Phase segregation in a system of active dumbbells

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A systems of self-propelled dumbbells interacting by a Weeks–Chandler–Anderson potential is considered. At sufficiently low temperatures the system phase separates into a dense phase and a gas-like phase. The kinetics of the cluster formation and the growth law for the average cluster size are analyzed.

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1. Introduction

Active matter generally refers to systems of self-propelled units, which move extracting energy from internal sources or from the environment. This leads to nonequilibrium systems with peculiar properties with no passive counterpart. An important difference with respect to more classic nonequilibrium systems is due to the different origin of nonequilibrium that is localized in each particle rather than in the system’s boundaries. Important examples of active matter are schools of fishes, bird flocks, bacterial colonies, insects, etc.1,2 They exhibit interesting collective properties like clustering,3–11 giant fluctuations,12,13 nonequilibrium effective
temperature, unexpected rheological properties and nontrivial behavior under shear.

In this paper, we will study a mesoscopic two-dimensional system of active particles immersed in an implicit solvent, ignoring hydrodynamic interactions. This approximation, better describing low density systems, permits a simplified treatment of the model, allowing to study collective properties of a large number of particles. In previous works, it has been shown that a suspension of self-propelled spherical particles phase separates into compact clusters and a gas-like phase under certain conditions of temperature and density. The behavior of swarms in systems of active rods has also been studied.

Our aim here is to analyze the effects of orientational order for the aggregation properties of active particles. Orientational order is very common in active matter and it is not taken into account in studying spherical objects. We consider a system of dumbbells, each consisting of two colloids linked by a spring and with a constant propulsive force acting along the direction connecting the two beads. This model is appropriate for describing bacterial systems and will be presented in Sec. 2. The length of the dumbbells will be really lower compared with that of the rods in the models so far considered. In particular, we expect that this length is not large enough to create clusters with parallel moving particles, like in Refs. 6 and 7, but sufficient to change significantly in both the phase diagram found for spherical particles and the behavior of the clusters. Our results for the phase behavior and the kinetics of aggregation will be given in Secs. 3 and 4, respectively.

2. Active Dumbbell Model

Our model consists of a system of $N$ dumbbells confined in a two-dimensional box with periodic boundary conditions and immersed in a solvent at temperature $T$. Each dumbbell is composed of two spheres of the same diameter $\sigma$ and mass $m$, which are linked via a finitely extensible nonlinear elastic (FENE) spring, described by the potential:

$$V_F(r) = -\frac{1}{2}kr_0^2 \ln \left[1 - \left(\frac{r}{r_0}\right)^2\right],$$

where $k$ is the spring constant and $r_0$ is the maximum extension distance between the two beads of the same dumbbell. Each bead also interacts with the other $2N - 1$ by a Weeks–Chandler–Anderson potential:

$$V_{WCA}(r) = \begin{cases} 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] - 4\epsilon \left[\left(\frac{\sigma}{r_c}\right)^{12} - \left(\frac{\sigma}{r_c}\right)^{6}\right], & r \leq r_c, \\ 0, & r > r_c, \end{cases}$$

which is a Lennard-Jones potential truncated in its minimum $r_c = 2^{1/6}\sigma$ and shifted by $\epsilon$, so that it does not present any attractive part. The bath is described by a
Langevin equation so that for each bead the equation of motion is

\[ m \ddot{r}_i(t) = -\gamma \dot{r}_i(t) - \frac{\partial V}{\partial r_i} + \sqrt{2k_B T} \xi_i(t) + F_a, \]

where \( r_i \) is the position of each bead, \( V = V_F + V_{WCA} \) is the total potential acting on each bead, \( \gamma \) is the friction coefficient, \( k_B \) is the Boltzmann constant, \( T \) is the temperature and \( \xi \) is a Gaussian white noise, with zero mean and variance \( \langle \xi_i(t)\xi_j(t') \rangle = \delta_{ij}\delta(t - t') \). \( F_a \) is a force which represents the self-propulsion: It is constant in modulus and is exerted along the direction of the line connecting the beads of each dumbbell. Each dumbbell is polar with a rear and a front bead and this completely defines the direction of self-propulsion.

Our simulations are performed using a second-order integrator for the Langevin equation introduced by Vanden-Eijnden and Ciccotti. Every constant is expressed in terms of Lennard-Jones reduced units \( m, \sigma \) and \( \epsilon \). The FENE parameters are set to \( k = 30\frac{\sigma}{\epsilon} \) and \( r_0 = 1.5\sigma \) and the friction to \( \gamma = 10\frac{m}{\tau} \), choosing \( k \) and \( \gamma \) so that the dumbbells are almost rigid. In the simulations we set \( m, \sigma \) and \( \epsilon \) equal to one using as time constant unit \( \tau = \sqrt{\frac{m\sigma^2}{\epsilon}} \) with maximum time-step \( \delta t = 10^{-2}\tau \).

We explore the behavior of our system by varying the temperature \( T \), the modulus of the active force \( F_a \) and the surface fraction \( \phi = \frac{N\sigma^2}{2A} \), which is the area fraction covered by the dumbbells with respect to the total area \( A \) of the system. An important parameter for this system is the Peclet number \( Pe = \frac{2F_a\sigma}{k_BT} \), defined in general as \( \frac{LU}{D} \), where \( L \) is a typical length of the system, here chosen as \( \sigma \), \( U \) is the advection velocity, given by \( \frac{F_a}{\gamma} \), and \( D \) is the diffusion constant, related only to the heat bath, in our case given by \( \frac{k_BT}{2\gamma} \). This number estimates the ratio between the advective transport rate and the diffusive transport rate. Another important parameter is the active Reynolds number \( Re_a = \frac{mF_a}{\gamma\nu\sigma} \), defined in general as \( \frac{LU}{\nu} \), where \( \nu \) is the kinematic viscosity, which represents the ratio between inertial and viscous forces. Here, we have set \( L = \sigma \), \( U = \frac{F_a}{\gamma} \) and \( \nu = \frac{3\sigma^2}{m} \). In our simulations, we always choose values of \( F_a \) such that \( Re_a \ll 1 \) in analogy with the Stokes regime.

3. Phase Behavior

When compared with the passive system, our first observation is that the presence of the active force generally gives rise to larger density fluctuations and different aggregation behavior, with more visible effects at increasing values of the Peclet number (see Fig. 1). A mechanism for the formation of clusters is schematically shown in Fig. 2. When dumbbells have directions pointing in average toward a common center, the active forces just nullify each other forcing the particles to remain close and a cluster is formed. This can happen only when the direction of motion is mainly due to the action of \( F_a \), and only slightly affected by thermal fluctuations (i.e. at large \( Pe \)). On the other hand, at small \( Pe \), or large \( T \) and fixed other parameters, dumbbells will not move toward the same center for a long time,
and stable clusters are not expected. Due to these different behaviors, one wonders if a phase transition occurs in this system.

In order to study the phase behavior we decided to evaluate the number $N_{\text{nd}}$ of pairs of dumbbells with their center of mass within a certain distance $r_{\text{nd}}$ (nearest dumbbells). We choose $r_{\text{nd}} = 1.1\sigma$, including only dumbbells which are parallel and very close (different choices for $r_{\text{nd}}$ would give similar results). The behavior of $N_{\text{nd}}$ is shown in Fig. 3 for a system with $\phi = 0.4$, $N = 15915$, $F_a = 1$, and different temperatures. We found a critical value $T_c \approx 0.03$ for the temperature, such that for $T > T_c$, $N_{\text{nd}}$ fluctuates around a fixed value, while $N_{\text{nd}}$ grows and becomes larger under $T_c$, indicating the formation of stable big clusters, instead of small and

![Fig. 1.](image1) (Color online) On the left: a typical configuration of a system without active force in equilibrium at $T = 0.01$ and $\phi = 0.4$ ($N = 2546$ dumbbells). On the right: a snapshot during the evolution of the same system with $F_a = 1$ (Pe = 200). The passive system shows small fluctuations and is generally uniform. Conversely, the active system presents large fluctuations. The size of the system is expressed in units of $\sigma$.

![Fig. 2.](image2) (Color online) Aggregation mechanism: The arrows represent the direction of active forces. If the Peclet number is sufficiently large, these also represent the direction of motion. Then, when a group of dumbbells collide moving toward a common center, active forces nullify each other and a small cluster can be formed.
unstable ones, as also confirmed by direct inspection of configurations (see the panels (1) and (3) of Fig. 4). These large clusters can sometimes partially break and reform, since there are no attractive forces among the beads, which could keep the cluster always compact. Therefore, we considered $N_{nd}$ as a useful parameter for identifying the different states of the system and the occurrence of a stationary behavior.

For a deeper understanding of the nature of the transition, we decided to measure the distribution of the local value of the surface fraction $\phi(r)$, coarse-graining this quantity over cells of size $10\sigma$, and taking 100 independent configurations under stationary conditions. From these data we constructed a histogram of $\phi(r)$ for different values of $T$ and overall concentration $\phi$. The results are shown in Fig. 4. Above $T_c$ the system fluctuates around the value of $\phi$, for any value of $\phi$, with the width of the distributions that decreases when $T$ increases. Under $T_c$ we observe the occurrence of bimodal distributions that indicates the presence of two different phases. Fixing the value of $T < T_c$ and varying $\phi$, we notice that the values of the two peaks remain the same. For values of $\phi$ external to the interval defined by the two peaks, the bimodal feature of the distributions is lost.

From the previous observations we conclude that for $T < T_c$ the system undergoes a phase separation, characterized by the coexistence of two phases with different densities, given by the values of the two peaks of density distributions, in some analogy with the behavior of a liquid–gas system. However, the behavior of the particle aggregates in the dense phase is typical of this active system and cannot be directly compared with the one of the usual liquid phase.

Fig. 3. (Color online) Evolution of the number of pairs of nearest dumbbells $N_{nd}$ at different temperatures. For $T > T_c \approx 0.03$ $N_{nd}$ remains constant with small fluctuations. For $T \approx T_c$ large fluctuations can be observed, still indicating a nonaggregated system. For $T < T_c$ $N_{nd}$ starts to grow larger and larger, reaching a stationary value around which, sometimes, large fluctuations are still observed. Time is expressed in units of $\tau$. 

Phase segregation in a system of active dumbbells
Finally, we studied the behavior of the cluster average size $L(\tau)$ during phase separation. The long time behavior of $L(\tau)$ has been previously studied for different kinds of active systems.\textsuperscript{21–25} For active colloids in two dimensions\textsuperscript{9,25} a power law $L(\tau) \sim \tau^{\alpha}$ is found with $\alpha \simeq 0.25 - 0.28$.

In our case we studied the kinetics of phase separation at concentrations $\phi = 0.4$ ($N = 267017$), 0.6 ($N = 400526$) with $T = 5 \cdot 10^{-3} < T_c$, starting from random initial configurations. Patterns at different times are shown in Fig. 5 for the two values of $\phi$. The clusters of dumbbells are identified by coarse-graining the system on square cells of side $4\sigma$ and denoting as filled cells the ones with local surface concentration $\phi(\mathbf{r}) \geq \phi_{\text{th}}$ where $\phi_{\text{th}} = 0.7$ is a threshold value. The value for the square cell size was fixed as the optimal one to have homogeneous clusters by using an eye-guided criterion.

Fig. 4. (Color online) First two rows: Distributions of the local surface concentration $\phi(\mathbf{r})$ for $\phi = 0.4$ (first row) and $\phi = 0.6$ (second row), respectively with $N = 15915$ and $N = 23873$, and three different temperatures ($T = 0.5$ (a), (b); $T = 0.05$ (c), (d); $T = 0.01$ (e), (f)). For $T > T_c$ the system is in a single phase, with mean value corresponding to $\phi$, Gaussian distributions for low $\phi$ ((a),(c)) and non-Gaussian for high $\phi$ ((b),(d)). Under $T_c$ the system phase separates into an aggregated phase and a gas-like phase. The peaks of the bimodal distributions are at the same position for different values of $\phi$. Last row: snapshots for the system with $\phi = 0.4$ and temperatures $T = 0.5$ (1), $T = 0.05$ (2), $T = 0.01$ (3).

4. Phase Separation Kinetics

Finally, we studied the behavior of the cluster average size $L(t)$ during phase separation. The long time behavior of $L(t)$ has been previously studied for different kinds of active systems.\textsuperscript{21–25} For active colloids in two dimensions\textsuperscript{9,25} a power law $L(t) \sim t^\alpha$ is found with $\alpha \simeq 0.25 - 0.28$.

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The coarse-grained system was then digitalized assigning the value $\rho(r, t) = 1$ to the pixels with $\phi(r, t) \geq \phi_{th}$ and $\rho(r, t) = -1$ to the remaining ones. The characteristic size $L(t)$ of clusters was computed as the inverse of the first moment of the spherically averaged structure factor

$$L(t) = 4\pi \int \frac{C(k, t) dk}{kC(k, t) dk},$$

where $k = |k|$ is the modulus of the wave vector in Fourier space and $C(k, t) = \langle \tilde{\rho}(k, t)\tilde{\rho}(-k, t) \rangle$

with $\tilde{\rho}(k, t)$ the spatial Fourier transform of $\rho(r, t)$. The angle brackets denote an average over a shell in $k$-space at fixed $k$. The prefactor 4 at the right-hand side of Eq. (4) takes into account the size, in units of $\sigma$, of the pixels.

We found a power law behavior $L(t) \sim t^\alpha$ with $\alpha$ depending on the surface concentrations (see Fig. 6): The best fits at long times give the values $\alpha = 0.90$ at $\phi = 0.4$ and $\alpha = 0.65$ at $\phi = 0.6$. We checked that the values of the growth exponents are not sensitive to the chosen value of the threshold concentration $\phi_{th}$.

We do not have a theoretical argument for explaining these exponents. However, we can relate their different values to the different cluster morphology observed by varying the concentration $\phi$ (see Fig. 5). Indeed, at lower $\phi$ phase separation is characterized by isolated clusters that can grow in size faster than the ones at higher values of $\phi$. In this latter case clusters are interconnected and this results in a slower growth rate. The observed values of $\alpha$ are in any case larger with respect to the ones found in active spherical colloids. It is not obvious how to relate this difference to the presence of orientational order in our model. For example, at high density, the steric

\[\text{Fig. 5. (Color online) Domain patterns at consecutive times for } \phi = 0.4 \text{ (upper row) and } \phi = 0.6 \text{ (lower row). Filled cells (see the text for details) were colored in yellow.}\]
constraints inhibit rotations and one could expect an aggregation mechanism with a cluster growth behavior similar to that observed for spherical colloids. However, this is not the case, as shown from the results at $\phi = 0.6$. Therefore, further numerical studies are needed to clarify this matter.

References