Freezing and phase separation of self-propelled disks

Yaouen Fily,1,2 Silke Henkes,1,3 and M. Cristina Marchetti1,4

1Physics Department, Syracuse University, Syracuse, NY 13244, USA
2Martin A. Fisher School of Physics, Brandeis University, Waltham, MA 02454, USA
3ICSMB, University of Aberdeen, Aberdeen AB24 3UE, UK
4Syracuse Biomaterials Institute, Syracuse University, Syracuse, NY 13244, USA

We study numerically a model of non-aligning self-propelled particles interacting through steric repulsion, which was recently shown to exhibit active phase separation in two dimensions in the absence of any attractive interaction or breaking of the orientational symmetry. We construct a phase diagram in terms of activity and packing fraction and identify three distinct regimes: a homogeneous liquid with anomalous cluster size distribution, a phase-separated state both at high and at low density, and a frozen phase. We provide a physical interpretation of the various regimes and develop scaling arguments for the boundaries separating them.

I. INTRODUCTION

Active materials, consisting of self-driven units capable of converting stored or ambient free energy into systematic movement, provide a model for the dynamics of living systems on many scales [1]. Examples range from the cytoskeleton that controls cell motion [2], to bacterial suspensions [3] and mammalian tissues [4,5], to animal groups [6]. For the physicist, active materials are an exciting new class of nonequilibrium systems in which the interplay of activity, noise and interactions gives rise to a wealth of novel phases with unusual structural, dynamical and mechanical properties. In recent years non-living analogues of active systems have been developed that allow controlled quantitative studies. These include self-propelled colloids [7,8] and droplets [9,10], as well as vibrated mechanical walkers [11]. It was recently demonstrated that even the simplest model of an active system, consisting of self-propelled disks with overdamped dynamics and purely repulsive interactions, exhibits surprising behavior: in a range of activity and density the disks phase separate into a dense fluid phase and a gas phase [12,13]. The phase separation resembles that obtained in an equilibrium van der Waals fluid, but occurs here in the absence of any attractive interactions and is a direct result of the activity of the system that breaks detailed balance [14-16]. Monodispersed active repulsive particles have also been shown to freeze at high density into unique active crystals [13,17].

In this paper, we explore systematically the phase diagram of purely repulsive, polydisperse active particles in two dimensions by covering a wide range of parameters in the regime where non-equilibrium effects are expected. We track the onset of freezing and phase separation by monitoring the mean square displacement and number fluctuations, supported by visual observations of the state of the system (see typical snapshots in Fig. 1).

We identify three regimes in the phase diagram of the system, as shown in Fig. 2: a homogeneous fluid, a phase separated fluid, and a glassy phase. Using scaling arguments combined with the mean-field model developed in a previous paper [12], we provide a phenomenological estimate for the low density boundary for the onset of phase separation which is in qualitative agreement with the data. As argued in the literature [12-17], this boundary may be interpreted as a spinodal line. This view is supported by the analysis of the cluster size distribution (CSD), which shows a diverging typical cluster size as the transition is approached. Non-thermal features in the CSD persist away from the transition and present similarities with what has been seen in other active systems [18,19].

The phase separated region, previously identified below close packing [12,13], is found to persist above close packing. In this case, in a reverse-clustering phenomenon, a low-density hole spontaneously forms while active forces push the rest of the system into an over-compressed state. This “hole” phase is separated from the glassy phase by a homogeneous liquid phase (see Fig. 3). As activity is increased at constant density above close packing, the system first goes through a melting transition from a frozen solid into a homogeneous fluid before reaching a distinct second transition to a phase separated state (see Fig. 5).

At very high activity, a weakly interacting limit is reached and clustering disappears. This crossover, however, is not generic as it depends on the type of repulsive interaction.

Section 2 introduces our model of self-propelled soft disks and provides a detailed discussion of the connection to thermal systems and to athermal soft sphere packings in the zero-activity limit. In Section 3 we identify various phases in terms of the behavior of the mean square displacement and of number fluctuations and describe the phase diagram of the model. We also discuss the behavior of the cluster size distribution near phase separation. Section 4 develops a mean-field theory of phase separation in the region below close packing, including predictions for the low-density portion of the spinodal line. We end the section with a discussion of the freezing and high-
II. MODEL

We consider a two-dimensional system of \( N \) colloidal particles in an area \( L \times L \), modeled as disks \([12]\). The dynamics of the \( i \)-th disk is described by the position \( \mathbf{r}_i \) of its center and the orientation \( \theta_i \) of a polar axis \( \mathbf{n}_i = (\cos \theta_i, \sin \theta_i) \). The dynamics is overdamped and is governed by the equations

\[
\frac{\partial \mathbf{r}_i}{\partial t} = v_0 \hat{n}_i + \mu \sum_{j \neq i} \mathbf{F}_{ij}, \quad \tag{1a}
\]

\[
\frac{\partial \theta_i}{\partial t} = \eta(t), \quad \tag{1b}
\]

with \( v_0 \) the single-particle self-propulsion speed and \( \mu \) the mobility. The angular dynamics is controlled entirely by the Gaussian white rotational noise \( \eta(t) \) with zero mean and correlations \( \langle \eta(t)\eta(t') \rangle = 2\nu_r \delta(t-t') \), where \( \nu_r \) is the rotational diffusion rate. For simplicity, we neglect translational noise in Eq. (1a), although its effect is described in the mean-field model below (see section \([IV A]\)). The \( i \)-th disk has radius \( a_i \) and the radii are uniformly distributed with mean \( a \) and 20% polydispersity. The particles interact through soft repulsive forces \( \mathbf{F}_{ij} = F_{ij} \hat{r}_{ij} \), with \( \hat{r}_{ij} = (\mathbf{r}_i - \mathbf{r}_j)/r_{ij} \), \( r_{ij} = |\mathbf{r}_i - \mathbf{r}_j| \), and \( F_{ij} = k(a_i + a_j - r_{ij}) \) if \( r_{ij} < a_i + a_j \) and \( F_{ij} = 0 \) otherwise. The interactions are radially symmetric and do not directly couple to the angular dynamics. The system is simulated in a square box with periodic boundary conditions, and the box size \( L \) is adjusted to obtain the desired packing fraction \( \phi = \sum_i \pi a_i^2/L^2 \).

The model contains three time scales: \( a/v_0 \) is the time it takes a free particle to travel its own radius, \( \tau_r \equiv \nu_r^{-1} \) is the correlation time of the orientation, and \( (\mu k)^{-1} \) is the elastic time scale. We render the equations of motion dimensionless by using \( a \) and \( (\mu k)^{-1} \) as units of length and time, respectively. The parameter space is then explored by varying the scaled single-particle self-propulsion speed \( \tilde{v} \equiv v_0/(a\mu k) \), which controls the typical overlap due to activity, the scaled rotational diffusion constant \( \tilde{\nu}_r \equiv \nu_r/(\mu k) \), and the packing fraction \( \tilde{\phi} \). A further important dimensionless quantity is the Péclet number \( \text{Pe} = v_0/(a\nu_r) = \tilde{v}/\tilde{\nu}_r \), which describes the distance travelled by a free particle before it loses its orientation. There are three limiting cases in which the system exhibits familiar behavior.

First, when \( \tilde{v} \gg 1 \) interactions are negligible compared to active forces. Our soft disks can then pass through each other, behaving as a collection of free self-propelled particles, each performing an independent persistent random walk.

Secondly, in the absence of activity (\( \tilde{v} \to 0 \)) the system reduces to an athermal packing of soft spheres. This system is well known to exhibit a kinetic arrest with increasing density \([20][22]\), although the onset of rigidity depends on the protocol used to generate the dense packing. Numerical studies of the rheology of packed spheres have shown that the onset of a glassy state at a packing fraction \( \phi_G \) upon cooling is distinct from density phase separation transitions and present scaling arguments for the corresponding phase boundaries.
the jamming obtained in the limit of zero strain rate at \( \phi_{\text{RCP}} > \phi G \). For polydisperse repulsive disks \( \phi G \simeq 0.8 \) and \( \phi_{\text{RCP}} \simeq 0.84 \). Recent numerical work on active repulsive particles in both two and three dimensions has shown that activity shifts the glass transition to higher packing fractions, allowing the study of packings close to \( \phi_{\text{RCP}} \).

Finally, when \( \nu_r \to \infty \) activity becomes equivalent to a white Gaussian translational noise [12]. The system then maps to an equilibrium thermal fluid with an effective temperature \( T_\phi = \nu_r^2/(2\nu_r) \). This limit is only realized, however, if the orientational correlation time \( \tau_r = \nu_r^{-1} \) is much smaller than all time scales present in the system. In particular, \( \tau_r \) must be small compared to the mean free time between collisions, \( \tau_c \approx (2a_{\text{vol}}\rho)^{-1} \), with \( \rho = N/L^2 \) the areal density. The thermal limit is obtained for \( \zeta = \tau_r/\tau_c \approx 2 Pe\phi/\pi \ll 1 \). We did not, however, simulate this range of parameters which is prohibitively time consuming. The onset of phase separation has also been interpreted in term of a critical value of \( \zeta \), and a recent study pointed out the crucial role played by \( \zeta \) in active suspensions, where hydrodynamic interactions are important [26]. Finally, the thermal limit also requires \( \tau_r \) to be much smaller than the elastic time scale \( \tau_e = (\mu k)^{-1} \), i.e., \( \nu_r = \tau_e/\tau_r \gg 1 \).

In the following we mainly explore parameter values in the regime \( \zeta > 1 \) where the non-equilibrium dynamics responsible for phase separation is expected to control the behavior. Typical runs simulate \( N = 2000 \) particles during a time \( t = 10^4 \) in scaled units, at densities 0.1 \( \leq \phi \leq 1.2 \), scaled velocities \( 10^{-3} \leq \tilde{v} \leq 10 \) and rotational diffusion \( 0 \leq \tilde{\nu}_r \leq 10^{-2} \). The quantities of interest are averaged over the second half of the run as well as over two independent configurations, i.e., two different realizations of the random initial positions, angles and radii of the particles, and angular noise. For the runs performed in the absence of angular noise (\( \tilde{\nu}_r = 0 \)), we lose ergodicity since time averaging does not average over particle orientations which are frozen for the whole duration of the run. This is addressed by using a higher number of independent configurations (10 instead of 2) for these runs. Ergodicity is also lost for glassy configurations, however as long as \( \tilde{\nu}_r \) is finite, the system still explores the local cage structure around each particle [27].

III. PHASE SEPARATION AND MELTING

The phase behavior of the system, as obtained from simulations of our model, is summarized in Fig. 2. We identify three regimes: a homogeneous fluid phase, a frozen state at high packing fraction and relatively low activity, and a regime where the system is phase separated. The phase separated regime exists in an intermediate range of packing fraction and activity and it changes continuously from a high density cluster surrounded by a gas at packing fractions below close-packing, as shown in Fig. 1b, to a “hole” of gas phase inside a densely packed liquid at packing fractions above close-packing, as shown in Fig. 1c.

![Color map of the exponents \( \alpha \) (MSD) and \( \beta_e \) (number fluctuations) in the \((\phi, \tilde{v})\) plane for \( \nu_r = 5 \times 10^{-4} \) showing the three phases of the system: homogeneous liquid, phase separated, and glassy. The boundary of the glassy (resp. phase separated) phase is defined as the set of points where \( \alpha = 0.5 \) (resp. \( \beta_e = 1.5 \)). The dotted line is the mean-field spinodal line given by Eq. (3) for \( D = 0 \) and corresponds to \( \phi = \phi_1 + \phi_2/Pe \) where \( Pe \) is the Péclet number. \( \phi_1 = 0.3 \) and \( \phi_2 = 2.2 \) are fitted to match the lower left side of the separated phase boundary (see section IV B). The dashed and dotted-dashed lines are linear fits to the melting line and lower right side of the separated phase boundary, respectively (see section IV B).](image)

A. Frozen state and active melting

To quantify the onset of the frozen state we have evaluated numerically the mean square displacement (MSD) \( \langle [\Delta r(t)]^2 \rangle = N^{-1} \sum_i \langle [r_i(t) - r_i(0)]^2 \rangle \) in the center of mass frame [23]. An individual self-propelled disk performs a persistent random walk, with MSD given by

\[
\langle [\Delta r(t)]^2 \rangle = 4D_0 \left[ t + \frac{e^{-\nu_r t}}{\nu_r} - 1 \right],
\]

with \( D_0 = \frac{v_0^2}{2\nu_r} \) the diffusion coefficient. The MSD is ballistic at short times and diffusive for \( t \gg \nu_r^{-1} \), where \( \langle [\Delta r(t)]^2 \rangle \sim 4D_0 t \). It was shown in Ref. [12] that at intermediate packing fractions, before the system phase separates, the MSD can still be fitted by the form given in Eq. (3), but with a renormalized local self-propulsion speed \( v_0 \to \nu(\rho) \) that accounts for the motility suppression due to caging by neighboring disks and an effective diffusivity \( D_r(\rho) = \frac{v_r(\rho)^2}{2\nu_r} \). This mean-field type approximation works well provided the self-propelled particles experience many collisions before their direction of persistent motion is randomized by rotational diffusion, i.e., in the regime \( \zeta >> 1 \).
The MSD evaluated numerically over a range of packing fractions is shown in Fig. 3 as a function of time. Although the effective diffusion constant is greatly suppressed at intermediate packing fraction, the long-time behavior remains diffusive. At high packing fraction and low activity, however, the MSD is bounded, indicating a frozen state. The boundary between fluid and frozen state is identified by measuring the exponent \( \alpha \) controlling the long-time behavior of the MSD, \( \langle \Delta r(t)^2 \rangle \sim t^\alpha \) and choosing a threshold value \( \alpha_x = 0.5 \) to separate the “frozen” state (\( \alpha < \alpha_x \)) from the liquid state (\( \alpha > \alpha_x \)).

We note that an identification of the transition based on a drop of the long time diffusion constant or simply the final value of the MSD would yield similar results. The results are displayed in the phase diagram of Fig. 2 in the form of a color plot of the exponent \( \alpha \) in the \((\phi, \tilde{v})\) plane. The blue solid line is the locus of points where \( \alpha = \alpha_x \).

**B. Phase separation**

To identify the phase separated region, we have measured the number fluctuations, i.e. the spatial variance \( \langle (\Delta N)^2 \rangle \) of the number of particles in a subsystem as a function of the average number \( N_s \) of particles in the subsystem. The results are shown in Fig. 4 for a range of packing fractions. For large subsystem sizes, a power law \( \langle (\Delta N)^2 \rangle \sim N_s^\beta \) is observed, with \( \beta = 1 \) at low density in the homogeneous fluid (ideal gas limit) and \( \beta = 2 \) in the phase separated state. It is known that jammed disordered packings of repulsive particles are hyperuniform, i.e., the number fluctuations inside a large window grow slower than the volume of the window (in three dimensions). This yields a value \( \beta < 1 \) in the frozen state obtained at low activity and high density. The inset of Figure 4 shows the exponent \( \beta \) as a function of packing fraction at finite activity \( \tilde{v} = 0.1 \) (solid line, blue online) and its thermal counterpart in the low temperature limit \( \beta_0 = \lim_{T \to 0} \beta \) with \( T = k_BT/(ka^2) \) (dashed line, green online). The latter clearly displays the hyperuniform nature of number fluctuations, also apparent in Fig. 4 at low \( \tilde{v} \). In fact, the exponent \( \beta_0 \) characterizing hyperuniformity in the passive limit can also be measured in the active system by taking the limit \( \tilde{v} \to 0 \), yielding similar results but at much greater computational cost. To account for hyperuniformity, we introduce an effective exponent \( \beta_x = \beta(\tilde{v}) - (\beta_0 - 1) \). The crossover between a homogeneous fluid and a phase separated state is of course smoothed out by finite size effects and we define a phase separated state as one with \( \beta_x > \beta_x = 1.5 \). This value is chosen as the one that best matches the results of direct visual observation of the state of the system.
FIG. 5. The long time MSD exponent $\alpha$ (dashed lines) and the number fluctuation exponent $\beta$ (solid lines) as functions of the self-propulsion speed $\tilde{v}$ for a range of packing fractions $\phi$ above random close packing. Note the convergence to $\beta \approx 0.8$ in the low $\tilde{v}$ limit due to hyperuniformity. The jump in the exponents signal the melting transition ($\alpha$) and the onset of phase separation ($\beta_s$). The figure shows that for each fixed value of $\phi$ melting and phase separation occur at different values of $\tilde{v}$.

C. Cluster Size Distribution

On Fig. [we further characterize the system by measuring the cluster size distribution (CSD), i.e. the average fraction $p(n)$ of clusters containing $n$ particles. At low density, we find that the CSD is well described by a power law with an exponential cut-off $n_0$: $p(n) = p(1) e^{-n/n_0}/n$. The cluster size cut-off $n_0$ increases with density and diverges at the onset of phase separation where the CSD reduces to $p(n) \sim n^{-1}$. In the phase separated region, the CSD exhibits a narrow peak at a value $N_c$ equal to the average number of particles in the dense phase while the dilute phase contributes the same cut-off power law found in the homogeneous state described above. As density is increased, $N_c$ increases until the dilute phase disappears completely ($N_c = N$) and a homogeneous dense phase is obtained, at which point $p(n)$ is simply $\delta_{n,N}$ where $\delta$ is the Kronecker symbol.

The presence of the $n^{-1}$ factor in the CSD contrasts with the exponential form $p(n) \sim e^{-n/n_0}$ we observe in the thermal case (data not shown), and proves that even well below the onset of phase separation, the system cannot be described by an effective temperature. At extreme dilution, when the particles' orientations decorrelate much faster than the mean free time ($\zeta \ll 1$, not explored in our simulations), one should recover athermal-like CSD.

Another striking feature is the extreme slowness of nucleation processes. Indeed, the onset of phase separation is akin to a first order equilibrium transition with distinct coexistence and spinodal curves, and macroscopic clusters can form through either nucleation or spinodal decomposition (the existence of nucleation-type growth was shown in Ref. [13] and the existence of hysteresis at the transition was confirmed in our simulations in the largest systems). Nucleation, however, requires such large seeds and long times that one can observe the divergent lengthscale associated with the spinodal transition, which would otherwise not be accessible.

Finally, the functional form of the CSD is similar to that obtained in Refs. [18, 19] by solving mean-field rate equations for cluster sizes. There is however a major difference: after the cut-off cluster size diverges, these models exhibit a bimodal CSD but no actual phase separation or hysteresis. Further, this remains true even if the rate equations, originally written for aligning particles, are modified to account for the fact that the average speed of a cluster decays with its size (data not shown).

IV. DISCUSSION

Several features of the phase diagram deserve comment. First we show on Fig. [the outline of the frozen and phase separated regions (i.e. the locus of points where $\alpha = \alpha_x$ and $\beta_x = \beta_x$, respectively) for various values of the dimensionless angular noise $\tilde{\nu}$, in the $\phi - \tilde{v}$ and $\phi - \tilde{v}$ planes.

At high activity ($\tilde{v} \geq 1$), self-propulsion dominates over repulsion and our soft disks can pass through each other. The system becomes a homogeneous fluid of independent self-propelled particles. This crossover clearly depends on the details of the repulsive interaction: it is pushed to higher velocities as the particles become stiffer and should disappear altogether for infinitely hard particles.

Conversely, the transition between homogeneous and phase separated fluid at low activity has features of a genuine critical point, although more work will be needed to establish this. When plotted in the $(\tilde{v}, \phi)$ plane (see right frame of Fig. [the phase boundaries seem to collapse on a critical point $\phi^* \simeq 0.6$ and $\tilde{v}^* \simeq 10$. This
A. Mean-Field Theory and Phase Separation Below Close Packing

The dynamics of a homogeneous fluid of self-propelled particles has been described by an effective continuum theory where motility suppression is incorporated in a density-dependent propulsion speed \( \nu(\rho) \). The mean-field model applies when particles experience many collisions before their directed motion becomes uncorrelated by rotational noise, i.e., for \( \zeta > > 1 \). In this regime the large-scale dynamics is described by continuum equations for the density \( \rho(r,t) \) and the polarization density field \( p(r,t) \) that describes the local orientation of the particles’ axis of self-propulsion. Although in the absence of alignment interactions, self-propelled disks cannot exhibit a state with orientational order, substantial correlations can build up in the local polarization for small values of the rotational diffusion rate. The continuum equations are given by

\[
\begin{align*}
\partial_t \rho &= -\nabla \cdot [\nu(\rho)p - D(\rho)\nabla \rho] , \\
\partial_t p &= -\nu_r p - \frac{1}{2} \nabla [\nu(\rho)p] + K\nabla^2 p ,
\end{align*}
\]

where for generality we have included a translational diffusion coefficient \( D(\rho) \) that would arise from thermal noise (not included in our numerics) or from interactions. For times \( t > \nu_r \), one can neglect the time derivative of the polarization in Eq. \( (3b) \) relative to the damping term, solve for \( p \), and eliminate \( p \) from Eq. \( (3a) \). To leading order in the gradients the dynamics is then described by a single nonlinear diffusion equation, given by

\[
\partial_t \rho = \nabla \cdot \left[ D(\rho) \nabla \rho \right] ,
\]

with effective diffusivity

\[
D(\rho) = D(\rho) + \frac{\nu^2(\rho)}{2\nu_r} \left( 1 + \frac{d \ln \nu}{d \ln \rho} \right) .
\]

The linear stability of a homogeneous state of constant density \( \rho = \bar{\rho} \) can be analyzed by examining the dynamics of density fluctuations, \( \delta \rho = \rho - \bar{\rho} \), that obey the linear diffusion equation

\[
\partial_t \delta \rho = D(\bar{\rho})\nabla^2 \delta \rho .
\]

The vanishing of \( D(\bar{\rho}) \) signals the instability against the growth of density fluctuations.

To obtain an explicit expression for the instability line, we need an estimate for the mean-field self-propulsion speed, \( \nu(\rho) \). At low density, the slowing down of particles is due to the time lost during binary collisions. The effective self-propulsion speed can then be written as \( \nu(\rho) \approx \nu_0(1 - \tau_c/\tau) \) where \( \tau_c = 1/(2\nu_0 \nu_r) \) is the mean-free time between collisions and \( \tau \) is the average delay caused by each collision. Considering for simplicity stiff particles (as appropriate for \( \bar{\nu} << 1 \)), we estimate \( \tau \) in two limiting cases. When particles maintain their orientation throughout the collision, the duration of a collision...
is simply the time it takes the particles to move around each other, or \( \tau_1 \sim a/v_0 \). If, on the other hand, particles reorient during the collision, the associated delay \( \tau_2 \) is the reorientation time \( \nu^{-1}_r \). Since the total collision time \( \tau \) is controlled by the faster of the two mechanisms, we assume additivity of the rates, obtaining \( \tau^{-1} \sim \tau_1^{-1} + \tau_2^{-1} \).

The effective velocity is then given by \( v(\rho) = v_0(1-\phi/\phi^*) \) where \( \phi \approx \rho/(\pi a^2) \) and \( \phi^*(Pe) = 2(\phi_1 + \phi_2/Pe) \), with \( \phi_1,2 \) constants of order 1 that depend on the details of the collisions. Inserting this estimate for \( v(\rho) \) in the expression for \( D(\rho) \), and setting \( D(\rho) = 0 \), yields the condition for the linear instability or mean-field spinodal line that can be written as

\[
D(\rho) = D(\rho) + \frac{v_0^2}{2\nu_r} (1 - \phi/\phi^*) (1 - 2\phi/\phi^*) . \tag{7}
\]

If we neglect \( D \), phase separation occurs at \( \phi_s = \phi^*(Pe)/2 = \phi_1 + \phi_2/Pe \), which further reduces to the constant value \( \phi = \phi_1 \) at high Péclet numbers or in the absence of angular noise. In this limit the transition line in the \( \phi - \nu \) plane would be a vertical line at \( \phi = \phi_1 \). This is indeed what we observe when \( \nu_r = 0 \) (see left frame of Fig. 7). Above \( \nu \approx 0.1 \) particle overlap becomes, however, significant and suppresses phase separation. A fit to the simple estimate \( \phi_s = \phi^*(Pe) \) is shown in Fig. 2 as a dotted line. We note that that close to the putative critical point, when the Pe\( ^{-1} \) term in \( \phi^* \) becomes dominant, our expression for the spinodal line reduces (up to numerical factors) to that obtained in Ref. 13 for the coexistence line via an analysis of the stability of a gas-cluster interface. This is not surprising as one expects the spinodal and the binodal lines to merge at the critical point.

A finite value of \( D \) yields a lower bound to the value of \( \nu \) required for the onset of phase separation, as discussed earlier. This can be seen by neglecting the density dependence of \( D(\rho) \). Eq. (7) is then easily solved for the spinodal boundary, with the result

\[
\phi_s = \frac{\phi^*(Pe)}{4} \left( 3 + \sqrt{1 - \left( \frac{Pe_m}{Pe} \right)^2} \right) , \tag{8}
\]

where \( Pe_m = 4\sqrt{D/(a^2\nu_r)} \) represents the a minimum value of \( Pe \) required for phase separation.

For finite orientational persistence time \( \nu_r^{-1} \), we need to retain the dynamics of polarization. The linear stability of the homogeneous state can then be examined by linearizing Eqs. (3) around \( \rho = \rho_0 \) and \( p = 0 \). Working in Fourier space, we let \( \{ \delta \rho (r, t), \delta p (r, t) \} = \sum_q \{ \delta \rho_q (t), p_q (t) \} e^{iq \cdot r} \). The time evolution of the Fourier amplitudes is governed by the coupled equations

\[
(\partial_t + Dq^2) \delta \rho_q + ivq \cdot p_q = 0 , \tag{9}
\]

\[
(\partial_t + \nu_r + Kq^2) p_q + \frac{1}{2} (v + \nu v^*) iq \delta \rho_q = 0 . \tag{10}
\]

where \( v' = dv/d\rho \) and all quantities are evaluated at the homogeneous density \( \rho_0 \). The decay/growth of fluctuations is governed by the eigenvalues of Eqs. (10). The stability is controlled by the eigenvalue \( s_+ (q) \), with dispersion relation

\[
s_+ (q) = -\frac{1}{2} \left[ \nu_r + (K + D)q^2 \right] + \frac{1}{2} \sqrt{\nu_r + (K - D)q^2} = 2q^2 (v + \nu v^*) . \tag{11}
\]

\[\text{FIG. 8. Schematic dispersion relation } s_+ (q) \text{ for } D > 0 \text{ and } D < 0.\]

For small wave vectors, the dispersion relation can be approximated as \( s_+ (q) \approx -q^2 D/\nu - q^4 B \), with \( B = 4\nu v^2 (v + \nu v^*) [2(K - D) - v(v + \nu v^*)/\nu] \). The rate \( s_+ \) becomes positive for \( D < 0 \), indicating the growth of a sinusoidal modulation of the density. The growth rate as a function of the wavevector \( q \) is shown in Fig. 8 and has the typical behavior expected in a spinodal regime. All modulations with \( q < q_0 = \sqrt{-D/B} \) are unstable. The maximum growth rate is obtained at \( q_{max} = q_0/\sqrt{2} \). At the onset of the instability modes of wavevector \( q_{max} = \sqrt{-D/(2KD)} \) will dominate experimental observations.

### B. Freezing and Phase Separation Above Close Packing

We observe an arrested phase at high density and low self propulsion speed. While the existence of dynamically arrested states of active systems has been reported before, the dynamics of the freezing transition has only started to attract interest recently. Berthier and Néel have reported a shift of the glass transition of active particles to packing fractions higher than those known for thermal systems, in both two and three dimensions. The shift grows with a parameter controlling the persistence time of the single-particle dynamics, essentially our \( \nu_r^{-1} \). Both simulations consider polydisperse hard particles, which differ from our soft-disk system in that they cannot be compressed beyond the random close packing (RCP) fraction, \( \phi_{RCP} \approx 0.522 \) in two dimensions. On the other hand, below RCP and in the limit \( k \to \infty \), the interparticle overlap for soft disks vanishes and hard and soft particles should exhibit similar behavior. More precisely, for \( \phi < \phi_{RCP} \) passive soft disks will behave like hard ones provided the interaction time scale \( (\mu k)^{-1} \) is short compared to the persistence
time $\nu^{-1}$, i.e., $\tilde{\nu} = \nu_r/(\mu k) \ll 1$. We then expect active soft disks to behave like hard ones provided $\tilde{\nu} \ll 1$ and $\tilde{v} = v_0/(a \mu k) \ll 1$. From Fig. 2, we extract the onset of a glassy state in the limit $\tilde{v} \rightarrow 0$ at $\phi_G(\tilde{v} \rightarrow 0) = 0.86 \pm 0.02$ for $\tilde{\nu} = 5 \times 10^{-4}$, above the thermal $\phi_G \approx 0.8$ and consistent with the value close to $\phi_{RCP}$ reported by Berthier.  
It is known that athermal homogeneously sheared systems jam at $\phi_{RCP} > \phi_G$ in the limit of vanishing strain rate. One can then speculate that activity, in spite of injecting energy locally rather than globally, be equivalent to a homogeneous shear in the limit $\tilde{\nu} \rightarrow 0$. Finally, we stress that a shift of the kinetic arrest to values of packing fractions above the glass transition was also reported for self-propelled disks with aligning interaction.

At finite $v_0$, the glass transition line shifts to higher packing fractions (Fig. 2). In addition, the phase separated state still exists at high $v_0$ and packing fraction above $\phi_{RCP}$, but is separated from the glassy phase by an intermediate region of homogeneous liquid. This gap between glass and phase separated state for $\phi > \phi_{RCP}$ is perhaps the most surprising feature of the phase diagrams in Figs. 2 and 7. Inspection of the dynamics in this region clearly shows no significant clustering and a substantial amount of local rearrangements, indicative of a fluid phase (see supplementary movie 1(d)). The gap is also apparent from Fig. 5 showing the behavior of the exponents $\alpha$ (MSD) and $\beta$ (number fluctuations) along vertical (i.e. constant $\phi$) slices of the phase diagram of Fig. 2 above close packing. Both the glass transition line and the phase separation at high density can be understood as arising from a balance between the passive pressure of a densely packed system and the active forces due to self-propulsion. In the absence of activity, the pressure of passive soft disks repelling via one-sided harmonic springs of stiffness $k$ scales linearly with the particle overlap $\delta$, which is positive at packing fractions above RCP, i.e., $p = k \delta$. Even though the packings are disordered and rearrangements are non-affine, the athermal equation of state in the solid phase remains linear with $p = p_0(\phi - \phi_{RCP})$ and $p_0 = 0.34$. In the active system, a pressure $p_a \approx v_0/2a\mu$ arises from self-propelled particles pushing against their neighbors. Balancing these two pressures yields a critical velocity in dimensionless units $\tilde{v}^* = v^*/(a \mu k) \sim u(\phi - \phi_{RCP})$, with $u$ a dimensionless parameter that should be compared to the full pressure balance at $u^* = 2p_0/k = 0.68$. The glass transition line can be fitted by this expression with $u = 0.07$, suggestive of a simple melting criterion where active particles squeeze through gaps between their neighbors at $\sim 10\%$ of the passive interparticle pressure. We stress that in the range of $\tilde{\nu}$ we explored ($\tilde{\nu} = 0$ to $10^{-2}$), the glass transition line is indeed nearly independent of $\tilde{\nu}$, and depends only on $\phi$.

In contrast, the boundary between the homogeneous liquid and the phase separated state at packing fractions above $\phi_{RCP}$ depends on both $\phi$ and $\tilde{\nu}$. When $\tilde{\nu} \rightarrow 0$, this boundary line and the glass transition line converge at $\phi_{RCP}$ when $\tilde{v} \rightarrow 0$ (see Fig. 7). The boundary line may again be interpreted as a pressure balance, this time at the interface that arises in the phase separated state between the dense liquid and the gas. First, we note that the surface of the dense phase consists of a highly polarized layer of particles pointing inwards. Indeed, particles pointing away from the dense phase immediately leave it. The active pressure exerted by this layer on the dense phase is $p_a \sim \gamma v_0/(2a\mu)$ where $v_0/\mu$ is the magnitude of the active force exerted by a single particle and $2a$ is the average distance between particles at the interface. The dimensionless factor $\gamma$, of order 1, captures information about the distribution of orientations in the interfacial layer and its thickness ($\gamma = 1$ for a single layer of particles all oriented normal to the surface). The passive pressure in the dense phase, on the other hand, is at least $p = p_0(\phi - \phi_{RCP})$ with $\phi$ the average packing fraction in the system. Balancing the two yields again a critical velocity $\tilde{v}^* = u(\phi - \phi_{RCP})$, where $u$ should now be compared to $u^*/\gamma$. It fits the phase separation boundary at $\tilde{\nu} = 0$ for $u = 0.7$, indicating that $\gamma \approx 1$. While melting requires overcoming only about $10\%$ of the passive pressure, phase separation occurs when activity is large enough to fully balance the passive pressure due to elastic forces. For $\tilde{\nu} > 0$, the gap for the onset of phase separation can be accounted for by using $\tilde{v}^* = u(\phi - \phi_{RCP}) + w(\tilde{\nu})$. The fit gives $u = 0.7$, independent of $\tilde{\nu}$, and $w \sim \tilde{\nu}^{1/2}$ at small $\tilde{\nu}$. More work is needed to understand whether the existence of a gap between melting and phase separation is generic for soft interparticle potentials.

V. SUMMARY

In this article, we present a numerical characterization of the phase diagram of self-propelled particles with only repulsive interactions and no alignment that shows the existence of three distinct phases in the system: a homogeneous liquid, a phase-separated liquid, and a glassy state. We show evidence that the phase separated region is bounded at low Péclet number by a critical point (Fig. 7), including scaling arguments for the spinodal line at both low and high packing fraction, consistent with the idea of a first order phase transition. Analysis of the CSD shows that the typical cluster size diverges as the spinodal line is approached, while non-thermal effects persist well below the transition. We also show the existence of a frozen phase at high packing fraction and low active self-propulsion and find a novel high density active liquid phase in the gap between the frozen and phase separated states. More work is required to provide a detailed characterization of the critical point at low Pe, in particular to differentiate spinodal and binodal lines taking nucleation and finite size effects into account. The existence of an active glass or jamming transition different from both its thermal and sheared counterparts is an intriguing result that deserves further exploration.
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