Can the self-propulsion of anisotropic microswimmers be described by using forces and torques?

Borge ten Hagen\textsuperscript{1}, Raphael Wittkowski\textsuperscript{2}, Daisuke Takagi\textsuperscript{3}, Felix Kümmel\textsuperscript{4}, Clemens Bechinger\textsuperscript{4,5} and Hartmut Löwen\textsuperscript{1}

\textsuperscript{1} Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf, Germany
\textsuperscript{2} SUPA, School of Physics and Astronomy, University of Edinburgh, Edinburgh, EH9 3FD, UK
\textsuperscript{3} Department of Mathematics, University of Hawaii at Manoa, Honolulu, Hawaii 96822, USA
\textsuperscript{4} 2. Physikalisches Institut, Universität Stuttgart, D-70569 Stuttgart, Germany
\textsuperscript{5} Max-Planck-Institut für Intelligente Systeme, D-70569 Stuttgart, Germany

E-mail: bhagen@thphy.uni-duesseldorf.de

Received 2 August 2014, revised 23 October 2014
Accepted for publication 4 November 2014
Published 29 April 2015

Abstract

The self-propulsion of artificial and biological microswimmers (or active colloidal particles) has often been modelled by using a force and a torque entering into the overdamped equations for the Brownian motion of passive particles. This seemingly contradicts the fact that a swimmer is force-free and torque-free, i.e. that the net force and torque on the particle vanish. Using different models for mechanical and diffusiophoretic self-propulsion, we demonstrate here that the equations of motion of microswimmers can be mapped onto those of passive particles with the shape-dependent grand resistance matrix and formally external effective forces and torques. This is consistent with experimental findings on the circular motion of artificial asymmetric microswimmers driven by self-diffusiophoresis. The concept of effective self-propulsion forces and torques significantly facilitates the understanding of the swimming paths, e.g. for a microswimmer under gravity. However, this concept has its limitations when the self-propulsion mechanism of a swimmer is disturbed either by another particle in its close vicinity or by interactions with obstacles, such as a wall.

Keywords: self-propelled particles, anisotropic microswimmers, active colloids

(Some figures may appear in colour only in the online journal)

1. Introduction

The basic interest in liquid matter research has shifted from passive simple liquids \cite{1} to complex liquids \cite{2} over the past decades. While the individual building blocks of the liquid are passive thermal particles in this case, a more recent topic concerns \textit{living liquids} which consist of self-propelling biological constituents, such as bacteria in a low-Reynolds-number fluid \cite{3,4,5,6}. Being perpetually driven by the consumption of energy needed for the self-propulsion, even a single swimmer represents already a complicated non-equilibrium situation. In this respect, artificial self-phoretically-driven colloidal particles serve as very helpful model systems to mimic the self-propulsion of biological microswimmers and enable particle-resolved insights into the one-particle and collective phenomena \cite{7,8,9,10,11,12,13,14}.

Regarding the modelling of microswimmer propulsion, there are basically two levels of description. The first coarse-grained approach does not resolve the details of the propagation but models the resulting propulsion velocity \( \mathbf{v} \) by the action of a formally external \textit{effective} self-propulsion force \( \mathbf{F} \) moving with the particle. This force then enters into the completely overdamped equations of motion for passive particles. In a demonstrative way, \( \mathbf{F} \) can be interpreted as the constraining force that is required to prevent the microswimmer from
moving, which can be achieved, e.g. by optical tweezers [15]. In its simplest form, i.e. for a sphere of hydrodynamic radius \( R \), the self-propulsion force \( \mathbf{F} \) is given by

\[
\gamma \mathbf{v} = \mathbf{F}
\]

with \( \gamma = 6\pi \eta R > 0 \) denoting a (scalar) Stokes friction coefficient for stick fluid boundary conditions on the surface of the particle and \( \eta \) denoting the dynamic (shear) viscosity of the fluid. There is plenty of literature by now in which this kind of force modelling was employed either in the context of single-particle motion [16–19] or to study various collective phenomena of self-propelled particles such as swarming [20–22], clustering [13, 23–29], and ratchet effects [30, 31].

The concept has also been used for several applications like particle separation [32, 33] or trapping [34–36] of self-propelled particles. Typically, the swimming direction is along a particle-fixed axis (usually a symmetry axis of the particle) denoted by a unit vector \( \hat{u} \). The direction of the self-propulsion force thus rotates with the particle orientation. Therefore it is called an ‘internal’ force. The particle orientation \( \hat{u} \) obeys an overdamped equation of motion with rotational friction. This makes the problem non-Hamiltonian and non-trivial, in particular in the presence of noise [37, 38]. However, throughout this article thermal fluctuations are neglected as they are not relevant for the present study.

From (1) it is evident how to generalize this equation towards an asymmetric microswimmer with an arbitrary non-spherical shape by using the \( 6 \times 6 \)-dimensional grand resistance matrix \( \mathbf{H} \) [39] (also called ‘hydrodynamic friction tensor’ [40]) and a six-dimensional generalized velocity \( \mathbf{V} = (v, \omega) \) composed of the translational velocity \( v \) and the angular velocity \( \omega \) of the particle. Corresponingly, the right-hand side of (1) is replaced by the six-dimensional generalized force \( \mathbf{K} = (\mathbf{F}, \mathbf{M}) \) composed of an internal force \( \mathbf{F} \) and an internal torque \( \mathbf{M} \), which are fixed in the particle frame, such that

\[
\eta \mathbf{H} \mathbf{V} = \mathbf{K}.
\]

Equation (2) comprises many different situations including circle swimming in two [12, 16] and helical swimming in three dimensions [18], which are induced by the simultaneous presence of a constant force and a torque in the particle frame. Many papers have adopted this formalism in order to describe the motion of microswimmers [15, 41–56]. On this coarse-grained level of modelling there is no explicit solvent velocity field, which is just disregarded.

The second level involves a more detailed description of the propulsion mechanism of an individual swimmer. At this level, several modes of propagation have to be distinguished. We shall discriminate in the following between mechanical self-propulsion and self-diffusiophoretic motion. Some type of mechanical self-propulsion is usually realized in biological microswimmers such as bacteria [57–59], algae [60, 61], or spermatozoa [62–65]. In particular,

[6] In two spatial dimensions the grand resistance matrix \( \mathbf{H} \) is only \( 3 \times 3 \)-dimensional and the generalized velocity \( \mathbf{V} \) as well as the generalized force \( \mathbf{K} \) are three-dimensional.
In this article we follow the alternative theoretical route: we model the swimmer motion explicitly according to the more detailed second level and check whether the resulting equation can be mapped onto the coarse-grained equation (2) using an effective force and torque. We do this explicitly for an asymmetric two-dimensional swimmer with an L-shape and discriminate between mechanical self-propulsion and self-diffusiophoretic propulsion in an unbounded fluid. In the first case, we consider an extension of the Golestanian swimmer [72, 89] towards an L-shaped particle. In the second case, we study slender biaxial particles consisting of two arms of different lengths that meet at a certain internal angle. To account for the diffusiophoretic self-propulsion mechanism, we consider an imposed slip velocity on one of the arms. The sense of rotation of the particles is found to depend on the internal angle. A previous but less general account for a rectangular internal angle was published elsewhere [14, 86]. For both the mechanical and the diffusiophoretic self-propulsion, we explicitly show that the matrix needed to describe the motion of the microswimmer is identical to the grand resistance matrix of the particle. This opens the way to think in terms of effective forces and torques, which is advantageous in order to get insights into the variety of swimming paths in more complicated situations. The benefit becomes most obvious when both external body forces and torques and internal effective self-propulsion forces and torques are present, such as in gravitaxis [14, 90, 91].

The paper is organized as follows: the mechanical self-propulsion mechanism and a generalization of the three-sphere swimmer of Golestanian towards an L-shaped microswimmer are discussed in section 2. Afterwards, in section 3, the self-propulsion of biaxial diffusiophoretic microswimmers is studied using slender body theory. Based on these considerations for two classes of microswimmers, section 4 contains general considerations for asymmetric particles with arbitrary shape and arbitrary self-propulsion. In section 5, we discuss limitations of the concept of effective forces and torques before we finally conclude in section 6.

2. Mechanical self-propulsion

Microswimmers with mechanical self-propulsion change their shapes in a non-reciprocal way [84] in order to propel themselves forward. These shape changes can be realized by deformations or—if the microswimmer consists of several individual parts—by translating or rotating different parts relative to each other through internal forces and torques \( k^{(a)} \) that are applied on the individual parts of the microswimmer. The noise-free equations of motion of such a mechanical microswimmer with \( n \) parts can be formulated through a modified force and torque balance (see, e.g. (42) and (45) in [92])

\[
K_{st} + K = 0, \quad K = \sum_{a=1}^{n} C^{(a)} k^{(a)}
\]

(3)

that ensures that the microswimmer is force-free and torque-free and that includes the Stokes friction force and torque

\[
K_{st} = -\eta \mathcal{H} \mathbf{V},
\]

which is proportional to the shape-dependent grand resistance matrix \( \mathcal{H} \) of the particle, and the rescaled internal forces and torques \( C^{(a)} k^{(a)} \) with rescaling matrices \( C^{(a)} \). For a specific particle shape, the rescaling matrices \( C^{(a)} \), which take into account the hydrodynamic interactions between the individual parts of the microswimmer, can in principle be calculated using the Green’s function approach [92, 93]. It is important to note that due to this rescaling the equations of motion of the microswimmer are given through a modified and not through a simple direct force and torque balance. The sum of the rescaled internal forces and torques is the formally external effective force and torque vector \( \mathbf{K} \).

The simplest mechanical microswimmer is the linear three-sphere swimmer of Najafi and Golestanian [72], which consists of three spheres one behind the other that are translated relative to each other (see (5) in [89] for the equation of motion). In the following, we generalize their theoretical approach to an L-shaped microswimmer in two spatial dimensions in order to provide a minimal microscopic model for an asymmetric mechanical microswimmer.

Our L-shaped Golestanian-like microswimmer consists of two very small spheres and a much larger L-shaped particle (see figure 1). The small spheres have distances \( d_1(t) \) and \( d_2(t) \) from the short arm of the L-shaped particle, which vary as a non-reciprocal function of time (see [72] for details) as a consequence of internal forces \( f^{(a)} \) with \( a \in \{1, 2\} \) that act on the two spheres. Note that the forces \( f^{(a)} \) are two-dimensional here as the motion is restricted to the \( x-y \) plane. We denote the length of the long arm of the L-shaped particle by \( a \) and its orientation by \( \mathbf{u}_L \). The length of the short arm of the particle is \( b \) and the width of the arms is \( b/2 \). The small spheres are only translated relative to the larger L-shaped particle. There are no internal torques that rotate the spheres and the L-shaped particle relative to each other. Nevertheless, the resulting effective (here three-dimensional) generalized self-propulsion force \( \mathbf{K} = (F, M) = C^{(1)} f^{(1)} + C^{(2)} f^{(2)} \) includes not only an effective self-propulsion force \( F \), but also an effective self-propulsion torque \( M \) that acts on the centre

Figure 1. Schematic of a force-free and torque-free L-shaped Golestanian-like microswimmer of size \( a \) and orientation \( \mathbf{u}_L \). To put the microswimmer in motion, the distances \( d_1(t) \) and \( d_2(t) \) of the two small spheres from the L-shaped particle vary as a non-reciprocal function of time. The effective lever arm \( l \) relates the effective force \( F \) to the effective torque \( M = ||M|| \) on the centre of mass \( S \).

\[
K_{st} = -\eta \mathcal{H} \mathbf{V},
\]

7 Note that the grand resistance matrix depends only on the shape but not on the activity of the particle. It is therefore the same for active and passive particles as long as the activity is not accompanied by a change of the shape.
of mass $S$ of the particle. Since the effective force $F$ acts perpendicularly on the middle of the short arm of the L-shaped particle, the effective torque is given by $M = lF\hat{e}_z$ with $\hat{e}_z = (0, 0, 1)$ and $F = |F|$. The effective self-propulsion torque $M$ can thus be expressed by the effective lever arm $l$, which denotes the distance in the direction of the short arm of the particle between the point on which the effective force acts and the point of reference for the calculation of the diffusion coefficients, which is the centre of mass in our case.

In two spatial dimensions, the grand resistance matrix of the L-shaped microswimmer, which in the limit of very small spheres is equal to the grand resistance matrix of the (passive) L-shaped part of the microswimmer, is $3 \times 3$-dimensional; the generalized velocity is the three-dimensional zero external torque, reduces to (3), which comprises the conditions of zero external force and dimensional. With this notation, the force and torque balance slip velocity on (parts of) the surface of the particle [73, 74].

Interestingly, such a hydrodynamic modelling leads to equations of motion for the self-propulsion mechanism that involves a prescribed slip velocity. As required by slender-body theory, the sum of effective forces and torques follows intrinsically from a self-propulsion model based on slender-body theory for Stokes flow [94, 95]. Applications of slender-body theory include Purcell’s three-link swimmer [84, 96] as well as the modelling of flagellar locomotion in general [66, 68]. In this section, we apply slender-body theory to a rigid slender particle with two arms of different lengths as sketched in figure 2. The two straight arms of lengths $a$ and $b$, the internal angle $\delta$, the centre of mass CM, and a prescribed fluid slip velocity $V_{sl}$ on the arm of length $b$. The particle-fixed rectangular coordinate system is indicated by the unit vectors $\hat{u}_1 = (\cos(\phi), \sin(\phi))$ and $\hat{u}_\perp = (-\sin(\phi), \cos(\phi))$, where $\hat{u}_1$ is parallel to the arm of length $b$, whereas the orientation of the arm of length $a$ is denoted by the unit vector $\hat{u}_a = (-\cos(\delta - \phi), \sin(\delta - \phi))$.

3. Diffusiophoretic self-propulsion

3.1. Slender rigid particles

In contrast to mechanical microswimmers, self-diffusiophoretic microswimmers do not change their shapes in order to propel themselves forward. They instead move as a consequence of a local concentration gradient, which they generate themselves. The self-propulsion of such self-diffusiophoretic microswimmers can be modelled by prescribing a non-vanishing slip velocity on (parts of) the surface of the particle [73, 74]. Interestingly, such a hydrodynamic modelling leads to equations of motion that are on a more coarse-grained model the same as the equations of motion of the corresponding passive particles complemented by effective forces and torques to model the self-propulsion. In the following, we prove this for biaxial particles with two arms of different lengths, which meet at a certain internal angle, through a hydrodynamic calculation based on slender-body theory for Stokes flow [94, 95]. Applications of slender-body theory include Purcell’s three-link swimmer [84, 96] as well as the modelling of flagellar locomotion in general [66, 68]. In this section, we apply slender-body theory to a rigid slender particle with two arms of different lengths as sketched in figure 2. The two straight arms of lengths $a$ and $b$ enclose the internal angle $\delta$ with $0 < \delta < \pi$. The special case $\delta = \pi/2$ corresponds to an L-shaped particle similar to what has been studied, using a different approach, in section 2. The results of the slender-body approach for this special case have already briefly been presented in [86]. Here, we provide a more general and detailed derivation, which shows that the concept of effective forces and torques follows intrinsically from a self-propulsion mechanism that involves a prescribed slip velocity. As required by slender-body theory, the sum $L = a + b$ of the lengths of the two arms of the particle is assumed to be significantly larger than the width $2\varepsilon$ of the arms. Although this is not always the case in related experiments, the physical structure of the equations of motion governing the dynamics of asymmetric microswimmers is clearly elucidated by the slenderness approximation $\epsilon \ll L$.

In order to describe the translational and rotational motion of the biaxial microswimmer, we define the centreline position

$$x(s) = r + rs' + as'$$

for $-b \leq s \leq a$. (6)

Here, $s$ is the arc length coordinate, $r$ is the particle’s centre-of-mass position, the vector $r_{CM} = (a^2u_a - b^2u_b)/(2L)$ is directed from the meeting point of the arms to the centre of mass CM (see figure 2), and $x' = dx/\partial s$ is the unit tangent,
which is $\dot{u}_l = (\cos(\delta), \sin(\delta))$ along the arm of length $b$ ($-b \leq s \leq 0$) and $\dot{u}_a = (-\cos(\delta - \phi), \sin(\delta - \phi))$ along the arm of length $a$ ($0 \leq s \leq a$). For slender arms with width $2\epsilon \ll L$, the fluid velocity at any point on the particle surface can be approximated by $x(s) + u_{sl}(s)$, where $\dot{x}(s) = \partial x/\partial t$ is the time derivative of $x$ and $u_{sl}$ is the local slip velocity averaged over the perimeter of the surface adjacent to $x(s)$. We consider a constant slip velocity $v_{sl} = -V_d \hat{u}_l$ pointing in the direction $-\hat{u}_l$ normal to the centreline along the arm of length $b$ and a vanishing slip velocity along the other arm. The fluid velocity on the particle surface is related to the local force per unit length $f(s)$ by the leading-order slender-body approximation

$$\dot{x} + v_{sl} = c (I + x' \otimes x') f,$$

where $c = \log(L/\epsilon)/(4\pi \eta)$ is a constant depending on the viscosity $\eta$ of the solvent, $I$ is the identity matrix, and $\otimes$ denotes the dyadic product. This approximation is valid as long as $\delta$ is not too small so that lubrication effects in the corner between the two arms are negligible. The total force on the particle is given by

$$F_{ext} = \int_{-b}^{a} f \, ds$$

and the total torque on the particle is

$$M_{ext} = \hat{e}_z \cdot \int_{-b}^{a} (-\hat{r}_{CM} + s\hat{x}) \times \dot{f} \, ds.$$

To define the vector product $\times$ in (9), we technically add a third (zero) component to the vectors $\hat{r}_{CM}$, $x'$, and $f$, which is indicated by the tilde. For force-free and torque-free microswimmers, $F_{ext}$ and $M_{ext}$ are zero, whereas they are non-zero for externally driven particles.

The integral constraints (8) and (9) lead to a system of three dynamic equations for $\dot{u}_l \cdot \hat{r}$, $\dot{u}_a \cdot \hat{r}$, and $\phi$. We begin by differentiating (6) with respect to time and multiplying with $\dot{u}_l$ and $\dot{u}_a$, respectively. This leads to

$$\dot{u}_l \cdot \hat{r} + \frac{a^2 \sin(\delta)}{2L} \phi$$

$$= \begin{cases} 2c\dot{u}_l \cdot f, & \text{if } -b \leq s \leq 0, \\ c(\dot{u}_l \cdot f - \cos(\delta) \dot{u}_a \cdot f) + s \sin(\delta) \phi, & \text{if } 0 < s \leq a \end{cases}$$

and

$$\dot{u}_a \cdot \hat{r} + \frac{b^2 \sin(\delta)}{2L} \phi$$

$$= \begin{cases} c(\dot{u}_a \cdot f - \cos(\delta) \dot{u}_l \cdot f) - s \sin(\delta) \phi + V_d \sin(\delta), & \text{if } -b \leq s \leq 0, \\ 2c\dot{u}_a \cdot f, & \text{if } 0 < s \leq a. \end{cases}$$

In order to eliminate the unknown $f$ from (10) and (11), the equations are integrated over $s$, separately from $-b$ to 0 and from 0 to $a$. After that, (8) and (9) are used to complete the system of differential equations. To apply the torque condition (9), equations (10) and (11) are first multiplied by $s$ before integrating over the two sections. Thus, one obtains eight equations altogether. Taking suitable linear combinations of these equations finally leads to the dynamic equations

$$\eta \mathbf{H} \begin{pmatrix} \dot{u}_l \cdot \hat{r} \\ \dot{u}_a \cdot \hat{r} \\ \phi \end{pmatrix} = \begin{pmatrix} \dot{u}_l \cdot F_{ext} \\ \dot{u}_a \cdot F_{ext} \\ M_{ext} \end{pmatrix} + V_d \begin{pmatrix} 0 \\ b \sin(\delta)/c \\ \frac{ab(a \cos(\delta) - b)}{(2cL)} \end{pmatrix}$$

with the grand resistance matrix

$$\mathbf{H} = \frac{1}{2c \eta} \begin{pmatrix} 2a + b & a \cos(\delta) & ab(a \cos(\delta) - b)/2L \\ b \cos(\delta) & a + 2b & \frac{ab(a \cos(\delta) - b)}{2L} \end{pmatrix}$$

and the constant

$$A = \left(\frac{a^3 + b^3}{3} - \frac{4b^2}{2L} \right) = \frac{a^3 + b^3 + 2a^2b^2 \cos(\delta)}{2L}.$$
Thus, the equations of motion of a force-free and torque-free L-shaped diffusiophoretic microswimmer read

\[ \eta \mathcal{H}_L \begin{pmatrix} \dot{u}_1 \\ \dot{u}_2 \\ \phi \end{pmatrix} = V_d \begin{pmatrix} 0 \\ b/c \\ -ab^2/(2cL) \end{pmatrix} \]  \hspace{1cm} (17)

in the particle frame. The grand resistance matrix \( \mathcal{H}_L \) in (17) can be expressed in terms of the generalized diffusion tensor

\[ \mathcal{D}_0 = \frac{1}{\beta \eta} \mathcal{H}^{-1}_L = \begin{pmatrix} D_\parallel & D_{\perp \parallel} & D_\perp \\ D_{\parallel \perp} & D_{\perp \perp} & D_{\perp \perp} \\ D_{\perp} & D_{\perp \perp} & D_R \end{pmatrix}. \]  \hspace{1cm} (18)

In order to transform the equations of motion (17) from the particle’s frame of reference to the laboratory frame, we use the rotation matrix

\[ \mathcal{M}(\phi) = \begin{pmatrix} \cos \phi & -\sin \phi & 0 \\ \sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix}. \]  \hspace{1cm} (19)

With this definition, the generalized diffusion tensor \( \mathcal{D}(\phi) \) in the laboratory frame of reference is given by

\[ \mathcal{D}(\phi) = \mathcal{M}(\phi) \mathcal{D}_0 \mathcal{M}^{-1}(\phi). \]  \hspace{1cm} (20)

Using the orientation vectors \( \hat{u}_1 \) and \( \hat{u}_\perp \), it can also be written as

\[ \mathcal{D}(\phi) = \begin{pmatrix} D_{\parallel}(\phi) & D_{\perp \parallel}(\phi) \\ D_{\parallel \perp}(\phi) & D_{\perp \perp}(\phi) \end{pmatrix}. \]  \hspace{1cm} (21)

with the translational short-time diffusion tensor \( \mathcal{D}_T(\phi) = D_\parallel \hat{u}_1 \otimes \hat{u}_1 + D_{\perp \parallel}(\hat{u}_1 \otimes \hat{u}_1 + \hat{u}_\perp \otimes \hat{u}_\perp) + D_{\parallel \perp} \hat{u}_\perp \otimes \hat{u}_\perp \) and its transpose \( D_{\parallel \perp}(\phi) \), the translational-rotational coupling vector \( D_{\perp \parallel}(\phi) = D_\parallel \hat{u}_1 + D_{\perp \perp} \hat{u}_\perp \) and the rotational diffusion coefficient \( D_R \). Thus, one finally obtains the equations of motion for an L-shaped self-propelled particle

\[ \begin{align*}
\vec{r} &= \beta F \left[ \mathcal{D}_T(\phi) \hat{u}_\perp + lD_{\perp \parallel}(\phi) \right], \\
\hat{\phi} &= \beta F \left[ D_R + lD_{\perp \parallel}(\phi) \right].
\end{align*} \]  \hspace{1cm} (22)

where \( F = bV_d/c \) is the effective self-propulsion force and \( l = -ab^2/(2cL) \) is an effective lever arm [12].

The above hydrodynamic calculation shows that also for an L-shaped self-propelled particle, \( \vec{u} \) and \( \sigma \) can be obtained directly and much more easily from the equations of motion of the corresponding passive particle to introducing effective forces and torques that model the self-propulsion.

### 3.2. General rigid particles

On top of the previous derivation for an L-shaped particle based on slender body theory, we now describe how the effective forces and torques can in principle be calculated for an arbitrarily shaped particle propelled by self-diffusiophoresis. The procedure is based on the Lorentz reciprocal theorem for low-Reynolds-number hydrodynamics [39]. It was similarly applied in [99] in order to relate the translational and rotational velocities of a swimming microorganism to its surface distortions [100, 101]. Such surface deformations and a streaming of the cell surface have been suggested as the swimming mechanism of cyanobacteria [102], for example. The modelling is similar to diffusiophoresis, where usually a slip velocity at the particle surface is assumed in the theoretical description [73, 74].

In order to calculate the effective forces and torques for an arbitrarily shaped rigid particle with a surface \( S \) and vectors \( s \) that define the points on \( S \), we first study how the slip velocity \( v_{sl}(s) \) on the surface affects the translational and rotational velocities \( v \) and \( \omega \) of the particle. On the one hand, we consider the velocity field \( u \) and the stress field \( \sigma \) around a rigid self-propelled particle that translates at velocity \( v \) due to some slip velocity \( v_{sl}(s) \) on the particle surface \( S \). On the other hand, we assume that \( \vec{u} \) and \( \vec{\sigma} \) are the velocity and stress fields around a corresponding passive particle that moves with velocity \( \vec{v} \) due to an external force \( F_{\text{ext}} \). The Lorentz reciprocal theorem states that

\[ \int_S n \cdot \vec{\sigma} \cdot \vec{u} \, dS = \int_S n \cdot \vec{\sigma} \cdot \vec{v}_{sl} \, dS, \]  \hspace{1cm} (23)

where \( n \) is the unit outward normal to the surface \( S \) and \( n \cdot \sigma \) is the stress exerted by the fluid on the surface. Note that the right-hand side of (23) vanishes because \( \vec{u} = \vec{v} \) is constant on the surface of the passive particle in the second case and \( \int_S n \cdot \sigma \, dS = 0 \) because the self-propelled particle in the first case is force-free. Setting \( u = v + v_{sl} \) on the surface of the self-propelled particle, we obtain

\[ \int_S n \cdot \vec{\sigma} \cdot (v + v_{sl}) \, dS = 0. \]  \hspace{1cm} (24)

This indicates that \( v \) is directly related to \( v_{sl} \). What is required is the stress \( n \cdot \vec{\sigma} \) on the passive particle, which can in principle be calculated by solving the Stokes equations for the flow around the particle. Equation (24) can also be written as

\[ F_{\text{ext}} \cdot v + \int_S n \cdot \vec{\sigma} \cdot v_{sl} \, dS = 0. \]  \hspace{1cm} (25)

Using a similar application of the Lorentz reciprocal theorem for a rigid self-propelled particle that rotates at angular velocity \( \omega \) due to some slip velocity \( v_{sl}(s) \) on the particle surface \( S \) and a corresponding passive particle that rotates with angular velocity \( \omega \) due to an external torque \( M_{\text{ext}} \), one can derive the relation

\[ M_{\text{ext}} \cdot \omega + \int_S n \cdot \vec{\sigma} \cdot v_{sl} \, dS = 0, \]  \hspace{1cm} (26)

where \( n \cdot \vec{\sigma} \) is the stress exerted by the fluid on the particle surface. By decomposing the slip velocity \( v_{sl} \) into the parts that translate and rotate the self-propelled particle, \( v_{sl} = v_{sl, t} + v_{sl, r} \), one could in principle predict the velocities \( v \) and \( \omega \). Although (25) is only a one-component equation, all components of \( v \) are accessible because different realizations of the external force \( F_{\text{ext}} \) and the corresponding stress fields \( \sigma \) can be inserted. Analogously, \( \omega \) can be obtained from (26). Once the translational and rotational velocities are known, the effective force \( F \) can be obtained by integrating the stress \( \vec{\sigma} \cdot n \) for the special case \( v = \vec{v} \) over the particle surface \( S \). Correspondingly, the effective torque \( M \) is the integral of \( (s - r_0) \times (\vec{\sigma} \cdot n) \) for the special case \( \vec{\omega} = \omega \) over the particle.
surface $S$, where $r_0$ is the reference point for the torque (e.g. the centre of mass of the particle). Following this procedure, the effective forces and torques for an arbitrarily shaped self-propelled particle can be calculated in principle.

4. Considerations for general self-propulsion

Based on the previous explicit investigations of active particles with either mechanical or diffusiophoretic self-propulsion, here we briefly present some general considerations about effective forces and torques on a rigid self-propelled particle. For these general considerations, the particle shape and the origin of the self-propulsion do not matter.

Assume that a rigid self-propelled particle with surface $S$ moves with translational velocity $v$ and angular velocity $\omega$. The only relevant condition is that the net force and the net torque vanish as required for swimmers [84]. On the other hand, we consider a passive rigid particle with the same surface $S$ but without self-propulsion. By applying a suitably chosen external force $F_{\text{ext}}$ and torque $M_{\text{ext}}$ one can drive the passive particle so that it moves with exactly the same translational and rotational velocities as the self-propelled particle. This is possible because $F_{\text{ext}}$ and $M_{\text{ext}}$ together have six independent components, which is sufficient for controlling the six degrees of freedom of the rigid particle. Thus, the motion of a force-free and torque-free self-propelled particle is equivalent to the motion of a passive particle with the same shape that is driven by an appropriate effective force $F = F_{\text{ext}}$ and torque $M = M_{\text{ext}}$. For run-and-tumble particles [103–105] the orientations of the effective force and torque are constant in the particle frame, whereas for active Brownian particles [18, 56, 104] also their magnitudes are constant in the particle frame.

Due to the linearity of Stokes flow, the generalized effective force and torque vector $K = (F, M)$ can be written in the form $\eta \mathbf{H} \mathbf{V}$ with the generalized velocity vector $\mathbf{V} = (v, \omega)$ and a $6 \times 6$-dimensional grand resistance matrix $\mathbf{H}$, which depends on the shape of the surface $S$. Thus, the validity of the concept of effective forces and torques is not affected by the specific type of self-propulsion of active particles. However, in order to relate these effective quantities directly to the physical process responsible for the self-propulsion, the details of the respective propulsion mechanism have to be known. The detailed calculations in sections 2 and 3 illustrate how the concept can be explicitly applied to specific situations.

5. Modifications and limitations of the concept of effective forces and torques

In the following, we address the questions when the concept of effective forces and torques has to be modified in order to still provide a valid theoretical model and when it finally reaches its limitations.

While we focused on particles with constant propulsion in this article, the concept can also be transferred to single active Brownian particles with time-dependent self-propulsion [55] in an unbounded fluid. This is particularly relevant in the context of run-and-tumble particles [60, 103] or when the swimming stroke itself results in variations of the propulsion speed.

The concept is also very useful if self-propelled particles in additional external fields such as gravity [14] are considered. All external body forces that do not affect the self-propulsion itself can easily be included in the generalized force vector $K$. However, if the intrinsic propulsion mechanism of an active particle is disturbed by the external field, the concept of effective forces and torques reaches its limitations. As an example, we refer to bimetallic nanorods driven by electrophoresis [106, 107] in an external electric field.

The situation becomes more complicated when the solvent flow field which is generated by the self-propelled particles governs the particle dynamics and has to be taken into account. The far-field behaviour of this solvent flow field is different from that for a passive particle exposed to a body force. While the latter corresponds to a force monopole, the former is a force dipole such that pusher- and puller-like swimmers can be distinguished. While the details of the solvent velocity field do not play any role for a single particle in an unbounded fluid, they affect the motion of a particle near system boundaries [108–110] and at high concentrations. In particular hydrodynamic interactions between different swimmers will depend on these solvent flow fields [111–114]. Therefore the concept of effective forces and torques cannot straightforwardly be applied in these situations. How exactly the effective forces and torques would change near walls or other particles is a matter of future research.

6. Conclusions

We have shown that effective forces and torques can be used to model the self-propulsion of microswimmers and that this concept is an appropriate and consistent theoretical framework to describe the dynamics of anisotropic active particles and to understand related experimental results. We have provided general arguments as well as specific examples for the concept of effective forces and torques. In particular, we have presented a fine-grained derivation for an L-shaped mechanical microswimmer and an explicit hydrodynamic derivation for a biaxial diffusiophoretic microswimmer. Although the detailed processes responsible for the self-propulsion of some artificial microswimmers are not fully understood yet [115], our general theoretical approach constitutes a powerful tool to describe the dynamics of self-propelled particles of arbitrary shape and turns out to be in good agreement with experimental observations [12, 14].

Acknowledgments

This work was supported by the Deutsche Forschungsgemeinschaft (DFG) through the priority programme SPP 1726 on microswimmers under contracts BE 1788/13-1 and LO 418/17-1, by the Marie Curie-Initial Training Network Complieds funded by the European Union Seventh Framework Program (FP7), by the ERC Advanced Grant INTERCOCOS (Grant No. 267499), and by EPSRC (Grant No. EP/J007404). RW gratefully acknowledges financial support through a Postdoctoral Research Fellowship (WI 4170/1-2) from the DFG.
References

[1] Hansen J-P and McDonald I R 2006 Theory of Simple Liquids 3rd edn (London: Academic)
[2] Barrat J-L and Hansen J-P 2003 Basic Concepts for Simple and Complex Liquids (Cambridge: Cambridge University Press)
[3] Cates M E 2012 Diffusive transport without detailed balance in motile bacteria: does microbiology need statistical physics? Rep. Prog. Phys. 75 042601
[4] Marchetti M C, Joanny J F, Bray P, Joanny J, Prost J,mos, and Simha R A 2013 Hydrodynamics of soft active matter Rev. Mod. Phys. 85 1143–89
[5] Wensink H H and L"owen H 2008 Self-propelled colloidal rods near confining walls Phys. Rev. E 78 031409
[6] Fily Y, Henkes S and Marchetti M C 2014 Freezing and phase separation of self-propelled disks Soft Matter 10 2132–40
[7] Angelani L, Costanzo A and Di Leonardo R 2011 Active ratchets Europhys. Lett. 96 68002
[8] Yang W, Misko V R, Nelissen K, Kom M and Peeters F M 2012 Using self-driven microswimmers for particle separation Soft Matter 8 5175–9
[9] Costanzo A, Elgeti J, Auth T, Gompper G and Ripoll M 2014 Motility-sorting of self-propelled particles in microchannels Europhys. Lett. 107 36003
[10] Kaiser A, Wensink H H and L"owen H 2012 How to capture active particles Phys. Rev. Lett. 108 268307
[11] Kaiser A, Popowa K, Wensink H H and L"owen H 2013 Capturing self-propelled particles in a moving microwedge Phys. Rev. E 88 022311
[12] Wang Z, Chen H-Y, Sheng Y-J and Tsao H-K 2014 Diffusion, sedimentation equilibrium, and harmonic trapping of run-and-tumble nanoswimmers Soft Matter 10 3209–17
[13] Howse J R, Jones R A L, Ryan A J, Gough T, Vafabakhsh R and Golestanian R 2007 Self-motile colloidal particles: from directed propulsion to random walk Phys. Rev. Lett. 99 048102
[14] ten Hagen B, van Teefelen S and L"owen H 2011 Brownian motion of a self-propelled particle J. Phys.: Condens. Matter 23 194119
[15] Happel J and Brenner H 1991 Low Reynolds Number Hydrodynamics: With Special Applications to Particulate Media (Mechanics of Fluids and Transport Processes vol 1) 2nd edn (Dordrecht: Kluwer)
[16] Kraft D J, Wittkowski R, ten Hagen B, Edmond K V, Pine D J and L"owen H 2013 Brownian motion and the hydrodynamic friction tensor for colloidal particles of complex shape Phys. Rev. E 88 050501
[17] van Teefelen S, Zimmermann U and L"owen H 2009 Clockwise-directional circle swimmer moves counter-clockwise in Petri dish- and ring-like confinements Soft Matter 5 4510–9
[18] C"ebers A 2011 Diffusion of magnetotactic bacteria in rotating magnetic field J. Magn. Magn. Mater. 323 279–82
[19] Gro"{o}mann R, Schimansky-Geier L and Romanzuk P 2012 Active Brownian particles with velocity-alignment and active fluctuations New J. Phys. 14 073033
[20] Radtke P K and Schimansky-Geier L 2012 Directed transport of confined Brownian particles with torque Phys. Rev. E 85 051110
[21] Si T 2012 The equation of motion for the trajectory of a circling particle with an overdamped circle center Physica A 391 3054–60
[93] Kim S and Karrila S J 1991 Microhydrodynamics: Principles and Selected Applications (Boston: Butterworth-Heinemann)

[94] Batchelor G K 1970 Slender-body theory for particles of arbitrary cross-section in Stokes flow J. Fluid Mech. 44 419–40

[95] Cox R G 1970 The motion of long slender bodies in a viscous fluid part 1. General theory J. Fluid Mech. 44 791–810

[96] Becker L E, Koehler S A and Stone H A 2003 On self-propulsion of micro-machines at low Reynolds number: Purcell’s three-link swimmer J. Fluid Mech. 490 15–35

[97] Ramachandran S, Sunil Kumar P B and Pagonabarraga I 2006 A Lattice-Boltzmann model for suspensions of self-propelling colloidal particles Eur. Phys. J. E 20 151–8

[98] Julicher F and Prost J 2009 Generic theory of colloidal transport Eur. Phys. J. E 29 27–36

[99] Stone H A and Samuel A D T 1996 Propulsion of microorganisms by surface distortions Phys. Rev. Lett. 77 4102–4

[100] Gonzalez-Rodriguez D and Lauga E 2009 Reciprocal locomotion of dense swimmers in Stokes flow J. Phys.: Condens. Matter 21 204103

[101] Lauga E 2014 Locomotion in complex fluids: integral theorems Phys. Fluids 26 081902

[102] Waterbury J B, Willey J M, Franks D G, Valois F W and Watson S W 1985 A cyanobacterium capable of swimming motility Science 230 74–6

[103] Taillieu J and Cates M E 2008 Statistical mechanics of interacting run-and-tumble bacteria Phys. Rev. Lett. 100 218103

[104] Cates M E and Taillieu J 2013 When are active Brownian particles and run-and-tumble particles equivalent? Consequences for motility-induced phase separation Europhys. Lett. 101 20010

[105] Paoluzzi M, Di Leonardo R and Angelani L 2013 Effective run-and-tumble dynamics of bacteria baths J. Phys.: Condens. Matter 25 415102

[106] Paxton W F, Kistler K C, Olmeda C C, Sen A, St Angelo S K, Cao Y, Mallouk T E, Lammert P E and Crespi V H 2004 Catalytic nanomotors: autonomous movement of striped nanorods J. Am. Chem. Soc. 126 13424–31

[107] Paxton W F, Baker P T, Kline T R, Wang Y, Mallouk T E and Sen A 2006 Catalytically induced electrodynamics for motors and micropumps J. Am. Chem. Soc. 128 14881–8

[108] Kreuter C, Siems U, Niehsa P, Leiderer P and Erbe A 2013 Transport phenomena and dynamics of externally and self-propelled colloids in confined geometry Eur. Phys. J. Spec. Top. 222 2923–39

[109] Takagi D, Palacci J, Braunschweig A B, Shelley M J and Zhang J 2014 Hydrodynamic capture of microswimmers into sphere-bound orbits Soft Matter 10 1784–9

[110] Chilukuri S, Collins C H and Underhill P T 2014 Impact of external flow on the dynamics of swimming microorganisms near surfaces J. Phys.: Condens. Matter 26 115101

[111] Kapral R 2008 Multiparticle collision dynamics: simulation of complex systems on mesoscales Adv. Chem. Phys. 140 89–146

[112] Gompper G, Ilhe T, Kroll D M and Winkler R G 2009 Multi-particle collision dynamics: a particle-based mesoscale simulation approach to the hydrodynamics of complex fluids Adv. Polym. Sci. 221 1–87

[113] Alexander G P, Pooley C M and Yeomans J M 2009 Hydrodynamics of linked sphere model swimmers J. Phys.: Condens. Matter 21 204108

[114] Reigh S Y, Winkler R G and Gompper G 2012 Synchronization and bundling of anchored bacterial flagella Soft Matter 8 4363–72

[115] Brown A and Poon W 2014 Ionic effects in self-propelled Pt-coated Janus swimmers Soft Matter 10 4016–27