$$

We find that $\tau$ does not depend on density and coincides with $\tau_r$ for all our runs (Fig. 7). Therefore, even though the time evolution of the pressure in the approach to the steady state is density dependent, once the steady state has been reached the only time scale for pressure fluctuations is given by the single-particle rotational diffusion.

V. CONCLUSIONS

We have examined the effects of finite system size and of the kinetics of MIPS on the pressure of ABPs in two dimensions. In a dilute gas of ABPs the finite-size effects on pressure for both open (periodic) and closed (particles in a square box) boundary conditions are quantitatively similar to what one would expect for a thermal gas. At finite density, finite-size effects are pronounced even for the periodic case. We find that the box size has to be several times larger than the persistence length of the particles to obtain results representative of bulk behavior. This has implications for studies in strip geometries [35], where a careful control is needed to avoid spurious anisotropies in the stresses.

For parameter values corresponding to MIPS, we have examined the correlation between the relaxation of the mean pressure to its steady state value and the kinetics of clustering and phase separation. In this regime, the interplay between the decreasing swim pressure and the increasing direct pressure from interaction in the incipient clusters results in long, density-dependent time scales for approach to the steady state. The phase separation process shows two distinct dynamical regimes: a rapid growth corresponding to the formation of small clusters, followed by a slower regime of cluster coalescence and coarsening. These two regimes are reflected in the time evolution of the pressure that first grows rapidly during the small cluster nucleation when it is mainly controlled by the swim pressure of the gas, even overshooting
The total pressure, has, however, been shown to remain equal across the two phases, confirming that this minimal model can be described in terms of an effective thermodynamics. The relationship between the kinetics of MIPS and the relaxation of pressure to its steady state value additionally validates the use of equilibrium-like ideas as done in Ref. [32] to describe the coarsening kinetics.

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At very high packing fraction, approaching or even surpassing the closed-packed limit, there are larger discrepancies, but we do not consider this regime here.

A particle $i$ is part of cluster $C$ if it is interacting with any other disks in that cluster (i.e., if $r_{ij} \leq 2a$ for any $j \in C$).

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