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# ABSTRACT

Using the tools of kinetic theory, we derive a hydrodynamic model for self-propelled particles of an arbitrary shape from first principles, in a sufficiently dilute suspension limit, moving in a 3-dimensional space inside a viscous solvent. The model is then restricted to particles with ellipsoidal geometry to quantify the interplay of the long-range excluded volume and the short range self-propulsion effects. The expression for the constitutive stresses, relating the kinetic theory with the momentum transport equations, are derived using a combination of the virtual work principle (for extra elastic stresses) and symmetry arguments (for active stresses).

Keywords: Kinetic theory, liquid crystal polymers, active materials, virtual work principle, excluded volume potential, collision operator, active stress

## **1. INTRODUCTION**

Self propelled particle (SPP) systems are a new and challenging class of complex fluids. Such systems are also termed as 'active materials' since they continuously burn energy, supplied by their internal or some external sources and dissipate it by moving through the system they inhabit. These systems are ubiquitous in biological contexts, such as bacterial swimmers, living cells moving on a substrate, ion pumps, self-propelled colloids [1] and cytoskeleton of eukariotic cells [2]. For example, the molecular motors associated with the cytoskeleton network, such as myosin and kinesin, use the chemical energy from the hydrolysis of adenosine triphosphate (ATP) to propel themselves and thus exert active stress on the network [3]. Similarly, non-biological counterparts may also be realized, for instance with vibrated granular rods [4].

Activity imparts peculiar physical characteristics in these systems such as swarming, chemotaxis and bio-convection [5]. Another striking phenomena exhibited by these systems is flocking, or the emergence of coherently moving macroscopic symmetry breaking structures such as radial arrays, esters, vortices and one dimensional bundles [6]. Spontaneous flow can occur in non-driven active materials [7], unlike their passive liquid crystalline counterparts which either need an external forcing [8, 9, 10, 11, 12] or the boundary effects [13] to drive them out of thermodynamic equilibrium. This is because the energy input that maintains these system out of equilibrium is on each unit rather than at the boundaries as in more conventional non-equilibrium situations [1]. Further, many active biological gels, such as actomyosin networks, thicken when sheared [7]. This is typically opposite of the behavior of viscous polymeric liquids which flows more easily when shear stress increases [14]. Physical characteristics, such as the persistence length, may also contribute to a different behavior of these gels [15].

Consequently various models have been proposed to understand the hydrodynamics and the rheology of active suspensions. Earliest continuum models have either ignored the particle diffusion or the interaction of the self-propulsion mechanism on the orientational dynamics [16]. Ramaswamy *et al.* [1, 17] generalized the Leslie-Erickson director theory of liquid crystals [18] and proposed the hydrodynamical equations in terms of a few course-grained field variables using symmetry considerations and conservation laws. A variation of this model was used by Prost *et al.* [6, 19] to describe the active dynamics of viscoelastic polar gels. Marenduzzo [7] studied the active nematics using lattice Boltzmann simulations and confirmed the existence of a phase transition from the passive to an active phase, characterized by a spontaneous flow in the steady state. Ishikawa [20] and Haines [21] performed simulations of dilute suspensions of self-propelled spheres and disks, respectively. They quantified the relationship between the decrease in the apparent viscosity and the increase in the alignment of these particles to the background flow. Cui performed the stability analysis to predict the

rheology of weakly sheared active suspension of rods, including an activity thickening / thinning behavior of the apparent viscosity, depending on the particle type, flow alignment and the boundary conditions [22]. However, self-propelled particles may come in a variety of shapes including spheres, rods and discs but these studies are only applicable to particles with a specific shape. Recently, Saintillan [15, 23] employed a mesoscopic kinetic theory to study the pattern formation in active suspensions similar to those found in experiments [5]. They found that the flow aligning rodlike particles are unstable at long wavelengths due to hydrodynamic fluctuations. But their results, while suggestive, do not include the spatial gradients of the hydrodynamic feedback.

Motivated by the above mentioned issues and recent experiments, we present a mesoscopic kinetic theory for semi-dilute active suspensions where the individual self-propelling units have an arbitrary shape. We hope to answer the following questions in our model: (1) How to effectively model the long range and the short range interactions due to self-propulsion? and (2) How does the particle shape effects the large scale dynamics of the system? We assume that the particles are apolar, i.e. apart from the contribution due to self-propulsion, an assembly of these particles can be approximated as a biaxial nematic liquid crystal polymer [12]. Our work is partly motivated by the classical theory of Kirkwood [24] who described the passive brownian motion of particles moving in a passive substrate, as well as the recent findings of Marchetti [25] describing the non-equilibrium statistical mechanics of SPPs.

The paper is organized as follows. In the next section, we detail the derivation of the generalized Smoluchowski equation describing the motion of self-propelled particles of arbitrary shapes. In section 3 we explore a specific case when these particles have ellipsoidal geometry and for this case we find out the translational velocities, angular velocities and other field variables of the system. Long range interactions in the system are modeled by the excluded volume potential with distortional elasticity terms (section 3.1), while the short range interactions due to self-propulsion are modeled as binary hard-core collisions (section 3.2). The governing system of equations for the SPP ensemble are then listed (section 4), followed by the derivation of various stresses (section 5) and a brief summary and the direction of our future work (section 6). An appendix (section 7) is added to aid in the derivation of these kinetic equations.

#### 2. HYDRODYNAMICAL KINETIC THEORY

In this section we describe the kinetic theory of a collection of self-propelled particles of an arbitrary shape moving in a passive solvent. This is realized by deriving a conservation equation in the generalized coordinate space. We assume a sufficiently dilute suspension of these particles in the solvent so that the dynamics of the system can be studied effectively by modeling the motion of a single particle interacting with its surroundings in a "mean field" sense. Let  $f(\mathbf{x}(t), \Omega(t), t)$  be the probability density function (PDF) of finding this particle such that its center of mass is at  $\mathbf{x}(t) = (x, y, z)$  and  $\Omega(t) = (\alpha(t), \beta(t), \gamma(t))$  denote the euler angle triplet describing the instantaneous orientation of its molecular axes ( $\mathbf{m}(t), \mathbf{n}(t), \mathbf{k}(t)$ ) with respect to an external fixed frame. The motion of the particle is followed by tracking an infinitesimal point on its surface. We refer this point as the mass point. A hydrodynamic force balance relation for these mass points is obtained, which is then summed up for all such points to arrive at the kinetic theory describing the motion of the entire body.

Let  $\mathbf{R}_i$  be the position vector of the *i*-th mass point in the fixed frame. Clearly  $\mathbf{R}_i = \mathbf{R}_i(\mathbf{Q})$ , where the generalized coordinates  $\mathbf{Q} = \{Q_a\}_{a=1}^6 \equiv \{x, y, z, \alpha, \beta, \gamma\}$  [14]. Let  $\mathbf{F}_i$  be the intermolecular force between the solvent and this mass point, approximated by a hydrodynamic drag force concentrated at the *i*-th mass point. A stokes expression is assumed to be valid for these forces and all the mass points have the same friction coefficient,  $\zeta$ . Then, the velocity of this mass point in the passive state,  $\mathbf{V}_i^{\text{pas}}$ , is

$$\mathbf{V}_{i}^{\text{pas}} = \mathbf{v}(\mathbf{R}_{i}) + \mathbf{F}_{i}/\zeta 
= K(t) \cdot \mathbf{R}_{i} + \mathbf{F}_{i}/\zeta,$$
(1)

where  $\mathbf{v}(\mathbf{r}) = K(t) \cdot \mathbf{r}$  is the unperturbed solvent velocity and K(t) is the velocity gradient tensor ( $K = \nabla \mathbf{v}$ ).

In the active state, a self propulsion force  $\mathbf{F}_0$  of constant magnitude acts on the center of mass of each particle and is directed along one of it's molecular axes (say m). In the viscous fluid limit this implies that the particle (and hence the mass point) moves with a constant speed  $v_0$  along this direction.

Further, on length scales comparable to the size of the particle, the intermolecular forces between these particles are predominantly due to hard-core collisions. The collisions are instantaneous implying

that probability that three or more particles being in contact at the same instant is of measure zero. These local and singular changes in the dynamics of self-propelling particles is modeled by the binary hard-core collision operator,  $T^{+}$ . We assume that the forces due to other physical or chemical processes apply on a timescale  $t \gg m/\zeta$  (*m* being the mass of the particle considered) and are therefore neglected. Hence the hydrodynamic relation for the *i*-th axes point, in the active state, is given by

$$\mathbf{V}_{i}^{\text{act}} = \mathbf{V}_{i}^{\text{pas}} + v_0 \mathbf{m} + T^+(v_0 \mathbf{m}).$$
<sup>(2)</sup>

To calculate the intermolecular force,  $\mathbf{F}_{i}$ , we note that the work done in 'hypothetically' deforming the mass points equals the change in the chemical potential of the system ( $\delta\mu$ ) [12, 26]. Thus

$$\delta \mu = \delta (\mathcal{U} + k_B T_A \ln f) = -\mathbf{F}_i \cdot \delta \mathbf{R}_i = -\mathbf{F}_i \cdot \frac{\partial \mathbf{R}_i}{\partial Q_a} \delta Q_a.$$
(3)

A repeated index in the above equation (and from now on) implies a summation over that index. U, the excluded volume potential, is energy penalty of a particle to occupy the area excluded by another particle (section 3.1),  $k_{\rm B}$  is the Boltzmann constant and  $T_A$  is the active temperature which is generally different from the thermodynamic temperature [4]. In the generalized coordinates, the work necessary to change  $Q_a$  by  $\delta Q_a$  is  $\delta \mu = \frac{\partial \mu}{\partial Q_a} \ \delta Q_a$ . From eqn (3), we have

$$\mathbf{F}_{i} \cdot \frac{\partial \mathbf{R}_{i}}{\partial Q_{a}} = -\frac{\partial \mu}{\partial Q_{a}} = -\frac{\partial}{\partial Q_{a}} (\mathcal{U} + k_{B}T_{A}\ln f).$$
(4)

The force  $\mathbf{F}_i$  can be found explicitly by solving eqn (2)

$$\mathbf{F}_{i} = \zeta (\mathbf{V}_{i} - K \cdot \mathbf{R}_{i} - v_{0}\mathbf{m} - T^{+}(v_{0}\mathbf{m}))$$
  
$$= \zeta \Big(\frac{\partial \mathbf{R}_{i}}{\partial Q_{a}} V_{a} - K \cdot \mathbf{R}_{i} - v_{0}\mathbf{m} - T^{+}_{i}(v_{0}\mathbf{m})\Big),$$
(5)

where  $\mathbf{V}_{i}^{act} = \mathbf{V}_{i} = \frac{\partial \mathbf{R}_{i}}{\partial Q_{a}} \mathbf{V}_{a}$ ,  $\mathbf{V}_{a}$  being the velocity of the generalized coordinate. Substituting eqn (5) in eqn (4), we have

$$\zeta \frac{\partial \mathbf{R}_i}{\partial Q_a} \cdot \left( \frac{\partial \mathbf{R}_i}{\partial Q_b} V_b - K \cdot \mathbf{R}_i - v_0 \mathbf{m} - T_i^+(v_0 \mathbf{m}) \right) = -\frac{\partial}{\partial Q_a} (\mathcal{U} + k_B T_A \ln f), \tag{6}$$

or,

$$h_{ab}^{-1}(V_b - V_b^D) = F_a^G,$$
(7)

where the shape matrix,  $h_{ab}$ , is such that  $h_{ab}^{-1} = \zeta \frac{\partial \mathbf{R}_i}{\partial Q_a} \cdot \frac{\partial \mathbf{R}_i}{\partial Q_b}$ .  $F_a^G = -\frac{\partial}{\partial Q_a} (\mathcal{U} + k_B T_A \ln f)$ , is the force in the generalized coordinate and the drift velocity of the system,  $\mathbf{V}^D = \mathbf{V}^K + \mathbf{V}^{SP} + \mathbf{V}^T$ , where the individual components due to deformation, self propulsion and collision, respectively, are

$$V_{a}^{K} = \zeta h_{ab} \frac{\partial \mathbf{R}_{i}}{\partial Q_{b}} \cdot K \cdot \mathbf{R}_{i}$$

$$V_{a}^{SP} = \zeta h_{ab} \frac{\partial \mathbf{R}_{i}}{\partial Q_{b}} \cdot (v_{0}\mathbf{m})$$

$$V_{a}^{T} = \zeta h_{ab} \frac{\partial \mathbf{R}_{i}}{\partial Q_{b}} \cdot T^{+}(v_{0}\mathbf{m}).$$
(8)

Hence, from eqn (7)

$$V_a = h_{ab}F_b^G + V_a^D = -h_{ab}\frac{\partial}{\partial Q_b}(\mathcal{U} + k_BT_A\ln f) + V_a^D.$$
(9)

Finally, the conservation (or the Smoluchowski) equation is given by [14]

$$\frac{\partial f}{\partial t} = -\sum_{i} \left(\frac{\partial}{\partial Q_{a}}\right)^{T} V_{a} f = \sum_{i} \left(\frac{\partial}{\partial Q_{a}}\right)^{T} \left[h_{ab} k_{B} T_{A} \frac{\partial \widehat{\mu}}{\partial Q_{b}} f - V_{a}^{D} f\right],\tag{10}$$

which describes the mean-field dynamics of a single self-propelled particle interacting with its surroundings in a dilute limit.  $\hat{\mu} = \mu/(k_B T_A)$  is the normalized chemical potential. In the next section we restrict this generalized theory to ellipsoids.

## 3. ELLIPSOIDS

We assume that the mass of the ellipsoidal particle is homogeneously distributed such that the center of mass coincides with its geometric center. Then the position vector of a mass point on its surface is  $\mathbf{R} = (\mathbf{r}^e + a \cos \theta \mathbf{m} + b \sin \theta \cos \phi \mathbf{n} + c \sin \theta \sin \phi \mathbf{k}), \theta \in [0, \pi], \phi \in [0, 2\pi]$ , where  $\mathbf{r}^e = (x, y, z)$  is instantaneous position of the center of mass in the fixed frame and (a, b, c) are the lengths of the respective semi-axes (m, n, k). We assume a > b > c, i.e. m represents the longest molecular axes or the major director. ((m, n, k) in terms of the euler angles ( $\alpha$ ,  $\beta$ ,  $\gamma$ ) are defined as

$$\mathbf{m} = (\cos\alpha\sin\beta, \sin\alpha\sin\beta, \cos\beta),$$
  

$$\mathbf{n} = (\cos\alpha\cos\beta\cos\gamma - \sin\alpha\sin\gamma, \sin\alpha\cos\beta\cos\gamma + \cos\alpha\sin\gamma, -\sin\beta\cos\gamma), \quad (11)$$
  

$$\mathbf{k} = (-\cos\alpha\cos\beta\sin\gamma - \sin\alpha\cos\gamma, -\sin\alpha\cos\beta\sin\gamma + \cos\alpha\cos\gamma, \sin\beta\sin\gamma)$$

To define the derivatives in the molecular frame, we introduce the angular momentum operator  $\mathbf{L} = \mathbf{m} \mathbf{L}_{m} + \mathbf{n} \mathbf{L}_{n} + \mathbf{k} \mathbf{L}_{k}$  [27] where

$$L_{m} = i\partial_{\gamma}$$

$$L_{n} = i(\cos\gamma\cot\beta\partial_{\gamma} + \sin\gamma\partial_{\beta} - \cos\gamma\csc\beta\partial_{\alpha})$$

$$L_{k} = i(-\sin\gamma\cot\beta\partial_{\gamma} + \cos\gamma\partial_{\beta} + \sin\gamma\csc\beta\partial_{\alpha}),$$
(12)

where  $i = \sqrt{-1}$ . The derivatives in the molecular frame are related to those in the fixed frame as follows

$$\begin{bmatrix} \partial_{x} \\ \partial_{y} \\ \partial_{z} \\ \partial_{\alpha} \\ \partial_{\beta} \\ \partial_{\gamma} \end{bmatrix} = \begin{bmatrix} \mathbf{I}_{3} & \mathbf{0}_{3} \\ & & \\ \mathbf{0}_{3} & A \end{bmatrix} \begin{bmatrix} \partial_{x} \\ \partial_{y} \\ \partial_{z} \\ \mathbf{L}_{m} \\ \mathbf{L}_{h} \\ \mathbf{L}_{k} \end{bmatrix}, \qquad (13)$$

where  $I_3$  is the 3  $\times$  3 identity matrix and the matrix A is

$$A = -i \begin{pmatrix} \cos\beta & -\sin\beta\cos\gamma & \sin\beta\sin\gamma \\ 0 & \sin\gamma & \cos\gamma \\ 1 & 0 & 0 \end{pmatrix}$$
(14)

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The shape matrix has the following form (see section 7)

$$h = \frac{1}{r_0 \zeta} \begin{bmatrix} \mathbf{I}_3/3 & 0\\ 0 & h_\Omega \end{bmatrix}, \tag{15}$$

where  $r_0 = \frac{4\pi}{3}$ . From eqns (10-15), the Smoluchowski equation for a self-propelling ellipsoid is

$$\frac{\partial f}{\partial t} = \nabla_{\mathbf{r}^e} \cdot D^T \cdot \left[ (\nabla_{\mathbf{r}^e} \widehat{\mu}) f \right] + \mathbf{L}^* \cdot D^R \cdot \left[ (\mathbf{L} \widehat{\mu}) f \right] 
- \nabla_{\mathbf{r}^e} \cdot \left( (\vec{g}_r^K + \vec{g}_r^{SP} + \vec{g}_r^T) f \right) - \mathbf{L}^* \cdot \left( (\vec{g}_\Omega^K + \vec{g}_\Omega^{SP} + \vec{g}_\Omega^T) f \right),$$
(16)

where  $\nabla_{\mathbf{r}e} = (\partial_x, \partial_y, \partial_z)$  is the gradient operator in the fixed frame,  $D^T = \frac{k_B T_A}{4\pi\zeta} \mathbf{I}_3$  and  $D^R = \frac{k_B T_A}{\zeta}$ diag  $(\frac{1}{b^2+c^2}, \frac{1}{c^2+a^2}, \frac{1}{a^2+b^2})$  are the translational and the rotational diffusivity matrices respectively and the conjugate operator  $\mathbf{L}^* = -\mathbf{L}^T$ . The translational velocities given by

$$\vec{g}_r^K = \hat{e}_x(K: \mathbf{r}^e \hat{e}_x) + \hat{e}_y(K: \mathbf{r}^e \hat{e}_y) + \hat{e}_z(K: \mathbf{r}^e \hat{e}_z), 
\vec{g}_r^{SP} = v_0 \mathbf{m}, 
\vec{g}_r^T = T^+(v_0 \mathbf{m}),$$
(17)

where  $(\hat{e}_x, \hat{e}_y, \hat{e}_z)$  are the unit vectors corresponding to the mutually orthogonal fixed frame and (:) is the contraction operator between two tensors and is defined as  $A:B = \sum_{ij} A_{ij} B_{ij}$ . The angular velocities are as follows

$$\vec{g}_{\Omega}^{K} = i \left[ \frac{\mathbf{m}}{b^{2} + c^{2}} K: (b^{2}\mathbf{n}\mathbf{k} - c^{2}\mathbf{k}\mathbf{n}) + \frac{\mathbf{n}}{c^{2} + a^{2}} K: (c^{2}\mathbf{k}\mathbf{m} - a^{2}\mathbf{m}\mathbf{k}) + \frac{\mathbf{k}}{a^{2} + b^{2}} K: (a^{2}\mathbf{m}\mathbf{n} - b^{2}\mathbf{n}\mathbf{m}) \right]$$
$$\vec{g}_{\Omega}^{SP} = \vec{g}_{\Omega}^{T} = 0, \qquad (18)$$

where nk, kn, mk, km, mn, nm are second order tensors given by, e.g. nk=n $\otimes$ k. The velocities described above are derived in section 7. Note that the angular velocities due to self-propulsion,  $\vec{g}_{\Omega}^{SP}, \vec{g}_{\Omega}^{T}$ , vanish. This observation is also discussed by Marchetti [25] for 2-D rods. The self-propulsion mechanism enters only in the form of a center of mass force. Further, we assume that the collisions are smooth and this suppresses the rotational degrees of freedom of the particle due to collisions (section 3.2). Therefore the rotational flux contains no information about the self-propulsion.

#### 3.1 Excluded volume potential: $\mathcal{U}$

On length scales larger than the size of the particle, these systems experience the long-range repulsive steric interaction. Due to a finite size of the particle, the other bodies cannot come inside a region occupied by the particle itself, termed as the excluded volume effect. To model this molecular interaction we propose a Marrucci-Greco mean-field biaxial nematic potential,  $\mathcal{U}(\mathbf{r}, \Omega, t)$  representing the second virial coefficient of these interactions in the mean field sense [28]

$$\mathcal{U} = -\frac{3}{2}Nk_BT_A \Big[\xi_0 \mathbf{M} : \mathbf{mm} + \gamma_0 (\mathbf{N} : \mathbf{mm} + \mathbf{M} : \mathbf{nn}) + \lambda_0 \mathbf{N} : \mathbf{nn} \\ + (\frac{\mathfrak{L}_m}{24}\nabla^2 \mathbf{M} + \frac{\mathfrak{L}_n}{24}\nabla^2 \mathbf{N}) : (\mathbf{mm} + \mathbf{nn})\Big],$$
(19)

where N is a dimensionless parameter measuring the strength of the potential, M = <mm> and N = <mn> are the second moment tensors of m and n with respect to the PDF,  $f(x, \Omega, t)$ , respectively. The ensemble average with respect to the PDF, is defined as

$$\left\langle (\cdot) \right\rangle = \int_{\Omega} (\cdot) f(\mathbf{x}, \mathbf{\Omega}, t) d\mathbf{\Omega},$$
 (20)

 $\mathfrak{L}_m$ ,  $\mathfrak{L}_n$  are the length scales characterizing the spatial interaction and are assumed to be larger than the particle size.  $(\xi_0, \gamma_0, \lambda_0)$  are the three material parameters related to the molecular geometry [26].

## 3.2 Collision operator: T<sup>+</sup>

The finite size of the self-propelled units give rise to a short range repulsive interaction, thereby introducing a singularity in the field variables, e.g. velocity. A collision operator is constructed to model the momentum exchanged in a binary hardcore collision of two self-propelled ellipsoids (see Figure 1).



Figure 1: Instantaneous collision between two ellipsoids with center of mass,  $r_i$  (i=1, 2), the vector between their center of mass and point of contact,  $\chi_i$ , and their molecular frames  $m_1 = (m, n, k)$  and  $m_2 = (m', n', k')$  respectively.  $\hat{k}_{12}$  is the normal at the point of contact, directed from ellipsoid 1 to ellipsoid 2.

The collisions are assumed to be smooth and elastic, implying that the angular velocities of the ellipsoids do not change [4]. Let the center of mass of the ellipsoids be  $\mathbf{r}_i$  (i=1, 2) and the vector between their respective center of mass and the point of contact be  $\chi_i = (a \cos \theta_i, b \sin \theta_i \cos \phi_i, c \sin \theta_i \sin \phi_i)$ , where the components are written in their respective molecular frames,  $M_1 = (\mathbf{m}, \mathbf{n}, \mathbf{k})$  and  $M_2 = (\mathbf{m}', \mathbf{n}', \mathbf{k}')$ . Since  $\chi_1$  lies on the surface of the ellipsoid, i.e.  $\sigma(\chi_1) = 0$  where  $\sigma(x, y, z) = \frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} - 1$ , the normal at the point of contact, directed from ellipsoid 1 to ellipsoid 2, is given by  $\mathbf{k}_{12} = \nabla \sigma(\chi_1)$ , i.e.

$$\mathbf{k}_{12} = \frac{2\cos\theta_1}{a}\mathbf{m} + \frac{2\sin\theta_1\cos\phi_1}{b}\mathbf{n} + \frac{2\sin\theta_1\sin\phi_1}{c}\mathbf{k},\tag{21}$$

and the unit vector  $\mathbf{\hat{k}}_{12} = \mathbf{k}_{12}/|\mathbf{k}_{12}|$ . If  $\mathbf{v}_1 (= v_0 \mathbf{m})$  and  $\mathbf{v}_2 (= v_0 \mathbf{m}')$  are initial velocities of the ellipsoids, then according to the collision rules governed by the conservation of energy and linear momentum, the final velocities,  $\mathbf{v'}_i$  (i=1, 2) are given by

$$\mathbf{v}'_{i} = \mathbf{v}_{i} \mp (\mathbf{v}_{12} \cdot \widehat{\mathbf{k}}_{12}) \widehat{\mathbf{k}}_{12} \qquad i = 1, 2,$$
(22)

where  $\mathbf{v}_{12} = \mathbf{v}_1 \cdot \mathbf{v}_2$ , and  $\mathbf{v}_{12} \cdot \widehat{\mathbf{k}}_{12} = v_0 \mathbf{k}_{12} \cdot (\mathbf{m} - \mathbf{m}') / |\mathbf{k}_{12}|$ .

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Using this information we capture the change in velocity by constructing the collision operator,  $T^+$ , which (a) changes the velocity at the time of collision, (b) acts only at the time of contact, and (c) acts only when the particles are approaching but not when they are receding.

From Figure 1, the condition of contact is  $\mathbf{r}_{12} + \chi_{12} = 0$ , where  $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$  and  $\chi_{12} = \chi_1 - \chi_2$ . Hence condition (b) is satisfied when  $T^*(\mathbf{v}_1) \propto \delta(\mathbf{r}_{12} + \chi_{12})$ . A '+' sign indicates the difference between the post-collisional and the pre-collisional velocity and not the other way round. The third condition demands that  $T^*(\mathbf{v}_1) \propto \Theta(-\mathbf{v}_{12} \cdot \mathbf{k}_{12})$ , where  $\Theta(\cdot)$  is the heavyside step function. The first condition is met when  $T^*(\mathbf{v}_1) \propto (\mathbf{v}'_1 - \mathbf{v}_1)$ . Finally, the probability of the second ellipsoid colliding with the first one is given by  $f(\mathbf{r}_2, M_2, t)$ . Since the point of contact  $(\chi_1, \chi_2)$  is arbitrary, the complete expression for the change in the velocity of the ellipsoid due to binary collisions is

$$T^{+}(\mathbf{v}_{1}) = \int_{\mathbf{r}_{2}} \int_{M_{2}} \int_{\chi_{1}} \int_{\chi_{2}} \delta(\mathbf{r}_{12} + \chi_{12}) \Theta(-\mathbf{v}_{12} \cdot \mathbf{k}_{12}) (\mathbf{v}'_{1} - \mathbf{v}_{1}) f d\chi_{2} d\chi_{1} dM_{2} d\mathbf{r}_{2}$$
  
$$= v_{0} \int_{\mathbf{r}_{2},\chi_{1},\chi_{2}} -\mathbf{k}_{12} \Big\langle \frac{\mathbf{k}_{12} \cdot (\mathbf{m} - \mathbf{m}')}{|\mathbf{k}_{12}|^{2}} \delta(\mathbf{r}_{12} + \chi_{12}) \Theta(-\mathbf{v}_{12} \cdot \mathbf{k}_{12}) \Big\rangle d\chi_{2} d\chi_{1} d\mathbf{r}_{2},$$
 (23)

## 4. GOVERNING SYSTEM OF EQUATIONS

In addition to the kinetic equation, the governing system of equations in the kinetic theory also include the continuity and the momentum transport equations. We assume that the solvent flow field is unperturbed in the presence of the particle and the velocity of the equivalent macroscopic continuum is equal to the solvent velocity, **v**, which is assumed to be incompressible. Thus we have

$$\nabla \cdot \mathbf{v} = 0,$$
  

$$\rho \frac{d}{dt} \mathbf{v} = \nabla \cdot (-p\mathbf{I} + \tau_e + \tau_v + \tau_a),$$
(24)

 $\rho$  is the density of the material, p is the hydrodynamic pressure and  $\tau_e$ ,  $\tau_a$ ,  $\tau_v$  are the constitutive stresses which are derived next.

## 5. STRESS CONSTITUTIVE EQUATIONS

The macroscopic stress tensor describing the dynamics of SPP ensemble consists of three parts: the extra elastic stress, the extra viscous stress and the active stress. The elastic stress,  $\tau_e$ , is due to the interaction between the self-propelled particles while the viscous stress,  $\tau_v$ , is the result of the interaction between the particles and the solvent molecules as well as among the solvent molecules. The activity of these moving particles exert local forces on the surrounding fluid which is measured by the active stresses,  $\tau_a$  [17]. In the next section, we derive the elastic stress, followed by an expression for the viscous stress (section 5.2) and active stress (section 5.3).

#### 5.1 Elastic stress

The extra elastic stress tensor is calculated by an extended virtual work principle [29, 30]. Let  $\delta u = \nabla v \delta t$  be the virtual deformation of the macroscopic system of active ellipsoidal suspensions. Then the variation in the free energy density, by invoking the first law of thermodynamics, equals the work done to the material volume by the elastic stress,  $\tau_e$ ,

$$\delta \mathcal{A} = \int_{G} \tau_e : \nabla \mathbf{v} \delta t dG, \tag{25}$$

where G is the control volume of the material under consideration. Work done by the surroundings on G is taken positive. Following deGennes [18], we eliminate the surface interactions by requiring the bounding surface of G to be stationary and the director orientation to be fixed on them, which is equivalent to using a virtual deformation of G that vanishes smoothly on its surface. The free energy

of this control volume is

$$\mathcal{A}[f] = \nu \int_{G} dG \int_{\Omega} \left[ k_B T_A(f \ln f - f) + \frac{\mathcal{U}}{2} \right] d\Omega,$$
(26)

where  $\nu$  is the number density of the suspension. The variation in the free energy is expressed as the rate of change of the PDF  $f(\mathbf{x}, \boldsymbol{\Omega}, t)$ 

$$\delta \mathcal{A} = \nu \int_{G} \int_{\Omega} (k_B T_A \ln f + \mathcal{U}) \delta f dG d\Omega = \nu \int_{G} \int_{\Omega} \mu \frac{\partial f}{\partial t} \delta t dG d\Omega.$$
(27)

For a rapid virtual deformation, i.e.  $K \to \infty$ , the diffusion and the self-propulsion terms can be neglected in eqn (10) [29]. Hence

$$\frac{\partial f}{\partial t} = -\nabla \cdot (\mathbf{g}_r^K) f - \mathbf{L}^* \cdot (\mathbf{g}_{\Omega}^K f)$$
(28)

From Eqs. (25)-(28),

$$\begin{split} \delta \mathcal{A} &= -\nu \int_{\mathbf{G}} \int_{\Omega} \mu \Big[ \nabla \cdot (\mathbf{g}_{r}^{K} f) + \mathbf{L}^{*} \cdot (\mathbf{g}_{\Omega}^{K} f) \Big] \delta t dG d\Omega \\ &= \nu \int_{G} \int_{\Omega} \Big( \mathbf{g}_{r}^{K} \cdot \nabla \mu + \mathbf{g}_{\Omega}^{*K} \cdot \mathbf{L} \mu \Big) f \delta t d\Omega dG \\ &= \nu \int_{G} \int_{\Omega} \Big( \mathbf{g}_{r}^{K} \cdot [k_{B} T_{A} \nabla f + (\nabla \mathcal{U}) f] + \mathbf{g}_{\Omega}^{*K} \cdot [k_{B} T_{A} \mathbf{L} f + (\mathbf{L} \mathcal{U}) f] \Big) \delta t d\Omega dG \\ &= \nu \int_{G} -k_{B} T_{A} \Big\langle \nabla \cdot \mathbf{g}_{r}^{K} + \mathbf{L} \cdot \mathbf{g}_{\Omega}^{*K} \Big\rangle + \Big\langle \mathbf{g}_{r}^{K} \cdot (\nabla \mathcal{U}) + \mathbf{g}_{\Omega}^{*K} \cdot (\mathbf{L} \mathcal{U}) \Big\rangle \end{split}$$
(29)

Using the equations for the flow vectors  $\mathbf{g}_r^K = \mathbf{K} : \gamma_m \hat{\mathbf{e}}_{\mathbf{x}} + \mathbf{K} : \gamma_y \hat{\mathbf{e}}_{\mathbf{y}} + \mathbf{K} : \gamma_z \hat{\mathbf{e}}_{\mathbf{z}}$  (eqn 17) and  $\mathbf{g}_{\Omega}^K = \mathbf{K} : \alpha_m \mathbf{m} + \mathbf{K} : \alpha_n \mathbf{n} + \mathbf{K} : \alpha_k \mathbf{k}$  (eqn 18), we get

$$\delta \mathcal{A} = \nabla \mathbf{v} : \int_{G} -\nu k_{B} T_{A} \left\langle \nabla \cdot \vec{\gamma}^{\alpha\beta} + \mathbf{L}^{*} \cdot \vec{\alpha}^{\alpha\beta} \right\rangle + \nu \left\langle \vec{\gamma}^{\alpha\beta} \cdot \nabla \mathcal{U} + \vec{\alpha}^{*\alpha\beta} \cdot \mathbf{L} \mathcal{U} \right\rangle$$
  
$$= \nabla \mathbf{v} : \int_{G} -\nu k_{B} T_{A} \left\langle \mathbf{I} + \mathbf{L}^{*} \cdot \vec{\alpha}^{\alpha\beta} \right\rangle + \nu \left\langle \vec{\gamma}^{\alpha\beta} \cdot \nabla \mathcal{U} + \vec{\alpha}^{*\alpha\beta} \cdot \mathbf{L} \mathcal{U} \right\rangle$$
(30)

where  $\vec{\gamma}^{\alpha\beta} = (\gamma_x^{\alpha\beta}, \gamma_y^{\alpha\beta}, \gamma_z^{\alpha\beta})$  and  $\vec{\alpha}^{\alpha\beta} = (\alpha_m^{\alpha\beta}, \alpha_n^{\alpha\beta}, \alpha_k^{\alpha\beta})$  are third order tensors. Comparing the terms containing  $\nabla v$  in Eqs. (25) and (30) we arrive at the expression for the elastic stress tensor

$$\tau_e^{\alpha\beta} = -\nu k_B T_A \left\langle \mathbf{I} + \mathbf{L}^* \cdot \vec{\alpha}^{\alpha\beta} \right\rangle + \nu \left\langle \vec{\gamma}^{\alpha\beta} \cdot \nabla \mathcal{U} + \vec{\alpha}^{*\alpha\beta} \cdot \mathbf{L} \mathcal{U} \right\rangle$$
(31)

In the above derivation, the definition of the chemical potential,  $\mu = \frac{\delta A}{\nu \delta f} = k_B T_A \ln f + \mathcal{U}$ , and the following identities have been used repeatedly

$$\int_{G} \int_{\Omega} \nabla f \cdot \mathbf{g} dG d\Omega = - \int_{G} \int_{\Omega} f \nabla \cdot \mathbf{g} dG d\Omega$$

$$\int_{G} \int_{\Omega} \mathbf{L} f \cdot \mathbf{g}^{*} dG d\Omega = - \int_{G} \int_{\Omega} f \mathbf{L}^{*} \cdot \mathbf{g} dG d\Omega$$
(32)

## 5.2 Viscous stress

The expression for the viscous stress follows from the work of Batchelor [31] and Roscoe [32]. They derived an expression for the viscous stress for ellipsoidal suspensions in viscous solvent,

$$\tau_v = 2\eta \mathbf{D} + 3\nu k T_a \zeta_0 \mathcal{B} : \mathbf{D}$$
(33)

where  $\eta$  is the viscosity of the solvent,  $\mathcal{B}$  is the fourth order strain rate concentration tensor,  $\mathbf{D}$  is the second order strain rate tensor, given by  $\mathbf{D} = \frac{1}{2}(\nabla \mathbf{v} + \nabla \mathbf{v}^T)$  and  $\zeta_0$  is a shape dependent friction coefficient proportional to the volume of the ellipsoidal suspension. Replacing the volume average by the ensemble average in [31], it follows that

$$\tau_{v} = 2\eta \mathbf{D} + \nu k T_{a} \zeta_{0} [\frac{4}{3(J_{1}J_{2}+J_{2}J_{3}+J_{1}J_{3})} ((J_{1}\langle \mathbf{mmmm} \rangle + J_{2}\langle \mathbf{nnnn} \rangle + J_{3}\langle \mathbf{kkkk} \rangle) : \mathbf{D} - \frac{\mathbf{I}}{3} (J_{1}\langle \mathbf{mm} \rangle + J_{2}\langle \mathbf{nn} \rangle + J_{3}\langle \mathbf{kk} \rangle) : \mathbf{D}) + \frac{2}{3} (\frac{1}{I_{1}} (\langle \mathbf{nk} + \mathbf{kn} \rangle) (\langle \mathbf{nk} + \mathbf{kn} \rangle) : \mathbf{D} + \frac{1}{I_{2}} (\langle \mathbf{mn} + \mathbf{nm} \rangle) (\langle \mathbf{mn} + \mathbf{nm} \rangle) : \mathbf{D} + \frac{1}{I_{3}} (\langle \mathbf{mk} + \mathbf{km} \rangle) (\langle \mathbf{mk} + \mathbf{km} \rangle) : \mathbf{D})].$$
(34)

Here, the shape constants  $(I_i, J_i)$ , i = 1, 2, 3 in Eqn. (34) are:

$$I_{1} = \int_{0}^{\infty} \frac{abc(a^{2}+c^{2})d\lambda}{\Delta(c^{2}+\lambda)(a^{2}+\lambda)}, I_{2} = \int_{0}^{\infty} \frac{abc(b^{2}+a^{2})d\lambda}{\Delta(b^{2}+\lambda)(a^{2}+\lambda)}, I_{3} = \int_{0}^{\infty} \frac{abc(b^{2}+c^{2})d\lambda}{\Delta(b^{2}+\lambda)(c^{2}+\lambda)}, J_{3} = \int_{0}^{\infty} \frac{abc\lambda d\lambda}{\Delta(b^{2}+\lambda)(c^{2}+\lambda)}, J_{4} = \int_{0}^{\infty} \frac{abc\lambda d\lambda}{\Delta(b^{2}+\lambda)(c^{2}+\lambda)}, J_{4} = \int_{0}^{\infty} \frac{abc\lambda d\lambda}{\Delta(b^{2}+\lambda)(c^{2}+\lambda)}, J_{4} = \int_{0}^{\infty} \frac{abc\lambda d\lambda}{\Delta(b^{2}+\lambda)(c^{2}+\lambda)}, J_{5} = \int_{0}^{\infty} \frac{abc\lambda d\lambda}{\Delta(b^{2}+\lambda)(c^{2}+\lambda)(c^{2}+\lambda)}, J_{5} = \int_{0}^{\infty} \frac{abc\lambda d\lambda}{\Delta(b^{2}+\lambda)(c^{2}+\lambda)(c^{2}+\lambda)(c^{2}+\lambda)}, J_{5} = \int_{0}^{\infty} \frac{abc\lambda d\lambda}{\Delta(b^{2}+\lambda)(c^{2}+\lambda)(c^{2}+\lambda)(c^{2}+\lambda)}, J_{5} = \int_{0}^{\infty} \frac{abc\lambda d\lambda}{\Delta(b^{2}+\lambda)(c^{2}+\lambda)(c^{2}+\lambda)(c^{2}+\lambda)(c^{2}+\lambda)(c^{2}+\lambda)}, J_{5} = \int_{0}^{\infty} \frac{abc\lambda d\lambda}{\Delta(b^{2}+\lambda)(c^{2}+\lambda)(c^{2}+\lambda)(c^{2}+\lambda)(c^{2}+\lambda)(c^{2}+\lambda)(c^{2}+\lambda)(c^{2}+\lambda)(c^{2}+\lambda)(c^{2}+\lambda)}, J_{5} = \int_{0}^{\infty} \frac{abc\lambda d\lambda}{\Delta(b^{2}+\lambda)(c^{2}+\lambda)($$

and  $\Delta^2 = (a^2 + \lambda)(b^2 + \lambda)(c^2 + \lambda)$ .

#### 5.3 Active stress

In swimmer literature it is reported that the activity in the self-propelled systems lowers the bulk viscosity of 'tensile' suspensions while it enhances the viscosity of 'contractile' systems [22]. This is because the particles in active suspensions exert forces on the surrounding fluid which lead to local tensile and contractile stresses. To calculate these local active stresses for apolar particles we adopt a phenomenological approach, based on symmetry [33].

Since the particle propulsion occurs only along one of the molecular axis, **m**, these local stresses are proportional to the orientation tensor  $\mathbf{M} = < \mathbf{mm} >$  which preserves the nematic symmetry ( $\mathbf{m} \rightarrow -\mathbf{m}$ ), i.e.

$$\tau_a = \gamma_m \mathbf{M},\tag{36}$$

 $\gamma_m$  is the amplitude of the force exerted on the fluid and measures the amount of activity. Tensile particles have  $\gamma_m < 0$  (e.g. *E. coli*) while contractile particles have  $\gamma_m > 0$  (e.g. *Chlamydomonas*) [33].

#### 6. SUMMARY

We have developed a kinetic theory to study the dynamics of ellipsoidal, self-propelled particles moving in a viscous solvent and in a sufficiently dilute concentration limit. The Smoluchowski

equation (16) describing the configurational PDF displays a broken nematic symmetry and differs from its passive counterpart [26] in three significant aspects: (1) the excluded volume potential,  $\mathcal{U}$ , accounts for the long-range hydrodynamic interactions in a "gradually varying" distorted orientational field, (2) the self-propulsion introduces a translation convective term,  $\vec{g}_r^{SP}$ , which models the movement of the particle along a direction of its long axis, and (2) the binary collisions that arise due to the momentum transfer leading to singular corrections in the field variables, provide another convective term,  $\vec{g}_r^T$ .

The model has been derived from first principles and provides a simple approach to capture the longrange molecular interactions as well as the short-range perturbations in the field variables. However, a semi-dilute limit in our model eludes any configurational interactions arising due to the concentration effects. Obviously a more dedicated effort, especially on the numerical front, to understand the various steady and dynamical states as well as their stability analysis at the different concentration, selfpropulsion velocities, material parameter regimes and the shape of the particle (in terms of its aspect ratios  $\frac{b}{a}, \frac{c}{a}$ ), is required. These various numerical predictions have to be tested with the existing experiments on living and artificial self-propelled particle systems. These are the results we look forward to explore in our forthcoming work.

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## 7. APPENDIX

This section supplements the derivation of the results given in section 3.

#### Shape Matrix

The shape matrix, h, (eqn (15), section 3) for ellipsoidal particles is given by  $h = \frac{1}{r_0\zeta} \operatorname{diag}[\mathbf{I}_3, \mathbf{h}_{\Omega}]$ where  $\mathbf{h}_{\Omega}$  is a symmetric second order tensor, given by

$$r_0(h_\Omega)_{ab}^{-1} = \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} \frac{\partial \mathbf{R}}{\partial \Lambda_a} \cdot \frac{\partial \mathbf{R}}{\partial \Lambda_b} \sin \theta d\theta d\phi, \tag{37}$$

where  $\mathbf{R} = (\mathbf{r}^e + a\cos\theta\mathbf{m} + b\sin\theta\cos\phi\mathbf{n} + c\sin\theta\sin\phi\mathbf{k}), \theta \in [0, \pi], \phi \in [0, 2\pi]$  and  $\Lambda = \{\alpha, \beta, \gamma\}$  and

$$(h_{\Omega})_{11} = \frac{a^2 + b^2 \cos^2 \gamma + c^2 \sin^2 \gamma}{(a^2 + b^2)(a^2 + c^2) \sin^2 \beta}, \qquad (h_{\Omega})_{12} = -\frac{(b^2 - c^2) \sin \gamma \cos \gamma}{(a^2 + b^2)(a^2 + c^2) \sin \beta},$$

$$(h_{\Omega})_{13} = -\cos \beta \frac{a^2 + b^2 \cos^2(\gamma) + c^2 \sin^2(\gamma)}{(a^2 + b^2)(a^2 + c^2) \sin^2 \beta}, \quad (h_{\Omega})_{22} = \frac{a^2 + b^2 \sin^2 \gamma + c^2 \cos^2 \gamma}{(a^2 + b^2)(a^2 + c^2)},$$

$$(h_{\Omega})_{23} = \frac{a^4 \sin^2 \beta + c^4 \cos^2 \beta \sin^2 \gamma + b^4 \cos^2 \beta \cos^2 \gamma + a^2 c^2 + a^2 b^2 + b^2 c^2}{\sin^2 \beta (a^2 + b^2)(c^2 + b^2)(c^2 + a^2)},$$

$$(h_{\Omega})_{33} = \frac{(b^2 - c^2) \sin \gamma \cos \gamma \cos \beta}{(a^2 + b^2)(a^2 + c^2) \sin \beta}, \qquad (38)$$

### **Brownian motion**

The first term on the right hand side of eqn (16) is the contribution due to the translational and rotational brownian motion of an SPP particle. Using the definition of shape matrix mentioned above, it can be simplified into

$$\begin{pmatrix} \frac{\partial}{\partial Q_a} \end{pmatrix}^T h_{ab} k_B T_a \frac{\partial \hat{\mu}}{\partial Q_a} f = \frac{\partial}{\partial \mathbf{r}_e}^T \left( \frac{k_B T_A}{\zeta} \frac{\mathbf{I}_3}{4\pi} \right) \frac{\partial \hat{\mu}}{\partial \mathbf{r}_e} f + \frac{\partial}{\partial \Lambda}^T \frac{k_B T_A}{\zeta} h_\Omega \frac{\partial \hat{\mu}}{\partial \Lambda} f$$

$$= \nabla_{\mathbf{r}_e} \cdot D^T \cdot \left[ (\nabla_{\mathbf{r}_e} \hat{\mu}) f \right] + \mathbf{L}^T \cdot \frac{k_B T_a}{\zeta} (A^T h_\Omega A) \cdot \left[ \mathbf{L} \hat{\mu} f \right]$$

$$= \nabla_{\mathbf{r}_e} \cdot D^T \cdot \left[ (\nabla_{\mathbf{r}_e} \hat{\mu}) f \right] + \mathbf{L}^* \cdot D^R \cdot \left[ (\mathbf{L} \hat{\mu}) f \right],$$

$$(39)$$

where the transformation matrix, A, is given by eqn (13),  $D^T = \frac{k_B T_A}{4\pi\zeta} \mathbf{I}_3$  and  $D^R = \frac{k_B T_A}{\zeta}$  and  $D^R = \frac{k_B T_A}{\zeta}$  diag  $\left[\frac{1}{b^2 + c^2}, \frac{1}{c^2 + a^2}, \frac{1}{a^2 + b^2}\right]$  are the translational and the rotational diffusivity matrices respectively.

# Drift due to external forcing

The second term on the rhs of eqn (16) is the drift due to the deformation of the solvent and is given by

$$\begin{aligned} \frac{\partial}{\partial Q_a}^T (V_a^K f) &= \frac{\partial}{\partial Q_a}^T \zeta h_{ab} \int_{\theta\phi} \left( \frac{\partial \mathbf{R}}{\partial Q_b} \cdot K \cdot \mathbf{R} f \right) \\ &= \frac{\partial}{\partial \mathbf{r}_e}^T \frac{\mathbf{I}_3}{4\pi} \int_{\theta\phi} \left( \frac{\partial \mathbf{R}}{\partial \mathbf{r}_e} \cdot K \cdot \mathbf{R} f \right) + \frac{\partial}{\partial \Lambda}^T \frac{h_\Omega}{r_0} \int_{\theta\phi} \left( \frac{\partial \mathbf{R}}{\partial \Lambda} \cdot K \cdot \mathbf{R} f \right) \\ &= \nabla_{\mathbf{r}_e} \cdot \frac{\mathbf{I}_3}{4\pi} K \colon \int_{\theta\phi} \left( \mathbf{R} \frac{\partial \mathbf{R}}{\partial \mathbf{r}_e} f \right) + \mathbf{L}^T \cdot \frac{(A^T h_\Omega A)}{r_0} \cdot \left[ K \colon \int_{\theta\phi} \left( \mathbf{R} (\mathbf{L} \mathbf{R}) f \right) \right], \\ &= \nabla_{\mathbf{r}_e} \cdot \left( (K \colon \mathbf{r}_e \hat{e}_x) \hat{e}_x + (K \colon \mathbf{r}_e \hat{e}_y) \hat{e}_y + (K \colon \mathbf{r}_e \hat{e}_z) \hat{e}_z \right) f + \\ &\mathbf{L}^* \cdot \left( \frac{i\mathbf{m}}{b^2 + c^2} K \colon (b^2 \mathbf{n} \mathbf{k} - c^2 \mathbf{k} \mathbf{n}) + \\ &\frac{i\mathbf{n}}{c^2 + a^2} K \colon (c^2 \mathbf{k} \mathbf{m} - a^2 \mathbf{m} \mathbf{k}) + \frac{i\mathbf{k}}{a^2 + b^2} (a^2 \mathbf{m} \mathbf{n} - b^2 \mathbf{n} \mathbf{m}) \right) f \\ &= \nabla_{\mathbf{r}_e} \cdot (\vec{g}_r^K f) + \mathbf{L}^* \cdot (\vec{g}_\Omega^K f), \end{aligned}$$

since

$$K: \int_{\theta\phi} \mathbf{R} \frac{\partial \mathbf{R}}{\partial \mathbf{r}_e} = 4\pi K: \Big( \mathbf{r}_e(\hat{\mathbf{e}_x}(\hat{\mathbf{e}_x}) + \hat{\mathbf{e}_y}(\hat{\mathbf{e}_y}) + \hat{\mathbf{e}_z}(\hat{\mathbf{e}_z})) \Big), \tag{41}$$

and

$$K: \int_{\theta\phi} \mathbf{R}(\mathbf{LR}) = K: \int_{\theta\phi} \mathbf{R} \Big( \cos\theta [(\mathbf{n}L_n + \mathbf{k}L_k)(a\mathbf{m})] + \sin\theta \cos\phi [(\mathbf{m}L_m + \mathbf{k}L_k)(b\mathbf{n})] \\ + \sin\theta \sin\phi [(\mathbf{m}L_m + \mathbf{n}L_n)(c\mathbf{k})] \Big) \\ = K: \int_{\theta\phi} i\mathbf{R} \Big( \cos\theta [(\mathbf{n}(-a\mathbf{k}) + \mathbf{k}(a\mathbf{n})] + \sin\theta \cos\phi [\mathbf{m}(b\mathbf{k}) + \mathbf{k}(-b\mathbf{m})] \\ + \sin\theta \sin\phi [\mathbf{m}(-c\mathbf{n}) + \mathbf{n}(c\mathbf{m})] \Big) \\ = r_0 i \Big( \mathbf{m}K: (b^2\mathbf{n}\mathbf{k} - c^2\mathbf{k}\mathbf{n}) + \mathbf{n}K: (c^2\mathbf{k}\mathbf{m} - a^2\mathbf{m}\mathbf{k}) \\ + \mathbf{k}K: (a^2\mathbf{m}\mathbf{n} - b^2\mathbf{n}\mathbf{m}) \Big).$$
(42)

In eqn (40) we have used the identity,  $\mathbf{a} \cdot K \cdot \mathbf{b} = K$ :  $\mathbf{ab}$ , while, in eqn (42) we have repeatedly used the rule,  $L_p(q) = i[p \times q]$ , where  $\{p, q\} = \mathbf{m}, \mathbf{n}, \mathbf{k}$ .

# Drift due to self propulsion

Similarly, the third term in the rhs of eqn (16) is the drift due to the self-propulsion mechanism of the particles, given by

$$\frac{\partial}{\partial Q_{a}}^{T}(V_{a}^{SP}f) = \frac{\partial}{\partial Q_{a}}^{T}\zeta h_{ab} \int_{\theta\phi} \left(\frac{\partial \mathbf{R}}{\partial Q_{b}} \cdot \mathbf{v}^{SP}f\right) \\
= \frac{\partial}{\partial \mathbf{r}_{e}}^{T} \frac{\mathbf{I}_{3}}{4\pi} \int_{\theta\phi} \left(\frac{\partial \mathbf{R}}{\partial \mathbf{r}_{e}} \cdot \mathbf{v}^{SP}f\right) + \frac{\partial}{\partial \Lambda}^{T} h_{\Omega} \int_{\theta\phi} \left(\frac{\partial \mathbf{R}}{\partial \Lambda} \cdot \mathbf{v}^{SP}f\right) \\
= \nabla_{\mathbf{r}_{e}} \cdot (v_{0}\mathbf{m}f) + \mathbf{L}^{T} \cdot \frac{(A^{T}h_{\Omega}A)}{r_{0}} \cdot \int_{\theta\phi} \left(\mathbf{v}^{SP} \cdot \mathbf{L}\mathbf{R}f\right) \\
= \nabla_{\mathbf{r}_{e}} \cdot (v_{0}\mathbf{m}f) \\
= \nabla_{\mathbf{r}_{e}} \cdot (\vec{g}_{r}^{SP}f) + \mathbf{L}^{*} \cdot (\vec{g}_{\Omega}^{SP}f),$$
(43)

where  $\mathbf{v}^{SP} = v_0 \mathbf{m}$ , and

$$\int_{\theta\phi} \mathbf{v}^{SP} \cdot (\mathbf{LR}) = \int_{\theta\phi} iv_0 \mathbf{m} \cdot \left(\cos\theta [(\mathbf{n}(-a\mathbf{k}) + \mathbf{k}(a\mathbf{n})] + \sin\theta\cos\phi [\mathbf{m}(b\mathbf{k}) + \mathbf{k}(-b\mathbf{m})] + \sin\theta\sin\phi [\mathbf{m}(-c\mathbf{n}) + \mathbf{n}(c\mathbf{m})]\right)$$

$$= 0.$$
(44)

## Drift due to collisions

The final term in eqn (16) arises due to the instantaneous collisions of self-propelled particles. Hence

$$\frac{\partial}{\partial Q_{a}}^{T}(V_{a}^{T}f) = \frac{\partial}{\partial Q_{a}}^{T}\zeta h_{ab} \int_{\theta\phi} \left(\frac{\partial \mathbf{R}}{\partial Q_{b}} \cdot T^{+}(v_{0}\mathbf{m})f\right) \\
= \frac{\partial}{\partial \mathbf{r}_{e}}^{T} \frac{\mathbf{I}_{3}}{4\pi} \int_{\theta\phi} \left(\frac{\partial \mathbf{R}}{\partial \mathbf{r}_{e}} \cdot T^{+}(v_{0}\mathbf{m})f\right) + \frac{\partial}{\partial \Lambda}^{T} h_{\Omega} \int_{\theta\phi} \left(\frac{\partial \mathbf{R}}{\partial \Lambda} \cdot T^{+}(v_{0}\mathbf{m})f\right) \\
= \nabla_{\mathbf{r}_{e}} \cdot \left((T^{+} \cdot \hat{e}_{x})\hat{e}_{x} + (T^{+} \cdot \hat{e}_{y})\hat{e}_{y} + (T^{+} \cdot \hat{e}_{z})\hat{e}_{z}\right)(v_{0}\mathbf{m})f \qquad (45) \\
= \nabla_{\mathbf{r}_{e}} \cdot \left(g_{r}^{T}f\right) + \mathbf{L}^{*} \cdot (g_{\Omega}^{T}f).$$

In deriving eqn (45), we use the following relation

$$\int_{\theta\phi} T^{+}(v_{0}\mathbf{m}) \cdot (\mathbf{LR}) = i \int_{\theta\phi} \left( \cos\theta [(\mathbf{n}(-a\mathbf{k}) + \mathbf{k}(a\mathbf{n})] \cdot T^{+} + \sin\theta \cos\phi [\mathbf{m}(b\mathbf{k}) + \mathbf{k}(-b\mathbf{m})] \cdot T^{+} + \sin\theta \sin\phi [\mathbf{m}(-c\mathbf{n}) + \mathbf{n}(c\mathbf{m})] \cdot T^{+} \right) (v_{0}\mathbf{m})$$

$$= 0 \qquad (46)$$

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