Anisotropic effective diffusion of torqued swimmers

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(Received 12 October 2012; revised manuscript received 12 January 2013; published 12 March 2013)

External torques affect the trajectories of swimming microorganisms. We calculate analytically the effective three-dimensional diffusivity of a spherical active particle subject to both a constant external torque and thermal noise. We find that the presence of a torque renders the effective diffusive behavior anisotropic. The analytical results are compared with Brownian dynamics simulations and we obtain excellent agreement. For steady swimmers an external torque always decreases the effective swimmer diffusivity whereas it may be enhanced for time-reversible swimmers.

DOI: 10.1103/PhysRevE.87.032708 PACS number(s): 87.10.−e

I. INTRODUCTION

The mechanics of swimming microorganisms [1–4], such as bacteria, plankton, spermatozoa, and synthetic microswimmers [5–7], is a very active research area [8–11]. Understanding small-scale locomotion enables us to gain insight into factors affecting many processes vital to biology, from human reproduction [12] to the marine life ecosystem [13]. Additionally, this understanding facilitates the development of novel synthetic microswimmers for a variety of applications ranging from diagnostics to drug delivery in the human body [14–16]. The small size of swimming cells leads to additional complications affecting the modeling of locomotory behavior and hence challenges in the design of their synthetic counterparts.

A critical complication is that microscopic swimmers are susceptible to thermal fluctuations which cause the microswimmers to lose their orientation due to this stochastic forcing [4,5,9,17–19], and then to perform Brownian motion. Classical work concerning Brownian motion includes isotropic passive particles in the absence [20–22] and presence of external fields [23–26]. Additionally, anisotropic passive particles undergoing Brownian motion in the absence [27,28] and presence of external fields [29] have been considered. More recently, and based on the previous classical works, the impact of thermal agitation on active particles (driven by an assumed internal mechanism) has received attention. For example, steadily swimming self-propelled bodies of simple shape, one sphere [5,8], multiple spheres [9], or ellipsoids [8] have been studied. An enhanced effective diffusive behavior has been obtained [17,18] and a recent extension to unsteady swimming showed that time-reversible motion could also lead to enhanced effective diffusion [30].

Another important issue is that both natural and artificial micro-swimmers, in addition to being affected by thermal forces, are often subject to external torques that potentially may affect the particle's trajectory. This would be the case, for example, for magnetotactic bacteria in the presence of an external magnetic field [31–34]. It has been shown [32] that these cells (like *Aquaspirillum magnetotacticum*) contain aligned cubic to octahedral magnetosomes (crystalline structures made of magnetite). Due to this alignment one can consider each cell as a single magnetic dipole, thus given there exists an angle between the cells' magnetic moment $\mathbf{m}$ and an external magnetic field $\mathbf{H}$, these microorganisms will experience a torque $\mathbf{L_m} = \mathbf{m} \times \mathbf{H}$ trying to align them along the magnetic field. Apart from magnetotactic bacteria, there exist in nature microorganisms whose center of mass are displaced from its geometric center (so-called bottom-heavy [19,35]) a distance h. If these cells of mass m have an orientation vector $\mathbf{e}$ and they are immersed in a gravitational field $\mathbf{g}$ then a torque $\mathbf{L_g} = mh\mathbf{e} \times \mathbf{g}$ will act on the cells tending to align them in the gravitational field direction. Another example where the presence of a torque proved to be a key factor, was in the motion of *Listeria monocytogenes* [36]. Here the inclusion of a torque in a deterministic dynamical model enabled to recover all the experimentally observed geometrical trajectories performed by *Listeria*.

Motivated by the latter scenarios and aware of the complicated and even stochastic relation between torque and time for those cases (see $\mathbf{L_m}$ and $\mathbf{L_g}$), in this work we consider the simplest case of having self-propelled particles in the presence of a constant torque and study its physical implications on the effective diffusion of swimming particles. Past work has addressed this problem only in two dimensions. A self-propelled particle moving in two dimensions subject to a constant and a time-dependent external torque was studied analytically in Ref. [37]. Similarly the two-dimensional effective diffusivity of a spherical self-propelled particle in a shear flow and subject to an external torque was studied in Ref. [38]. Anisotropic active particles subject to a constant torque and where its propulsion direction is different to its orientation, have also been considered in Ref. [10]. Moreover, the case of a constant external torque has already experimentally achieved [39]. In order to artificially generate a constant torque on a swimmer, Ebbens *et al.* [39] built doublets of Janus beads (allowed to move in two dimensions) with catalytic patches positioned on each bead at different angle. The patches reacted in peroxide fuel and water, thus generating translation and rotation to the doublets. Its dynamics was well described following a Langevin approach.

In this paper, we consider a self-propelled particle swimming in three dimensions, free to rotate in any direction, and subject to both a constant external torque and thermal

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fluctuations, hence this paper can be seen as a generalization of the work in Ref. [37]. Using a change of frame, we derive the probability distribution function for the swimmer orientation which we then exploit to calculate the effective swimmer diffusivity. The presence of an external torque is seen to render the effective diffusion anisotropic, a result not seen before since active particles under an external torque were confined to move in a plane. Our theoretical results are applied to two specific cases. For steady swimming we see that an external torque always leads to a decrease of the effective diffusion constant. In contrast, for time-reversible swimming an external torque may enhance diffusion. Finally, our analytical results are validated using Brownian dynamics simulations.

II. PHYSICAL MODEL

Consider a spherical particle of radius a that self-propels (swims) in a three-dimensional fluctuating environment. This sphere orientation is described by the most general two rotational degrees of freedom (φ,θ), where φ and θ are, respectively, the azimuthal and polar angle in a spherical coordinates system. The particle is also subject to a constant external torque, $\mathbf{M} = M\mathbf{k}$, where $\mathbf{k}$ is the unit vector along the z direction. The dynamics of this particle is described by its translational velocity, $\mathbf{U}(t)$, and angular velocity, $\boldsymbol{\Omega}(t)$, which in the Brownian dynamics formalism follow

$$\mathbf{R}_U(\mathbf{U} - \mathbf{U}_s) = \widetilde{\mathbf{f}}, \tag{1a}$$

$$\mathbf{R}_\Omega \boldsymbol{\Omega} - \mathbf{M} = \widetilde{\mathbf{g}}, \tag{1b}$$

where $\mathbf{U}_s(t)$ is the (imposed) swimming velocity, and $\mathbf{R}_U = R_U \mathbf{I}$, and $\mathbf{R}_\Omega = R_\Omega \mathbf{I}$ are, respectively, the viscous resistances to translation and rotation ($R_U = 6\pi\eta a$, $R_\Omega = 8\pi\eta a^3$ and $\mathbf{I}$ is the identity tensor). In Eq. (1) $\widetilde{\mathbf{f}}$ and $\widetilde{\mathbf{g}}$ are zero-mean Brownian random force and torque whose correlations are given by $\langle \widetilde{f}_i(t)\widetilde{f}_j(t')\rangle = 2k_BTR_U\delta_{ij}\delta(t-t')$ and $\langle \widetilde{g}_i(t)\widetilde{g}_j(t')\rangle = 2k_BTR_\Omega\delta_{ij}\delta(t-t')$ according to the fluctuation-dissipation theorem (here $\langle\cdot\rangle$ represent ensemble averaging) [40].

From Eq. (1a), we see that the equation of motion for the sphere position, $\mathbf{x}(t)$, is given by

$$\dot{\mathbf{x}}(t) = U_s(t)\mathbf{e}(t) + \mathbf{f}(t), \tag{2}$$

where we denote by $\mathbf{e}(t)$ the instantaneous unit vector in the direction of swimming with origin at the center of the sphere, $U_s(t)$ the instantaneous magnitude of the swimming velocity along $\mathbf{e}(t)$, $\mathbf{f} = R_U^{-1}\widetilde{\mathbf{f}}$ and where the dot represents a time derivative.

III. DERIVATION OF EFFECTIVE DIFFUSION

From Eq. (2), the trajectory of the active particle is given by

$$\mathbf{x}(t) = \int_0^t U_s(t')\mathbf{e}(t')dt' + \int_0^t \mathbf{f}(t')dt', \tag{3}$$

hence by combining Eqs. (2) and (3) we get

$$\mathbf{x}\cdot\dot{\mathbf{x}} = U_s(t)\int_0^t U_s(t')\mathbf{e}(t)\cdot\mathbf{e}(t')dt' + \int_0^t \mathbf{e}(t)\cdot\mathbf{f}(t')dt' + \int_0^t U_s(t')\mathbf{f}(t)\cdot\mathbf{e}(t')dt' + \int_0^t \mathbf{f}(t)\cdot\mathbf{f}(t')dt'. \tag{4}$$

By taking ensemble average of Eq. (4), one finds that

$$\langle \mathbf{x}\cdot\dot{\mathbf{x}}\rangle = U_s(t)\int_0^t U_s(t')\langle\mathbf{e}(t)\cdot\mathbf{e}(t')\rangle dt' + \int_0^t \langle\mathbf{f}(t)\cdot\mathbf{f}(t')\rangle dt', \tag{5}$$

where we used that the random force and swimming direction are not correlated.

Anticipating on the anisotropy of the effective diffusion, we define

$$\mathbf{x} = \mathbf{x}_\parallel + \mathbf{x}_\perp, \quad \mathbf{e} = \mathbf{e}_\parallel + \mathbf{e}_\perp, \quad \mathbf{f} = \mathbf{f}_\parallel + \mathbf{f}_\perp, \tag{6}$$

where, for any vector $\mathbf{v}$ (=$\mathbf{e}$, $\mathbf{x}$ or $\mathbf{f}$), parallel refers to the component along the axis where the torque is applied, $\mathbf{v}_\parallel = (\mathbf{v}\cdot\mathbf{k})\mathbf{k}$, and perpendicular, $\mathbf{v}_\perp = \mathbf{v} - \mathbf{v}_\parallel$, refers to the other two. Hence combining Eq. (5) with Eq. (6) we obtain

$$\langle \mathbf{x}_\beta\cdot\dot{\mathbf{x}}_\beta\rangle = U_s(t)\int_0^t U_s(t')\langle\mathbf{e}_\beta(t)\cdot\mathbf{e}_\beta(t')\rangle dt' + \int_0^t \langle\mathbf{f}_\beta(t)\cdot\mathbf{f}_\beta(t')\rangle dt'. \tag{7}$$

where $\beta = \parallel$ or $\perp$. In three dimensions, we expect a long-time effective diffusive behavior as $\langle\mathbf{x}_\parallel\cdot\mathbf{x}_\parallel\rangle = 2D_\parallel t$ and $\langle\mathbf{x}_\perp\cdot\mathbf{x}_\perp\rangle = 4D_\perp t$ in the limit $t\to\infty$, thus the effective diffusion constants can be obtained as

$$D_\parallel = \lim_{t\to\infty}\langle\mathbf{x}_\parallel\cdot\dot{\mathbf{x}}_\parallel\rangle, \quad D_\perp = \tfrac{1}{2}\lim_{t\to\infty}\langle\mathbf{x}_\perp\cdot\dot{\mathbf{x}}_\perp\rangle. \tag{8}$$

The fluctuation-dissipation theorem expressed along both directions is $\langle\mathbf{f}_\parallel(t)\cdot\mathbf{f}_\parallel(t')\rangle = 2D_B\delta(t-t')$ and $\langle\mathbf{f}_\perp(t)\cdot\mathbf{f}_\perp(t')\rangle = 4D_B\delta(t-t')$, where D_B is the Brownian diffusion constant, $D_B = k_BT/R_U$. Plugging these results into Eq. (7) and using the definitions in Eq. (8) we finally obtain the effective long-time diffusion constants parallel ($D_\parallel$) and perpendicular ($D_\perp$) to the torque direction as

$$D_\parallel = D_B + \lim_{t\to\infty}\int_0^t U_s(t)U_s(t')\langle\mathbf{e}_\parallel(t)\cdot\mathbf{e}_\parallel(t')\rangle dt', \tag{9}$$

$$D_\perp = D_B + \frac{1}{2}\lim_{t\to\infty}\int_0^t U_s(t)U_s(t')\langle\mathbf{e}_\perp(t)\cdot\mathbf{e}_\perp(t')\rangle dt'. \tag{10}$$

IV. ORIENTATION PROBABILITY DISTRIBUTION FUNCTION

In order to evaluate $D_\parallel$ and $D_\perp$ we need to determine the correlations in swimmer orientations. From Eq. (1b), we get

$$\boldsymbol{\Omega}(t) = \Lambda\mathbf{k} + \mathbf{g}(t), \tag{11}$$

where we have defined $\Lambda = M/R_\Omega$ and $\mathbf{g} = R_\Omega^{-1}\widetilde{\mathbf{g}}$. Equation (11) provides the physical meaning of adding an external torque to an active particle, that is, the constant external torque generates that the particle rotates with a constant angular velocity. The term $\mathbf{g}(t)$ in Eq. (11) represents thermal forces. Equation (11) may also be a connection for a possible experiment. For example, Ebbens *et. al* [39] made doublets of Janus particles with catalytic patches whose chemical reaction generated a constant angular velocity.

From vectorial mechanics [41], it can be shown that the dynamics of $\mathbf{e}(t)$ satisfies $\dot{\mathbf{e}}(t) = \mathbf{\Omega}(t)\times\mathbf{e}(t)$. Thus explicitly substituting the value of $\mathbf{\Omega}(t)$ in the latter equation we get

$$\dot{\mathbf{e}}(t) = [\Lambda\mathbf{k} + \mathbf{g}(t)]\times\mathbf{e}(t). \qquad (12)$$

The probability distribution function (pdf), $P(\theta,\varphi,t)$, governing the swimmer orientation, $\mathbf{e}(t)$, in the absence of torque follows a diffusion equation, $\partial P(\theta,\varphi,t)/\partial t = D_\Omega \nabla^2_{\theta,\varphi} P(\theta,\varphi,t)$, where $\nabla^2_{\theta,\varphi}$ is the angular diffusion operator and D_Ω is the rotational diffusion coefficient ($D_\Omega = k_B T/R_\Omega$).

In the presence of an external torque, a diffusion-type equation for $P(\theta,\varphi,t)$ should be formulated and solved including a rotational transport term. Alternatively, we introduce the rotational transformation $\mathbb{R}(t)$, that is,

$$\mathbf{v}(t) = \mathbb{R}(t)\mathbf{v}'(t), \quad \mathbb{R}(t) = \begin{bmatrix} \cos\Lambda t & -\sin\Lambda t & 0 \\ \sin\Lambda t & \cos\Lambda t & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad (13)$$

where $\mathbf{v}$ (=$\mathbf{e}$ or $\mathbf{g}$), and the prime represents a vector in the rotated frame. Applying this transformation to Eq. (12) gives

$$\dot{\mathbf{e}}'(t) = \mathbf{g}'(t)\times\mathbf{e}'(t). \qquad (14)$$

Thus in the prime coordinate system the pdf is already known and given by a sum of spherical harmonics [42]. Using the transformation $\theta' = \theta$, $\varphi' = \varphi - \Lambda t$ into the pdf expressed in the rotated frame we obtain the pdf in the laboratory frame as

$$P = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} e^{-D_\Omega l(l+1)t}\, Y_l^{m*}(\theta_0,\varphi_0)\, Y_l^m(\theta,\varphi)\, e^{-im\Lambda t}, \qquad (15)$$

where Y_l^m are the spherical harmonics, Y_l^{m*} their complex conjugates, and θ_0 and φ_0 the angular coordinates of $\mathbf{e}(t=0) \equiv \mathbf{e}_0$. With the knowledge of the pdf, the correlation of swimmer orientation may then be evaluated. It is defined as [42]

$$\langle \mathbf{e}_\beta(t)\cdot\mathbf{e}_\beta(0)\rangle = \int d^2e_0 \int d^2e\, \mathbf{e}_\beta(t)\cdot\mathbf{e}_\beta(0)\, G(\mathbf{e},t;\mathbf{e}_0,0), \qquad (16)$$

where $\beta = \parallel$ or $\perp$, and $G(\mathbf{e},t;\mathbf{e}_0,0)$ is the joint probability distribution for an orientation $\mathbf{e}_0$ at $t = 0$ and $\mathbf{e}$ at time t. This joint probability may be expressed as $G(\mathbf{e},t;\mathbf{e}_0,0) = P(\theta,\varphi,t)P_{eq}$, where $P_{eq} = \lim_{t\to\infty} P(\theta,\varphi,t) = 1/4\pi$. By solving directly Eq. (16) for both components, the orientation correlations are finally obtained as

$$\langle \mathbf{e}_\parallel(t)\cdot\mathbf{e}_\parallel(0)\rangle = \frac{e^{-2D_\Omega t}}{3}, \qquad (17)$$

$$\langle \mathbf{e}_\perp(t)\cdot\mathbf{e}_\perp(0)\rangle = e^{-2D_\Omega t}\left[\frac{2}{3}\cos\Lambda t\right]. \qquad (18)$$

The difference in correlations in the two directions as seen in Eqs. (17) and (18) is at the origin of the anisotropy in the effective diffusion. Whereas the swimmer orientation along the torque direction follows a Brownian exponential loss, the orientation in the plane perpendicular to it undergoes an exponential loss of direction modulated by a harmonic function. If we set $\Lambda = 0$ in Eq. (17), we recover by adding to Eqs. (17) and (18) the classical Brownian exponential decay, $\langle \mathbf{e}(t)\cdot\mathbf{e}(0)\rangle = e^{-2D_\Omega t}$ [40].

V. ANISOTROPIC DIFFUSION

A. General results

Substituting Eqs. (17) and (18) into Eqs. (9) and (10) we finally obtain the general formula for the parallel and perpendicular effective long time diffusivities as

$$D_\parallel = D_B + \frac{1}{3}\lim_{t\to\infty}\int_0^t U_s(t)U_s(t')e^{-2D_\Omega(t-t')}dt', \qquad (19)$$

and

$$D_\perp = D_B + \frac{1}{3}\lim_{t\to\infty}\int_0^t [U_s(t)U_s(t')e^{-2D_\Omega(t-t')} \times \cos\Lambda(t-t')]dt'. \qquad (20)$$

We see that the presence of a torque has no influence on the diffusion coefficient along its direction ($D_\parallel$ is independent of Λ). From Eqs. (19) and (20), the total effective diffusion D can then be obtained as $D = (D_\parallel + 2D_\perp)/3$.

B. Steady swimming

Let us now evaluate $D_\parallel$ and $D_\perp$ for two specific swimming kinematics. The simplest case is that of a self-propelled particle swimming at constant speed, $U_s(t) = U$, along $\mathbf{e}(t)$. Solving Eqs. (19) and (20) leads to

$$D_\parallel = D_B + \frac{U^2}{6D_\Omega}, \qquad (21)$$

$$D_\perp = D_B + \frac{U^2}{6D_\Omega(1+\alpha^2/4)}, \qquad (22)$$

where the dimensionless parameter $\alpha = 2\Lambda\tau$ measures the typical ratio between the thermal time scale for loss of orientation ($\tau = 1/2D_\Omega$) and the rotation time scale from the external torque (Λ^{-1}). Clearly we always have the anisotropy $D_\perp < D_\parallel$. In the large-torque limit, $\alpha \gg 1$, we see that $D_\perp \to D_B$; in that case, swimming excursions in the plane perpendicular to the applied torque are inhibited so the enhanced diffusion from swimming only acts along one direction, that of the applied torque. Note that the total effective diffusion constant, D, is

$$D = D_B + \frac{U^2}{6D_\Omega}\left[\frac{1+\alpha^2/12}{1+\alpha^2/4}\right], \qquad (23)$$

and setting $\alpha = 0$ in Eq. (23) reduces to the classic formula for the diffusivity of a self-propelled particle [17,18]. Note that using a similar mathematical framework we can evaluate the off-diagonal terms of the mean-square displacement dyadic, and obtain here $\langle xy\rangle = \langle xz\rangle = \langle yz\rangle = 0$.

In order to validate our theoretical results, we compare them with Brownian dynamics simulations [43]. To do so, we consider a spherical swimmer of radius $a = 1$ μm, immersed in water at $T = 300$ K, and simulate two different scenarios, with results illustrated in Fig. 1: (a) steady swimming at speed $U_s(t) = U = 5$ μm/s with no torque; (b) steady swimming at same speed but under an external torque $\mathbf{M} = M\mathbf{k}$ with $\Lambda = M/R_\Omega = 1$ s^{-1} (equivalent to $\alpha \approx 6$). Note that the above parameters were chosen arbitrarily. The results shown in

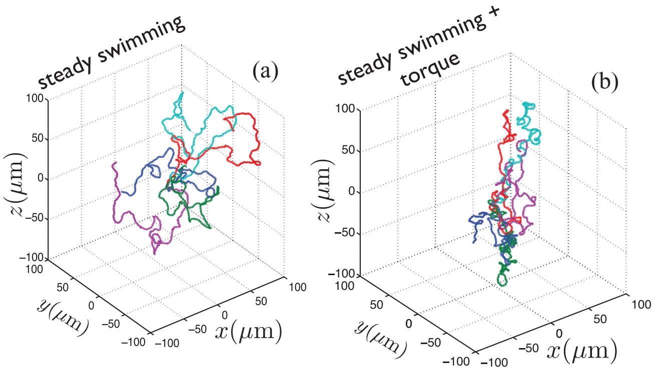

FIG. 1. (Color online) Brownian dynamics simulations showing the superposition of five realizations during 100 s of a spherical swimmer (radius $a = 1\ \mu$m) in water at 300 K for two different scenarios: (a) steady swimming at speed $U_s = 5\ \mu$m/s; (b) steady swimming plus external torque corresponding to $\alpha \approx 6$. A comparison between (a) and (b) visually shows that the overall diffusivity decreases for a torqued particle, and becomes anisotropic (diffusion mainly taking place along the z direction).

Fig. 1 reproduce the superposition of five realizations for both cases during 100 s. When comparing Fig. 1(a) to Fig. 1(b) we see that the presence of an external torque leads to a diffusive motion taking place mainly along the z direction, confirming our theoretical prediction of increased anisotropy with an increase of the external torque. The overall diffusion constant is also observed to go down, in agreement with our analytical results. In Fig. 2 we display the mean square displacement along the torque direction, $\langle \mathbf{x}_\parallel \cdot \mathbf{x}_\parallel \rangle$, and in the plane perpendicular to it, $\langle \mathbf{x}_\perp \cdot \mathbf{x}_\perp \rangle$. The simulations confirm

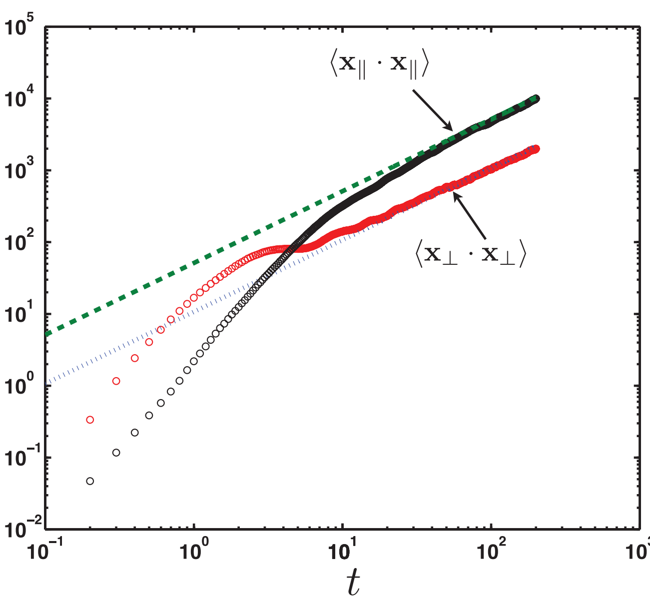

FIG. 2. (Color online) Brownian dynamics simulations for 500 realizations during a period of 200 s (circles) showing the mean square displacement along the torque direction, $\langle \mathbf{x}_\parallel \cdot \mathbf{x}_\parallel \rangle$, and perpendicular to it, $\langle \mathbf{x}_\perp \cdot \mathbf{x}_\perp \rangle$, for steady swimming with same parameters as in Fig. 1 and with $\alpha \approx 6$. The theoretical results are shown as straight lines. This figure clearly shows the generated anisotropy.

the anisotropy, $D_\perp < D_\parallel$, and agree quantitatively with the theoretical predictions from Eqs. (21) and (22) shown as straight lines in Fig. 2.

C. Reciprocal swimming

The next case of interest is an active particle displaying a time-reversible (so-called reciprocal [44]) motion of the form $U_s(t) = \mathcal{U}\cos\omega t$. Its effective diffusion constants in both directions and averaged over a period are then

$$D_\parallel = D_B + \frac{\mathcal{U}^2}{12 D_\Omega}\frac{1}{1+\gamma^2}, \tag{24}$$

$$D_\perp = D_B + \frac{\mathcal{U}^2}{12 D_\Omega}\left[\frac{2}{4+(\alpha-2\gamma)^2} + \frac{2}{4+(\alpha+2\gamma)^2}\right], \tag{25}$$

where the dimensionless parameter $\gamma = \omega\tau$ quantifies the ratio between the thermal time scale and the time scale of the periodic swimming. Here again, Eqs. (24) and (25) confirm the anisotropic diffusion induced by the external torque. Isotropy is recovered by setting $\alpha = 0$, in which case the results agree with Ref. [30]. The total effective diffusion constant, D, is in this case

$$D = D_B + \frac{\mathcal{U}^2}{36 D_\Omega}\left[\frac{4}{4+(\alpha-2\gamma)^2} + \frac{1}{(1+\gamma^2)} + \frac{4}{4+(\alpha+2\gamma)^2}\right]. \tag{26}$$

Can the presence of a torque ever enhance diffusion? When $\gamma < 1/\sqrt{3}$, the maximum of the bracket term $[\ldots]$ in Eq. (26) occurs at $\alpha = 0$ (no torque); in this case, the presence of any finite torque always decreases the effective diffusion constant. In contrast, when $\gamma > 1/\sqrt{3}$, the maximum of the bracket term is obtained at $\alpha = 2\sqrt{2\gamma\sqrt{1+\gamma^2} - (1+\gamma^2)}$, which corresponds to a finite torque; in this case, a range of torques exists (from $\alpha = 0$ up to $\alpha = 2\sqrt{3\gamma^2 - 1}$) leading to an enhancement of the diffusion constant compared to the no-torque case. Physically, this enhancement comes from the rotation from the applied torque which allows the trajectory to deviate from the reciprocal small-amplitude motion and increase its effective swimming amplitude in the $\mathbf{x}_\perp$ direction. This enhancement can be visually observed by using Brownian dynamics simulations. Once more, we consider a spherical swimmer (radius $a = 1\ \mu$m, in water at $T = 300$ K) and simulate: (a) reciprocal swimming, $U_s(t) = \mathcal{U}\cos\omega t$, with $\mathcal{U} = 5\ \mu$m/s, $\omega = 1$ rad/s (equivalent to $\gamma \approx 3$) [Fig. 3(a)]; (b) reciprocal swimming with the same parameters but under an external torque $\mathbf{M} = M\mathbf{k}$ with $\alpha \approx 6$ [Fig. 3(b)]. The results shown in Fig. 3 reproduce the superposition of five realizations for each case during 100 s. The comparison of Figs. 3(a) and 3(b) visually shows that for a reciprocal motion, diffusion is enhanced by the presence of the external torque hence in agreement with our theoretical predictions.

Finally to make our comparison quantitative we plot in Fig. 4 the mean-square displacement of 500 realizations during a period of 200 s (circles) together with our theoretical results (shown as straight lines) for the same all four scenarios and with the same parameters described in Figs. 1 and 3.

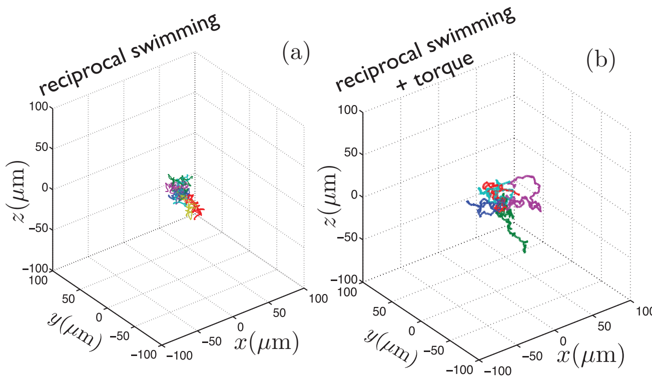

FIG. 3. (Color online) Brownian dynamics simulations showing the superposition of five realizations during 100 s of a spherical swimmer (radius a, 1 μm) in water at 300 K for two scenarios: (a) pure reciprocal swimming with amplitude $\mathcal{U} = 5$ μm/s and frequency $\omega = 1$ rad/s, corresponding to $\gamma \approx 3$; (b) reciprocal swimming plus external torque corresponding to $\alpha \approx 6$. The figure visually shows that the inclusion of an external torque for the reciprocal swimming case may enhance its effective diffusivity.

Figure 4 shows basically two time regimes, that is, $t \leqslant 10$ s where the Brownian simulations show that the particle has been just released from the origin, hence its mean-square displacement is small, and $t > 10$ s where the theoretical and numerical results start to converge, here the linear behavior of the mean-square displacement with time for all scenarios can be observed. We can also see an oscillatory behavior for $t \leqslant 10$ s (short time scales) in the case of reciprocal swimming, which is due to the fact that its mean-square displacement contains harmonic functions multiplied by an exponentially time decaying term namely, $\exp(-t/\tau)$. For longer time scales, this decaying term tends to zero, thus disappearing the oscillatory behavior.

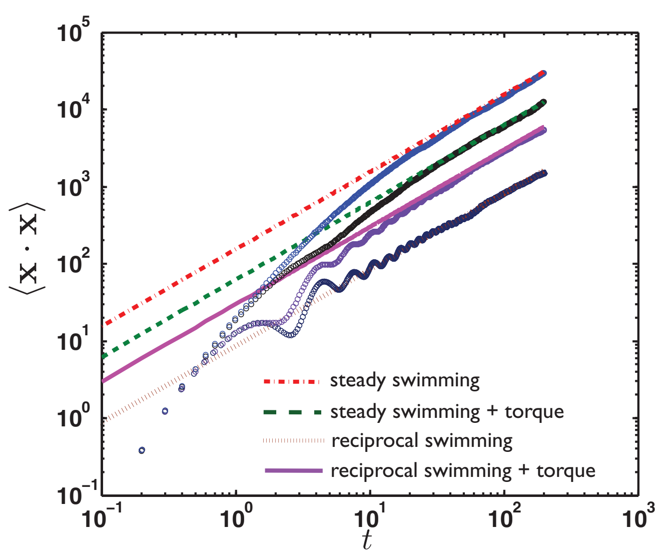

FIG. 4. (Color online) Brownian dynamics simulations for 500 realizations during a period of 200 s (circles) showing a quantitative comparison among the total effective diffusion for the four scenarios and same parameters described in Figs. 1 and 3. The theoretical results are shown as straight lines.

Figure 4 also shows an excellent quantitative agreement between the computational results and our analytical results. Additionally, one can easily see from this figure that an external torque may enhance the total effective diffusion of an active particle performing reciprocal motion (compared to the no-torque case). As predicted by theory, this enhancement occurs as long as $\gamma > 1/\sqrt{3}$. Note that in this plot $\gamma \approx 3$, thus in agreement with the theoretical results. On the other hand, we observe that an external torque decreases the total effective diffusivity for steady swimming as it is also predicted by our developed theory.

VI. CONCLUDING REMARKS

In this paper we characterized theoretically the effective three-dimensional diffusivity of a spherical active particle, free to rotate in any direction, and subject to both a constant external torque and thermal agitation. Thus this paper spatially generalized the work in Ref. [37]. By means of a rotational transformation to the equation governing the dynamics of the swimmer orientation, we obtained analytically the swimmer orientation probability distribution function. This allowed us to find by hand the swimmer orientation correlations, hence an analytical prediction, Eqs. (19) and (20), for the effective diffusivity was derived. These general equations revealed that the presence of an external torque leads in general to an anisotropic diffusive motion, and they were applied for two types of swimming (steady and reciprocal swimming). For steady swimmers the external torque always decreases the effective swimmer diffusivity whereas for time-reversible swimmers it may actually be enhanced. To validate our theoretical results we also performed Brownian dynamics simulations that showed excellent agreement between theory and numerical experiments. We conclude mentioning that the inclusion in our model of a simple constant external torque, generated two important physical effects namely, anisotropy and reduction or enhancement (depending on the type of motion) on the swimmer diffusion. These effects surely should be taken into account or even exploited when designing novel microswimming devices. As it has already been shown, the reciprocal motion performed by some bacteria in nature and thought to be useless [44], has a reason, that is, the enhancement of the bacteria diffusivity [30], now we have also shown that another possible reason may be that the combination of reciprocal motion with an external torque (a very typical scenario in the microworld) may also enhance the swimmers diffusivity, thus another possible strategy for active particles to sample more space at low energetic cost.

ACKNOWLEDGMENTS

This work was funded in part by CONACYT, Mexico, and the University of California San Diego. M.S. acknowledges fruitful discussions with E. Lauga and G. Elfring, and thanks Professors R. M. Velasco, H. Morales, N. Aquino, and the Complex Systems Group from UAM-I for their invaluable support.

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