Enhanced Diffusion and Ordering of Self-Propelled Rods

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(Received 27 June 2008; published 22 December 2008)

Starting from a minimal physical model of self-propelled hard rods on a substrate in two dimensions, we derive a modified Smoluchowski equation for the system. Self-propulsion enhances longitudinal diffusion and modifies the mean-field excluded volume interaction. From the Smoluchowski equation we obtain hydrodynamic equations for rod concentration, polarization and nematic order parameter. New results at large scales are a lowering of the density of the isotropic-nematic transition and a strong enhancement of boundary effects in confined self-propelled systems.

DOI: 10.1103/PhysRevLett.101.268101
PACS numbers: 87.18.Ed, 05.65.+b, 47.54.–r

Self-propelled particles consume energy from internal or external sources and dissipate it by actively moving through the medium that they inhabit. Assemblies of interacting self-propelled particles (SPP) exhibit rich collective behavior, such as nonequilibrium phase transitions between disordered and ordered (possibly moving) states and novel long-range correlations. Biologically relevant systems that belong to this class include fish schools, bird flocks [1], bacterial colonies [2], and cell extracts of cytoskeletal filaments and associated motor proteins [3]. A nonliving realization may be a vibrated monolayer of granular rods [4]. Collections of SPP have been the focus of extensive experimental [3–5] and theoretical studies in recent years. A number of distinct theoretical approaches have proved fruitful for understanding the complex dynamics of these nonequilibrium systems. These include numerical studies of simple models [6–9], inspired by the seminal work of Vicsek [10], and phenomenological continuum theories based on general symmetry arguments [11]. Recent work on deriving the hydrodynamic equations from specific microscopic models has led to some insight into the origin of the collective behavior of these systems [12–16]. An important open question that we address here is the modification induced by self-propulsion in the sterically effects arising from the shape of the particle and the signature of this modification in the large scale physics of the system.

In this Letter we consider a physical model of self-propelled hard rods that interact with each other solely through excluded volume. The rods move on a passive substrate. Self-propulsion is modeled as a nonequilibrium velocity \( v_0 \) along the direction of the rods' long axes. The goal of our work is to understand how self-propulsion modifies the diffusion processes and the mean-field Onsager excluded volume interaction [17]. Using the tools of nonequilibrium statistical mechanics we derive a modified Smoluchowski equation that differs from the familiar version for thermal hard rods [17] in three respects. The first and obvious modification is a convective mass flux at the self-propulsion speed \( v_0 \) along the direction of orientation of the rod. Second, self-propulsion enhances the longitudinal diffusion constant \( D_L \) of the rods, according to \( D_L \to D_L (1 + v_0^2/k_BT) \). This enhancement arises because self-propelled particles perform a persistent random walk [18]. Living cells also exhibit modified Brownian dynamics [19] that can be modeled as a biased random walk on suitably coarse-grained scales. Finally, the momentum exchanged by two rods upon collision is rendered highly anisotropic by self-propulsion thus modifying the Onsager form of the excluded volume interaction. This leads to novel anisotropic forces and torques from steric repulsion in the Smoluchowski equation.

These modifications of the Smoluchowski equation have dramatic consequences for the properties of the system on hydrodynamic scales. This is illustrated by two examples. First, we show that the additional momentum transfer from self-propulsion lowers the density of the isotropic-nematic transition, thereby providing a microscopic identification for the physical mechanism responsible for the enhancement of orientational order observed in numerical simulations of motility assays [8]. Second, we demonstrate that self-propulsion greatly enhances the effect of confinement and the role of boundaries.

The microscopic model.—We consider quasi two-dimensional hard rods of length \( \ell \) and thickness \( 2R \) confined to a plane, as shown in Fig. 1. The \( i \)th rod is characterized by the position \( r_i \) of its center of mass and a unit vector \( \hat{u}_i = (\cos \theta_i, \sin \theta_i) \) directed along its long axis. Each rod free-streams on the substrate, until it collides with another rod. The collision results in instantaneous linear and angular momentum transfer such that the total energy, linear and angular momenta of the two rods are conserved [20]. The microdynamics of the system is governed by coupled Langevin equations.

\[ \dot{u}_i = \frac{1}{m_i} \left( F_i + \xi_i \right) \text{ and } \dot{\theta}_i = \frac{1}{I_i} \left( \Gamma_i + \eta_i \right) \]
from the center of mass, and $R$ is the moment of inertia of the rod and $T_{a}$ an effective temperature defined by these relationships. Finally, the collision operator $T(i,j)$ generates the instantaneous momentum transfer between rods at contact and is given by

$$T(1,2) = \int_{s_{12}}^{s_{12}^0} \int_{\hat{k}} |V_{12} \cdot \hat{k}| \Theta(-V_{12} \cdot \hat{k})(b_{12} - 1),$$

where $\hat{k}$ is the unit normal at the point of contact directed from rod 2 to rod 1, $s_{12} \in [-\ell/2, \ell/2]$ parameterize the distance of points along the axis of each rod from the center of mass, and $\int_{s_{12}}^{s_{12}^0} \int_{s_{12}^0}^{t/2} ds_{1} \times \int_{t/2}^{t_{12}} ds_{2} \delta(R_{12}) \ldots$, where $R_{12} = 0$ corresponds to the condition that the two rods be in contact at one point, as for instance in Fig. 1, where $R_{12} = r_{1} - r_{2} + s_{1} \hat{u}_{1} - (\ell/2)\hat{u}_{2} - 2R\hat{k}$. Also, $V_{12} = v_{1} - v_{2} + \omega_{1} \times \xi_{1} - \omega_{2} \times \xi_{2}$, with $\xi_{j} = s_{j} \hat{u}_{j} \pm R\hat{k}$, is the relative velocity of the two rods at the point of contact. The operator $b_{12}$ replaces precollisional velocities with their postcollisional values, e.g., $b(1, 2)v_{1,2} = v_{1,2} \mp \hat{k}A$, where the momentum exchange $A$ is obtained by requiring energy and momentum conservation. The explicit calculation of the $T$ operator is given in [21].

**Modified Smoluchowski equation.**—We are interested here in the overdamped limit, when inertial effects are negligible and the low density dynamics is described by a Smoluchowski equation for the probability distribution $c(x, t)$ of rods at $r$ oriented in the direction $\theta$, with $x = (r, \theta)$. The derivation of the Smoluchowski equation is rather technical and will not be presented here. It can be carried out in analogy to the case of thermal hard rods and we only outline the key steps and approximations. (i) First, using formal statistical physics techniques [22], the noise averaged dynamics described by the coupled Langevin Eqs. (1) and (2) can be recast into a hierarchy of coupled equations for reduced distribution functions, analogous to the BBGKY hierarchy for Hamiltonian systems. Assuming a low density of rods, we then neglect two particle correlations and obtain a closed Boltzmann-Fokker-Planck equation for the one particle distribution function $f(x, p, t)$, with $p = (v, \omega)$. (ii) The probability distribution is $c(x, t) = \int_{p} f(x, p, t)$. If the friction between the rods and a solvent or substrate is large, the velocities of the rods decay to a stationary value on microscopic time scales, much shorter than those controlling the relaxation of the spatial probability distribution, $c(x, t)$. In this regime we assume $f(x, p, t) \approx c(x, t)f_{M}(p|\theta)$, with $f_{M} \sim \exp(-\frac{1}{k_{B}T_{a}}(v - v_{0}\hat{u})^{2} - \frac{1}{2k_{B}T_{a}}\omega^{2})$ a Maxwellian distribution centered at the self-propulsion velocity $v_{0}\hat{u}$. This product form is an approximate solution of the noninteracting Fokker-Planck equation for large friction. Inserting this ansatz for $f(x, p, t)$ in the Boltzmann-Fokker-Planck equation and averaging over the velocities $p$, we obtain the Smoluchowski equation for $c(x, t)$. We stress that it is essential to explicitly derive the Smoluchowski equation from the Fokker-Planck equation to capture the enhancement of longitudinal diffusion ($D_{x}$) in Eq. (4). (iii) When carrying out the average over $p$ a further approximation is required to evaluate the mean force $\langle T(1,2)v_{1}\rangle_{M}$ and torque $\langle T(1,2)\omega_{1}\rangle_{M}$ on a given rod due to all other rods in the fluid, where $\langle \ldots \rangle_{M} = \int f_{p1} \cdots f_{p2} f_{M}(p_{1}|\theta_{1})f_{M}(p_{2}|\theta_{2})$. When $v_{0} = 0$, this average can be carried out exactly and yields the Onsager excluded volume interaction. For $v_{0} \neq 0$, $f_{M}$ depends on the angular coordinate $\hat{u}$. Hence, averaging over velocities induces orientational correlations that cannot be incorporated exactly. To make progress, we neglect the coupling between velocity and angular correlations in calculating velocity-averaged forces and torques.

The result is the modified Smoluchowski equation:

$$\begin{align*}
\partial_{t}c + v_{0}\partial_{\parallel}c &= D_{R}\partial_{\parallel}c + (D_{\parallel} + D_{\perp})\partial_{\perp}c + D_{\perp}\partial_{\perp}c \\
&- \frac{1}{I_{KR}}\partial_{\theta}\tau_{ex} - \nabla \cdot \xi^{-1} \cdot F_{ex} - \frac{1}{I_{KR}}\partial_{\theta}\tau_{sp} \\
&- \nabla \cdot \xi^{-1} \cdot F_{sp},
\end{align*}$$

(4)
where $\partial_{||} = \hat{u} \cdot \nabla$ and $\partial_{\perp} = \nabla - \hat{u}(\hat{u} \cdot \nabla)$. The convective term on the left hand side of (4) is a trivial consequence of self-propulsion and describes mass flux along the long axis of the rod. The first three terms on the right hand side of the equation describe translational diffusion longitudinal ($D_{||}$) and transverse ($D_{\perp}$) to the rod’s long axis and rotational diffusion ($D_{R}$). For long thin rods $D_{||} = 2D_{\perp} = D$. At low density $D = k_{B}T_{a}/\xi_{||}$ and $D_{R} = 6D_{\perp}/c^{2}$. A novel consequence of self-propulsion is the enhancement of longitudinal diffusion by the anisotropic steric forces and torques in Eq. (5).

$$\begin{align*}
\tau_{\text{SP}} &= \nu_{0}^{2} \int_{x_{1}, t_{1}} \int_{x_{2}, t_{2}} \left( \theta \cdot (\xi_{1} \times \hat{k}) \right) \left[ \hat{z} \cdot (\hat{u}_{1} \times \hat{u}_{2}) \right]^{2} \\
&\times \Theta(-\hat{u}_{12} \cdot \hat{k})c(x_{1}, t)c(x_{2}, t),
\end{align*}$$

(5)

with $\hat{u}_{12} = \hat{u}_{1} - \hat{u}_{2}$. In Onsager’s mean-field model, two thin rods of length $\ell$ exchange an average momentum $\langle |\Delta v| \rangle \nu_{\text{coll}} \approx k_{B}T_{a}/\ell$ per unit time upon collision, with $\langle |\Delta v| \rangle \sim \sqrt{k_{B}T_{a}}$ and $\nu_{\text{coll}} = v_{th}/\ell \sim \sqrt{k_{B}T_{a}}/\ell$. When rods are self-propelled there are anisotropic contributions to both the momentum exchanged (\langle |\Delta v| \rangle \sim v_{0}(|\hat{u}_{1} \times \hat{u}_{2}|)/\ell) and the collision rate ($\nu_{\text{coll}} \sim v_{0}(|\hat{u}_{1} \times \hat{u}_{2}|)/\ell$). These yield the new anisotropic steric forces and torques in Eq. (5).

Hydrodynamics.—We now use the modified Smoluchowski equation to obtain coarse-grained equations that describe the dynamics on length and time scales long compared to the rod length and the collision time. In this regime the dynamics is controlled by the “slow variables” corresponding to the conserved densities (here only the concentration of filaments $\rho = \int_{a} c(x, t)$) and the fields associated with possible broken symmetries. In a liquid of self-propelled rods, both polar and nematic order are possible, described by a polarization vector $\mathbf{P}(r, t) = \int_{a} \mathbf{u}c(x, t)$ and the nematic alignment tensor $Q_{\alpha\beta}(r, t) = \int_{a} (\hat{u}_{\alpha} \hat{u}_{\beta} - \frac{1}{2} \delta_{\alpha\beta})c(x, t)$, respectively. Since each rod has a self-propulsion velocity $v_{0}\mathbf{u}$, the polarization is also proportional to the self-propulsion flow field. The equations for these continuum fields are obtained by taking the corresponding moments of the Smoluchowski equation (4) and are given by

$$\begin{align*}
\partial_{t}\rho + v_{0}\nabla \cdot \mathbf{P} &= D_{p} \nabla^{2} \rho + D_{Q} \nabla \cdot \rho \mathbf{Q}, \\
\partial_{t} \mathbf{Q} + 4D_{R} \left(1 - \frac{\rho}{\rho_{\text{IN}}}\right) \mathbf{Q} + v_{0} \mathbf{F} &= -\lambda \left[ 3(\mathbf{P} \cdot \nabla) \mathbf{P} - \frac{1}{2} \nabla \rho^{2} - \mathbf{P} \cdot \nabla \mathbf{P} \right] = D_{b} \nabla^{2} \mathbf{P} + (D_{\text{spl}} - D_{b}) \nabla \cdot \mathbf{P},
\end{align*}$$

(6)

(7)

where $F_{\alpha\beta} = (\partial_{\alpha}P_{\beta} + \partial_{\beta}P_{\alpha} - \delta_{\alpha\beta} \nabla \cdot \mathbf{P})$ and $G_{\alpha\beta} = Q_{\alpha\gamma} \partial_{\gamma}P_{\beta} + Q_{\beta\gamma} \partial_{\gamma}P_{\alpha} - \delta_{\alpha\beta}Q_{\gamma\gamma} \partial_{\gamma}P_{\alpha}$. All $\lambda$ parameters in Eqs. (7) and (8) are proportional to $v_{0}^{2}$ and vanish in the absence of self-Propulsion. All diffusion constants are enhanced by self-propulsion via additive terms proportional to $D_{S}$. Finally, we have suppressed in Eqs. (6)–(8) excluded volume corrections to the diffusive terms, non-linear terms of second order in gradients, and corrections to the convective terms beyond linear in $v_{0}$. The complete hydrodynamic equations with explicit expressions for the various coefficients can be found in Ref. [21].

The stable homogeneous stationary solution of Eqs. (6)–(8) are the bulk states of the self-propelled system. Two such states are possible: an isotropic state, with $\rho = \text{constant}$, $\mathbf{P} = 0$, $Q_{\alpha\beta} = 0$, and a nematic state, with $\rho = \text{constant}$, $\mathbf{P} = 0$ and $Q_{\alpha\beta} \neq 0$. We find that hard core interactions and self-propulsion modeled simply as a body force do not to generate a bulk polar state, with $\mathbf{P} \neq 0$. This result is corroborated by numerical simulations of self-propelled rods on a substrate, that have observed large correlated regions of finite polarization, but not an ordered bulk state [9]. Other effects, such as shape or mass distribution asymmetry of the driven particles or many-body hydrodynamic interactions not included in our model, may lead to a macroscopic polar (moving) state. To this day no microscopic mechanism capable of giving rise to polar long-range order of self-propelled units in bulk has been convincingly demonstrated.

Self-propulsion does have a profound effect on the isotropic-nematic transition which occurs at the density $\rho_{\text{IN}}(v_{0}) = \rho_{N}/(1 + v_{0}^{2})$, where $\rho_{N} = 3/(\pi \ell^{2})$ is the Onsager transition density. The transition occurs where
the coefficient of the term linear in $Q_{ab}$ on the right-hand side of Eq. (8) changes sign, signaling the unstable growth of nematic fluctuations. This enhancement of orientational order has been observed in numerical simulations of actin motor assays, where actin filaments move on a substrate grafted with motor proteins [8]. It arises from the additional torque $\tau_{32}$ that self-propelled rods experience upon collision as compared to thermal rods. This enhances entropic ordering and aligns the rods [23].

Although no bulk polar order is possible in our system, self-propulsion greatly enhances the length scale over which polarization fluctuations decay. As a result, boundaries are very important in self-propelled systems. To illustrate this we consider a self-propelled 2d hard rod fluid confined in a channel of width $L$, as shown in Fig. 2. We assume that the boundaries induce polarity by forcing all rods to align in the same direction, i.e., $P_y(-L/2) = P_y(L/2) = P_0$. In this geometry the density is constant. One can easily solve for the polarization profile across the channel with the result $P_y(y) = P_0 \cosh(y/\delta)/\cosh(L/2\delta)$, where $\delta = \sqrt{D_\|/D_\perp} = \ell/2\sqrt{5/2 + v_0^2/k_BT}$ is the boundary layer width over which the polarization penetrates in the channel. In the absence of self-propulsion $\delta \sim \ell$, i.e., a finite polarization at the boundary decays (via rotational diffusion) over a length $\sim \ell$. For large self-propulsion velocity, $\delta \sim |v_0|$. If $L \sim \delta$ the entire channel is effectively polarized. We expect that the boundary layer length $\delta$ also sets the scale of correlations in bulk systems. Finally, as shown in [15], Eqs. (6)–(8) yield two important properties of fluctuations in self-propelled systems. First, the isotropic state can support soundlike propagating density waves for a range of wave vectors above a critical value of $v_0$. Second, large number fluctuations always destabilize the homogeneous nematic state. We refer the reader to Ref. [15] for a description of both results.

In summary, we have analyzed a simple model that captures two crucial properties of self-propelled systems: the orientable shape of the particles and the self-propulsion. Using the tools of nonequilibrium statistical mechanics we have derived a modified Smoluchowski equation for SPP and used it to identify the microscopic origin of several observed or observable large scale phenomena.

This work was supported by the NSF on Grants DMR-0705105 and DMR-0806511.

References

[20] Although the substrate acts as a momentum sink, hard particle collisions, which are instantaneous, can still be treated as binary and energy-momentum conserving.
[21] A. Baskaran and M.C. Marchetti (to be published).
[23] No enhancement of orientational order occurs if the self-propulsion velocity is normal to the rods’ long axis.