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Minimal model of active colloids highlights the role of mechanical interactions in controlling the emergent behavior of active matter

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ABSTRACT

Minimal models of active Brownian colloids consisting of self-propelled spherical particles with purely repulsive interactions have recently been identified as excellent quantitative testing grounds for theories of active matter and have been the subject of extensive numerical and analytical investigation. These systems do not exhibit aligned or flocking states but do have a rich phase diagram, forming active gases, liquids, and solids with novel mechanical properties. This article reviews recent advances in the understanding of such models, including the description of the active gas and its swim pressure, the motility-induced phase separation and the high-density crystalline and glassy behavior.

1. Introduction

Living entities, on scales from birds to individual cells, organize in complex patterns with collective behaviors that serve important biological functions. Examples range from the flocking of birds [1] to the sorting and organization of cells in morphogenesis [2]. Work over the last 10 years has shown that many aspects of this complex organization can be captured by physical models based on a minimal set of rules or interactions, leading to the emergence of the new field of active matter [3•]. This is defined as a distinct category of nonequilibrium matter in which energy uptake, dissipation, and movement take place at the level of discrete microscopic constituents. The active matter paradigm has additionally inspired the development of ingenious synthetic chemical and mechanical analogs, such as "active" colloids: micron-size spheres partly coated with a catalyst that promotes the decomposition of one of the components of the ambient fluid, resulting in self-propulsion of the colloidal particles [4,5,6,7]. Collections of such active synthetic particles have been shown to spontaneously assemble in coherent mesoscale structures with remarkable life-like properties [8•,9].

Active systems exhibit rich emergent behaviors, where a collection of many interacting entities show large-scale spatial or temporal organization in states with novel macroscopic properties. For instance, a dense swarm of bacteria can behave collectively as a living fluid with novel rheology [10,11], self-organize in complex regular patterns [12], exhibit turbulent motion [13], or 'freeze' into a solid-like biofilm [14]. This type of behavior is of course well known in inert inanimate matter that exhibits transitions between different phases upon the tuning of an external parameter, such as temperature, or the application of external forces that perturb the system at its boundaries (e.g., shear stresses) or globally (e.g., an electric or magnetic field). It acquires, however, a new unexplored richness in active systems that are tuned out of equilibrium by energy generated internally by each unit. The active matter paradigm aims at describing and classifying the behavior of this new class of nonequilibrium systems. It does so by drawing on our understanding of familiar states of matter and of the transitions between them as controlled by interactions between atoms and molecules. New states of matter arise when we put together many units that are individually driven or motile. How are these new states formed? Are they controlled solely by local interactions among the active particles or is chemical signaling required to understand the emergence of these new states? Can we classify and describe them and control the transitions between such states as we know how to do with familiar inert matter?

Recently, a number of ingenious synthetic systems have been engineered that show the emergent behavior of living active systems. These include autophoretic colloids [5,6,17], rollers [18], and droplets [19]. The simplest realization of such 'colloidal microswimmers' is obtained by immersing spherical Janus colloids created by coating a hemisphere of a gold bead with platinum in a solution rich in hydrogen

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peroxide (H_2O_2) [4]. The difference in the consumption rate of H_2O_2 at the gold and platinum sides maintains an asymmetric concentration of solute on the two hemispheres, resulting in propulsion of the particles along their symmetry axis. In this and other catalytic colloidal swimmers interactions and propulsion can be tuned in a controlled way, allowing systematic studies up to moderate densities (see Fig. 2(b)). One remarkable phenomenon shown by these systems is spontaneous assembly in macroscopic clusters [17,8]. This phenomenon is distinct from equilibrium assembly that arises from attractive interactions between the particles and has been shown to be driven by the nonequilibrium interplay of motility and crowding. The nonequilibrium pressure equation of state of active colloids has been probed experimentally via sedimentation measurements [30•], revealing a motility-induced effective adhesion that can strongly suppress the pressure at moderate density. A review of recent experimental findings can be found in Ref. [21] and is beyond the scope of the present article that focuses on minimal models of active colloids that have in many cases predicted and then qualitatively reproduced many of the experimental observations.

Colloids have played a key role in condensed matter physics as model systems for atomic materials where pair interaction can be customized and equilibrium phase transitions and glassy behavior can be investigated with optical microscopy [16]. Although many active entities, from bacteria to birds, are elongated in shape and order in states with local or global liquid crystalline order leading to collective flocking, the growing body of work on synthetic active systems has shown that even spherical active particles can exhibit novel behaviors arising from the irreversible dynamics of each constituent, providing an excellent system for the quantitative testing of active matter theories. This has led to extensive theoretical and numerical studies of minimal models consisting of self-propelled spheres with purely repulsive interactions known as active Brownian particles (ABP) [20•,21]. These systems do not exhibit aligned or flocking states but form active gases, liquids, and solids, as summarized in the phase diagram shown in Fig. 1. The interplay between motility and steric effects is responsible for intriguing new phenomena, including motility-induced phase separation in the absence of any attractive interactions [22•,20•], Casimir-type forces [23], and ratchet effects [24]. The complexity of behavior that arises in these minimal models is truly remarkable. Importantly, the ABP model has demonstrated that many aspects of the emergent behavior of active systems do not require biochemical signaling but are captured by physical contact interactions. It has additionally provided an excellent playground for addressing fundamental questions about the nonequilibrium statistical mechanics of active systems and whether equilibrium-like notions, such as effective temperature or equations of state, may be useful to describe them.

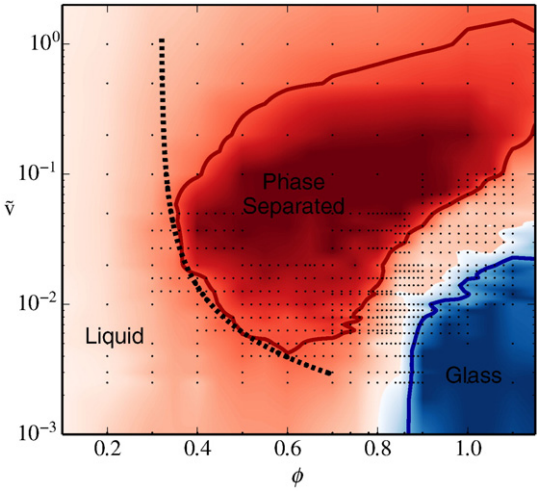

Fig. 1. Numerical phase diagram of a polydisperse active suspension with soft repulsion obtained by integrating Eqs. (1)–(2) for $D_r/(\mu k) = 5 \times 10^{-4}$ and $D_t = 0$, reproduced from Ref. [15] with permission from the Royal Society of Chemistry. The red region corresponds to a phase-separated system. The blue region corresponds to a glass as characterized by the behavior of the MSD. The glass would be replaced by a crystalline state in a monodisperse suspension. The dotted line is the mean-field spinodal line given by $\rho_c^-(\mathrm{Pe}_r)$ from Eq. (15) for $D_t = 0$ using a two-parameter variant of Eq. (10) (see Ref. [15]).

In this article, we review recent advances on the theoretical description of collections of active Brownian particles (ABP) defined as spherical self-propelled particles with purely repulsive interactions by organizing their behaviors in terms of the new active gas, liquid, and solid phases formed by these systems. The work described demonstrates that some key aspects of the emergent behavior of active systems, such as the tendency to spontaneously cluster in large compact structures and to accumulate at surfaces exerting organized forces on the environment, can be described in terms of the nonequilibrium interplay of motility and crowding, without invoking attractive interactions nor biochemical signaling. We believe that minimal models of the type described here will continue to provide important tools for advancing our understanding of the nonequilibrium statistical mechanics of active matter.

The rest of this paper is organized as follows. In Section 2, the minimal model of ABP is presented, emphasizing its parameters, limiting cases, and critical values. Next, in Section 3, we consider the properties of active gases in the context of recent work characterizing their mechanical properties and defining a pressure equation of state. From the dilute ideal active gas limit, tuning the rotational Péclet number and increasing density beyond a critical value results in phase separation, where significant groups of active particles find their self-propulsion velocity caged due to increased interactions, yielding an active liquid coexisting with the active gas. This has been characterized by equations of mean velocity and critical density, which are presented and supported by simulation. This motility-induced phase separation (MIPS) is analyzed in Section 4 using continuum equations. The high-density limit, discussed in Section 5, is one in which solids and glasses of active colloids are formed, and this is distinguished from the glasses or crystalline states that result from high-density collections of passive colloids. Finally, a discussion and outlook is provided in Section 6, raising current questions regarding the interplay of noise and damping in the current models of active systems.

2. A minimal model of active colloids

The rich behavior of active colloids has been studied using a minimal model of self-propelled particles (SPPs) that allows for both analytical and numerical progress. In this model, hydrodynamic interactions are neglected and the ambient fluid is assumed to only provide friction, rendering the dynamics overdamped. Each colloid is modeled as a spherical particle of radius a_i, with an orientation defined by the axis of self-propulsion. In the following, we will discuss both monodisperse systems, where all disks have the same radius a, and polydisperse systems, where a will denote the mean radius and the radii are uniformly distributed with 20% polydispersity. While most of the work on this model known in the literature as ABP has been carried out in two dimensions ($2d$), and we will restrict ourselves to this case here, many of the results described also hold in three dimensions [25]. Each particle is characterized by the position $\boldsymbol{r}_i$ of its center and its orientation $\boldsymbol{e}_i = (\cos\theta_i, \sin\theta_i)$, which in $2d$ corresponds to a single angle θ_i. The dynamics is then described by coupled Langevin equations (see Fig. 2)

$$\partial_t \boldsymbol{r}_i = \mathrm{v}_0 \boldsymbol{e}_i + \mu \sum_j \boldsymbol{f}_{ij} + \boldsymbol{\eta}_i(t) \ , \tag{1}$$

$$\partial_t \theta_i = \eta_i^r(t) \ , \tag{2}$$

where v_0 is the active (self-propulsion) speed and μ the mobility. The particles interact via short-range radial repulsive forces $\boldsymbol{f}_{ij} = -\frac{\partial U(|\boldsymbol{r}_{ij}|)}{\partial \boldsymbol{r}_i}$, where