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(Dated: February 19, 2010)

Using tools of nonequilibirum mechanics, we study a model of self-propelled hard rods on a substrate in two dimensions to quantify the interplay of self-propulsion and excluded-volume effects. We derive of a Smoluchowski equation for the configurational probability density of self-propelled rods that contains several modifications as compared to the familiar Smoluchowski equation for thermal rods. As a side-product of our work, we also present a purely dynamical derivation of the Onsager form of the mean field excluded volume interaction among thermal hard rods.

I. INTRODUCTION

Self-propelled particles draw energy from internal or external sources and dissipate this energy by moving through the medium they inhabit. A wide class of systems, including fish schools, bacterial colonies, and monolayers of vibrated granular rods can be described within this paradigm. These systems exhibit rich collective behavior, such as nonequilibrium phase transitions between disordered and ordered (possibly moving) states and novel long-range correlations and have been the subject of extensive theoretical [1–3], numerical [4–6] and experimental investigations [7–10] in recent years.

Self-propelled particles are elongated in shape and have a self-replenishing momentum along one direction of their long body axis. They generally experience attractive and repulsive interactions, both of a direct nature and mediated by the medium. One generic interaction that is relevant to all self-propelled systems is the short-range repulsive interaction arising from the finite size of the self-propelled units. Our goal here is to understand the interplay of self-propulsion and short range repulsive interactions in controlling the collective dynamics of the system. To this end, we consider the simplest implementation of short range steric repulsion, which is the hard particle limit, and consider a minimal model of self-propelled hard rods moving on a substrate in two dimensions. We will show that self-propulsion modifies the momentum exchanged by hard rods upon collision and the resulting mean-field excluded volume interaction as compared to the Onsager result for passive rods [14, 18].

The simplest model of equilibrium nematic liquid crystals is a collection of long, thin hard rods [14]. In the overdamped regime and at low density, the dynamical properties of the system are described by a Smoluchowski equation for the configurational probability density, $c(\mathbf{r}_1, \hat{\mathbf{u}}_1, t)$, of finding a rod with center of mass at $\mathbf{r}_1$ and long axis oriented along the unit vector $\hat{\mathbf{u}}_1$ at time t, given by

$$\frac{\partial c}{\partial t} + \boldsymbol{\nabla}_1 \cdot \mathbf{J} + \mathcal{R}_1 \cdot \mathbf{J}^R = 0 \ , \tag{1}$$

where $\mathcal{R}_1 = \hat{\mathbf{u}}_1 \times \partial_{\hat{\mathbf{u}}_1}$ is a rotation operator and $\mathbf{J}$ and $\mathbf{J}^R$ are translational and rotational currents, respectively, given by

$$J_\alpha = -D_{\alpha\beta}\left[\partial_{1\beta}c + \frac{1}{k_B T}\left(\partial_{1\beta}V_{ex}\right)c\right] \ , \tag{2a}$$

$$\mathbf{J}^R = -D_R\left[\mathcal{R}_1 c + \frac{1}{k_B T}\left(\mathcal{R}_1 V_{ex}\right)c\right] \ , \tag{2b}$$

with

$$D_{\alpha\beta} = D_\perp \delta_{\alpha\beta} + (D_\parallel - D_\perp)\hat{u}_{1\alpha}\hat{u}_{1\beta} \tag{3}$$

a diffusion tensor that incorporates the anisotropy of translational diffusion of elongated objects, with $D_\parallel > D_\perp$, and D_R the rate of rotational diffusion. The currents given in Eqs. (2a) and (2b) incorporate both diffusion and binary interactions. The latter are described by a mean field excluded volume potential, V_{ex}, given by

$$V_{ex} = k_B T \int_{\hat{\mathbf{u}}_2} \int_{\mathbf{s}} |\hat{\mathbf{u}}_1 \times \hat{\mathbf{u}}_2|\, c\,(\mathbf{r}_1 + \mathbf{s}, \hat{\mathbf{u}}_2, t) \ , \tag{4}$$

with m the mass of a rod, T the temperature, and $\mathbf{s} = \mathbf{r}_2 - \mathbf{r}_1$ the separation between the cnters of mass of the two rods when they are at contact (Fig.). If the thickness of the rods is negligible compared to their length, we can
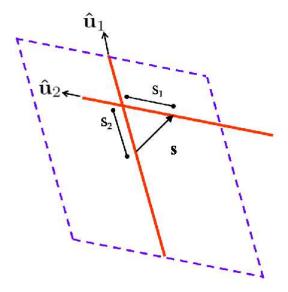
FIG. 1: (color online) Long, thin rods of length ℓ are parametrized by the position $\mathbf{r}_i$ of their center of mass and a unit vector $\hat{\mathbf{u}}_i$ denoting the rod's orientation in the plane. The position along the i-th rod measured from the center of mass is denoted by s_i, with $-\ell/2 \leq s_i \leq \ell/2$. The overlap situation shown in the figure requires $\mathbf{r}_1 + \hat{\mathbf{u}}_1 s_1 \simeq \mathbf{r}_2 + \hat{\mathbf{u}}_2 s_2$, so that $\mathbf{s} = s_1 \hat{\mathbf{u}}_1 - s_2 \hat{\mathbf{u}}_2$. The area excluded by rod 2 to rod 1 is the area of the dashed parallelogram spanned by the unit vectors $\hat{\mathbf{u}}_1$ and $\hat{\mathbf{u}}_2$, given by $\ell^2 |\hat{\mathbf{u}}_1 \times \hat{\mathbf{u}}_2|$.

approximate $\mathbf{s} \simeq s_1 \hat{\mathbf{u}}_1 - s_2 \hat{\mathbf{u}}_2$, where $-\ell/2 \leq s_i \leq \ell/2$ for $i = 1, 2$, parametrizes the position along the i-th rod of length ℓ measured from its center of mass. The integral over the vector $\mathbf{s}$ spans the area excluded to rod 1 by a second rod with center of mass at $\mathbf{r}_2$, oriented in the direction $\hat{\mathbf{u}}_2$. The excluded volume potential represents the second virial coefficient of the static structure factor and was first derived by Onsager [18].

In this paper we present the derivation of a *modified* Smoluchowski equation that describes the low density, over-damped dynamics of a collection of *self-propelled* hard rods. We consider long, thin hard rods moving on a substrate characterized by a friction constant ζ. Self propulsion is modeled by assuming that each rod moves along one direction of its long axis with a constant speed v_0. In addition, the rods experience binary hard-core collisions. This is the simplest model for a "living nematic liquid crystal", a terminology that has been used to describe the collective behavior of a variety of intrinsically self-propelled systems, from bacterial suspensions to monolayers of vibrated granular rods. Since the rods have a purely dynamical self-replenishing momentum, the statistical mechanics needs to be derived from the underlying trajectory dynamics. The details of the derivation are described in this paper. The outcome is a modified Smoluchowski equation for the configurational probability density of the form given in Eq. (1), but where the translational and rotational currents acquire additional contributions due to self propulsion and take the form

$$J_\alpha = v_0 \hat{u}_{1\alpha} c - D_{\alpha\beta}^{SP} \partial_{1\beta} c - \frac{D_{\alpha\beta}}{k_B T} \left(\partial_{1\beta} V_{ex} \right) c - \frac{D_\parallel m v_0^2}{2 k_B T_a} I_\alpha^{SP} , \tag{5a}$$

$$\mathbf{J}^R = -D_R \left[\mathcal{R}_1 c + \frac{1}{k_B T} \left(\mathcal{R}_1 V_{ex} \right) c \right] - \frac{D_R m v_0^2}{2 k_B T_a} \mathbf{I}_R^{SP} , \tag{5b}$$

where

$$D_{\alpha\beta}^{SP} \quad = D_{\alpha\beta} + D_S \ \hat{u}_{1\alpha}\hat{u}_{1\beta}$$
$$= D_\perp \delta_{\alpha\beta} + (D_\parallel + D_S - D_\perp)\hat{u}_{1\alpha}\hat{u}_{1\beta} \ , \tag{6}$$

with $D_S = v_0^2/\zeta$, is the diffusion tensor. Self-propulsion modifies the familiar Smoluchowski equation for hard rods in several important ways. The first modification is the convective mass flux at the self-propulsion speed v_0 along the axis of the rod, described by the first term on the right hand side of Eq. (5a). Secondly, self-propulsion enhances the longitudinal diffusion constant $D_\parallel$ of the rods, according to $D_\parallel \to D_\parallel + D_S = D_\parallel(1 + mv_0^2/k_B T_a)$, as shown in eq. (6) This enhancement arises because self-propelled particles perform a *persistent random walk*, as recently pointed out by other authors [19, 20]. Finally, the momentum exchanged by two rods upon collision is rendered highly anisotropic by self-propulsion. This yields the additional collisional contributions to the excluded volume interaction described by the last terms in Eqs. (5a) and (5b). The precise form of these contributions can be found in Section IV.B. The Smoluchowski equation for self-propelled hard rods is the central result of this work. It has also been shown by us that the novel terms arising from self-propulsion have important consequences for the long-wavelength, long-time behavior of the system by introducing new terms in the coarse-grained equations for the dynamics of conserved quantities and broken symmetry variables. These hydrodynamic signatures have been reported in earlier work [12]. Finally, an additional result of the work presented here is a purely dynamical derivation of the familiar Onsager excluded volume potential for equilibrium hard rods, given in Section IV.A.

The layout of this paper is as follows. In Section II we analyze the trajectory of hard rods moving on a substrate in two dimensions. Using the fact that their trajectories are piece-wise differentiable, with singularities at the time of each collision, we derive an expression for the collision operator governing the momentum exchanged in a binary collision. In Section III we derive a formal hierarchy of Fokker-Planck equations governing the noise-averaged dynamics of a collections of self-propelled hard rods. In section IV we consider the limit of high friction with the substrate that yields a fast relaxation of the linear and angular momentum degrees of freedom, relative to that of the configurational degrees of freedom. This approximation, together with a low density closure of the Fokker-Planck hierarchy, allows us to derive the Smoluchowski equation. We conclude with a brief discussion.

II. BINARY COLLISION OF HARD RODS

Our model is a collection of self-propelled thin hard rods of length ℓ and mass m, confined to two dimensions. Although we will focus below on the limit of long, thin rods, to describe a binary collision we need to incorporate their finite thickness of the rods. We model each rod as a capped rectangle of uniform mass density, consisting of a rectangle of length ℓ and thickness $2R \ll \ell$, capped at the two short sides by semicircles of radius R, as shown in Fig. (2). Each rod is described by the position $\mathbf{r}$ of its center of mass and a unit vector $\hat{\mathbf{u}} = \cos\theta\hat{\mathbf{x}} + \sin\theta\hat{\mathbf{y}}$ directed along its long axis. The rods have head/tail, i.e., nematic symmetry. This symmetry is broken by self-propulsion that is implemented by assuming that a force $\mathbf{F}$ of constant magnitude and directed along the rod's long axis acts on the center of mass of each rod. The direction of the self-propulsion force will be referred to as the "head" of the rod and the unit vector $\hat{\mathbf{u}}$ is chosen to point in the direction of the head, so that $\mathbf{F} = F\hat{\mathbf{u}}$.

The rods move on a passive medium that provides frictional damping to their motion. Any other physical or chemical process that may be present in the system is assumed to occur on a fast time scale, such that it can be modeled as an additive Markovian white noise. The dynamics of a self propelled rod is then described by Langevin equations for the center of mass velocity $\mathbf{v} = \partial_t\mathbf{r}$ and the angular velocity $\boldsymbol{\omega} = \hat{\mathbf{z}}\omega = \hat{\mathbf{z}}\partial_t\theta$, where $\hat{\mathbf{z}}$ is normal to the plane of motion. The equations of motion are given by

$$m\partial_t v_\alpha = -\zeta_{\alpha\beta}v_\beta + F\hat{u}_\alpha + \eta_\alpha(t) \ , \tag{7a}$$

$$\partial_t\omega = -\zeta^R\omega + \eta_R(t), \tag{7b}$$

where $\zeta_{\alpha\beta} = \zeta_\parallel \hat{u}_\alpha\hat{u}_\beta + \zeta_\perp(\delta_{\alpha\beta} - \hat{u}_\alpha\hat{u}_\beta)$ is a translational friction tensor with $\zeta_\parallel < \zeta_\perp$ reflecting the fact that frictional damping is smaller for motion along the long axis of the rod, ζ_R is a rotational friction constant, and $\boldsymbol{\eta}$ and η_R are white noise terms with zero mean and correlations

$$\langle \eta_\alpha(t)\,\eta_\beta(t')\rangle = \Delta_{\alpha\beta}(\hat{\mathbf{u}})\ \delta(t - t') \ , \tag{8a}$$

$$\langle \eta_R(t)\,\eta_R(t')\rangle = \Delta_R\ \delta(t - t') \ . \tag{8b}$$

For simplicity, we assume that the noise amplitudes $\Delta_{\alpha\beta}$ and Δ_R have the same form as in equilibrium,

$$\Delta_{\alpha\beta}(\hat{\mathbf{u}}) = 2k_B T_a \zeta_{\alpha\beta}(\hat{\mathbf{u}})/m \ , \tag{9a}$$
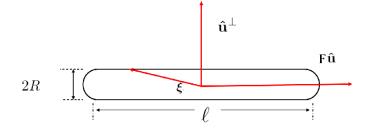
$$\Delta_R = 2k_B T_a \zeta_R/I \ , \tag{9b}$$

FIG. 2: (color online) Each self-propelled particle is modeled as a capped rectangle of uniform mass density, consisting of a rectangle of length ℓ and thickness $2R$ capped at the two short sides by semicircles of radius R (the width of the rod is exaggerated for clarity). Self-propulsion is provided by a force of constant magnitude F directed along the "head" of the rod. The vector $\boldsymbol{\xi}$ locates points on the boundary of the rod relative to the center of mass. The unit vector $\hat{\mathbf{u}}_\perp$ is defined as $\hat{\mathbf{u}}_\perp = \hat{\mathbf{z}} \times \hat{\mathbf{u}}$, where $\hat{\mathbf{z}}$ points out of the plane.

with T_a an active temperature and I the component of the moment of inertia tensor $\mathbf{I}$ of the rod along the long axis,

$$I = \frac{m}{2\ell + \pi R}\left[\frac{2\ell}{3}\left(3R^2 + \frac{\ell^2}{4}\right) + \pi R\left(\frac{R^2}{2} + \frac{\ell^2}{4}\right)\right] \sim \frac{m\ell^2}{12} . \tag{10}$$

The last approximate equality in Eq. (10) holds in the limits $\ell \gg 2R$ of long, thin rods. The active temperature T_a is generally different from the thermodynamic temperature of the system and is a measure of the noise amplitude.

The rods interact with each other exclusively via hard-core interactions. The collisions are instantaneous and conserve energy and momentum of the colliding rods. To incorporate these interactions in the Langevin equations for the particles, we need to construct a collision operator that generates the instantaneous collision. We consider two rods and denote by $t = 0$ the origin of time. The two rods travel freely with linear and angular velocities $x_1 = (\mathbf{v}_1, \boldsymbol{\omega}_1)$ and $x_2 = (\mathbf{v}_2, \boldsymbol{\omega}_2)$ until a time $\tau(\Gamma_1, \Gamma_2)$ when they come into contact, where $\Gamma_i = \{\mathbf{r}_i, \hat{\mathbf{u}}_i, \mathbf{v}_i, \boldsymbol{\omega}\}$ is the phase point of each rod. Denoting by a prime the post-collisional velocities, $x_i' = (\mathbf{v}_i', \boldsymbol{\omega}_i')_{i=1,2}$, the time dependence of the observables x_i can be written as

$$x_i(t) = x_i \Theta\left(\tau\left(\Gamma_1, \Gamma_2\right) - t\right) + x_i' \Theta\left(t - \tau\left(\Gamma_1, \Gamma_2\right)\right) . \tag{11}$$

The equation of motion for x_i is then

$$\partial_t x_i = \Delta x_i \, \delta\left(t - \tau\left(\Gamma_1, \Gamma_2\right)\right) , \tag{12}$$

with $\Delta x_i = x_i - x_i'$. The post-collisional velocities are easily calculated by imposing conservation of energy and of linear and angular momentum, $\mathbf{p}_i = m\mathbf{v}_i$ and $\mathbf{L}_i = I\boldsymbol{\omega}_i$, with the result [15, 16]

$$\mathbf{p}_i' = \mathbf{p}_i - \hat{\mathbf{k}}_{ji} A , \tag{13a}$$

$$\mathbf{L}_i' = \mathbf{L}_i - \boldsymbol{\xi}_i \times \hat{\mathbf{k}}_{ji} A , \tag{13b}$$

where $\widehat{\mathbf{k}}_{ji}$ is the unit normal at the point of contact of the two rods and is directed from rod j to rod i, and $\boldsymbol{\xi}_i$ is the vector from the center of mass of rod i to the point of contact of the two rods, as shown in Fig. 3. The magnitude of the momentum transfer A is

$$A = \frac{m\hat{\mathbf{k}}_{21} \cdot \mathbf{V}_{12}}{1 + \frac{m}{2}\left(\boldsymbol{\xi}_1 \times \hat{\mathbf{k}}_{21}\right) \cdot \mathbf{I}^{-1} \cdot \left(\boldsymbol{\xi}_1 \times \hat{\mathbf{k}}_{21}\right) + \frac{m}{2}\left(\boldsymbol{\xi}_2 \times \hat{\mathbf{k}}_{21}\right) \cdot \mathbf{I}^{-1} \cdot \left(\boldsymbol{\xi}_2 \times \hat{\mathbf{k}}_{21}\right)} \tag{14}$$

with $\mathbf{V}_{12} = \mathbf{v}_{12} + \boldsymbol{\omega}_1 \times \boldsymbol{\xi}_1 - \boldsymbol{\omega}_2 \times \boldsymbol{\xi}_2$ the relative velocity of the two rods at the point of contact, and $\mathbf{v}_{12} = \mathbf{v}_1 - \mathbf{v}_2$. To render Eq. (12) explicit we need an expression for the time $\tau(\Gamma_1, \Gamma_2)$. The condition of contact can be written as the requirement that $\mathbf{r}_1(\tau) + \boldsymbol{\xi}_1(\tau) = \mathbf{r}_2(\tau) + \boldsymbol{\xi}_2(\tau)$ for some value of $\boldsymbol{\xi}_1$ and $\boldsymbol{\xi}_2$ on the surface of the two rods, where
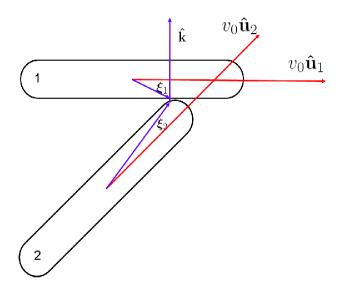
FIG. 3: (color online) A cap-to-side collision of two self-propelled hard rods (the width of the rod is exaggerated for clarity). $\hat{\mathbf{k}}$ is a unit vector from rod 2 to rod 1 normal to the point of contact. Points on the side of the rods are identified by vectors $\boldsymbol{\xi}_i$.

$\mathbf{r}_i(\tau) = \mathbf{r}_i + \mathbf{v}_i\tau$ and $\hat{\mathbf{u}}_i(\tau) = \cos(\theta_i + \omega_i\tau)\,\hat{\mathbf{x}} + \sin(\theta_i + \omega_i\tau)\,\hat{\mathbf{y}}$. It is apparent from Fig. 3 that $\mathbf{r}_{12} + \boldsymbol{\xi}_1 - \boldsymbol{\xi}_2$ must lie along $\hat{\mathbf{k}}_{21}$. The condition of contact can then be written as two scalar equations, given by

$$(\mathbf{r}_{12} + \boldsymbol{\xi}_1 - \boldsymbol{\xi}_2) \cdot \hat{\mathbf{k}}_{21} = |\mathbf{r}_{12} + \boldsymbol{\xi}_1 - \boldsymbol{\xi}_2| = 0 \ , \tag{15a}$$

$$(\mathbf{r}_{12} + \boldsymbol{\xi}_1 - \boldsymbol{\xi}_2) \cdot \left(\hat{\mathbf{z}} \times \hat{\mathbf{k}}_{21}\right) = 0 \ , \tag{15b}$$

where all variables are evaluated at time τ. Equations (15a) and (15b) are implicit equations for $\tau(\Gamma_1, \Gamma_2)$. The first condition, Eq. (15a), imposes that two rods be in contact at any point along their surface. The second condition, Eq. (15b), determines the precise point on the surface of each rod. As an illustration we consider the collision shown in Fig. 3 when the cap of rod 2 comes into contact with a side of rod 1. In this case, $\hat{\mathbf{k}}_{12} \equiv \hat{\mathbf{u}}_1^{\perp} = \hat{\mathbf{z}} \times \hat{\mathbf{u}}_1$ and the surface of the rod 1 is parametrized by $\boldsymbol{\xi}_1 = s_1\hat{\mathbf{u}}_1 - R\hat{\mathbf{u}}_1^{\perp}$, with $\hat{\mathbf{u}}_i^{\perp} = \hat{\mathbf{z}} \times \hat{\mathbf{u}}_i$. The point of contact on rod 2 is simply $\boldsymbol{\xi}_2 = \frac{\ell}{2}\hat{\mathbf{u}}_2 + R\hat{\mathbf{u}}_1^{\perp}$. The contact conditions Eqs. (15a) and (15b) become

$$\mathbf{r}_{12} \cdot \hat{\mathbf{u}}_1^{\perp} - \frac{\ell}{2}\hat{\mathbf{u}}_2 \cdot \hat{\mathbf{u}}_1^{\perp} - 2R = 0 \ , \tag{16a}$$

$$\mathbf{r}_{12} \cdot \hat{\mathbf{u}}_1 - \frac{\ell}{2}\hat{\mathbf{u}}_2 \cdot \hat{\mathbf{u}}_1 + s_1 = 0 \ . \tag{16b}$$

Eq. (16a) requires the rods to be at contact at any point along the side of rod 1, while Eq. (16b) determines the position of contact along the side of rod 1.

To obtain an expression that can be used to eliminate $\tau(\Gamma_1, \Gamma_2)$ from the equation of motion, Eq. (12) we use the identity

$$\delta(f(x) - f_0) = \frac{\delta(x - x_0)}{\left|\frac{\partial f}{\partial x}\big|_{x_0}\right|} \ . \tag{17}$$

Using Eq. (17), together with

$$\frac{\partial}{\partial t}(\mathbf{r}_{12} + \boldsymbol{\xi}_1 - \boldsymbol{\xi}_2) \cdot \hat{\mathbf{k}}_{21}\big|_{t=\tau} = \mathbf{V}_{12}(\tau) \cdot \hat{\mathbf{k}}_{21} \tag{18}$$

we can rewrite the temporal δ function in the equation of motion, Eq. (12) as

$$\delta \left(t - \tau \left(\Gamma_1, \Gamma_2\right)\right) = \delta \left(\left(\mathbf{r}_{12} + \boldsymbol{\xi}_1 - \boldsymbol{\xi}_2\right) \cdot \hat{\mathbf{k}}_{21}\right) \left|\mathbf{V}_{12} \cdot \hat{\mathbf{k}}_{21}\right| . \tag{19}$$

Finally, although Eqs. (15a-15b) determine the contact condition, an actual collision results from the contact only if the pre-collisional velocities at the point of contact are such that the two particles are moving towards each other, i.e., $\mathbf{V}_{12} \cdot \hat{\mathbf{k}}_{21} < 0$. Putting all of these results together, the equation of motion for the observable x_i can be written in the form

$$\partial_t x_i = T\left(1, 2\right) x_i , \tag{20}$$

where $T(1, 2)$ is a binary collision operator, given by

$$T\left(1, 2\right) = \int_{\boldsymbol{\xi}_1, \boldsymbol{\xi}_2} \int_{\hat{\mathbf{k}}_{21}} \Theta\left(-\mathbf{V}_{12} \cdot \hat{\mathbf{k}}_{21}\right) \left|\mathbf{V}_{12} \cdot \hat{\mathbf{k}}_{21}\right| \delta\left(\left(\mathbf{r}_{12} + \boldsymbol{\xi}_1 - \boldsymbol{\xi}_2\right) \cdot \hat{\mathbf{k}}_{21}\right) \delta\left(\left(\mathbf{r}_{12} + \boldsymbol{\xi}_1 - \boldsymbol{\xi}_2\right) \cdot \left(\hat{\mathbf{z}} \times \hat{\mathbf{k}}_{21}\right)\right) \left(\hat{b}_{12} - 1\right) , \tag{21}$$

with $\hat{b}_{12}$ a substitution operator such that $\hat{b}_{12} x_i = x_i'$. The integration in Eq. (21) ranges over all physical collision geometries. In the following, we will focus on the case of rods of large aspect ratio ($\ell \gg 2R$). In this limit, cap-on-cap collisions are rare relative to to cap-on-side collisions and will be neglected. For cap-on-side collisions, the $\int_{\boldsymbol{\xi}_1, \boldsymbol{\xi}_2} \int_{\hat{\mathbf{k}}_{21}}$ can be given an explicit representation of the form

$$
\begin{aligned}
\int_{\boldsymbol{\xi}_1, \boldsymbol{\xi}_2} \int_{\hat{\mathbf{k}}_{21}} ... = \quad & \int_{s_1, s_2} \int_{\hat{\mathbf{k}}_{21}} ... \left\{ \left[\delta\left(s_2 + \frac{\ell}{2}\right) + \delta\left(s_2 - \frac{\ell}{2}\right)\right] \left[\delta\left(\hat{\mathbf{k}}_{21} - \hat{\mathbf{u}}_1^\perp\right) + \delta\left(\hat{\mathbf{k}}_{21} + \hat{\mathbf{u}}_1^\perp\right)\right] \right. \\
& \left. + \left[\delta\left(s_1 + \frac{\ell}{2}\right) + \delta\left(s_1 - \frac{\ell}{2}\right)\right] \left[\delta\left(\hat{\mathbf{k}}_{21} - \hat{\mathbf{u}}_2^\perp\right) + \delta\left(\hat{\mathbf{k}}_{21} + \hat{\mathbf{u}}_2^\perp\right)\right] \right\} \\
\equiv \quad & \int_{s_1, s_2} \int_{\hat{\mathbf{k}}_{21}} ... \, \delta\left(\Gamma_{cont}(s_1, s_2, \hat{\mathbf{k}}_{21})\right) .
\end{aligned} \tag{22}
$$

where $\int_s ... = \int_{-\ell/2}^{\ell/2} ds...$ and the last line simply defines a compact notation for the condition of contact. Equation (21), with the expression given in Eq. (22) for the range of integration, is the generator of collisional dynamics that will be used in the rest of this work.

The above considerations are readily generalized to a system of N rods by considering only binary collisions since collisions among particles with hard core interactions are instantaneous and the probability of three or more particles being at contact at the same instant is of measure zero. In addition, the dynamics arising from the white noise due to the interaction with the substrate is described by a continuous generator and does not lead to any additional singularity. The derivation of the collision trajectory can then be carried out as before. The dynamics of a system of N self-propelled hard rods moving on a passive substrate in the N-rod phase space $\Gamma = \{\Gamma_1, \Gamma_2, ..., \Gamma_N\}$ is controlled by a set of coupled Langevin equations for the linear velocities $\partial_t \mathbf{r}_i = \mathbf{v}_i$ and angular velocities $\boldsymbol{\omega}_i = \hat{\mathbf{u}}_i \times \partial_t \hat{\mathbf{u}}_i = \hat{\mathbf{z}} \omega_i$, given by

$$m\partial_t \mathbf{v}_i = m \sum_{j \neq i} T\left(i, j\right) \mathbf{v}_i - \boldsymbol{\zeta}_i \cdot \mathbf{v}_i + F\hat{\mathbf{u}}_i + \boldsymbol{\eta}_i \tag{23a}$$

$$\partial_t \omega_i = \sum_{j \neq i} T\left(i, j\right) \omega_i - \zeta_R \omega_i + \eta_i^R \tag{23b}$$

where $\boldsymbol{\zeta}_i$ is a friction tensor with components $\zeta_{i,\alpha\beta} = (\zeta_\parallel - \zeta_\perp)\hat{u}_{i\alpha}\hat{u}_{i\beta} + \zeta_\perp \delta_{\alpha\beta}$, $\boldsymbol{\eta}_i$ and η_i^R are Gaussian random forces with zero mean and correlations as defined in Eqs. (8a-8b). Noise sources associated with different values of the rod index i are uncorrelated.

III. NON-EQUILIBRIUM STATISTICAL MECHANICS

We are interested in the collective behavior of self-propelled rods in the limit of large friction with the substrate. In this limit one can consider a description that applies on time scales $t \gg m\zeta_\parallel^{-1}$ that neglects the fast dynamics of the linear and angular velocities and only considers the dynamics of the coordinate degrees of freedom, $\{\mathbf{r}_i, \hat{\mathbf{u}}_i\}_{i=1}^N$. The derivation of the overdamped dynamics must, however, be carried out carefully when dealing with the singular limit of hard particles, where the interactions, even though conservative, depend on the velocities of the particles.

With this goal in mind, we consider an observable of the system $\hat{A}(\Gamma)$, where Γ is an N-rod phase point. Using Ito calculus [17], the stochastic equation of motion for the observable $\hat{A}$ can be derived from the equations of motion, Eq. (23a) and (23b), for the phase space variables, with the result

$$\frac{\partial \hat{A}(\Gamma, t)}{\partial t} = \hat{L}\hat{A}(\Gamma, t) , \tag{24}$$

where the operator $\hat{L}$ is given by

$$\begin{aligned}
\hat{L} = \sum_{i=1}^{N} &\left\{ \mathbf{v}_i \cdot \nabla_{\mathbf{r}_i} + \boldsymbol{\omega}_i \cdot \mathcal{R}_i + \frac{F}{m}\widehat{\mathbf{u}}_i \cdot \nabla_{\mathbf{v}_i} - \frac{1}{m}\zeta_{\alpha\beta}^i v_{i\beta}\partial_{v_{i\alpha}} - \zeta^R \omega_i \partial_{\omega_i} \right. \\
&\left. + \frac{1}{m}\boldsymbol{\eta}_i \cdot \nabla_{\mathbf{v}_i} + \eta_i^R \partial_{\omega_i} - \frac{1}{2m}\Delta_{\alpha\beta}^{iT}\partial_{v_{i\alpha}}\partial_{v_{i\beta}} - \frac{1}{2}\Delta^R \partial_{\omega_i}^2 f \right\} + \frac{1}{2}\sum_{i,j\neq i} T(i,j) ,
\end{aligned} \tag{25}$$

where $\mathcal{R}_i = \widehat{\mathbf{u}}_i \times \partial_{\widehat{\mathbf{u}}_i}$. The binary substitution operator $\hat{b}_{ij}$ contained in $T(i,j) \equiv T(\Gamma_i, \Gamma_j)$ replaces the velocities of the (i,j) pair with their post-collisional values, according to $\hat{b}_{ij}\hat{A}(\mathbf{v}_i, \mathbf{v}_j, \boldsymbol{\omega}_i, \boldsymbol{\omega}_j) = \hat{A}(\mathbf{v}_i', \mathbf{v}_j', \boldsymbol{\omega}_i', \boldsymbol{\omega}_j')$, leaving the velocities of all other particles unchanged. Equation (24) describes the stochastic dynamics of any observable $\hat{A}(\Gamma)$ for given initial conditions in phase space. The quantity of interest here, however, is not the stochastic observable itself, but rather its ensemble averaged value for a given ensemble of initial conditions, $\hat{\rho}_N(\Gamma)$, i.e.,

$$\left\langle \hat{A}(t) \right\rangle_{ens} = \int d\Gamma \hat{\rho}_N(\Gamma) \hat{A}(\Gamma, t) . \tag{26}$$

Equivalently, we can treat the phase space density as the dynamical quantity and write the ensemble average of an observable as

$$\left\langle \hat{A}(t) \right\rangle_{ens} = \int d\Gamma \hat{\rho}_N(\Gamma, t) \hat{A}(\Gamma) . \tag{27}$$

Equation (27) *defines* the dynamics of the phase space probability density, $\hat{\rho}_N(\Gamma, t)$. Taking the time derivative of both Eqs. (26) and (27) and defining an adjoint operator $\hat{\mathcal{L}}$,

$$\begin{aligned}
\int d\Gamma \, \partial_t \hat{\rho}(\Gamma, t) A(\Gamma) &= \int d\Gamma \, \hat{\rho}_N(\Gamma) \partial_t \hat{A}(\Gamma, t) \\
&= \int d\Gamma \, \hat{\rho}_N(\Gamma) \hat{L}\hat{A}(\Gamma, t) \\
&= -\int d\Gamma \left[\hat{\mathcal{L}}\hat{\rho}_N(\Gamma, t) \right] \hat{A}(\Gamma) ,
\end{aligned} \tag{28}$$

we obtain a Liouville-like equation describing the time evolution of of the phase space probability density,

$$\left(\frac{\partial}{\partial t} + \hat{\mathcal{L}} \right) \rho_N(\Gamma, t) = 0 , \tag{29}$$

where

$$\begin{aligned}
\hat{L} = \sum_{i=1}^{N} &\left\{ \mathbf{v}_i \cdot \nabla_{\mathbf{r}_i} + \boldsymbol{\omega}_i \cdot \mathcal{R}_i + \frac{F}{m}\widehat{\mathbf{u}}_i \cdot \nabla_{\mathbf{v}_i} - \frac{1}{m}\zeta_{\alpha\beta}^i v_{i\beta}\partial_{v_{i\alpha}} - \zeta^R \omega_i \partial_{\omega_i} \right. \\
&\left. + \frac{1}{m}\boldsymbol{\eta}_i \cdot \nabla_{\mathbf{v}_i} + \eta_i^R \partial_{\omega_i} - \frac{1}{2m}\Delta_{\alpha\beta}^{iT}\partial_{v_{i\alpha}}\partial_{v_{i\beta}} - \frac{1}{2}\Delta^R \partial_{\omega_i}^2 f \right\} - \frac{1}{2}\sum_{i,j\neq i} \bar{T}(i,j) .
\end{aligned} \tag{30}$$

The single-particle part of $\hat{\mathcal{L}}$ is identified by a simple integration by parts. To determine the binary collision operator $\bar{T}(i,j)$ one needs to explicitly construct the restituting collision, with the result

$$\overline{T}(1,2)\hat{\rho} = \int_{s_1 s_2} \int_{\widehat{\mathbf{k}}} \delta\left(\Gamma_{cont}\left(s_1, s_2, \widehat{\mathbf{k}} \right) \right) \left(\hat{b}_{12}^{-1} - 1 \right) \left| \mathbf{V}_{12} \cdot \widehat{\mathbf{k}} \right| \Theta\left(-\mathbf{V}_{12} \cdot \widehat{\mathbf{k}} \right) \hat{\rho} , \tag{31}$$

where $\hat{b}_{ij}^{-1}$ is the generator of restituting collisions, i.e., $\hat{b}_{ij}^{-1} A\left(x_i', x_j'\right) = A\left(x_i, x_j\right)$, i.e., it replaces the post-collisional velocities of the pair with their pre-collisional values, and $\delta\left(\Gamma_{cont}\left(s_1, s_2, \widehat{\mathbf{k}}\right)\right)$, defined in Eq. (22), enforces the condition of contact.

Finally, we average over the noise and define $\rho_N = \langle \hat{\rho} \rangle$. The dynamical equation describing the evolution of the noise-averaged density is

$$\left(\frac{\partial}{\partial t} + \mathcal{L}\right) \rho_N\left(\Gamma, t\right) = 0 , \tag{32}$$

where $\mathcal{L}$ is the Liouville Fokker Planck operator, given by

$$\begin{aligned}
\mathcal{L} = \sum_{i=1}^N &\left\{ \mathbf{v}_i \cdot \nabla_{\mathbf{r}_i} + \boldsymbol{\omega}_i \cdot \left(\hat{\mathbf{u}}_i \times \frac{\partial}{\partial \hat{\mathbf{u}}_i} \right) + \frac{F}{m} \widehat{\mathbf{u}}_i \cdot \boldsymbol{\nabla}_{\mathbf{v}_i} - \frac{\zeta_{\alpha\beta}^i}{m} \partial_{v_{i\alpha}} v_{i\beta} - \zeta^R \partial_{\omega_i} \omega_i \right. \\
&\left. - \frac{1}{2m} \Delta_{\alpha\beta}^{iT} \partial_{v_{i\alpha}} \partial_{v_{i\beta}} - \frac{1}{2} \Delta^R \partial_{\omega_i}^2 f \right\} - \frac{1}{2} \sum_{i,j \neq i} \overline{T}\left(i,j\right) .
\end{aligned} \tag{33}$$

The formulation just described is exact and can be used, for instance, to evaluate time correlation functions for the system. To proceed, we will now restrict our attention to a low-density collections of self-propelled rods. In this case one can make systematic approximations to obtain the effective coarse-grained theory in the form of a Smoluchowski equation.

IV. LOW DENSITY EFFECTIVE STATISTICAL MECHANICS

In order to carry out systematic approximations in the low density limit, it is convenient to define a hierarchy of reduced distribution functions as

$$f_m\left(\Gamma_1, ..., \Gamma_m, t\right) = V^m \int d\Gamma_{m+1}...d\Gamma_N \, \rho_N\left(\Gamma, t\right) . \tag{34}$$

The Liouville Fokker-Planck equation, Eq. (32), can then be rewritten as an infinite hierarchy of equations for the reduced distribution functions. The m-th equation for f_m couples to f_{m+1}. The resulting Fokker-Planck hierarchy is analogous to the BBGKY hierarchy for Hamiltonian systems and forms the starting point for constructing approximate theories to describe the system in various regimes of interest.

At low density, we consider the first equation of the hierarchy for the one-particle distribution function $f_1\left(\Gamma_1, t\right)$, given by

$$\frac{\partial f_1(\Gamma_1, t)}{\partial t} + \mathcal{D} f_1(\Gamma_1, t) = \int d\Gamma_2 \, \overline{T}\left(1, 2\right) f_2(\Gamma_1, \Gamma_2, t) , \tag{35}$$

where the one-particle operator $\mathcal{D}$ is given by

$$\mathcal{D} f_1 = \mathbf{v}_1 \cdot \nabla_{\mathbf{r}_1} f_1 + \boldsymbol{\omega}_1 \cdot \mathcal{R}_1 f_1 + \frac{F}{m} \widehat{\mathbf{u}_1} \cdot \boldsymbol{\nabla}_{\mathbf{v}_1} f_1 - \frac{1}{m} \zeta_{\alpha\beta}^1 \partial_{v_{1\alpha}} \left(v_{1\beta} f_1\right) - \zeta^R \partial_{\omega_1} \left(\omega_1 f_1\right) - \frac{1}{2m} \Delta_{\alpha\beta}^{1T} \partial_{v_{1\alpha}} \partial_{v_{1\beta}} f_1 - \frac{1}{2} \Delta^R \partial_{\omega_1}^2 f_1 . \tag{36}$$

Equation (35) is a generalized Fokker-Planck equation that includes binary collisions. We are interested in the limit of large friction, where linear and angular velocities relax on fast time scales. Our goal is to construct an approximate closed equation for a local concentration field $c\left(\mathbf{r}, \hat{\mathbf{u}}, t\right)$, defined as

$$c\left(\mathbf{r}_1, \hat{\mathbf{u}}_1, t\right) = \int_{\mathbf{v}_1, \boldsymbol{\omega}_1} f_1\left(\mathbf{r}_1, \mathbf{v}_1, \hat{\mathbf{u}}_1, \boldsymbol{\omega}_1, t\right) . \tag{37}$$

Specifically, we seek to derive a kinetic equation for self propelled particles that is analogous to the mean field Smoluchowski equation for thermal nematics. In the remainder of this section we present a systematic method for deriving such a closed kinetic equation for c in the limit of low density.

We adopt the simplest phenomenological closure of the Fokker-Planck equation (35) of the form $f_2\left(\Gamma_1, \Gamma_2, t\right) = f_1\left(\Gamma_1, t\right) f_1\left(\Gamma_2, t\right)$. With this closure, Eq. (35) becomes a Boltzmann-Fokker-Planck equation for the one-particle distribution function,

$$\frac{\partial f_1}{\partial t} + \mathcal{D} f_1 = \int d\Gamma_2 \, \overline{T}\left(1, 2\right) f_1(\Gamma_1, t) f_1(\Gamma_2, t) \tag{38}$$

To derive the Smoluchowski equation, in addition to the concentration field $c\left(\mathbf{r}, \hat{\mathbf{u}}, t\right)$ given in Eq. (37), we introduce translational and rotational currents $\mathbf{J}^T$ and $\mathbf{J}^R$, defined as velocity moments of the one particle distribution function, with

$$\mathbf{J}^T\left(\mathbf{r}_1, \hat{\mathbf{u}}_1, t\right) = \int_{\mathbf{v}_1, \boldsymbol{\omega}_1} \mathbf{v}_1 \; f_1\left(\mathbf{r}_1, \hat{\mathbf{u}}_1, \mathbf{v}_1, \boldsymbol{\omega}_1, t\right) \; , \tag{39a}$$

$$\mathbf{J}^R\left(\mathbf{r}_1, \hat{\mathbf{u}}_1, t\right) = \int_{\mathbf{v}_1, \boldsymbol{\omega}_1} \boldsymbol{\omega}_1 \; f_1\left(\mathbf{r}_1, \hat{\mathbf{u}}_1, \mathbf{v}_1, \boldsymbol{\omega}_1, t\right) \; . \tag{39b}$$

The dynamical equations for the concentration c and the translational and rotational currents are obtained by taking moments of Eq. (38), with the result,

$$\frac{\partial c}{\partial t} + \boldsymbol{\nabla}_{\mathbf{r}_1} \cdot \mathbf{J}^T + \mathcal{R}_1 \cdot \mathbf{J}^R = 0 \tag{40a}$$

$$\frac{\partial J_\alpha^T}{\partial t} + \frac{\zeta_{\alpha\beta}^1}{m} J_\beta^T - \frac{F}{m} \widehat{u}_{1\alpha} c + \partial_{1\beta} \langle v_\alpha v_\beta \rangle c + \mathcal{R}_{1\beta} \langle \omega_\alpha v_\beta \rangle c = -I_\alpha^T \tag{40b}$$

$$\frac{\partial J_\alpha^R}{\partial t} + \zeta^R J_\alpha^R + \partial_{1\beta} \langle \omega_\alpha v_\beta \rangle c + \mathcal{R}_{1\beta} \langle \omega_\alpha \omega_\beta \rangle c = -I_\alpha^R \tag{40c}$$

where

$$\langle v_\alpha v_\beta \rangle = \frac{1}{c} \int_{\mathbf{v}_1, \boldsymbol{\omega}_1} v_{1\alpha} v_{1\beta} \; f_1(\Gamma_1, t) \tag{41a}$$

$$\langle \omega_\alpha v_\beta \rangle = \frac{1}{c} \int_{\mathbf{v}_1, \boldsymbol{\omega}_1} \omega_{1\alpha} v_{1\beta} \; f_1(\Gamma_1, t) \tag{41b}$$

$$\langle \omega_\alpha \omega_\beta \rangle = \frac{1}{c} \int_{\mathbf{v}_1, \boldsymbol{\omega}_1} \omega_{1\alpha} \omega_{1\beta} \; f_1(\Gamma_1, t) \tag{41c}$$

are the second moments of f_1 with respect to the translational and rotational velocities, and

$$I_\alpha^T = \int d\Gamma_2 \; [T\left(1, 2\right) v_{1\alpha}] \, f_1(\Gamma_1, t) f_1(\Gamma_2, t) \tag{42a}$$

$$I_\alpha^R = \int d\Gamma_2 \; [T\left(1, 2\right) \omega_{1\alpha}] \, f_1(\Gamma_1, t) f_1(\Gamma_2, t) \tag{42b}$$

are the linear and angular momentum transfers, respectively, due to collisions with the other particles in the system.

The equations for the translational and rotational currents contain frictional damping and relax on time scales of order $m/\zeta_\parallel$ due to the interaction with the substrate. On time scales $t \gg m\zeta_\parallel^{-1}$ the fluxes can be approximated as

$$\lim_{t \gg m/\zeta_\parallel} J_\alpha^T = -m(\zeta_{\alpha\beta}^1)^{-1} \left[-\frac{F}{m} \widehat{u}_{1\beta} c + \partial_{1\beta} \langle v_\alpha v_\beta \rangle c + \mathcal{R}_{1\beta} \langle \omega_\alpha v_\beta \rangle c + I_\alpha^T \right] \; , \tag{43a}$$

$$\lim_{t \gg \zeta_R^{-1}} J_\alpha^R = -\zeta_R^{-1} \left[\partial_{1\beta} \langle \omega_\alpha v_\beta \rangle c + \mathcal{R}_{1\beta} \langle \omega_\alpha \omega_\beta \rangle c + I_\alpha^R \right] \; . \tag{43b}$$

In this regime we can fully describe the system's dynamics in terms of the one-particle configurational probability $c(\mathbf{r}, \hat{\mathbf{u}}, t)$. To obtain a closed equation, we must express the currents as functionals of the configurational probability.

A. Thermal Hard Rods: Derivation of the Onsager Excluded Volume Interaction

Before deriving the Smoluchwski equation for self-propelled hard rods, we show in this section how this method can be implemented to provide a derivation of the Smoluchowski equation for thermal hard rods, with the well-known mean field Onsager excluded volume interaction. We set the self-propulsion force $F = 0$ and assume the noise is thermal, i.e. $T_a = T$.

For large friction the relaxation of the linear and angular velocities of the rods is controlled primarily by the interaction of the rods with the substrate, rather than by interparticle collisions. We can then assume that the for

times $t >> m/\zeta_\parallel$ the velocity distribution has relaxed to its noninteracting value. In the absence of collisions, the Fokker-Planck equation, Eq. (35), for the one-particle distribution function takes the form

$$\frac{m}{\zeta_\parallel} \left(\partial_t + \mathbf{v}_1 \cdot \nabla_{\mathbf{r}_1} + \boldsymbol{\omega}_1 \cdot \mathcal{R}_1\right) f_1 \quad + \left[\frac{\zeta_\perp}{\zeta_\parallel}\delta_{\alpha\beta} - \left(1 - \frac{\zeta_\perp}{\zeta_\parallel}\right) \hat{u}_{1\alpha}\hat{u}_{1\beta}\right] \left(\partial_{v_{1\alpha}} v_{1\beta} + \frac{k_B T}{m}\partial_{v_{1\alpha}} \partial_{v_{1\beta}}\right) f_1$$

$$+ \frac{m\zeta^R}{\zeta_\parallel} \left(\partial_{\omega_1} \omega_1 + \frac{k_B T}{I}\partial^2_{\omega_1}\right) f_1 = 0 \ , \tag{44}$$

where we have used the form of the noise amplitude in Eq. (8a-8b) to eliminate it in favor of the temperature T. The first term on the left hand side of Eq. (44) can be neglected for $t >> m/\zeta_\parallel$. The solution of the non-interacting Fokker-Planck equation can then be written in a factorized form as

$$f_1 \left(\mathbf{r}_1, \mathbf{v}_1, \hat{\mathbf{u}}_1, \boldsymbol{\omega}_1, t\right) = c \left(\mathbf{r}_1, \hat{\mathbf{u}}_1, t\right) f_M(v_1, \omega_1) \ , \tag{45}$$

with

$$f_M(v_1, \omega_1) = A \exp\left(-mv_1^2/2k_B T\right) \exp(-I\omega_1^2/2k_B T) \ , \tag{46}$$

and A a normalization constant. In other words, we assume that on the time scales of interest the linear and angular velocity distributions have relaxed to their equilibrium forms. Using this expression, the velocity moments defined in Eqs. (41a-42b) can be immediately calculated with the result,

$$\langle v_\alpha v_\beta \rangle = \frac{k_B T}{m}\delta_{\alpha\beta} \ , \tag{47a}$$

$$\langle v_\alpha \omega_\beta \rangle = 0 \ , \tag{47b}$$

$$\langle \omega_\alpha \omega_\beta \rangle = \frac{k_B T}{I}\delta_{\alpha\beta} \ . \tag{47c}$$

Next, we need to evaluate the collisional transfer contributions, I_α^T and I_α^R defined in Eqs. (42a) and (42b). This requires calculating the mean linear and angular velocity transferred in a collision, $\langle T(1,2) v_{1\alpha}\rangle_M$ and $\langle T(1,2) \omega_{1\alpha}\rangle_M$ where

$$\langle X \rangle_M = \int_{\mathbf{v}_1, \boldsymbol{\omega}_1} \int_{\mathbf{v}_2, \boldsymbol{\omega}_2} X \ f_M (v_1, \omega_1) f_M (v_2, \omega_2) \ . \tag{48}$$

Using the explicit form of the momentum transfer in a binary hard rod collision given in Eq. (14), we find

$$\langle T(1,2)\mathbf{v}_{1\alpha}\rangle_M = -\int_{s_1 s_2 \hat{k}} \left\langle \left(\mathbf{V}_{12} \cdot \hat{\mathbf{k}}\right)^2 \Theta \left(-\mathbf{V}_{12} \cdot \hat{\mathbf{k}}\right) \right\rangle_M$$

$$\times \frac{1}{1 + \frac{m}{2I}\left(\boldsymbol{\xi}_1 \times \hat{\mathbf{k}}\right)^2 + \frac{m}{2I}\left(\boldsymbol{\xi}_2 \times \hat{\mathbf{k}}\right)^2} \delta\left(\Gamma_{cont}\left(s_1, s_2, \hat{\mathbf{k}}\right)\right) \hat{k}_\alpha \ . \tag{49}$$

The Θ function in Eq. (49) selects only those values of the pre-collision velocities that will actually result in a collision. In the mean field limit of interest here, we assume that on average half the particles in the flux will have initial velocities that will yield a collision and approximate the velocity average in Eq. (49) as

$$\left\langle \left(\mathbf{V}_{12} \cdot \hat{\mathbf{k}}\right)^2 \Theta \left(-\mathbf{V}_{12} \cdot \hat{\mathbf{k}}\right) \right\rangle_M \sim \frac{1}{2} \left\langle \left(\mathbf{V}_{12} \cdot \hat{\mathbf{k}}\right)^2 \right\rangle_M$$

$$= \frac{1}{2} \left[\frac{2k_B T}{m} + \frac{k_B T}{I}\left(\boldsymbol{\xi}_1 \times \hat{\mathbf{k}}\right)^2 + \frac{k_B T}{I}\left(\boldsymbol{\xi}_2 \times \hat{\mathbf{k}}\right)^2\right] \ . \tag{50}$$

Substituting Eq. (50) in Eq. (49) we find

$$\langle T(1,2)\mathbf{v}_{1\alpha}\rangle_M \simeq -\frac{k_B T}{m} \int_{s_1 s_2} \int_{\hat{\mathbf{k}}} \delta\left(\Gamma_{cont}\left(s_1, s_2, \hat{\mathbf{k}}\right)\right) \hat{k}_\alpha \ . \tag{51}$$

Similarly, it is easy to show that

$$\langle T(1,2)\omega_{1\alpha}\rangle_M = -\frac{k_B T}{I} \int_{s_1 s_2} \int_{\hat{\mathbf{k}}} \delta\left(\Gamma_{cont}\left(s_1, s_2, \hat{\mathbf{k}}\right)\right) \left(\mathbf{s} \times \hat{\mathbf{k}}\right)_\alpha \ , \tag{52}$$

where $\mathbf{s}$ is defined in Fig. 1. In the thin rod limit, i.e., $R \to 0$, the contact delta function in Eqs. (51) and (52) is non zero on the perimeter of a parallelogram centered at the position $\mathbf{r}_1$ rod 1 with sides of length ℓ directed along $\hat{\mathbf{u}}_1$ and $\hat{\mathbf{u}}_2$ (Fig. 1). The area of such a parallelogram can be written as

$$A_{\|gram}(\mathbf{r}_1, \hat{\mathbf{u}}_1) = \ell^2 \int_{s_1, s_2} \Theta \left(0^+ - |\mathbf{r}_{12} + s_1 \hat{\mathbf{u}}_1 - s_2 \hat{\mathbf{u}}_2| \right) . \tag{53}$$

It is easy to verify that

$$\nabla_{\mathbf{r}_1} A_{\|gram} = -\ell^2 \int_{s_1, s_2} \int_{\hat{\mathbf{k}}_{21}} \delta \left(\Gamma_{cont} \left(s_1, s_2, \hat{\mathbf{k}}_{21} \right) \right) \hat{\mathbf{k}}_{21} , \tag{54a}$$

$$\mathcal{R}_1 A_{\|gram} = -\ell^2 \int_{s_1, s_2} \int_{\hat{\mathbf{k}}_{21}} \delta \left(\Gamma_{cont} \left(s_1, s_2, \hat{\mathbf{k}} \right) \right) \left(\mathbf{s} \times \hat{\mathbf{k}}_{21} \right) . \tag{54b}$$

Finally, combining all these results we obtain the familiar Smoluchowski equation for hard given in Eqs. (1), (2b) and (2a) with $D_{\alpha\beta} = \zeta_{\alpha\beta}^{-1} k_B T / m$ and $D_R = k_B T / (\zeta_R I)$. The excluded volume interaction can be written in the familiar Onsager form by noting that the area of the collisional parallelogram is simply given by $A^{\|gram} = \ell^2 |\hat{\mathbf{u}}_1 \times \hat{\mathbf{u}}_2|$ as illustrated in Fig. (1). This gives Eq. (4), where the integral over $\mathbf{s}$ spans the area of the parallelogram shown in Fig. (1) for fixed orientation of rod 2, while the integral over $\hat{\mathbf{u}}_2$ averages over all possible orientations of the second rod. The Onsager excluded volume interaction has a purely entropic interpretation as the free energy cost for a rod to occupy the area excluded by another rod. Here the same result has been derived from dynamical considerations and has the alternate interpretation of mean-field momentum transfer in a binary collision of two rods, each carrying an average momentum of magnitude $\sqrt{m k_B T}$. The orientational correlations arise then from the anisotropy of the collision frequency due to the fact that head to head collisions are of measure zero with respect to head to side collisions.

In summary, we have shown in this subsection that for thermal (non self-propelled) hard rods the method described in this paper can be used to derive the familiar Smoluchowski equation with the Onsager expression for the excluded volume interaction. In the next section we apply the same procedure to self-propelled hard rods and show that self-propulsion modifies the Smoluchowski equation in several ways.

B. Self-propelled hard rods

As for the case of thermal hard rods, the derivation of the Smoluchowski equation for self propelled rods consists of two steps: (i) we identify a stationary normal solution of the noninteracting Boltzmann-Fokker Plank equation, and (ii) we use this functional form to close the equations for the translational and rotational fluxes in a quasi-static approximation.

In the absence of interactions, the Fokker-Planck equation for self-propelled rods is given by

$$\frac{m}{\zeta_{\|}} \left(\partial_t + \mathbf{v}_1 \cdot \nabla_{\mathbf{r}_1} + \boldsymbol{\omega}_1 \cdot \mathcal{R}_1 \right) f_1 + v_0 \hat{\mathbf{u}}_1 \cdot \nabla_{\mathbf{v}_1} + \left[\frac{\zeta_\perp}{\zeta_{\|}} \delta_{\alpha\beta} - \left(1 - \frac{\zeta_\perp}{\zeta_{\|}} \right) \hat{u}_{1\alpha} \hat{u}_{1\beta} \right] \left(\partial_{v_{1\alpha}} v_{1\beta} + \frac{k_B T}{m} \partial_{v_{1\alpha}} \partial_{v_{1\beta}} \right) f_1$$
$$+ \frac{m \zeta^R}{\zeta_{\|}} \left(\partial_{\omega_1} \omega_1 + \frac{k_B T}{I} \partial_{\omega_1}^2 \right) f_1 = 0 \tag{55}$$

with $v_0 = \frac{F}{\zeta_{\|}}$ the self propulsion velocity. On time scales large compared to $m/\zeta_{\|}$, we neglect the first term on the left hand side of Eq. (55). The stationary normal solution then has the form

$$f_1 \left(\mathbf{r}_1, \hat{\mathbf{u}}_1, \mathbf{v}_1, \boldsymbol{\omega}_1, t \right) = c \left(\mathbf{r}_1, \hat{\mathbf{u}}_1, t \right) f_S \left(\mathbf{v}_1, \boldsymbol{\omega}_1 | \hat{\mathbf{u}}_1 \right) , \tag{56}$$

with

$$f_S = A \exp \left(-\frac{1}{2 k_B T} m \left(\mathbf{v}_1 - v_0 \hat{\mathbf{u}}_1 \right)^2 - \frac{1}{2 k_B T} I \omega_1^2 \right) , \tag{57}$$

and A a normalization constant. Inserting this stationary normal solution in Eqs. (43), we obtain

$$J_\alpha^T = v_0 \hat{u}_{1\alpha} c - D_S \hat{u}_{1\alpha} \hat{\mathbf{u}}_1 \cdot \nabla_{\mathbf{r}_1} c - D_{\alpha\beta} \partial_{r_{1\beta}} c - m \zeta_{\alpha\beta}^{-1} \left(\int d\mathbf{r}_2 d\hat{\mathbf{u}}_2 \left\langle T(1,2) v_{1\beta} \right\rangle_S c \left(\mathbf{r}_2, \hat{\mathbf{u}}_2, t \right) \right) c \left(\mathbf{r}_1, \hat{\mathbf{u}}_1, t \right) , \tag{58a}$$

$$\mathbf{J}^R = -D_R \mathcal{R}_1 c - \frac{1}{\zeta^R} \left(\int d\mathbf{r}_2 d\hat{\mathbf{u}}_2 \left\langle T(1,2) \boldsymbol{\omega}_1 \right\rangle_S c \left(\mathbf{r}_2, \hat{\mathbf{u}}_2, t \right) \right) c \left(\mathbf{r}_1, \hat{\mathbf{u}}_1, t \right) , \tag{58b}$$

where the angular brackets $\langle ... \rangle_S$ denote the average over the linear and angular velocities with weigh f_S. The diffusion coefficients $D_{\alpha\beta}$ and D_R are as given in the previous subsection, but with $T = T_a$, and $D_S = \frac{v_0^2}{\zeta_\parallel}$.

The next step is the evaluation of the average linear and angular momentum transfer in a collision,

$$\langle T(1,2) \mathbf{v}_1 \rangle_S = \int_{\mathbf{v}_1, \boldsymbol{\omega}_1} \int_{\mathbf{v}_2, \boldsymbol{\omega}_2} T(1,2) \mathbf{v}_1 \, f_S(\mathbf{v}_1, \boldsymbol{\omega}_1 | \hat{\mathbf{u}}_1) f_S(\mathbf{v}_2, \boldsymbol{\omega}_2 | \hat{\mathbf{u}}_2) \,, \tag{59a}$$

$$\langle T(1,2) \boldsymbol{\omega}_1 \rangle_S = \int_{\mathbf{v}_1, \boldsymbol{\omega}_1} \int_{\mathbf{v}_2, \boldsymbol{\omega}_2} T(1,2) \boldsymbol{\omega}_1 \, f_S(\mathbf{v}_1, \boldsymbol{\omega}_1 | \hat{\mathbf{u}}_1) f_S(\mathbf{v}_2, \boldsymbol{\omega}_2 | \hat{\mathbf{u}}_2) \,. \tag{59b}$$

When deriving the Onsager excluded volume interaction in the previous subsection, we neglected dynamical velocity correlations by approximating $\left\langle (\mathbf{V}_{12} \cdot \hat{\mathbf{k}})^2 \Theta(-\mathbf{V}_{12} \cdot \hat{\mathbf{k}}) \right\rangle \sim \frac{1}{2} \left\langle (\mathbf{V}_{12} \cdot \hat{\mathbf{k}})^2 \right\rangle$. This approximation is not valid for self-propelled rods as the dynamical velocity correlations induced by the self propulsion velocity, which is directed along $\hat{\mathbf{u}}$, are also *orientational* correlations. On the other hand, an approximation is required to make the problem tractable.

The Smoluchowski equation is a mean field model and only describes the average momentum transfer in a collision. We then assume

$$\langle T(1,2) \mathbf{v}_1 \rangle_S \simeq \langle T(1,2) \mathbf{v}_1 \rangle_{M_a} + \langle T(1,2) \mathbf{v}_1 \rangle_{SP} \,, \tag{60a}$$

$$\langle T(1,2) \boldsymbol{\omega}_1 \rangle_S \simeq \langle T(1,2) \boldsymbol{\omega}_1 \rangle_{M_a} + \langle T(1,2) \boldsymbol{\omega}_1 \rangle_{SP} \,, \tag{60b}$$

where $\langle X \rangle_{M_a}$ denotes velocity averages with the Maxwellian distribution given in Eq. (46) at temperature $T = T_a$ and $\langle X \rangle_{SP}$ denotes velocity averages in a regime where all particles are moving at velocity $v_0 \hat{\mathbf{u}}$ and the one-rod velocity distribution is given by $f_{SP} \sim \delta(\mathbf{v} - v_0 \hat{\mathbf{u}}) \delta(\boldsymbol{\omega})$. The first terms on the right hand side of Eqs. (60) are then evaluated as in the previous section by neglecting the dynamical velocity correlations and yield again the Onsager excluded volume potential given in Eq. (4). The second terms on the right hand side of Eqs. (60) are evaluated by neglecting static orientational correlations arising from the term $\left[1 + (m/2I)(\boldsymbol{\xi}_1 \times \hat{\mathbf{k}})^2 + (m/2I)(\boldsymbol{\xi}_2 \times \hat{\mathbf{k}})^2 \right]^{-1}$ in Eq. (14) as these correlations are already incorporated in the noise. It can be shown that this approximation becomes exact if we replace the rod by a string of beads in contact with each other and calculate the momentum transfer between the two specific beads that participate in the collision. With these approximations, the average momentum transfer is given by

$$\left(\int_2 \langle T(1,2) \mathbf{v}_{1\beta} \rangle_S c(2) \right) c(1) \simeq \frac{1}{m} (\nabla_{\mathbf{r}_{1\alpha}} V_{ex}) c + v_0^2 I_\alpha^{SP} \tag{61a}$$

$$\left(\int_2 \langle T(1,2) \boldsymbol{\omega}_1 \rangle_S c(2) \right) c(1) \simeq \frac{1}{I} \mathcal{R}_1 V_{ex} c + \frac{v_0^2}{2I} I_R^{SP} \,, \tag{61b}$$

with

$$I^{SP} = \int_s \int_{\hat{\mathbf{u}}_2} \sin^2(\theta_1 - \theta_2) \left[\Theta(\sin(\theta_1 - \theta_2)) - \Theta(-\sin(\theta_1 - \theta_2)) \right]$$

$$\times \left[\hat{\mathbf{u}}_1^\perp \, c\left(\mathbf{r}_1 + s\hat{\mathbf{u}}_1 - \frac{\ell}{2}\hat{\mathbf{u}}_2, \hat{\mathbf{u}}_2, t \right) + \hat{\mathbf{u}}_2^\perp \, c\left(\mathbf{r}_1 + s\hat{\mathbf{u}}_2 - \frac{\ell}{2}\hat{\mathbf{u}}_1, \hat{\mathbf{u}}_2, t \right) \right] \,, \tag{62}$$

$$\mathbf{I}_R^{SP} = \hat{\mathbf{z}} \int_s \int_{\hat{\mathbf{u}}_2} \sin^2(\theta_1 - \theta_2) \left[\Theta(\sin(\theta_1 - \theta_2)) - \Theta(-\sin(\theta_1 - \theta_2)) \right]$$

$$\times \left[s \, c\left(\mathbf{r}_1 + s\hat{\mathbf{u}}_1 - \frac{\ell}{2}\hat{\mathbf{u}}_2, \hat{\mathbf{u}}_2, t \right) + \frac{\ell}{2} \cos(\theta_1 - \theta_2) \, c\left(\mathbf{r}_1 + s\hat{\mathbf{u}}_2 - \frac{\ell}{2}\hat{\mathbf{u}}_1, \hat{\mathbf{u}}_2, t \right) \right] \,. \tag{63}$$

Finally, when these results are substituted into Eq. (58a) and (58b), we obtain the modified Smoluchowski equation given in Eq. (5).

There are three important modifications of the Smoluchowski equation for self-propelled particles when compared to its equilibrium counterpart for thermal particles.

1. The translational current $\mathbf{J}^T$ in Eq. (5a) contains a convective term $v_0 \hat{\mathbf{u}}_1 c$ that arises because self-propelled particles move in the direction of their long axis. This is a signature of the polar nature of the microdynamics of the system.

2. Self propulsion yields an additional longitudinal diffusion current $D_S \hat{u}_{1\alpha} \hat{u}_{1\beta} \partial_{1\beta} c$, with $D_S \sim v_0^2$. This can be understood as follows. A Brownian particle subject to a frictional damping ζ takes Brownian steps of mean length $\Delta \sim \sqrt{m k_B T}/\zeta$, with $\sqrt{k_B T/m}$ the thermal speed of the particle and m/ζ the frictional time scale over which the velocity relaxes to zero. This yields the simple estimate $D \sim \Delta^2/(m/\zeta) \sim k_B T/\zeta$ for the diffusion coefficient. A Brownian rod experiences anisotropic friction $\zeta_\parallel$ and $\zeta_\perp$, yielding mean steps $\Delta_\parallel \sim \sqrt{m k_B T}/\zeta_\parallel$ and $\Delta_\perp \sim \sqrt{m k_B T}/\zeta_\perp$ in the directions longitudinal and transverse to its long axis, respectively. This gives anisotropic diffusion constants $D_\parallel \sim k_B T \zeta_\parallel$ and $D_\perp \sim k_B T/\zeta_\perp$. When the rod is self propelled it performs a persistent random walk along its long axis controlled by the competition between ballistic motion at speed v_0 and rotational diffusion at rate $D_R \sim D_\parallel/\ell^2$. As a result, the mean square velocity is approximately $\langle v^2 \rangle \sim \frac{k_B T}{m} + v_0^2$. For small values of v_0 this gives $\langle v^2 \rangle^{1/2} \sim \frac{k_B T}{m} \left[1 + \frac{m v_0^2}{2 k_B T} \right]$. This yields an additional contribution of order v_0^2 to the longitudinal diffusion, corresponding to the second term of Eq. (6).

3. Both the translational and rotational fluxes in Eq. (5) contain additional active contributions arising from the momentum transfer associated with self propulsion. Collisions among particle induce dynamical velocity correlations. These are negligible for a mean-field description of overdamped thermal hard rods that only seeks to capture the dynamics of the translational and orientational degrees of freedom. When the rods are self-propelled with a physical velocity directed along their long axis, collisions induce *both* velocity and orientational correlations since the two are intimately coupled. These additional collision-induced orientational correlations have been shown to affect the physics of the system even on hydrodynamic scales [12].

Our work demonstrates that orientational fluctuations have a profound effect on mass transport in self-propelled particle systems. Furthermore this observation is not limited to the specific hard rod model considered here, but holds generically for all collections of self-propelled units. Our result relies solely on the presence of short-range excluded volume interactions that are present in all physical systems, but not on the specific implementation of such interaction in the hard particle limit.

V. DISCUSSION

In this paper we have analyzed the microscopic dynamics and statistical mechanics of a collection of self-propelled particles modeled as long thin polar rods that move along one direction of their long axis. The formalism developed here is general and of wide applicability. It can be used to study fluctuations and response functions in fluids of self-propelled particles by building on techniques developed for traditional fluids. In addition, the formalism can readily be generalized to particles of arbitrary shape and to higher dimensions, making it also relevant for applications to granular fluids.

As a particular application of the general formalism, we have derived the Smoluchowski equation that governs the dynamics of the one particle configuration probability density in the overdamped regime, for both thermal and self propelled particles. For thermal rods, this provides a purely dynamical derivation of the familiar Onsager excluded volume interaction and is useful for identifying the limitations of this widely used effective interaction in capturing the physics of out-of-equilibrium systems. For self propelled hard rods, the modified Smoluchowski equation presented here is the first tractable theory of the dynamics of self-propelled particles that captures the physics of contact interactions and their modifications due to the presence of self propulsion. In a separate work we have used this Smoluchowski equation as the starting point for deriving a coarse grained (hydrodynamic) description of the system in terms of conserved quantities and broken symmetry variables [12, 13]. Self propulsion has profound effects on the system on hydrodynamic scales, including enhanced orientational order arising from the orientational correlations induced dynamically via collisions, instabilities of the ordered phases, and the existence of propagating sound-like density waves in this otherwise overdamped system.

Having derived the Smoluchowski equation from first principles, we can also identify its scope and limitations. Our theory captures the fluctuations in velocity induced by orientational fluctuations and the associated modifications to the mass flux that characterize this inherently nonequilibrium system. These effects yield the convective and diffusive terms in Eq. (5). The theory also captures some of the orientational correlations induced by collisional interactions through the additional momentum transfer contributions to the fluxes. These correlations are important as evidenced by the enhanced ordering identified in [12] and observed in numerical simulations of motility assays [6]. The derivation is, however, based on a low-density kinetic theory that neglects two-particle velocity correlations. While this is a reasonable approximation for overdamped thermal particles that have an underlying equilibrium state, in the case of self propelled particles, these correlations will generate additional orientational correlations that are neglected in the present approximation. The Fokker-Planck hierarchy derived here can serve as the starting point for analyzing the effect of these two-particle correlations. This is left for future work.

In summary, we have constructed the non-equilibrium statistical mechanics of a system of self propelled particles and derived a modified Smoluchowski equation for the system. We have discussed the content of the resulting theory and identified its scope, limitations and potential for future applications.

Acknowledgments

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